Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:01 AM GMT

PDB ID	:	3GLC
Title	:	Crystal Structure of E. coli LsrF in complex with Ribose-5-phosphate
Authors	:	Miller, S.T.; Diaz, Z.C.
Deposited on	:	2009-03-11
Resolution	:	2.50 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:

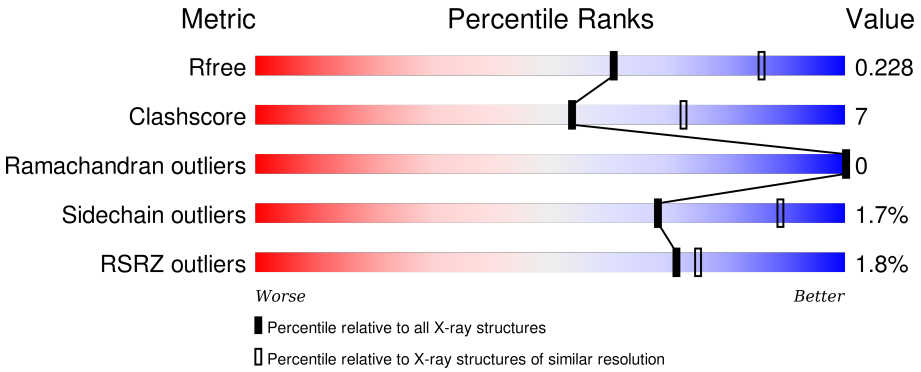
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	295	80% 13% 6%
1	B	295	83% 10% 6%
1	C	295	84% 9% 6%
1	D	295	81% 13% 6%
1	E	295	82% 11% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	295	2% 82% 12% 6%
1	G	295	81% 13% 6%
1	H	295	% 80% 13% 6%
1	I	295	2% 80% 13% 6%
1	J	295	3% 80% 13% 6%
1	K	295	% 83% 11% 6%
1	L	295	3% 82% 11% 6%
1	M	295	2% 84% 9% 6%
1	N	295	2% 80% 14% 6%
1	O	295	% 82% 11% 6%
1	P	295	3% 79% 14% 6%
1	Q	295	2% 80% 12% 6%
1	R	295	% 80% 14% 6%
1	S	295	2% 82% 11% 6%
1	T	295	2% 80% 13% 6%

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	R5P	A	400	-	-	-	X
2	R5P	B	400	-	-	-	X
2	R5P	C	400	-	-	-	X
2	R5P	D	400	-	-	-	X
2	R5P	E	400	-	-	-	X
2	R5P	G	400	-	-	-	X
2	R5P	H	400	-	-	-	X
2	R5P	I	400	-	-	-	X
2	R5P	J	400	-	-	-	X
2	R5P	K	400	-	-	-	X
2	R5P	M	400	-	-	-	X
2	R5P	N	400	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	R5P	O	400	-	-	-	X
2	R5P	P	400	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 42874 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 Aldolase lsrF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	B	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	C	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	D	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	E	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	F	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	G	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	H	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	I	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	J	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	K	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	L	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	M	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	N	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	O	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	P	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	R	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	S	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			
1	T	276	Total	C	N	O	S	0	0	0
			2113	1331	373	392	17			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P76143
A	-2	SER	-	EXPRESSION TAG	UNP P76143
A	-1	PHE	-	EXPRESSION TAG	UNP P76143
A	0	THR	-	EXPRESSION TAG	UNP P76143
B	-3	GLY	-	EXPRESSION TAG	UNP P76143
B	-2	SER	-	EXPRESSION TAG	UNP P76143
B	-1	PHE	-	EXPRESSION TAG	UNP P76143
B	0	THR	-	EXPRESSION TAG	UNP P76143
C	-3	GLY	-	EXPRESSION TAG	UNP P76143
C	-2	SER	-	EXPRESSION TAG	UNP P76143
C	-1	PHE	-	EXPRESSION TAG	UNP P76143
C	0	THR	-	EXPRESSION TAG	UNP P76143
D	-3	GLY	-	EXPRESSION TAG	UNP P76143
D	-2	SER	-	EXPRESSION TAG	UNP P76143
D	-1	PHE	-	EXPRESSION TAG	UNP P76143
D	0	THR	-	EXPRESSION TAG	UNP P76143
E	-3	GLY	-	EXPRESSION TAG	UNP P76143
E	-2	SER	-	EXPRESSION TAG	UNP P76143
E	-1	PHE	-	EXPRESSION TAG	UNP P76143
E	0	THR	-	EXPRESSION TAG	UNP P76143
F	-3	GLY	-	EXPRESSION TAG	UNP P76143
F	-2	SER	-	EXPRESSION TAG	UNP P76143
F	-1	PHE	-	EXPRESSION TAG	UNP P76143
F	0	THR	-	EXPRESSION TAG	UNP P76143
G	-3	GLY	-	EXPRESSION TAG	UNP P76143
G	-2	SER	-	EXPRESSION TAG	UNP P76143
G	-1	PHE	-	EXPRESSION TAG	UNP P76143
G	0	THR	-	EXPRESSION TAG	UNP P76143
H	-3	GLY	-	EXPRESSION TAG	UNP P76143
H	-2	SER	-	EXPRESSION TAG	UNP P76143
H	-1	PHE	-	EXPRESSION TAG	UNP P76143

Continued on next page...

Continued from previous page...

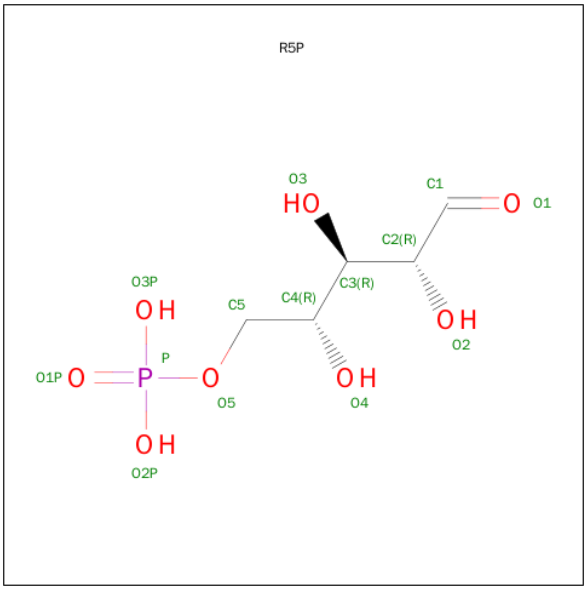
Chain	Residue	Modelled	Actual	Comment	Reference
H	0	THR	-	EXPRESSION TAG	UNP P76143
I	-3	GLY	-	EXPRESSION TAG	UNP P76143
I	-2	SER	-	EXPRESSION TAG	UNP P76143
I	-1	PHE	-	EXPRESSION TAG	UNP P76143
I	0	THR	-	EXPRESSION TAG	UNP P76143
J	-3	GLY	-	EXPRESSION TAG	UNP P76143
J	-2	SER	-	EXPRESSION TAG	UNP P76143
J	-1	PHE	-	EXPRESSION TAG	UNP P76143
J	0	THR	-	EXPRESSION TAG	UNP P76143
K	-3	GLY	-	EXPRESSION TAG	UNP P76143
K	-2	SER	-	EXPRESSION TAG	UNP P76143
K	-1	PHE	-	EXPRESSION TAG	UNP P76143
K	0	THR	-	EXPRESSION TAG	UNP P76143
L	-3	GLY	-	EXPRESSION TAG	UNP P76143
L	-2	SER	-	EXPRESSION TAG	UNP P76143
L	-1	PHE	-	EXPRESSION TAG	UNP P76143
L	0	THR	-	EXPRESSION TAG	UNP P76143
M	-3	GLY	-	EXPRESSION TAG	UNP P76143
M	-2	SER	-	EXPRESSION TAG	UNP P76143
M	-1	PHE	-	EXPRESSION TAG	UNP P76143
M	0	THR	-	EXPRESSION TAG	UNP P76143
N	-3	GLY	-	EXPRESSION TAG	UNP P76143
N	-2	SER	-	EXPRESSION TAG	UNP P76143
N	-1	PHE	-	EXPRESSION TAG	UNP P76143
N	0	THR	-	EXPRESSION TAG	UNP P76143
O	-3	GLY	-	EXPRESSION TAG	UNP P76143
O	-2	SER	-	EXPRESSION TAG	UNP P76143
O	-1	PHE	-	EXPRESSION TAG	UNP P76143
O	0	THR	-	EXPRESSION TAG	UNP P76143
P	-3	GLY	-	EXPRESSION TAG	UNP P76143
P	-2	SER	-	EXPRESSION TAG	UNP P76143
P	-1	PHE	-	EXPRESSION TAG	UNP P76143
P	0	THR	-	EXPRESSION TAG	UNP P76143
Q	-3	GLY	-	EXPRESSION TAG	UNP P76143
Q	-2	SER	-	EXPRESSION TAG	UNP P76143
Q	-1	PHE	-	EXPRESSION TAG	UNP P76143
Q	0	THR	-	EXPRESSION TAG	UNP P76143
R	-3	GLY	-	EXPRESSION TAG	UNP P76143
R	-2	SER	-	EXPRESSION TAG	UNP P76143
R	-1	PHE	-	EXPRESSION TAG	UNP P76143
R	0	THR	-	EXPRESSION TAG	UNP P76143
S	-3	GLY	-	EXPRESSION TAG	UNP P76143

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	SER	-	EXPRESSION TAG	UNP P76143
S	-1	PHE	-	EXPRESSION TAG	UNP P76143
S	0	THR	-	EXPRESSION TAG	UNP P76143
T	-3	GLY	-	EXPRESSION TAG	UNP P76143
T	-2	SER	-	EXPRESSION TAG	UNP P76143
T	-1	PHE	-	EXPRESSION TAG	UNP P76143
T	0	THR	-	EXPRESSION TAG	UNP P76143

- Molecule 2 is SUGAR (RIBOSE-5-PHOSPHATE) (three-letter code: R5P) (formula: $C_5H_{11}O_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 14 5 8 1	0	0
2	B	1	Total C O P 14 5 8 1	0	0
2	C	1	Total C O P 14 5 8 1	0	0
2	D	1	Total C O P 14 5 8 1	0	0
2	E	1	Total C O P 14 5 8 1	0	0
2	F	1	Total C O P 14 5 8 1	0	0
2	G	1	Total C O P 14 5 8 1	0	0
2	H	1	Total C O P 14 5 8 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total C O P 14 5 8 1	0	0
2	J	1	Total C O P 14 5 8 1	0	0
2	K	1	Total C O P 14 5 8 1	0	0
2	L	1	Total C O P 14 5 8 1	0	0
2	M	1	Total C O P 14 5 8 1	0	0
2	N	1	Total C O P 14 5 8 1	0	0
2	O	1	Total C O P 14 5 8 1	0	0
2	P	1	Total C O P 14 5 8 1	0	0
2	Q	1	Total C O P 14 5 8 1	0	0
2	R	1	Total C O P 14 5 8 1	0	0
2	S	1	Total C O P 14 5 8 1	0	0
2	T	1	Total C O P 14 5 8 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	15	Total O 15 15	0	0
3	B	9	Total O 9 9	0	0
3	C	16	Total O 16 16	0	0
3	D	28	Total O 28 28	0	0
3	E	23	Total O 23 23	0	0
3	F	19	Total O 19 19	0	0
3	G	11	Total O 11 11	0	0

Continued on next page...

Continued from previous page...

