Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:58 PM GMT

PDB ID	:	1YRQ
Title	:	Structure of the ready oxidized form of [NiFe]-hydrogenase
Authors	:	Volbeda, A.; Martin, L.; Cavazza, C.; Matho, M.; Faber, B.W.; Roseboom, W.; Albracht, S.P.; Garcin, E.; Rousset, M.; Fontecilla-Camps, J.C.
Deposited on	:	2005-02-04
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

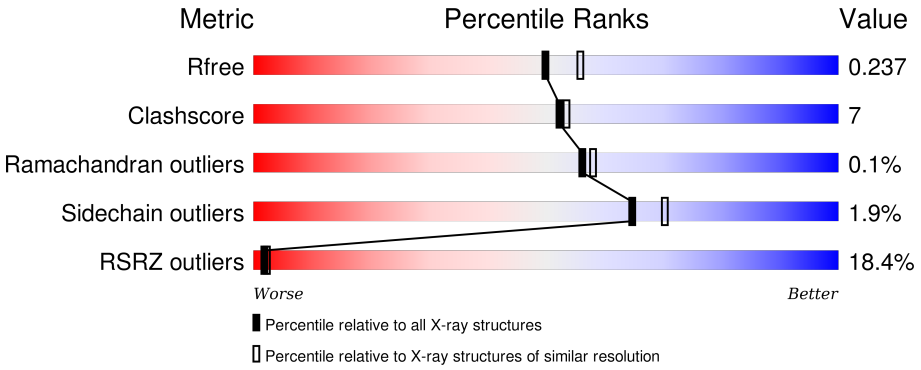
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk26765
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	264	2% 80% 19%
1	1-B	264	15% 83% 16%
1	1-C	264	% 86% 11%
1	1-D	264	% 83% 17%
1	1-F	264	2% 84% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	1-G	264	96% 67% 31%
1	2-A	264	2% 81% 19%
1	2-B	264	15% 83% 16%
1	2-C	264	% 86% 11%
1	2-D	264	% 83% 17%
1	2-F	264	2% 83% 15%
1	2-G	264	96% 66% 32%
2	1-H	549	2% 84% 14%
2	1-I	549	5% 85% 14%
2	1-J	549	4% 82% 16%
2	1-K	549	2% 83% 15%
2	1-M	549	4% 81% 17%
2	1-N	549	93% 81% 17%
2	2-H	549	2% 84% 14%
2	2-I	549	5% 85% 14%
2	2-J	549	4% 82% 16%
2	2-K	549	2% 83% 15%
2	2-M	549	4% 81% 17%
2	2-N	549	93% 81% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SF4	1-G	267	-	-	-	X
5	SF4	2-G	267	-	-	-	X
7	FCO	1-N	550	-	-	X	-
7	FCO	2-N	550	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 77694 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Periplasmic [NiFe] hydrogenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	262	Total	C	N	O	S	0	0	0
			1970	1254	330	371	15			
1	2-A	262	Total	C	N	O	S	0	0	0
			1970	1254	330	371	15			
1	1-B	262	Total	C	N	O	S	0	0	0
			1971	1255	330	371	15			
1	2-B	262	Total	C	N	O	S	0	0	0
			1971	1255	330	371	15			
1	1-C	260	Total	C	N	O	S	0	0	0
			1952	1243	325	369	15			
1	2-C	260	Total	C	N	O	S	0	0	0
			1952	1243	325	369	15			
1	1-D	262	Total	C	N	O	S	0	0	0
			1971	1255	330	371	15			
1	2-D	262	Total	C	N	O	S	0	0	0
			1971	1255	330	371	15			
1	1-F	260	Total	C	N	O	S	0	0	0
			1952	1243	325	369	15			
1	2-F	260	Total	C	N	O	S	0	0	0
			1952	1243	325	369	15			
1	1-G	262	Total	C	N	O	S	0	0	0
			1970	1254	330	371	15			
1	2-G	262	Total	C	N	O	S	0	0	0
			1970	1254	330	371	15			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	ALA	THR	SEE REMARK 999	UNP P18187
A	56	ALA	SER	SEE REMARK 999	UNP P18187
A	112	GLY	ARG	SEE REMARK 999	UNP P18187
A	113	THR	HIS	SEE REMARK 999	UNP P18187
A	114	CYS	LEU	SEE REMARK 999	UNP P18187

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	SER	PRO	SEE REMARK 999	UNP P18187
A	116	ALA	HIS	SEE REMARK 999	UNP P18187
A	117	TYR	-	INSERTION	UNP P18187
A	171	SER	GLU	SEE REMARK 999	UNP P18187
B	55	ALA	THR	SEE REMARK 999	UNP P18187
B	56	ALA	SER	SEE REMARK 999	UNP P18187
B	112	GLY	ARG	SEE REMARK 999	UNP P18187
B	113	THR	HIS	SEE REMARK 999	UNP P18187
B	114	CYS	LEU	SEE REMARK 999	UNP P18187
B	115	SER	PRO	SEE REMARK 999	UNP P18187
B	116	ALA	HIS	SEE REMARK 999	UNP P18187
B	117	TYR	-	INSERTION	UNP P18187
B	171	SER	GLU	SEE REMARK 999	UNP P18187
C	55	ALA	THR	SEE REMARK 999	UNP P18187
C	56	ALA	SER	SEE REMARK 999	UNP P18187
C	112	GLY	ARG	SEE REMARK 999	UNP P18187
C	113	THR	HIS	SEE REMARK 999	UNP P18187
C	114	CYS	LEU	SEE REMARK 999	UNP P18187
C	115	SER	PRO	SEE REMARK 999	UNP P18187
C	116	ALA	HIS	SEE REMARK 999	UNP P18187
C	117	TYR	-	INSERTION	UNP P18187
C	171	SER	GLU	SEE REMARK 999	UNP P18187
D	55	ALA	THR	SEE REMARK 999	UNP P18187
D	56	ALA	SER	SEE REMARK 999	UNP P18187
D	112	GLY	ARG	SEE REMARK 999	UNP P18187
D	113	THR	HIS	SEE REMARK 999	UNP P18187
D	114	CYS	LEU	SEE REMARK 999	UNP P18187
D	115	SER	PRO	SEE REMARK 999	UNP P18187
D	116	ALA	HIS	SEE REMARK 999	UNP P18187
D	117	TYR	-	INSERTION	UNP P18187
D	171	SER	GLU	SEE REMARK 999	UNP P18187
F	55	ALA	THR	SEE REMARK 999	UNP P18187
F	56	ALA	SER	SEE REMARK 999	UNP P18187
F	112	GLY	ARG	SEE REMARK 999	UNP P18187
F	113	THR	HIS	SEE REMARK 999	UNP P18187
F	114	CYS	LEU	SEE REMARK 999	UNP P18187
F	115	SER	PRO	SEE REMARK 999	UNP P18187
F	116	ALA	HIS	SEE REMARK 999	UNP P18187
F	117	TYR	-	INSERTION	UNP P18187
F	171	SER	GLU	SEE REMARK 999	UNP P18187
G	55	ALA	THR	SEE REMARK 999	UNP P18187
G	56	ALA	SER	SEE REMARK 999	UNP P18187

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	112	GLY	ARG	SEE REMARK 999	UNP P18187
G	113	THR	HIS	SEE REMARK 999	UNP P18187
G	114	CYS	LEU	SEE REMARK 999	UNP P18187
G	115	SER	PRO	SEE REMARK 999	UNP P18187
G	116	ALA	HIS	SEE REMARK 999	UNP P18187
G	117	TYR	-	INSERTION	UNP P18187
G	171	SER	GLU	SEE REMARK 999	UNP P18187

- Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1-H	545	Total	C	N	O	S	0	0	0
			4167	2654	725	766	22			
2	2-H	545	Total	C	N	O	S	0	0	0
			4167	2654	725	766	22			
2	1-I	545	Total	C	N	O	S	0	0	0
			4166	2653	725	766	22			
2	2-I	545	Total	C	N	O	S	0	0	0
			4166	2653	725	766	22			
2	1-J	544	Total	C	N	O	S	0	0	0
			4162	2651	724	765	22			
2	2-J	544	Total	C	N	O	S	0	0	0
			4162	2651	724	765	22			
2	1-K	544	Total	C	N	O	S	0	0	0
			4162	2651	724	765	22			
2	2-K	544	Total	C	N	O	S	0	0	0
			4162	2651	724	765	22			
2	1-M	545	Total	C	N	O	S	0	0	0
			4166	2653	725	766	22			
2	2-M	545	Total	C	N	O	S	0	0	0
			4166	2653	725	766	22			
2	1-N	545	Total	C	N	O	S	4	0	0
			4167	2654	725	766	22			
2	2-N	545	Total	C	N	O	S	0	0	0
			4167	2654	725	766	22			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	149	ALA	ASP	SEE REMARK 999	UNP P18188
H	150	PRO	THR	SEE REMARK 999	UNP P18188
H	153	PRO	THR	SEE REMARK 999	UNP P18188

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	157	ALA	GLU	SEE REMARK 999	UNP P18188
H	303	SER	GLU	SEE REMARK 999	UNP P18188
H	353	GLY	CYS	SEE REMARK 999	UNP P18188
H	478	ALA	SER	SEE REMARK 999	UNP P18188
H	508	ALA	PRO	SEE REMARK 999	UNP P18188
I	149	ALA	ASP	SEE REMARK 999	UNP P18188
I	150	PRO	THR	SEE REMARK 999	UNP P18188
I	153	PRO	THR	SEE REMARK 999	UNP P18188
I	157	ALA	GLU	SEE REMARK 999	UNP P18188
I	303	SER	GLU	SEE REMARK 999	UNP P18188
I	353	GLY	CYS	SEE REMARK 999	UNP P18188
I	478	ALA	SER	SEE REMARK 999	UNP P18188
I	508	ALA	PRO	SEE REMARK 999	UNP P18188
J	149	ALA	ASP	SEE REMARK 999	UNP P18188
J	150	PRO	THR	SEE REMARK 999	UNP P18188
J	153	PRO	THR	SEE REMARK 999	UNP P18188
J	157	ALA	GLU	SEE REMARK 999	UNP P18188
J	303	SER	GLU	SEE REMARK 999	UNP P18188
J	353	GLY	CYS	SEE REMARK 999	UNP P18188
J	478	ALA	SER	SEE REMARK 999	UNP P18188
J	508	ALA	PRO	SEE REMARK 999	UNP P18188
K	149	ALA	ASP	SEE REMARK 999	UNP P18188
K	150	PRO	THR	SEE REMARK 999	UNP P18188
K	153	PRO	THR	SEE REMARK 999	UNP P18188
K	157	ALA	GLU	SEE REMARK 999	UNP P18188
K	303	SER	GLU	SEE REMARK 999	UNP P18188
K	353	GLY	CYS	SEE REMARK 999	UNP P18188
K	478	ALA	SER	SEE REMARK 999	UNP P18188
K	508	ALA	PRO	SEE REMARK 999	UNP P18188
M	149	ALA	ASP	SEE REMARK 999	UNP P18188
M	150	PRO	THR	SEE REMARK 999	UNP P18188
M	153	PRO	THR	SEE REMARK 999	UNP P18188
M	157	ALA	GLU	SEE REMARK 999	UNP P18188
M	303	SER	GLU	SEE REMARK 999	UNP P18188
M	353	GLY	CYS	SEE REMARK 999	UNP P18188
M	478	ALA	SER	SEE REMARK 999	UNP P18188
M	508	ALA	PRO	SEE REMARK 999	UNP P18188
N	149	ALA	ASP	SEE REMARK 999	UNP P18188
N	150	PRO	THR	SEE REMARK 999	UNP P18188
N	153	PRO	THR	SEE REMARK 999	UNP P18188
N	157	ALA	GLU	SEE REMARK 999	UNP P18188
N	303	SER	GLU	SEE REMARK 999	UNP P18188

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	353	GLY	CYS	SEE REMARK 999	UNP P18188
N	478	ALA	SER	SEE REMARK 999	UNP P18188
N	508	ALA	PRO	SEE REMARK 999	UNP P18188

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	2-I	1	Total Ni 1 1	0	0
3	1-J	1	Total Ni 1 1	0	0
3	2-H	1	Total Ni 1 1	0	0
3	1-K	1	Total Ni 1 1	0	0
3	1-H	1	Total Ni 1 1	0	0
3	1-I	1	Total Ni 1 1	0	0
3	2-N	1	Total Ni 1 1	0	0
3	2-M	1	Total Ni 1 1	0	0
3	1-N	1	Total Ni 1 1	0	0
3	2-K	1	Total Ni 1 1	0	0
3	2-J	1	Total Ni 1 1	0	0
3	1-M	1	Total Ni 1 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

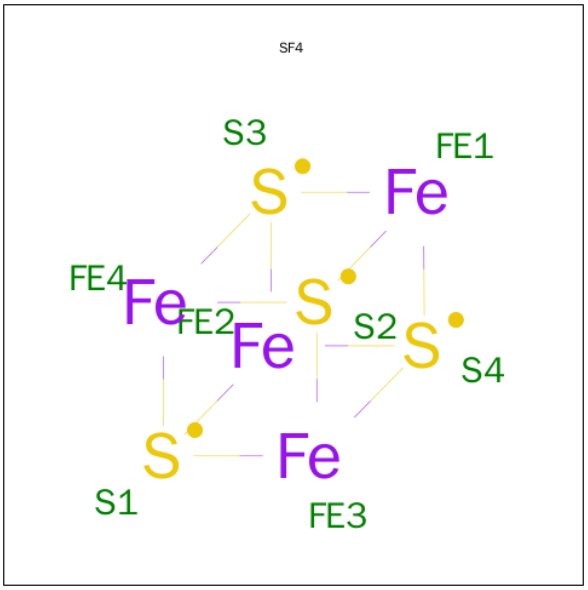
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	2-I	1	Total Mg 1 1	0	0
4	1-J	1	Total Mg 1 1	0	0
4	2-H	1	Total Mg 1 1	0	0
4	1-K	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-H	1	Total Mg 1 1	0	0
4	1-I	1	Total Mg 1 1	0	0
4	2-N	1	Total Mg 1 1	0	0
4	2-M	1	Total Mg 1 1	0	0
4	1-N	1	Total Mg 1 1	0	0
4	2-K	1	Total Mg 1 1	0	0
4	2-J	1	Total Mg 1 1	0	0
4	1-M	1	Total Mg 1 1	0	0

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



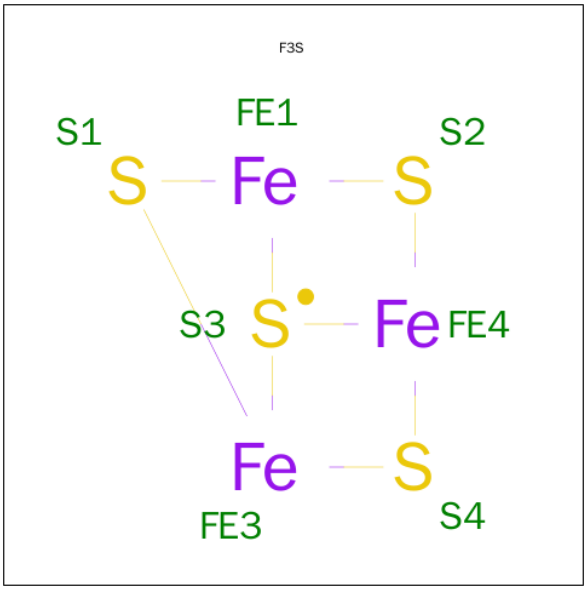
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1-A	1	Total Fe S 8 4 4	0	0
5	2-A	1	Total Fe S 8 4 4	0	0
5	1-A	1	Total Fe S 8 4 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	2-A	1	Total Fe S 8 4 4	0	0
5	1-B	1	Total Fe S 8 4 4	0	0
5	2-B	1	Total Fe S 8 4 4	0	0
5	1-B	1	Total Fe S 8 4 4	0	0
5	2-B	1	Total Fe S 8 4 4	0	0
5	1-C	1	Total Fe S 8 4 4	0	0
5	2-C	1	Total Fe S 8 4 4	0	0
5	1-C	1	Total Fe S 8 4 4	0	0
5	2-C	1	Total Fe S 8 4 4	0	0
5	1-D	1	Total Fe S 8 4 4	0	0
5	2-D	1	Total Fe S 8 4 4	0	0
5	1-D	1	Total Fe S 8 4 4	0	0
5	2-D	1	Total Fe S 8 4 4	0	0
5	1-F	1	Total Fe S 8 4 4	0	0
5	2-F	1	Total Fe S 8 4 4	0	0
5	1-F	1	Total Fe S 8 4 4	0	0
5	2-F	1	Total Fe S 8 4 4	0	0
5	1-G	1	Total Fe S 8 4 4	0	0
5	2-G	1	Total Fe S 8 4 4	0	0
5	1-G	1	Total Fe S 8 4 4	0	0
5	2-G	1	Total Fe S 8 4 4	0	0

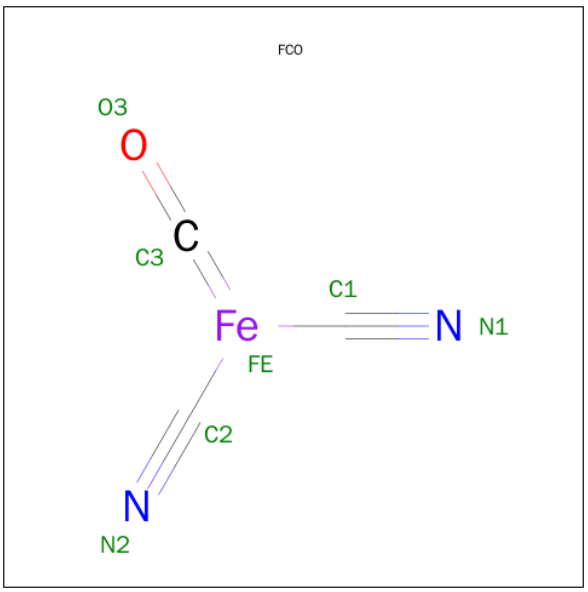
- Molecule 6 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1-A	1	Total Fe S 7 3 4	0	0
6	2-A	1	Total Fe S 7 3 4	0	0
6	1-B	1	Total Fe S 7 3 4	0	0
6	2-B	1	Total Fe S 7 3 4	0	0
6	1-C	1	Total Fe S 7 3 4	0	0
6	2-C	1	Total Fe S 7 3 4	0	0
6	1-D	1	Total Fe S 7 3 4	0	0
6	2-D	1	Total Fe S 7 3 4	0	0
6	1-F	1	Total Fe S 7 3 4	0	0
6	2-F	1	Total Fe S 7 3 4	0	0
6	1-G	1	Total Fe S 7 3 4	0	0
6	2-G	1	Total Fe S 7 3 4	0	0

- Molecule 7 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula:

C_3FeN_2O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	1-H	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	2-H	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	1-I	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	2-I	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	1-J	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	2-J	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	1-K	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	2-K	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	1-M	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	2-M	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	1-N	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	2-N	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	1-A	122	Total O 122 122	0	0
8	2-A	122	Total O 122 122	0	0
8	1-B	83	Total O 83 83	0	0
8	2-B	84	Total O 84 84	0	0
8	1-C	120	Total O 120 120	0	0
8	2-C	120	Total O 120 120	0	0
8	1-D	149	Total O 149 149	0	0
8	2-D	148	Total O 148 148	0	0
8	1-F	108	Total O 108 108	0	0
8	2-F	109	Total O 109 109	0	0
8	1-G	59	Total O 59 59	0	0
8	2-G	58	Total O 58 58	0	0
8	1-H	245	Total O 245 245	0	0
8	2-H	245	Total O 245 245	0	0
8	1-I	218	Total O 218 218	0	0
8	2-I	218	Total O 218 218	0	0
8	1-J	208	Total O 208 208	0	0
8	2-J	208	Total O 208 208	0	0
8	1-K	253	Total O 253 253	0	0
8	2-K	253	Total O 253 253	0	0
8	1-M	183	Total O 183 183	0	0
8	2-M	183	Total O 183 183	0	0

Continued on next page...

Continued from previous page...

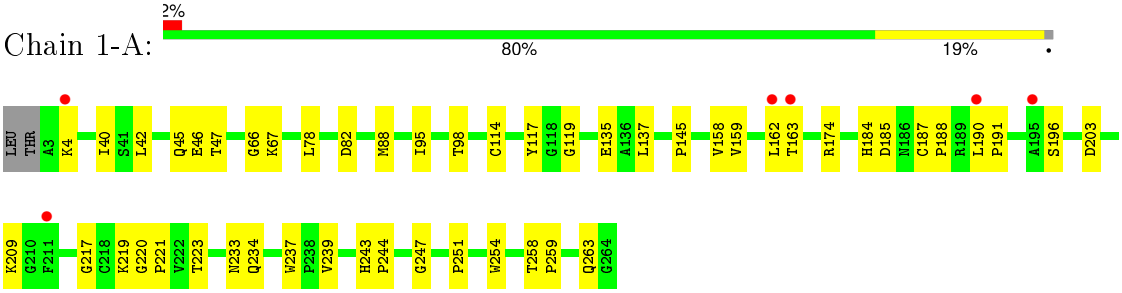
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	1-N	138	Total O 138 138	0	0
8	2-N	124	Total O 124 124	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

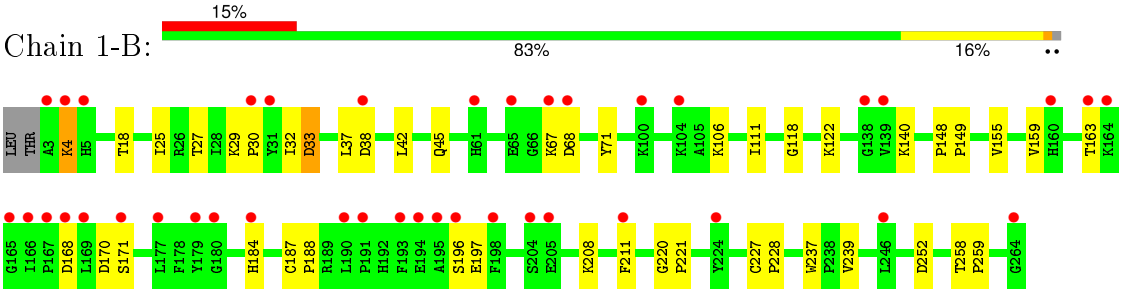
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 1-A:



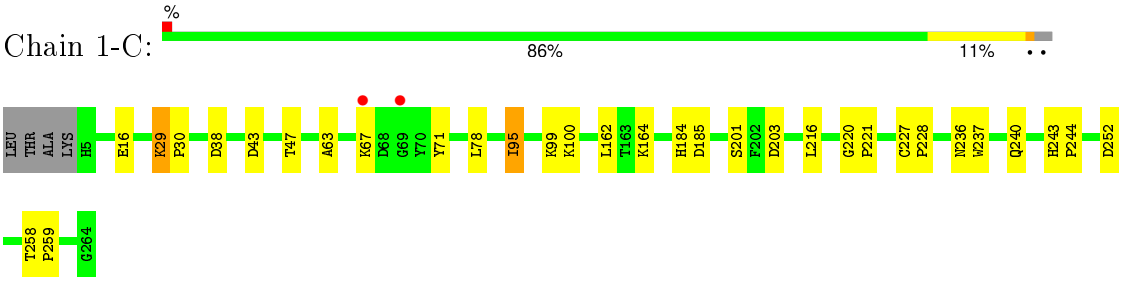
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 1-B:



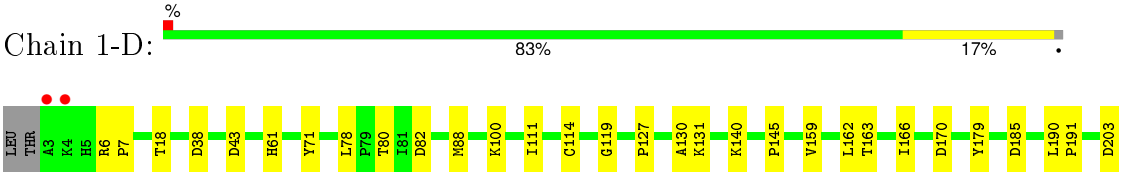
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 1-C:



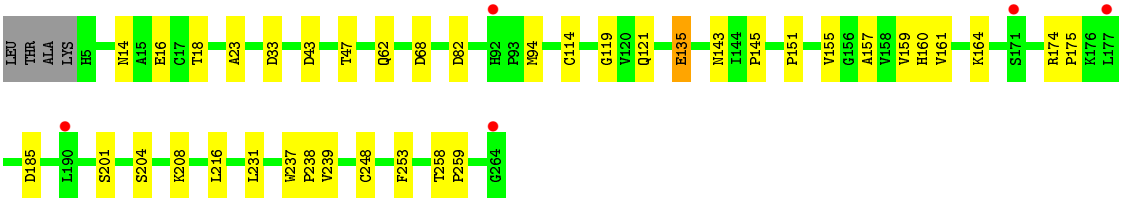
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 1-D:



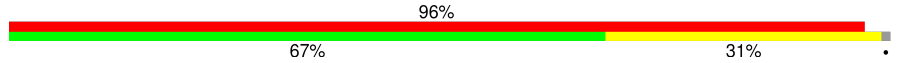
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

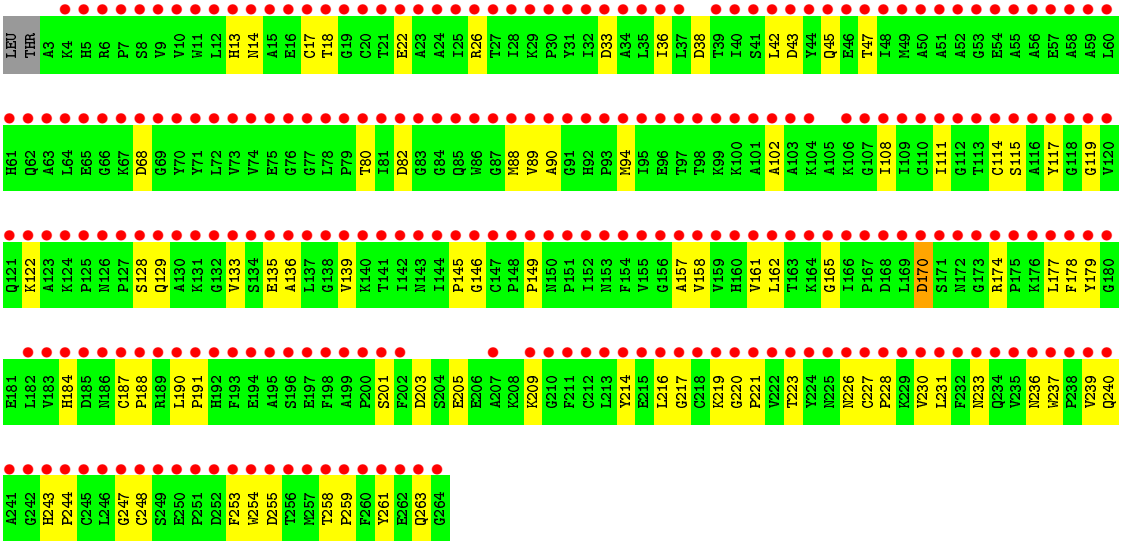
Chain 1-F:



• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

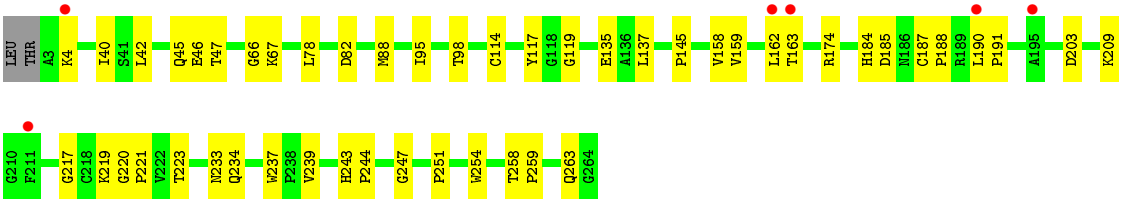
Chain 1-G:





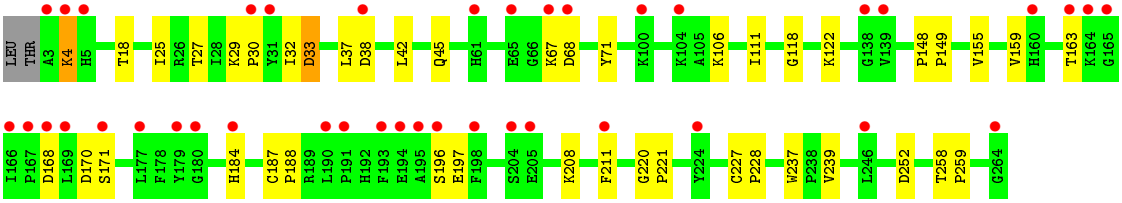
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 2-A:



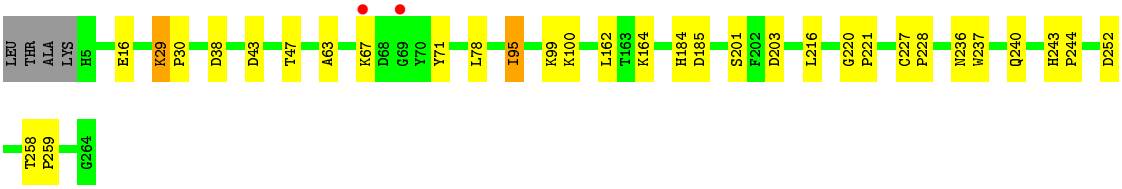
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 2-B:



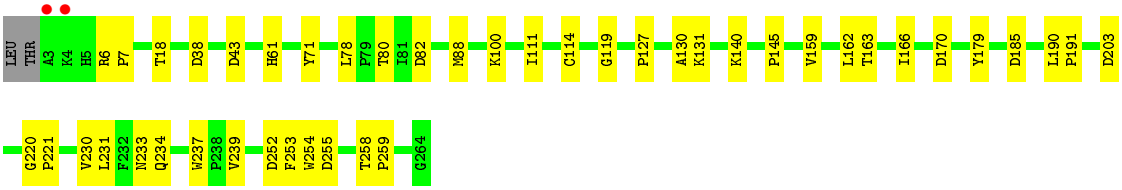
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 2-C:



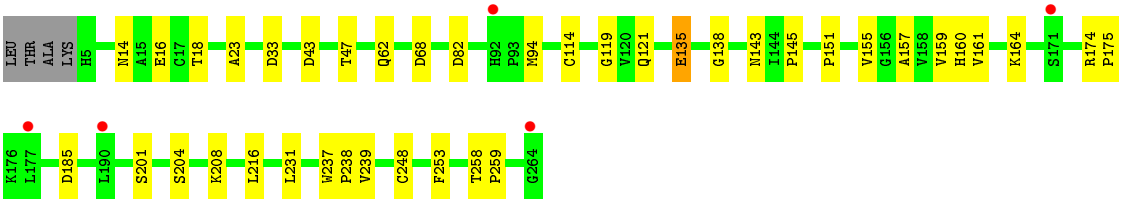
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 2-D:



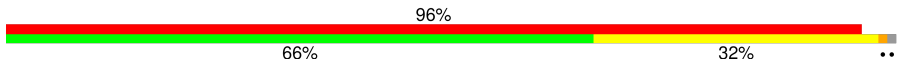
• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

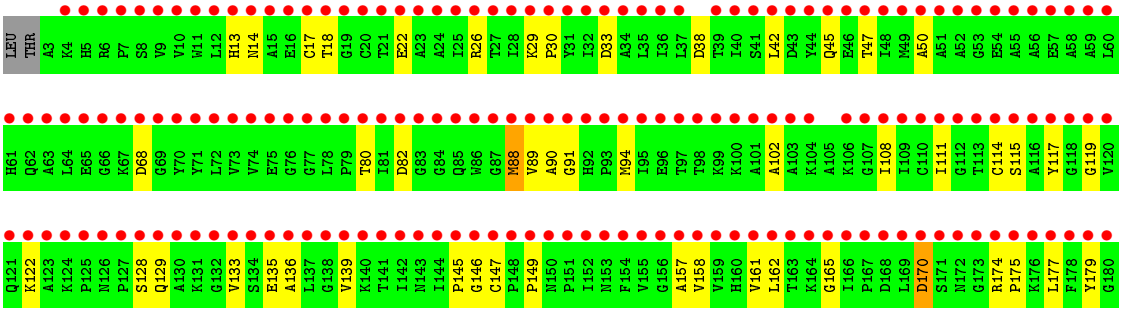
Chain 2-F:

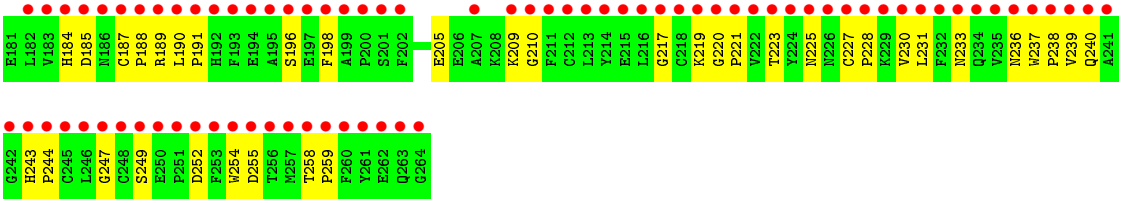


• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain 2-G:

