Full wwPDB X-ray Structure Validation Report (i)

Apr 12, 2016 – 12:17 PM EDT

PDB ID	:	5B0L
Title	:	Structure of MoeN5-Sso7d fusion protein in complex with beta-nonyl glucoside
Authors	:	Ko, T.-P.; Zhang, L.; Chen, C.-C.; Guo, R.-T.; Oldfield, E.O.
Deposited on	:	2015-11-02
Resolution	:	2.80 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:

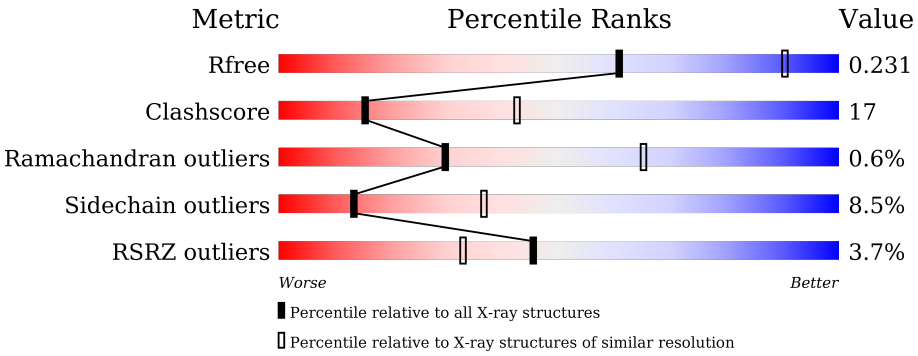
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 2.80 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.



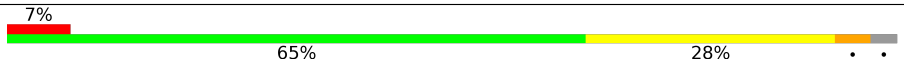
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	A	343	% 56% 18% • • 23%
1	B	343	5% 62% 32% • •
1	C	343	% 57% 17% • 23%
1	D	343	5% 66% 28% • •
1	E	343	% 52% 24% • 22%
1	F	343	6% 62% 29% 5% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	343	
1	H	343	

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
2	BNG	A	502	-	-	-	X
2	BNG	C	502	-	-	-	X
2	BNG	D	501	-	-	-	X
2	BNG	D	502	-	-	-	X
2	BNG	E	401	-	-	-	X
2	BNG	F	401	-	-	-	X
2	BNG	G	401	-	-	-	X
2	BNG	H	501	-	-	-	X
2	BNG	H	502	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19608 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 MoeN5,DNA-binding protein 7d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2010	1240	374	385	11			
1	B	334	Total	C	N	O	S	0	0	0
			2549	1582	466	487	14			
1	C	265	Total	C	N	O	S	0	0	0
			2017	1245	375	386	11			
1	D	333	Total	C	N	O	S	0	0	0
			2540	1576	464	486	14			
1	E	269	Total	C	N	O	S	0	0	0
			2057	1269	387	390	11			
1	F	332	Total	C	N	O	S	0	0	0
			2534	1573	464	483	14			
1	G	263	Total	C	N	O	S	0	0	0
			2003	1237	373	382	11			
1	H	333	Total	C	N	O	S	0	0	0
			2542	1577	465	486	14			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A0A010
A	-12	ALA	-	expression tag	UNP A0A010
A	-11	HIS	-	expression tag	UNP A0A010
A	-10	HIS	-	expression tag	UNP A0A010
A	-9	HIS	-	expression tag	UNP A0A010
A	-8	HIS	-	expression tag	UNP A0A010
A	-7	HIS	-	expression tag	UNP A0A010
A	-6	HIS	-	expression tag	UNP A0A010
A	-5	VAL	-	expression tag	UNP A0A010
A	-4	ASP	-	expression tag	UNP A0A010
A	-3	ASP	-	expression tag	UNP A0A010
A	-2	ASP	-	expression tag	UNP A0A010
A	-1	ASP	-	expression tag	UNP A0A010

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	LYS	-	expression tag	UNP A0A010
A	261	ALA	-	linker	UNP A0A010
A	262	GLY	-	linker	UNP A0A010
A	263	ALA	-	linker	UNP A0A010
A	264	GLY	-	linker	UNP A0A010
A	265	ALA	-	linker	UNP A0A010
B	-13	MET	-	expression tag	UNP A0A010
B	-12	ALA	-	expression tag	UNP A0A010
B	-11	HIS	-	expression tag	UNP A0A010
B	-10	HIS	-	expression tag	UNP A0A010
B	-9	HIS	-	expression tag	UNP A0A010
B	-8	HIS	-	expression tag	UNP A0A010
B	-7	HIS	-	expression tag	UNP A0A010
B	-6	HIS	-	expression tag	UNP A0A010
B	-5	VAL	-	expression tag	UNP A0A010
B	-4	ASP	-	expression tag	UNP A0A010
B	-3	ASP	-	expression tag	UNP A0A010
B	-2	ASP	-	expression tag	UNP A0A010
B	-1	ASP	-	expression tag	UNP A0A010
B	0	LYS	-	expression tag	UNP A0A010
B	261	ALA	-	linker	UNP A0A010
B	262	GLY	-	linker	UNP A0A010
B	263	ALA	-	linker	UNP A0A010
B	264	GLY	-	linker	UNP A0A010
B	265	ALA	-	linker	UNP A0A010
C	-13	MET	-	expression tag	UNP A0A010
C	-12	ALA	-	expression tag	UNP A0A010
C	-11	HIS	-	expression tag	UNP A0A010
C	-10	HIS	-	expression tag	UNP A0A010
C	-9	HIS	-	expression tag	UNP A0A010
C	-8	HIS	-	expression tag	UNP A0A010
C	-7	HIS	-	expression tag	UNP A0A010
C	-6	HIS	-	expression tag	UNP A0A010
C	-5	VAL	-	expression tag	UNP A0A010
C	-4	ASP	-	expression tag	UNP A0A010
C	-3	ASP	-	expression tag	UNP A0A010
C	-2	ASP	-	expression tag	UNP A0A010
C	-1	ASP	-	expression tag	UNP A0A010
C	0	LYS	-	expression tag	UNP A0A010
C	261	ALA	-	linker	UNP A0A010
C	262	GLY	-	linker	UNP A0A010
C	263	ALA	-	linker	UNP A0A010

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	264	GLY	-	linker	UNP A0A010
C	265	ALA	-	linker	UNP A0A010
D	-13	MET	-	expression tag	UNP A0A010
D	-12	ALA	-	expression tag	UNP A0A010
D	-11	HIS	-	expression tag	UNP A0A010
D	-10	HIS	-	expression tag	UNP A0A010
D	-9	HIS	-	expression tag	UNP A0A010
D	-8	HIS	-	expression tag	UNP A0A010
D	-7	HIS	-	expression tag	UNP A0A010
D	-6	HIS	-	expression tag	UNP A0A010
D	-5	VAL	-	expression tag	UNP A0A010
D	-4	ASP	-	expression tag	UNP A0A010
D	-3	ASP	-	expression tag	UNP A0A010
D	-2	ASP	-	expression tag	UNP A0A010
D	-1	ASP	-	expression tag	UNP A0A010
D	0	LYS	-	expression tag	UNP A0A010
D	261	ALA	-	linker	UNP A0A010
D	262	GLY	-	linker	UNP A0A010
D	263	ALA	-	linker	UNP A0A010
D	264	GLY	-	linker	UNP A0A010
D	265	ALA	-	linker	UNP A0A010
E	-13	MET	-	expression tag	UNP A0A010
E	-12	ALA	-	expression tag	UNP A0A010
E	-11	HIS	-	expression tag	UNP A0A010
E	-10	HIS	-	expression tag	UNP A0A010
E	-9	HIS	-	expression tag	UNP A0A010
E	-8	HIS	-	expression tag	UNP A0A010
E	-7	HIS	-	expression tag	UNP A0A010
E	-6	HIS	-	expression tag	UNP A0A010
E	-5	VAL	-	expression tag	UNP A0A010
E	-4	ASP	-	expression tag	UNP A0A010
E	-3	ASP	-	expression tag	UNP A0A010
E	-2	ASP	-	expression tag	UNP A0A010
E	-1	ASP	-	expression tag	UNP A0A010
E	0	LYS	-	expression tag	UNP A0A010
E	261	ALA	-	linker	UNP A0A010
E	262	GLY	-	linker	UNP A0A010
E	263	ALA	-	linker	UNP A0A010
E	264	GLY	-	linker	UNP A0A010
E	265	ALA	-	linker	UNP A0A010
F	-13	MET	-	expression tag	UNP A0A010
F	-12	ALA	-	expression tag	UNP A0A010

Continued on next page...

Continued from previous page...

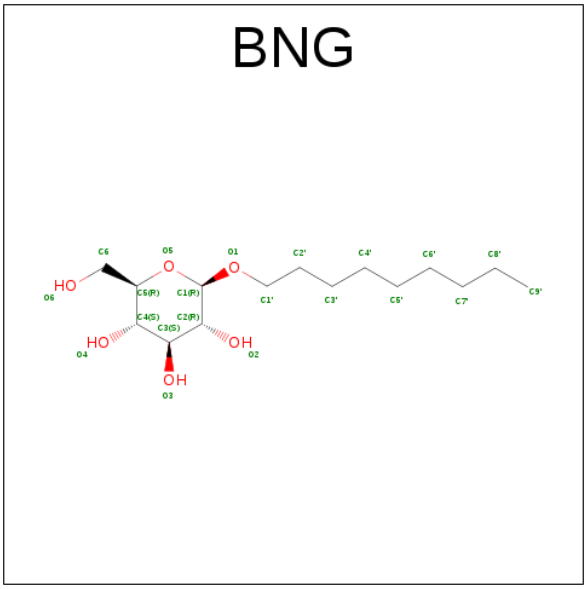
Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	HIS	-	expression tag	UNP A0A010
F	-10	HIS	-	expression tag	UNP A0A010
F	-9	HIS	-	expression tag	UNP A0A010
F	-8	HIS	-	expression tag	UNP A0A010
F	-7	HIS	-	expression tag	UNP A0A010
F	-6	HIS	-	expression tag	UNP A0A010
F	-5	VAL	-	expression tag	UNP A0A010
F	-4	ASP	-	expression tag	UNP A0A010
F	-3	ASP	-	expression tag	UNP A0A010
F	-2	ASP	-	expression tag	UNP A0A010
F	-1	ASP	-	expression tag	UNP A0A010
F	0	LYS	-	expression tag	UNP A0A010
F	261	ALA	-	linker	UNP A0A010
F	262	GLY	-	linker	UNP A0A010
F	263	ALA	-	linker	UNP A0A010
F	264	GLY	-	linker	UNP A0A010
F	265	ALA	-	linker	UNP A0A010
G	-13	MET	-	expression tag	UNP A0A010
G	-12	ALA	-	expression tag	UNP A0A010
G	-11	HIS	-	expression tag	UNP A0A010
G	-10	HIS	-	expression tag	UNP A0A010
G	-9	HIS	-	expression tag	UNP A0A010
G	-8	HIS	-	expression tag	UNP A0A010
G	-7	HIS	-	expression tag	UNP A0A010
G	-6	HIS	-	expression tag	UNP A0A010
G	-5	VAL	-	expression tag	UNP A0A010
G	-4	ASP	-	expression tag	UNP A0A010
G	-3	ASP	-	expression tag	UNP A0A010
G	-2	ASP	-	expression tag	UNP A0A010
G	-1	ASP	-	expression tag	UNP A0A010
G	0	LYS	-	expression tag	UNP A0A010
G	261	ALA	-	linker	UNP A0A010
G	262	GLY	-	linker	UNP A0A010
G	263	ALA	-	linker	UNP A0A010
G	264	GLY	-	linker	UNP A0A010
G	265	ALA	-	linker	UNP A0A010
H	-13	MET	-	expression tag	UNP A0A010
H	-12	ALA	-	expression tag	UNP A0A010
H	-11	HIS	-	expression tag	UNP A0A010
H	-10	HIS	-	expression tag	UNP A0A010
H	-9	HIS	-	expression tag	UNP A0A010
H	-8	HIS	-	expression tag	UNP A0A010

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	HIS	-	expression tag	UNP A0A010
H	-6	HIS	-	expression tag	UNP A0A010
H	-5	VAL	-	expression tag	UNP A0A010
H	-4	ASP	-	expression tag	UNP A0A010
H	-3	ASP	-	expression tag	UNP A0A010
H	-2	ASP	-	expression tag	UNP A0A010
H	-1	ASP	-	expression tag	UNP A0A010
H	0	LYS	-	expression tag	UNP A0A010
H	261	ALA	-	linker	UNP A0A010
H	262	GLY	-	linker	UNP A0A010
H	263	ALA	-	linker	UNP A0A010
H	264	GLY	-	linker	UNP A0A010
H	265	ALA	-	linker	UNP A0A010

- Molecule 2 is B-NONYLGLUCOSIDE (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 21 15 6	0	0
2	A	1	Total C O 21 15 6	0	0
2	B	1	Total C O 21 15 6	0	0
2	B	1	Total C O 21 15 6	0	0
2	C	1	Total C O 21 15 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 21 15 6	0	0
2	D	1	Total C O 21 15 6	0	0
2	D	1	Total C O 21 15 6	0	0
2	E	1	Total C O 21 15 6	0	0
2	F	1	Total C O 21 15 6	0	0
2	G	1	Total C O 21 15 6	0	0
2	H	1	Total C O 21 15 6	0	0
2	H	1	Total C O 21 15 6	0	0

- Molecule 3 is water.