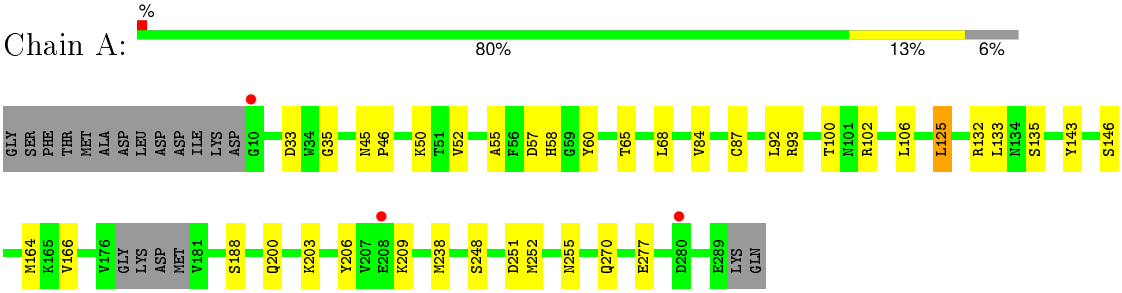
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	23	Total O 23 23	0	0
3	I	18	Total O 18 18	0	0
3	J	11	Total O 11 11	0	0
3	K	16	Total O 16 16	0	0
3	L	10	Total O 10 10	0	0
3	M	18	Total O 18 18	0	0
3	N	22	Total O 22 22	0	0
3	O	20	Total O 20 20	0	0
3	P	21	Total O 21 21	0	0
3	Q	17	Total O 17 17	0	0
3	R	13	Total O 13 13	0	0
3	S	11	Total O 11 11	0	0
3	T	13	Total O 13 13	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.

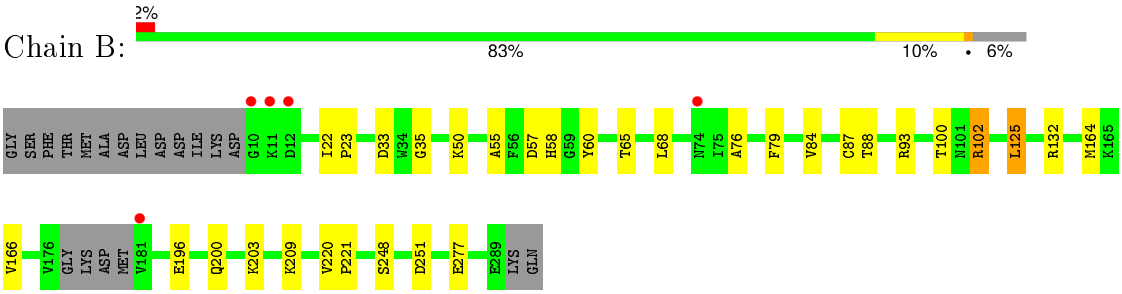
- Molecule 1: Aldolase lsrF

Chain A:



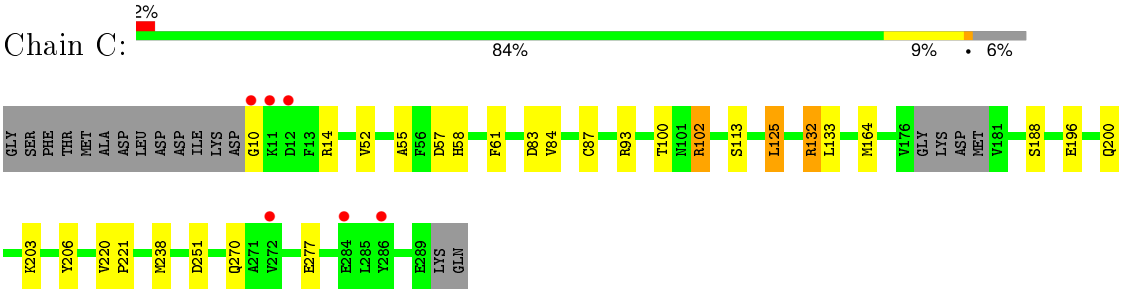
- Molecule 1: Aldolase lsrF

Chain B:



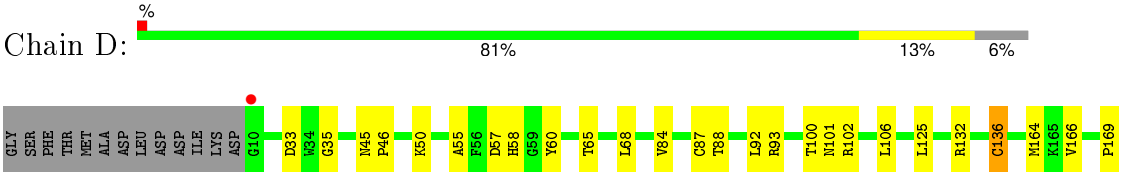
- Molecule 1: Aldolase lsrF

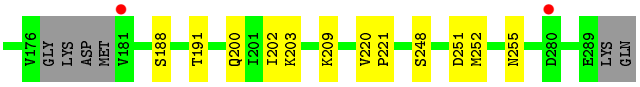
Chain C:



- Molecule 1: Aldolase lsrF

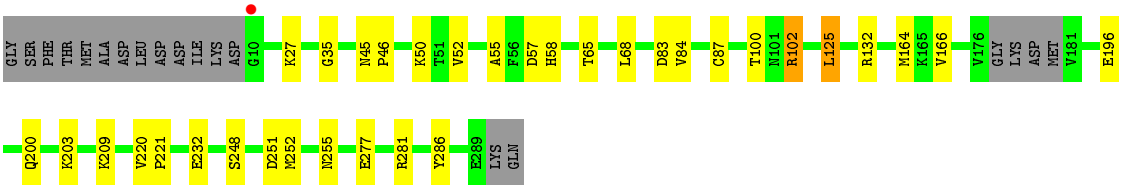
Chain D:





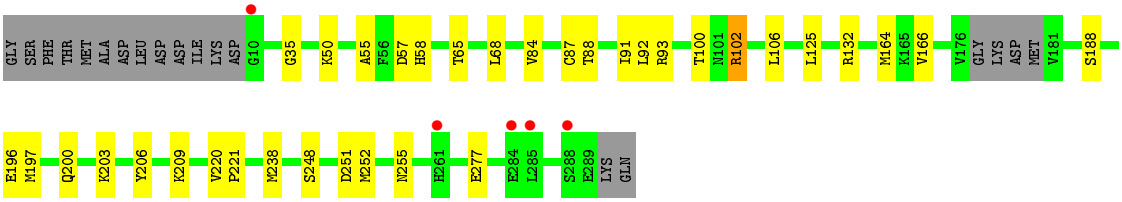
• Molecule 1: Aldolase lsrF

Chain E:



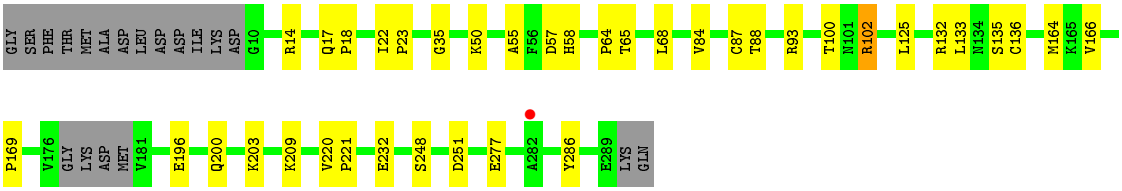
• Molecule 1: Aldolase lsrF

Chain F:



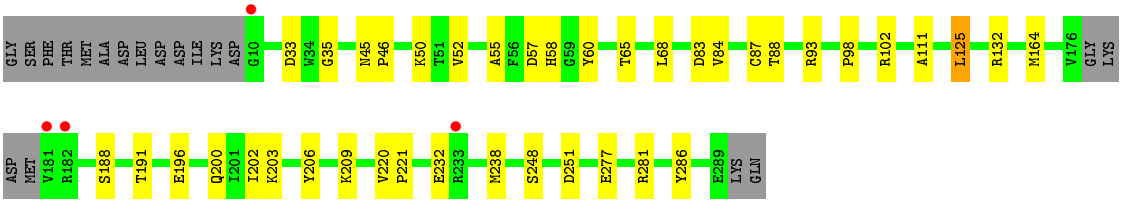
• Molecule 1: Aldolase lsrF

Chain G:



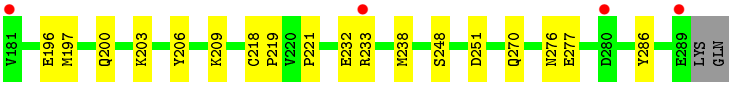
• Molecule 1: Aldolase lsrF

Chain H:



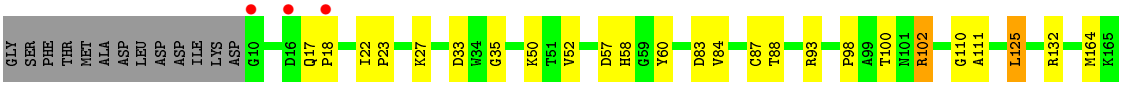
• Molecule 1: Aldolase lsrF

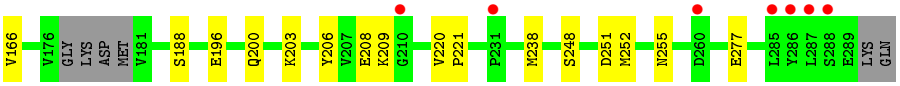
Chain I:



• Molecule 1: Aldolase lsrF

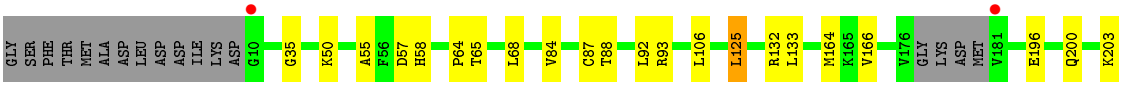
Chain J:

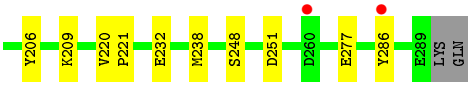




• Molecule 1: Aldolase lsrF

Chain K:



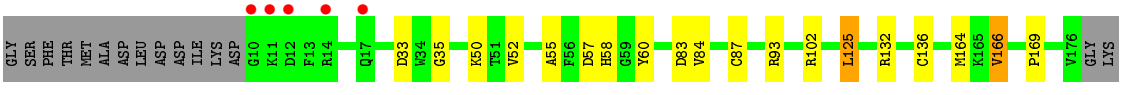


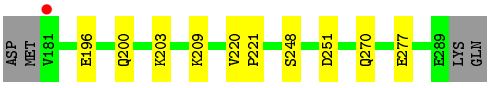
• Molecule 1: Aldolase lsrF

Chain L:

• Molecule 1: Aldolase lsrF

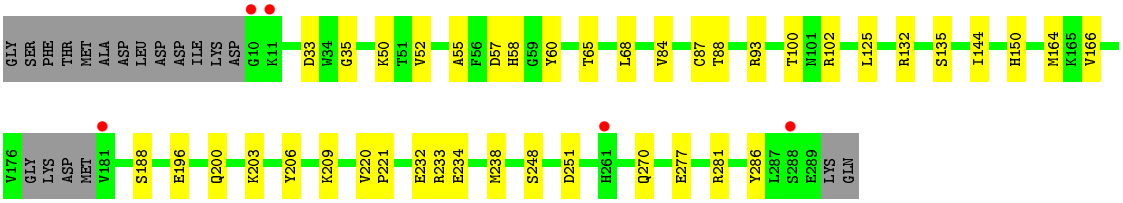
Chain M:





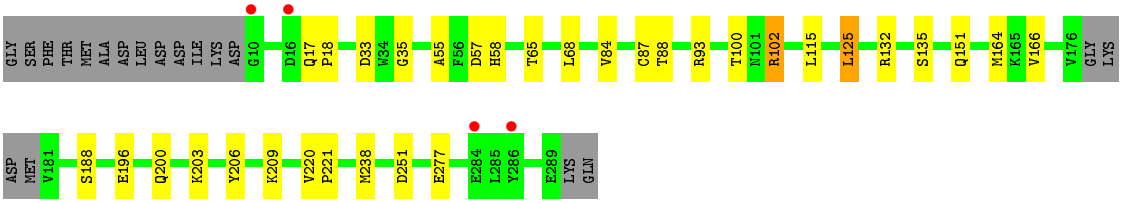
• Molecule 1: Aldolase lsrF

Chain N:



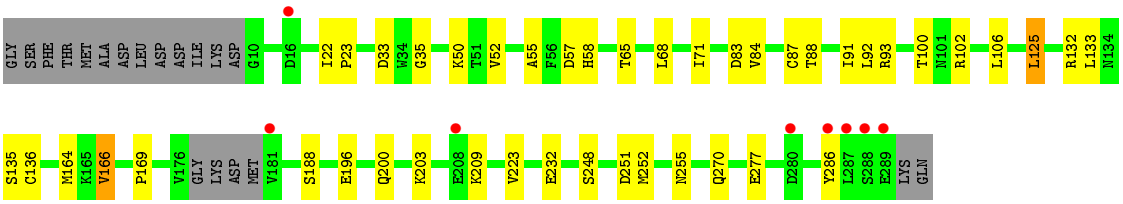
• Molecule 1: Aldolase lsrF

Chain O:



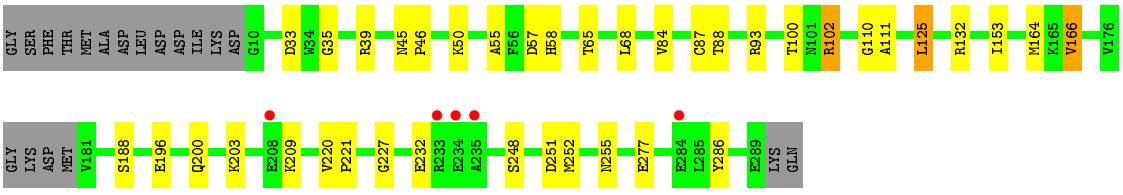
• Molecule 1: Aldolase lsrF

Chain P:



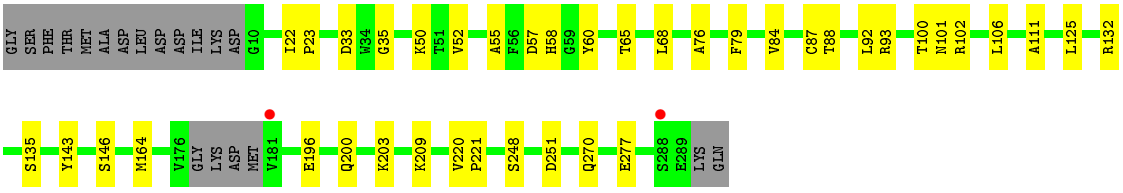
• Molecule 1: Aldolase lsrF

Chain Q:



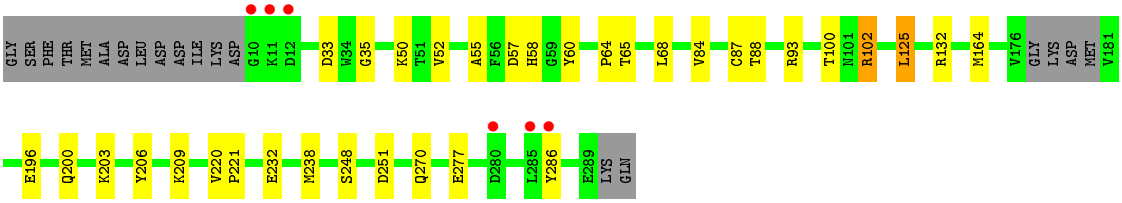
• Molecule 1: Aldolase lsrF

Chain R:

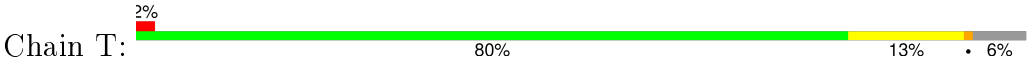


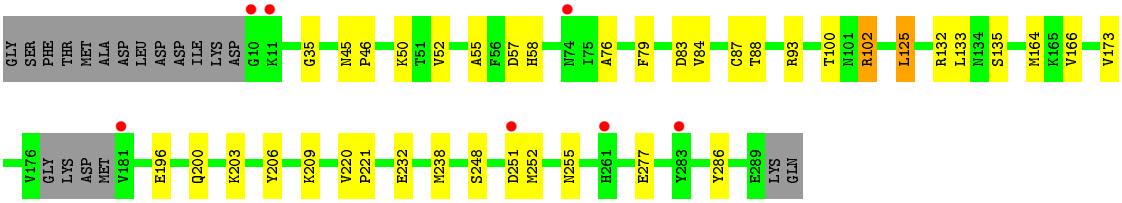
• Molecule 1: Aldolase lsrF

Chain S:



- Molecule 1: Aldolase lsrF





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.35Å 105.45Å 173.41Å 89.51° 79.79° 90.34°	Depositor
Resolution (Å)	55.73 – 2.50 39.13 – 2.50	Depositor EDS
% Data completeness (in resolution range)	67.4 (55.73-2.50) 67.3 (39.13-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.205 , 0.235 0.199 , 0.228	Depositor DCC
R_{free} test set	7743 reflections (6.39%)	DCC
Wilson B-factor (Å^2)	39.6	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.6	EDS
Estimated twinning fraction	0.025 for h,-k,h-l 0.032 for -h,k,-l 0.013 for -h,-k,-h+l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 127454 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	42874	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: R5P

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	0.69	0/2151	0.67	0/2910
1	B	0.67	0/2151	0.68	0/2910
1	C	0.65	0/2151	0.68	1/2910 (0.0%)
1	D	0.68	1/2151 (0.0%)	0.68	0/2910
1	E	0.65	0/2151	0.67	0/2910
1	F	0.67	0/2151	0.66	0/2910
1	G	0.67	0/2151	0.67	0/2910
1	H	0.68	0/2151	0.68	0/2910
1	I	0.68	0/2151	0.70	1/2910 (0.0%)
1	J	0.69	0/2151	0.66	0/2910
1	K	0.66	0/2151	0.68	0/2910
1	L	0.66	0/2151	0.66	0/2910
1	M	0.66	0/2151	0.66	0/2910
1	N	0.68	0/2151	0.68	0/2910
1	O	0.67	0/2151	0.66	0/2910
1	P	0.66	0/2151	0.67	0/2910
1	Q	0.65	0/2151	0.68	1/2910 (0.0%)
1	R	0.68	0/2151	0.67	0/2910
1	S	0.70	0/2151	0.67	0/2910
1	T	0.67	0/2151	0.67	0/2910
All	All	0.67	1/43020 (0.0%)	0.67	3/58200 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	136	CYS	CB-SG	-6.97	1.70	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	39	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	I	39	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	132	ARG	NE-CZ-NH2	-5.26	117.67	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2113	0	2122	28	0
1	B	2113	0	2122	30	0
1	C	2113	0	2122	27	0
1	D	2113	0	2122	30	0
1	E	2113	0	2122	39	0
1	F	2113	0	2122	31	0
1	G	2113	0	2122	32	1
1	H	2113	0	2122	35	0
1	I	2113	0	2122	28	2
1	J	2113	0	2122	36	0
1	K	2113	0	2122	28	0
1	L	2113	0	2122	29	0
1	M	2113	0	2122	29	0
1	N	2113	0	2122	39	1
1	O	2113	0	2122	30	0
1	P	2113	0	2122	36	0
1	Q	2113	0	2122	34	0
1	R	2113	0	2122	33	0
1	S	2113	0	2122	29	0
1	T	2113	0	2122	32	0
2	A	14	0	9	2	0
2	B	14	0	9	2	0
2	C	14	0	9	2	0
2	D	14	0	9	2	0
2	E	14	0	9	1	0
2	F	14	0	9	2	0
2	G	14	0	9	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	14	0	9	2	0
2	I	14	0	9	1	0
2	J	14	0	9	2	0
2	K	14	0	9	1	0
2	L	14	0	9	2	0
2	M	14	0	9	2	0
2	N	14	0	9	2	0
2	O	14	0	9	2	0
2	P	14	0	9	2	0
2	Q	14	0	9	3	0
2	R	14	0	9	2	0
2	S	14	0	9	2	0
2	T	14	0	9	1	0
3	A	15	0	0	0	0
3	B	9	0	0	1	0
3	C	16	0	0	1	0
3	D	28	0	0	2	0
3	E	23	0	0	1	0
3	F	19	0	0	0	0
3	G	11	0	0	0	0
3	H	23	0	0	0	0
3	I	18	0	0	0	0
3	J	11	0	0	1	0
3	K	16	0	0	0	0
3	L	10	0	0	0	0
3	M	18	0	0	0	0
3	N	22	0	0	1	0
3	O	20	0	0	1	0
3	P	21	0	0	1	0
3	Q	17	0	0	0	0
3	R	13	0	0	1	0
3	S	11	0	0	1	0
3	T	13	0	0	0	0
All	All	42874	0	42620	557	2