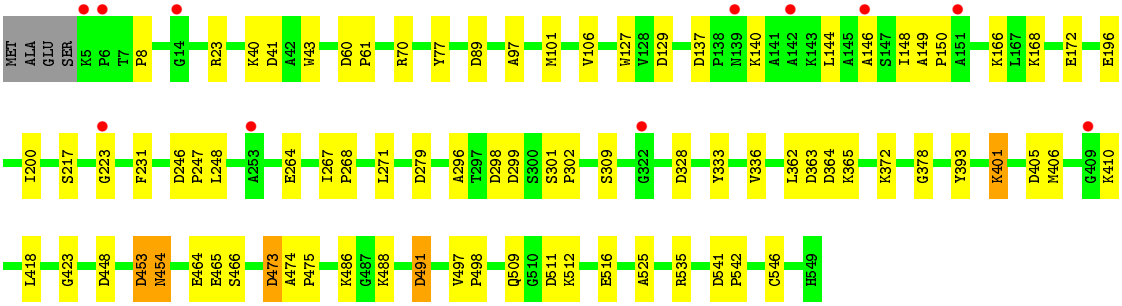






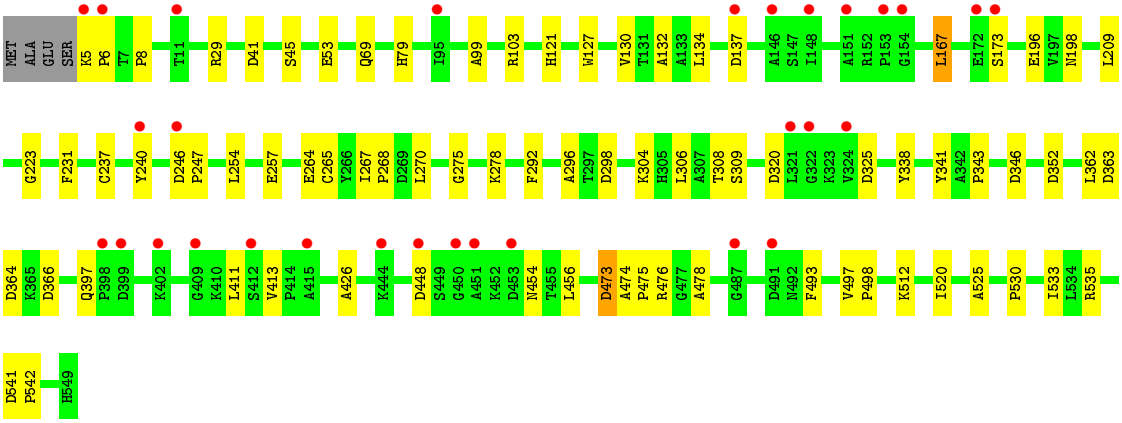
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 1-H:



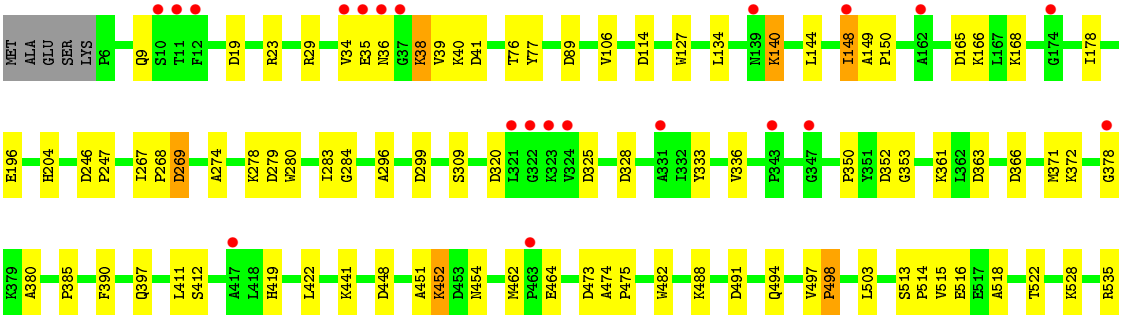
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

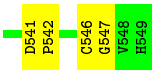
Chain 1-I:



• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

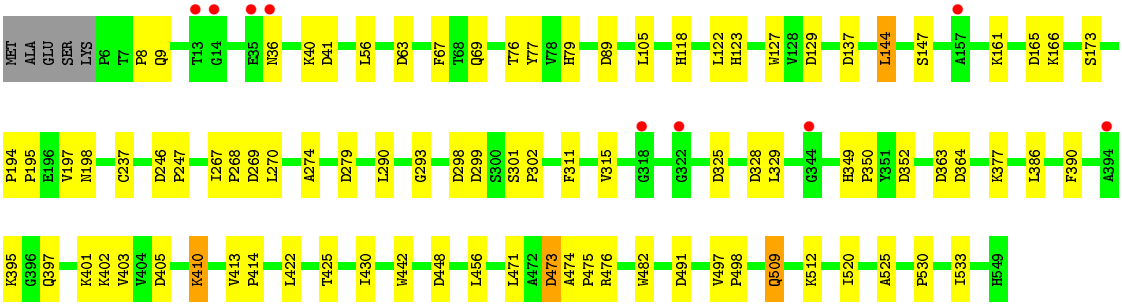
Chain 1-J:





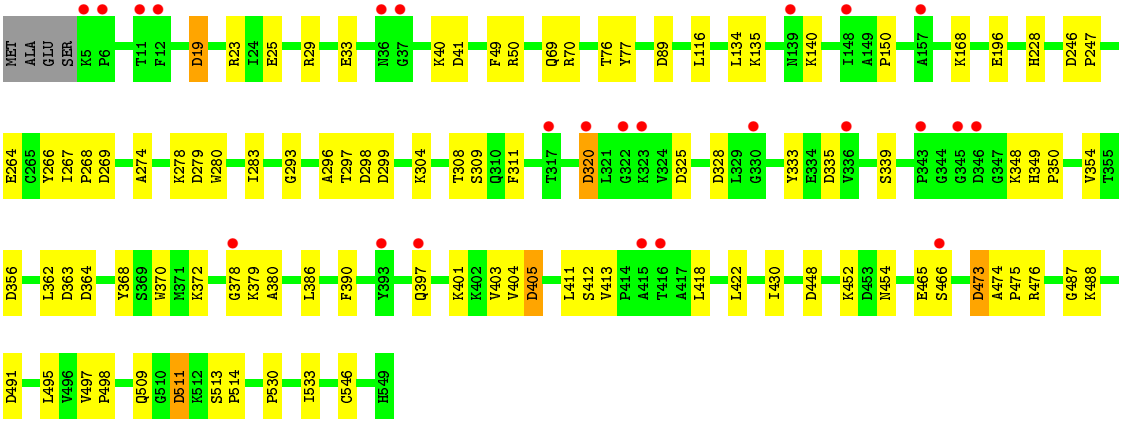
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 1-K:



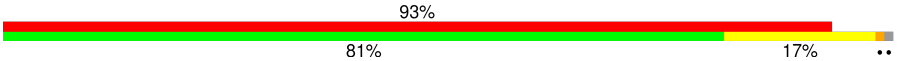
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

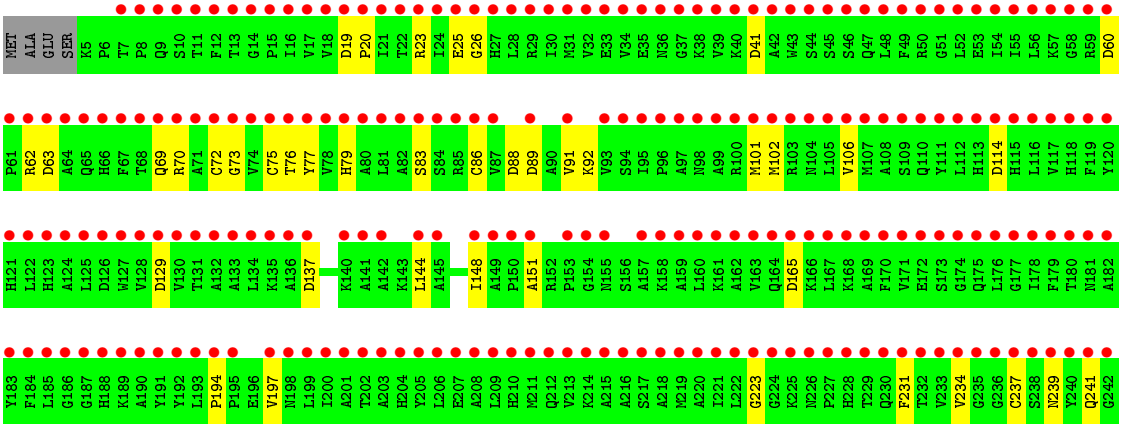
Chain 1-M:

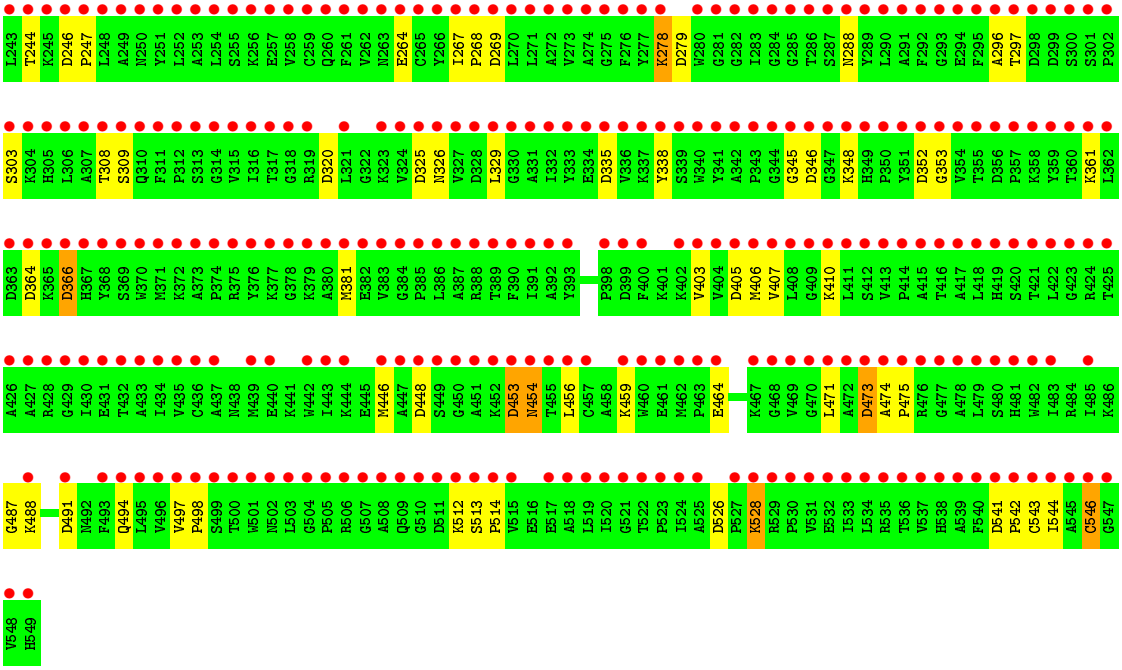


• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

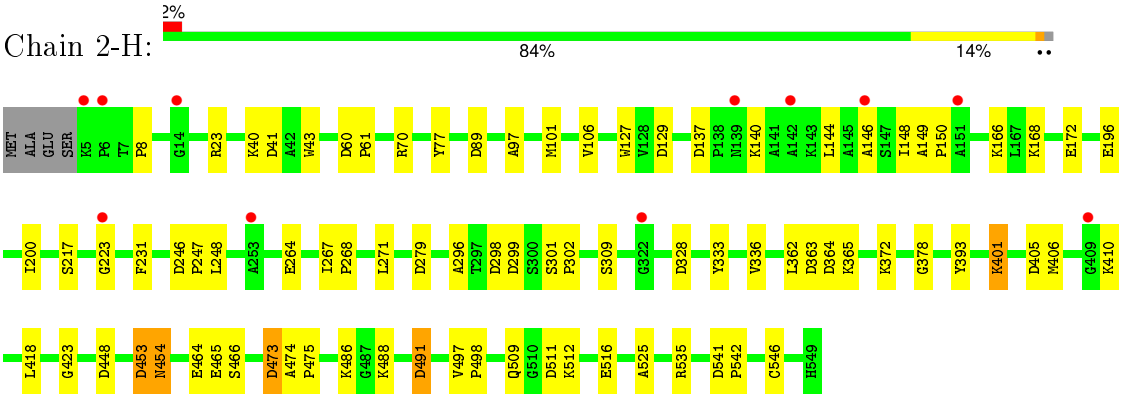
Chain 1-N:



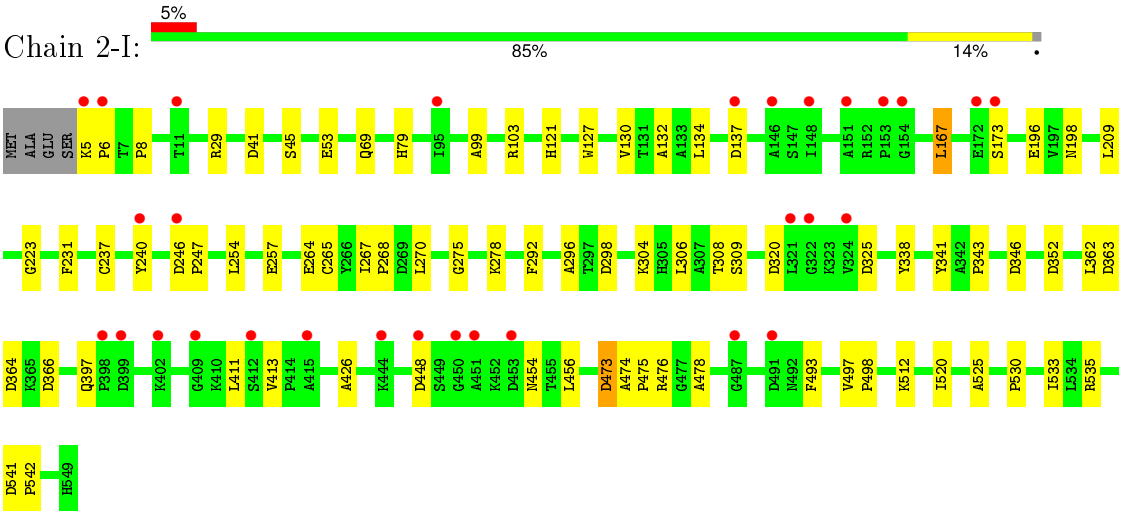




• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

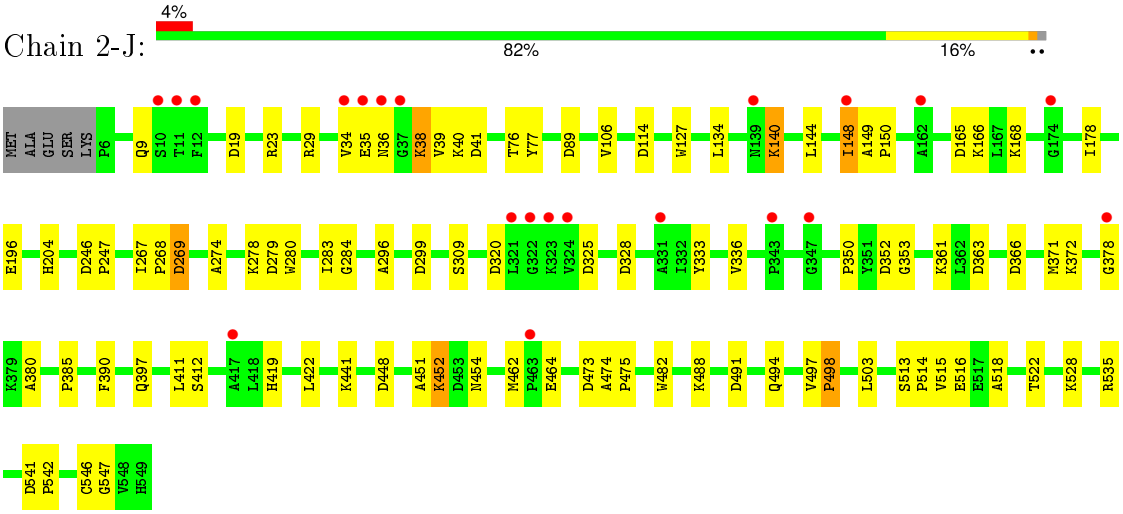


• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit



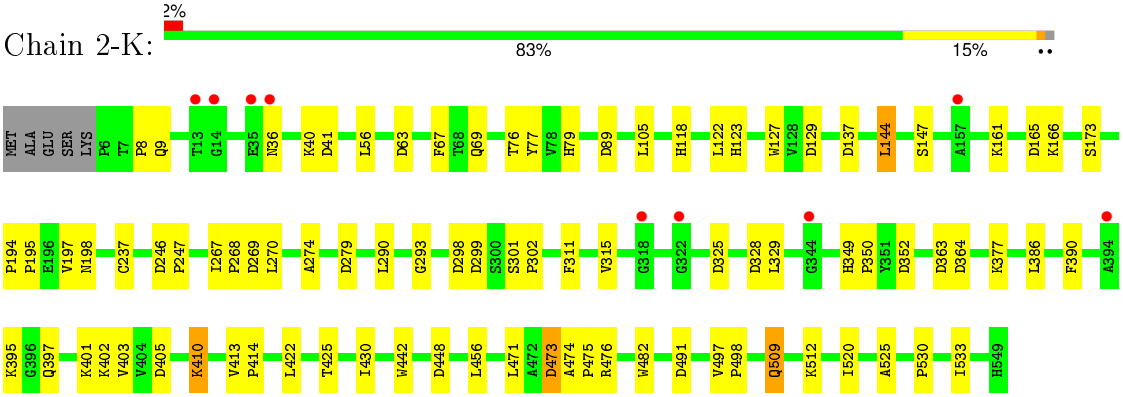
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 2-J:



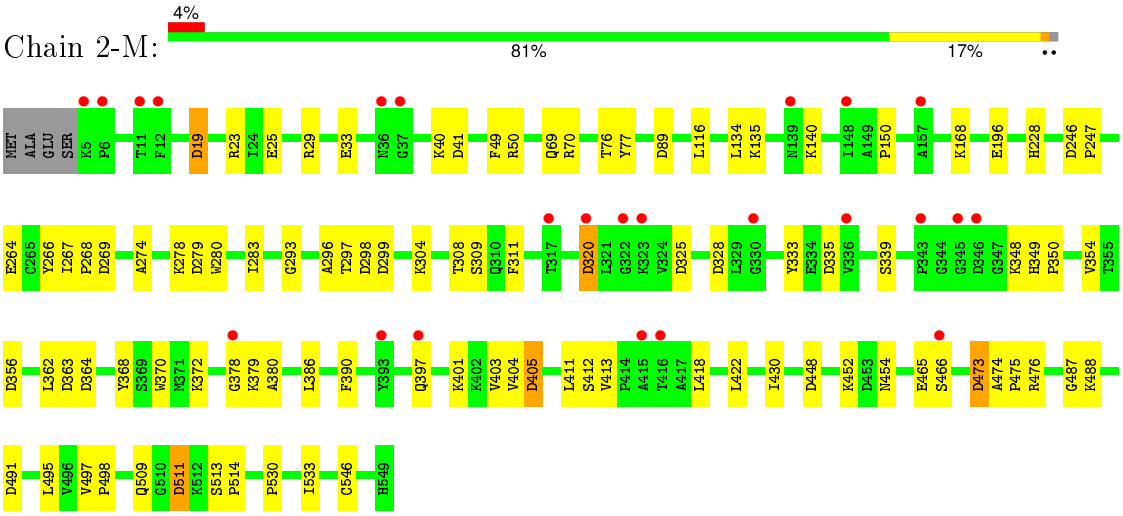
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 2-K:



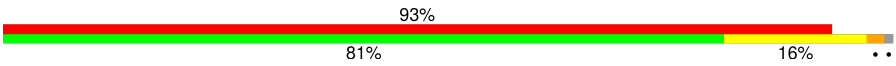
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

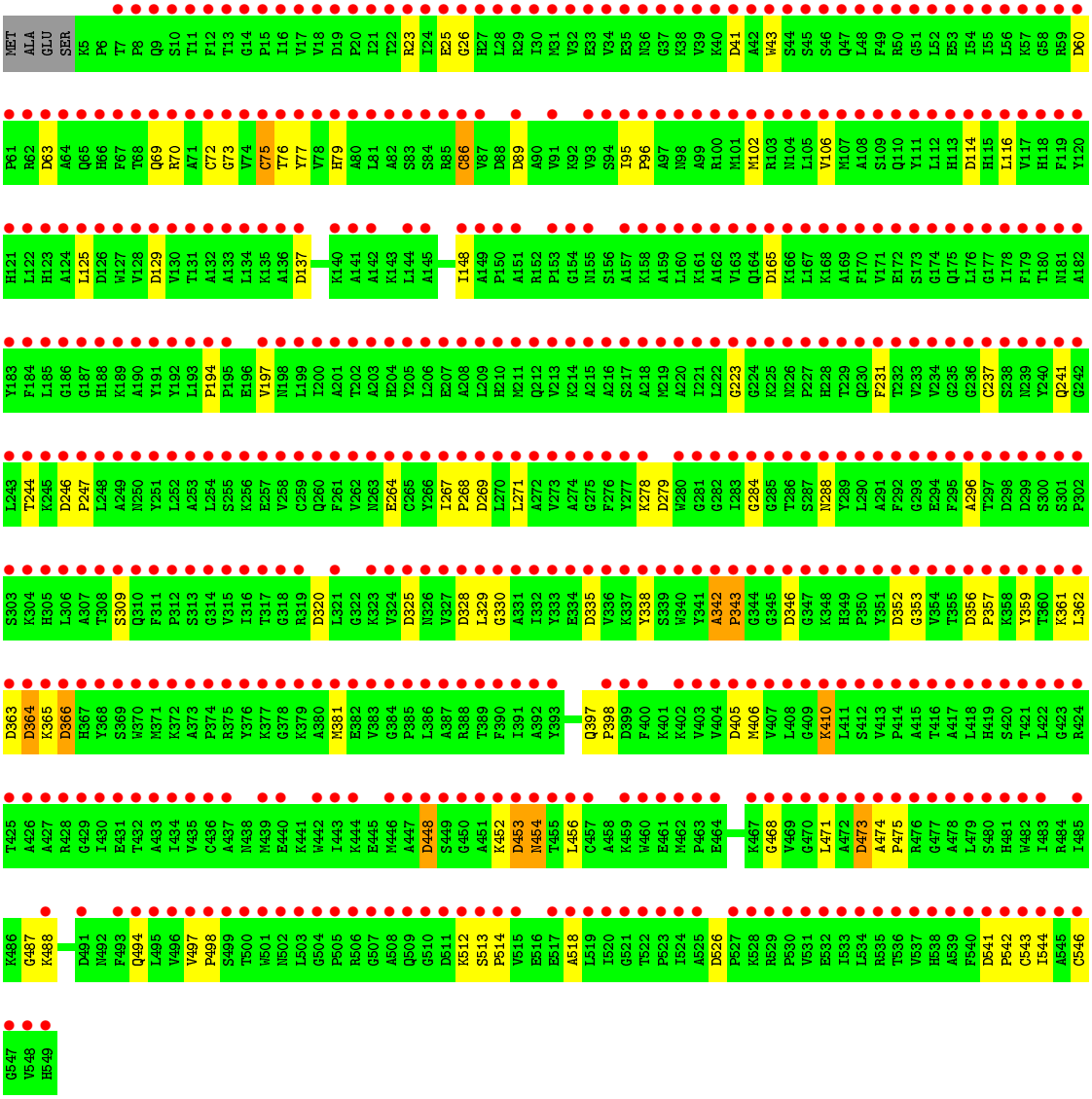
Chain 2-M:



• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain 2-N:




MET ALA GLU SER K5 P6 T7 P8 Q9 S10 T11 F12 T13 G14 P15 I16 V17 V18 D19 P20 I21 T22 R23 I24 E25 G26 H27 L28 R29 I30 M31 V32 E33 V34 E35 N36 G37 K38 V39 K40 D41 A42 W43 S44 S45 S46 Q47 L48 F49 R50 G51 L52 E53 I54 I55 L56 K57 G58 R59 D60
P61 R62 D63 A64 Q65 H66 F67 T68 Q69 R70 A71 C72 G73 V74 C75 T76 Y77 V78 H79 A80 L81 A82 S83 S84 R85 C86 V87 D88 D89 A90 V91 K92 V93 S94 I95 P96 A97 N98 A99 R100 M101 M102 R103 N104 L105 V106 M107 A108 S109 Q110 Y111 L112 H113 D114 H115 L116 V117 H118 F119 Y120
H121 L122 H123 A124 L125 D126 W127 Y128 D129 V130 T131 A132 A133 L134 K135 A136 D137 K140 A141 A142 K143 L144 A145 I148 A149 P150 A151 R152 P153 G154 N155 S156 A157 K158 A159 L160 K161 A162 V163 Q164 D165 K166 L167 K168 A169 F170 V171 E172 S173 G174 Q175 L176 G177 I178 F179 T180 N181 A182
Y183 F184 L185 G186 G187 H188 K189 A190 Y191 Y192 L193 P194 P195 E196 V197 N198 L199 I200 A201 T202 A203 H204 Y205 L206 E207 A208 L209 H210 M211 Q212 V213 K214 A215 A216 S217 A218 M219 A220 I221 L222 G223 G224 K225 N226 P227 H228 T229 Q230 F231 T232 V233 V234 G235 G236 C237 S238 N239 Y240 Q241 G242
L243 T244 K245 D246 P247 L248 A249 N250 Y251 L252 A253 L254 S255 K256 E257 V258 C259 Q260 F261 V262 N263 E264 C265 Y266 I267 P268 D269 L270 L271 A272 V273 A274 G275 F276 Y277 K278 D279 W280 G281 G282 I283 G284 G285 T286 S287 N288 Y289 L290 A291 F292 G293 E294 F295 A296 T297 D298 D299 S300 S301 P302
S303 K304 H305 L306 A307 T308 S309 Q310 F311 P312 S313 G314 V315 I316 T317 G318 R319 D320 L321 G322 K323 V324 D325 N326 V327 D328 L329 G330 A331 I332 Y333 E334 D335 V336 K337 Y338 S339 W340 Y341 A342 P343 G344 G345 D346 G347 K348 H349 P350 Y351 D352 G353 V354 T355 D356 P357 K358 Y359 T360 K361 L362
D363 D364 K365 D366 H367 Y368 S369 W370 M371 K372 A373 P374 R375 Y376 K377 G378 K379 A380 M381 E382 V383 G384 P385 L386 A387 R388 T389 F390 I391 A392 Y393 Q397 P398 D399 F400 K401 K402 V403 V404 D405 M406 V407 L408 G409 K410 L411 S412 V413 P414 A415 T416 A417 L418 H419 S420 T421 L422 G423 R424
T425 A426 A427 R428 G429 I430 E431 T432 A433 I434 V435 C436 A437 N438 M439 E440 K441 W442 I443 K444 E445 M446 A447 D448 S449 G450 A451 K452 D453 N454 T455 L456 C457 A458 K459 W460 E461 M462 P463 E464 K467 G468 V469 G470 L471 A472 D473 A474 P475 R476 G477 A478 L479 S480 H481 W482 I483 R484 I485
K486 G487 K488 D491 N492 F493 Q494 L495 V496 V497 P498 S499 T500 W501 N502 L503 G504 P505 R506 G507 A508 Q509 G510 D511 K512 S513 P514 V515 E516 E517 A518 I519 I520 G521 T522 F523 I524 A525 D526 F527 K528 R529 P530 V531 E532 I533 L534 R535 T536 V537 H538 A539 F540 D541 F542 C543 I544 A545 G546
G547 V548 H549

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	127.50Å 99.70Å 183.20Å 90.00° 91.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 29.51 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.6 (20.00-2.10) 87.7 (29.51-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.27	Depositor
R, R_{free}	0.171 , 0.220 0.194 , 0.237	Depositor DCC
R_{free} test set	11803 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.60 , 44.8	EDS
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 233861 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	77694	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.05 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3614e-06.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, MG, F3S, SF4, FCO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1-A	0.58	0/2024	0.76	3/2755 (0.1%)
1	1-B	0.46	0/2025	0.70	6/2757 (0.2%)
1	1-C	0.52	0/2005	0.73	5/2731 (0.2%)
1	1-D	0.63	0/2025	0.78	8/2757 (0.3%)
1	1-F	0.52	0/2005	0.73	4/2731 (0.1%)
1	1-G	0.31	0/2024	0.63	8/2755 (0.3%)
1	2-A	0.58	0/2024	0.76	3/2755 (0.1%)
1	2-B	0.46	0/2025	0.70	6/2757 (0.2%)
1	2-C	0.52	0/2005	0.73	5/2731 (0.2%)
1	2-D	0.63	0/2025	0.78	8/2757 (0.3%)
1	2-F	0.52	0/2005	0.73	4/2731 (0.1%)
1	2-G	0.27	0/2024	0.61	8/2755 (0.3%)
2	1-H	0.57	0/4272	0.81	16/5800 (0.3%)
2	1-I	0.53	0/4271	0.78	11/5798 (0.2%)
2	1-J	0.51	0/4267	0.78	13/5792 (0.2%)
2	1-K	0.56	0/4267	0.81	19/5792 (0.3%)
2	1-M	0.50	0/4271	0.77	18/5798 (0.3%)
2	1-N	0.39	2/4272 (0.0%)	0.69	25/5800 (0.4%)
2	2-H	0.57	0/4272	0.81	16/5800 (0.3%)
2	2-I	0.53	0/4271	0.78	11/5798 (0.2%)
2	2-J	0.51	0/4267	0.78	13/5792 (0.2%)
2	2-K	0.56	0/4267	0.81	19/5792 (0.3%)
2	2-M	0.50	0/4271	0.77	18/5798 (0.3%)
2	2-N	0.30	1/4272 (0.0%)	0.68	22/5800 (0.4%)
All	All	0.51	3/75456 (0.0%)	0.76	269/102532 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-N	361	LYS	CB-CG	10.38	1.80	1.52
2	1-N	459	LYS	C-O	5.89	1.34	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2-N	75	CYS	CB-SG	5.08	1.90	1.82