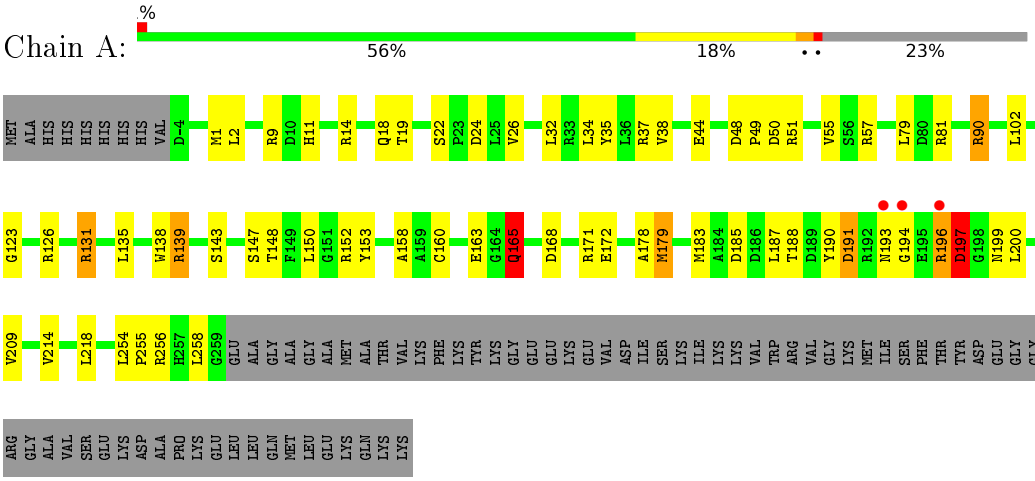
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	149	Total O 149 149	0	0
3	B	144	Total O 144 144	0	0
3	C	138	Total O 138 138	0	0
3	D	142	Total O 142 142	0	0
3	E	94	Total O 94 94	0	0
3	F	167	Total O 167 167	0	0
3	G	99	Total O 99 99	0	0
3	H	150	Total O 150 150	0	0

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.

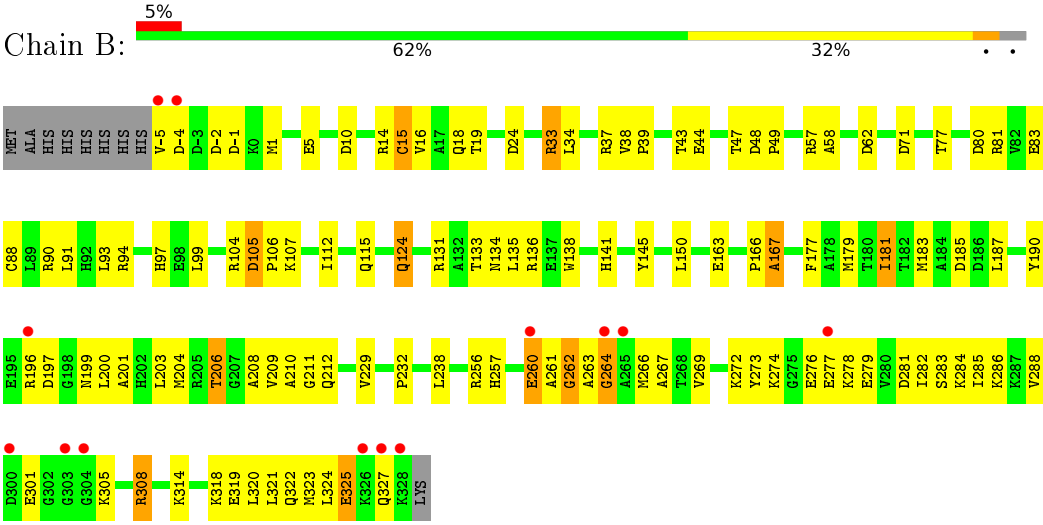
- Molecule 1: MoeN5,DNA-binding protein 7d

Chain A:



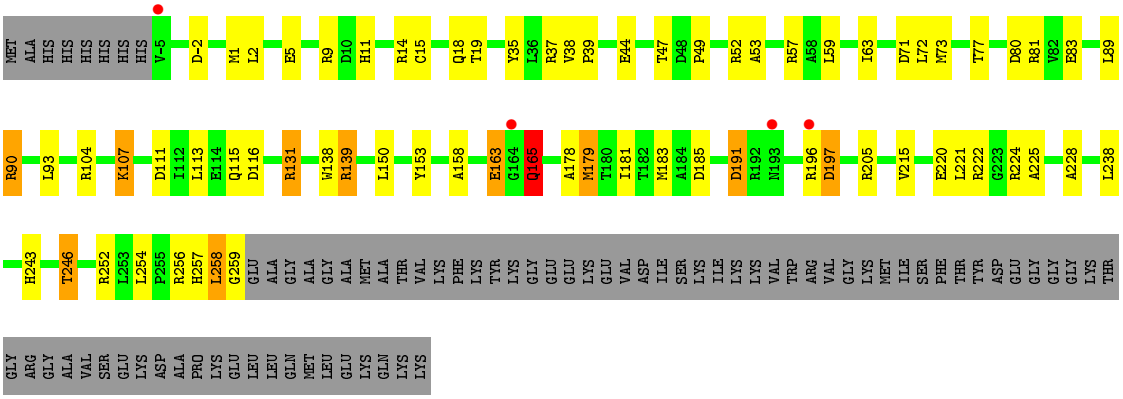
- Molecule 1: MoeN5,DNA-binding protein 7d

Chain B:



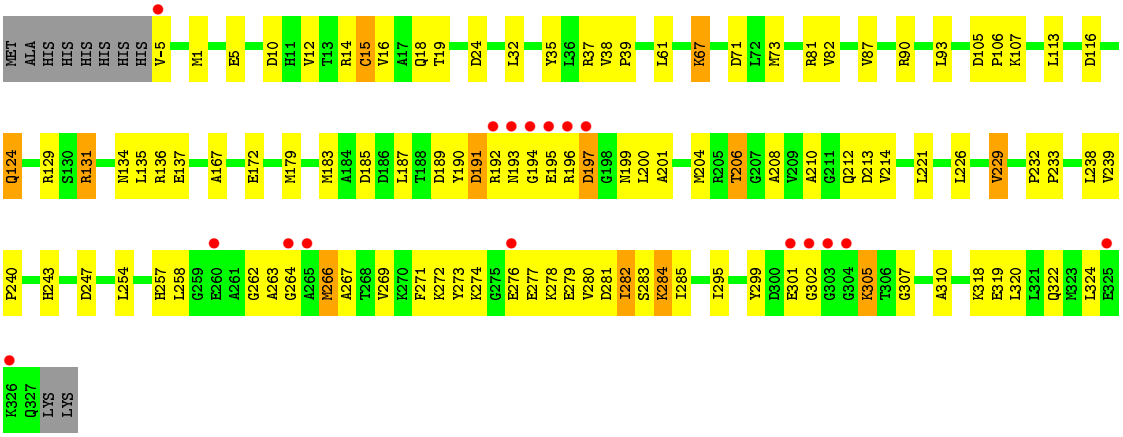
- Molecule 1: MoeN5,DNA-binding protein 7d

Chain C:



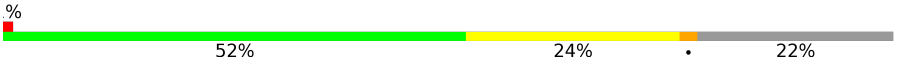
• Molecule 1: MoeN5,DNA-binding protein 7d

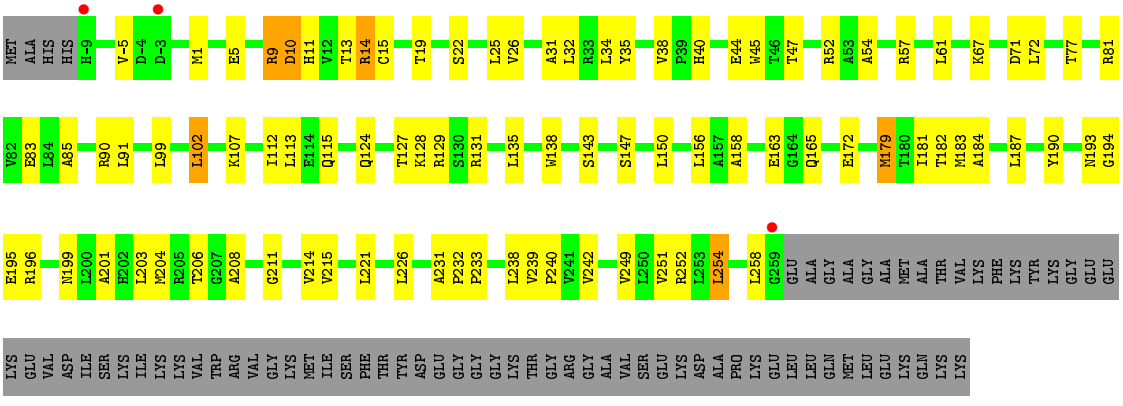
Chain D:



• Molecule 1: MoeN5,DNA-binding protein 7d

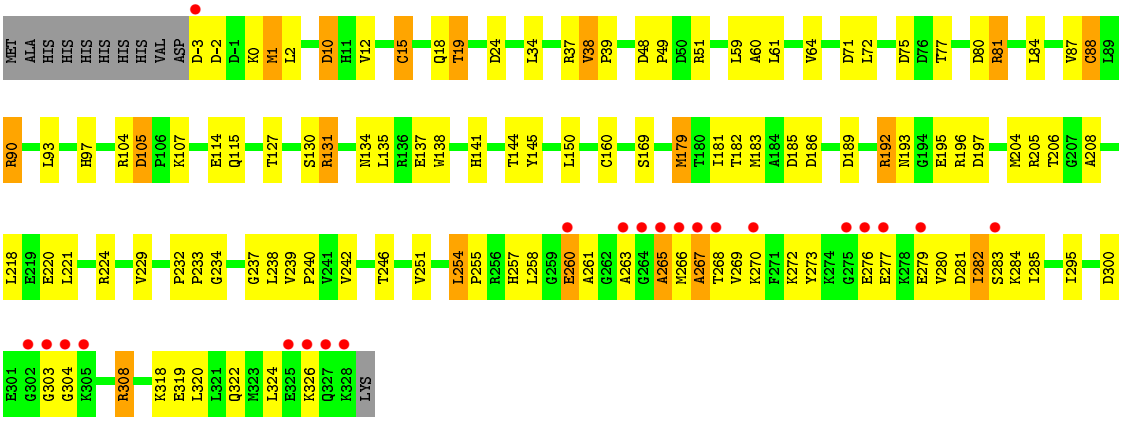
Chain E:





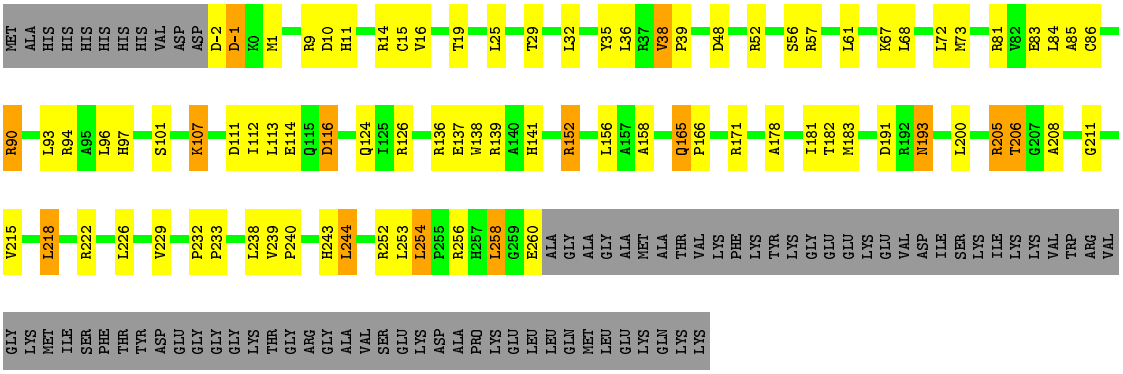
• Molecule 1: MoeN5,DNA-binding protein 7d