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 (557) 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:E:281:ARG:HD2	1:N:233:ARG:NH2	1.30	1.43
1:E:281:ARG:CD	1:N:233:ARG:HH22	1.51	1.22
1:E:281:ARG:HH12	1:N:234:GLU:HG3	1.30	0.96
1:H:164:MET:HE2	1:H:200:GLN:HE22	1.29	0.95
1:E:281:ARG:HH12	1:N:234:GLU:CG	1.79	0.95
1:F:164:MET:HE2	1:F:200:GLN:HE22	1.40	0.86
1:E:164:MET:HE2	1:E:200:GLN:HE22	1.40	0.86
1:M:164:MET:HE2	1:M:200:GLN:HE22	1.42	0.84
1:I:164:MET:HE2	1:I:200:GLN:HE22	1.42	0.83
1:S:164:MET:HE2	1:S:200:GLN:HE22	1.42	0.81
1:C:164:MET:CE	1:C:200:GLN:HE22	1.93	0.81
1:C:164:MET:HE2	1:C:200:GLN:HE22	1.47	0.80
1:H:164:MET:HE2	1:H:200:GLN:NE2	1.96	0.80
1:D:164:MET:HE2	1:D:200:GLN:HE22	1.44	0.80
1:H:164:MET:CE	1:H:200:GLN:HE22	1.94	0.79
1:R:164:MET:CE	1:R:200:GLN:HE22	1.95	0.79
1:E:281:ARG:CD	1:N:233:ARG:NH2	2.25	0.79
1:R:164:MET:HE2	1:R:200:GLN:HE22	1.47	0.79
1:E:164:MET:CE	1:E:200:GLN:HE22	1.96	0.78
1:T:164:MET:HE2	1:T:200:GLN:HE22	1.49	0.77
1:J:164:MET:HE2	1:J:200:GLN:HE22	1.48	0.77
1:N:164:MET:HE2	1:N:200:GLN:HE22	1.50	0.76
1:M:164:MET:CE	1:M:200:GLN:HE22	1.98	0.76
1:K:164:MET:CE	1:K:200:GLN:HE22	1.98	0.76
1:I:164:MET:CE	1:I:200:GLN:HE22	1.97	0.76
1:Q:164:MET:CE	1:Q:200:GLN:HE22	1.98	0.76
1:B:164:MET:HE2	1:B:200:GLN:HE22	1.49	0.75
1:F:164:MET:CE	1:F:200:GLN:HE22	1.99	0.75
1:G:164:MET:HE2	1:G:200:GLN:HE22	1.50	0.75
1:T:203:LYS:NZ	2:T:400:R5P:O4	2.19	0.75
1:L:164:MET:HE2	1:L:200:GLN:HE22	1.52	0.75
1:C:164:MET:CE	1:C:200:GLN:NE2	2.48	0.75
1:J:164:MET:CE	1:J:200:GLN:HE22	2.00	0.74
1:A:164:MET:HE2	1:A:200:GLN:HE22	1.53	0.74
1:E:125:LEU:O	1:E:125:LEU:HD12	1.88	0.73
1:K:125:LEU:O	1:K:125:LEU:HD12	1.88	0.73
1:P:164:MET:CE	1:P:200:GLN:HE22	2.01	0.73
1:S:164:MET:CE	1:S:200:GLN:HE22	2.00	0.73
1:I:203:LYS:NZ	2:I:400:R5P:O4	2.21	0.73
1:O:164:MET:HE2	1:O:200:GLN:HE22	1.53	0.73
1:B:164:MET:CE	1:B:200:GLN:HE22	2.02	0.72
1:F:125:LEU:O	1:F:125:LEU:HD12	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:125:LEU:O	1:J:125:LEU:HD12	1.90	0.72
1:N:164:MET:CE	1:N:200:GLN:HE22	2.02	0.71
1:A:164:MET:CE	1:A:200:GLN:HE22	2.04	0.71
1:D:164:MET:CE	1:D:200:GLN:HE22	2.03	0.71
1:H:164:MET:CE	1:H:200:GLN:NE2	2.53	0.71
1:F:164:MET:CE	1:F:200:GLN:NE2	2.54	0.71
1:K:164:MET:HE2	1:K:200:GLN:HE22	1.55	0.70
1:T:125:LEU:HD12	1:T:125:LEU:O	1.92	0.70
1:B:125:LEU:HD12	1:B:125:LEU:O	1.91	0.70
1:S:164:MET:HE2	1:S:200:GLN:NE2	2.06	0.70
1:L:164:MET:CE	1:L:200:GLN:HE22	2.05	0.70
1:E:164:MET:CE	1:E:200:GLN:NE2	2.54	0.70
1:C:58:HIS:CD2	1:C:58:HIS:H	2.09	0.69
1:P:164:MET:HE2	1:P:200:GLN:HE22	1.56	0.69
1:B:203:LYS:NZ	2:B:400:R5P:O4	2.22	0.69
1:D:164:MET:HE2	1:D:200:GLN:NE2	2.07	0.69
1:K:164:MET:CE	1:K:200:GLN:NE2	2.56	0.69
1:G:164:MET:CE	1:G:200:GLN:HE22	2.04	0.69
1:J:203:LYS:NZ	2:J:400:R5P:O4	2.24	0.68
1:O:125:LEU:O	1:O:125:LEU:HD12	1.93	0.68
1:M:164:MET:HE2	1:M:200:GLN:NE2	2.09	0.68
1:C:164:MET:HE2	1:C:200:GLN:NE2	2.08	0.68
1:G:203:LYS:NZ	2:G:400:R5P:O4	2.27	0.68
1:J:164:MET:CE	1:J:200:GLN:NE2	2.56	0.67
1:E:281:ARG:NH1	1:N:234:GLU:CG	2.57	0.67
1:Q:164:MET:HE2	1:Q:200:GLN:HE22	1.57	0.67
1:A:125:LEU:O	1:A:125:LEU:HD12	1.94	0.67
1:H:203:LYS:NZ	2:H:400:R5P:O4	2.26	0.67
1:F:164:MET:HE2	1:F:200:GLN:NE2	2.08	0.67
1:C:125:LEU:HD12	1:C:125:LEU:O	1.94	0.67
1:A:203:LYS:NZ	2:A:400:R5P:O4	2.26	0.67
1:T:164:MET:CE	1:T:200:GLN:HE22	2.08	0.66
1:B:164:MET:CE	1:B:200:GLN:NE2	2.59	0.66
1:R:203:LYS:NZ	2:R:400:R5P:O4	2.24	0.66
1:P:164:MET:CE	1:P:200:GLN:NE2	2.59	0.66
1:L:125:LEU:HD12	1:L:125:LEU:O	1.95	0.66
1:P:203:LYS:NZ	2:P:400:R5P:O4	2.26	0.66
1:Q:164:MET:CE	1:Q:200:GLN:NE2	2.59	0.65
1:D:164:MET:CE	1:D:200:GLN:NE2	2.59	0.65
1:E:281:ARG:NH1	1:N:234:GLU:HG3	2.07	0.65
1:O:164:MET:CE	1:O:200:GLN:HE22	2.09	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:203:LYS:NZ	2:K:400:R5P:O4	2.27	0.65
1:I:164:MET:HE2	1:I:200:GLN:NE2	2.11	0.65
1:N:164:MET:CE	1:N:200:GLN:NE2	2.60	0.65
1:R:164:MET:CE	1:R:200:GLN:NE2	2.61	0.64
1:M:203:LYS:NZ	2:M:400:R5P:O4	2.30	0.64
1:T:58:HIS:CD2	1:T:58:HIS:H	2.15	0.64
1:F:203:LYS:NZ	2:F:400:R5P:O4	2.29	0.64
1:E:203:LYS:NZ	2:E:400:R5P:O4	2.27	0.64
1:O:58:HIS:H	1:O:58:HIS:CD2	2.16	0.64
1:T:164:MET:CE	1:T:200:GLN:NE2	2.61	0.64
1:L:58:HIS:H	1:L:58:HIS:CD2	2.15	0.64
1:J:58:HIS:H	1:J:58:HIS:CD2	2.16	0.64
1:L:164:MET:CE	1:L:200:GLN:NE2	2.62	0.63
1:S:203:LYS:NZ	2:S:400:R5P:O4	2.28	0.63
1:S:164:MET:CE	1:S:200:GLN:NE2	2.61	0.63
1:M:164:MET:CE	1:M:200:GLN:NE2	2.60	0.63
1:K:58:HIS:CD2	1:K:58:HIS:H	2.15	0.63
1:O:203:LYS:NZ	2:O:400:R5P:O4	2.30	0.62
1:I:164:MET:CE	1:I:200:GLN:NE2	2.62	0.62
1:F:58:HIS:H	1:F:58:HIS:CD2	2.17	0.61
1:E:58:HIS:CD2	1:E:58:HIS:H	2.16	0.61
1:A:58:HIS:CD2	1:A:58:HIS:H	2.17	0.61
1:I:58:HIS:H	1:I:58:HIS:CD2	2.17	0.61
1:O:164:MET:CE	1:O:200:GLN:NE2	2.63	0.61
1:J:164:MET:HE2	1:J:200:GLN:NE2	2.13	0.61
1:A:164:MET:CE	1:A:200:GLN:NE2	2.63	0.61
1:S:58:HIS:CD2	1:S:58:HIS:H	2.17	0.61
1:R:58:HIS:H	1:R:58:HIS:CD2	2.19	0.60
1:H:58:HIS:H	1:H:58:HIS:CD2	2.16	0.60
1:B:132:ARG:O	1:J:35:GLY:HA3	2.02	0.60
1:M:125:LEU:HD12	1:M:125:LEU:O	2.01	0.60
1:Q:164:MET:HE2	1:Q:200:GLN:NE2	2.15	0.60
1:E:164:MET:HE2	1:E:200:GLN:NE2	2.11	0.60
1:E:35:GLY:HA3	1:G:132:ARG:O	2.01	0.59
1:Q:58:HIS:CD2	1:Q:58:HIS:H	2.20	0.59
1:D:58:HIS:CD2	1:D:58:HIS:H	2.21	0.59
1:N:58:HIS:H	1:N:58:HIS:CD2	2.18	0.59
1:M:58:HIS:CD2	1:M:58:HIS:H	2.19	0.59
1:C:203:LYS:NZ	2:C:400:R5P:O4	2.30	0.59
1:H:125:LEU:HD12	1:H:125:LEU:O	2.03	0.59
1:D:88:THR:HG21	1:E:196:GLU:HG3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:LEU:HD12	1:D:125:LEU:O	2.02	0.58
1:M:57:ASP:HB3	1:M:87:CYS:HA	1.86	0.57
1:P:58:HIS:CD2	1:P:58:HIS:H	2.21	0.57
1:E:281:ARG:HH22	1:N:234:GLU:HG2	1.70	0.57
1:G:164:MET:CE	1:G:200:GLN:NE2	2.67	0.57
1:L:203:LYS:NZ	2:L:400:R5P:O4	2.34	0.57
1:P:125:LEU:O	1:P:125:LEU:HD12	2.04	0.57
1:N:33:ASP:OD1	1:R:93:ARG:NH1	2.37	0.57
1:B:58:HIS:CD2	1:B:58:HIS:H	2.21	0.57
1:P:52:VAL:O	1:P:83:ASP:HB2	2.04	0.56
1:K:164:MET:HE2	1:K:200:GLN:NE2	2.19	0.56
1:D:33:ASP:OD1	1:H:93:ARG:NH1	2.38	0.56
1:I:57:ASP:HB3	1:I:87:CYS:HA	1.86	0.56
1:B:93:ARG:NH1	1:J:33:ASP:OD1	2.38	0.56
1:N:203:LYS:NZ	2:N:400:R5P:O4	2.32	0.56
1:N:93:ARG:NH1	1:R:33:ASP:OD1	2.38	0.56
1:N:57:ASP:HB3	1:N:87:CYS:HA	1.88	0.56
1:A:55:ALA:HB2	1:A:251:ASP:OD1	2.05	0.56
1:M:196:GLU:HG3	1:N:88:THR:HG21	1.88	0.56
1:E:55:ALA:HB2	1:E:251:ASP:OD1	2.06	0.56
1:O:164:MET:HE2	1:O:200:GLN:NE2	2.21	0.55
1:N:125:LEU:O	1:N:125:LEU:HD12	2.06	0.55
1:G:57:ASP:HB3	1:G:87:CYS:HA	1.88	0.55
1:C:164:MET:HE1	1:C:200:GLN:NE2	2.22	0.55
1:T:57:ASP:HB3	1:T:87:CYS:HA	1.89	0.55
1:A:35:GLY:HA3	1:F:132:ARG:O	2.06	0.54
1:N:164:MET:HE1	1:N:200:GLN:NE2	2.21	0.54
1:Q:55:ALA:HB2	1:Q:251:ASP:OD1	2.07	0.54
1:I:125:LEU:HD12	1:I:125:LEU:O	2.08	0.54
1:G:125:LEU:O	1:G:125:LEU:HD12	2.08	0.54
1:R:125:LEU:HD12	1:R:125:LEU:O	2.08	0.54
1:Q:196:GLU:HG2	1:R:60:TYR:HA	1.88	0.54
1:E:125:LEU:C	1:E:125:LEU:HD12	2.28	0.53
1:J:110:GLY:O	1:J:111:ALA:HB3	2.09	0.53
1:K:164:MET:HE1	1:K:200:GLN:NE2	2.22	0.53
1:C:57:ASP:HB3	1:C:87:CYS:HA	1.90	0.53
1:G:58:HIS:H	1:G:58:HIS:CD2	2.27	0.53
1:R:164:MET:HE1	1:R:200:GLN:NE2	2.24	0.53
1:B:164:MET:HE2	1:B:200:GLN:NE2	2.20	0.53
1:A:164:MET:HE1	1:A:200:GLN:NE2	2.24	0.52
1:B:125:LEU:C	1:B:125:LEU:HD12	2.29	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:MET:HE1	1:E:200:GLN:NE2	2.24	0.52
1:I:50:LYS:HA	1:I:248:SER:O	2.10	0.52
1:A:57:ASP:HB3	1:A:87:CYS:HA	1.92	0.52
1:B:35:GLY:HA3	1:J:132:ARG:O	2.08	0.52
1:A:125:LEU:C	1:A:125:LEU:HD12	2.29	0.52
1:L:57:ASP:HB3	1:L:87:CYS:HA	1.90	0.52
1:N:35:GLY:HA3	1:R:132:ARG:O	2.09	0.52
1:H:57:ASP:HB3	1:H:87:CYS:HA	1.92	0.52
1:S:57:ASP:HB3	1:S:87:CYS:HA	1.91	0.52
1:P:164:MET:HE2	1:P:200:GLN:NE2	2.22	0.52
1:F:50:LYS:HA	1:F:248:SER:O	2.10	0.52
1:K:125:LEU:C	1:K:125:LEU:HD12	2.30	0.52
1:M:196:GLU:HG2	1:N:60:TYR:HA	1.92	0.51
1:D:57:ASP:HB3	1:D:87:CYS:HA	1.93	0.51
1:Q:125:LEU:HD12	1:Q:125:LEU:O	2.10	0.51
1:P:166:VAL:HG13	1:P:166:VAL:O	2.09	0.51
1:P:164:MET:HE1	1:P:200:GLN:NE2	2.25	0.51
1:C:93:ARG:NH1	1:I:33:ASP:OD1	2.43	0.51
1:L:164:MET:HE1	1:L:200:GLN:NE2	2.26	0.51
1:K:35:GLY:HA3	1:P:132:ARG:O	2.09	0.51
1:Q:196:GLU:HG3	1:R:88:THR:HG21	1.93	0.51
1:A:277:GLU:OE1	1:A:277:GLU:HA	2.09	0.51
1:T:164:MET:HE2	1:T:200:GLN:NE2	2.20	0.51
1:B:164:MET:HE1	1:B:200:GLN:NE2	2.25	0.51
1:L:50:LYS:HA	1:L:248:SER:O	2.10	0.51
1:E:132:ARG:O	1:G:35:GLY:HA3	2.11	0.51
1:F:164:MET:HE1	1:F:200:GLN:NE2	2.26	0.51
1:N:55:ALA:HB2	1:N:251:ASP:OD1	2.10	0.51
1:R:164:MET:HE2	1:R:200:GLN:NE2	2.21	0.50
1:P:57:ASP:HB3	1:P:87:CYS:HA	1.94	0.50
1:F:100:THR:HG22	1:F:102:ARG:HB2	1.93	0.50
1:O:151:GLN:HG2	3:O:305:HOH:O	2.10	0.50
1:T:50:LYS:HA	1:T:248:SER:O	2.11	0.50
1:H:277:GLU:HA	1:H:277:GLU:OE1	2.11	0.50
1:O:220:VAL:HB	1:O:221:PRO:HD2	1.94	0.50
1:Q:50:LYS:HA	1:Q:248:SER:O	2.11	0.50
1:M:52:VAL:O	1:M:83:ASP:HB2	2.12	0.50
1:K:57:ASP:HB3	1:K:87:CYS:HA	1.94	0.50
1:L:55:ALA:HB2	1:L:251:ASP:OD1	2.11	0.50
1:J:164:MET:HE1	1:J:200:GLN:NE2	2.26	0.50
1:M:125:LEU:C	1:M:125:LEU:HD12	2.32	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:55:ALA:HB2	1:T:251:ASP:OD1	2.12	0.50
1:R:55:ALA:HB2	1:R:251:ASP:OD1	2.12	0.50
1:O:65:THR:CG2	1:O:68:LEU:HD12	2.42	0.50
1:S:50:LYS:HA	1:S:248:SER:O	2.12	0.50
1:J:100:THR:HG22	1:J:102:ARG:HB2	1.93	0.50
1:O:220:VAL:HB	1:O:221:PRO:CD	2.42	0.49
1:O:55:ALA:HB2	1:O:251:ASP:OD1	2.11	0.49
1:S:125:LEU:HD12	1:S:125:LEU:O	2.11	0.49
1:P:232:GLU:HG2	1:P:286:TYR:CZ	2.48	0.49
1:B:33:ASP:OD1	1:J:93:ARG:NH1	2.45	0.49
1:B:57:ASP:HB3	1:B:87:CYS:HA	1.95	0.49
1:M:132:ARG:O	1:S:35:GLY:HA3	2.11	0.49
1:D:203:LYS:NZ	2:D:400:R5P:O4	2.35	0.49
1:L:35:GLY:HA3	1:T:132:ARG:O	2.11	0.49
1:K:196:GLU:HG3	1:L:88:THR:HG21	1.94	0.49
1:O:277:GLU:HA	1:O:277:GLU:OE1	2.13	0.49
1:N:132:ARG:O	1:R:35:GLY:HA3	2.12	0.49
1:H:50:LYS:HA	1:H:248:SER:O	2.13	0.49
1:G:277:GLU:OE1	1:G:277:GLU:HA	2.12	0.49
1:I:125:LEU:HD12	1:I:125:LEU:C	2.33	0.49
1:K:93:ARG:NH1	1:P:33:ASP:OD1	2.46	0.49
1:Q:166:VAL:HG13	1:Q:166:VAL:O	2.12	0.49
1:G:65:THR:CG2	1:G:68:LEU:HD12	2.42	0.49
1:L:93:ARG:CZ	1:L:133:LEU:HD21	2.43	0.49
1:P:50:LYS:HA	1:P:248:SER:O	2.12	0.49
3:B:295:HOH:O	1:J:98:PRO:HD2	2.12	0.49
1:Q:277:GLU:HA	1:Q:277:GLU:OE1	2.13	0.49
1:I:52:VAL:HG21	1:I:270:GLN:HG2	1.93	0.49
1:T:164:MET:HE1	1:T:200:GLN:NE2	2.28	0.48
1:C:125:LEU:HD12	1:C:125:LEU:C	2.34	0.48
1:F:57:ASP:HB3	1:F:87:CYS:HA	1.95	0.48
1:J:125:LEU:C	1:J:125:LEU:HD12	2.33	0.48
1:P:125:LEU:HD12	1:P:125:LEU:C	2.33	0.48
1:N:150:HIS:HB3	3:N:312:HOH:O	2.13	0.48
1:P:93:ARG:CZ	1:P:133:LEU:HD21	2.43	0.48
1:A:33:ASP:OD1	1:F:93:ARG:NH1	2.45	0.48
1:N:277:GLU:OE1	1:N:277:GLU:HA	2.13	0.48
1:P:88:THR:HG21	1:T:196:GLU:HG3	1.96	0.48
1:D:136:CYS:O	1:D:169:PRO:HD2	2.13	0.48
1:S:57:ASP:OD1	2:S:400:R5P:O3	2.29	0.48
1:H:65:THR:CG2	1:H:68:LEU:HD12	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:166:VAL:CG1	1:P:166:VAL:O	2.60	0.48
1:R:100:THR:HG22	1:R:102:ARG:HB2	1.96	0.48
1:Q:232:GLU:HG2	1:Q:286:TYR:CZ	2.49	0.48
1:B:88:THR:HG21	1:C:196:GLU:HG3	1.96	0.48
1:O:57:ASP:HB3	1:O:87:CYS:HA	1.96	0.48
1:G:220:VAL:HB	1:G:221:PRO:CD	2.44	0.48
1:J:57:ASP:HB3	1:J:87:CYS:HA	1.95	0.48
1:Q:220:VAL:HB	1:Q:221:PRO:HD2	1.95	0.48
1:T:220:VAL:HB	1:T:221:PRO:CD	2.44	0.48
1:S:100:THR:HG22	1:S:102:ARG:HB2	1.95	0.47
1:E:220:VAL:HB	1:E:221:PRO:HD2	1.96	0.47
1:E:50:LYS:HA	1:E:248:SER:O	2.14	0.47
1:C:55:ALA:HB2	1:C:251:ASP:OD1	2.13	0.47
1:E:277:GLU:OE1	1:E:277:GLU:HA	2.14	0.47
1:R:277:GLU:OE1	1:R:277:GLU:HA	2.13	0.47
1:G:232:GLU:HG2	1:G:286:TYR:CZ	2.50	0.47
1:O:35:GLY:HA3	1:Q:132:ARG:O	2.14	0.47
1:K:209:LYS:HE3	1:K:209:LYS:HB2	1.68	0.47
1:T:52:VAL:O	1:T:83:ASP:HB2	2.14	0.47
1:F:125:LEU:C	1:F:125:LEU:HD12	2.34	0.47
1:E:166:VAL:HG13	1:E:166:VAL:O	2.14	0.47
1:H:88:THR:HG21	1:I:196:GLU:HG3	1.96	0.47
1:G:164:MET:HE1	1:G:200:GLN:NE2	2.29	0.47
1:K:55:ALA:HB2	1:K:251:ASP:OD1	2.15	0.47
1:O:209:LYS:HE3	1:O:209:LYS:HB2	1.70	0.47
1:B:50:LYS:HA	1:B:248:SER:O	2.14	0.47
1:N:65:THR:CG2	1:N:68:LEU:HD12	2.45	0.47
1:T:206:TYR:HB3	1:T:238:MET:CE	2.44	0.47
1:E:57:ASP:HB3	1:E:87:CYS:HA	1.96	0.47
1:E:102:ARG:NH1	3:E:306:HOH:O	2.48	0.47
1:K:88:THR:OG1	1:O:196:GLU:HG3	2.14	0.47