All (269) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	185	ASP	CB-CG-OD2	8.28	125.75	118.30
1	2-A	185	ASP	CB-CG-OD2	8.28	125.75	118.30
2	1-H	279	ASP	CB-CG-OD2	8.05	125.54	118.30
2	2-H	279	ASP	CB-CG-OD2	8.05	125.54	118.30
2	1-K	129	ASP	CB-CG-OD2	8.00	125.50	118.30
2	2-K	129	ASP	CB-CG-OD2	8.00	125.50	118.30
2	1-H	89	ASP	CB-CG-OD2	7.94	125.45	118.30
2	2-H	89	ASP	CB-CG-OD2	7.94	125.45	118.30
2	1-H	129	ASP	CB-CG-OD2	7.83	125.34	118.30
2	2-H	129	ASP	CB-CG-OD2	7.83	125.34	118.30
2	1-M	89	ASP	CB-CG-OD2	7.77	125.29	118.30
2	2-M	89	ASP	CB-CG-OD2	7.77	125.29	118.30
2	1-K	165	ASP	CB-CG-OD2	7.24	124.82	118.30
2	2-K	165	ASP	CB-CG-OD2	7.24	124.82	118.30
2	1-I	364	ASP	CB-CG-OD2	7.24	124.82	118.30
2	2-I	364	ASP	CB-CG-OD2	7.24	124.82	118.30
2	2-N	86	CYS	CA-CB-SG	-7.23	100.98	114.00
1	1-D	170	ASP	CB-CG-OD2	7.05	124.65	118.30
1	2-D	170	ASP	CB-CG-OD2	7.05	124.65	118.30
1	1-A	82	ASP	CB-CG-OD2	7.01	124.61	118.30
1	2-A	82	ASP	CB-CG-OD2	7.01	124.61	118.30
2	1-N	361	LYS	CA-CB-CG	-6.99	98.02	113.40
2	1-I	448	ASP	CB-CG-OD2	6.90	124.51	118.30
2	2-I	448	ASP	CB-CG-OD2	6.90	124.51	118.30
1	1-B	252	ASP	CB-CG-OD2	6.87	124.48	118.30
1	2-B	252	ASP	CB-CG-OD2	6.87	124.48	118.30
2	1-K	137	ASP	CB-CG-OD2	6.77	124.39	118.30
2	2-K	137	ASP	CB-CG-OD2	6.77	124.39	118.30
1	1-G	255	ASP	CB-CG-OD2	6.76	124.38	118.30
1	1-D	82	ASP	CB-CG-OD2	6.75	124.38	118.30
1	2-D	82	ASP	CB-CG-OD2	6.75	124.38	118.30
2	1-H	41	ASP	CB-CG-OD2	6.59	124.23	118.30
2	2-H	41	ASP	CB-CG-OD2	6.59	124.23	118.30
2	1-K	473	ASP	CB-CG-OD2	6.57	124.22	118.30
2	2-K	473	ASP	CB-CG-OD2	6.57	124.22	118.30
2	1-J	366	ASP	CB-CG-OD2	6.55	124.20	118.30
2	2-J	366	ASP	CB-CG-OD2	6.55	124.20	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1-I	320	ASP	CB-CG-OD2	6.47	124.12	118.30
2	2-I	320	ASP	CB-CG-OD2	6.47	124.12	118.30
2	1-H	328	ASP	CB-CG-OD2	6.45	124.10	118.30
2	2-H	328	ASP	CB-CG-OD2	6.45	124.10	118.30
1	1-B	33	ASP	CB-CG-OD2	6.44	124.10	118.30
1	2-B	33	ASP	CB-CG-OD2	6.44	124.10	118.30
2	1-J	279	ASP	CB-CG-OD2	6.41	124.07	118.30
2	2-J	279	ASP	CB-CG-OD2	6.41	124.07	118.30
2	1-K	448	ASP	CB-CG-OD2	6.41	124.07	118.30
2	2-K	448	ASP	CB-CG-OD2	6.41	124.07	118.30
2	1-I	473	ASP	CB-CG-OD2	6.37	124.03	118.30
2	2-I	473	ASP	CB-CG-OD2	6.37	124.03	118.30
2	1-J	320	ASP	CB-CG-OD2	6.36	124.02	118.30
2	2-J	320	ASP	CB-CG-OD2	6.36	124.02	118.30
2	1-J	325	ASP	CB-CG-OD2	6.33	123.99	118.30
2	2-J	325	ASP	CB-CG-OD2	6.33	123.99	118.30
2	1-H	363	ASP	CB-CG-OD2	6.32	123.99	118.30
2	2-H	363	ASP	CB-CG-OD2	6.32	123.99	118.30
2	1-K	279	ASP	CB-CG-OD2	6.31	123.97	118.30
2	2-K	279	ASP	CB-CG-OD2	6.31	123.97	118.30
2	1-K	328	ASP	CB-CG-OD2	6.30	123.97	118.30
2	2-K	328	ASP	CB-CG-OD2	6.30	123.97	118.30
2	1-M	279	ASP	CB-CG-OD2	6.28	123.95	118.30
2	2-M	279	ASP	CB-CG-OD2	6.28	123.95	118.30
2	1-M	405	ASP	CB-CG-OD2	6.24	123.92	118.30
2	2-M	405	ASP	CB-CG-OD2	6.24	123.92	118.30
2	1-M	320	ASP	CB-CG-OD2	6.19	123.87	118.30
2	2-M	320	ASP	CB-CG-OD2	6.19	123.87	118.30
2	1-H	491	ASP	CB-CG-OD2	6.16	123.84	118.30
2	2-H	491	ASP	CB-CG-OD2	6.16	123.84	118.30
2	1-N	114	ASP	CB-CG-OD2	6.15	123.83	118.30
2	1-K	41	ASP	CB-CG-OD2	6.13	123.82	118.30
2	2-K	41	ASP	CB-CG-OD2	6.13	123.82	118.30
2	1-J	165	ASP	CB-CG-OD2	6.13	123.81	118.30
2	2-J	165	ASP	CB-CG-OD2	6.13	123.81	118.30
1	1-B	68	ASP	CB-CG-OD2	6.12	123.80	118.30
1	2-B	68	ASP	CB-CG-OD2	6.12	123.80	118.30
2	1-J	363	ASP	CB-CG-OD2	6.11	123.80	118.30
2	2-J	363	ASP	CB-CG-OD2	6.11	123.80	118.30
2	1-N	335	ASP	CB-CG-OD2	6.10	123.79	118.30
2	1-H	137	ASP	CB-CG-OD2	6.05	123.75	118.30
2	2-H	137	ASP	CB-CG-OD2	6.05	123.75	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2-N	279	ASP	CB-CG-OD2	6.05	123.75	118.30
2	1-N	279	ASP	CB-CG-OD2	6.04	123.73	118.30
2	1-N	269	ASP	CB-CG-OD2	6.03	123.72	118.30
2	1-N	366	ASP	CB-CG-OD2	6.03	123.72	118.30
1	2-G	82	ASP	CB-CG-OD2	6.01	123.71	118.30
1	1-D	43	ASP	CB-CG-OD2	5.98	123.68	118.30
1	2-D	43	ASP	CB-CG-OD2	5.98	123.68	118.30
2	1-M	299	ASP	CB-CG-OD2	5.96	123.66	118.30
2	2-M	299	ASP	CB-CG-OD2	5.96	123.66	118.30
2	1-J	299	ASP	CB-CG-OD2	5.94	123.64	118.30
2	2-J	299	ASP	CB-CG-OD2	5.94	123.64	118.30
2	1-J	89	ASP	CB-CG-OD2	5.93	123.64	118.30
2	2-J	89	ASP	CB-CG-OD2	5.93	123.64	118.30
1	1-A	203	ASP	CB-CG-OD2	5.93	123.64	118.30
1	2-A	203	ASP	CB-CG-OD2	5.93	123.64	118.30
2	1-H	298	ASP	CB-CG-OD2	5.90	123.61	118.30
2	2-H	298	ASP	CB-CG-OD2	5.90	123.61	118.30
2	1-I	325	ASP	CB-CG-OD2	5.90	123.61	118.30
2	2-I	325	ASP	CB-CG-OD2	5.90	123.61	118.30
2	1-N	137	ASP	CB-CG-OD2	5.88	123.59	118.30
2	1-K	325	ASP	CB-CG-OD2	5.85	123.57	118.30
2	2-K	325	ASP	CB-CG-OD2	5.85	123.57	118.30
1	2-G	255	ASP	CB-CG-OD2	5.83	123.55	118.30
2	2-N	269	ASP	CB-CG-OD2	5.82	123.54	118.30
1	1-F	185	ASP	CB-CG-OD2	5.82	123.54	118.30
1	2-F	185	ASP	CB-CG-OD2	5.82	123.54	118.30
1	1-G	170	ASP	CB-CG-OD2	5.82	123.54	118.30
1	2-G	170	ASP	CB-CG-OD2	5.79	123.51	118.30
2	2-N	114	ASP	CB-CG-OD2	5.78	123.50	118.30
1	1-D	38	ASP	CB-CG-OD2	5.78	123.50	118.30
1	2-D	38	ASP	CB-CG-OD2	5.78	123.50	118.30
1	1-G	82	ASP	CB-CG-OD2	5.77	123.49	118.30
2	2-N	335	ASP	CB-CG-OD2	5.75	123.48	118.30
2	1-N	320	ASP	CB-CG-OD2	5.75	123.47	118.30
2	1-M	356	ASP	CB-CG-OD2	5.74	123.46	118.30
2	2-M	356	ASP	CB-CG-OD2	5.74	123.46	118.30
2	1-K	298	ASP	CB-CG-OD2	5.72	123.45	118.30
2	2-K	298	ASP	CB-CG-OD2	5.72	123.45	118.30
2	1-N	448	ASP	CB-CG-OD2	5.71	123.44	118.30
2	1-N	325	ASP	CB-CG-OD2	5.69	123.42	118.30
2	1-N	364	ASP	CB-CG-OD2	5.67	123.40	118.30
2	1-M	473	ASP	CB-CG-OD2	5.66	123.39	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2-M	473	ASP	CB-CG-OD2	5.66	123.39	118.30
2	2-N	473	ASP	CB-CG-OD2	5.66	123.39	118.30
1	2-G	38	ASP	CB-CG-OD2	5.65	123.38	118.30
2	1-I	137	ASP	CB-CG-OD2	5.64	123.38	118.30
2	2-I	137	ASP	CB-CG-OD2	5.64	123.38	118.30
1	1-F	43	ASP	CB-CG-OD2	5.64	123.37	118.30
1	2-F	43	ASP	CB-CG-OD2	5.64	123.37	118.30
2	1-H	364	ASP	CB-CG-OD2	5.63	123.37	118.30
1	1-B	168	ASP	CB-CG-OD2	5.63	123.37	118.30
2	2-H	364	ASP	CB-CG-OD2	5.63	123.37	118.30
1	2-B	168	ASP	CB-CG-OD2	5.63	123.37	118.30
2	2-N	352	ASP	CB-CG-OD2	5.63	123.36	118.30
1	1-D	185	ASP	CB-CG-OD2	5.62	123.36	118.30
1	2-D	185	ASP	CB-CG-OD2	5.62	123.36	118.30
2	2-N	63	ASP	CB-CG-OD2	5.62	123.36	118.30
2	1-N	129	ASP	CB-CG-OD2	5.61	123.35	118.30
2	1-J	114	ASP	CB-CG-OD2	5.59	123.33	118.30
2	2-J	114	ASP	CB-CG-OD2	5.59	123.33	118.30
2	2-N	405	ASP	CB-CG-OD2	5.54	123.28	118.30
2	1-N	346	ASP	CB-CG-OD2	5.51	123.26	118.30
2	1-H	405	ASP	CB-CG-OD2	5.51	123.26	118.30
2	2-H	405	ASP	CB-CG-OD2	5.51	123.26	118.30
2	1-J	41	ASP	CB-CG-OD2	5.50	123.25	118.30
2	2-J	41	ASP	CB-CG-OD2	5.50	123.25	118.30
2	1-N	89	ASP	CB-CG-OD2	5.49	123.24	118.30
2	2-N	165	ASP	CB-CG-OD2	5.47	123.23	118.30
2	1-K	363	ASP	CB-CG-OD2	5.46	123.22	118.30
2	2-K	363	ASP	CB-CG-OD2	5.46	123.22	118.30
2	2-N	325	ASP	CB-CG-OD2	5.46	123.22	118.30
2	2-N	137	ASP	CB-CG-OD2	5.45	123.20	118.30
1	2-G	33	ASP	CB-CG-OD2	5.45	123.20	118.30
2	1-I	346	ASP	CB-CG-OD2	5.45	123.20	118.30
2	2-I	346	ASP	CB-CG-OD2	5.45	123.20	118.30
2	2-N	320	ASP	CB-CG-OD2	5.44	123.19	118.30
2	1-J	491	ASP	CB-CG-OD2	5.44	123.19	118.30
2	2-J	491	ASP	CB-CG-OD2	5.44	123.19	118.30
2	1-H	448	ASP	CB-CG-OD2	5.43	123.19	118.30
2	2-H	448	ASP	CB-CG-OD2	5.43	123.19	118.30
2	1-H	299	ASP	CB-CG-OD2	5.41	123.17	118.30
2	1-M	335	ASP	CB-CG-OD2	5.41	123.17	118.30
2	2-H	299	ASP	CB-CG-OD2	5.41	123.17	118.30
2	2-M	335	ASP	CB-CG-OD2	5.41	123.17	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-G	185	ASP	CB-CG-OD2	5.40	123.16	118.30
1	1-C	252	ASP	CB-CG-OD2	5.39	123.15	118.30
1	2-C	252	ASP	CB-CG-OD2	5.39	123.15	118.30
1	1-C	43	ASP	CB-CG-OD2	5.38	123.14	118.30
1	2-C	43	ASP	CB-CG-OD2	5.38	123.14	118.30
1	2-G	252	ASP	CB-CG-OD2	5.38	123.14	118.30
2	1-M	363	ASP	CB-CG-OD2	5.38	123.14	118.30
2	2-M	363	ASP	CB-CG-OD2	5.38	123.14	118.30
1	1-B	38	ASP	CB-CG-OD2	5.37	123.14	118.30
1	2-B	38	ASP	CB-CG-OD2	5.37	123.14	118.30
2	1-M	511	ASP	CB-CG-OD2	5.35	123.12	118.30
2	2-M	511	ASP	CB-CG-OD2	5.35	123.12	118.30
2	1-H	473	ASP	CB-CG-OD2	5.35	123.11	118.30
2	2-H	473	ASP	CB-CG-OD2	5.35	123.11	118.30
1	1-B	170	ASP	CB-CG-OD2	5.34	123.11	118.30
1	2-B	170	ASP	CB-CG-OD2	5.34	123.11	118.30
2	2-N	129	ASP	CB-CG-OD2	5.34	123.10	118.30
2	2-N	41	ASP	CB-CG-OD2	5.33	123.10	118.30
1	1-C	185	ASP	CB-CG-OD2	5.33	123.10	118.30
1	2-C	185	ASP	CB-CG-OD2	5.33	123.10	118.30
2	1-K	269	ASP	CB-CG-OD2	5.32	123.09	118.30
2	2-K	269	ASP	CB-CG-OD2	5.32	123.09	118.30
1	1-G	38	ASP	CB-CG-OD2	5.31	123.08	118.30
1	1-C	38	ASP	CB-CG-OD2	5.30	123.07	118.30
1	2-C	38	ASP	CB-CG-OD2	5.30	123.07	118.30
2	1-N	473	ASP	CB-CG-OD2	5.29	123.06	118.30
2	1-N	41	ASP	CB-CG-OD2	5.28	123.06	118.30
1	1-G	203	ASP	CB-CG-OD2	5.27	123.05	118.30
2	1-H	453	ASP	CB-CG-OD2	5.27	123.04	118.30
2	2-H	453	ASP	CB-CG-OD2	5.27	123.04	118.30
1	1-G	43	ASP	CB-CG-OD2	5.27	123.04	118.30
2	1-N	453	ASP	CB-CG-OD2	5.26	123.04	118.30
2	1-N	352	ASP	CB-CG-OD2	5.26	123.03	118.30
2	1-M	328	ASP	CB-CG-OD2	5.25	123.03	118.30
2	2-M	328	ASP	CB-CG-OD2	5.25	123.03	118.30
2	1-J	328	ASP	CB-CG-OD2	5.25	123.02	118.30
2	2-J	328	ASP	CB-CG-OD2	5.25	123.02	118.30
1	1-F	68	ASP	CB-CG-OD2	5.23	123.01	118.30
1	2-F	68	ASP	CB-CG-OD2	5.23	123.01	118.30
2	1-I	352	ASP	CB-CG-OD2	5.23	123.00	118.30
2	1-K	89	ASP	CB-CG-OD2	5.23	123.00	118.30
2	2-I	352	ASP	CB-CG-OD2	5.23	123.00	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2-K	89	ASP	CB-CG-OD2	5.23	123.00	118.30
1	2-G	68	ASP	CB-CG-OD2	5.22	123.00	118.30
2	1-M	448	ASP	CB-CG-OD2	5.22	122.99	118.30
2	1-M	491	ASP	CB-CG-OD2	5.22	122.99	118.30
2	2-M	448	ASP	CB-CG-OD2	5.22	122.99	118.30
2	2-M	491	ASP	CB-CG-OD2	5.22	122.99	118.30
1	1-D	203	ASP	CB-CG-OD2	5.21	122.99	118.30
1	2-D	203	ASP	CB-CG-OD2	5.21	122.99	118.30
2	2-N	526	ASP	CB-CG-OD2	5.20	122.98	118.30
2	2-N	453	ASP	CB-CG-OD2	5.20	122.98	118.30
1	1-G	33	ASP	CB-CG-OD2	5.20	122.98	118.30
2	1-K	299	ASP	CB-CG-OD2	5.19	122.97	118.30
2	2-K	299	ASP	CB-CG-OD2	5.19	122.97	118.30
2	1-N	60	ASP	CB-CG-OD2	5.19	122.97	118.30
2	1-M	325	ASP	CB-CG-OD2	5.18	122.96	118.30
2	2-M	325	ASP	CB-CG-OD2	5.18	122.96	118.30
2	1-N	405	ASP	CB-CG-OD2	5.18	122.96	118.30
2	1-K	352	ASP	CB-CG-OD2	5.16	122.95	118.30
2	2-K	352	ASP	CB-CG-OD2	5.16	122.95	118.30
2	2-N	89	ASP	CB-CG-OD2	5.16	122.94	118.30
2	1-K	491	ASP	CB-CG-OD2	5.15	122.94	118.30
2	2-K	491	ASP	CB-CG-OD2	5.15	122.94	118.30
2	1-J	269	ASP	CB-CG-OD2	5.15	122.94	118.30
1	1-G	68	ASP	CB-CG-OD2	5.15	122.94	118.30
2	2-J	269	ASP	CB-CG-OD2	5.15	122.94	118.30
2	2-N	448	ASP	CB-CG-OD2	5.15	122.94	118.30
2	2-N	346	ASP	CB-CG-OD2	5.13	122.92	118.30
1	1-F	33	ASP	CB-CG-OD2	5.13	122.92	118.30
1	2-F	33	ASP	CB-CG-OD2	5.13	122.92	118.30
2	1-N	526	ASP	CB-CG-OD2	5.12	122.91	118.30
2	1-M	298	ASP	CB-CG-OD2	5.12	122.91	118.30
2	2-M	298	ASP	CB-CG-OD2	5.12	122.91	118.30
2	2-N	363	ASP	CB-CG-OD2	5.12	122.91	118.30
2	1-N	165	ASP	CB-CG-OD2	5.12	122.90	118.30
2	2-N	60	ASP	CB-CG-OD2	5.11	122.90	118.30
2	1-H	511	ASP	CB-CG-OD2	5.11	122.90	118.30
2	2-H	511	ASP	CB-CG-OD2	5.11	122.90	118.30
2	1-I	363	ASP	CB-CG-OD2	5.11	122.90	118.30
2	2-I	363	ASP	CB-CG-OD2	5.11	122.90	118.30
1	1-D	252	ASP	CB-CG-OD2	5.10	122.89	118.30
2	1-N	88	ASP	CB-CG-OD2	5.10	122.89	118.30
1	2-D	252	ASP	CB-CG-OD2	5.10	122.89	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1-K	364	ASP	CB-CG-OD2	5.09	122.88	118.30
2	1-N	491	ASP	CB-CG-OD2	5.09	122.88	118.30
2	2-K	364	ASP	CB-CG-OD2	5.09	122.88	118.30
2	1-K	405	ASP	CB-CG-OD2	5.07	122.86	118.30
2	1-M	19	ASP	CB-CG-OD2	5.07	122.86	118.30
2	2-K	405	ASP	CB-CG-OD2	5.07	122.86	118.30
2	2-M	19	ASP	CB-CG-OD2	5.07	122.86	118.30
1	1-C	203	ASP	CB-CG-OD2	5.06	122.86	118.30
1	2-C	203	ASP	CB-CG-OD2	5.06	122.86	118.30
2	1-M	41	ASP	CB-CG-OD2	5.06	122.85	118.30
2	1-N	63	ASP	CB-CG-OD2	5.06	122.85	118.30
2	2-M	41	ASP	CB-CG-OD2	5.06	122.85	118.30
2	1-I	41	ASP	CB-CG-OD2	5.05	122.85	118.30
2	2-I	41	ASP	CB-CG-OD2	5.05	122.85	118.30
2	1-M	269	ASP	CB-CG-OD2	5.02	122.82	118.30
2	2-M	269	ASP	CB-CG-OD2	5.02	122.82	118.30
1	1-D	255	ASP	CB-CG-OD2	5.01	122.81	118.30
1	2-D	255	ASP	CB-CG-OD2	5.01	122.81	118.30
2	1-I	298	ASP	CB-CG-OD2	5.00	122.80	118.30
2	1-K	63	ASP	CB-CG-OD2	5.00	122.80	118.30
2	2-I	298	ASP	CB-CG-OD2	5.00	122.80	118.30
2	2-K	63	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1970	0	1910	30	1
1	1-B	1971	0	1914	22	0
1	1-C	1952	0	1891	14	0
1	1-D	1971	0	1914	26	0
1	1-F	1952	0	1891	25	0
1	1-G	1970	0	1910	62	0
1	2-A	1970	0	1910	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2-B	1971	0	1914	21	0
1	2-C	1952	0	1891	14	0
1	2-D	1971	0	1914	26	0
1	2-F	1952	0	1891	28	0
1	2-G	1970	0	1910	67	0
2	1-H	4167	0	4140	52	0
2	1-I	4166	0	4139	45	0
2	1-J	4162	0	4139	57	0
2	1-K	4162	0	4139	52	0
2	1-M	4166	0	4139	57	0
2	1-N	4167	0	4140	60	1
2	2-H	4167	0	4140	52	0
2	2-I	4166	0	4139	45	0
2	2-J	4162	0	4139	57	0
2	2-K	4162	0	4139	52	0
2	2-M	4166	0	4139	57	0
2	2-N	4167	0	4140	80	0
3	1-H	1	0	0	0	0
3	1-I	1	0	0	0	0
3	1-J	1	0	0	0	0
3	1-K	1	0	0	0	0
3	1-M	1	0	0	0	0
3	1-N	1	0	0	0	0
3	2-H	1	0	0	0	0
3	2-I	1	0	0	0	0
3	2-J	1	0	0	0	0
3	2-K	1	0	0	0	0
3	2-M	1	0	0	0	0
3	2-N	1	0	0	0	0
4	1-H	1	0	0	0	0
4	1-I	1	0	0	0	0
4	1-J	1	0	0	0	0
4	1-K	1	0	0	0	0
4	1-M	1	0	0	0	0
4	1-N	1	0	0	0	0
4	2-H	1	0	0	0	0
4	2-I	1	0	0	0	0
4	2-J	1	0	0	0	0
4	2-K	1	0	0	0	0
4	2-M	1	0	0	0	0
4	2-N	1	0	0	0	0
5	1-A	16	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1-B	16	0	0	0	0
5	1-C	16	0	0	0	0
5	1-D	16	0	0	0	0
5	1-F	16	0	0	0	0
5	1-G	16	0	0	0	0
5	2-A	16	0	0	0	0
5	2-B	16	0	0	0	0
5	2-C	16	0	0	0	0
5	2-D	16	0	0	0	0
5	2-F	16	0	0	0	0
5	2-G	16	0	0	1	0
6	1-A	7	0	0	0	0
6	1-B	7	0	0	0	0
6	1-C	7	0	0	0	0
6	1-D	7	0	0	0	0
6	1-F	7	0	0	0	0
6	1-G	7	0	0	0	0
6	2-A	7	0	0	0	0
6	2-B	7	0	0	0	0
6	2-C	7	0	0	0	0
6	2-D	7	0	0	0	0
6	2-F	7	0	0	0	0
6	2-G	7	0	0	0	0
7	1-H	7	0	0	0	0
7	1-I	7	0	0	0	0
7	1-J	7	0	0	0	0
7	1-K	7	0	0	0	0
7	1-M	7	0	0	1	0
7	1-N	7	0	0	2	0
7	2-H	7	0	0	0	0
7	2-I	7	0	0	0	0
7	2-J	7	0	0	0	0
7	2-K	7	0	0	0	0
7	2-M	7	0	0	1	0
7	2-N	7	0	0	3	0
8	1-A	122	0	0	3	0
8	1-B	83	0	0	1	0
8	1-C	120	0	0	1	0
8	1-D	149	0	0	4	0
8	1-F	108	0	0	2	0
8	1-G	59	0	0	10	0
8	1-H	245	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	1-I	218	0	0	3	0
8	1-J	208	0	0	3	0
8	1-K	253	0	0	6	0
8	1-M	183	0	0	2	0
8	1-N	138	0	0	1	0
8	2-A	122	0	0	3	0
8	2-B	84	0	0	1	0
8	2-C	120	0	0	1	0
8	2-D	148	0	0	4	0
8	2-F	109	0	0	2	0
8	2-G	58	0	0	8	0
8	2-H	245	0	0	2	0
8	2-I	218	0	0	3	0
8	2-J	208	0	0	3	0
8	2-K	253	0	0	6	0
8	2-M	183	0	0	2	0
8	2-N	124	0	0	2	0
All	All	77694	0	72532	977	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (977) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:342:ALA:HB1	2:N:343:PRO:CD	1.55	1.33
1:G:177:LEU:HD23	1:G:178:PHE:CE2	1.78	1.17
1:G:177:LEU:HD23	1:G:178:PHE:CZ	1.79	1.16
2:N:342:ALA:CB	2:N:343:PRO:HD2	1.79	1.12
2:N:43:TRP:CZ2	2:N:365:LYS:HE2	1.84	1.10
2:N:342:ALA:O	8:N:5596:HOH:O	1.77	1.02
2:J:448:ASP:O	2:J:452:LYS:HE3	1.62	0.99
2:J:448:ASP:O	2:J:452:LYS:HE3	1.62	0.99
2:N:342:ALA:CB	2:N:343:PRO:CD	2.37	0.99
2:N:342:ALA:HB1	2:N:343:PRO:HD2	1.02	0.99
2:N:497:VAL:HG11	2:N:546:CYS:SG	2.07	0.95
1:G:88:MET:CE	2:N:362:LEU:HD13	2.01	0.91
1:D:61:HIS:HE1	1:D:100:LYS:NZ	1.69	0.89
1:D:61:HIS:HE1	1:D:100:LYS:NZ	1.69	0.89
2:J:497:VAL:CG1	2:J:498:PRO:HD2	2.05	0.86
2:J:497:VAL:CG1	2:J:498:PRO:HD2	2.05	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:497:VAL:CG1	2:I:498:PRO:HD2	2.06	0.85
2:I:497:VAL:CG1	2:I:498:PRO:HD2	2.06	0.85
1:F:135:GLU:HA	2:N:328:ASP:CG	1.97	0.85
1:G:135:GLU:OE1	8:G:5276:HOH:O	1.95	0.85
2:N:543:CYS:SG	2:N:546:CYS:HB2	2.18	0.83
2:J:448:ASP:O	2:J:452:LYS:CE	2.26	0.83
2:J:448:ASP:O	2:J:452:LYS:CE	2.26	0.83
1:G:177:LEU:CD2	1:G:178:PHE:CZ	2.62	0.82
2:J:497:VAL:HG13	2:J:498:PRO:HD2	1.60	0.82
2:J:497:VAL:HG13	2:J:498:PRO:HD2	1.60	0.82
1:G:135:GLU:OE1	8:G:5276:HOH:O	1.97	0.82
2:J:178:ILE:HG23	8:J:2690:HOH:O	1.80	0.82
2:J:178:ILE:HG23	8:J:695:HOH:O	1.80	0.82
2:H:406:MET:HE3	2:H:410:LYS:HG3	1.62	0.81
2:H:406:MET:HE3	2:H:410:LYS:HG3	1.62	0.81
2:N:342:ALA:HB1	2:N:343:PRO:HD3	1.60	0.80
1:G:88:MET:HE2	2:N:362:LEU:HD13	1.63	0.79
2:K:497:VAL:CG1	2:K:498:PRO:HD2	2.12	0.79
2:K:497:VAL:CG1	2:K:498:PRO:HD2	2.12	0.79
1:D:140:LYS:HE3	8:D:3422:HOH:O	1.83	0.79
1:D:140:LYS:HE3	8:D:3422:HOH:O	1.83	0.79
1:G:115:SER:O	1:G:133:VAL:HG23	1.82	0.78
2:N:497:VAL:CG1	2:N:498:PRO:HD2	2.13	0.78
2:I:5:LYS:N	2:I:6:PRO:HD2	2.00	0.77
2:I:5:LYS:N	2:I:6:PRO:HD2	2.00	0.77
2:N:43:TRP:CZ2	2:N:365:LYS:CE	2.66	0.76
1:G:115:SER:O	1:G:133:VAL:HG23	1.86	0.76
2:N:497:VAL:CG1	2:N:498:PRO:HD2	2.15	0.76
1:G:136:ALA:O	8:G:5287:HOH:O	2.03	0.76
1:F:14:ASN:ND2	1:F:94:MET:HB3	2.01	0.76
1:F:14:ASN:ND2	1:F:94:MET:HB3	2.01	0.76
2:J:333:TYR:OH	2:J:378:GLY:HA2	1.87	0.75
2:J:333:TYR:OH	2:J:378:GLY:HA2	1.87	0.75
1:G:177:LEU:CD2	1:G:178:PHE:CE2	2.66	0.75
1:G:217:GLY:O	1:G:219:LYS:HD3	1.87	0.74
2:N:25:GLU:OE1	2:N:543:CYS:SG	2.46	0.73
2:J:267:ILE:HB	2:J:268:PRO:HD3	1.70	0.73
2:J:267:ILE:HB	2:J:268:PRO:HD3	1.70	0.73
2:I:497:VAL:HG13	2:I:498:PRO:HD2	1.69	0.73
2:I:497:VAL:HG13	2:I:498:PRO:HD2	1.69	0.73
2:M:497:VAL:CG1	2:M:498:PRO:HD2	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:497:VAL:CG1	2:M:498:PRO:HD2	2.18	0.73
2:J:353:GLY:HA3	2:J:494:GLN:HG3	1.71	0.73
2:J:353:GLY:HA3	2:J:494:GLN:HG3	1.71	0.73
2:J:134:LEU:HD22	2:J:168:LYS:HG3	1.71	0.72
2:J:134:LEU:HD22	2:J:168:LYS:HG3	1.71	0.72
2:N:497:VAL:HG13	2:N:498:PRO:HD2	1.69	0.72
1:A:223:THR:HG21	1:A:247:GLY:HA2	1.71	0.72
1:A:223:THR:HG21	1:A:247:GLY:HA2	1.71	0.72
1:F:135:GLU:OE1	8:F:4279:HOH:O	2.06	0.71
1:F:135:GLU:OE1	8:F:4279:HOH:O	2.06	0.71
1:D:61:HIS:HE1	1:D:100:LYS:HZ2	1.37	0.71
1:D:61:HIS:HE1	1:D:100:LYS:HZ2	1.37	0.71
2:K:497:VAL:HG12	2:K:498:PRO:HD2	1.72	0.70
2:K:497:VAL:HG12	2:K:498:PRO:HD2	1.72	0.70
1:F:135:GLU:HG2	2:N:328:ASP:HB2	1.72	0.70
2:N:497:VAL:HG13	2:N:498:PRO:HD2	1.71	0.70
1:G:236:ASN:OD1	1:G:240:GLN:HB3	1.91	0.69
2:N:364:ASP:OD2	2:N:366:ASP:N	2.26	0.69
1:G:128:SER:OG	8:G:5272:HOH:O	2.11	0.68
2:M:19:ASP:OD2	2:M:29:ARG:HD2	1.93	0.68
2:M:19:ASP:OD2	2:M:29:ARG:HD2	1.93	0.68
1:G:136:ALA:O	8:G:5287:HOH:O	2.11	0.68
1:G:145:PRO:HG3	1:G:174:ARG:CD	2.24	0.68
2:H:406:MET:CE	2:H:410:LYS:HG3	2.23	0.68
2:H:406:MET:CE	2:H:410:LYS:HG3	2.23	0.68
1:D:61:HIS:HE1	1:D:100:LYS:HZ1	1.40	0.68
1:D:61:HIS:HE1	1:D:100:LYS:HZ1	1.40	0.68
2:K:144:LEU:HD23	2:K:144:LEU:O	1.94	0.67
2:K:144:LEU:HD23	2:K:144:LEU:O	1.94	0.67
2:N:72:CYS:HB3	2:N:75:CYS:SG	2.35	0.67
2:N:271:LEU:HD13	2:N:410:LYS:HD3	1.77	0.67
1:D:61:HIS:CE1	1:D:100:LYS:NZ	2.59	0.67
1:D:61:HIS:CE1	1:D:100:LYS:NZ	2.59	0.67
2:H:497:VAL:CG1	2:H:498:PRO:HD2	2.24	0.66
2:H:497:VAL:CG1	2:H:498:PRO:HD2	2.24	0.66
2:M:497:VAL:HG12	2:M:498:PRO:HD2	1.78	0.66
2:M:497:VAL:HG12	2:M:498:PRO:HD2	1.78	0.66
2:I:497:VAL:HG12	2:I:498:PRO:HD2	1.78	0.65
2:I:497:VAL:HG12	2:I:498:PRO:HD2	1.78	0.65
2:I:5:LYS:N	2:I:6:PRO:CD	2.59	0.65
2:I:5:LYS:N	2:I:6:PRO:CD	2.59	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:PRO:HG3	1:G:174:ARG:CD	2.25	0.65
2:N:497:VAL:CG1	2:N:546:CYS:SG	2.83	0.65
2:H:223:GLY:HA2	2:H:231:PHE:CD2	2.32	0.64
2:H:223:GLY:HA2	2:H:231:PHE:CD2	2.32	0.64
8:I:1650:HOH:O	2:K:410:LYS:HE3	1.97	0.64
1:G:237:TRP:CZ2	1:G:239:VAL:HB	2.33	0.64
1:G:13:HIS:ND1	8:G:5316:HOH:O	2.30	0.64
8:I:655:HOH:O	2:K:410:LYS:HE3	1.97	0.64
2:N:72:CYS:SG	2:N:75:CYS:SG	2.96	0.63
1:G:214:TYR:CE2	1:G:263:GLN:NE2	2.67	0.63
2:J:127:TRP:CZ2	2:J:535:ARG:HG2	2.34	0.62
1:A:237:TRP:CH2	1:A:239:VAL:HB	2.33	0.62
2:J:127:TRP:CZ2	2:J:535:ARG:HG2	2.34	0.62
1:A:237:TRP:CH2	1:A:239:VAL:HB	2.33	0.62
2:M:530:PRO:HB2	2:M:533:ILE:HD12	1.81	0.62
2:M:530:PRO:HB2	2:M:533:ILE:HD12	1.81	0.62
2:N:364:ASP:C	2:N:364:ASP:OD2	2.38	0.62
2:K:395:LYS:HE3	8:K:3787:HOH:O	2.00	0.62
2:K:395:LYS:HE3	8:K:797:HOH:O	2.00	0.62
1:A:98:THR:HG22	1:A:137:LEU:HD11	1.82	0.61
1:A:98:THR:HG22	1:A:137:LEU:HD11	1.82	0.61
2:M:411:LEU:O	2:M:413:VAL:HG13	1.99	0.61
2:M:411:LEU:O	2:M:413:VAL:HG13	1.99	0.61
1:F:157:ALA:O	1:F:161:VAL:HG23	2.00	0.61
1:G:258:THR:HA	1:G:259:PRO:C	2.19	0.61
1:F:157:ALA:O	1:F:161:VAL:HG23	2.00	0.61
2:J:497:VAL:HG12	2:J:498:PRO:HD2	1.83	0.61
2:J:497:VAL:HG12	2:J:498:PRO:HD2	1.83	0.61
2:M:511:ASP:HA	8:M:4721:HOH:O	1.99	0.61
1:G:205:GLU:O	1:G:209:LYS:HG3	2.00	0.61
2:M:511:ASP:HA	8:M:731:HOH:O	1.99	0.61
2:K:497:VAL:HG13	2:K:498:PRO:HD2	1.83	0.61
2:K:270:LEU:HD11	2:K:425:THR:HG22	1.83	0.61
2:K:497:VAL:HG13	2:K:498:PRO:HD2	1.83	0.61
1:G:220:GLY:N	1:G:221:PRO:CD	2.64	0.61
2:K:270:LEU:HD11	2:K:425:THR:HG22	1.83	0.61
2:H:393:TYR:CE1	2:H:401:LYS:HD3	2.36	0.61
2:H:393:TYR:CE1	2:H:401:LYS:HD3	2.36	0.61
2:H:454:ASN:H	2:H:454:ASN:HD22	1.49	0.60
2:H:454:ASN:HD22	2:H:454:ASN:H	1.49	0.60
2:H:127:TRP:CZ3	2:H:535:ARG:HD3	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:127:TRP:CZ3	2:H:535:ARG:HD3	2.36	0.60
2:N:278:LYS:NZ	2:N:278:LYS:HB3	2.16	0.60
1:G:258:THR:HA	1:G:259:PRO:C	2.21	0.60
1:G:220:GLY:N	1:G:221:PRO:CD	2.63	0.60
1:D:61:HIS:CE1	1:D:100:LYS:HZ2	2.19	0.60
1:D:61:HIS:CE1	1:D:100:LYS:HZ2	2.19	0.60
1:G:18:THR:O	1:G:18:THR:HG22	2.02	0.60
2:I:474:ALA:HB1	2:I:475:PRO:HD2	1.84	0.60
2:I:474:ALA:HB1	2:I:475:PRO:HD2	1.84	0.60
1:F:138:GLY:HA2	2:N:330:GLY:N	2.16	0.60
2:H:97:ALA:O	2:H:101:MET:HG3	2.02	0.59
2:H:97:ALA:O	2:H:101:MET:HG3	2.02	0.59
1:G:128:SER:OG	8:G:5272:HOH:O	2.17	0.59
1:G:18:THR:O	1:G:18:THR:HG22	2.02	0.59
1:G:13:HIS:ND1	8:G:5316:HOH:O	2.31	0.59
1:G:227:CYS:N	1:G:228:PRO:HD2	2.18	0.59
2:K:386:LEU:HD11	2:K:390:PHE:CE1	2.37	0.59
2:M:69:GLN:OE1	2:M:228:HIS:HA	2.03	0.59
2:K:386:LEU:HD11	2:K:390:PHE:CE1	2.37	0.59
2:M:69:GLN:OE1	2:M:228:HIS:HA	2.03	0.59
2:M:386:LEU:HD11	2:M:390:PHE:CE1	2.37	0.59
2:M:386:LEU:HD11	2:M:390:PHE:CE1	2.37	0.59
2:N:72:CYS:CB	2:N:75:CYS:SG	2.91	0.59
2:I:304:LYS:O	2:I:308:THR:HG23	2.02	0.59
2:I:304:LYS:O	2:I:308:THR:HG23	2.02	0.59
2:N:101:MET:HB2	2:N:446:MET:HG3	1.84	0.58
1:G:157:ALA:O	1:G:161:VAL:HG23	2.03	0.58
2:I:246:ASP:HB2	2:I:247:PRO:HD3	1.86	0.58
1:F:135:GLU:OE2	2:N:326:ASN:ND2	2.37	0.58
2:I:246:ASP:HB2	2:I:247:PRO:HD3	1.86	0.58
2:H:149:ALA:HB1	2:H:150:PRO:CD	2.34	0.58
1:A:254:TRP:HH2	2:H:70:ARG:HD3	1.68	0.58
2:H:149:ALA:HB1	2:H:150:PRO:CD	2.34	0.58
1:A:254:TRP:HH2	2:H:70:ARG:HD3	1.68	0.58
2:N:403:VAL:O	2:N:407:VAL:HG23	2.03	0.58
2:J:296:ALA:HA	2:J:309:SER:HA	1.85	0.58
2:M:140:LYS:HG2	2:M:196:GLU:HG2	1.85	0.58
2:M:296:ALA:HA	2:M:309:SER:HA	1.84	0.58
1:A:135:GLU:OE1	8:A:279:HOH:O	2.17	0.58
1:G:230:VAL:O	1:G:231:LEU:HB2	2.04	0.58
2:J:296:ALA:HA	2:J:309:SER:HA	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:140:LYS:HG2	2:M:196:GLU:HG2	1.85	0.58
2:M:296:ALA:HA	2:M:309:SER:HA	1.84	0.58
1:A:135:GLU:OE1	8:A:279:HOH:O	2.17	0.58
2:I:275:GLY:O	2:I:278:LYS:HG3	2.03	0.58
2:I:275:GLY:O	2:I:278:LYS:HG3	2.03	0.58
2:K:274:ALA:CB	2:K:422:LEU:HD11	2.34	0.58
2:K:274:ALA:HB1	2:K:422:LEU:HD11	1.86	0.58
1:G:17:CYS:HB2	2:N:73:GLY:N	2.19	0.58
2:K:274:ALA:CB	2:K:422:LEU:HD11	2.34	0.58
2:K:274:ALA:HB1	2:K:422:LEU:HD11	1.86	0.58
1:F:135:GLU:HA	2:N:328:ASP:OD2	2.04	0.58
2:I:29:ARG:HB3	2:I:45:SER:HB3	1.85	0.57
2:I:29:ARG:HB3	2:I:45:SER:HB3	1.85	0.57
1:D:61:HIS:CE1	1:D:100:LYS:HZ1	2.20	0.57
1:D:61:HIS:CE1	1:D:100:LYS:HZ1	2.20	0.57
1:G:157:ALA:O	1:G:161:VAL:HG23	2.03	0.57
2:J:451:ALA:HB3	2:J:452:LYS:HE2	1.85	0.57
2:H:336:VAL:HG12	2:H:372:LYS:HG2	1.86	0.57
2:J:451:ALA:HB3	2:J:452:LYS:HE2	1.85	0.57
2:H:336:VAL:HG12	2:H:372:LYS:HG2	1.86	0.57
1:G:88:MET:CE	2:N:362:LEU:CD1	2.78	0.57
2:H:140:LYS:NZ	2:J:464:GLU:OE1	2.38	0.57
2:M:474:ALA:HB1	2:M:475:PRO:HD2	1.87	0.57
2:H:140:LYS:NZ	2:J:464:GLU:OE1	2.38	0.57
2:M:474:ALA:HB1	2:M:475:PRO:HD2	1.87	0.57
2:N:246:ASP:HB2	2:N:247:PRO:HD3	1.87	0.57
2:I:530:PRO:HB2	2:I:533:ILE:HD12	1.85	0.57
2:I:530:PRO:HB2	2:I:533:ILE:HD12	1.85	0.57
1:A:223:THR:CG2	1:A:247:GLY:HA2	2.35	0.57
2:H:144:LEU:C	2:H:144:LEU:HD23	2.25	0.57
1:G:139:VAL:HG11	8:G:5293:HOH:O	2.03	0.57
1:A:223:THR:CG2	1:A:247:GLY:HA2	2.35	0.57
2:H:144:LEU:C	2:H:144:LEU:HD23	2.25	0.57
2:H:246:ASP:HB2	2:H:247:PRO:HD3	1.86	0.57
2:H:246:ASP:HB2	2:H:247:PRO:HD3	1.86	0.57
1:G:225:ASN:HD22	1:G:249:SER:HB3	1.70	0.57
1:G:227:CYS:N	1:G:228:PRO:HD2	2.19	0.57
2:N:454:ASN:H	2:N:454:ASN:HD22	1.53	0.56
1:B:4:LYS:O	1:B:4:LYS:HD3	2.05	0.56
1:G:237:TRP:CD1	1:G:240:GLN:HB2	2.40	0.56
1:B:140:LYS:NZ	2:N:151:ALA:HB2	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LYS:HD3	1:B:4:LYS:O	2.05	0.56
2:M:349:HIS:ND1	2:M:350:PRO:HD2	2.21	0.56
2:M:134:LEU:HD22	2:M:168:LYS:HG3	1.88	0.56
2:M:349:HIS:ND1	2:M:350:PRO:HD2	2.21	0.56
2:M:134:LEU:HD22	2:M:168:LYS:HG3	1.88	0.56
2:N:246:ASP:HB2	2:N:247:PRO:HD3	1.87	0.56
1:G:223:THR:HG21	1:G:247:GLY:HA2	1.85	0.56
2:J:462:MET:O	2:J:488:LYS:HE3	2.05	0.56
2:J:462:MET:O	2:J:488:LYS:HE3	2.05	0.56
2:M:497:VAL:HG13	2:M:498:PRO:HD2	1.86	0.56
2:H:149:ALA:HB1	2:H:150:PRO:HD2	1.86	0.56
2:K:246:ASP:HB2	2:K:247:PRO:HD3	1.87	0.56
2:M:497:VAL:HG13	2:M:498:PRO:HD2	1.86	0.56
2:H:149:ALA:HB1	2:H:150:PRO:HD2	1.86	0.56
2:K:246:ASP:HB2	2:K:247:PRO:HD3	1.87	0.56
2:K:166:LYS:HE3	8:K:3741:HOH:O	2.05	0.56
2:K:166:LYS:HE3	8:K:751:HOH:O	2.05	0.56
1:F:47:THR:O	2:M:23:ARG:HA	2.05	0.55
1:F:47:THR:O	2:M:23:ARG:HA	2.05	0.55
2:J:144:LEU:O	2:J:148:ILE:HG12	2.05	0.55
2:N:72:CYS:HB3	2:N:75:CYS:SG	2.46	0.55
2:J:144:LEU:O	2:J:148:ILE:HG12	2.05	0.55
2:I:267:ILE:HD13	2:I:267:ILE:N	2.22	0.55
1:G:17:CYS:HB2	2:N:72:CYS:HA	1.88	0.55
2:I:267:ILE:N	2:I:267:ILE:HD13	2.22	0.55
1:G:117:TYR:HE2	1:G:145:PRO:HB3	1.71	0.55
2:I:474:ALA:HB1	2:I:475:PRO:CD	2.37	0.55
2:N:264:GLU:O	2:N:268:PRO:HG2	2.07	0.55
2:M:401:LYS:NZ	2:M:405:ASP:OD2	2.40	0.55
2:I:474:ALA:HB1	2:I:475:PRO:CD	2.37	0.55
2:M:401:LYS:NZ	2:M:405:ASP:OD2	2.40	0.55
1:D:145:PRO:HD2	1:D:179:TYR:CZ	2.40	0.55
2:I:265:CYS:C	2:I:268:PRO:HD2	2.27	0.55
1:D:145:PRO:HD2	1:D:179:TYR:CZ	2.40	0.55
2:I:265:CYS:C	2:I:268:PRO:HD2	2.27	0.55
1:G:17:CYS:HB2	2:N:73:GLY:N	2.22	0.55
2:H:497:VAL:HG13	2:H:498:PRO:HD2	1.87	0.55
2:H:497:VAL:HG13	2:H:498:PRO:HD2	1.87	0.55
2:M:380:ALA:HB1	2:M:514:PRO:HD3	1.87	0.55
2:M:380:ALA:HB1	2:M:514:PRO:HD3	1.87	0.55
1:G:117:TYR:HE2	1:G:145:PRO:HB3	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:474:ALA:HB1	2:N:475:PRO:HD2	1.89	0.55
2:M:349:HIS:CE1	2:M:350:PRO:HD2	2.43	0.54
2:M:349:HIS:CE1	2:M:350:PRO:HD2	2.43	0.54
1:G:254:TRP:HH2	2:N:70:ARG:HD3	1.71	0.54
1:G:189:ARG:HD3	1:G:210:GLY:O	2.06	0.54
2:J:77:TYR:CD2	2:J:106:VAL:HG12	2.43	0.54
1:F:18:THR:OG1	2:M:25:GLU:HG2	2.07	0.54
2:J:77:TYR:CD2	2:J:106:VAL:HG12	2.43	0.54
1:F:18:THR:OG1	2:M:25:GLU:HG2	2.07	0.54
2:N:338:TYR:HA	2:N:366:ASP:O	2.08	0.54
2:N:474:ALA:HB1	2:N:475:PRO:HD2	1.88	0.54
2:J:353:GLY:HA3	2:J:494:GLN:CG	2.38	0.54
2:I:8:PRO:HB2	2:I:525:ALA:HB2	1.89	0.54
2:J:353:GLY:HA3	2:J:494:GLN:CG	2.38	0.54
2:I:8:PRO:HB2	2:I:525:ALA:HB2	1.89	0.54
1:A:258:THR:HA	1:A:259:PRO:C	2.29	0.54
1:A:258:THR:HA	1:A:259:PRO:C	2.29	0.54
1:G:190:LEU:N	1:G:191:PRO:CD	2.71	0.53
2:N:239:ASN:OD1	8:N:590:HOH:O	2.18	0.53
1:C:47:THR:O	2:J:23:ARG:HA	2.08	0.53
2:K:267:ILE:HB	2:K:268:PRO:HD3	1.89	0.53
1:C:47:THR:O	2:J:23:ARG:HA	2.08	0.53
2:K:267:ILE:HB	2:K:268:PRO:HD3	1.89	0.53
2:K:329:LEU:HD11	2:K:471:LEU:HD11	1.91	0.53
2:K:329:LEU:HD11	2:K:471:LEU:HD11	1.91	0.53
1:G:14:ASN:ND2	1:G:94:MET:HB3	2.23	0.53
1:B:118:GLY:HA3	1:B:122:LYS:HD3	1.90	0.53
1:G:17:CYS:HB2	2:N:73:GLY:H	1.73	0.53
1:B:118:GLY:HA3	1:B:122:LYS:HD3	1.90	0.53
2:K:144:LEU:C	2:K:144:LEU:CD2	2.77	0.53
2:K:144:LEU:CD2	2:K:144:LEU:C	2.77	0.53
2:N:448:ASP:O	2:N:452:LYS:HG3	2.08	0.53
1:B:208:LYS:HG2	2:I:240:TYR:CE1	2.44	0.53
1:B:208:LYS:HG2	2:I:240:TYR:CE1	2.44	0.53
2:M:372:LYS:NZ	8:M:4592:HOH:O	2.31	0.53
2:M:267:ILE:HB	2:M:268:PRO:HD3	1.91	0.53
1:B:258:THR:HA	1:B:259:PRO:C	2.29	0.53
2:M:403:VAL:HG12	2:M:430:ILE:HG23	1.90	0.53
2:I:541:ASP:N	2:I:542:PRO:HD3	2.23	0.53
2:M:372:LYS:NZ	8:M:606:HOH:O	2.31	0.53
2:M:267:ILE:HB	2:M:268:PRO:HD3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:THR:HA	1:B:259:PRO:C	2.29	0.53
2:M:403:VAL:HG12	2:M:430:ILE:HG23	1.90	0.53
2:I:541:ASP:N	2:I:542:PRO:HD3	2.23	0.53
1:A:66:GLY:O	8:A:287:HOH:O	2.18	0.53
1:G:243:HIS:CG	1:G:244:PRO:HD2	2.44	0.53
1:A:66:GLY:O	8:A:287:HOH:O	2.18	0.53
1:G:91:GLY:HA2	2:N:362:LEU:HD21	1.90	0.53
2:M:348:LYS:HG3	2:M:354:VAL:HG23	1.90	0.52
2:M:348:LYS:HG3	2:M:354:VAL:HG23	1.90	0.52
2:I:223:GLY:HA2	2:I:231:PHE:CD2	2.45	0.52
1:D:78:LEU:O	1:D:130:ALA:HA	2.10	0.52
2:I:223:GLY:HA2	2:I:231:PHE:CD2	2.45	0.52
1:D:78:LEU:O	1:D:130:ALA:HA	2.10	0.52
2:H:144:LEU:O	2:H:144:LEU:HD23	2.10	0.52
1:G:42:LEU:HD21	1:G:45:GLN:HG3	1.91	0.52
2:H:144:LEU:O	2:H:144:LEU:HD23	2.10	0.52
1:D:159:VAL:O	1:D:163:THR:HG23	2.09	0.52