Chain F:



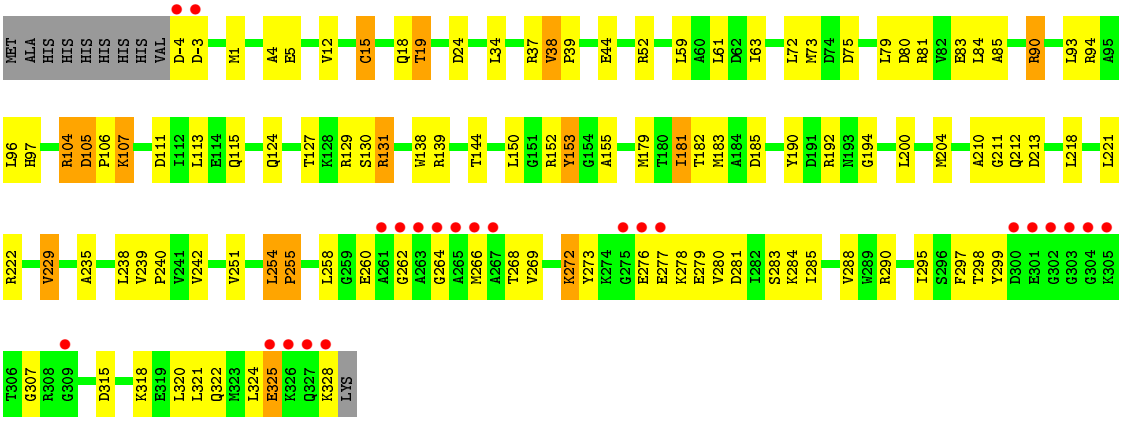
• Molecule 1: MoeN5,DNA-binding protein 7d

Chain G:



• Molecule 1: MoeN5,DNA-binding protein 7d

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	142.17Å 205.81Å 220.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80 24.89 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.1 (25.00-2.80) 97.0 (24.89-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.57 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.170 , 0.232 0.170 , 0.231	Depositor DCC
R_{free} test set	3906 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 77211 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19608	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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 43.72 % 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 1.6927e-04.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: BNG

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	A	0.84	0/2042	0.95	1/2775 (0.0%)
1	B	0.81	1/2588 (0.0%)	0.94	3/3499 (0.1%)
1	C	0.91	1/2049 (0.0%)	1.00	4/2785 (0.1%)
1	D	0.78	0/2579	0.90	1/3488 (0.0%)
1	E	0.85	0/2093	0.96	2/2845 (0.1%)
1	F	0.82	1/2573 (0.0%)	0.94	3/3478 (0.1%)
1	G	0.85	1/2035 (0.0%)	1.00	4/2765 (0.1%)
1	H	0.83	1/2581 (0.0%)	0.94	3/3489 (0.1%)
All	All	0.83	5/18540 (0.0%)	0.95	21/25124 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	H	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	15	CYS	CB-SG	-7.38	1.69	1.82
1	B	15	CYS	CB-SG	-6.94	1.70	1.82
1	G	15	CYS	CB-SG	-6.85	1.70	1.82
1	H	15	CYS	CB-SG	-6.50	1.71	1.82
1	C	15	CYS	CB-SG	-5.21	1.73	1.81

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	81	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	G	-1	ASP	C-N-CA	7.72	140.99	121.70
1	F	80	ASP	CB-CG-OD1	6.78	124.40	118.30
1	F	10	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	H	111	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	C	165	GLN	N-CA-C	-5.95	94.94	111.00
1	C	252	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	B	256	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	B	197	ASP	N-CA-C	-5.68	95.66	111.00
1	E	9	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	C	52	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	G	73	MET	CA-CB-CG	5.48	122.61	113.30
1	G	111	ASP	CB-CG-OD1	5.39	123.15	118.30
1	H	111	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	165	GLN	N-CA-C	-5.28	96.74	111.00
1	G	171	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	E	9	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	H	222	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	57	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	C	14	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	D	73	MET	CG-SD-CE	5.11	108.38	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	TYR	Sidechain
1	C	153	TYR	Sidechain
1	H	153	TYR	Sidechain

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	A	2010	0	1990	67	0
1	B	2549	0	2554	99	0
1	C	2017	0	1999	59	0
1	D	2540	0	2541	98	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2057	0	2027	80	0
1	F	2534	0	2541	104	0
1	G	2003	0	1988	76	0
1	H	2542	0	2545	85	0
2	A	42	0	60	4	0
2	B	42	0	60	3	0
2	C	42	0	60	6	0
2	D	42	0	60	7	0
2	E	21	0	30	2	0
2	F	21	0	30	3	0
2	G	21	0	30	2	0
2	H	42	0	60	7	0
3	A	149	0	0	7	0
3	B	144	0	0	2	0
3	C	138	0	0	5	0
3	D	142	0	0	3	0
3	E	94	0	0	1	0
3	F	167	0	0	6	0
3	G	99	0	0	2	0
3	H	150	0	0	2	0
All	All	19608	0	18575	641	0

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 17.