1:C:100:THR:HG22	1:C:102:ARG:HB2	1.95	0.47
1:D:125:LEU:HD12	1:D:125:LEU:C	2.36	0.47
1:Q:100:THR:HG22	1:Q:102:ARG:HB2	1.97	0.47
1:S:232:GLU:HG2	1:S:286:TYR:CZ	2.50	0.47
1:D:132:ARG:O	1:H:35:GLY:HA3	2.15	0.47
1:S:65:THR:CG2	1:S:68:LEU:HD12	2.45	0.46
1:R:50:LYS:HA	1:R:248:SER:O	2.14	0.46
1:C:52:VAL:O	1:C:83:ASP:HB2	2.15	0.46
1:C:57:ASP:OD1	2:C:400:R5P:O3	2.30	0.46
1:T:277:GLU:HA	1:T:277:GLU:OE1	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:232:GLU:HG2	1:H:286:TYR:CZ	2.50	0.46
1:T:252:MET:HG2	1:T:255:ASN:HB2	1.97	0.46
1:K:206:TYR:HB3	1:K:238:MET:CE	2.46	0.46
1:M:55:ALA:HB2	1:M:251:ASP:OD1	2.16	0.46
1:M:220:VAL:HB	1:M:221:PRO:CD	2.45	0.46
1:I:206:TYR:HB3	1:I:238:MET:CE	2.45	0.46
1:M:277:GLU:HA	1:M:277:GLU:OE1	2.16	0.46
1:M:50:LYS:HA	1:M:248:SER:O	2.15	0.46
1:F:209:LYS:HB2	1:F:209:LYS:HE3	1.67	0.46
1:G:209:LYS:HB2	1:G:209:LYS:HE3	1.69	0.46
1:H:52:VAL:O	1:H:83:ASP:HB2	2.15	0.46
1:O:164:MET:HE1	1:O:200:GLN:NE2	2.31	0.46
1:M:93:ARG:NH1	1:S:33:ASP:OD1	2.49	0.46
1:E:65:THR:CG2	1:E:68:LEU:HD12	2.45	0.46
1:J:27:LYS:O	1:J:221:PRO:HD3	2.15	0.46
1:P:92:LEU:HD22	1:P:106:LEU:HD21	1.97	0.46
1:L:92:LEU:HD22	1:L:106:LEU:HD21	1.97	0.46
1:D:252:MET:HG2	1:D:255:ASN:HB2	1.97	0.46
1:S:55:ALA:HB2	1:S:251:ASP:OD1	2.15	0.46
1:M:35:GLY:HA3	1:S:132:ARG:O	2.15	0.46
1:G:100:THR:HG22	1:G:102:ARG:HB2	1.97	0.46
1:G:88:THR:OG1	1:H:196:GLU:HG3	2.16	0.46
1:B:57:ASP:OD1	2:B:400:R5P:O3	2.32	0.46
1:R:57:ASP:HB3	1:R:87:CYS:HA	1.98	0.46
1:R:92:LEU:HD22	1:R:106:LEU:HD21	1.97	0.46
1:G:50:LYS:HA	1:G:248:SER:O	2.16	0.46
1:O:132:ARG:O	1:Q:35:GLY:HA3	2.16	0.46
1:A:143:TYR:HB3	1:A:146:SER:HB2	1.98	0.46
1:P:100:THR:HG22	1:P:102:ARG:HB2	1.97	0.46
1:L:57:ASP:OD1	2:L:400:R5P:O3	2.29	0.46
1:D:191:THR:HG22	1:D:202:ILE:HG21	1.97	0.46
1:G:55:ALA:HB2	1:G:251:ASP:OD1	2.16	0.46
1:I:93:ARG:CZ	1:I:133:LEU:HD21	2.45	0.46
1:R:65:THR:CG2	1:R:68:LEU:HD12	2.46	0.46
1:N:232:GLU:HG2	1:N:286:TYR:CZ	2.51	0.46
1:B:88:THR:OG1	1:C:196:GLU:HG3	2.16	0.45
1:L:132:ARG:O	1:T:35:GLY:HA3	2.15	0.45
1:E:281:ARG:NH2	1:N:234:GLU:HG2	2.30	0.45
1:R:220:VAL:HB	1:R:221:PRO:CD	2.45	0.45
1:D:35:GLY:HA3	1:H:132:ARG:O	2.15	0.45
1:H:57:ASP:OD1	2:H:400:R5P:O3	2.28	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:206:TYR:HB3	1:J:238:MET:CE	2.47	0.45
1:Q:209:LYS:HE3	1:Q:209:LYS:HB2	1.74	0.45
1:S:209:LYS:HE3	1:S:209:LYS:HB2	1.73	0.45
1:Q:220:VAL:HB	1:Q:221:PRO:CD	2.47	0.45
1:R:57:ASP:OD1	2:R:400:R5P:O3	2.28	0.45
1:P:88:THR:OG1	1:T:196:GLU:HG3	2.16	0.45
1:P:65:THR:CG2	1:P:68:LEU:HD12	2.46	0.45
1:R:52:VAL:HG21	1:R:270:GLN:HG2	1.98	0.45
1:N:50:LYS:HA	1:N:248:SER:O	2.17	0.45
1:J:277:GLU:OE1	1:J:277:GLU:HA	2.16	0.45
1:B:76:ALA:HA	1:B:79:PHE:CE2	2.52	0.45
1:E:52:VAL:O	1:E:83:ASP:HB2	2.17	0.45
1:T:209:LYS:HE3	1:T:209:LYS:HB2	1.66	0.45
1:D:220:VAL:HB	1:D:221:PRO:CD	2.46	0.45
1:K:65:THR:CG2	1:K:68:LEU:HD12	2.47	0.45
1:Q:57:ASP:HB3	1:Q:87:CYS:HA	1.98	0.45
1:C:10:GLY:N	3:C:299:HOH:O	2.49	0.45
1:L:125:LEU:HD12	1:L:125:LEU:C	2.36	0.45
1:H:281:ARG:NH1	1:M:277:GLU:OE2	2.50	0.45
1:Q:203:LYS:NZ	2:Q:400:R5P:O4	2.35	0.45
1:B:65:THR:CG2	1:B:68:LEU:HD12	2.47	0.45
1:Q:65:THR:CG2	1:Q:68:LEU:HD12	2.47	0.45
1:C:132:ARG:O	1:I:35:GLY:HA3	2.17	0.45
1:M:209:LYS:HE3	1:M:209:LYS:HB2	1.66	0.45
1:P:55:ALA:HB2	1:P:251:ASP:OD1	2.16	0.45
1:D:93:ARG:NH1	1:H:33:ASP:OD1	2.50	0.44
1:Q:166:VAL:O	1:Q:166:VAL:CG1	2.64	0.44
1:N:206:TYR:HB3	1:N:238:MET:CE	2.47	0.44
1:O:206:TYR:HB3	1:O:238:MET:CE	2.47	0.44
1:H:220:VAL:HB	1:H:221:PRO:CD	2.47	0.44
1:D:100:THR:HG22	1:D:102:ARG:HB2	2.00	0.44
1:L:164:MET:HE2	1:L:200:GLN:NE2	2.23	0.44
1:F:196:GLU:HG2	1:J:60:TYR:HA	2.00	0.44
1:K:232:GLU:HG2	1:K:286:TYR:CZ	2.52	0.44
1:S:125:LEU:HD12	1:S:125:LEU:C	2.38	0.44
1:G:220:VAL:HB	1:G:221:PRO:HD2	2.00	0.44
1:G:88:THR:HG21	1:H:196:GLU:HG3	1.98	0.44
1:Q:57:ASP:OD1	2:Q:400:R5P:O3	2.30	0.44
1:F:206:TYR:HB3	1:F:238:MET:CE	2.47	0.44
1:O:125:LEU:HD12	1:O:125:LEU:C	2.38	0.44
1:H:125:LEU:HD12	1:H:125:LEU:C	2.37	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:101:ASN:HA	3:R:302:HOH:O	2.17	0.44
1:T:125:LEU:HD12	1:T:125:LEU:C	2.37	0.44
1:D:65:THR:CG2	1:D:68:LEU:HD12	2.48	0.44
1:S:277:GLU:OE1	1:S:277:GLU:HA	2.16	0.44
1:E:209:LYS:HE3	1:E:209:LYS:HB2	1.74	0.44
1:J:50:LYS:HA	1:J:248:SER:O	2.18	0.44
1:K:220:VAL:HB	1:K:221:PRO:CD	2.47	0.44
1:K:132:ARG:O	1:P:35:GLY:HA3	2.17	0.44
1:H:191:THR:HG22	1:H:202:ILE:HG21	2.00	0.44
1:C:277:GLU:OE1	1:C:277:GLU:HA	2.17	0.44
1:E:27:LYS:O	1:E:221:PRO:HD3	2.18	0.44
1:S:52:VAL:HG21	1:S:270:GLN:HG2	2.00	0.44
1:E:166:VAL:CG1	1:E:166:VAL:O	2.64	0.44
1:C:52:VAL:HG21	1:C:270:GLN:HG2	2.00	0.44
1:B:277:GLU:HA	1:B:277:GLU:OE1	2.18	0.44
1:A:209:LYS:HE3	1:A:209:LYS:HB2	1.66	0.44
1:K:196:GLU:HG3	1:L:88:THR:OG1	2.18	0.43
1:T:220:VAL:HB	1:T:221:PRO:HD2	1.99	0.43
1:T:206:TYR:HB3	1:T:238:MET:HE3	1.99	0.43
1:N:196:GLU:HG3	1:O:88:THR:HG21	1.98	0.43
1:I:55:ALA:HB2	1:I:251:ASP:OD1	2.19	0.43
1:A:60:TYR:HA	1:B:196:GLU:HG2	1.99	0.43
1:L:277:GLU:HA	1:L:277:GLU:OE1	2.17	0.43
1:D:57:ASP:OD1	2:D:400:R5P:O3	2.31	0.43
1:S:196:GLU:HG3	1:T:88:THR:HG21	2.00	0.43
1:A:45:ASN:HA	1:A:46:PRO:HD3	1.88	0.43
1:A:52:VAL:HG21	1:A:270:GLN:HG2	2.00	0.43
1:G:136:CYS:O	1:G:169:PRO:HD2	2.18	0.43
1:D:45:ASN:HA	1:D:46:PRO:HD3	1.93	0.43
1:L:33:ASP:OD1	1:T:93:ARG:NH1	2.51	0.43
1:G:125:LEU:HD12	1:G:125:LEU:C	2.39	0.43
1:M:220:VAL:HB	1:M:221:PRO:HD2	2.01	0.43
1:M:33:ASP:OD1	1:S:93:ARG:NH1	2.52	0.43
1:J:52:VAL:O	1:J:83:ASP:HB2	2.18	0.43
1:E:252:MET:HG2	1:E:255:ASN:HB2	2.01	0.43
1:F:220:VAL:HB	1:F:221:PRO:CD	2.48	0.43
1:I:209:LYS:HB2	1:I:209:LYS:HE3	1.62	0.43
1:J:209:LYS:HB2	1:J:209:LYS:HE3	1.67	0.43
1:K:50:LYS:HA	1:K:248:SER:O	2.18	0.43
1:A:206:TYR:HB3	1:A:238:MET:CE	2.49	0.43
1:H:220:VAL:HB	1:H:221:PRO:HD2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:33:ASP:OD1	1:Q:93:ARG:NH1	2.52	0.43
1:A:50:LYS:HA	1:A:248:SER:O	2.18	0.43
1:B:166:VAL:HG13	1:B:166:VAL:O	2.19	0.43
1:G:93:ARG:CZ	1:G:133:LEU:HD21	2.48	0.43
1:O:57:ASP:OD1	2:O:400:R5P:O3	2.35	0.43
1:I:232:GLU:HG2	1:I:286:TYR:CZ	2.54	0.43
1:P:277:GLU:OE1	1:P:277:GLU:HA	2.18	0.43
1:D:209:LYS:HB2	1:D:209:LYS:HE3	1.63	0.43
1:N:164:MET:HE2	1:N:200:GLN:NE2	2.23	0.43
1:Q:164:MET:HE1	1:Q:200:GLN:NE2	2.34	0.43
1:P:52:VAL:HG21	1:P:270:GLN:HG2	2.01	0.43
1:M:52:VAL:HG21	1:M:270:GLN:HG2	2.01	0.43
1:L:52:VAL:HG21	1:L:270:GLN:HG2	1.99	0.43
1:J:252:MET:HG2	1:J:255:ASN:HB2	2.00	0.43
1:L:220:VAL:HB	1:L:221:PRO:CD	2.49	0.43
1:A:93:ARG:CZ	1:A:133:LEU:HD21	2.49	0.43
1:E:220:VAL:HB	1:E:221:PRO:CD	2.49	0.42
1:C:220:VAL:HB	1:C:221:PRO:CD	2.48	0.42
1:L:65:THR:CG2	1:L:68:LEU:HD12	2.49	0.42
1:P:196:GLU:HG3	1:Q:88:THR:OG1	2.18	0.42
1:A:65:THR:CG2	1:A:68:LEU:HD12	2.48	0.42
1:L:209:LYS:HE3	1:L:209:LYS:HB2	1.64	0.42
1:B:60:TYR:HA	1:C:196:GLU:HG2	2.01	0.42
1:B:22:ILE:HA	1:B:23:PRO:HD3	1.94	0.42
1:F:65:THR:CG2	1:F:68:LEU:HD12	2.49	0.42
1:J:17:GLN:HA	1:J:18:PRO:HD3	1.94	0.42
1:B:220:VAL:HB	1:B:221:PRO:CD	2.49	0.42
1:H:60:TYR:HA	1:I:196:GLU:HG2	2.01	0.42
1:A:100:THR:HG22	1:A:102:ARG:HB2	2.01	0.42
1:S:206:TYR:HB3	1:S:238:MET:CE	2.49	0.42
1:G:64:PRO:HG2	1:H:188:SER:HB3	2.01	0.42
1:H:251:ASP:C	1:H:251:ASP:OD1	2.58	0.42
1:Q:252:MET:HG2	1:Q:255:ASN:HB2	2.02	0.42
1:N:57:ASP:OD1	2:N:400:R5P:O3	2.31	0.42
1:J:251:ASP:C	1:J:251:ASP:OD1	2.57	0.42
1:A:132:ARG:O	1:F:35:GLY:HA3	2.18	0.42
1:K:206:TYR:HB3	1:K:238:MET:HE2	2.02	0.42
1:B:209:LYS:HE3	1:B:209:LYS:HB2	1.69	0.42
1:I:88:THR:OG1	1:J:196:GLU:HG3	2.18	0.42
1:M:166:VAL:O	1:M:166:VAL:CG1	2.67	0.42
1:J:166:VAL:O	1:J:166:VAL:HG13	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:144:ILE:HG22	1:O:115:LEU:HD12	2.02	0.42
1:D:251:ASP:OD1	1:D:251:ASP:C	2.58	0.42
1:D:55:ALA:HB2	1:D:251:ASP:OD1	2.18	0.42
1:G:57:ASP:OD1	2:G:400:R5P:O3	2.35	0.42
1:P:203:LYS:HA	1:P:223:VAL:O	2.20	0.42
1:K:92:LEU:HD22	1:K:106:LEU:HD21	2.02	0.42
1:N:220:VAL:HB	1:N:221:PRO:CD	2.50	0.42
1:Q:125:LEU:C	1:Q:125:LEU:HD12	2.40	0.42
1:C:93:ARG:CZ	1:C:133:LEU:HD21	2.50	0.42
1:H:55:ALA:HB2	1:H:251:ASP:OD1	2.20	0.42
1:I:218:CYS:HA	1:I:219:PRO:HD3	1.96	0.42
1:Q:110:GLY:O	1:Q:111:ALA:HB3	2.19	0.42
1:K:277:GLU:HA	1:K:277:GLU:OE1	2.18	0.42
1:P:209:LYS:HE3	1:P:209:LYS:HB2	1.73	0.42
1:P:57:ASP:OD1	2:P:400:R5P:O3	2.32	0.42
1:G:102:ARG:HA	1:G:102:ARG:HD3	1.88	0.42
1:J:22:ILE:HA	1:J:23:PRO:HD3	1.93	0.42
1:H:45:ASN:HA	1:H:46:PRO:HD3	1.94	0.42
1:R:209:LYS:HB2	1:R:209:LYS:HE3	1.73	0.42
1:M:166:VAL:O	1:M:166:VAL:HG13	2.19	0.41
1:N:52:VAL:HG21	1:N:270:GLN:HG2	2.01	0.41
1:F:277:GLU:OE1	1:F:277:GLU:HA	2.20	0.41
3:D:297:HOH:O	1:H:98:PRO:HD2	2.20	0.41
1:A:164:MET:HE2	1:A:200:GLN:NE2	2.25	0.41
1:J:57:ASP:OD1	2:J:400:R5P:O3	2.34	0.41
1:F:197:MET:HE3	1:J:111:ALA:H	1.86	0.41
1:R:196:GLU:HG3	1:S:88:THR:HG21	2.02	0.41
1:P:252:MET:HG2	1:P:255:ASN:HB2	2.03	0.41
1:Q:153:ILE:HG21	1:R:111:ALA:HA	2.02	0.41
1:N:209:LYS:HE3	1:N:209:LYS:HB2	1.67	0.41
1:I:277:GLU:OE1	1:I:277:GLU:HA	2.19	0.41
1:T:93:ARG:CZ	1:T:133:LEU:HD21	2.50	0.41
1:E:45:ASN:HA	1:E:46:PRO:HD3	1.91	0.41
1:O:93:ARG:NH1	1:Q:33:ASP:OD1	2.54	0.41
1:F:55:ALA:HB2	1:F:251:ASP:OD1	2.20	0.41
1:F:206:TYR:HB3	1:F:238:MET:HE2	2.02	0.41
1:S:220:VAL:HB	1:S:221:PRO:CD	2.50	0.41
1:N:100:THR:HG22	1:N:102:ARG:HB2	2.02	0.41
1:C:14:ARG:HE	1:C:14:ARG:HB3	1.53	0.41
1:A:92:LEU:HD22	1:A:106:LEU:HD21	2.01	0.41
1:T:173:VAL:HG13	1:T:203:LYS:HD2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:125:LEU:C	1:N:125:LEU:HD12	2.40	0.41
1:E:100:THR:HG22	1:E:102:ARG:HB2	2.03	0.41
1:J:220:VAL:HB	1:J:221:PRO:HD2	2.02	0.41
1:P:71:ILE:HG12	3:P:311:HOH:O	2.20	0.41
1:G:22:ILE:HA	1:G:23:PRO:HD3	1.95	0.41
1:P:91:ILE:HD13	1:P:91:ILE:HA	1.91	0.41
1:Q:45:ASN:HA	1:Q:46:PRO:HD3	1.92	0.41
1:P:136:CYS:O	1:P:169:PRO:HD2	2.21	0.41
1:T:45:ASN:HA	1:T:46:PRO:HD3	1.92	0.41
1:L:196:GLU:HG2	1:M:60:TYR:HA	2.02	0.41
1:P:22:ILE:HA	1:P:23:PRO:HD3	1.97	0.41
1:F:91:ILE:HD13	1:F:91:ILE:HA	1.88	0.41
1:D:101:ASN:HA	3:D:318:HOH:O	2.20	0.41
1:H:209:LYS:HE3	1:H:209:LYS:HB2	1.60	0.41
1:T:232:GLU:HG2	1:T:286:TYR:CZ	2.56	0.41
1:I:206:TYR:HB3	1:I:238:MET:HE2	2.02	0.41
1:M:136:CYS:O	1:M:169:PRO:HD2	2.21	0.41
1:I:27:LYS:O	1:I:221:PRO:HD3	2.21	0.41
1:G:166:VAL:O	1:G:166:VAL:HG13	2.20	0.41
1:T:76:ALA:HA	1:T:79:PHE:CE2	2.56	0.41
1:G:14:ARG:HE	1:G:14:ARG:HB3	1.50	0.41
1:R:22:ILE:HA	1:R:23:PRO:HD3	1.92	0.41
1:D:60:TYR:HA	1:E:196:GLU:HG2	2.03	0.41
1:L:220:VAL:HB	1:L:221:PRO:HD2	2.02	0.41
1:I:143:TYR:HB3	1:I:146:SER:HB2	2.03	0.41
1:C:206:TYR:HB3	1:C:238:MET:CE	2.51	0.41
1:B:251:ASP:OD1	1:B:251:ASP:C	2.58	0.41
1:R:143:TYR:HB3	1:R:146:SER:HB2	2.03	0.41
1:O:100:THR:HG22	1:O:102:ARG:HB2	2.01	0.41
1:D:50:LYS:HA	1:D:248:SER:O	2.21	0.41
1:O:17:GLN:HA	1:O:18:PRO:HD3	1.93	0.41
1:H:111:ALA:H	1:I:197:MET:HE3	1.86	0.41
1:S:200:GLN:NE2	3:S:299:HOH:O	2.54	0.41
1:M:57:ASP:OD1	2:M:400:R5P:O3	2.36	0.41
1:B:55:ALA:HB2	1:B:251:ASP:OD1	2.21	0.41
1:J:208:GLU:HG2	3:J:301:HOH:O	2.21	0.41
1:H:206:TYR:HB3	1:H:238:MET:CE	2.51	0.41
1:F:252:MET:HG2	1:F:255:ASN:HB2	2.03	0.41
1:C:61:PHE:HB2	1:C:113:SER:HA	2.03	0.41
1:A:57:ASP:OD1	2:A:400:R5P:O3	2.31	0.40
1:K:93:ARG:CZ	1:K:133:LEU:HD21	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:GLU:HG3	1:J:88:THR:OG1	2.22	0.40
1:D:92:LEU:HD22	1:D:106:LEU:HD21	2.03	0.40
1:I:22:ILE:HA	1:I:23:PRO:HD3	1.98	0.40
1:E:232:GLU:HG2	1:E:286:TYR:CZ	2.56	0.40
1:J:58:HIS:N	1:J:58:HIS:CD2	2.87	0.40
1:S:251:ASP:C	1:S:251:ASP:OD1	2.59	0.40
1:D:220:VAL:HB	1:D:221:PRO:HD2	2.03	0.40
1:Q:227:GLY:N	2:Q:400:R5P:O1P	2.53	0.40
1:A:252:MET:HG2	1:A:255:ASN:HB2	2.03	0.40
1:L:206:TYR:HB3	1:L:238:MET:CE	2.51	0.40
1:O:166:VAL:O	1:O:166:VAL:HG13	2.21	0.40
1:F:92:LEU:HD22	1:F:106:LEU:HD21	2.03	0.40
1:F:57:ASP:OD1	2:F:400:R5P:O3	2.32	0.40
1:K:88:THR:HG21	1:O:196:GLU:HG3	2.02	0.40
1:R:220:VAL:HB	1:R:221:PRO:HD2	2.03	0.40
1:F:220:VAL:HB	1:F:221:PRO:HD2	2.02	0.40
1:F:88:THR:OG1	1:G:196:GLU:HG3	2.21	0.40
1:B:100:THR:HG22	1:B:102:ARG:HB2	2.02	0.40
1:R:196:GLU:HG2	1:S:60:TYR:HA	2.03	0.40
1:G:17:GLN:HA	1:G:18:PRO:HD3	1.95	0.40
1:R:76:ALA:HA	1:R:79:PHE:CE2	2.57	0.40
1:T:100:THR:HG22	1:T:102:ARG:HB2	2.03	0.40
1:L:232:GLU:HG2	1:L:286:TYR:CZ	2.56	0.40