1:D:258:THR:HA	1:D:259:PRO:C	2.30	0.52
1:D:159:VAL:O	1:D:163:THR:HG23	2.09	0.52
1:D:258:THR:HA	1:D:259:PRO:C	2.30	0.52
1:G:226:ASN:O	1:G:230:VAL:HG22	2.09	0.52
1:C:258:THR:HA	1:C:259:PRO:C	2.30	0.52
1:B:220:GLY:N	1:B:221:PRO:CD	2.73	0.52
1:C:258:THR:HA	1:C:259:PRO:C	2.30	0.52
1:B:220:GLY:N	1:B:221:PRO:CD	2.73	0.52
2:H:497:VAL:HG12	2:H:498:PRO:HD2	1.92	0.52
2:H:146:ALA:HB2	8:H:718:HOH:O	2.08	0.52
2:H:497:VAL:HG12	2:H:498:PRO:HD2	1.92	0.52
2:H:146:ALA:HB2	8:H:716:HOH:O	2.08	0.52
2:I:254:LEU:O	2:I:257:GLU:HB3	2.09	0.52
2:I:254:LEU:O	2:I:257:GLU:HB3	2.09	0.52
1:G:114:CYS:HA	1:G:119:GLY:HA3	1.91	0.51
2:K:8:PRO:HB2	2:K:525:ALA:HB2	1.93	0.51
1:G:114:CYS:HA	1:G:119:GLY:HA3	1.91	0.51
2:K:8:PRO:HB2	2:K:525:ALA:HB2	1.93	0.51
2:N:267:ILE:HB	2:N:268:PRO:HD3	1.93	0.51
2:N:454:ASN:H	2:N:454:ASN:HD22	1.58	0.51
2:M:513:SER:HB2	2:M:514:PRO:HD2	1.93	0.51
2:M:513:SER:HB2	2:M:514:PRO:HD2	1.93	0.51
1:F:135:GLU:CG	2:N:328:ASP:HB2	2.38	0.51
1:G:236:ASN:OD1	1:G:240:GLN:HB3	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:139:VAL:HG11	8:G:5293:HOH:O	2.10	0.51
2:J:390:PHE:CZ	2:J:419:HIS:CE1	2.99	0.51
2:J:390:PHE:CZ	2:J:419:HIS:CE1	2.99	0.51
1:A:217:GLY:O	1:A:219:LYS:HD3	2.11	0.51
1:A:233:ASN:HB3	2:H:217:SER:HA	1.92	0.51
2:N:101:MET:CB	2:N:446:MET:HG3	2.40	0.51
1:A:217:GLY:O	1:A:219:LYS:HD3	2.11	0.51
1:A:233:ASN:HB3	2:H:217:SER:HA	1.92	0.51
1:G:145:PRO:HG3	1:G:174:ARG:HD3	1.91	0.51
2:M:76:THR:O	2:M:77:TYR:HB3	2.11	0.51
2:N:513:SER:HB2	2:N:514:PRO:HD2	1.93	0.51
1:C:63:ALA:O	8:C:2311:HOH:O	2.19	0.51
2:N:498:PRO:HG2	7:N:550:FCO:N1	2.25	0.51
2:M:76:THR:O	2:M:77:TYR:HB3	2.11	0.51
1:C:63:ALA:O	8:C:2311:HOH:O	2.19	0.51
2:J:336:VAL:HG12	2:J:372:LYS:HG2	1.93	0.51
1:G:17:CYS:O	1:G:18:THR:HB	2.11	0.51
2:J:336:VAL:HG12	2:J:372:LYS:HG2	1.93	0.51
2:N:498:PRO:HG2	7:N:550:FCO:N1	2.25	0.50
2:M:349:HIS:CG	2:M:350:PRO:HD2	2.46	0.50
2:H:196:GLU:N	2:H:196:GLU:OE1	2.43	0.50
2:M:349:HIS:CG	2:M:350:PRO:HD2	2.46	0.50
2:H:196:GLU:OE1	2:H:196:GLU:N	2.43	0.50
1:F:145:PRO:HG3	1:F:174:ARG:HD3	1.93	0.50
1:G:205:GLU:O	1:G:209:LYS:HG3	2.12	0.50
2:K:350:PRO:HB2	2:K:482:TRP:CG	2.46	0.50
1:F:145:PRO:HG3	1:F:174:ARG:HD3	1.93	0.50
2:K:350:PRO:HB2	2:K:482:TRP:CG	2.46	0.50
2:M:150:PRO:HG2	2:M:264:GLU:HG2	1.92	0.50
1:F:62:GLN:NE2	8:F:4356:HOH:O	2.39	0.50
2:M:150:PRO:HG2	2:M:264:GLU:HG2	1.92	0.50
2:N:338:TYR:HA	2:N:366:ASP:O	2.11	0.50
1:F:62:GLN:NE2	8:F:4356:HOH:O	2.39	0.50
2:J:77:TYR:CE2	2:J:106:VAL:HG12	2.46	0.50
2:J:77:TYR:CE2	2:J:106:VAL:HG12	2.46	0.50
1:A:145:PRO:HG3	1:A:174:ARG:HD3	1.92	0.50
1:G:233:ASN:HA	8:G:5270:HOH:O	2.12	0.50
1:A:145:PRO:HG3	1:A:174:ARG:HD3	1.92	0.50
2:N:513:SER:HB2	2:N:514:PRO:HD2	1.94	0.50
1:G:17:CYS:HB2	2:N:72:CYS:HA	1.94	0.50
2:H:406:MET:HE3	2:H:410:LYS:CG	2.37	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:TRP:CH2	1:B:239:VAL:HB	2.46	0.50
1:D:237:TRP:CH2	1:D:239:VAL:HB	2.47	0.50
2:H:406:MET:HE3	2:H:410:LYS:CG	2.37	0.50
1:B:237:TRP:CH2	1:B:239:VAL:HB	2.46	0.50
1:D:237:TRP:CH2	1:D:239:VAL:HB	2.47	0.50
1:G:17:CYS:O	1:G:18:THR:HB	2.11	0.50
2:N:267:ILE:HB	2:N:268:PRO:HD3	1.93	0.50
1:D:230:VAL:O	1:D:231:LEU:HB2	2.12	0.50
1:D:230:VAL:O	1:D:231:LEU:HB2	2.12	0.50
1:G:146:GLY:O	1:G:149:PRO:HD3	2.12	0.50
1:G:158:VAL:O	1:G:162:LEU:HG	2.12	0.49
2:K:474:ALA:HB1	2:K:475:PRO:HD2	1.94	0.49
1:B:42:LEU:HD21	1:B:45:GLN:HG3	1.94	0.49
2:K:474:ALA:HB1	2:K:475:PRO:HD2	1.94	0.49
1:B:42:LEU:HD21	1:B:45:GLN:HG3	1.94	0.49
2:N:498:PRO:HG2	7:N:550:FCO:C1	2.42	0.49
2:K:144:LEU:C	2:K:144:LEU:HD23	2.31	0.49
8:I:1650:HOH:O	2:K:410:LYS:CE	2.57	0.49
1:B:71:TYR:CE1	1:B:106:LYS:HD2	2.47	0.49
2:K:144:LEU:HD23	2:K:144:LEU:C	2.31	0.49
8:I:655:HOH:O	2:K:410:LYS:CE	2.57	0.49
1:G:190:LEU:N	1:G:191:PRO:CD	2.74	0.49
1:B:71:TYR:CE1	1:B:106:LYS:HD2	2.47	0.49
1:C:201:SER:HA	1:C:216:LEU:HD21	1.94	0.49
1:G:47:THR:O	2:N:23:ARG:HA	2.13	0.49
1:C:201:SER:HA	1:C:216:LEU:HD21	1.94	0.49
1:B:208:LYS:HG2	2:I:240:TYR:CZ	2.47	0.49
1:G:102:ALA:HB1	1:G:108:ILE:HD11	1.95	0.49
1:B:208:LYS:HG2	2:I:240:TYR:CZ	2.47	0.49
2:N:264:GLU:O	2:N:268:PRO:HG2	2.11	0.49
1:G:42:LEU:HD21	1:G:45:GLN:HG3	1.94	0.49
2:J:497:VAL:CG1	2:J:498:PRO:CD	2.86	0.49
2:K:237:CYS:HB2	2:K:456:LEU:HG	1.93	0.49
2:J:497:VAL:CG1	2:J:498:PRO:CD	2.86	0.49
2:N:278:LYS:HZ2	2:N:278:LYS:HB3	1.78	0.49
2:N:288:ASN:HB3	2:N:381:MET:CE	2.43	0.49
2:N:296:ALA:HA	2:N:309:SER:HA	1.94	0.49
2:K:237:CYS:HB2	2:K:456:LEU:HG	1.93	0.49
2:J:513:SER:HB2	2:J:514:PRO:HD2	1.94	0.49
2:J:474:ALA:HB1	2:J:475:PRO:HD2	1.94	0.49
2:J:513:SER:HB2	2:J:514:PRO:HD2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:474:ALA:HB1	2:J:475:PRO:HD2	1.94	0.49
2:I:512:LYS:HE2	2:I:520:ILE:HD11	1.95	0.49
2:I:512:LYS:HE2	2:I:520:ILE:HD11	1.95	0.49
2:N:83:SER:O	2:N:86:CYS:HB3	2.13	0.49
1:F:135:GLU:HA	2:N:328:ASP:OD1	2.13	0.49
2:K:301:SER:HB2	2:K:302:PRO:HD2	1.95	0.49
1:F:114:CYS:HA	1:F:119:GLY:HA3	1.94	0.49
2:K:301:SER:HB2	2:K:302:PRO:HD2	1.95	0.49
1:F:114:CYS:HA	1:F:119:GLY:HA3	1.94	0.49
2:N:359:TYR:O	8:N:5637:HOH:O	2.20	0.49
2:N:237:CYS:HB2	2:N:456:LEU:HG	1.94	0.49
1:B:159:VAL:O	1:B:163:THR:HG23	2.13	0.48
2:H:541:ASP:N	2:H:542:PRO:HD3	2.28	0.48
2:N:288:ASN:HB3	2:N:381:MET:CE	2.43	0.48
2:H:296:ALA:HA	2:H:309:SER:HA	1.93	0.48
2:J:38:LYS:HB3	2:J:40:LYS:HE2	1.94	0.48
1:B:159:VAL:O	1:B:163:THR:HG23	2.13	0.48
2:H:541:ASP:N	2:H:542:PRO:HD3	2.28	0.48
2:H:296:ALA:HA	2:H:309:SER:HA	1.93	0.48
2:J:38:LYS:HB3	2:J:40:LYS:HE2	1.94	0.48
1:F:135:GLU:HG2	2:N:328:ASP:CB	2.42	0.48
2:M:474:ALA:HB1	2:M:475:PRO:CD	2.43	0.48
2:M:474:ALA:HB1	2:M:475:PRO:CD	2.43	0.48
2:H:301:SER:HB2	2:H:302:PRO:HD2	1.95	0.48
2:H:301:SER:HB2	2:H:302:PRO:HD2	1.95	0.48
1:G:47:THR:O	2:N:23:ARG:HA	2.13	0.48
1:B:18:THR:O	1:B:18:THR:HG22	2.14	0.48
1:B:18:THR:HG22	1:B:18:THR:O	2.14	0.48
2:I:121:HIS:CE1	2:I:209:LEU:HD23	2.49	0.48
2:J:140:LYS:HD3	2:J:196:GLU:HG2	1.95	0.48
2:I:121:HIS:CE1	2:I:209:LEU:HD23	2.49	0.48
2:J:140:LYS:HD3	2:J:196:GLU:HG2	1.95	0.48
2:N:43:TRP:CH2	2:N:365:LYS:HE2	2.43	0.48
2:K:301:SER:HB2	2:K:302:PRO:CD	2.44	0.48
2:I:130:VAL:HG12	2:I:167:LEU:HD21	1.95	0.48
2:K:301:SER:HB2	2:K:302:PRO:CD	2.44	0.48
2:I:130:VAL:HG12	2:I:167:LEU:HD21	1.95	0.48
2:N:345:GLY:O	2:N:348:LYS:HG2	2.13	0.48
2:H:454:ASN:HD22	2:H:454:ASN:N	2.10	0.48
2:K:512:LYS:HE2	2:K:520:ILE:HD11	1.96	0.48
2:H:333:TYR:OH	2:H:378:GLY:HA2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD21	1:A:45:GLN:HG3	1.96	0.48
1:F:121:GLN:HB3	2:M:50:ARG:HG2	1.96	0.48
1:A:114:CYS:HA	1:A:119:GLY:HA3	1.96	0.48
1:G:145:PRO:HD2	1:G:179:TYR:CE1	2.49	0.48
2:H:454:ASN:HD22	2:H:454:ASN:N	2.10	0.48
2:K:512:LYS:HE2	2:K:520:ILE:HD11	1.96	0.48
2:H:333:TYR:OH	2:H:378:GLY:HA2	2.13	0.48
1:A:42:LEU:HD21	1:A:45:GLN:HG3	1.96	0.48
1:F:121:GLN:HB3	2:M:50:ARG:HG2	1.96	0.48
1:A:114:CYS:HA	1:A:119:GLY:HA3	1.96	0.48
1:C:71:TYR:CE1	1:C:162:LEU:CD2	2.97	0.48
1:C:71:TYR:CE1	1:C:162:LEU:CD2	2.97	0.48
2:N:497:VAL:HG12	2:N:498:PRO:HD2	1.95	0.48
2:I:99:ALA:O	2:I:103:ARG:HG3	2.13	0.48
1:A:47:THR:O	2:H:23:ARG:HA	2.14	0.48
2:H:474:ALA:HB1	2:H:475:PRO:HD2	1.95	0.48
1:F:135:GLU:OE2	2:N:326:ASN:CB	2.62	0.48
2:I:99:ALA:O	2:I:103:ARG:HG3	2.13	0.48
1:A:47:THR:O	2:H:23:ARG:HA	2.14	0.48
2:H:474:ALA:HB1	2:H:475:PRO:HD2	1.95	0.48
1:F:14:ASN:HD22	1:F:94:MET:HB3	1.74	0.48
1:F:14:ASN:HD22	1:F:94:MET:HB3	1.74	0.48
1:G:254:TRP:HH2	2:N:70:ARG:HD3	1.79	0.48
1:G:223:THR:CG2	1:G:247:GLY:HA2	2.44	0.47
2:N:498:PRO:HG2	7:N:550:FCO:C1	2.44	0.47
1:B:33:ASP:O	1:B:37:LEU:HG	2.14	0.47
1:F:160:HIS:CE1	1:F:164:LYS:HB2	2.50	0.47
1:B:33:ASP:O	1:B:37:LEU:HG	2.14	0.47
1:F:160:HIS:CE1	1:F:164:LYS:HB2	2.50	0.47
2:M:134:LEU:HD22	2:M:168:LYS:CG	2.43	0.47
2:M:403:VAL:CG1	2:M:430:ILE:HG23	2.44	0.47
1:D:114:CYS:HA	1:D:119:GLY:HA3	1.96	0.47
2:M:274:ALA:CB	2:M:422:LEU:HD11	2.45	0.47
1:F:135:GLU:CD	2:N:326:ASN:HB2	2.33	0.47
2:M:134:LEU:HD22	2:M:168:LYS:CG	2.43	0.47
2:M:403:VAL:CG1	2:M:430:ILE:HG23	2.44	0.47
1:D:114:CYS:HA	1:D:119:GLY:HA3	1.96	0.47
2:M:274:ALA:CB	2:M:422:LEU:HD11	2.45	0.47
1:G:196:SER:HA	1:G:198:PHE:CZ	2.49	0.47
2:H:464:GLU:HA	2:H:488:LYS:HG3	1.96	0.47
1:C:228:PRO:HB3	1:C:237:TRP:CZ2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:166:LYS:NZ	8:H:562:HOH:O	2.35	0.47
2:K:530:PRO:HB2	2:K:533:ILE:HD12	1.97	0.47
2:H:464:GLU:HA	2:H:488:LYS:HG3	1.96	0.47
1:C:228:PRO:HB3	1:C:237:TRP:CZ2	2.50	0.47
2:H:166:LYS:NZ	8:H:560:HOH:O	2.35	0.47
2:K:530:PRO:HB2	2:K:533:ILE:HD12	1.97	0.47
2:H:196:GLU:O	2:H:200:ILE:HG13	2.15	0.47
1:G:14:ASN:ND2	1:G:94:MET:HB3	2.29	0.47
1:A:158:VAL:O	1:A:162:LEU:HG	2.14	0.47
2:I:69:GLN:HA	2:I:79:HIS:HB2	1.97	0.47
1:G:187:CYS:HA	1:G:188:PRO:HD3	1.82	0.47
2:N:474:ALA:HB1	2:N:475:PRO:CD	2.45	0.47
2:H:196:GLU:O	2:H:200:ILE:HG13	2.15	0.47
1:A:158:VAL:O	1:A:162:LEU:HG	2.14	0.47
2:I:69:GLN:HA	2:I:79:HIS:HB2	1.97	0.47
2:N:102:MET:O	2:N:106:VAL:HG23	2.15	0.47
1:G:145:PRO:HG3	1:G:174:ARG:HD3	1.93	0.47
2:I:264:GLU:O	2:I:268:PRO:HG2	2.15	0.47
1:D:220:GLY:N	1:D:221:PRO:CD	2.77	0.47
2:N:541:ASP:N	2:N:542:PRO:HD3	2.29	0.47
2:J:34:VAL:HG12	2:J:35:GLU:N	2.29	0.47
1:A:78:LEU:HD22	1:A:95:ILE:HA	1.97	0.47
2:I:264:GLU:O	2:I:268:PRO:HG2	2.15	0.47
1:D:220:GLY:N	1:D:221:PRO:CD	2.77	0.47
2:J:34:VAL:HG12	2:J:35:GLU:N	2.29	0.47
1:A:78:LEU:HD22	1:A:95:ILE:HA	1.97	0.47
2:H:127:TRP:CH2	2:H:535:ARG:HD3	2.49	0.47
2:H:267:ILE:HB	2:H:268:PRO:HD3	1.96	0.47
2:H:127:TRP:CH2	2:H:535:ARG:HD3	2.49	0.47
1:G:36:ILE:O	8:G:5282:HOH:O	2.20	0.47
2:H:267:ILE:HB	2:H:268:PRO:HD3	1.96	0.47
2:M:264:GLU:O	2:M:268:PRO:HG2	2.15	0.46
2:I:132:ALA:HB3	2:I:198:ASN:ND2	2.29	0.46
2:M:264:GLU:O	2:M:268:PRO:HG2	2.15	0.46
2:I:132:ALA:HB3	2:I:198:ASN:ND2	2.29	0.46
2:N:76:THR:O	2:N:77:TYR:HB3	2.15	0.46
1:G:50:ALA:HB2	2:N:125:LEU:HD13	1.96	0.46
1:G:243:HIS:CG	1:G:244:PRO:HD2	2.50	0.46
2:N:194:PRO:HG2	2:N:197:VAL:HG23	1.97	0.46
2:M:70:ARG:N	2:M:70:ARG:HD2	2.30	0.46
1:G:233:ASN:HA	8:G:5270:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:541:ASP:N	2:N:542:PRO:HD3	2.29	0.46
2:M:70:ARG:N	2:M:70:ARG:HD2	2.30	0.46
2:N:474:ALA:HB1	2:N:475:PRO:CD	2.44	0.46
2:N:237:CYS:HB2	2:N:456:LEU:HG	1.96	0.46
2:J:278:LYS:NZ	2:J:411:LEU:O	2.44	0.46
2:J:284:GLY:HA2	2:J:518:ALA:O	2.16	0.46
1:F:135:GLU:CD	2:N:326:ASN:HD22	2.18	0.46
2:J:278:LYS:NZ	2:J:411:LEU:O	2.44	0.46
2:J:284:GLY:HA2	2:J:518:ALA:O	2.16	0.46
2:J:371:MET:CE	2:J:547:GLY:HA3	2.46	0.46
2:J:371:MET:CE	2:J:547:GLY:HA3	2.46	0.46
2:J:497:VAL:HG12	2:J:498:PRO:CD	2.45	0.46
1:B:148:PRO:HB2	1:B:149:PRO:HD2	1.98	0.46
2:J:497:VAL:HG12	2:J:498:PRO:CD	2.45	0.46
1:G:14:ASN:HD22	1:G:94:MET:HB3	1.80	0.46
1:B:148:PRO:HB2	1:B:149:PRO:HD2	1.98	0.46
2:N:69:GLN:HA	2:N:79:HIS:HB2	1.98	0.46
2:M:497:VAL:CG1	2:M:498:PRO:CD	2.90	0.46
1:D:131:LYS:CE	8:D:3421:HOH:O	2.62	0.46
2:M:293:GLY:HA2	2:M:311:PHE:O	2.16	0.46
2:M:497:VAL:CG1	2:M:498:PRO:CD	2.90	0.46
1:D:131:LYS:CE	8:D:3421:HOH:O	2.62	0.46
2:M:293:GLY:HA2	2:M:311:PHE:O	2.16	0.46
1:A:190:LEU:HB3	1:A:191:PRO:HD3	1.97	0.46
2:K:509:GLN:HB2	2:K:509:GLN:HE21	1.63	0.46
1:A:190:LEU:HB3	1:A:191:PRO:HD3	1.97	0.46
2:K:509:GLN:HB2	2:K:509:GLN:HE21	1.63	0.46
1:G:136:ALA:HA	8:G:5287:HOH:O	2.15	0.46
1:A:237:TRP:CZ2	1:A:239:VAL:HB	2.50	0.46
1:B:184:HIS:HB2	1:B:220:GLY:C	2.35	0.46
1:F:237:TRP:CH2	1:F:239:VAL:HB	2.51	0.46
1:A:237:TRP:CZ2	1:A:239:VAL:HB	2.50	0.46
1:B:184:HIS:HB2	1:B:220:GLY:C	2.35	0.46
1:G:223:THR:HG21	1:G:247:GLY:HA2	1.98	0.46
1:F:237:TRP:CH2	1:F:239:VAL:HB	2.51	0.46
1:G:17:CYS:HB2	2:N:73:GLY:H	1.81	0.46
2:J:515:VAL:HG13	2:J:516:GLU:N	2.30	0.46
2:M:333:TYR:OH	2:M:378:GLY:HA2	2.16	0.46
2:J:515:VAL:HG13	2:J:516:GLU:N	2.30	0.46
2:M:333:TYR:OH	2:M:378:GLY:HA2	2.16	0.46
2:J:76:THR:O	2:J:77:TYR:HB3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:246:ASP:HB2	2:M:247:PRO:HD3	1.97	0.45
2:J:76:THR:O	2:J:77:TYR:HB3	2.16	0.45
2:M:246:ASP:HB2	2:M:247:PRO:HD3	1.97	0.45
1:D:190:LEU:N	1:D:191:PRO:CD	2.79	0.45
1:D:190:LEU:N	1:D:191:PRO:CD	2.79	0.45
1:G:88:MET:HE3	2:N:362:LEU:CD1	2.46	0.45
1:F:145:PRO:HG3	1:F:174:ARG:CD	2.46	0.45
2:K:413:VAL:HB	2:K:414:PRO:HD2	1.98	0.45
2:N:296:ALA:HA	2:N:309:SER:HA	1.99	0.45
1:F:145:PRO:HG3	1:F:174:ARG:CD	2.46	0.45
1:G:158:VAL:O	1:G:162:LEU:HG	2.15	0.45
2:K:413:VAL:HB	2:K:414:PRO:HD2	1.98	0.45
1:A:159:VAL:O	1:A:163:THR:HG23	2.15	0.45
1:A:159:VAL:O	1:A:163:THR:HG23	2.15	0.45
2:K:118:HIS:HD2	2:K:122:LEU:HD12	1.81	0.45
2:K:118:HIS:HD2	2:K:122:LEU:HD12	1.81	0.45
1:G:227:CYS:N	1:G:228:PRO:CD	2.79	0.45
2:I:476:ARG:HD2	8:I:552:HOH:O	2.16	0.45
2:I:476:ARG:HD2	8:I:557:HOH:O	2.16	0.45
1:C:227:CYS:HB2	1:C:228:PRO:HD3	1.98	0.45
1:C:164:LYS:HE3	1:C:164:LYS:HB3	1.65	0.45
1:A:220:GLY:N	1:A:221:PRO:CD	2.80	0.45
1:G:161:VAL:HA	1:G:165:GLY:O	2.16	0.45
1:C:227:CYS:HB2	1:C:228:PRO:HD3	1.98	0.45
2:N:25:GLU:HB3	2:N:543:CYS:SG	2.56	0.45
1:C:164:LYS:HE3	1:C:164:LYS:HB3	1.65	0.45
1:A:220:GLY:N	1:A:221:PRO:CD	2.80	0.45
1:B:27:THR:CB	1:B:155:VAL:HG21	2.47	0.45
2:I:292:PHE:CD1	2:I:478:ALA:HB1	2.52	0.45
1:B:27:THR:CB	1:B:155:VAL:HG21	2.47	0.45
2:I:292:PHE:CD1	2:I:478:ALA:HB1	2.52	0.45
2:N:497:VAL:CG1	2:N:498:PRO:CD	2.92	0.45
1:G:220:GLY:N	1:G:221:PRO:HD3	2.32	0.45
2:H:418:LEU:O	2:H:423:GLY:HA3	2.17	0.45
2:H:418:LEU:O	2:H:423:GLY:HA3	2.17	0.45
2:N:487:GLY:O	2:N:488:LYS:HB2	2.17	0.45
1:A:254:TRP:CH2	2:H:70:ARG:HD3	2.50	0.44
2:M:280:TRP:HA	2:M:283:ILE:HD12	1.99	0.44
2:J:9:GLN:NE2	2:J:36:ASN:O	2.48	0.44
1:G:146:GLY:O	1:G:149:PRO:HD3	2.17	0.44
1:A:254:TRP:CH2	2:H:70:ARG:HD3	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:223:GLY:HA2	2:N:231:PHE:CD2	2.52	0.44
2:M:280:TRP:HA	2:M:283:ILE:HD12	1.99	0.44
2:J:9:GLN:NE2	2:J:36:ASN:O	2.48	0.44
1:G:161:VAL:HA	1:G:165:GLY:O	2.16	0.44
1:F:204:SER:O	1:F:208:LYS:HG3	2.17	0.44
1:F:204:SER:O	1:F:208:LYS:HG3	2.17	0.44
1:D:131:LYS:HE2	8:D:3421:HOH:O	2.17	0.44
1:D:131:LYS:HE2	8:D:3421:HOH:O	2.17	0.44
2:H:8:PRO:HB2	2:H:525:ALA:HB2	2.00	0.44
1:B:111:ILE:O	1:B:111:ILE:HG23	2.18	0.44
2:N:497:VAL:HG12	2:N:498:PRO:HD2	1.97	0.44
2:H:8:PRO:HB2	2:H:525:ALA:HB2	2.00	0.44
1:B:111:ILE:O	1:B:111:ILE:HG23	2.18	0.44
2:J:448:ASP:O	2:J:452:LYS:HE2	2.11	0.44
2:N:512:LYS:HB2	2:N:512:LYS:HE2	1.84	0.44
2:J:448:ASP:O	2:J:452:LYS:HE2	2.11	0.44
1:A:190:LEU:N	1:A:191:PRO:CD	2.80	0.44
2:N:329:LEU:HD11	2:N:471:LEU:HD11	1.99	0.44
1:G:111:ILE:HG23	1:G:111:ILE:O	2.18	0.44
1:D:18:THR:O	1:D:18:THR:HG22	2.18	0.44
1:A:190:LEU:N	1:A:191:PRO:CD	2.80	0.44
1:G:261:TYR:CD2	2:N:62:ARG:HB3	2.53	0.44
1:G:111:ILE:O	1:G:111:ILE:HG23	2.18	0.44
1:D:18:THR:O	1:D:18:THR:HG22	2.18	0.44
1:G:258:THR:HB	1:G:259:PRO:HA	1.98	0.44
1:D:80:THR:HG21	1:D:131:LYS:HD2	1.99	0.44
2:K:195:PRO:O	2:K:198:ASN:HB2	2.18	0.44
2:N:76:THR:O	2:N:77:TYR:HB3	2.17	0.44
1:D:80:THR:HG21	1:D:131:LYS:HD2	1.99	0.44
2:K:195:PRO:O	2:K:198:ASN:HB2	2.18	0.44
2:N:487:GLY:O	2:N:488:LYS:HB2	2.18	0.44
2:N:69:GLN:HA	2:N:79:HIS:HB2	1.98	0.44
2:J:497:VAL:HG11	2:J:546:CYS:HB3	2.00	0.44
2:H:474:ALA:HB1	2:H:475:PRO:CD	2.48	0.44
2:K:194:PRO:HG2	2:K:197:VAL:HG23	2.00	0.44
2:H:512:LYS:HD2	2:H:516:GLU:HB3	2.00	0.44
2:M:40:LYS:HD2	2:M:40:LYS:HA	1.85	0.44
2:J:497:VAL:HG11	2:J:546:CYS:HB3	2.00	0.44
2:H:474:ALA:HB1	2:H:475:PRO:CD	2.48	0.44
2:K:194:PRO:HG2	2:K:197:VAL:HG23	2.00	0.44
2:H:512:LYS:HD2	2:H:516:GLU:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:40:LYS:HD2	2:M:40:LYS:HA	1.85	0.44
2:J:352:ASP:O	2:J:353:GLY:C	2.55	0.43
1:G:227:CYS:HB2	1:G:228:PRO:HD3	2.00	0.43
2:M:487:GLY:O	2:M:488:LYS:HB2	2.17	0.43
2:J:352:ASP:O	2:J:353:GLY:C	2.55	0.43
1:G:187:CYS:HA	1:G:188:PRO:HD3	1.85	0.43
2:M:487:GLY:O	2:M:488:LYS:HB2	2.17	0.43
1:G:170:ASP:C	1:G:170:ASP:OD1	2.56	0.43
2:J:385:PRO:HD2	8:J:2751:HOH:O	2.17	0.43
1:G:80:THR:OG1	1:G:129:GLN:O	2.29	0.43
2:J:385:PRO:HD2	8:J:756:HOH:O	2.17	0.43
2:N:497:VAL:HG12	2:N:498:PRO:CD	2.49	0.43
1:C:78:LEU:HD13	1:C:95:ILE:HD12	1.99	0.43
2:N:223:GLY:HA2	2:N:231:PHE:CD2	2.53	0.43
2:M:49:PHE:HB2	2:M:370:TRP:CD2	2.52	0.43
2:K:161:LYS:HG3	2:K:161:LYS:O	2.19	0.43
2:H:77:TYR:CD2	2:H:106:VAL:HG12	2.52	0.43
1:C:78:LEU:HD13	1:C:95:ILE:HD12	1.99	0.43
2:M:49:PHE:HB2	2:M:370:TRP:CD2	2.52	0.43
2:K:161:LYS:O	2:K:161:LYS:HG3	2.19	0.43
2:H:77:TYR:CD2	2:H:106:VAL:HG12	2.52	0.43
2:H:150:PRO:HG2	2:H:264:GLU:HA	2.00	0.43
2:I:209:LEU:HD23	2:I:209:LEU:HA	1.90	0.43
2:K:293:GLY:HA2	2:K:311:PHE:O	2.18	0.43
1:B:187:CYS:HA	1:B:188:PRO:HD3	1.77	0.43
2:I:362:LEU:HA	2:I:362:LEU:HD12	1.77	0.43
2:K:9:GLN:NE2	2:K:36:ASN:O	2.51	0.43
2:H:150:PRO:HG2	2:H:264:GLU:HA	2.00	0.43
2:I:209:LEU:HA	2:I:209:LEU:HD23	1.90	0.43
2:K:293:GLY:HA2	2:K:311:PHE:O	2.18	0.43
1:B:187:CYS:HA	1:B:188:PRO:HD3	1.77	0.43
2:N:194:PRO:HG2	2:N:197:VAL:HG23	1.99	0.43
2:I:362:LEU:HD12	2:I:362:LEU:HA	1.77	0.43
2:K:9:GLN:NE2	2:K:36:ASN:O	2.51	0.43
1:F:237:TRP:HB2	1:F:238:PRO:CD	2.48	0.43
1:G:184:HIS:HA	5:G:265:SF4:S1	2.58	0.43
1:C:243:HIS:CG	1:C:244:PRO:HD2	2.54	0.43
2:K:290:LEU:HD12	2:K:315:VAL:HG22	2.01	0.43
2:I:127:TRP:CZ3	2:I:535:ARG:HD3	2.53	0.43
2:H:43:TRP:CE2	2:H:365:LYS:HE2	2.53	0.43
2:N:102:MET:O	2:N:106:VAL:HG23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:173:SER:HB2	8:K:3670:HOH:O	2.17	0.43
1:F:237:TRP:HB2	1:F:238:PRO:CD	2.48	0.43
1:C:243:HIS:CG	1:C:244:PRO:HD2	2.54	0.43
2:K:290:LEU:HD12	2:K:315:VAL:HG22	2.01	0.43
2:I:127:TRP:CZ3	2:I:535:ARG:HD3	2.53	0.43
2:H:43:TRP:CE2	2:H:365:LYS:HE2	2.53	0.43
2:K:173:SER:HB2	8:K:681:HOH:O	2.17	0.43
2:M:390:PHE:CZ	2:M:418:LEU:HB2	2.54	0.43
2:M:297:THR:OG1	2:M:308:THR:HB	2.19	0.43
1:G:237:TRP:CZ2	1:G:239:VAL:HB	2.54	0.43
2:M:390:PHE:CZ	2:M:418:LEU:HB2	2.54	0.43
2:N:241:GLN:O	2:N:244:THR:OG1	2.34	0.43
2:M:297:THR:OG1	2:M:308:THR:HB	2.19	0.43
2:N:328:ASP:OD1	2:N:328:ASP:C	2.57	0.43
2:J:353:GLY:HA3	2:J:494:GLN:CD	2.39	0.43
2:M:404:VAL:HG22	2:M:430:ILE:HD13	2.00	0.43
1:G:237:TRP:HB2	1:G:238:PRO:HD2	2.00	0.43
2:M:116:LEU:HA	2:M:116:LEU:HD23	1.75	0.43
2:J:353:GLY:HA3	2:J:494:GLN:CD	2.39	0.43
2:M:404:VAL:HG22	2:M:430:ILE:HD13	2.00	0.43
2:M:116:LEU:HD23	2:M:116:LEU:HA	1.75	0.43
8:G:5321:HOH:O	2:N:234:VAL:HG23	2.18	0.43
2:I:296:ALA:HA	2:I:309:SER:HA	2.01	0.43
2:K:105:LEU:HD21	2:K:442:TRP:HB3	2.00	0.43
1:G:29:LYS:HA	1:G:30:PRO:HA	1.79	0.43
2:I:296:ALA:HA	2:I:309:SER:HA	2.01	0.43
2:K:105:LEU:HD21	2:K:442:TRP:HB3	2.00	0.43
2:N:512:LYS:HB2	2:N:512:LYS:HE2	1.87	0.43
1:G:122:LYS:NZ	8:G:5276:HOH:O	2.36	0.43
1:G:145:PRO:HD2	1:G:179:TYR:CE1	2.54	0.43
2:M:354:VAL:O	2:M:372:LYS:NZ	2.51	0.43
2:J:246:ASP:HB2	2:J:247:PRO:HD3	2.00	0.43
2:I:306:LEU:HA	2:I:306:LEU:HD23	1.90	0.43
2:M:354:VAL:O	2:M:372:LYS:NZ	2.51	0.43
2:J:246:ASP:HB2	2:J:247:PRO:HD3	2.00	0.43
2:I:306:LEU:HD23	2:I:306:LEU:HA	1.90	0.43
2:K:270:LEU:CD1	2:K:425:THR:HG22	2.49	0.42
2:K:377:LYS:CE	8:K:3778:HOH:O	2.67	0.42
2:M:364:ASP:O	2:M:368:TYR:HB3	2.19	0.42
2:N:497:VAL:CG1	2:N:498:PRO:CD	2.93	0.42
2:K:270:LEU:CD1	2:K:425:THR:HG22	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:377:LYS:CE	8:K:788:HOH:O	2.67	0.42
2:M:364:ASP:O	2:M:368:TYR:HB3	2.19	0.42
2:H:168:LYS:O	2:H:172:GLU:HG3	2.19	0.42
2:K:123:HIS:CD2	2:K:127:TRP:HE1	2.37	0.42
2:H:168:LYS:O	2:H:172:GLU:HG3	2.19	0.42
2:K:123:HIS:CD2	2:K:127:TRP:HE1	2.37	0.42
1:G:89:VAL:O	1:G:90:ALA:HB3	2.19	0.42
2:J:127:TRP:CH2	2:J:535:ARG:HG2	2.54	0.42
1:G:190:LEU:N	1:G:191:PRO:HD2	2.34	0.42
2:J:411:LEU:O	2:J:412:SER:HB2	2.19	0.42
2:J:127:TRP:CH2	2:J:535:ARG:HG2	2.54	0.42
2:J:411:LEU:O	2:J:412:SER:HB2	2.19	0.42
1:G:102:ALA:HB1	1:G:108:ILE:HD11	1.99	0.42
2:H:271:LEU:HD13	2:H:410:LYS:CE	2.49	0.42
2:I:237:CYS:HB2	2:I:456:LEU:HG	2.02	0.42
2:M:465:GLU:O	2:M:466:SER:HB2	2.19	0.42
2:K:403:VAL:CG1	2:K:430:ILE:HG23	2.49	0.42
1:F:248:CYS:HA	1:F:253:PHE:CD1	2.55	0.42
2:H:271:LEU:HD13	2:H:410:LYS:CE	2.49	0.42
2:I:237:CYS:HB2	2:I:456:LEU:HG	2.02	0.42
2:M:465:GLU:O	2:M:466:SER:HB2	2.19	0.42
2:K:403:VAL:CG1	2:K:430:ILE:HG23	2.49	0.42
1:F:248:CYS:HA	1:F:253:PHE:CD1	2.55	0.42
2:I:343:PRO:HG2	2:K:147:SER:HB3	2.01	0.42
1:D:111:ILE:HG23	1:D:111:ILE:O	2.20	0.42
2:H:362:LEU:HA	2:H:362:LEU:HD12	1.85	0.42
2:J:166:LYS:HE3	2:J:166:LYS:HB2	1.77	0.42
1:B:197:GLU:HB3	1:B:211:PHE:CE1	2.54	0.42
1:F:258:THR:HA	1:F:259:PRO:C	2.39	0.42
2:I:53:GLU:HG2	2:I:493:PHE:O	2.20	0.42
2:I:343:PRO:HG2	2:K:147:SER:HB3	2.01	0.42
1:D:111:ILE:HG23	1:D:111:ILE:O	2.20	0.42
2:H:362:LEU:HD12	2:H:362:LEU:HA	1.85	0.42
2:J:166:LYS:HE3	2:J:166:LYS:HB2	1.77	0.42
2:N:297:THR:OG1	2:N:308:THR:HB	2.19	0.42
1:B:197:GLU:HB3	1:B:211:PHE:CE1	2.54	0.42
1:F:258:THR:HA	1:F:259:PRO:C	2.39	0.42
2:I:53:GLU:HG2	2:I:493:PHE:O	2.20	0.42
2:K:349:HIS:CG	2:K:350:PRO:HD2	2.55	0.42
1:A:46:GLU:HG3	8:A:289:HOH:O	2.19	0.42
2:M:320:ASP:C	2:M:320:ASP:OD1	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:349:HIS:CG	2:K:350:PRO:HD2	2.55	0.42
2:N:26:GLY:HA3	2:N:544:ILE:HB	2.02	0.42
1:A:46:GLU:HG3	8:A:289:HOH:O	2.19	0.42
2:M:320:ASP:OD1	2:M:320:ASP:C	2.58	0.42
2:J:40:LYS:HA	2:J:40:LYS:HD3	1.83	0.42
2:J:350:PRO:HB2	2:J:482:TRP:CG	2.54	0.42
2:J:441:LYS:NZ	8:J:2644:HOH:O	2.51	0.42
2:M:495:LEU:N	2:M:495:LEU:HD12	2.35	0.42
2:J:40:LYS:HD3	2:J:40:LYS:HA	1.83	0.42
2:J:350:PRO:HB2	2:J:482:TRP:CG	2.54	0.42
2:J:441:LYS:NZ	8:J:651:HOH:O	2.51	0.42
2:M:495:LEU:N	2:M:495:LEU:HD12	2.35	0.42
1:A:184:HIS:NE2	1:A:190:LEU:CD1	2.83	0.42
2:K:476:ARG:HD2	8:K:552:HOH:O	2.19	0.42
2:K:69:GLN:OE1	2:K:77:TYR:HA	2.19	0.42
2:H:486:LYS:HB3	2:H:491:ASP:HB2	2.02	0.42
1:A:184:HIS:NE2	1:A:190:LEU:CD1	2.83	0.42
2:N:91:VAL:O	2:N:92:LYS:HB2	2.20	0.42
2:K:476:ARG:HD2	8:K:557:HOH:O	2.19	0.42
2:K:69:GLN:OE1	2:K:77:TYR:HA	2.19	0.42
2:N:19:ASP:HA	2:N:20:PRO:HA	1.85	0.42
2:H:486:LYS:HB3	2:H:491:ASP:HB2	2.02	0.42
2:N:454:ASN:N	2:N:454:ASN:HD22	2.14	0.42
2:J:380:ALA:HB1	2:J:514:PRO:HD3	2.02	0.42
2:M:476:ARG:HD2	7:M:550:FCO:C2	2.50	0.42
2:J:380:ALA:HB1	2:J:514:PRO:HD3	2.02	0.42
2:M:476:ARG:HD2	7:M:550:FCO:C2	2.50	0.42
1:A:40:ILE:HG22	1:A:162:LEU:CD1	2.50	0.42
2:K:76:THR:O	2:K:77:TYR:HB3	2.19	0.42
1:A:40:ILE:HG22	1:A:162:LEU:CD1	2.50	0.42
2:K:76:THR:O	2:K:77:TYR:HB3	2.19	0.42
2:N:328:ASP:OD1	2:N:330:GLY:N	2.53	0.41
2:K:246:ASP:N	2:K:247:PRO:CD	2.83	0.41
2:N:241:GLN:O	2:N:244:THR:OG1	2.37	0.41
2:I:411:LEU:O	2:I:413:VAL:HG13	2.20	0.41
2:K:246:ASP:N	2:K:247:PRO:CD	2.83	0.41
2:I:411:LEU:O	2:I:413:VAL:HG13	2.20	0.41
2:J:515:VAL:CG1	2:J:516:GLU:N	2.83	0.41
1:G:80:THR:OG1	1:G:129:GLN:O	2.29	0.41
2:K:402:LYS:HB2	2:K:402:LYS:HE3	1.85	0.41
2:J:515:VAL:CG1	2:J:516:GLU:N	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:402:LYS:HB2	2:K:402:LYS:HE3	1.85	0.41
1:G:201:SER:HA	1:G:216:LEU:HD21	2.02	0.41
2:J:274:ALA:CB	2:J:422:LEU:HD11	2.51	0.41
1:C:29:LYS:HA	1:C:30:PRO:HA	1.83	0.41
1:G:147:CYS:SG	1:G:147:CYS:O	2.78	0.41
1:G:122:LYS:NZ	8:G:5276:HOH:O	2.41	0.41
1:G:117:TYR:CE2	1:G:145:PRO:HB3	2.54	0.41
2:J:274:ALA:CB	2:J:422:LEU:HD11	2.51	0.41
1:C:29:LYS:HA	1:C:30:PRO:HA	1.83	0.41
2:H:60:ASP:HA	2:H:61:PRO:HD3	1.98	0.41
2:I:196:GLU:OE1	2:I:196:GLU:N	2.50	0.41
2:N:543:CYS:SG	2:N:546:CYS:HB2	2.60	0.41
2:H:60:ASP:HA	2:H:61:PRO:HD3	1.98	0.41
2:I:196:GLU:N	2:I:196:GLU:OE1	2.50	0.41
1:A:233:ASN:O	1:A:234:GLN:HB2	2.21	0.41
2:I:134:LEU:HD21	2:I:167:LEU:HB3	2.02	0.41
1:G:22:GLU:O	1:G:26:ARG:HG2	2.20	0.41
2:N:26:GLY:HA3	2:N:544:ILE:HB	2.01	0.41
1:A:263:GLN:HA	1:A:263:GLN:OE1	2.20	0.41
1:A:233:ASN:O	1:A:234:GLN:HB2	2.21	0.41
2:I:134:LEU:HD21	2:I:167:LEU:HB3	2.02	0.41
1:G:223:THR:CG2	1:G:247:GLY:HA2	2.50	0.41
2:N:329:LEU:HD11	2:N:471:LEU:HD11	2.02	0.41
1:A:263:GLN:OE1	1:A:263:GLN:HA	2.20	0.41
2:M:76:THR:OG1	2:M:228:HIS:N	2.49	0.41
1:G:237:TRP:CH2	1:G:239:VAL:HB	2.56	0.41
1:D:253:PHE:CZ	1:D:254:TRP:CE2	3.09	0.41
2:J:204:HIS:ND1	2:J:269:ASP:OD2	2.35	0.41
2:M:76:THR:OG1	2:M:228:HIS:N	2.49	0.41
2:N:454:ASN:N	2:N:454:ASN:HD22	2.17	0.41
1:D:253:PHE:CZ	1:D:254:TRP:CE2	3.09	0.41
2:J:204:HIS:ND1	2:J:269:ASP:OD2	2.35	0.41
2:H:144:LEU:CD2	2:H:144:LEU:C	2.89	0.41
1:D:127:PRO:HD2	8:D:3268:HOH:O	2.20	0.41
1:C:236:ASN:OD1	1:C:240:GLN:HB3	2.20	0.41
2:N:284:GLY:HA2	2:N:518:ALA:O	2.21	0.41
2:H:465:GLU:O	2:H:466:SER:HB2	2.21	0.41
2:N:353:GLY:HA3	2:N:494:GLN:HG3	2.02	0.41
2:H:248:LEU:HA	2:H:248:LEU:HD23	1.77	0.41
1:G:89:VAL:O	1:G:90:ALA:HB3	2.20	0.41
2:H:144:LEU:C	2:H:144:LEU:CD2	2.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:464:GLU:HA	2:N:488:LYS:HG3	2.03	0.41
1:D:127:PRO:HD2	8:D:3268:HOH:O	2.20	0.41
1:C:236:ASN:OD1	1:C:240:GLN:HB3	2.20	0.41
2:H:465:GLU:O	2:H:466:SER:HB2	2.21	0.41
2:H:248:LEU:HD23	2:H:248:LEU:HA	1.77	0.41
1:G:174:ARG:HA	1:G:175:PRO:HD3	1.85	0.41
2:K:350:PRO:HB2	2:K:482:TRP:CD2	2.55	0.41
2:K:474:ALA:HB1	2:K:475:PRO:CD	2.51	0.41
2:K:69:GLN:HA	2:K:79:HIS:HB2	2.03	0.41
1:C:184:HIS:HB2	1:C:220:GLY:C	2.41	0.41
2:N:497:VAL:HG12	2:N:498:PRO:CD	2.50	0.41
2:K:350:PRO:HB2	2:K:482:TRP:CD2	2.55	0.41
2:K:474:ALA:HB1	2:K:475:PRO:CD	2.51	0.41
2:K:69:GLN:HA	2:K:79:HIS:HB2	2.03	0.41
1:C:184:HIS:HB2	1:C:220:GLY:C	2.41	0.41
2:H:497:VAL:HG11	2:H:546:CYS:HB3	2.02	0.41
1:G:190:LEU:HB3	1:G:191:PRO:HD3	2.03	0.41
1:B:227:CYS:N	1:B:228:PRO:HD2	2.35	0.41
1:D:6:ARG:HA	1:D:7:PRO:HD3	1.93	0.41
1:B:29:LYS:HA	1:B:30:PRO:HA	1.83	0.41
2:J:541:ASP:N	2:J:542:PRO:HD3	2.36	0.41
1:D:233:ASN:O	1:D:234:GLN:HB2	2.20	0.41
1:B:25:ILE:HG22	1:B:32:ILE:HG12	2.01	0.41
2:J:39:VAL:CG2	2:J:522:THR:HB	2.51	0.41
1:G:170:ASP:C	1:G:170:ASP:OD1	2.58	0.41
1:A:243:HIS:CG	1:A:244:PRO:HD2	2.56	0.41
1:A:187:CYS:HA	1:A:188:PRO:HD3	1.90	0.41
1:F:155:VAL:O	1:F:159:VAL:HG23	2.21	0.41
2:H:497:VAL:HG11	2:H:546:CYS:HB3	2.02	0.41
1:G:230:VAL:O	1:G:231:LEU:HB2	2.21	0.41
1:G:190:LEU:HB3	1:G:191:PRO:HD3	2.02	0.41
1:B:227:CYS:N	1:B:228:PRO:HD2	2.35	0.41
1:D:6:ARG:HA	1:D:7:PRO:HD3	1.93	0.41
1:B:29:LYS:HA	1:B:30:PRO:HA	1.83	0.41
2:J:541:ASP:N	2:J:542:PRO:HD3	2.36	0.41
1:D:233:ASN:O	1:D:234:GLN:HB2	2.20	0.41
1:B:25:ILE:HG22	1:B:32:ILE:HG12	2.01	0.41
2:J:39:VAL:CG2	2:J:522:THR:HB	2.51	0.41
1:A:243:HIS:CG	1:A:244:PRO:HD2	2.56	0.41
1:A:187:CYS:HA	1:A:188:PRO:HD3	1.90	0.41
2:N:353:GLY:HA3	2:N:494:GLN:HG3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:155:VAL:O	1:F:159:VAL:HG23	2.21	0.41
2:N:75:CYS:CB	7:N:550:FCO:C2	2.99	0.41
2:M:349:HIS:CG	2:M:350:PRO:CD	3.04	0.41
2:I:341:TYR:O	2:I:343:PRO:HD3	2.21	0.41
2:K:56:LEU:HD21	2:K:67:PHE:HB2	2.03	0.41
2:M:349:HIS:CG	2:M:350:PRO:CD	3.04	0.41
2:I:341:TYR:O	2:I:343:PRO:HD3	2.21	0.41
2:K:56:LEU:HD21	2:K:67:PHE:HB2	2.03	0.41
2:N:95:ILE:HA	2:N:96:PRO:HD3	1.92	0.40
1:F:201:SER:HA	1:F:216:LEU:HD21	2.04	0.40
1:A:117:TYR:CD2	1:A:251:PRO:HA	2.57	0.40
2:N:116:LEU:HD23	2:N:116:LEU:HA	1.97	0.40
2:H:509:GLN:HE21	2:H:509:GLN:HB2	1.69	0.40
1:F:23:ALA:O	1:F:151:PRO:HB3	2.20	0.40
1:G:261:TYR:HD2	2:N:62:ARG:HB3	1.86	0.40
1:F:201:SER:HA	1:F:216:LEU:HD21	2.04	0.40
1:A:117:TYR:CD2	1:A:251:PRO:HA	2.57	0.40
2:H:509:GLN:HE21	2:H:509:GLN:HB2	1.69	0.40
1:F:23:ALA:O	1:F:151:PRO:HB3	2.20	0.40
2:M:267:ILE:N	2:M:268:PRO:CD	2.84	0.40
2:N:513:SER:HB2	2:N:514:PRO:CD	2.52	0.40
2:I:270:LEU:HD21	2:I:426:ALA:HA	2.03	0.40
1:D:71:TYR:CE1	1:D:162:LEU:CD2	3.04	0.40
2:M:267:ILE:N	2:M:268:PRO:CD	2.84	0.40
2:I:270:LEU:HD21	2:I:426:ALA:HA	2.03	0.40
1:D:71:TYR:CE1	1:D:162:LEU:CD2	3.04	0.40
2:I:246:ASP:N	2:I:247:PRO:CD	2.84	0.40
2:M:274:ALA:HA	2:M:422:LEU:HD11	2.03	0.40
1:F:143:ASN:O	1:F:175:PRO:HD3	2.21	0.40
2:N:356:ASP:HA	2:N:357:PRO:HD2	1.93	0.40
2:I:338:TYR:HA	2:I:366:ASP:O	2.21	0.40
1:G:136:ALA:HA	8:G:5287:HOH:O	2.21	0.40
1:G:184:HIS:HB2	1:G:220:GLY:C	2.42	0.40
2:I:246:ASP:N	2:I:247:PRO:CD	2.84	0.40
2:M:274:ALA:HA	2:M:422:LEU:HD11	2.03	0.40
1:G:217:GLY:O	1:G:219:LYS:HD3	2.20	0.40
1:G:248:CYS:HA	1:G:253:PHE:CD2	2.56	0.40
1:F:143:ASN:O	1:F:175:PRO:HD3	2.21	0.40
2:I:338:TYR:HA	2:I:366:ASP:O	2.21	0.40
2:M:497:VAL:HG11	2:M:546:CYS:HB3	2.03	0.40
2:J:441:LYS:HE2	2:J:441:LYS:HB3	1.84	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:149:ALA:HB1	2:J:150:PRO:HD2	2.03	0.40
8:B:1742:HOH:O	2:I:173:SER:HB2	2.20	0.40
2:M:497:VAL:HG11	2:M:546:CYS:HB3	2.03	0.40
2:J:441:LYS:HB3	2:J:441:LYS:HE2	1.84	0.40
2:J:149:ALA:HB1	2:J:150:PRO:HD2	2.03	0.40
8:B:1742:HOH:O	2:I:173:SER:HB2	2.20	0.40
2:N:144:LEU:C	2:N:144:LEU:HD23	2.41	0.40
2:K:377:LYS:NZ	8:K:3778:HOH:O	2.47	0.40
1:C:220:GLY:N	1:C:221:PRO:CD	2.84	0.40
2:N:86:CYS:SG	2:N:468:GLY:O	2.80	0.40
2:J:19:ASP:CG	2:J:29:ARG:HB2	2.42	0.40
2:J:280:TRP:HA	2:J:283:ILE:HD12	2.03	0.40
2:N:397:GLN:HA	2:N:398:PRO:HD3	1.85	0.40
2:K:377:LYS:NZ	8:K:788:HOH:O	2.47	0.40
1:C:220:GLY:N	1:C:221:PRO:CD	2.84	0.40
1:G:22:GLU:O	1:G:26:ARG:HG2	2.21	0.40
2:J:19:ASP:CG	2:J:29:ARG:HB2	2.42	0.40
2:J:280:TRP:HA	2:J:283:ILE:HD12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:SER:OG	2:N:528:LYS:NZ[2_656]	1.95	0.25