All (641) 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)
1:B:183:MET:CE	1:B:183:MET:SD	2.03	1.47
2:A:501:BNG:H4'1	2:A:501:BNG:H9'3	1.32	1.04
1:G:126:ARG:NH1	3:G:501:HOH:O	1.93	0.99
1:C:158:ALA:HA	1:C:165:GLN:HG2	1.48	0.96
2:D:501:BNG:H4'1	2:D:501:BNG:H9'2	1.47	0.95
1:E:158:ALA:HA	1:E:165:GLN:HG2	1.46	0.95
1:D:266:MET:HE3	1:D:267:ALA:H	1.30	0.94
1:E:211:GLY:O	1:E:215:VAL:HG23	1.67	0.94
1:C:89:LEU:HD23	2:D:502:BNG:H9'2	1.47	0.94
1:B:124:GLN:HE21	1:B:124:GLN:HA	1.28	0.93
1:D:124:GLN:HA	1:D:124:GLN:HE21	1.35	0.91
1:E:25:LEU:HB2	1:E:83:GLU:OE2	1.72	0.89
1:B:183:MET:HB3	1:B:183:MET:HE2	1.56	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:TYR:O	1:B:276:GLU:HB2	1.74	0.87
1:B:269:VAL:HG21	1:B:285:ILE:HD11	1.55	0.87
1:E:131:ARG:HH11	1:E:131:ARG:HG2	1.38	0.85
1:F:254:LEU:HD22	1:F:258:LEU:HG	1.57	0.85
1:H:295:ILE:HD12	1:H:324:LEU:HD11	1.59	0.85
1:D:229:VAL:HG21	1:D:238:LEU:HB2	1.59	0.84
1:D:269:VAL:HG21	1:D:285:ILE:HD11	1.59	0.84
1:C:81:ARG:HD3	3:C:649:HOH:O	1.76	0.84
1:F:295:ILE:HD12	1:F:324:LEU:HD11	1.61	0.83
1:B:272:LYS:HE3	1:B:277:GLU:OE2	1.80	0.82
1:B:33:ARG:HH21	1:B:33:ARG:HG2	1.45	0.82
1:D:285:ILE:HD13	1:D:320:LEU:HD13	1.62	0.82
1:A:81:ARG:HD3	3:A:664:HOH:O	1.78	0.81
1:G:10:ASP:HB3	1:G:14:ARG:NH2	1.95	0.81
1:C:89:LEU:CD2	2:D:502:BNG:H9'2	2.10	0.81
1:H:251:VAL:O	1:H:255:PRO:HG2	1.79	0.81
1:D:266:MET:CE	1:D:267:ALA:H	1.93	0.81
2:F:401:BNG:H61	3:F:508:HOH:O	1.79	0.80
1:F:251:VAL:O	1:F:255:PRO:HG2	1.81	0.80
1:C:139:ARG:HD3	1:C:179:MET:HE1	1.64	0.79
1:D:134:ASN:ND2	1:D:137:GLU:HG3	1.97	0.79
1:B:285:ILE:HD13	1:B:320:LEU:HD13	1.64	0.79
1:F:179:MET:HG2	1:F:221:LEU:HD11	1.65	0.78
1:D:272:LYS:HE3	1:D:277:GLU:OE2	1.84	0.77
1:B:33:ARG:NH2	1:B:33:ARG:HG2	1.98	0.77
1:D:179:MET:HG2	1:D:221:LEU:HD11	1.65	0.77
1:B:80:ASP:OD2	1:B:83:GLU:HG3	1.86	0.77
1:C:1:MET:SD	1:C:37:ARG:HD2	2.25	0.76
1:A:158:ALA:HA	1:A:165:GLN:HG2	1.67	0.76
1:E:124:GLN:HE21	2:E:401:BNG:H6'2	1.49	0.76
1:F:285:ILE:HD13	1:F:320:LEU:HD13	1.68	0.75
1:A:168:ASP:O	1:A:172:GLU:HG3	1.87	0.75
1:B:200:LEU:HG	1:B:204:MET:CE	2.17	0.75
1:D:196:ARG:HG2	1:D:197:ASP:N	2.02	0.74
1:C:222:ARG:HG3	1:C:246:THR:HG21	1.69	0.74
1:E:179:MET:HG2	1:E:221:LEU:HD11	1.70	0.74
2:D:501:BNG:H4'1	2:D:501:BNG:C9'	2.17	0.74
1:F:237:GLY:O	1:F:240:PRO:HD2	1.86	0.74
1:F:38:VAL:HG12	1:F:39:PRO:HD3	1.70	0.74
1:D:318:LYS:O	1:D:322:GLN:HG3	1.87	0.74
1:B:71:ASP:HB3	1:B:77:THR:HG21	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:TRP:CH2	1:B:183:MET:HG2	2.24	0.73
1:F:1:MET:HE3	1:F:37:ARG:HD3	1.69	0.73
1:G:205:ARG:HG2	1:G:205:ARG:HH11	1.52	0.73
1:G:86:CYS:HA	2:H:502:BNG:H9'1	1.70	0.73
1:A:258:LEU:HA	3:A:666:HOH:O	1.89	0.73
1:D:124:GLN:HG2	2:D:502:BNG:H8'1	1.70	0.72
1:E:45:TRP:HB2	1:E:165:GLN:NE2	2.03	0.72
2:F:401:BNG:O3	3:F:501:HOH:O	2.06	0.72
1:F:267:ALA:HB1	1:F:282:ILE:CG1	2.19	0.72
1:E:158:ALA:CA	1:E:165:GLN:HG2	2.18	0.72
1:F:60:ALA:O	1:F:64:VAL:HG23	1.89	0.72
1:A:191:ASP:HB3	1:E:81:ARG:HH21	1.55	0.71
1:B:285:ILE:CD1	1:B:320:LEU:HD13	2.20	0.71
1:F:234:GLY:O	3:F:502:HOH:O	2.07	0.71
1:H:38:VAL:HG12	1:H:39:PRO:HD3	1.71	0.71
1:B:183:MET:HB3	1:B:183:MET:CE	2.20	0.71
2:A:501:BNG:H9'3	2:A:501:BNG:C4'	2.15	0.71
1:D:214:VAL:HG11	1:D:254:LEU:HD21	1.71	0.71
1:F:72:LEU:O	1:F:81:ARG:NH1	2.24	0.71
1:E:34:LEU:HD21	1:E:181:ILE:HD12	1.72	0.71
1:H:288:VAL:HG23	1:H:297:PHE:HB3	1.71	0.71
1:D:285:ILE:CD1	1:D:320:LEU:HD13	2.21	0.70
2:D:501:BNG:H5'1	2:D:502:BNG:H62	1.73	0.70
1:B:318:LYS:O	1:B:322:GLN:HG3	1.91	0.70
1:F:269:VAL:HG21	1:F:285:ILE:HD11	1.73	0.70
1:G:113:LEU:O	1:G:152:ARG:NH1	2.25	0.70
1:H:179:MET:HG2	1:H:221:LEU:HD11	1.74	0.70
1:D:131:ARG:NH1	1:D:196:ARG:HH11	1.90	0.69
1:E:99:LEU:HD13	1:E:156:LEU:HD13	1.74	0.69
1:F:265:ALA:C	1:F:267:ALA:H	1.96	0.69
1:E:19:THR:HG22	1:E:19:THR:O	1.93	0.69
1:H:273:TYR:HB3	1:H:278:LYS:HE2	1.74	0.68
1:B:124:GLN:NE2	1:B:124:GLN:HA	2.06	0.68
1:C:19:THR:OG1	1:C:90:ARG:HG3	1.93	0.68
1:D:187:LEU:HD23	1:D:201:ALA:HB2	1.75	0.68
1:A:191:ASP:HB3	1:E:81:ARG:NH2	2.09	0.68
1:D:273:TYR:HB3	1:D:278:LYS:HE2	1.73	0.68
2:H:501:BNG:H3'1	2:H:502:BNG:H5	1.74	0.68
1:A:81:ARG:HH22	1:B:81:ARG:HD2	1.60	0.67
1:G:38:VAL:HG12	1:G:39:PRO:HD3	1.76	0.67
3:A:618:HOH:O	1:B:107:LYS:HG2	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ALA:O	1:D:282:ILE:HG12	1.95	0.67
1:A:256:ARG:HA	1:F:130:SER:HB3	1.76	0.67
1:A:258:LEU:HD12	1:A:258:LEU:O	1.93	0.67
1:H:295:ILE:CD1	1:H:324:LEU:HD11	2.25	0.67
1:F:267:ALA:HB1	1:F:282:ILE:HG12	1.76	0.66
1:G:-2:ASP:OD1	1:G:-1:ASP:N	2.29	0.66
1:F:1:MET:CE	1:F:37:ARG:HH11	2.08	0.66
1:F:1:MET:HE1	1:F:37:ARG:HH11	1.60	0.66
1:H:238:LEU:O	1:H:242:VAL:HG23	1.95	0.66
1:A:11:HIS:CG	1:A:57:ARG:HD2	2.30	0.66
1:D:192:ARG:O	1:D:195:GLU:HB2	1.96	0.65
1:C:179:MET:HG2	1:C:221:LEU:HD11	1.76	0.65
1:C:38:VAL:HG12	1:C:39:PRO:HD3	1.78	0.65
1:B:112:ILE:HA	1:B:115:GLN:NE2	2.11	0.65
1:H:72:LEU:HD21	1:H:85:ALA:HB2	1.79	0.65
1:G:96:LEU:HD11	1:H:96:LEU:HD11	1.79	0.65
1:D:266:MET:CE	1:D:267:ALA:N	2.59	0.64
1:E:131:ARG:NH1	1:E:131:ARG:HG2	2.04	0.64
1:F:1:MET:CE	1:F:37:ARG:HD3	2.26	0.64
1:A:55:VAL:HG22	1:A:102:LEU:HD13	1.80	0.64
1:B:267:ALA:HB2	1:B:319:GLU:OE2	1.98	0.63
1:H:204:MET:O	1:H:262:GLY:HA3	1.99	0.63
1:F:1:MET:SD	1:F:37:ARG:HD3	2.38	0.63
1:E:195:GLU:HG2	1:E:199:ASN:HB2	1.78	0.63
1:H:80:ASP:HB3	1:H:83:GLU:HG2	1.81	0.63
2:B:501:BNG:H9'3	2:B:501:BNG:H3'2	1.81	0.63
1:G:205:ARG:NH2	1:G:260:GLU:HG3	2.14	0.63
1:H:12:VAL:HG22	1:H:61:LEU:HD23	1.82	0.62
1:G:205:ARG:NH1	1:G:205:ARG:HG2	2.14	0.62
1:D:273:TYR:O	1:D:276:GLU:HB2	1.99	0.62
1:E:72:LEU:O	1:F:81:ARG:NH2	2.32	0.62
1:H:260:GLU:C	1:H:262:GLY:H	2.00	0.62
1:G:138:TRP:CH2	1:G:182:THR:HG22	2.34	0.62
1:G:166:PRO:HD3	1:G:233:PRO:HD2	1.81	0.62
1:B:134:ASN:OD1	1:B:136:ARG:HB3	1.99	0.62
1:H:324:LEU:O	1:H:328:LYS:HG2	2.00	0.62
1:H:269:VAL:HG21	1:H:285:ILE:HD11	1.81	0.62
1:B:185:ASP:OD2	2:B:502:BNG:H61	1.99	0.61
1:E:138:TRP:CH2	1:E:182:THR:HG22	2.34	0.61
1:D:295:ILE:HD12	1:D:324:LEU:HD11	1.83	0.61
1:F:265:ALA:C	1:F:267:ALA:N	2.54	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:THR:HB	1:F:279:GLU:HG2	1.82	0.61
1:C:258:LEU:O	1:C:258:LEU:HD22	2.01	0.61
1:H:104:ARG:NH1	1:H:104:ARG:HB2	2.16	0.61
1:F:138:TRP:CH2	1:F:182:THR:HG22	2.35	0.61
1:B:131:ARG:NH1	1:B:196:ARG:HD2	2.16	0.61
1:B:187:LEU:HD23	1:B:201:ALA:HB2	1.81	0.60
1:F:270:LYS:HG2	1:F:279:GLU:HG3	1.83	0.60
1:A:131:ARG:HH11	1:A:131:ARG:HG2	1.66	0.60
1:A:107:LYS:NZ	1:B:97:HIS:ND1	2.49	0.60
1:D:206:THR:HG22	1:D:208:ALA:H	1.65	0.60
1:F:205:ARG:HA	1:F:261:ALA:HB2	1.83	0.60
1:G:11:HIS:CD2	1:G:57:ARG:HD2	2.36	0.60
1:D:179:MET:HG2	1:D:221:LEU:CD1	2.32	0.60
1:F:135:LEU:O	1:F:135:LEU:HD12	2.01	0.60
1:E:113:LEU:HB3	1:F:93:LEU:HD22	1.83	0.60
1:G:206:THR:HG22	1:G:208:ALA:H	1.66	0.60
1:H:273:TYR:O	1:H:276:GLU:HB2	2.02	0.60
1:E:81:ARG:HD2	1:F:81:ARG:NH1	2.17	0.60
1:G:239:VAL:HB	1:G:240:PRO:HD3	1.82	0.60
1:H:181:ILE:HG22	1:H:182:THR:N	2.16	0.60
1:D:210:ALA:HB3	1:D:213:ASP:OD2	2.01	0.60
1:D:14:ARG:NH1	1:F:192:ARG:HA	2.17	0.60
1:F:1:MET:HE1	1:F:37:ARG:NH1	2.17	0.59
1:B:206:THR:HG22	1:B:208:ALA:H	1.67	0.59
1:C:131:ARG:HH11	1:C:131:ARG:HG2	1.67	0.59
1:G:10:ASP:HB3	1:G:14:ARG:HH21	1.65	0.59
1:D:14:ARG:NH1	3:D:602:HOH:O	2.35	0.59
1:E:206:THR:HG23	1:E:208:ALA:H	1.67	0.59
1:H:183:MET:HE1	1:H:218:LEU:HG	1.85	0.59
1:H:183:MET:CE	1:H:218:LEU:HG	2.33	0.59
1:C:73:MET:SD	1:D:82:VAL:HG22	2.42	0.59
1:G:94:ARG:HH21	1:G:97:HIS:CD2	2.21	0.59
1:F:1:MET:HG3	1:F:2:LEU:N	2.17	0.58
1:D:12:VAL:HG22	1:D:61:LEU:HD23	1.85	0.58
1:C:81:ARG:CD	3:C:649:HOH:O	2.41	0.58
1:F:238:LEU:O	1:F:242:VAL:HG23	2.04	0.58
1:D:15:CYS:O	1:D:19:THR:HG22	2.04	0.58
1:G:1:MET:HE2	3:G:536:HOH:O	2.04	0.58
1:B:1:MET:SD	1:B:37:ARG:HD3	2.44	0.57
1:F:285:ILE:CD1	1:F:320:LEU:HD13	2.32	0.57
1:G:107:LYS:HD3	1:G:107:LYS:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:TRP:CH2	1:C:183:MET:HG2	2.39	0.57
1:E:44:GLU:HG2	1:E:238:LEU:HG	1.85	0.57
1:C:256:ARG:HA	1:H:130:SER:HB3	1.85	0.57
1:H:268:THR:HB	1:H:279:GLU:HG2	1.86	0.57
1:C:163:GLU:OE2	3:C:601:HOH:O	2.17	0.57
1:B:183:MET:CB	1:B:183:MET:HE2	2.31	0.57
1:B:131:ARG:CZ	1:B:196:ARG:HH11	2.18	0.57
1:B:266:MET:HE2	1:B:282:ILE:N	2.20	0.57
1:G:11:HIS:CG	1:G:57:ARG:HD2	2.39	0.57
1:E:201:ALA:HA	1:E:204:MET:HE2	1.87	0.56
1:F:1:MET:CE	1:F:37:ARG:NH1	2.68	0.56
1:D:67:LYS:HE3	1:D:71:ASP:OD1	2.06	0.56
1:A:165:GLN:O	3:A:601:HOH:O	2.18	0.56
1:B:135:LEU:HB2	1:B:209:VAL:HG13	1.86	0.56
1:H:124:GLN:HG2	2:H:502:BNG:H7'1	1.86	0.56
1:A:22:SER:O	1:A:26:VAL:HG23	2.05	0.56
1:A:90:ARG:HD3	1:A:90:ARG:C	2.26	0.56
1:D:124:GLN:HA	1:D:124:GLN:NE2	2.13	0.56
1:F:272:LYS:HE3	1:F:277:GLU:OE2	2.06	0.56
1:C:259:GLY:HA2	1:H:131:ARG:HH12	1.69	0.56
1:E:201:ALA:HA	1:E:204:MET:CE	2.36	0.56
1:A:1:MET:SD	1:A:37:ARG:HD3	2.46	0.56
1:E:179:MET:HG2	1:E:221:LEU:CD1	2.36	0.56
1:G:116:ASP:OD1	1:G:152:ARG:NE	2.30	0.56
1:H:104:ARG:CZ	1:H:104:ARG:CB	2.84	0.56
1:C:1:MET:CE	1:C:37:ARG:HD2	2.35	0.56
1:D:134:ASN:CG	1:D:137:GLU:HG3	2.25	0.56
1:B:124:GLN:HE22	1:B:145:TYR:HB3	1.71	0.55
1:E:38:VAL:HG11	1:E:150:LEU:HD11	1.88	0.55
1:H:75:ASP:HB2	1:H:81:ARG:NH1	2.21	0.55
1:C:38:VAL:CG1	1:C:39:PRO:HD3	2.36	0.55
1:C:139:ARG:HB2	1:C:179:MET:HE3	1.89	0.55
1:E:183:MET:HE1	1:E:214:VAL:HG13	1.89	0.55
1:G:229:VAL:HG12	1:G:238:LEU:HD12	1.88	0.55
1:B:301:GLU:HG2	1:B:301:GLU:O	2.06	0.55