All (2) 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:I:276:ASN:ND2	1:N:281:ARG:NH1[1_565]	2.06	0.14
1:G:277:GLU:OE1	1:I:233:ARG:NH2[1_545]	2.16	0.04

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	272/295 (92%)	264 (97%)	8 (3%)	0	100	100
1	B	272/295 (92%)	262 (96%)	10 (4%)	0	100	100
1	C	272/295 (92%)	263 (97%)	9 (3%)	0	100	100
1	D	272/295 (92%)	262 (96%)	10 (4%)	0	100	100
1	E	272/295 (92%)	264 (97%)	8 (3%)	0	100	100
1	F	272/295 (92%)	265 (97%)	7 (3%)	0	100	100
1	G	272/295 (92%)	264 (97%)	8 (3%)	0	100	100
1	H	272/295 (92%)	264 (97%)	8 (3%)	0	100	100
1	I	272/295 (92%)	262 (96%)	10 (4%)	0	100	100
1	J	272/295 (92%)	262 (96%)	10 (4%)	0	100	100
1	K	272/295 (92%)	263 (97%)	9 (3%)	0	100	100
1	L	272/295 (92%)	266 (98%)	6 (2%)	0	100	100
1	M	272/295 (92%)	260 (96%)	12 (4%)	0	100	100
1	N	272/295 (92%)	265 (97%)	7 (3%)	0	100	100
1	O	272/295 (92%)	263 (97%)	9 (3%)	0	100	100
1	P	272/295 (92%)	266 (98%)	6 (2%)	0	100	100
1	Q	272/295 (92%)	264 (97%)	8 (3%)	0	100	100
1	R	272/295 (92%)	264 (97%)	8 (3%)	0	100	100
1	S	272/295 (92%)	264 (97%)	8 (3%)	0	100	100
1	T	272/295 (92%)	261 (96%)	11 (4%)	0	100	100
All	All	5440/5900 (92%)	5268 (97%)	172 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	224/240 (93%)	219 (98%)	5 (2%)	60	84
1	B	224/240 (93%)	221 (99%)	3 (1%)	76	92
1	C	224/240 (93%)	220 (98%)	4 (2%)	66	88
1	D	224/240 (93%)	221 (99%)	3 (1%)	76	92
1	E	224/240 (93%)	221 (99%)	3 (1%)	76	92
1	F	224/240 (93%)	220 (98%)	4 (2%)	66	88
1	G	224/240 (93%)	221 (99%)	3 (1%)	76	92
1	H	224/240 (93%)	221 (99%)	3 (1%)	76	92
1	I	224/240 (93%)	221 (99%)	3 (1%)	76	92
1	J	224/240 (93%)	220 (98%)	4 (2%)	66	88
1	K	224/240 (93%)	220 (98%)	4 (2%)	66	88
1	L	224/240 (93%)	221 (99%)	3 (1%)	76	92
1	M	224/240 (93%)	220 (98%)	4 (2%)	66	88
1	N	224/240 (93%)	220 (98%)	4 (2%)	66	88
1	O	224/240 (93%)	219 (98%)	5 (2%)	60	84
1	P	224/240 (93%)	219 (98%)	5 (2%)	60	84
1	Q	224/240 (93%)	219 (98%)	5 (2%)	60	84
1	R	224/240 (93%)	222 (99%)	2 (1%)	84	95
1	S	224/240 (93%)	220 (98%)	4 (2%)	66	88
1	T	224/240 (93%)	219 (98%)	5 (2%)	60	84
All	All	4480/4800 (93%)	4404 (98%)	76 (2%)	68	89