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	260/264 (98%)	254 (98%)	6 (2%)	0	100	100
1	1-B	260/264 (98%)	250 (96%)	10 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-C	258/264 (98%)	247 (96%)	11 (4%)	0	100	100
1	1-D	260/264 (98%)	251 (96%)	9 (4%)	0	100	100
1	1-F	258/264 (98%)	245 (95%)	12 (5%)	1 (0%)	39	37
1	1-G	260/264 (98%)	250 (96%)	10 (4%)	0	100	100
1	2-A	260/264 (98%)	254 (98%)	6 (2%)	0	100	100
1	2-B	260/264 (98%)	250 (96%)	10 (4%)	0	100	100
1	2-C	258/264 (98%)	247 (96%)	11 (4%)	0	100	100
1	2-D	260/264 (98%)	251 (96%)	9 (4%)	0	100	100
1	2-F	258/264 (98%)	245 (95%)	12 (5%)	1 (0%)	39	37
1	2-G	260/264 (98%)	249 (96%)	11 (4%)	0	100	100
2	1-H	543/549 (99%)	527 (97%)	16 (3%)	0	100	100
2	1-I	543/549 (99%)	526 (97%)	17 (3%)	0	100	100
2	1-J	542/549 (99%)	525 (97%)	17 (3%)	0	100	100
2	1-K	542/549 (99%)	530 (98%)	12 (2%)	0	100	100
2	1-M	543/549 (99%)	523 (96%)	20 (4%)	0	100	100
2	1-N	543/549 (99%)	524 (96%)	18 (3%)	1 (0%)	52	53
2	2-H	543/549 (99%)	527 (97%)	16 (3%)	0	100	100
2	2-I	543/549 (99%)	526 (97%)	17 (3%)	0	100	100
2	2-J	542/549 (99%)	525 (97%)	17 (3%)	0	100	100
2	2-K	542/549 (99%)	530 (98%)	12 (2%)	0	100	100
2	2-M	543/549 (99%)	523 (96%)	20 (4%)	0	100	100
2	2-N	543/549 (99%)	521 (96%)	19 (4%)	3 (1%)	30	24
All	All	9624/9756 (99%)	9300 (97%)	318 (3%)	6 (0%)	56	58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2-N	343	PRO
2	2-N	342	ALA
1	1-F	231	LEU
1	2-F	231	LEU
2	1-N	148	ILE
2	2-N	148	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	208/210 (99%)	204 (98%)	4 (2%)	65	70
1	1-B	208/210 (99%)	204 (98%)	4 (2%)	65	70
1	1-C	206/210 (98%)	200 (97%)	6 (3%)	50	53
1	1-D	208/210 (99%)	206 (99%)	2 (1%)	82	87
1	1-F	206/210 (98%)	203 (98%)	3 (2%)	72	78
1	1-G	208/210 (99%)	207 (100%)	1 (0%)	92	95
1	2-A	208/210 (99%)	204 (98%)	4 (2%)	65	70
1	2-B	208/210 (99%)	204 (98%)	4 (2%)	65	70
1	2-C	206/210 (98%)	200 (97%)	6 (3%)	50	53
1	2-D	208/210 (99%)	206 (99%)	2 (1%)	82	87
1	2-F	206/210 (98%)	203 (98%)	3 (2%)	72	78
1	2-G	208/210 (99%)	206 (99%)	2 (1%)	82	87
2	1-H	435/439 (99%)	429 (99%)	6 (1%)	74	80
2	1-I	435/439 (99%)	431 (99%)	4 (1%)	84	89
2	1-J	435/439 (99%)	424 (98%)	11 (2%)	55	59
2	1-K	435/439 (99%)	428 (98%)	7 (2%)	70	76
2	1-M	435/439 (99%)	421 (97%)	14 (3%)	46	48
2	1-N	435/439 (99%)	426 (98%)	9 (2%)	61	66
2	2-H	435/439 (99%)	429 (99%)	6 (1%)	74	80
2	2-I	435/439 (99%)	431 (99%)	4 (1%)	84	89
2	2-J	435/439 (99%)	424 (98%)	11 (2%)	55	59
2	2-K	435/439 (99%)	428 (98%)	7 (2%)	70	76
2	2-M	435/439 (99%)	421 (97%)	14 (3%)	46	48
2	2-N	435/439 (99%)	426 (98%)	9 (2%)	61	66
All	All	7708/7788 (99%)	7565 (98%)	143 (2%)	65	70