1:F:285:ILE:HD13	1:F:320:LEU:CD1	2.34	0.55
1:H:44:GLU:HG3	1:H:44:GLU:O	2.06	0.54
1:H:73:MET:HE1	2:H:502:BNG:H8'2	1.88	0.54
1:D:196:ARG:HG2	1:D:197:ASP:H	1.72	0.54
1:E:71:ASP:HB3	1:E:77:THR:HG21	1.90	0.54
1:H:260:GLU:C	1:H:262:GLY:N	2.59	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ARG:NH1	1:D:196:ARG:NH1	2.56	0.54
1:C:131:ARG:NH1	1:C:131:ARG:HG2	2.22	0.54
1:C:181:ILE:HD11	2:C:501:BNG:H7'2	1.90	0.54
1:E:195:GLU:O	1:E:196:ARG:HD3	2.08	0.54
1:E:61:LEU:HD22	1:E:91:LEU:HD23	1.90	0.54
1:G:72:LEU:HD13	1:G:84:LEU:HB3	1.89	0.54
1:E:203:LEU:O	1:E:206:THR:HG22	2.08	0.54
1:B:263:ALA:HB3	3:B:645:HOH:O	2.08	0.54
1:F:260:GLU:OE1	1:F:326:LYS:NZ	2.41	0.54
1:B:322:GLN:HA	1:B:325:GLU:OE2	2.08	0.53
1:E:81:ARG:HD2	1:F:81:ARG:HH12	1.72	0.53
1:G:244:LEU:HD12	1:G:244:LEU:O	2.08	0.53
1:H:104:ARG:CZ	1:H:104:ARG:HB3	2.38	0.53
1:C:80:ASP:OD2	1:C:83:GLU:HG3	2.08	0.53
1:D:239:VAL:N	1:D:240:PRO:HD2	2.24	0.53
1:E:25:LEU:CB	1:E:83:GLU:OE2	2.52	0.53
1:F:51:ARG:NH2	1:F:160:CYS:O	2.41	0.53
1:F:195:GLU:O	1:F:196:ARG:NH1	2.40	0.53
1:F:75:ASP:HB2	1:F:81:ARG:HH11	1.73	0.53
1:H:285:ILE:HD13	1:H:320:LEU:HD13	1.90	0.53
1:C:191:ASP:HB3	1:G:81:ARG:NH2	2.22	0.53
1:D:281:ASP:O	1:D:283:SER:N	2.42	0.53
1:H:318:LYS:O	1:H:322:GLN:HG3	2.07	0.53
1:C:-2:ASP:O	1:C:2:LEU:HG	2.09	0.53
1:D:281:ASP:C	1:D:283:SER:N	2.62	0.53
1:D:214:VAL:CG1	1:D:254:LEU:HD21	2.39	0.53
1:B:183:MET:CB	1:B:183:MET:CE	2.85	0.53
1:C:9:ARG:HD2	3:C:654:HOH:O	2.08	0.53
1:G:19:THR:O	1:G:19:THR:HG22	2.08	0.53
1:A:131:ARG:NH1	1:A:131:ARG:HG2	2.23	0.53
1:A:205:ARG:HB3	1:F:131:ARG:HH21	1.74	0.53
1:F:267:ALA:HB1	1:F:282:ILE:HG13	1.90	0.53
1:D:226:LEU:O	1:D:229:VAL:HG12	2.08	0.52
1:C:205:ARG:NH1	1:H:131:ARG:HG3	2.24	0.52
1:C:44:GLU:HG2	1:C:238:LEU:HG	1.90	0.52
1:B:295:ILE:HD12	1:B:324:LEU:HD11	1.91	0.52
1:G:112:ILE:HD12	1:G:156:LEU:HD23	1.91	0.52
1:B:138:TRP:HH2	1:B:183:MET:HG2	1.74	0.52
1:H:285:ILE:CD1	1:H:320:LEU:HD13	2.40	0.52
1:A:190:TYR:O	1:A:191:ASP:HB2	2.09	0.52
1:A:258:LEU:HD22	3:A:720:HOH:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:THR:O	1:A:152:ARG:HG3	2.09	0.52
1:F:265:ALA:O	1:F:267:ALA:N	2.43	0.52
1:H:105:ASP:C	1:H:105:ASP:OD2	2.48	0.52
1:A:32:LEU:HB3	1:A:35:TYR:CD2	2.45	0.52
1:A:81:ARG:NH2	1:B:81:ARG:HD2	2.25	0.52
1:H:59:LEU:O	1:H:63:ILE:HG13	2.10	0.52
1:D:190:TYR:O	1:D:191:ASP:HB2	2.10	0.52
1:D:266:MET:HE2	1:D:267:ALA:O	2.10	0.52
1:F:138:TRP:HH2	1:F:182:THR:HG22	1.74	0.52
1:A:139:ARG:HD3	1:A:179:MET:HE3	1.92	0.51
1:H:1:MET:O	1:H:4:ALA:N	2.40	0.51
1:H:181:ILE:CG2	2:H:501:BNG:H2'2	2.39	0.51
1:A:138:TRP:CH2	1:A:183:MET:HG2	2.44	0.51
1:D:196:ARG:CG	1:D:197:ASP:N	2.74	0.51
1:E:138:TRP:CZ2	1:E:182:THR:HG22	2.46	0.51
1:E:143:SER:HA	1:E:147:SER:HB2	1.93	0.51
1:F:204:MET:O	1:F:261:ALA:HB1	2.11	0.51
1:G:9:ARG:HB2	1:G:36:LEU:HD13	1.91	0.51
1:A:185:ASP:OD2	2:A:502:BNG:H61	2.11	0.51
1:C:185:ASP:OD2	2:C:502:BNG:O4	2.19	0.51
1:F:268:THR:HA	1:F:280:VAL:O	2.10	0.51
1:G:244:LEU:HD12	1:G:244:LEU:C	2.30	0.51
1:B:200:LEU:O	1:B:204:MET:HB2	2.11	0.51
1:E:11:HIS:CE1	1:E:57:ARG:HD2	2.45	0.51
1:G:183:MET:HE1	1:G:218:LEU:CD1	2.40	0.51
1:B:183:MET:CE	1:B:183:MET:CG	2.88	0.51
1:C:11:HIS:CG	1:C:57:ARG:HD2	2.46	0.51
1:D:282:ILE:HG21	1:D:319:GLU:HB3	1.93	0.51
1:D:302:GLY:O	1:D:305:LYS:HB2	2.11	0.51
1:F:308:ARG:HG2	1:F:308:ARG:HH11	1.75	0.51
1:A:123:GLY:HA2	1:A:126:ARG:NH2	2.25	0.51
1:A:44:GLU:HG3	1:A:44:GLU:O	2.11	0.51
1:B:85:ALA:O	1:B:88:CYS:HB3	2.11	0.51
1:B:16:VAL:HG22	1:B:87:VAL:CG1	2.41	0.51
1:E:22:SER:O	1:E:26:VAL:HG23	2.10	0.51
1:F:105:ASP:OD1	1:F:107:LYS:N	2.41	0.51
1:F:38:VAL:N	1:F:39:PRO:CD	2.73	0.51
1:D:10:ASP:HB3	1:D:14:ARG:HH22	1.75	0.51
1:D:206:THR:HG22	1:D:208:ALA:N	2.26	0.51
1:F:206:THR:HG22	1:F:208:ALA:H	1.76	0.51
1:B:261:ALA:O	1:B:262:GLY:O	2.29	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:67:LYS:HD3	1:G:67:LYS:O	2.11	0.50
1:C:257:HIS:O	1:C:258:LEU:C	2.46	0.50
1:F:254:LEU:HD13	1:F:258:LEU:HD11	1.94	0.50
1:A:204:MET:HE1	1:A:214:VAL:HG11	1.93	0.50
1:A:81:ARG:NH2	1:B:81:ARG:CD	2.75	0.50
1:F:205:ARG:HA	1:F:261:ALA:CB	2.41	0.50
1:H:5:GLU:OE1	1:H:37:ARG:CZ	2.60	0.50
1:B:286:LYS:HE2	1:B:299:TYR:C	2.32	0.50
1:G:61:LEU:HD13	1:G:94:ARG:HG2	1.94	0.50
1:A:139:ARG:HD3	1:A:179:MET:CE	2.41	0.50
1:B:267:ALA:O	1:B:282:ILE:HG12	2.12	0.50
1:F:254:LEU:N	1:F:255:PRO:CD	2.75	0.50
1:D:200:LEU:HG	1:D:204:MET:CE	2.43	0.49
1:A:258:LEU:O	1:A:258:LEU:CD1	2.59	0.49
1:E:203:LEU:C	1:E:206:THR:HG22	2.33	0.49
1:F:269:VAL:O	1:F:279:GLU:HA	2.12	0.49
1:G:38:VAL:N	1:G:39:PRO:CD	2.76	0.49
1:B:39:PRO:O	1:B:43:THR:HG23	2.12	0.49
1:E:107:LYS:NZ	1:F:97:HIS:ND1	2.60	0.49
1:E:239:VAL:HB	1:E:240:PRO:HD3	1.93	0.49
1:G:183:MET:HE1	1:G:218:LEU:HD12	1.94	0.49
1:B:288:VAL:HG12	1:B:327:GLN:HE22	1.77	0.49
1:G:68:LEU:HD22	1:G:84:LEU:CD2	2.42	0.49
1:B:131:ARG:HH12	1:B:196:ARG:HD2	1.76	0.49
1:D:105:ASP:OD1	1:D:106:PRO:CD	2.61	0.49
1:E:72:LEU:HD21	1:E:85:ALA:HB2	1.95	0.49
1:A:171:ARG:NH1	3:A:605:HOH:O	2.41	0.49
1:F:12:VAL:HG22	1:F:61:LEU:HD23	1.93	0.49
1:G:114:GLU:CD	1:H:94:ARG:HH11	2.16	0.49
1:A:55:VAL:CG2	1:A:102:LEU:HD13	2.42	0.49
1:A:203:LEU:HB3	1:A:209:VAL:HG23	1.94	0.49
1:A:81:ARG:HH22	1:B:81:ARG:CD	2.23	0.49
1:F:206:THR:O	1:F:206:THR:CG2	2.61	0.49
1:D:271:PHE:CE2	1:D:278:LYS:HD2	2.47	0.49
1:E:226:LEU:HD21	1:E:239:VAL:HG13	1.94	0.48
1:G:211:GLY:O	1:G:215:VAL:HG23	2.13	0.48
1:E:10:ASP:OD2	1:E:14:ARG:NH2	2.46	0.48
1:D:267:ALA:HB2	1:D:319:GLU:OE2	2.11	0.48
1:E:5:GLU:OE2	1:E:9:ARG:NH1	2.46	0.48
1:D:281:ASP:C	1:D:283:SER:H	2.15	0.48
1:E:-5:VAL:HG12	3:E:549:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:THR:CG2	1:B:87:VAL:HG22	2.43	0.48
1:E:158:ALA:CB	1:E:165:GLN:HG2	2.43	0.48
1:F:229:VAL:HG21	1:F:238:LEU:HB2	1.94	0.48
1:G:10:ASP:O	1:G:14:ARG:HB2	2.13	0.48
1:A:2:LEU:HD22	1:E:31:ALA:HB2	1.95	0.48
1:F:318:LYS:O	1:F:322:GLN:HG3	2.13	0.48
1:B:212:GLN:HA	1:B:263:ALA:HB1	1.94	0.48
1:C:139:ARG:HD3	1:C:179:MET:CE	2.38	0.48
1:C:150:LEU:HD13	2:C:501:BNG:H8'2	1.95	0.48
1:D:14:ARG:CZ	1:D:14:ARG:HB2	2.44	0.48
1:A:19:THR:OG1	1:A:90:ARG:HG3	2.14	0.48
1:C:93:LEU:HD22	1:D:113:LEU:HB3	1.96	0.48
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.66	0.48
1:C:183:MET:HB3	1:C:183:MET:HE3	1.83	0.48
1:D:232:PRO:HA	1:D:233:PRO:C	2.34	0.48
1:C:113:LEU:HB3	1:D:93:LEU:HD22	1.95	0.48
1:E:190:TYR:O	1:E:194:GLY:HA2	2.14	0.48
1:B:138:TRP:NE1	1:B:200:LEU:HB2	2.28	0.47
1:B:177:PHE:CE2	1:B:181:ILE:HD13	2.49	0.47
1:E:249:VAL:O	1:E:254:LEU:HB2	2.14	0.47
1:H:179:MET:HG2	1:H:221:LEU:CD1	2.42	0.47
1:B:285:ILE:HD13	1:B:320:LEU:CD1	2.39	0.47
1:B:-5:VAL:HG12	1:B:-5:VAL:O	2.13	0.47
1:C:205:ARG:HB3	1:H:131:ARG:NH2	2.28	0.47
1:F:127:THR:HG21	1:F:145:TYR:CD2	2.49	0.47
1:H:239:VAL:N	1:H:240:PRO:HD2	2.28	0.47
1:D:301:GLU:O	1:D:301:GLU:HG2	2.14	0.47
1:H:288:VAL:O	1:H:328:LYS:NZ	2.43	0.47
1:A:35:TYR:CD1	2:A:501:BNG:H9'1	2.49	0.47
1:B:288:VAL:HG11	1:B:323:MET:HB2	1.96	0.47
1:H:138:TRP:CH2	1:H:182:THR:HG22	2.50	0.47
1:B:166:PRO:O	1:B:167:ALA:C	2.52	0.47
1:B:58:ALA:HB1	1:B:99:LEU:HG	1.96	0.47
1:D:5:GLU:OE1	1:D:37:ARG:NH1	2.48	0.47
1:D:185:ASP:OD1	2:D:501:BNG:H1'2	2.14	0.47
1:E:112:ILE:HD12	1:E:156:LEU:HD23	1.97	0.47
1:H:322:GLN:HA	1:H:325:GLU:OE2	2.14	0.47
1:H:105:ASP:OD2	1:H:106:PRO:N	2.48	0.47
1:B:105:ASP:OD1	1:B:106:PRO:HD2	2.15	0.47
1:D:32:LEU:HB3	1:D:35:TYR:CD2	2.50	0.47
1:G:124:GLN:HG2	2:G:401:BNG:H8'1	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ASP:C	1:B:283:SER:N	2.68	0.47
1:E:11:HIS:CG	1:E:57:ARG:HD3	2.49	0.47
1:B:16:VAL:HG22	1:B:87:VAL:HG11	1.96	0.47
1:D:-5:VAL:HG22	1:D:-5:VAL:O	2.15	0.47
1:F:131:ARG:HG3	1:F:131:ARG:NH1	2.30	0.47
1:C:5:GLU:OE1	1:C:37:ARG:HD3	2.15	0.47
1:E:1:MET:HA	1:E:40:HIS:CD2	2.50	0.47
1:G:138:TRP:CZ2	1:G:182:THR:HG22	2.49	0.46
1:H:150:LEU:HD12	1:H:150:LEU:HA	1.69	0.46
2:B:502:BNG:H2	3:B:634:HOH:O	2.15	0.46
1:B:212:GLN:HB2	1:B:264:GLY:H	1.80	0.46
1:E:9:ARG:O	1:E:13:THR:HG23	2.15	0.46
1:F:90:ARG:C	1:F:90:ARG:HD3	2.36	0.46
1:G:35:TYR:OH	2:G:401:BNG:H1	2.15	0.46
1:A:143:SER:HA	1:A:147:SER:HB2	1.97	0.46
1:C:81:ARG:HH11	1:C:81:ARG:HG2	1.81	0.46
1:D:266:MET:HE2	1:D:267:ALA:N	2.30	0.46
1:D:299:TYR:CE1	1:D:307:GLY:HA3	2.51	0.46
2:F:401:BNG:C6	3:F:508:HOH:O	2.47	0.46
1:A:205:ARG:HB3	1:F:131:ARG:NH2	2.31	0.46
1:F:281:ASP:C	1:F:283:SER:H	2.18	0.46
1:F:282:ILE:HG13	1:F:319:GLU:HB2	1.97	0.46
1:A:150:LEU:CB	1:A:178:ALA:HB2	2.45	0.46
1:C:196:ARG:O	1:C:197:ASP:C	2.54	0.46
1:D:274:LYS:C	1:D:276:GLU:H	2.19	0.46
1:D:280:VAL:HG12	1:D:284:LYS:HB2	1.97	0.46
1:E:19:THR:CG2	1:E:19:THR:O	2.63	0.46
1:A:187:LEU:HD21	1:A:204:MET:HE3	1.97	0.46
1:G:193:ASN:C	1:G:193:ASN:HD22	2.19	0.46
1:G:93:LEU:HD22	1:H:113:LEU:HB3	1.96	0.46
1:A:193:ASN:HB3	1:A:194:GLY:H	1.62	0.46
1:C:81:ARG:HH22	1:D:81:ARG:HD2	1.82	0.46
1:C:71:ASP:HB3	1:C:77:THR:HG21	1.98	0.45
1:F:71:ASP:HB3	1:F:77:THR:HG21	1.97	0.45
1:D:16:VAL:HG22	1:D:87:VAL:HG11	1.99	0.45
1:F:273:TYR:O	1:F:276:GLU:HB2	2.16	0.45
1:G:113:LEU:HB3	1:H:93:LEU:HD22	1.98	0.45
2:C:501:BNG:H4'1	2:C:501:BNG:H9'3	1.97	0.45
1:F:204:MET:HE1	1:F:257:HIS:HB2	1.98	0.45
1:F:72:LEU:HD12	1:F:72:LEU:HA	1.71	0.45
1:H:272:LYS:HE2	1:H:277:GLU:OE2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ILE:HD13	1:D:320:LEU:CD1	2.37	0.45
1:F:48:ASP:OD1	1:F:49:PRO:HD2	2.16	0.45
1:D:37:ARG:HH11	1:D:37:ARG:HG3	1.81	0.45