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	125	LEU
1	A	135	SER
1	A	166	VAL
1	A	188	SER
1	B	84	VAL
1	B	102	ARG
1	B	125	LEU
1	C	84	VAL
1	C	102	ARG
1	C	125	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	188	SER
1	D	84	VAL
1	D	166	VAL
1	D	188	SER
1	E	84	VAL
1	E	102	ARG
1	E	125	LEU
1	F	84	VAL
1	F	102	ARG
1	F	166	VAL
1	F	188	SER
1	G	84	VAL
1	G	102	ARG
1	G	135	SER
1	H	84	VAL
1	H	102	ARG
1	H	125	LEU
1	I	84	VAL
1	I	125	LEU
1	I	166	VAL
1	J	84	VAL
1	J	102	ARG
1	J	125	LEU
1	J	188	SER
1	K	64	PRO
1	K	84	VAL
1	K	125	LEU
1	K	166	VAL
1	L	84	VAL
1	L	125	LEU
1	L	188	SER
1	M	84	VAL
1	M	102	ARG
1	M	125	LEU
1	M	166	VAL
1	N	84	VAL
1	N	135	SER
1	N	166	VAL
1	N	188	SER
1	O	84	VAL
1	O	102	ARG
1	O	125	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	135	SER
1	O	188	SER
1	P	84	VAL
1	P	125	LEU
1	P	135	SER
1	P	166	VAL
1	P	188	SER
1	Q	84	VAL
1	Q	102	ARG
1	Q	125	LEU
1	Q	166	VAL
1	Q	188	SER
1	R	84	VAL
1	R	135	SER
1	S	64	PRO
1	S	84	VAL
1	S	102	ARG
1	S	125	LEU
1	T	84	VAL
1	T	102	ARG
1	T	125	LEU
1	T	135	SER
1	T	166	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	200	GLN
1	B	58	HIS
1	B	200	GLN
1	C	58	HIS
1	C	200	GLN
1	D	58	HIS
1	D	200	GLN
1	E	58	HIS
1	E	200	GLN
1	E	275	HIS
1	F	58	HIS
1	F	200	GLN
1	G	58	HIS
1	G	200	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	58	HIS
1	H	200	GLN
1	I	58	HIS
1	I	200	GLN
1	J	58	HIS
1	J	200	GLN
1	K	58	HIS
1	K	200	GLN
1	L	58	HIS
1	L	200	GLN
1	M	58	HIS
1	M	200	GLN
1	N	58	HIS
1	N	200	GLN
1	O	58	HIS
1	O	200	GLN
1	P	58	HIS
1	P	200	GLN
1	Q	58	HIS
1	Q	200	GLN
1	R	58	HIS
1	R	200	GLN
1	S	58	HIS
1	S	200	GLN
1	T	58	HIS
1	T	200	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)