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	4	LYS
1	1-A	67	LYS
1	1-A	88	MET
1	1-A	209	LYS
2	1-H	40	LYS
2	1-H	148	ILE
2	1-H	401	LYS
2	1-H	453	ASP
2	1-H	454	ASN
2	1-H	473	ASP
1	1-B	4	LYS
1	1-B	67	LYS
1	1-B	171	SER
1	1-B	196	SER
2	1-I	167	LEU
2	1-I	397	GLN
2	1-I	454	ASN
2	1-I	473	ASP
1	1-C	16	GLU
1	1-C	29	LYS
1	1-C	67	LYS
1	1-C	95	ILE
1	1-C	99	LYS
1	1-C	100	LYS
2	1-J	38	LYS
2	1-J	140	LYS
2	1-J	148	ILE
2	1-J	361	LYS
2	1-J	397	GLN
2	1-J	452	LYS
2	1-J	454	ASN
2	1-J	473	ASP
2	1-J	498	PRO
2	1-J	503	LEU
2	1-J	528	LYS
1	1-D	88	MET
1	1-D	166	ILE
2	1-K	40	LYS
2	1-K	144	LEU
2	1-K	397	GLN
2	1-K	401	LYS
2	1-K	410	LYS
2	1-K	473	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1-K	509	GLN
1	1-F	16	GLU
1	1-F	82	ASP
1	1-F	135	GLU
2	1-M	33	GLU
2	1-M	135	LYS
2	1-M	266	TYR
2	1-M	278	LYS
2	1-M	304	LYS
2	1-M	339	SER
2	1-M	362	LEU
2	1-M	379	LYS
2	1-M	397	GLN
2	1-M	412	SER
2	1-M	452	LYS
2	1-M	454	ASN
2	1-M	473	ASP
2	1-M	509	GLN
1	1-G	88	MET
2	1-N	278	LYS
2	1-N	303	SER
2	1-N	406	MET
2	1-N	410	LYS
2	1-N	453	ASP
2	1-N	454	ASN
2	1-N	473	ASP
2	1-N	528	LYS
2	1-N	546	CYS
1	2-A	4	LYS
1	2-A	67	LYS
1	2-A	88	MET
1	2-A	209	LYS
2	2-H	40	LYS
2	2-H	148	ILE
2	2-H	401	LYS
2	2-H	453	ASP
2	2-H	454	ASN
2	2-H	473	ASP
1	2-B	4	LYS
1	2-B	67	LYS
1	2-B	171	SER
1	2-B	196	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2-I	167	LEU
2	2-I	397	GLN
2	2-I	454	ASN
2	2-I	473	ASP
1	2-C	16	GLU
1	2-C	29	LYS
1	2-C	67	LYS
1	2-C	95	ILE
1	2-C	99	LYS
1	2-C	100	LYS
2	2-J	38	LYS
2	2-J	140	LYS
2	2-J	148	ILE
2	2-J	361	LYS
2	2-J	397	GLN
2	2-J	452	LYS
2	2-J	454	ASN
2	2-J	473	ASP
2	2-J	498	PRO
2	2-J	503	LEU
2	2-J	528	LYS
1	2-D	88	MET
1	2-D	166	ILE
2	2-K	40	LYS
2	2-K	144	LEU
2	2-K	397	GLN
2	2-K	401	LYS
2	2-K	410	LYS
2	2-K	473	ASP
2	2-K	509	GLN
1	2-F	16	GLU
1	2-F	82	ASP
1	2-F	135	GLU
2	2-M	33	GLU
2	2-M	135	LYS
2	2-M	266	TYR
2	2-M	278	LYS
2	2-M	304	LYS
2	2-M	339	SER
2	2-M	362	LEU
2	2-M	379	LYS
2	2-M	397	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2-M	412	SER
2	2-M	452	LYS
2	2-M	454	ASN
2	2-M	473	ASP
2	2-M	509	GLN
1	2-G	88	MET
1	2-G	177	LEU
2	2-N	278	LYS
2	2-N	361	LYS
2	2-N	364	ASP
2	2-N	366	ASP
2	2-N	406	MET
2	2-N	410	LYS
2	2-N	453	ASP
2	2-N	454	ASN
2	2-N	473	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	14	ASN
1	1-A	62	GLN
2	1-H	250	ASN
2	1-H	454	ASN
2	1-H	509	GLN
1	1-B	14	ASN
1	1-B	62	GLN
1	1-B	172	ASN
2	1-I	454	ASN
1	1-C	62	GLN
1	1-C	172	ASN
2	1-J	454	ASN
1	1-D	14	ASN
1	1-D	61	HIS
1	1-D	172	ASN
2	1-K	509	GLN
1	1-F	14	ASN
2	1-M	454	ASN
2	1-M	509	GLN
1	1-G	14	ASN
1	1-G	172	ASN
2	1-N	123	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1-N	326	ASN
2	1-N	454	ASN
2	1-N	509	GLN
1	2-A	14	ASN
1	2-A	62	GLN
2	2-H	250	ASN
2	2-H	454	ASN
2	2-H	509	GLN
1	2-B	14	ASN
1	2-B	62	GLN
1	2-B	172	ASN
2	2-I	454	ASN
1	2-C	62	GLN
1	2-C	172	ASN
2	2-J	454	ASN
1	2-D	14	ASN
1	2-D	61	HIS
1	2-D	172	ASN
2	2-K	509	GLN
1	2-F	14	ASN
2	2-M	454	ASN
2	2-M	509	GLN
1	2-G	14	ASN
2	2-N	123	HIS
2	2-N	454	ASN
2	2-N	509	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 72 ligands modelled in this entry, 24 are monoatomic - leaving 48 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SF4	1-A	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	1-A	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	1-A	267	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SF4	1-B	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	1-B	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	1-B	267	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SF4	1-C	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	1-C	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	1-C	267	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SF4	1-D	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	1-D	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	1-D	267	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SF4	1-F	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	1-F	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	1-F	267	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SF4	1-G	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	1-G	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	1-G	267	1	0,12,12	0.00	-	0,24,24	0.00	-
7	FCO	1-H	550	8,2	0,6,6	0.00	-	0,6,6	0.00	-
7	FCO	1-I	550	8,2	0,6,6	0.00	-	0,6,6	0.00	-
7	FCO	1-J	550	8,2	0,6,6	0.00	-	0,6,6	0.00	-
7	FCO	1-K	550	8,2	0,6,6	0.00	-	0,6,6	0.00	-
7	FCO	1-M	550	8,2	0,6,6	0.00	-	0,6,6	0.00	-
7	FCO	1-N	550	8,2	0,6,6	0.00	-	0,6,6	0.00	-
5	SF4	2-A	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	2-A	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	2-A	267	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SF4	2-B	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	2-B	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	2-B	267	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SF4	2-C	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	2-C	266	1	0,9,9	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SF4	2-C	267	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SF4	2-D	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	2-D	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	2-D	267	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SF4	2-F	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	2-F	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	2-F	267	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SF4	2-G	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	2-G	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	2-G	267	1	0,12,12	0.00	-	0,24,24	0.00	-
7	FCO	2-H	550	8,2	0,6,6	0.00	-	0,6,6	0.00	-
7	FCO	2-I	550	8,2	0,6,6	0.00	-	0,6,6	0.00	-
7	FCO	2-J	550	8,2	0,6,6	0.00	-	0,6,6	0.00	-
7	FCO	2-K	550	8,2	0,6,6	0.00	-	0,6,6	0.00	-
7	FCO	2-M	550	8,2	0,6,6	0.00	-	0,6,6	0.00	-
7	FCO	2-N	550	8,2	0,6,6	0.00	-	0,6,6	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF4	1-A	265	1	-	0/0/48/48	0/6/5/5
6	F3S	1-A	266	1	-	0/0/24/24	0/0/3/3
5	SF4	1-A	267	1	-	0/0/48/48	0/6/5/5
5	SF4	1-B	265	1	-	0/0/48/48	0/6/5/5
6	F3S	1-B	266	1	-	0/0/24/24	0/0/3/3
5	SF4	1-B	267	1	-	0/0/48/48	0/6/5/5
5	SF4	1-C	265	1	-	0/0/48/48	0/6/5/5
6	F3S	1-C	266	1	-	0/0/24/24	0/0/3/3
5	SF4	1-C	267	1	-	0/0/48/48	0/6/5/5
5	SF4	1-D	265	1	-	0/0/48/48	0/6/5/5
6	F3S	1-D	266	1	-	0/0/24/24	0/0/3/3
5	SF4	1-D	267	1	-	0/0/48/48	0/6/5/5
5	SF4	1-F	265	1	-	0/0/48/48	0/6/5/5
6	F3S	1-F	266	1	-	0/0/24/24	0/0/3/3
5	SF4	1-F	267	1	-	0/0/48/48	0/6/5/5
5	SF4	1-G	265	1	-	0/0/48/48	0/6/5/5
6	F3S	1-G	266	1	-	0/0/24/24	0/0/3/3
5	SF4	1-G	267	1	-	0/0/48/48	0/6/5/5
7	FCO	1-H	550	8,2	-	0/0/6/6	0/0/0/0
7	FCO	1-I	550	8,2	-	0/0/6/6	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FCO	1-J	550	8,2	-	0/0/6/6	0/0/0/0
7	FCO	1-K	550	8,2	-	0/0/6/6	0/0/0/0
7	FCO	1-M	550	8,2	-	0/0/6/6	0/0/0/0
7	FCO	1-N	550	8,2	-	0/0/6/6	0/0/0/0
5	SF4	2-A	265	1	-	0/0/48/48	0/6/5/5
6	F3S	2-A	266	1	-	0/0/24/24	0/0/3/3
5	SF4	2-A	267	1	-	0/0/48/48	0/6/5/5
5	SF4	2-B	265	1	-	0/0/48/48	0/6/5/5
6	F3S	2-B	266	1	-	0/0/24/24	0/0/3/3
5	SF4	2-B	267	1	-	0/0/48/48	0/6/5/5
5	SF4	2-C	265	1	-	0/0/48/48	0/6/5/5
6	F3S	2-C	266	1	-	0/0/24/24	0/0/3/3
5	SF4	2-C	267	1	-	0/0/48/48	0/6/5/5
5	SF4	2-D	265	1	-	0/0/48/48	0/6/5/5
6	F3S	2-D	266	1	-	0/0/24/24	0/0/3/3
5	SF4	2-D	267	1	-	0/0/48/48	0/6/5/5
5	SF4	2-F	265	1	-	0/0/48/48	0/6/5/5
6	F3S	2-F	266	1	-	0/0/24/24	0/0/3/3
5	SF4	2-F	267	1	-	0/0/48/48	0/6/5/5
5	SF4	2-G	265	1	-	0/0/48/48	0/6/5/5
6	F3S	2-G	266	1	-	0/0/24/24	0/0/3/3
5	SF4	2-G	267	1	-	0/0/48/48	0/6/5/5
7	FCO	2-H	550	8,2	-	0/0/6/6	0/0/0/0
7	FCO	2-I	550	8,2	-	0/0/6/6	0/0/0/0
7	FCO	2-J	550	8,2	-	0/0/6/6	0/0/0/0
7	FCO	2-K	550	8,2	-	0/0/6/6	0/0/0/0
7	FCO	2-M	550	8,2	-	0/0/6/6	0/0/0/0
7	FCO	2-N	550	8,2	-	0/0/6/6	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	1-M	550	FCO	1	0
7	1-N	550	FCO	2	0
5	2-G	265	SF4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	2-M	550	FCO	1	0
7	2-N	550	FCO	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1-A	262/264 (99%)	-0.20	6 (2%) 64 70	5, 9, 18, 28	8 (3%)
1	1-B	262/264 (99%)	0.64	40 (15%) 3 4	4, 10, 18, 25	6 (2%)
1	1-C	260/264 (98%)	-0.32	2 (0%) 87 90	4, 9, 16, 23	6 (2%)
1	1-D	262/264 (99%)	-0.44	2 (0%) 87 90	3, 9, 16, 30	5 (1%)
1	1-F	260/264 (98%)	-0.09	5 (1%) 70 75	4, 10, 17, 24	6 (2%)
1	1-G	262/264 (99%)	5.49	253 (96%) 0 0	6, 10, 10, 11	262 (100%)
1	2-A	262/264 (99%)	-0.20	6 (2%) 64 70	5, 9, 18, 28	8 (3%)
1	2-B	262/264 (99%)	0.64	40 (15%) 3 4	4, 10, 18, 25	6 (2%)
1	2-C	260/264 (98%)	-0.32	2 (0%) 87 90	4, 9, 16, 23	6 (2%)
1	2-D	262/264 (99%)	-0.44	2 (0%) 87 90	3, 9, 16, 30	5 (1%)
1	2-F	260/264 (98%)	-0.09	5 (1%) 70 75	4, 10, 17, 24	6 (2%)
1	2-G	262/264 (99%)	5.49	253 (96%) 0 0	6, 10, 10, 11	262 (100%)
2	1-H	545/549 (99%)	-0.21	11 (2%) 68 73	4, 9, 16, 27	11 (2%)
2	1-I	545/549 (99%)	0.04	30 (5%) 29 37	3, 9, 16, 24	6 (1%)
2	1-J	544/549 (99%)	-0.06	21 (3%) 43 52	4, 9, 17, 23	12 (2%)
2	1-K	544/549 (99%)	-0.18	9 (1%) 73 78	3, 9, 17, 24	12 (2%)
2	1-M	545/549 (99%)	0.09	24 (4%) 38 47	3, 10, 16, 31	12 (2%)
2	1-N	545/549 (99%)	4.55	510 (93%) 0 0	6, 10, 11, 12	545 (100%)
2	2-H	545/549 (99%)	-0.21	11 (2%) 68 73	4, 9, 16, 27	11 (2%)
2	2-I	545/549 (99%)	0.04	30 (5%) 29 37	3, 9, 16, 24	6 (1%)
2	2-J	544/549 (99%)	-0.06	21 (3%) 43 52	4, 9, 17, 23	12 (2%)
2	2-K	544/549 (99%)	-0.18	9 (1%) 73 78	3, 9, 17, 24	12 (2%)
2	2-M	545/549 (99%)	0.09	24 (4%) 38 47	3, 10, 16, 31	12 (2%)
2	2-N	545/549 (99%)	4.55	510 (93%) 0 0	6, 10, 11, 12	545 (100%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	9672/9756 (99%)	0.75	1826 (18%)	2	2	3, 9, 16, 31	1782 (18%)