1:F:84:LEU:O	1:F:88:CYS:HB3	2.17	0.45
1:G:48:ASP:C	1:G:48:ASP:OD1	2.55	0.45
1:G:94:ARG:NH2	1:G:97:HIS:CD2	2.84	0.45
1:A:204:MET:HE2	1:A:214:VAL:HG21	1.99	0.45
1:B:93:LEU:HA	1:B:93:LEU:HD23	1.79	0.45
1:E:11:HIS:NE2	1:E:61:LEU:HD11	2.32	0.45
1:F:134:ASN:C	1:F:134:ASN:OD1	2.54	0.45
1:F:303:GLY:HA3	3:F:503:HOH:O	2.17	0.45
1:G:229:VAL:HG11	1:G:238:LEU:CB	2.47	0.45
1:G:258:LEU:HD12	1:G:258:LEU:HA	1.68	0.45
1:A:135:LEU:O	1:A:139:ARG:HB3	2.17	0.45
1:G:25:LEU:O	1:G:29:THR:HG23	2.17	0.45
1:H:229:VAL:HG22	1:H:235:ALA:HB3	1.99	0.45
1:H:211:GLY:HA3	1:H:258:LEU:HD21	1.97	0.45
1:B:260:GLU:HG3	1:G:137:GLU:OE2	2.17	0.45
1:G:158:ALA:HA	1:G:165:GLN:HG2	1.99	0.45
1:C:104:ARG:HD3	1:C:163:GLU:OE1	2.16	0.45
1:F:131:ARG:HH11	1:F:131:ARG:HG3	1.82	0.45
1:F:281:ASP:O	1:F:283:SER:N	2.50	0.45
1:H:229:VAL:HG13	1:H:235:ALA:O	2.15	0.45
1:B:190:TYR:O	1:B:191:ASP:HB2	2.17	0.44
1:D:192:ARG:NH2	1:F:75:ASP:O	2.50	0.44
1:F:179:MET:HG2	1:F:221:LEU:CD1	2.42	0.44
1:F:281:ASP:C	1:F:283:SER:N	2.70	0.44
1:G:226:LEU:HA	1:G:226:LEU:HD23	1.61	0.44
1:G:232:PRO:HA	1:G:233:PRO:C	2.38	0.44
1:E:226:LEU:HD23	1:E:226:LEU:HA	1.63	0.44
1:C:35:TYR:CE2	2:C:501:BNG:H1'2	2.52	0.44
1:C:53:ALA:O	1:C:57:ARG:HG2	2.18	0.44
1:D:193:ASN:HB3	1:D:194:GLY:H	1.29	0.44
1:D:201:ALA:HB1	1:D:257:HIS:CE1	2.52	0.44
1:D:299:TYR:HE1	1:D:301:GLU:HB2	1.83	0.44
1:H:84:LEU:HA	1:H:84:LEU:HD23	1.73	0.44
1:B:38:VAL:N	1:B:39:PRO:CD	2.80	0.44
1:E:251:VAL:HG12	1:E:252:ARG:N	2.29	0.44
1:E:61:LEU:CD2	1:E:91:LEU:CD2	2.95	0.44
1:G:191:ASP:OD2	1:G:256:ARG:NH1	2.51	0.44
1:A:114:GLU:OE2	1:B:94:ARG:NH1	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-4:ASP:O	1:B:-1:ASP:HB2	2.18	0.44
1:B:288:VAL:HG12	1:B:327:GLN:NE2	2.32	0.44
1:E:32:LEU:HD22	1:E:35:TYR:CE2	2.52	0.44
1:G:101:SER:HA	1:H:107:LYS:HE2	1.98	0.44
1:B:105:ASP:OD1	1:B:106:PRO:CD	2.66	0.44
1:E:238:LEU:O	1:E:242:VAL:HG23	2.18	0.44
1:F:282:ILE:HG21	1:F:319:GLU:HB3	2.00	0.44
1:G:254:LEU:HA	1:G:254:LEU:HD23	1.69	0.44
1:H:79:LEU:HD23	1:H:79:LEU:HA	1.86	0.44
1:F:34:LEU:HD11	1:F:181:ILE:HG12	2.00	0.44
1:A:200:LEU:HG	1:A:204:MET:HE3	2.00	0.44
1:A:11:HIS:CE1	1:A:57:ARG:HE	2.36	0.44
1:A:9:ARG:HB2	1:A:9:ARG:NH2	2.33	0.44
1:D:134:ASN:HD21	1:D:137:GLU:HG3	1.78	0.44
1:B:321:LEU:O	1:B:325:GLU:OE2	2.36	0.43
1:A:107:LYS:HD3	1:A:107:LYS:O	2.17	0.43
1:A:48:ASP:HA	1:A:49:PRO:HD2	1.85	0.43
1:D:67:LYS:HE3	1:D:71:ASP:CG	2.38	0.43
1:H:254:LEU:O	1:H:255:PRO:C	2.55	0.43
1:E:183:MET:O	1:E:187:LEU:HG	2.19	0.43
1:E:32:LEU:HB3	1:E:35:TYR:HD2	1.83	0.43
1:G:165:GLN:HB2	1:G:165:GLN:HE21	1.57	0.43
1:H:106:PRO:HA	3:H:632:HOH:O	2.19	0.43
1:H:63:ILE:HG12	1:H:153:TYR:CE2	2.53	0.43
1:B:308:ARG:HG2	1:B:308:ARG:HH11	1.83	0.43
1:E:131:ARG:NH1	1:E:131:ARG:CG	2.77	0.43
1:B:201:ALA:HB1	1:B:257:HIS:CE1	2.53	0.43
1:D:243:HIS:O	1:D:247:ASP:HB2	2.18	0.43
1:F:232:PRO:HA	1:F:233:PRO:C	2.38	0.43
1:F:266:MET:O	1:F:266:MET:HG3	2.19	0.43
1:H:104:ARG:HH11	1:H:104:ARG:HB2	1.84	0.43
1:H:254:LEU:N	1:H:255:PRO:CD	2.81	0.43
1:H:298:THR:HA	1:H:307:GLY:O	2.18	0.43
1:E:112:ILE:CD1	1:E:156:LEU:HD23	2.49	0.43
1:F:127:THR:HG23	1:F:141:HIS:HB3	2.01	0.43
1:B:229:VAL:HG11	1:B:238:LEU:HB2	2.00	0.43
1:C:111:ASP:O	1:C:115:GLN:HB2	2.19	0.43
1:D:299:TYR:CE1	1:D:301:GLU:HB2	2.53	0.43
1:H:210:ALA:HB3	1:H:213:ASP:HB2	2.00	0.43
1:B:44:GLU:HG2	1:B:238:LEU:HG	2.01	0.43
1:G:226:LEU:HD11	1:G:243:HIS:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:GLU:HA	3:C:601:HOH:O	2.19	0.43
1:D:107:LYS:HG2	3:D:645:HOH:O	2.17	0.43
1:E:124:GLN:OE1	1:E:124:GLN:HA	2.19	0.43
1:E:129:ARG:HH11	1:E:129:ARG:HG2	1.84	0.43
1:A:14:ARG:HD2	3:A:655:HOH:O	2.18	0.43
1:A:51:ARG:NH2	1:A:160:CYS:O	2.51	0.43
1:D:136:ARG:HH21	1:D:136:ARG:HG2	1.83	0.43
1:F:220:GLU:O	1:F:224:ARG:HG2	2.18	0.43
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.83	0.42
1:C:150:LEU:HD23	1:C:178:ALA:HB2	2.00	0.42
1:D:226:LEU:HD23	1:D:226:LEU:HA	1.72	0.42
1:G:25:LEU:HD22	1:G:83:GLU:HB3	2.01	0.42
1:G:90:ARG:HD3	1:G:90:ARG:C	2.39	0.42
1:A:1:MET:SD	1:A:37:ARG:CD	3.07	0.42
1:D:14:ARG:HH12	1:F:192:ARG:HA	1.82	0.42
1:G:67:LYS:HD3	1:G:67:LYS:C	2.39	0.42
1:H:290:ARG:O	3:H:601:HOH:O	2.21	0.42
1:A:90:ARG:O	1:A:90:ARG:HD3	2.19	0.42
1:C:215:VAL:HG22	1:C:254:LEU:HD11	2.01	0.42
1:D:295:ILE:O	1:D:310:ALA:HA	2.20	0.42
1:E:67:LYS:O	1:E:67:LYS:HD3	2.19	0.42
1:F:-2:ASP:HB3	1:F:1:MET:HG2	2.01	0.42
1:F:304:GLY:N	3:F:503:HOH:O	2.40	0.42
1:B:48:ASP:HA	1:B:49:PRO:HD2	1.85	0.42
1:C:222:ARG:HD3	1:C:243:HIS:CE1	2.54	0.42
1:D:183:MET:HE1	1:D:214:VAL:HG13	2.02	0.42
1:E:187:LEU:HD21	1:E:204:MET:HE1	2.02	0.42
1:H:190:TYR:O	1:H:194:GLY:HA2	2.20	0.42
1:D:10:ASP:HB3	1:D:14:ARG:NH2	2.34	0.42
1:D:113:LEU:HA	1:D:113:LEU:HD23	1.84	0.42
1:D:135:LEU:HA	1:D:135:LEU:HD12	1.77	0.42
1:F:114:GLU:O	1:F:115:GLN:C	2.58	0.42
1:E:81:ARG:CD	1:F:81:ARG:NH1	2.83	0.42
1:F:218:LEU:HD23	1:F:218:LEU:HA	1.93	0.42
1:G:72:LEU:HD21	1:G:85:ALA:HB2	2.02	0.42
1:H:280:VAL:HG12	1:H:281:ASP:N	2.35	0.42
1:B:203:LEU:HB3	1:B:209:VAL:HG23	2.02	0.42
1:C:72:LEU:HD12	1:C:81:ARG:NH1	2.34	0.42
1:D:124:GLN:HE21	1:D:124:GLN:CA	2.14	0.42
1:F:75:ASP:HB2	1:F:81:ARG:NH1	2.35	0.42
1:G:238:LEU:HD23	1:G:238:LEU:HA	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:129:ARG:HD3	1:H:129:ARG:HA	1.81	0.42
1:H:152:ARG:O	1:H:155:ALA:HB3	2.20	0.42
1:H:181:ILE:HG23	2:H:501:BNG:H2'2	2.01	0.42
1:G:107:LYS:NZ	1:H:97:HIS:ND1	2.65	0.42
1:A:254:LEU:HB2	1:A:255:PRO:HD3	2.02	0.42
1:D:1:MET:SD	1:D:37:ARG:HD3	2.60	0.42
1:A:165:GLN:HB2	1:A:165:GLN:HE21	1.49	0.42
1:B:273:TYR:HB3	1:B:278:LYS:HE2	2.01	0.42
1:C:225:ALA:O	1:C:228:ALA:HB3	2.19	0.42
1:D:269:VAL:O	1:D:279:GLU:HA	2.20	0.42
1:E:184:ALA:HB2	1:E:249:VAL:CG2	2.50	0.42
1:E:54:ALA:HB1	1:E:102:LEU:HD11	2.02	0.42
1:F:229:VAL:HG21	1:F:238:LEU:CB	2.50	0.42
1:G:252:ARG:CZ	1:G:253:LEU:HD21	2.50	0.42
1:G:68:LEU:HD22	1:G:84:LEU:HD22	2.01	0.42
1:B:206:THR:HG23	1:B:206:THR:O	2.20	0.42
1:D:116:ASP:N	1:D:116:ASP:OD1	2.53	0.42
1:B:179:MET:O	1:B:183:MET:HG3	2.21	0.41
1:C:179:MET:HG2	1:C:221:LEU:CD1	2.46	0.41
1:D:106:PRO:HA	3:D:638:HOH:O	2.19	0.41
1:E:124:GLN:NE2	2:E:401:BNG:H6'2	2.27	0.41
1:E:67:LYS:HD3	1:E:67:LYS:C	2.41	0.41
1:F:239:VAL:N	1:F:240:PRO:CD	2.83	0.41
1:G:229:VAL:CG1	1:G:238:LEU:HD12	2.50	0.41
1:A:150:LEU:HD12	1:A:150:LEU:HA	1.66	0.41
1:B:133:THR:HA	1:B:203:LEU:HD21	2.02	0.41
1:D:38:VAL:N	1:D:39:PRO:CD	2.84	0.41
1:C:81:ARG:NH2	1:D:81:ARG:HD2	2.33	0.41
1:G:178:ALA:O	1:G:181:ILE:HB	2.20	0.41
1:H:285:ILE:HD13	1:H:320:LEU:CD1	2.50	0.41
1:H:280:VAL:HG21	1:H:299:TYR:CD2	2.54	0.41
1:B:14:ARG:NH2	1:H:192:ARG:HG3	2.35	0.41
1:E:203:LEU:HA	1:E:206:THR:CG2	2.51	0.41
1:E:258:LEU:HD23	1:E:258:LEU:HA	1.69	0.41
1:H:321:LEU:O	1:H:325:GLU:OE2	2.38	0.41
1:H:75:ASP:HB2	1:H:81:ARG:HH12	1.83	0.41
1:A:196:ARG:O	1:A:197:ASP:C	2.59	0.41
1:B:141:HIS:HB3	1:B:145:TYR:HE2	1.86	0.41
1:D:14:ARG:HG3	1:D:14:ARG:HH11	1.85	0.41
1:D:38:VAL:O	1:D:39:PRO:C	2.59	0.41
1:E:158:ALA:HA	1:E:165:GLN:CG	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:LEU:HA	1:E:187:LEU:HD23	1.83	0.41
1:G:29:THR:HA	1:G:32:LEU:CD1	2.50	0.41
1:G:61:LEU:CD1	1:G:94:ARG:HG2	2.51	0.41
1:H:19:THR:CG2	1:H:90:ARG:HG3	2.50	0.41
1:B:124:GLN:HE21	1:B:124:GLN:CA	2.08	0.41
1:B:48:ASP:OD1	1:B:48:ASP:C	2.59	0.41
2:C:502:BNG:H8'2	2:C:502:BNG:H5'2	1.75	0.41
1:F:150:LEU:HA	1:F:150:LEU:HD12	1.90	0.41
1:G:96:LEU:HD11	1:H:96:LEU:CD1	2.47	0.41
1:H:212:GLN:H	1:H:264:GLY:CA	2.33	0.41
1:B:10:ASP:O	1:B:14:ARG:HB2	2.20	0.41
1:C:107:LYS:HD3	1:C:107:LYS:O	2.21	0.41
1:B:150:LEU:HA	1:B:150:LEU:HD12	1.53	0.41
1:B:5:GLU:OE1	1:B:37:ARG:NH2	2.50	0.41
1:C:139:ARG:NH1	1:C:220:GLU:OE2	2.51	0.41
1:E:254:LEU:HD22	1:E:258:LEU:HG	2.02	0.41
2:H:502:BNG:O2	2:H:502:BNG:H1'1	2.21	0.41
1:B:269:VAL:O	1:B:279:GLU:HA	2.20	0.41
1:B:267:ALA:HB2	1:B:319:GLU:CD	2.41	0.41
1:D:212:GLN:HA	1:D:263:ALA:HB1	2.02	0.41
1:H:115:GLN:HA	1:H:115:GLN:OE1	2.20	0.41
1:H:200:LEU:O	1:H:204:MET:HE2	2.21	0.41
1:H:1:MET:SD	1:H:37:ARG:HD3	2.60	0.41
1:B:210:ALA:O	1:B:211:GLY:C	2.58	0.41
1:B:274:LYS:C	1:B:276:GLU:H	2.24	0.41
1:F:276:GLU:HB3	1:F:277:GLU:H	1.73	0.41
1:G:222:ARG:HD2	1:G:243:HIS:CE1	2.56	0.41
1:E:231:ALA:HA	1:E:232:PRO:HD3	1.84	0.41
1:G:29:THR:HA	1:G:32:LEU:HD12	2.03	0.41
1:A:11:HIS:CD2	1:A:57:ARG:HD2	2.56	0.40
1:B:281:ASP:O	1:B:283:SER:N	2.54	0.40
1:B:269:VAL:CG2	1:B:285:ILE:HD11	2.38	0.40
1:F:189:ASP:HB3	1:F:193:ASN:HD22	1.86	0.40
1:G:183:MET:HB3	1:G:183:MET:HE3	1.79	0.40
1:H:281:ASP:C	1:H:283:SER:N	2.73	0.40
1:H:72:LEU:HD21	1:H:85:ALA:CB	2.50	0.40
1:A:258:LEU:CG	1:A:258:LEU:O	2.68	0.40
1:B:133:THR:HA	1:B:203:LEU:CD2	2.51	0.40
1:D:271:PHE:HE1	1:D:280:VAL:HG23	1.86	0.40
1:E:203:LEU:HA	1:E:206:THR:HG22	2.03	0.40
1:F:183:MET:CE	1:F:218:LEU:HG	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:VAL:HG21	1:G:29:THR:HG21	2.02	0.40
1:A:258:LEU:HD11	1:F:137:GLU:OE2	2.21	0.40
1:B:200:LEU:HG	1:B:204:MET:HE1	2.02	0.40
1:C:1:MET:SD	1:C:37:ARG:CD	3.05	0.40
1:E:135:LEU:HA	1:E:135:LEU:HD12	1.65	0.40
1:F:59:LEU:O	1:F:60:ALA:C	2.58	0.40
1:G:200:LEU:HD12	1:G:200:LEU:HA	1.87	0.40
1:F:280:VAL:HG12	1:F:281:ASP:N	2.36	0.40
1:A:188:THR:HG22	1:A:190:TYR:CE1	2.56	0.40
1:C:59:LEU:O	1:C:63:ILE:HG13	2.21	0.40
1:D:229:VAL:CG2	1:D:238:LEU:HB2	2.40	0.40
1:F:19:THR:HB	1:F:87:VAL:HG22	2.03	0.40
1:F:272:LYS:HE2	1:F:272:LYS:HB3	1.69	0.40

There are no symmetry-related clashes.

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	A	262/343 (76%)	251 (96%)	10 (4%)	1 (0%)	39 74
1	B	332/343 (97%)	314 (95%)	15 (4%)	3 (1%)	21 55
1	C	263/343 (77%)	256 (97%)	7 (3%)	0	100 100
1	D	331/343 (96%)	312 (94%)	14 (4%)	5 (2%)	13 40
1	E	267/343 (78%)	258 (97%)	9 (3%)	0	100 100
1	F	330/343 (96%)	312 (94%)	14 (4%)	4 (1%)	16 47
1	G	261/343 (76%)	247 (95%)	14 (5%)	0	100 100
1	H	331/343 (96%)	312 (94%)	18 (5%)	1 (0%)	46 79
All	All	2377/2744 (87%)	2262 (95%)	101 (4%)	14 (1%)	30 65

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	263	ALA
1	F	267	ALA
1	B	262	GLY
1	B	264	GLY
1	D	262	GLY
1	D	264	GLY
1	A	197	ASP
1	D	167	ALA
1	H	266	MET
1	B	167	ALA
1	F	265	ALA
1	D	258	LEU
1	F	282	ILE
1	D	282	ILE

5.3.2 Protein sidechains

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	A	207/270 (77%)	192 (93%)	15 (7%)	18 45
1	B	262/270 (97%)	238 (91%)	24 (9%)	11 32
1	C	208/270 (77%)	192 (92%)	16 (8%)	16 41
1	D	261/270 (97%)	243 (93%)	18 (7%)	19 48
1	E	212/270 (78%)	196 (92%)	16 (8%)	17 43
1	F	260/270 (96%)	233 (90%)	27 (10%)	9 25
1	G	206/270 (76%)	188 (91%)	18 (9%)	13 35
1	H	261/270 (97%)	235 (90%)	26 (10%)	9 27
All	All	1877/2160 (87%)	1717 (92%)	160 (8%)	13 36