All (1826) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	1-N	171	VAL	16.5
2	2-N	171	VAL	16.5
2	1-N	186	GLY	15.6
2	2-N	186	GLY	15.6
1	1-G	137	LEU	14.1
1	2-G	137	LEU	14.1
2	1-N	185	LEU	13.2
2	2-N	185	LEU	13.2
2	1-N	451	ALA	12.9
2	2-N	451	ALA	12.9
1	1-G	196	SER	12.3
1	2-G	196	SER	12.3
1	1-G	254	TRP	12.1
1	2-G	254	TRP	12.1
1	1-G	145	PRO	12.1
1	2-G	145	PRO	12.1
2	1-N	181	ASN	11.9
2	2-N	181	ASN	11.9
2	1-N	134	LEU	11.6
2	2-N	134	LEU	11.6
2	1-N	324	VAL	11.4
2	2-N	324	VAL	11.4
2	1-N	199	LEU	11.4
2	2-N	199	LEU	11.4
2	1-N	247	PRO	11.3
2	2-N	247	PRO	11.3
1	1-G	12	LEU	11.1
1	1-G	79	PRO	11.1
1	2-G	12	LEU	11.1
1	2-G	79	PRO	11.1
1	1-G	64	LEU	11.1
1	2-G	64	LEU	11.1
1	1-G	138	GLY	11.0
1	2-G	138	GLY	11.0
1	1-G	10	VAL	10.9
1	2-G	10	VAL	10.9
2	1-N	347	GLY	10.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	347	GLY	10.9
1	1-G	114	CYS	10.8
1	2-G	114	CYS	10.8
1	1-G	169	LEU	10.7
1	2-G	169	LEU	10.7
2	1-N	49	PHE	10.5
2	1-N	155	ASN	10.5
2	2-N	49	PHE	10.5
2	2-N	155	ASN	10.5
2	1-N	176	LEU	10.5
2	2-N	176	LEU	10.5
2	1-N	289	TYR	10.5
2	2-N	289	TYR	10.5
2	1-N	154	GLY	10.5
2	2-N	154	GLY	10.5
1	1-G	58	ALA	10.4
1	2-G	58	ALA	10.4
2	1-N	213	VAL	10.2
2	2-N	213	VAL	10.2
2	1-N	174	GLY	10.2
2	2-N	174	GLY	10.2
2	1-N	327	VAL	10.2
2	2-N	327	VAL	10.2
2	1-N	341	TYR	10.1
2	2-N	341	TYR	10.1
2	1-N	184	PHE	9.9
2	2-N	184	PHE	9.9
2	1-N	175	GLN	9.9
2	2-N	175	GLN	9.9
1	1-G	237	TRP	9.7
1	2-G	237	TRP	9.7
1	1-G	213	LEU	9.6
1	2-G	213	LEU	9.6
1	1-G	157	ALA	9.6
1	2-G	157	ALA	9.6
1	1-G	74	VAL	9.4
1	2-G	74	VAL	9.4
1	1-G	248	CYS	9.4
1	2-G	248	CYS	9.4
1	1-G	49	MET	9.4
1	2-G	49	MET	9.4
2	1-N	187	GLY	9.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	187	GLY	9.3
1	1-G	11	TRP	9.3
1	2-G	11	TRP	9.3
2	1-N	51	GLY	9.3
2	2-N	51	GLY	9.3
1	1-G	136	ALA	9.2
1	2-G	136	ALA	9.2
2	1-N	246	ASP	9.2
2	2-N	246	ASP	9.2
2	1-N	178	ILE	9.1
2	2-N	178	ILE	9.1
1	1-G	158	VAL	8.9
1	2-G	158	VAL	8.9
2	1-N	180	THR	8.9
2	2-N	180	THR	8.9
2	1-N	393	TYR	8.9
2	2-N	393	TYR	8.9
2	1-N	130	VAL	8.9
2	2-N	130	VAL	8.9
1	1-G	108	ILE	8.8
1	2-G	108	ILE	8.8
2	1-N	177	GLY	8.7
2	2-N	177	GLY	8.7
1	1-G	17	CYS	8.7
1	2-G	17	CYS	8.7
1	1-G	47	THR	8.6
1	2-G	47	THR	8.6
1	1-G	110	CYS	8.6
1	2-G	110	CYS	8.6
2	1-N	366	ASP	8.5
2	2-N	366	ASP	8.5
1	1-G	190	LEU	8.5
1	2-G	190	LEU	8.5
2	1-N	518	ALA	8.4
2	2-N	518	ALA	8.4
1	1-G	166	ILE	8.4
1	2-G	166	ILE	8.4
1	1-G	168	ASP	8.3
1	2-G	168	ASP	8.3
1	1-G	32	ILE	8.3
1	1-G	154	PHE	8.3
1	2-G	32	ILE	8.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2-G	154	PHE	8.3
2	1-N	67	PHE	8.3
2	2-N	67	PHE	8.3
1	1-G	72	LEU	8.2
1	2-G	72	LEU	8.2
2	1-N	344	GLY	8.2
2	2-N	344	GLY	8.2
2	1-N	54	ILE	8.2
2	2-N	54	ILE	8.2
1	1-G	199	ALA	8.1
1	2-G	199	ALA	8.1
2	1-N	131	THR	8.1
2	2-N	131	THR	8.1
2	1-N	206	LEU	8.1
2	2-N	206	LEU	8.1
2	1-N	377	LYS	8.0
2	2-N	377	LYS	8.0
1	1-G	52	ALA	7.9
1	2-G	52	ALA	7.9
2	1-N	42	ALA	7.9
2	2-N	42	ALA	7.9
1	1-G	61	HIS	7.8
1	2-G	61	HIS	7.8
2	1-N	508	ALA	7.8
2	2-N	508	ALA	7.8
2	1-N	182	ALA	7.7
2	2-N	182	ALA	7.7
2	1-N	132	ALA	7.7
2	2-N	132	ALA	7.7
1	1-G	44	TYR	7.7
1	2-G	44	TYR	7.7
2	1-N	227	PRO	7.7
2	2-N	227	PRO	7.7
2	1-N	370	TRP	7.7
2	2-N	370	TRP	7.7
1	1-G	42	LEU	7.6
1	2-G	42	LEU	7.6
1	1-G	109	ILE	7.6
1	2-G	109	ILE	7.6
1	1-G	133	VAL	7.6
1	2-G	133	VAL	7.6
1	1-G	77	GLY	7.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2-G	77	GLY	7.6
1	1-G	207	ALA	7.6
1	2-G	207	ALA	7.6
1	1-G	144	ILE	7.6
1	2-G	144	ILE	7.6
1	1-G	246	LEU	7.5
1	2-G	246	LEU	7.5
1	1-G	261	TYR	7.5
1	2-G	261	TYR	7.5
1	1-G	20	CYS	7.5
1	2-G	20	CYS	7.5
2	1-N	359	TYR	7.5
2	2-N	359	TYR	7.5
1	1-G	91	GLY	7.5
1	2-G	91	GLY	7.5
2	1-N	106	VAL	7.5
2	2-N	106	VAL	7.5
2	1-N	183	TYR	7.4
2	2-N	183	TYR	7.4
1	1-G	120	VAL	7.4
1	2-G	120	VAL	7.4
2	1-N	321	LEU	7.4
2	2-N	321	LEU	7.4
1	1-G	15	ALA	7.4
1	2-G	15	ALA	7.4
2	1-N	254	LEU	7.4
2	2-N	254	LEU	7.4
2	1-N	221	ILE	7.3
2	2-N	221	ILE	7.3
2	1-N	72	CYS	7.3
2	2-N	72	CYS	7.3
1	1-G	73	VAL	7.3
1	2-G	73	VAL	7.3
1	1-G	45	GLN	7.3
1	2-G	45	GLN	7.3
2	1-N	76	THR	7.3
2	2-N	76	THR	7.3
2	1-N	403	VAL	7.2
2	2-N	403	VAL	7.2
1	1-G	90	ALA	7.2
1	1-G	117	TYR	7.2
1	2-G	90	ALA	7.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2-G	117	TYR	7.2
2	1-N	330	GLY	7.2
2	2-N	330	GLY	7.2
1	1-G	148	PRO	7.2
1	2-G	148	PRO	7.2
1	1-G	155	VAL	7.2
1	2-G	155	VAL	7.2
1	1-G	118	GLY	7.2
1	2-G	118	GLY	7.2
1	1-G	62	GLN	7.2
1	2-G	62	GLN	7.2
2	1-N	326	ASN	7.2
2	2-N	326	ASN	7.2
1	1-G	232	PHE	7.2
1	2-G	232	PHE	7.2
1	1-G	48	ILE	7.1
1	2-G	48	ILE	7.1
2	1-N	229	THR	7.1
2	2-N	229	THR	7.1
1	1-G	46	GLU	7.1
1	2-G	46	GLU	7.1
2	1-N	135	LYS	7.1
2	2-N	135	LYS	7.1
1	1-G	159	VAL	7.0
1	2-G	159	VAL	7.0
1	1-G	7	PRO	7.0
1	2-G	7	PRO	7.0
1	1-G	239	VAL	7.0
1	2-G	239	VAL	7.0
1	1-G	262	GLU	7.0
1	2-G	262	GLU	7.0
1	1-G	260	PHE	7.0
1	2-G	260	PHE	7.0
2	1-N	99	ALA	6.9
2	1-N	331	ALA	6.9
2	2-N	99	ALA	6.9
2	2-N	331	ALA	6.9
1	1-G	86	TRP	6.9
1	2-G	86	TRP	6.9
1	1-G	43	ASP	6.9
1	2-G	43	ASP	6.9
2	1-N	369	SER	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	369	SER	6.9
1	1-G	149	PRO	6.9
1	2-G	149	PRO	6.9
1	1-G	171	SER	6.9
1	2-G	171	SER	6.9
2	1-N	228	HIS	6.9
2	2-N	228	HIS	6.9
1	1-G	9	VAL	6.9
1	2-G	9	VAL	6.9
2	1-N	546	CYS	6.9
2	2-N	546	CYS	6.9
1	1-G	25	ILE	6.8
1	2-G	25	ILE	6.8
2	1-N	336	VAL	6.8
2	2-N	336	VAL	6.8
2	1-N	75	CYS	6.7
2	2-N	75	CYS	6.7
1	1-G	258	THR	6.7
1	2-G	258	THR	6.7
2	1-N	172	GLU	6.7
2	2-N	172	GLU	6.7
1	1-G	13	HIS	6.7
1	2-G	13	HIS	6.7
2	1-N	80	ALA	6.7
2	2-N	80	ALA	6.7
2	1-N	376	TYR	6.7
2	2-N	376	TYR	6.7
1	1-G	23	ALA	6.7
1	2-G	23	ALA	6.7
1	1-G	177	LEU	6.7
1	2-G	177	LEU	6.7
1	1-G	253	PHE	6.7
1	2-G	253	PHE	6.7
2	1-N	350	PRO	6.7
2	2-N	350	PRO	6.7
2	1-N	179	PHE	6.6
2	2-N	179	PHE	6.6
1	1-G	95	ILE	6.6
1	2-G	95	ILE	6.6
1	1-G	53	GLY	6.6
1	2-G	53	GLY	6.6
2	1-N	71	ALA	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	1-N	112	LEU	6.6
2	2-N	71	ALA	6.6
2	2-N	112	LEU	6.6
2	1-N	543	CYS	6.6
2	2-N	543	CYS	6.6
1	1-G	24	ALA	6.5
1	2-G	24	ALA	6.5
1	1-G	70	TYR	6.5
1	2-G	70	TYR	6.5
2	1-N	66	HIS	6.5
2	2-N	66	HIS	6.5
1	1-G	21	THR	6.5
1	2-G	21	THR	6.5
2	1-N	253	ALA	6.5
2	2-N	253	ALA	6.5
2	1-N	125	LEU	6.5
2	2-N	125	LEU	6.5
1	1-G	227	CYS	6.5
1	2-G	227	CYS	6.5
2	1-N	332	ILE	6.5
2	2-N	332	ILE	6.5
2	1-N	149	ALA	6.4
2	2-N	149	ALA	6.4
1	1-G	238	PRO	6.4
1	2-G	238	PRO	6.4
1	1-G	198	PHE	6.4
1	2-G	198	PHE	6.4
2	1-N	410	LYS	6.4
2	2-N	410	LYS	6.4
2	1-N	77	TYR	6.4
2	2-N	77	TYR	6.4
2	1-N	544	ILE	6.4
2	2-N	544	ILE	6.4
2	1-N	400	PHE	6.4
2	2-N	400	PHE	6.4
2	1-N	205	TYR	6.3
2	2-N	205	TYR	6.3
2	1-N	501	TRP	6.3
2	2-N	501	TRP	6.3
2	1-N	329	LEU	6.3
2	2-N	329	LEU	6.3
2	1-N	21	ILE	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	21	ILE	6.3
1	1-G	161	VAL	6.3
1	2-G	161	VAL	6.3
1	1-G	147	CYS	6.3
1	2-G	147	CYS	6.3
2	1-N	34	VAL	6.3
2	2-N	34	VAL	6.3
2	1-N	342	ALA	6.2
2	2-N	342	ALA	6.2
1	1-G	229	LYS	6.2
1	2-G	229	LYS	6.2
1	1-G	214	TYR	6.2
1	2-G	214	TYR	6.2
2	1-N	74	VAL	6.2
2	2-N	74	VAL	6.2
2	1-N	167	LEU	6.1
2	1-N	333	TYR	6.1
2	1-N	418	LEU	6.1
2	2-N	167	LEU	6.1
2	2-N	333	TYR	6.1
2	2-N	418	LEU	6.1
2	1-N	338	TYR	6.1
2	2-N	338	TYR	6.1
1	1-G	67	LYS	6.1
1	2-G	67	LYS	6.1
2	1-N	105	LEU	6.1
2	2-N	105	LEU	6.1
1	1-G	215	GLU	6.1
1	2-G	215	GLU	6.1
2	1-N	223	GLY	6.0
2	2-N	223	GLY	6.0
1	1-G	40	ILE	6.0
1	2-G	40	ILE	6.0
1	1-G	218	CYS	6.0
1	2-G	218	CYS	6.0
2	1-N	340	TRP	6.0
2	2-N	340	TRP	6.0
1	1-G	165	GLY	6.0
1	2-G	165	GLY	6.0
2	1-N	122	LEU	6.0
2	2-N	122	LEU	6.0
2	1-N	281	GLY	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	281	GLY	5.9
2	1-N	52	LEU	5.9
2	2-N	52	LEU	5.9
2	1-N	443	ILE	5.9
2	2-N	443	ILE	5.9
1	1-G	179	TYR	5.9
1	2-G	179	TYR	5.9
1	1-G	225	ASN	5.9
1	2-G	225	ASN	5.9
2	1-N	117	VAL	5.9
2	1-N	406	MET	5.9
2	2-N	117	VAL	5.9
2	2-N	406	MET	5.9
2	1-N	297	THR	5.9
2	1-N	432	THR	5.9
2	2-N	297	THR	5.9
2	2-N	432	THR	5.9
1	1-G	222	VAL	5.9
1	2-G	222	VAL	5.9
2	1-N	258	VAL	5.9
2	2-N	258	VAL	5.9
2	1-N	43	TRP	5.9
2	2-N	43	TRP	5.9
2	1-N	291	ALA	5.8
2	1-N	415	ALA	5.8
2	1-N	433	ALA	5.8
2	2-N	291	ALA	5.8
2	2-N	415	ALA	5.8
2	2-N	433	ALA	5.8
1	1-G	163	THR	5.8
1	2-G	163	THR	5.8
1	1-G	189	ARG	5.8
1	2-G	189	ARG	5.8
2	1-N	209	LEU	5.8
2	2-N	209	LEU	5.8
2	1-N	73	GLY	5.8
2	2-N	73	GLY	5.8
2	1-N	17	VAL	5.8
2	1-N	24	ILE	5.8
2	2-N	17	VAL	5.8
2	2-N	24	ILE	5.8
1	1-G	97	THR	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-G	178	PHE	5.8
1	2-G	97	THR	5.8
1	2-G	178	PHE	5.8
1	1-G	51	ALA	5.7
1	2-G	51	ALA	5.7
2	1-N	226	ASN	5.7
2	2-N	226	ASN	5.7
1	1-G	180	GLY	5.7
1	2-G	180	GLY	5.7
2	1-N	28	LEU	5.7
2	2-N	28	LEU	5.7
2	1-N	360	THR	5.7
2	1-N	510	GLY	5.7
2	1-N	548	VAL	5.7
2	2-N	360	THR	5.7
2	2-N	510	GLY	5.7
2	2-N	548	VAL	5.7
2	1-N	220	ALA	5.7
2	1-N	447	ALA	5.7
2	2-N	220	ALA	5.7
2	2-N	447	ALA	5.7
2	1-N	509	GLN	5.7
2	2-N	509	GLN	5.7
1	1-G	78	LEU	5.7
1	2-G	78	LEU	5.7
1	1-G	245	CYS	5.7
1	2-G	245	CYS	5.7
2	1-N	456	LEU	5.7
2	2-N	456	LEU	5.7
2	1-N	435	VAL	5.7
2	2-N	435	VAL	5.7
1	1-G	50	ALA	5.7
1	2-G	50	ALA	5.7
2	1-N	261	PHE	5.6
2	1-N	390	PHE	5.6
2	2-N	261	PHE	5.6
2	2-N	390	PHE	5.6
2	1-N	69	GLN	5.6
2	2-N	69	GLN	5.6
1	1-G	36	ILE	5.6
1	2-G	36	ILE	5.6
2	1-N	343	PRO	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	343	PRO	5.6
1	1-G	54	GLU	5.6
1	2-G	54	GLU	5.6
2	1-N	230	GLN	5.6
2	2-N	230	GLN	5.6
2	1-N	290	LEU	5.6
2	2-N	290	LEU	5.6
2	1-N	250	ASN	5.6
2	2-N	250	ASN	5.6
1	1-G	30	PRO	5.6
1	2-G	30	PRO	5.6
2	1-N	417	ALA	5.6
2	2-N	417	ALA	5.6
1	1-B	165	GLY	5.6
1	1-G	217	GLY	5.6
1	2-B	165	GLY	5.6
1	2-G	217	GLY	5.6
2	1-N	265	CYS	5.6
2	2-N	265	CYS	5.6
1	1-G	4	LYS	5.6
1	2-G	4	LYS	5.6
2	1-N	354	VAL	5.6
2	2-N	354	VAL	5.6
1	1-G	18	THR	5.6
1	1-G	71	TYR	5.6
1	2-G	18	THR	5.6
1	2-G	71	TYR	5.6
1	1-G	60	LEU	5.6
1	2-G	60	LEU	5.6
2	1-N	11	THR	5.6
2	2-N	11	THR	5.6
2	1-N	46	SER	5.6
2	1-N	170	PHE	5.6
2	2-N	46	SER	5.6
2	2-N	170	PHE	5.6
2	1-N	386	LEU	5.6
2	2-N	386	LEU	5.6
1	1-G	127	PRO	5.5
1	2-G	127	PRO	5.5
1	1-G	216	LEU	5.5
1	2-G	216	LEU	5.5
2	1-N	13	THR	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	13	THR	5.5
2	1-N	430	ILE	5.5
2	2-N	430	ILE	5.5
1	1-G	41	SER	5.5
1	2-G	41	SER	5.5
1	1-G	172	ASN	5.5
1	2-G	172	ASN	5.5
2	1-N	266	TYR	5.5
2	2-N	266	TYR	5.5
2	1-N	378	GLY	5.5
2	2-N	378	GLY	5.5
2	1-N	316	ILE	5.5
2	2-N	316	ILE	5.5
2	1-N	216	ALA	5.5
2	2-N	216	ALA	5.5
2	1-N	70	ARG	5.5
2	2-N	70	ARG	5.5
2	1-N	457	CYS	5.5
2	2-N	457	CYS	5.5
1	1-G	193	PHE	5.5
1	2-G	193	PHE	5.5
2	1-N	116	LEU	5.5
2	2-N	116	LEU	5.5
2	1-N	374	PRO	5.4
2	2-N	374	PRO	5.4
2	1-N	389	THR	5.4
2	2-N	389	THR	5.4
1	1-G	194	GLU	5.4
1	2-G	194	GLU	5.4
2	1-N	356	ASP	5.4
2	2-N	356	ASP	5.4
2	1-N	16	ILE	5.4
2	1-N	533	ILE	5.4
2	2-N	16	ILE	5.4
2	2-N	533	ILE	5.4
1	1-G	257	MET	5.4
1	2-G	257	MET	5.4
2	1-N	78	VAL	5.4
2	2-N	78	VAL	5.4
2	1-N	460	TRP	5.4
2	2-N	460	TRP	5.4
1	1-G	231	LEU	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2-G	231	LEU	5.4
2	1-N	63	ASP	5.4
2	1-N	365	LYS	5.4
2	2-N	63	ASP	5.4
2	2-N	365	LYS	5.4
2	1-N	232	THR	5.4
2	2-N	232	THR	5.4
1	1-G	150	ASN	5.4
1	2-G	150	ASN	5.4
1	1-G	55	ALA	5.4
1	2-G	55	ALA	5.4
2	1-N	429	GLY	5.4
2	2-N	429	GLY	5.4
1	1-G	259	PRO	5.4
1	2-G	259	PRO	5.4
2	1-N	150	PRO	5.4
2	2-N	150	PRO	5.4
1	1-G	113	THR	5.4
1	2-G	113	THR	5.4
1	1-G	123	ALA	5.4
1	2-G	123	ALA	5.4
1	1-G	167	PRO	5.4
1	1-G	228	PRO	5.4
1	2-G	167	PRO	5.4
1	2-G	228	PRO	5.4
2	1-N	22	THR	5.4
2	2-N	22	THR	5.4
1	1-G	35	LEU	5.4
1	2-G	35	LEU	5.4
1	1-G	69	GLY	5.4
1	2-G	69	GLY	5.4
1	1-G	92	HIS	5.3
1	2-G	92	HIS	5.3
2	1-N	479	LEU	5.3
2	2-N	479	LEU	5.3
2	1-N	36	ASN	5.3
2	2-N	36	ASN	5.3
1	1-G	8	SER	5.3
1	2-G	8	SER	5.3
1	1-G	66	GLY	5.3
1	2-G	66	GLY	5.3
2	1-N	107	MET	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	107	MET	5.3
2	1-N	231	PHE	5.3
2	2-N	231	PHE	5.3
1	1-G	57	GLU	5.3
1	2-G	57	GLU	5.3
2	1-N	426	ALA	5.3
2	2-N	426	ALA	5.3
1	1-G	132	GLY	5.3
1	2-G	132	GLY	5.3
1	1-G	88	MET	5.3
1	2-G	88	MET	5.3
2	1-N	219	MET	5.3
2	2-N	219	MET	5.3
2	1-N	65	GLN	5.3
2	2-N	65	GLN	5.3
1	1-G	107	GLY	5.3
1	2-G	107	GLY	5.3
1	1-G	87	GLY	5.3
1	2-G	87	GLY	5.3
1	1-G	244	PRO	5.3
1	2-G	244	PRO	5.3
2	1-N	56	LEU	5.3
2	2-N	56	LEU	5.3
2	1-N	346	ASP	5.3
2	2-N	346	ASP	5.3
2	1-N	120	TYR	5.2
2	2-N	120	TYR	5.2
2	1-N	163	VAL	5.2
2	2-N	163	VAL	5.2
1	1-G	115	SER	5.2
1	2-G	115	SER	5.2
1	1-G	116	ALA	5.2
1	2-G	116	ALA	5.2
2	1-N	64	ALA	5.2
2	2-N	64	ALA	5.2
2	1-N	30	ILE	5.2
2	2-N	30	ILE	5.2
2	1-N	286	THR	5.2
2	2-N	286	THR	5.2
2	1-N	295	PHE	5.2
2	2-N	295	PHE	5.2
1	1-G	76	GLY	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2-G	76	GLY	5.2
1	1-G	151	PRO	5.2
1	2-G	151	PRO	5.2
1	1-G	63	ALA	5.2
1	2-G	63	ALA	5.2
2	1-N	81	LEU	5.2
2	2-N	81	LEU	5.2
2	1-N	292	PHE	5.2
2	2-N	292	PHE	5.2
2	1-N	225	LYS	5.1
2	2-N	225	LYS	5.1
2	1-N	68	THR	5.1
2	2-N	68	THR	5.1
2	1-N	482	TRP	5.1
2	2-N	482	TRP	5.1
2	1-N	315	VAL	5.1
2	2-N	315	VAL	5.1
1	1-G	247	GLY	5.1
1	2-G	247	GLY	5.1
1	1-G	103	ALA	5.1
1	2-G	103	ALA	5.1
1	1-G	19	GLY	5.1
1	2-G	19	GLY	5.1
2	1-N	530	PRO	5.1
2	2-N	530	PRO	5.1
2	1-N	173	SER	5.1
2	2-N	173	SER	5.1
1	1-G	202	PHE	5.1
1	2-G	202	PHE	5.1
1	1-G	56	ALA	5.0
1	2-G	56	ALA	5.0
1	1-G	111	ILE	5.0
1	2-G	111	ILE	5.0
1	1-G	98	THR	5.0
1	2-G	98	THR	5.0
2	1-N	119	PHE	5.0
2	2-N	119	PHE	5.0
1	1-G	104	LYS	5.0
1	2-G	104	LYS	5.0
2	1-N	514	PRO	5.0
2	2-N	514	PRO	5.0
1	1-G	142	ILE	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2-G	142	ILE	5.0
2	1-N	517	GLU	5.0
2	2-N	517	GLU	5.0
1	1-G	243	HIS	5.0
1	2-G	243	HIS	5.0
2	1-N	520	ILE	5.0
2	2-N	520	ILE	5.0
2	1-N	128	VAL	5.0
2	1-N	251	TYR	5.0
2	2-N	128	VAL	5.0
2	2-N	251	TYR	5.0
1	1-B	169	LEU	5.0
1	2-B	169	LEU	5.0
2	1-N	379	LYS	5.0
2	2-N	379	LYS	5.0
2	1-N	244	THR	4.9
2	2-N	244	THR	4.9
1	1-G	89	VAL	4.9
1	2-G	89	VAL	4.9
2	1-N	240	TYR	4.9
2	2-N	240	TYR	4.9
2	1-N	367	HIS	4.9
2	2-N	367	HIS	4.9
1	1-G	195	ALA	4.9
1	2-G	195	ALA	4.9
2	1-N	20	PRO	4.9
2	1-N	547	GLY	4.9
2	2-N	20	PRO	4.9
2	2-N	547	GLY	4.9
1	1-G	27	THR	4.9
1	2-G	27	THR	4.9
2	1-N	293	GLY	4.9
2	2-N	293	GLY	4.9
2	1-N	402	LYS	4.9
2	2-N	402	LYS	4.9
2	1-N	260	GLN	4.8
2	1-N	272	ALA	4.8
2	2-N	260	GLN	4.8
2	2-N	272	ALA	4.8
2	1-N	311	PHE	4.8
2	2-N	311	PHE	4.8
2	1-N	141	ALA	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	141	ALA	4.8
2	1-N	383	VAL	4.8
2	1-N	407	VAL	4.8
2	2-N	383	VAL	4.8
2	2-N	407	VAL	4.8
2	1-M	322	GLY	4.8
2	2-M	322	GLY	4.8
2	1-N	373	ALA	4.8
2	2-N	373	ALA	4.8
1	1-G	200	PRO	4.8
1	2-G	200	PRO	4.8
2	1-N	539	ALA	4.8
2	2-N	539	ALA	4.8
1	1-G	121	GLN	4.8
1	1-G	263	GLN	4.8
1	2-G	121	GLN	4.8
1	2-G	263	GLN	4.8
1	1-G	226	ASN	4.8
1	2-G	226	ASN	4.8
2	1-N	452	LYS	4.8
2	2-N	452	LYS	4.8
1	1-G	230	VAL	4.8
1	2-G	230	VAL	4.8
2	1-N	137	ASP	4.8
2	1-N	521	GLY	4.8
2	2-N	137	ASP	4.8
2	2-N	521	GLY	4.8
2	1-N	531	VAL	4.7
2	2-N	531	VAL	4.7
2	1-N	133	ALA	4.7
2	1-N	307	ALA	4.7
2	2-N	133	ALA	4.7
2	2-N	307	ALA	4.7
1	1-B	67	LYS	4.7
1	2-B	67	LYS	4.7
2	1-N	224	GLY	4.7
2	2-N	224	GLY	4.7
2	1-N	148	ILE	4.7
2	2-N	148	ILE	4.7
2	1-N	425	THR	4.7
2	2-N	425	THR	4.7
2	1-N	248	LEU	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	248	LEU	4.7
2	1-N	27	HIS	4.7
2	1-N	409	GLY	4.7
2	2-N	27	HIS	4.7
2	2-N	409	GLY	4.7
1	1-G	16	GLU	4.7
1	2-G	16	GLU	4.7
1	1-G	81	ILE	4.7
1	2-G	81	ILE	4.7
1	1-G	185	ASP	4.7
1	2-G	185	ASP	4.7
2	1-N	32	VAL	4.7
2	2-N	32	VAL	4.7
2	1-N	160	LEU	4.7
2	2-N	160	LEU	4.7
2	1-N	348	LYS	4.7
2	2-N	348	LYS	4.7
2	1-N	113	HIS	4.6
2	2-N	113	HIS	4.6
1	1-G	264	GLY	4.6
1	2-G	264	GLY	4.6
2	1-N	362	LEU	4.6
2	2-N	362	LEU	4.6
1	1-G	211	PHE	4.6
1	2-G	211	PHE	4.6
2	1-N	527	PRO	4.6
2	2-N	527	PRO	4.6
1	1-G	235	VAL	4.6
1	2-G	235	VAL	4.6
2	1-N	41	ASP	4.6
2	2-N	41	ASP	4.6
1	1-G	251	PRO	4.6
1	2-G	251	PRO	4.6
2	1-N	267	ILE	4.6
2	2-N	267	ILE	4.6
2	1-N	422	LEU	4.6
2	2-N	422	LEU	4.6
2	1-N	287	SER	4.6
2	2-N	287	SER	4.6
2	1-M	415	ALA	4.6
2	2-M	415	ALA	4.6
1	1-G	153	ASN	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2-G	153	ASN	4.6
2	1-N	208	ALA	4.6
2	2-N	208	ALA	4.6
2	1-N	280	TRP	4.6
2	2-N	280	TRP	4.6
2	1-N	83	SER	4.6
2	2-N	83	SER	4.6
1	1-G	93	PRO	4.5
1	2-G	93	PRO	4.5
1	1-G	135	GLU	4.5
1	2-G	135	GLU	4.5
2	1-N	108	ALA	4.5
2	2-N	108	ALA	4.5
1	1-G	223	THR	4.5
1	2-G	223	THR	4.5
2	1-N	437	ALA	4.5
2	2-N	437	ALA	4.5
1	1-G	99	LYS	4.5
1	1-G	219	LYS	4.5
1	1-G	256	THR	4.5
1	2-G	99	LYS	4.5
1	2-G	219	LYS	4.5
1	2-G	256	THR	4.5
2	1-N	233	VAL	4.5
2	2-N	233	VAL	4.5
2	1-N	427	ALA	4.5
2	2-N	427	ALA	4.5
2	1-N	499	SER	4.5
2	2-N	499	SER	4.5
1	1-G	252	ASP	4.5
1	2-G	252	ASP	4.5
2	1-N	391	ILE	4.5
2	2-N	391	ILE	4.5
1	1-G	6	ARG	4.5
1	2-G	6	ARG	4.5
2	1-N	262	VAL	4.5
2	2-N	262	VAL	4.5
2	1-N	129	ASP	4.5
2	1-N	222	LEU	4.5
2	2-N	129	ASP	4.5
2	2-N	222	LEU	4.5
2	1-N	157	ALA	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	157	ALA	4.5
2	1-I	153	PRO	4.5
2	1-N	23	ARG	4.5
2	2-I	153	PRO	4.5
2	2-N	23	ARG	4.5
2	1-N	111	TYR	4.5
2	1-N	368	TYR	4.5
2	2-N	111	TYR	4.5
2	2-N	368	TYR	4.5
2	1-N	242	GLY	4.5
2	2-N	242	GLY	4.5
2	1-N	86	CYS	4.5
2	2-N	86	CYS	4.5
2	1-N	420	SER	4.5
2	2-N	420	SER	4.5
2	1-N	363	ASP	4.4
2	2-N	363	ASP	4.4
1	1-G	191	PRO	4.4
1	2-G	191	PRO	4.4
2	1-N	153	PRO	4.4
2	2-N	153	PRO	4.4
1	1-G	249	SER	4.4
1	2-G	249	SER	4.4
2	1-N	361	LYS	4.4
2	2-N	361	LYS	4.4
2	1-N	237	CYS	4.4
2	2-N	237	CYS	4.4
2	1-N	496	VAL	4.4
2	2-N	496	VAL	4.4
2	1-N	202	THR	4.4
2	2-N	202	THR	4.4
2	1-N	188	HIS	4.4
2	2-N	188	HIS	4.4
2	1-N	472	ALA	4.4
2	2-N	472	ALA	4.4
1	1-G	29	LYS	4.4
1	2-G	29	LYS	4.4
2	1-N	392	ALA	4.4
2	2-N	392	ALA	4.4
2	1-N	534	LEU	4.4
2	2-N	534	LEU	4.4
2	1-N	39	VAL	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	39	VAL	4.4
1	1-G	141	THR	4.4
1	2-G	141	THR	4.4
2	1-N	211	MET	4.4
2	2-N	211	MET	4.4
2	1-N	145	ALA	4.3
2	2-N	145	ALA	4.3
1	1-G	146	GLY	4.3
1	2-G	146	GLY	4.3
2	1-N	470	GLY	4.3
2	2-N	470	GLY	4.3
2	1-N	121	HIS	4.3
2	2-N	121	HIS	4.3
2	1-N	349	HIS	4.3
2	2-N	349	HIS	4.3
1	1-G	242	GLY	4.3
1	2-G	242	GLY	4.3
2	1-N	33	GLU	4.3
2	2-N	33	GLU	4.3
2	1-N	296	ALA	4.3
2	2-N	296	ALA	4.3
1	1-G	234	GLN	4.3
1	2-G	234	GLN	4.3
2	1-N	419	HIS	4.3
2	2-N	419	HIS	4.3
2	1-N	325	ASP	4.3
2	1-N	381	MET	4.3
2	1-N	453	ASP	4.3
2	2-N	325	ASP	4.3
2	2-N	381	MET	4.3
2	2-N	453	ASP	4.3
1	1-G	112	GLY	4.3
1	1-G	156	GLY	4.3
1	1-G	175	PRO	4.3
1	2-G	112	GLY	4.3
1	2-G	156	GLY	4.3
1	2-G	175	PRO	4.3
2	1-N	385	PRO	4.3
2	2-N	385	PRO	4.3
1	1-G	65	GLU	4.3
1	2-G	65	GLU	4.3
2	1-N	102	MET	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	102	MET	4.3
2	1-N	26	GLY	4.3
2	2-N	26	GLY	4.3
1	1-G	100	LYS	4.3
1	2-G	100	LYS	4.3
2	1-N	411	LEU	4.3
2	1-N	519	LEU	4.3
2	2-N	411	LEU	4.3
2	2-N	519	LEU	4.3
1	1-G	152	ILE	4.3
1	2-G	152	ILE	4.3
2	1-N	190	ALA	4.3
2	2-N	190	ALA	4.3
1	1-G	31	TYR	4.2
1	2-G	31	TYR	4.2
2	1-N	48	LEU	4.2
2	2-N	48	LEU	4.2
1	1-G	59	ALA	4.2
1	2-G	59	ALA	4.2
2	1-N	136	ALA	4.2
2	1-N	413	VAL	4.2
2	2-N	136	ALA	4.2
2	2-N	413	VAL	4.2
1	1-B	167	PRO	4.2
1	1-G	125	PRO	4.2
1	2-B	167	PRO	4.2
1	2-G	125	PRO	4.2
2	1-I	322	GLY	4.2
2	2-I	322	GLY	4.2
1	1-G	233	ASN	4.2
1	2-G	233	ASN	4.2
2	1-N	243	LEU	4.2
2	2-N	243	LEU	4.2
2	1-N	234	VAL	4.2
2	2-N	234	VAL	4.2
2	1-N	249	ALA	4.2
2	1-N	387	ALA	4.2
2	2-N	249	ALA	4.2
2	2-N	387	ALA	4.2
2	1-N	195	PRO	4.2
2	2-N	195	PRO	4.2
1	1-G	82	ASP	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2-G	82	ASP	4.2
1	1-G	14	ASN	4.2
1	1-G	143	ASN	4.2
1	2-G	14	ASN	4.2
1	2-G	143	ASN	4.2
2	1-J	36	ASN	4.2
2	2-J	36	ASN	4.2
2	1-N	317	THR	4.1
2	2-N	317	THR	4.1
2	1-N	239	ASN	4.1
2	2-N	239	ASN	4.1
2	1-N	127	TRP	4.1
2	2-N	127	TRP	4.1
1	1-G	224	TYR	4.1
1	2-G	224	TYR	4.1
2	1-N	306	LEU	4.1
2	2-N	306	LEU	4.1
2	1-N	498	PRO	4.1
2	2-N	498	PRO	4.1
2	1-I	453	ASP	4.1
2	2-I	453	ASP	4.1
1	1-G	94	MET	4.1
1	2-G	94	MET	4.1
2	1-N	495	LEU	4.1
2	2-N	495	LEU	4.1
2	1-N	115	HIS	4.1
2	2-N	115	HIS	4.1
2	1-N	109	SER	4.1
2	2-N	109	SER	4.1
2	1-N	448	ASP	4.0
2	2-N	448	ASP	4.0
2	1-N	201	ALA	4.0
2	2-N	201	ALA	4.0
2	1-N	31	MET	4.0
2	1-N	62	ARG	4.0
2	2-N	31	MET	4.0
2	2-N	62	ARG	4.0
2	1-N	428	ARG	4.0
2	2-N	428	ARG	4.0