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	24	ASP
1	A	34	LEU
1	A	38	VAL
1	A	50	ASP
1	A	90	ARG
1	A	131	ARG
1	A	139	ARG
1	A	163	GLU
1	A	165	GLN
1	A	179	MET
1	A	191	ASP
1	A	196	ARG
1	A	197	ASP
1	A	199	ASN
1	B	-2	ASP
1	B	15	CYS
1	B	18	GLN
1	B	24	ASP
1	B	33	ARG
1	B	34	LEU
1	B	47	THR
1	B	62	ASP
1	B	90	ARG
1	B	91	LEU
1	B	104	ARG
1	B	105	ASP
1	B	124	GLN
1	B	163	GLU
1	B	181	ILE
1	B	199	ASN
1	B	206	THR
1	B	232	PRO
1	B	260	GLU
1	B	284	LYS
1	B	305	LYS
1	B	308	ARG
1	B	314	LYS
1	B	325	GLU
1	C	18	GLN
1	C	47	THR
1	C	49	PRO
1	C	90	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	107	LYS
1	C	116	ASP
1	C	131	ARG
1	C	139	ARG
1	C	163	GLU
1	C	165	GLN
1	C	179	MET
1	C	191	ASP
1	C	197	ASP
1	C	224	ARG
1	C	246	THR
1	C	258	LEU
1	D	15	CYS
1	D	18	GLN
1	D	24	ASP
1	D	67	LYS
1	D	90	ARG
1	D	124	GLN
1	D	129	ARG
1	D	131	ARG
1	D	172	GLU
1	D	189	ASP
1	D	191	ASP
1	D	197	ASP
1	D	199	ASN
1	D	206	THR
1	D	229	VAL
1	D	266	MET
1	D	284	LYS
1	D	305	LYS
1	E	10	ASP
1	E	14	ARG
1	E	15	CYS
1	E	47	THR
1	E	52	ARG
1	E	90	ARG
1	E	102	LEU
1	E	115	GLN
1	E	127	THR
1	E	128	LYS
1	E	163	GLU
1	E	172	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	179	MET
1	E	193	ASN
1	E	233	PRO
1	E	254	LEU
1	F	-3	ASP
1	F	0	LYS
1	F	1	MET
1	F	10	ASP
1	F	15	CYS
1	F	18	GLN
1	F	19	THR
1	F	24	ASP
1	F	38	VAL
1	F	88	CYS
1	F	90	ARG
1	F	104	ARG
1	F	105	ASP
1	F	131	ARG
1	F	144	THR
1	F	169	SER
1	F	179	MET
1	F	185	ASP
1	F	186	ASP
1	F	192	ARG
1	F	197	ASP
1	F	246	THR
1	F	254	LEU
1	F	260	GLU
1	F	284	LYS
1	F	300	ASP
1	F	308	ARG
1	G	38	VAL
1	G	52	ARG
1	G	56	SER
1	G	90	ARG
1	G	107	LYS
1	G	116	ASP
1	G	136	ARG
1	G	139	ARG
1	G	141	HIS
1	G	152	ARG
1	G	165	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	193	ASN
1	G	205	ARG
1	G	206	THR
1	G	218	LEU
1	G	244	LEU
1	G	254	LEU
1	G	258	LEU
1	H	-4	ASP
1	H	-3	ASP
1	H	15	CYS
1	H	18	GLN
1	H	19	THR
1	H	24	ASP
1	H	34	LEU
1	H	38	VAL
1	H	52	ARG
1	H	90	ARG
1	H	104	ARG
1	H	105	ASP
1	H	107	LYS
1	H	127	THR
1	H	131	ARG
1	H	139	ARG
1	H	144	THR
1	H	181	ILE
1	H	185	ASP
1	H	229	VAL
1	H	254	LEU
1	H	255	PRO
1	H	272	LYS
1	H	284	LYS
1	H	315	ASP
1	H	325	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	165	GLN
1	A	202	HIS
1	B	18	GLN
1	B	40	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	115	GLN
1	B	124	GLN
1	B	165	GLN
1	C	18	GLN
1	C	40	HIS
1	C	165	GLN
1	D	119	HIS
1	D	124	GLN
1	D	199	ASN
1	E	40	HIS
1	F	40	HIS
1	F	193	ASN
1	G	97	HIS
1	G	165	GLN
1	G	193	ASN
1	H	165	GLN
1	H	193	ASN

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

13 ligands are modelled in this entry.

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	$\#\|Z\|>2$
2	BNG	A	501	-	21,21,21	1.04	1 (4%)	26,26,26	0.73	1 (3%)
2	BNG	A	502	-	21,21,21	0.86	1 (4%)	26,26,26	0.93	1 (3%)
2	BNG	B	501	-	21,21,21	1.15	1 (4%)	26,26,26	0.84	1 (3%)
2	BNG	B	502	-	21,21,21	0.85	1 (4%)	26,26,26	0.92	1 (3%)
2	BNG	C	501	-	21,21,21	1.16	1 (4%)	26,26,26	0.89	1 (3%)
2	BNG	C	502	-	21,21,21	0.83	1 (4%)	26,26,26	0.76	1 (3%)
2	BNG	D	501	-	21,21,21	1.04	1 (4%)	26,26,26	0.94	2 (7%)
2	BNG	D	502	-	21,21,21	0.97	1 (4%)	26,26,26	1.65	3 (11%)
2	BNG	E	401	-	21,21,21	0.97	1 (4%)	26,26,26	0.79	1 (3%)
2	BNG	F	401	-	21,21,21	0.94	1 (4%)	26,26,26	1.44	3 (11%)
2	BNG	G	401	-	21,21,21	0.88	1 (4%)	26,26,26	0.89	1 (3%)
2	BNG	H	501	-	21,21,21	1.21	1 (4%)	26,26,26	1.04	2 (7%)
2	BNG	H	502	-	21,21,21	0.81	1 (4%)	26,26,26	0.92	2 (7%)

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
2	BNG	A	501	-	-	0/12/32/32	0/1/1/1
2	BNG	A	502	-	-	0/12/32/32	0/1/1/1
2	BNG	B	501	-	-	0/12/32/32	0/1/1/1
2	BNG	B	502	-	-	0/12/32/32	0/1/1/1
2	BNG	C	501	-	-	0/12/32/32	0/1/1/1
2	BNG	C	502	-	-	0/12/32/32	0/1/1/1
2	BNG	D	501	-	-	0/12/32/32	0/1/1/1
2	BNG	D	502	-	-	0/12/32/32	0/1/1/1
2	BNG	E	401	-	-	0/12/32/32	0/1/1/1
2	BNG	F	401	-	-	0/12/32/32	0/1/1/1
2	BNG	G	401	-	-	0/12/32/32	0/1/1/1
2	BNG	H	501	-	-	0/12/32/32	0/1/1/1
2	BNG	H	502	-	-	0/12/32/32	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	502	BNG	O1-C1'	3.12	1.51	1.42
2	F	401	BNG	O1-C1'	3.24	1.51	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	BNG	O1-C1'	3.29	1.52	1.42
2	A	502	BNG	O1-C1'	3.34	1.52	1.42
2	C	502	BNG	O1-C1'	3.35	1.52	1.42
2	B	502	BNG	O1-C1'	3.41	1.52	1.42
2	A	501	BNG	O1-C1'	3.57	1.52	1.42
2	D	502	BNG	O1-C1'	3.71	1.53	1.42
2	E	401	BNG	O1-C1'	3.87	1.53	1.42
2	D	501	BNG	O1-C1'	3.89	1.53	1.42
2	C	501	BNG	O1-C1'	4.07	1.54	1.42
2	B	501	BNG	O1-C1'	4.17	1.54	1.42
2	H	501	BNG	O1-C1'	4.22	1.54	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	502	BNG	C1'-O1-C1	-5.41	104.55	114.00
2	F	401	BNG	C1'-O1-C1	-3.72	107.50	114.00
2	B	502	BNG	C1'-O1-C1	-3.06	108.66	114.00
2	A	502	BNG	C1'-O1-C1	-3.05	108.67	114.00
2	H	501	BNG	C1'-O1-C1	-2.99	108.78	114.00
2	E	401	BNG	C1'-O1-C1	-2.92	108.90	114.00
2	G	401	BNG	C1'-O1-C1	-2.81	109.08	114.00
2	H	502	BNG	C6-C5-C4	-2.58	106.51	112.99
2	D	501	BNG	C1'-O1-C1	-2.53	109.58	114.00
2	D	502	BNG	C1-O5-C5	-2.40	109.03	113.74
2	C	502	BNG	C1'-O1-C1	-2.03	110.46	114.00
2	H	502	BNG	C3-C4-C5	2.00	113.80	110.23
2	A	501	BNG	O1-C1-C2	2.23	110.74	108.00
2	F	401	BNG	C4-C3-C2	2.63	115.62	110.79
2	B	501	BNG	O1-C1-C2	2.66	111.27	108.00
2	D	501	BNG	O1-C1-C2	2.78	111.42	108.00
2	C	501	BNG	O1-C1-C2	2.88	111.55	108.00
2	H	501	BNG	O1-C1-C2	3.47	112.28	108.00
2	F	401	BNG	C1-C2-C3	4.08	118.08	109.98
2	D	502	BNG	O1-C1-C2	4.49	113.52	108.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	BNG	3	0
2	A	502	BNG	1	0
2	B	501	BNG	1	0
2	B	502	BNG	2	0
2	C	501	BNG	4	0
2	C	502	BNG	2	0
2	D	501	BNG	4	0
2	D	502	BNG	4	0
2	E	401	BNG	2	0
2	F	401	BNG	3	0
2	G	401	BNG	2	0
2	H	501	BNG	3	0
2	H	502	BNG	5	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	A	264/343 (76%)	-0.76	3 (1%) 82 74	18, 33, 61, 89	0
1	B	334/343 (97%)	-0.43	16 (4%) 34 23	21, 41, 93, 103	0
1	C	265/343 (77%)	-0.68	4 (1%) 76 68	23, 35, 61, 92	0
1	D	333/343 (97%)	-0.40	17 (5%) 32 21	20, 44, 93, 105	0
1	E	269/343 (78%)	-0.67	3 (1%) 82 74	21, 41, 64, 98	0
1	F	332/343 (96%)	-0.36	22 (6%) 22 13	18, 38, 112, 133	0
1	G	263/343 (76%)	-0.69	0 100 100	21, 39, 57, 95	0
1	H	333/343 (97%)	-0.29	23 (6%) 20 11	19, 39, 116, 140	0
All	All	2393/2744 (87%)	-0.52	88 (3%) 45 33	18, 38, 94, 140	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	264	GLY	8.4
1	H	265	ALA	8.2
1	F	266	MET	7.3
1	F	263	ALA	5.5
1	H	266	MET	5.4
1	F	302	GLY	4.7
1	H	276	GLU	4.7
1	H	261	ALA	4.6
1	H	263	ALA	4.6
1	B	-5	VAL	4.4
1	F	264	GLY	4.3
1	F	276	GLU	4.3
1	H	303	GLY	4.3
1	H	326	LYS	4.1
1	C	193	ASN	3.9
1	H	305	LYS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	196	ARG	3.8
1	H	275	GLY	3.7
1	D	-5	VAL	3.7
1	D	193	ASN	3.7
1	H	262	GLY	3.7
1	F	303	GLY	3.7
1	D	194	GLY	3.6
1	B	193	ASN	3.6
1	F	325	GLU	3.6
1	B	194	GLY	3.6
1	H	325	GLU	3.6
1	D	303	GLY	3.5
1	D	302	GLY	3.5
1	H	327	GLN	3.5
1	H	-3	ASP	3.5
1	B	328	LYS	3.4
1	H	302	GLY	3.4
1	D	260	GLU	3.4
1	B	326	LYS	3.4
1	H	328	LYS	3.3
1	H	304	GLY	3.3
1	H	277	GLU	3.3
1	F	305	LYS	3.2
1	B	260	GLU	3.2
1	F	327	GLN	3.1
1	F	275	GLY	3.0
1	D	192	ARG	3.0
1	F	265	ALA	3.0
1	D	197	ASP	3.0
1	F	304	GLY	2.9
1	H	300	ASP	2.9
1	F	-3	ASP	2.9
1	B	303	GLY	2.8
1	F	326	LYS	2.8
1	H	267	ALA	2.8
1	F	270	LYS	2.7
1	F	328	LYS	2.7
1	E	259	GLY	2.6
1	E	-9	HIS	2.6
1	D	326	LYS	2.6
1	F	268	THR	2.6
1	F	267	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	264	GLY	2.5
1	B	192	ARG	2.5
1	B	327	GLN	2.5
1	B	300	ASP	2.5
1	A	194	GLY	2.5
1	B	304	GLY	2.5
1	D	264	GLY	2.4
1	D	304	GLY	2.4
1	B	277	GLU	2.4
1	D	325	GLU	2.4
1	H	309	GLY	2.3
1	A	196	ARG	2.3
1	D	195	GLU	2.3
1	H	-4	ASP	2.2
1	B	265	ALA	2.2
1	C	164	GLY	2.2
1	A	193	ASN	2.1
1	E	-3	ASP	2.1
1	C	196	ARG	2.1
1	F	277	GLU	2.1
1	D	265	ALA	2.1
1	B	-4	ASP	2.1
1	D	276	GLU	2.1
1	F	283	SER	2.1
1	F	260	GLU	2.1
1	F	279	GLU	2.0
1	C	-5	VAL	2.0
1	B	196	ARG	2.0
1	D	301	GLU	2.0
1	H	301	GLU	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

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
2	BNG	H	501	21/21	0.74	0.30	5.02	84,108,116,117	0
2	BNG	H	502	21/21	0.92	0.21	4.87	56,70,80,83	0
2	BNG	G	401	21/21	0.88	0.24	3.37	56,79,90,93	0
2	BNG	E	401	21/21	0.91	0.22	3.12	58,88,94,96	0
2	BNG	C	502	21/21	0.92	0.20	3.01	48,66,69,69	0
2	BNG	D	501	21/21	0.90	0.22	2.60	74,80,84,85	0
2	BNG	D	502	21/21	0.93	0.20	2.48	41,65,75,76	0
2	BNG	A	502	21/21	0.94	0.19	2.43	38,65,74,76	0
2	BNG	F	401	21/21	0.92	0.17	2.18	55,69,76,76	0
2	BNG	A	501	21/21	0.91	0.20	1.41	55,66,75,77	0
2	BNG	B	501	21/21	0.92	0.19	1.29	69,75,81,82	0
2	BNG	B	502	21/21	0.94	0.16	1.00	46,71,76,79	0
2	BNG	C	501	21/21	0.93	0.18	0.85	62,70,72,74	0

6.5 Other polymers

There are no such residues in this entry.