2	1-N	416	THR	4.0
2	2-N	416	THR	4.0
1	1-G	5	HIS	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2-G	5	HIS	4.0
2	1-N	118	HIS	4.0
2	1-N	305	HIS	4.0
2	2-N	118	HIS	4.0
2	2-N	305	HIS	4.0
2	1-N	536	THR	4.0
2	2-N	536	THR	4.0
2	1-N	399	ASP	4.0
2	2-N	399	ASP	4.0
1	1-G	119	GLY	4.0
1	2-G	119	GLY	4.0
2	1-N	217	SER	4.0
2	2-N	217	SER	4.0
2	1-N	312	PRO	4.0
2	2-N	312	PRO	4.0
1	1-G	37	LEU	3.9
1	2-G	37	LEU	3.9
2	1-N	284	GLY	3.9
2	2-N	284	GLY	3.9
2	1-N	203	ALA	3.9
2	2-N	203	ALA	3.9
1	1-G	183	VAL	3.9
1	2-G	183	VAL	3.9
2	1-I	148	ILE	3.9
2	2-I	148	ILE	3.9
2	1-N	504	GLY	3.9
2	2-N	504	GLY	3.9
2	1-N	273	VAL	3.9
2	2-N	273	VAL	3.9
1	1-G	241	ALA	3.9
1	2-G	241	ALA	3.9
2	1-N	50	ARG	3.9
2	2-N	50	ARG	3.9
2	1-N	540	PHE	3.9
2	2-N	540	PHE	3.9
2	1-N	423	GLY	3.9
2	2-N	423	GLY	3.9
2	1-N	480	SER	3.9
2	2-N	480	SER	3.9
2	1-N	35	GLU	3.9
2	2-N	35	GLU	3.9
2	1-N	98	ASN	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	98	ASN	3.9
2	1-M	378	GLY	3.9
2	1-N	282	GLY	3.9
2	2-M	378	GLY	3.9
2	2-N	282	GLY	3.9
2	1-N	469	VAL	3.9
2	2-N	469	VAL	3.9
2	1-N	164	GLN	3.8
2	2-N	164	GLN	3.8
2	1-N	538	HIS	3.8
2	2-N	538	HIS	3.8
2	1-N	18	VAL	3.8
2	2-N	18	VAL	3.8
2	1-J	37	GLY	3.8
2	2-J	37	GLY	3.8
2	1-N	446	MET	3.8
2	2-N	446	MET	3.8
2	1-N	114	ASP	3.8
2	2-N	114	ASP	3.8
2	1-N	408	LEU	3.8
2	2-N	408	LEU	3.8
2	1-N	473	ASP	3.8
2	2-N	473	ASP	3.8
2	1-N	87	VAL	3.8
2	1-N	537	VAL	3.8
2	2-N	87	VAL	3.8
2	2-N	537	VAL	3.8
2	1-N	44	SER	3.8
2	1-N	84	SER	3.8
2	2-N	44	SER	3.8
2	2-N	84	SER	3.8
2	1-N	19	ASP	3.8
2	2-N	19	ASP	3.8
2	1-N	270	LEU	3.8
2	2-N	270	LEU	3.8
2	1-N	337	LYS	3.8
2	2-N	337	LYS	3.8
2	1-N	12	PHE	3.8
2	2-N	12	PHE	3.8
1	1-G	101	ALA	3.7
1	2-G	101	ALA	3.7
2	1-H	146	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-H	146	ALA	3.7
2	1-M	343	PRO	3.7
2	2-M	343	PRO	3.7
2	1-N	29	ARG	3.7
2	2-N	29	ARG	3.7
2	1-N	478	ALA	3.7
2	1-N	545	ALA	3.7
2	2-N	478	ALA	3.7
2	2-N	545	ALA	3.7
2	1-N	158	LYS	3.7
2	2-N	158	LYS	3.7
1	1-G	26	ARG	3.7
1	2-G	26	ARG	3.7
2	1-N	271	LEU	3.7
2	1-N	471	LEU	3.7
2	2-N	271	LEU	3.7
2	2-N	471	LEU	3.7
2	1-N	238	SER	3.7
2	2-N	238	SER	3.7
2	1-N	475	PRO	3.7
2	2-N	475	PRO	3.7
2	1-N	388	ARG	3.7
2	2-N	388	ARG	3.7
2	1-N	256	LYS	3.7
2	2-N	256	LYS	3.7
2	1-N	95	ILE	3.7
2	2-N	95	ILE	3.7
2	1-N	421	THR	3.7
2	2-N	421	THR	3.7
2	1-N	309	SER	3.7
2	2-N	309	SER	3.7
2	1-N	245	LYS	3.7
2	2-N	245	LYS	3.7
1	1-G	187	CYS	3.7
1	2-G	187	CYS	3.7
2	1-N	328	ASP	3.7
2	2-N	328	ASP	3.7
2	1-N	274	ALA	3.7
2	2-N	274	ALA	3.7
2	1-N	497	VAL	3.6
2	2-N	497	VAL	3.6
2	1-N	299	ASP	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	299	ASP	3.6
2	1-N	434	ILE	3.6
2	2-N	434	ILE	3.6
2	1-N	285	GLY	3.6
2	2-N	285	GLY	3.6
1	1-G	75	GLU	3.6
1	2-G	75	GLU	3.6
2	1-N	58	GLY	3.6
2	1-N	384	GLY	3.6
2	2-N	58	GLY	3.6
2	2-N	384	GLY	3.6
2	1-N	124	ALA	3.6
2	1-N	193	LEU	3.6
2	2-N	124	ALA	3.6
2	2-N	193	LEU	3.6
2	1-N	300	SER	3.6
2	2-N	300	SER	3.6
2	1-N	308	THR	3.6
2	2-N	308	THR	3.6
2	1-N	268	PRO	3.6
2	2-N	268	PRO	3.6
1	1-B	194	GLU	3.6
1	2-B	194	GLU	3.6
2	1-H	6	PRO	3.6
2	2-H	6	PRO	3.6
2	1-N	503	LEU	3.6
2	2-N	503	LEU	3.6
2	1-N	442	TRP	3.6
2	2-N	442	TRP	3.6
2	1-N	144	LEU	3.5
2	1-N	524	ILE	3.5
2	2-N	144	LEU	3.5
2	2-N	524	ILE	3.5
2	1-N	298	ASP	3.5
2	2-N	298	ASP	3.5
2	1-N	375	ARG	3.5
2	2-N	375	ARG	3.5
1	1-A	163	THR	3.5
1	1-G	39	THR	3.5
1	2-A	163	THR	3.5
1	2-G	39	THR	3.5
2	1-N	276	PHE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	276	PHE	3.5
2	1-N	215	ALA	3.5
2	2-N	215	ALA	3.5
1	1-G	83	GLY	3.5
1	2-G	83	GLY	3.5
2	1-N	61	PRO	3.5
2	1-N	351	TYR	3.5
2	2-N	61	PRO	3.5
2	2-N	351	TYR	3.5
2	1-N	335	ASP	3.5
2	2-N	335	ASP	3.5
1	1-B	139	VAL	3.5
1	2-B	139	VAL	3.5
1	1-G	236	ASN	3.5
1	2-G	236	ASN	3.5
2	1-N	505	PRO	3.5
2	2-N	505	PRO	3.5
2	1-N	101	MET	3.5
2	1-N	151	ALA	3.5
2	2-N	101	MET	3.5
2	2-N	151	ALA	3.5
1	1-B	264	GLY	3.5
1	1-G	173	GLY	3.5
1	2-B	264	GLY	3.5
1	2-G	173	GLY	3.5
2	1-N	318	GLY	3.5
2	2-N	318	GLY	3.5
2	1-N	110	GLN	3.5
2	2-N	110	GLN	3.5
1	1-B	61	HIS	3.5
1	2-B	61	HIS	3.5
2	1-N	259	CYS	3.5
2	2-N	259	CYS	3.5
2	1-N	529	ARG	3.5
2	2-N	529	ARG	3.5
2	1-J	343	PRO	3.4
2	1-N	79	HIS	3.4
2	2-J	343	PRO	3.4
2	2-N	79	HIS	3.4
2	1-N	450	GLY	3.4
2	2-N	450	GLY	3.4
2	1-N	194	PRO	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	194	PRO	3.4
2	1-N	198	ASN	3.4
2	2-N	198	ASN	3.4
2	1-N	191	TYR	3.4
2	2-N	191	TYR	3.4
2	1-N	357	PRO	3.4
2	2-N	357	PRO	3.4
2	1-N	528	LYS	3.4
2	2-N	528	LYS	3.4
1	1-B	168	ASP	3.4
1	2-B	168	ASP	3.4
2	1-N	511	ASP	3.4
2	2-N	511	ASP	3.4
2	1-N	55	ILE	3.4
2	2-N	55	ILE	3.4
2	1-N	352	ASP	3.4
2	2-N	352	ASP	3.4
2	1-N	439	MET	3.4
2	2-N	439	MET	3.4
2	1-H	151	ALA	3.4
2	1-N	382	GLU	3.4
2	2-H	151	ALA	3.4
2	2-N	382	GLU	3.4
2	1-N	45	SER	3.4
2	2-N	45	SER	3.4
2	1-N	477	GLY	3.4
2	2-N	477	GLY	3.4
2	1-J	11	THR	3.4
2	2-J	11	THR	3.4
2	1-N	494	GLN	3.4
2	1-N	549	HIS	3.4
2	2-N	494	GLN	3.4
2	2-N	549	HIS	3.4
2	1-H	139	ASN	3.3
2	2-H	139	ASN	3.3
1	1-G	85	GLN	3.3
1	2-G	85	GLN	3.3
2	1-N	502	ASN	3.3
2	2-N	502	ASN	3.3
2	1-N	542	PRO	3.3
2	2-N	542	PRO	3.3
2	1-N	294	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	1-N	455	THR	3.3
2	2-N	294	GLU	3.3
2	2-N	455	THR	3.3
1	1-B	224	TYR	3.3
1	2-B	224	TYR	3.3
1	1-G	128	SER	3.3
1	2-G	128	SER	3.3
2	1-N	40	LYS	3.3
2	2-N	40	LYS	3.3
2	1-I	398	PRO	3.3
2	2-I	398	PRO	3.3
2	1-N	474	ALA	3.3
2	2-N	474	ALA	3.3
2	1-N	345	GLY	3.3
2	1-N	436	CYS	3.3
2	2-N	345	GLY	3.3
2	2-N	436	CYS	3.3
1	1-C	67	LYS	3.3
1	2-C	67	LYS	3.3
2	1-N	512	LYS	3.3
2	2-N	512	LYS	3.3
1	1-B	138	GLY	3.3
1	2-B	138	GLY	3.3
2	1-I	146	ALA	3.3
2	1-N	507	GLY	3.3
2	2-I	146	ALA	3.3
2	2-N	507	GLY	3.3
2	1-N	210	HIS	3.3
2	2-N	210	HIS	3.3
2	1-N	449	SER	3.3
2	2-N	449	SER	3.3
1	1-G	22	GLU	3.3
1	2-G	22	GLU	3.3
1	1-G	212	CYS	3.3
1	2-G	212	CYS	3.3
2	1-I	451	ALA	3.2
2	1-N	60	ASP	3.2
2	2-I	451	ALA	3.2
2	2-N	60	ASP	3.2
2	1-N	304	LYS	3.2
2	2-N	304	LYS	3.2
2	1-N	371	MET	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	371	MET	3.2
2	1-J	148	ILE	3.2
2	2-J	148	ILE	3.2
2	1-N	500	THR	3.2
2	2-N	500	THR	3.2
2	1-N	269	ASP	3.2
2	2-N	269	ASP	3.2
2	1-N	9	GLN	3.2
2	2-N	9	GLN	3.2
1	1-G	28	ILE	3.2
1	2-G	28	ILE	3.2
2	1-M	148	ILE	3.2
2	2-M	148	ILE	3.2
2	1-N	372	LYS	3.2
2	2-N	372	LYS	3.2
2	1-J	162	ALA	3.2
2	2-J	162	ALA	3.2
2	1-N	10	SER	3.2
2	1-N	283	ILE	3.2
2	2-N	10	SER	3.2
2	2-N	283	ILE	3.2
2	1-N	168	LYS	3.2
2	2-N	168	LYS	3.2
1	1-G	102	ALA	3.2
1	2-G	102	ALA	3.2
2	1-N	339	SER	3.2
2	2-N	339	SER	3.2
2	1-N	7	THR	3.2
2	2-N	7	THR	3.2
2	1-N	459	LYS	3.2
2	2-N	459	LYS	3.2
1	1-G	129	GLN	3.2
1	2-G	129	GLN	3.2
2	1-N	303	SER	3.1
2	2-N	303	SER	3.1
2	1-K	157	ALA	3.1
2	1-N	162	ALA	3.1
2	2-K	157	ALA	3.1
2	2-N	162	ALA	3.1
2	1-I	6	PRO	3.1
2	2-I	6	PRO	3.1
1	1-B	166	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2-B	166	ILE	3.1
2	1-N	200	ILE	3.1
2	2-N	200	ILE	3.1
2	1-N	47	GLN	3.1
2	2-N	47	GLN	3.1
2	1-I	448	ASP	3.1
2	2-I	448	ASP	3.1
1	1-G	184	HIS	3.1
1	2-G	184	HIS	3.1
1	1-G	255	ASP	3.1
1	2-G	255	ASP	3.1
2	1-N	541	ASP	3.1
2	2-N	541	ASP	3.1
2	1-N	288	ASN	3.1
2	2-N	288	ASN	3.1
2	1-N	212	GLN	3.1
2	2-N	212	GLN	3.1
2	1-M	157	ALA	3.1
2	2-M	157	ALA	3.1
2	1-N	313	SER	3.1
2	2-N	313	SER	3.1
2	1-N	123	HIS	3.1
2	2-N	123	HIS	3.1
1	1-A	195	ALA	3.1
1	2-A	195	ALA	3.1
2	1-N	355	THR	3.1
2	2-N	355	THR	3.1
2	1-N	461	GLU	3.1
2	2-N	461	GLU	3.1
1	1-G	106	LYS	3.1
1	2-G	106	LYS	3.1
2	1-M	37	GLY	3.1
2	2-M	37	GLY	3.1
2	1-N	523	PRO	3.1
2	2-N	523	PRO	3.1
2	1-I	415	ALA	3.0
2	1-N	218	ALA	3.0
2	2-I	415	ALA	3.0
2	2-N	218	ALA	3.0
2	1-N	93	VAL	3.0
2	1-N	197	VAL	3.0
2	2-N	93	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	197	VAL	3.0
1	1-G	131	LYS	3.0
1	2-G	131	LYS	3.0
2	1-N	364	ASP	3.0
2	2-N	364	ASP	3.0
1	1-B	31	TYR	3.0
1	2-B	31	TYR	3.0
1	1-G	174	ARG	3.0
1	2-G	174	ARG	3.0
2	1-N	334	GLU	3.0
2	2-N	334	GLU	3.0
1	1-G	201	SER	3.0
1	2-G	201	SER	3.0
2	1-N	264	GLU	3.0
2	1-N	277	TYR	3.0
2	2-N	264	GLU	3.0
2	2-N	277	TYR	3.0
1	1-G	176	LYS	3.0
1	2-G	176	LYS	3.0
2	1-N	476	ARG	3.0
2	2-N	476	ARG	3.0
1	1-G	34	ALA	3.0
1	2-G	34	ALA	3.0
2	1-N	515	VAL	3.0
2	2-N	515	VAL	3.0
2	1-N	8	PRO	3.0
2	2-N	8	PRO	3.0
2	1-N	94	SER	3.0
2	2-N	94	SER	3.0
1	1-D	4	LYS	3.0
1	2-D	4	LYS	3.0
2	1-N	506	ARG	3.0
2	2-N	506	ARG	3.0
2	1-N	301	SER	3.0
2	2-N	301	SER	3.0
2	1-N	25	GLU	2.9
2	2-N	25	GLU	2.9
2	1-N	236	GLY	2.9
2	2-N	236	GLY	2.9
2	1-N	483	ILE	2.9
2	2-N	483	ILE	2.9
1	1-B	5	HIS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2-B	5	HIS	2.9
2	1-J	378	GLY	2.9
2	1-N	235	GLY	2.9
2	1-N	314	GLY	2.9
2	2-J	378	GLY	2.9
2	2-N	235	GLY	2.9
2	2-N	314	GLY	2.9
2	1-N	522	THR	2.9
2	2-N	522	THR	2.9
1	1-G	192	HIS	2.9
1	2-G	192	HIS	2.9
2	1-N	169	ALA	2.9
2	1-N	380	ALA	2.9
2	2-N	169	ALA	2.9
2	2-N	380	ALA	2.9
2	1-N	103	ARG	2.9
2	2-N	103	ARG	2.9
2	1-I	412	SER	2.9
2	2-I	412	SER	2.9
1	1-B	164	LYS	2.9
1	1-G	209	LYS	2.9
1	2-B	164	LYS	2.9
1	2-G	209	LYS	2.9
2	1-N	412	SER	2.9
2	1-N	481	HIS	2.9
2	2-N	412	SER	2.9
2	2-N	481	HIS	2.9
2	1-I	487	GLY	2.9
2	1-N	275	GLY	2.9
2	2-I	487	GLY	2.9
2	2-N	275	GLY	2.9
1	1-B	190	LEU	2.9
1	1-G	182	LEU	2.9
1	2-B	190	LEU	2.9
1	2-G	182	LEU	2.9
2	1-N	100	ARG	2.9
2	2-N	100	ARG	2.9
1	1-D	3	ALA	2.9
1	2-D	3	ALA	2.9
1	1-B	171	SER	2.8
1	2-B	171	SER	2.8
2	1-N	255	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	255	SER	2.8
2	1-N	59	ARG	2.8
2	2-N	59	ARG	2.8
1	1-G	68	ASP	2.8
1	2-G	68	ASP	2.8
2	1-N	85	ARG	2.8
2	1-N	513	SER	2.8
2	2-N	85	ARG	2.8
2	2-N	513	SER	2.8
2	1-K	35	GLU	2.8
2	1-N	37	GLY	2.8
2	2-K	35	GLU	2.8
2	2-N	37	GLY	2.8
2	1-M	5	LYS	2.8
2	2-M	5	LYS	2.8
1	1-G	197	GLU	2.8
1	2-G	197	GLU	2.8
2	1-N	252	LEU	2.8
2	2-N	252	LEU	2.8
1	1-B	163	THR	2.8
1	2-B	163	THR	2.8
2	1-I	11	THR	2.8
2	1-M	317	THR	2.8
2	2-I	11	THR	2.8
2	2-M	317	THR	2.8
2	1-H	5	LYS	2.8
2	2-H	5	LYS	2.8
2	1-N	398	PRO	2.8
2	2-N	398	PRO	2.8
2	1-N	405	ASP	2.8
2	2-N	405	ASP	2.8
1	1-G	221	PRO	2.7
1	2-G	221	PRO	2.7
2	1-N	444	LYS	2.7
2	2-N	444	LYS	2.7
2	1-I	450	GLY	2.7
2	2-I	450	GLY	2.7
2	1-J	10	SER	2.7
2	1-N	126	ASP	2.7
2	2-J	10	SER	2.7
2	2-N	126	ASP	2.7
2	1-M	139	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-M	139	ASN	2.7
2	1-I	151	ALA	2.7
2	1-N	97	ALA	2.7
2	2-I	151	ALA	2.7
2	2-N	97	ALA	2.7
2	1-N	241	GLN	2.7
2	2-N	241	GLN	2.7
1	1-G	33	ASP	2.7
1	2-G	33	ASP	2.7
1	1-G	188	PRO	2.7
1	2-G	188	PRO	2.7
1	1-G	134	SER	2.7
1	2-G	134	SER	2.7
2	1-N	82	ALA	2.7
2	2-N	82	ALA	2.7
1	1-B	211	PHE	2.7
1	2-B	211	PHE	2.7
2	1-K	36	ASN	2.7
2	1-N	263	ASN	2.7
2	2-K	36	ASN	2.7
2	2-N	263	ASN	2.7
1	1-F	177	LEU	2.7
1	2-F	177	LEU	2.7
1	1-B	3	ALA	2.7
1	2-B	3	ALA	2.7
2	1-N	192	TYR	2.7
2	2-N	192	TYR	2.7
1	1-B	198	PHE	2.7
1	2-B	198	PHE	2.7
1	1-G	210	GLY	2.7
1	2-G	210	GLY	2.7
2	1-K	318	GLY	2.6
2	1-N	14	GLY	2.6
2	2-K	318	GLY	2.6
2	2-N	14	GLY	2.6
1	1-G	122	LYS	2.6
1	2-G	122	LYS	2.6
1	1-G	170	ASP	2.6
1	2-G	170	ASP	2.6
2	1-I	5	LYS	2.6
2	1-N	214	LYS	2.6
2	2-I	5	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	214	LYS	2.6
1	1-G	220	GLY	2.6
1	2-G	220	GLY	2.6
1	1-G	240	GLN	2.6
1	2-G	240	GLN	2.6
1	1-B	191	PRO	2.6
1	2-B	191	PRO	2.6
1	1-B	180	GLY	2.6
1	2-B	180	GLY	2.6
2	1-I	409	GLY	2.6
2	2-I	409	GLY	2.6
2	1-N	104	ASN	2.6
2	2-N	104	ASN	2.6
1	1-B	104	LYS	2.6
1	1-G	140	LYS	2.6
1	2-B	104	LYS	2.6
1	2-G	140	LYS	2.6
2	1-N	493	PHE	2.6
2	2-N	493	PHE	2.6
2	1-H	322	GLY	2.6
2	2-H	322	GLY	2.6
1	1-G	186	ASN	2.6
1	2-G	186	ASN	2.6
2	1-J	139	ASN	2.6
2	1-N	454	ASN	2.6
2	2-J	139	ASN	2.6
2	2-N	454	ASN	2.6
2	1-M	323	LYS	2.6
2	1-N	189	LYS	2.6
2	2-M	323	LYS	2.6
2	2-N	189	LYS	2.6
1	1-B	246	LEU	2.6
1	2-B	246	LEU	2.6
2	1-J	322	GLY	2.6
2	1-M	11	THR	2.6
2	2-J	322	GLY	2.6
2	2-M	11	THR	2.6
1	1-A	4	LYS	2.6
1	2-A	4	LYS	2.6
2	1-M	36	ASN	2.6
2	2-M	36	ASN	2.6
1	1-G	124	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2-G	124	LYS	2.5
2	1-N	431	GLU	2.5
2	2-N	431	GLU	2.5
2	1-M	12	PHE	2.5
2	1-N	424	ARG	2.5
2	2-M	12	PHE	2.5
2	2-N	424	ARG	2.5
1	1-B	195	ALA	2.5
1	2-B	195	ALA	2.5
2	1-N	462	MET	2.5
2	2-N	462	MET	2.5
1	1-G	139	VAL	2.5
1	2-G	139	VAL	2.5
2	1-N	485	ILE	2.5
2	2-N	485	ILE	2.5
1	1-B	68	ASP	2.5
1	1-B	205	GLU	2.5
1	2-B	68	ASP	2.5
1	2-B	205	GLU	2.5
2	1-H	142	ALA	2.5
2	2-H	142	ALA	2.5
1	1-B	177	LEU	2.5
1	2-B	177	LEU	2.5
2	1-I	173	SER	2.5
2	2-I	173	SER	2.5
1	1-B	179	TYR	2.5
1	1-B	193	PHE	2.5
1	2-B	179	TYR	2.5
1	2-B	193	PHE	2.5
2	1-J	35	GLU	2.5
2	2-J	35	GLU	2.5
2	1-I	321	LEU	2.5
2	2-I	321	LEU	2.5
2	1-M	397	GLN	2.5
2	2-M	397	GLN	2.5
1	1-G	130	ALA	2.4
1	2-G	130	ALA	2.4
2	1-N	57	LYS	2.4
2	1-N	358	LYS	2.4
2	2-N	57	LYS	2.4
2	2-N	358	LYS	2.4
2	1-N	165	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	1-N	404	VAL	2.4
2	2-N	165	ASP	2.4
2	2-N	404	VAL	2.4
1	1-G	84	GLY	2.4
1	1-G	164	LYS	2.4
1	2-G	84	GLY	2.4
1	2-G	164	LYS	2.4
2	1-N	319	ARG	2.4
2	2-N	319	ARG	2.4
2	1-N	204	HIS	2.4
2	1-N	414	PRO	2.4
2	2-N	204	HIS	2.4
2	2-N	414	PRO	2.4
1	1-G	126	ASN	2.4
1	2-G	126	ASN	2.4
2	1-N	257	GLU	2.4
2	2-N	257	GLU	2.4
1	1-B	204	SER	2.4
1	2-B	204	SER	2.4
2	1-N	91	VAL	2.4
2	2-N	91	VAL	2.4
2	1-N	525	ALA	2.4
2	2-N	525	ALA	2.4
1	1-C	69	GLY	2.4
1	2-C	69	GLY	2.4
2	1-H	223	GLY	2.4
2	2-H	223	GLY	2.4
2	1-N	166	LYS	2.3
2	1-N	440	GLU	2.3
2	2-N	166	LYS	2.3
2	2-N	440	GLU	2.3
1	1-G	162	LEU	2.3
1	2-G	162	LEU	2.3
2	1-N	15	PRO	2.3
2	1-N	302	PRO	2.3
2	2-N	15	PRO	2.3
2	2-N	302	PRO	2.3
2	1-I	324	VAL	2.3
2	2-I	324	VAL	2.3
1	1-F	171	SER	2.3
1	2-F	171	SER	2.3
2	1-K	322	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-K	322	GLY	2.3
1	1-B	184	HIS	2.3
1	2-B	184	HIS	2.3
1	1-A	162	LEU	2.3
1	2-A	162	LEU	2.3
2	1-K	13	THR	2.3
2	2-K	13	THR	2.3
2	1-M	393	TYR	2.3
2	2-M	393	TYR	2.3
2	1-I	491	ASP	2.3
1	1-G	160	HIS	2.3
1	2-G	160	HIS	2.3
2	1-M	466	SER	2.3
2	1-N	491	ASP	2.3
2	2-I	491	ASP	2.3
2	2-M	466	SER	2.3
2	2-N	491	ASP	2.3
2	1-I	402	LYS	2.3
2	2-I	402	LYS	2.3
2	1-H	253	ALA	2.3
2	1-J	417	ALA	2.3
2	2-H	253	ALA	2.3
2	2-J	417	ALA	2.3
2	1-N	161	LYS	2.3
2	1-N	353	GLY	2.3
2	1-N	467	LYS	2.3
2	2-N	161	LYS	2.3
2	2-N	353	GLY	2.3
2	2-N	467	LYS	2.3
2	1-K	394	ALA	2.3
2	1-N	159	ALA	2.3
2	2-K	394	ALA	2.3
2	2-N	159	ALA	2.3
1	1-F	190	LEU	2.3
1	2-F	190	LEU	2.3
2	1-J	12	PHE	2.2
2	2-J	12	PHE	2.2
1	1-B	100	LYS	2.2
1	2-B	100	LYS	2.2
2	1-N	38	LYS	2.2
2	2-N	38	LYS	2.2
2	1-N	89	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	89	ASP	2.2
2	1-N	310	GLN	2.2
2	2-N	310	GLN	2.2
1	1-F	264	GLY	2.2
1	2-F	264	GLY	2.2
2	1-N	323	LYS	2.2
2	2-N	323	LYS	2.2
2	1-I	246	ASP	2.2
2	2-I	246	ASP	2.2
2	1-M	416	THR	2.2
2	2-M	416	THR	2.2
1	1-B	160	HIS	2.2
1	2-B	160	HIS	2.2
2	1-I	444	LYS	2.2
2	1-M	330	GLY	2.2
2	2-I	444	LYS	2.2
2	2-M	330	GLY	2.2
2	1-N	535	ARG	2.2
2	2-N	535	ARG	2.2
1	1-B	65	GLU	2.2
1	2-B	65	GLU	2.2
2	1-N	532	GLU	2.2
2	2-N	532	GLU	2.2
2	1-N	140	LYS	2.2
2	2-N	140	LYS	2.2
2	1-I	154	GLY	2.2
2	1-K	14	GLY	2.2
2	2-I	154	GLY	2.2
2	2-K	14	GLY	2.2
1	1-B	38	ASP	2.2
1	2-B	38	ASP	2.2
1	1-G	96	GLU	2.2
1	2-G	96	GLU	2.2
2	1-I	399	ASP	2.2
2	2-I	399	ASP	2.2
1	1-B	4	LYS	2.2
1	2-B	4	LYS	2.2
1	1-A	190	LEU	2.1
1	1-F	92	HIS	2.1
1	2-A	190	LEU	2.1
1	2-F	92	HIS	2.1
2	1-J	174	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	1-N	464	GLU	2.1
2	2-J	174	GLY	2.1
2	2-N	464	GLU	2.1
1	1-A	211	PHE	2.1
1	2-A	211	PHE	2.1
1	1-B	30	PRO	2.1
1	2-B	30	PRO	2.1
2	1-I	172	GLU	2.1
2	1-J	331	ALA	2.1
2	2-I	172	GLU	2.1
2	2-J	331	ALA	2.1
2	1-M	6	PRO	2.1
2	2-M	6	PRO	2.1
2	1-I	137	ASP	2.1
2	2-I	137	ASP	2.1
2	1-N	468	GLY	2.1
2	2-N	468	GLY	2.1
2	1-N	463	PRO	2.1
2	2-N	463	PRO	2.1
2	1-H	14	GLY	2.1
2	1-J	324	VAL	2.1
2	1-M	336	VAL	2.1
2	2-H	14	GLY	2.1
2	2-J	324	VAL	2.1
2	2-M	336	VAL	2.1
2	1-I	95	ILE	2.1
2	2-I	95	ILE	2.1
2	1-J	463	PRO	2.1
2	2-J	463	PRO	2.1
2	1-J	34	VAL	2.1
2	1-J	323	LYS	2.1
2	2-J	34	VAL	2.1
2	2-J	323	LYS	2.1
2	1-N	278	LYS	2.1
2	2-N	278	LYS	2.1
1	1-G	80	THR	2.0
1	2-G	80	THR	2.0
1	1-G	250	GLU	2.0
1	2-G	250	GLU	2.0
2	1-N	53	GLU	2.0
2	2-N	53	GLU	2.0
2	1-N	96	PRO	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2-N	96	PRO	2.0
2	1-J	321	LEU	2.0
2	2-J	321	LEU	2.0
2	1-I	240	TYR	2.0
2	2-I	240	TYR	2.0
2	1-J	347	GLY	2.0
2	1-K	344	GLY	2.0
2	2-J	347	GLY	2.0
2	2-K	344	GLY	2.0
1	1-B	196	SER	2.0
1	2-B	196	SER	2.0
2	1-M	320	ASP	2.0
2	1-M	346	ASP	2.0
2	1-N	142	ALA	2.0
2	2-M	320	ASP	2.0
2	2-M	346	ASP	2.0
2	2-N	142	ALA	2.0
2	1-H	409	GLY	2.0
2	1-M	345	GLY	2.0
2	1-N	207	GLU	2.0
2	2-H	409	GLY	2.0
2	2-M	345	GLY	2.0
2	2-N	207	GLU	2.0
2	1-N	488	LYS	2.0
2	2-N	488	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	MG	2-M	553	1/1	0.95	0.13	0.54	8,8,8,8	0
4	MG	1-M	553	1/1	0.95	0.13	0.54	8,8,8,8	0
7	FCO	2-N	550	7/7	0.97	0.37	0.34	5,6,7,9	7
7	FCO	1-N	550	7/7	0.97	0.37	0.34	5,6,7,9	7
7	FCO	2-M	550	7/7	0.99	0.10	-0.39	4,6,7,12	0
7	FCO	1-M	550	7/7	0.99	0.10	-0.39	4,6,7,12	0
4	MG	1-J	553	1/1	0.98	0.09	-0.42	5,5,5,5	0
4	MG	2-J	553	1/1	0.98	0.09	-0.42	5,5,5,5	0
5	SF4	1-G	265	8/8	0.85	0.32	-0.56	4,6,7,8	8
5	SF4	2-G	265	8/8	0.85	0.32	-0.56	8,10,11,12	8
5	SF4	1-G	267	8/8	0.96	0.41	-0.62	7,10,10,12	8
5	SF4	2-G	267	8/8	0.96	0.41	-0.62	7,10,10,12	8
4	MG	1-I	553	1/1	0.99	0.07	-0.66	6,6,6,6	0
4	MG	2-I	553	1/1	0.99	0.07	-0.66	6,6,6,6	0
7	FCO	1-K	550	7/7	0.99	0.07	-0.92	6,8,10,12	0
7	FCO	2-K	550	7/7	0.99	0.07	-0.92	6,8,10,12	0
7	FCO	1-J	550	7/7	1.00	0.08	-0.94	7,7,11,12	0
7	FCO	2-J	550	7/7	1.00	0.08	-0.94	7,7,11,12	0
7	FCO	1-I	550	7/7	1.00	0.06	-1.02	3,5,8,9	0
7	FCO	2-I	550	7/7	1.00	0.06	-1.02	3,5,8,9	0
7	FCO	1-H	550	7/7	0.99	0.06	-1.12	8,9,11,13	0
7	FCO	2-H	550	7/7	0.99	0.06	-1.12	8,9,11,13	0
6	F3S	1-G	266	7/7	0.92	0.36	-1.12	8,9,11,11	7
6	F3S	2-G	266	7/7	0.92	0.36	-1.19	10,10,11,11	7
4	MG	2-H	553	1/1	0.96	0.06	-1.24	8,8,8,8	0
5	SF4	2-F	265	8/8	0.98	0.06	-1.24	6,7,10,10	0
4	MG	1-H	553	1/1	0.96	0.06	-1.24	8,8,8,8	0
5	SF4	1-F	265	8/8	0.98	0.06	-1.24	6,7,10,10	0
5	SF4	1-B	265	8/8	0.98	0.09	-1.53	5,6,9,9	0
5	SF4	2-B	265	8/8	0.98	0.09	-1.53	5,6,9,9	0
4	MG	2-K	553	1/1	0.97	0.07	-1.76	3,3,3,3	0
4	MG	1-K	553	1/1	0.97	0.07	-1.76	3,3,3,3	0
6	F3S	1-B	266	7/7	0.98	0.06	-1.79	9,10,10,10	0
6	F3S	2-B	266	7/7	0.98	0.06	-1.79	9,10,10,10	0
6	F3S	1-C	266	7/7	0.99	0.04	-1.89	9,10,11,12	0
6	F3S	2-C	266	7/7	0.99	0.04	-1.89	9,10,11,12	0
6	F3S	1-A	266	7/7	0.98	0.05	-1.98	6,7,10,13	0
6	F3S	2-A	266	7/7	0.98	0.05	-1.98	6,7,10,13	0
5	SF4	2-B	267	8/8	0.98	0.05	-1.99	4,8,9,10	0
5	SF4	1-B	267	8/8	0.98	0.05	-1.99	4,8,9,10	0
5	SF4	1-D	267	8/8	0.99	0.04	-2.00	3,7,9,9	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	SF4	2-D	267	8/8	0.99	0.04	-2.00	3,7,9,9	0
5	SF4	2-C	265	8/8	0.99	0.04	-2.04	6,6,8,9	0
5	SF4	1-C	265	8/8	0.99	0.04	-2.04	6,6,8,9	0
5	SF4	1-C	267	8/8	0.99	0.04	-2.05	5,9,10,10	0
5	SF4	2-C	267	8/8	0.99	0.04	-2.05	5,9,10,10	0
5	SF4	2-A	265	8/8	0.97	0.05	-2.16	7,9,10,12	0
5	SF4	1-A	265	8/8	0.97	0.05	-2.16	7,9,10,12	0
3	NI	1-M	551	1/1	1.00	0.06	-2.24	8,8,8,8	0
3	NI	2-M	551	1/1	1.00	0.06	-2.24	8,8,8,8	0
3	NI	1-I	551	1/1	0.99	0.03	-2.30	10,10,10,10	0
3	NI	2-I	551	1/1	0.99	0.03	-2.30	10,10,10,10	0
4	MG	1-N	553	1/1	0.86	0.27	-2.32	8,8,8,8	1
4	MG	2-N	553	1/1	0.86	0.27	-2.32	8,8,8,8	1
6	F3S	2-D	266	7/7	0.98	0.04	-2.37	7,8,10,10	0
6	F3S	1-D	266	7/7	0.98	0.04	-2.37	7,8,10,10	0
5	SF4	1-D	265	8/8	0.99	0.03	-2.41	6,8,9,9	0
5	SF4	2-D	265	8/8	0.99	0.03	-2.41	6,8,9,9	0
3	NI	2-J	551	1/1	1.00	0.05	-2.43	9,9,9,9	0
3	NI	1-J	551	1/1	1.00	0.05	-2.43	9,9,9,9	0
3	NI	1-K	551	1/1	1.00	0.04	-2.66	11,11,11,11	0
3	NI	2-K	551	1/1	1.00	0.04	-2.66	11,11,11,11	0
5	SF4	1-A	267	8/8	0.98	0.05	-2.68	7,8,10,11	0
5	SF4	2-A	267	8/8	0.98	0.05	-2.68	7,8,10,11	0
3	NI	1-N	551	1/1	0.99	0.32	-2.74	13,13,13,13	1
3	NI	2-N	551	1/1	0.99	0.32	-2.74	12,12,12,12	1
3	NI	1-H	551	1/1	1.00	0.02	-2.99	9,9,9,9	0
3	NI	2-H	551	1/1	1.00	0.02	-2.99	9,9,9,9	0
5	SF4	1-F	267	8/8	0.98	0.05	-3.20	4,8,9,10	0
5	SF4	2-F	267	8/8	0.98	0.05	-3.20	4,8,9,10	0
6	F3S	2-F	266	7/7	0.98	0.05	-3.42	7,9,12,12	0
6	F3S	1-F	266	7/7	0.98	0.05	-3.42	7,9,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.