20 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	R5P	A	400	-	13,13,13	2.10	5 (38%)	15,18,18	1.44	1 (6%)
2	R5P	B	400	-	13,13,13	1.98	4 (30%)	15,18,18	1.56	1 (6%)
2	R5P	C	400	-	13,13,13	2.13	6 (46%)	15,18,18	1.52	1 (6%)
2	R5P	D	400	-	13,13,13	2.07	6 (46%)	15,18,18	1.51	1 (6%)
2	R5P	E	400	-	13,13,13	2.05	3 (23%)	15,18,18	1.50	1 (6%)
2	R5P	F	400	-	13,13,13	1.99	4 (30%)	15,18,18	1.39	1 (6%)
2	R5P	G	400	-	13,13,13	2.12	5 (38%)	15,18,18	1.54	2 (13%)
2	R5P	H	400	-	13,13,13	2.07	4 (30%)	15,18,18	1.47	1 (6%)
2	R5P	I	400	-	13,13,13	1.99	5 (38%)	15,18,18	1.61	2 (13%)
2	R5P	J	400	-	13,13,13	2.09	6 (46%)	15,18,18	1.43	1 (6%)
2	R5P	K	400	-	13,13,13	2.11	6 (46%)	15,18,18	1.43	1 (6%)
2	R5P	L	400	-	13,13,13	2.08	6 (46%)	15,18,18	1.39	1 (6%)
2	R5P	M	400	-	13,13,13	2.02	5 (38%)	15,18,18	1.58	1 (6%)
2	R5P	N	400	-	13,13,13	2.03	6 (46%)	15,18,18	1.60	1 (6%)
2	R5P	O	400	-	13,13,13	2.09	6 (46%)	15,18,18	1.41	1 (6%)
2	R5P	P	400	-	13,13,13	2.10	5 (38%)	15,18,18	1.34	1 (6%)
2	R5P	Q	400	-	13,13,13	1.95	3 (23%)	15,18,18	1.50	1 (6%)
2	R5P	R	400	-	13,13,13	2.02	6 (46%)	15,18,18	1.49	1 (6%)
2	R5P	S	400	-	13,13,13	2.02	5 (38%)	15,18,18	1.58	1 (6%)
2	R5P	T	400	-	13,13,13	2.08	4 (30%)	15,18,18	1.47	1 (6%)

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	R5P	A	400	-	-	0/14/16/16	0/0/0/0
2	R5P	B	400	-	-	0/14/16/16	0/0/0/0
2	R5P	C	400	-	-	0/14/16/16	0/0/0/0
2	R5P	D	400	-	-	0/14/16/16	0/0/0/0
2	R5P	E	400	-	-	0/14/16/16	0/0/0/0
2	R5P	F	400	-	-	0/14/16/16	0/0/0/0
2	R5P	G	400	-	-	0/14/16/16	0/0/0/0
2	R5P	H	400	-	-	0/14/16/16	0/0/0/0
2	R5P	I	400	-	-	0/14/16/16	0/0/0/0
2	R5P	J	400	-	-	0/14/16/16	0/0/0/0
2	R5P	K	400	-	-	0/14/16/16	0/0/0/0
2	R5P	L	400	-	-	0/14/16/16	0/0/0/0
2	R5P	M	400	-	-	0/14/16/16	0/0/0/0
2	R5P	N	400	-	-	0/14/16/16	0/0/0/0
2	R5P	O	400	-	-	0/14/16/16	0/0/0/0
2	R5P	P	400	-	-	0/14/16/16	0/0/0/0
2	R5P	Q	400	-	-	0/14/16/16	0/0/0/0
2	R5P	R	400	-	-	0/14/16/16	0/0/0/0
2	R5P	S	400	-	-	0/14/16/16	0/0/0/0
2	R5P	T	400	-	-	0/14/16/16	0/0/0/0

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	400	R5P	P-O2P	-2.69	1.45	1.54
2	G	400	R5P	P-O2P	-2.52	1.45	1.54
2	N	400	R5P	P-O2P	-2.49	1.45	1.54
2	H	400	R5P	P-O3P	-2.46	1.45	1.54
2	O	400	R5P	P-O2P	-2.44	1.45	1.54
2	O	400	R5P	P-O3P	-2.39	1.46	1.54
2	T	400	R5P	P-O2P	-2.38	1.46	1.54
2	K	400	R5P	P-O3P	-2.37	1.46	1.54
2	S	400	R5P	P-O3P	-2.36	1.46	1.54
2	M	400	R5P	P-O2P	-2.34	1.46	1.54
2	P	400	R5P	P-O2P	-2.32	1.46	1.54
2	L	400	R5P	P-O2P	-2.31	1.46	1.54
2	J	400	R5P	P-O3P	-2.30	1.46	1.54
2	M	400	R5P	P-O3P	-2.30	1.46	1.54
2	A	400	R5P	P-O3P	-2.29	1.46	1.54
2	E	400	R5P	P-O2P	-2.27	1.46	1.54
2	R	400	R5P	P-O2P	-2.26	1.46	1.54
2	F	400	R5P	P-O2P	-2.22	1.46	1.54
2	A	400	R5P	P-O2P	-2.22	1.46	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	400	R5P	P-O3P	-2.21	1.46	1.54
2	B	400	R5P	P-O2P	-2.21	1.46	1.54
2	T	400	R5P	P-O3P	-2.20	1.46	1.54
2	C	400	R5P	P-O3P	-2.20	1.46	1.54
2	D	400	R5P	P-O2P	-2.20	1.46	1.54
2	N	400	R5P	P-O3P	-2.20	1.46	1.54
2	D	400	R5P	P-O3P	-2.18	1.46	1.54
2	K	400	R5P	P-O2P	-2.18	1.46	1.54
2	J	400	R5P	P-O2P	-2.17	1.46	1.54
2	S	400	R5P	P-O2P	-2.15	1.47	1.54
2	B	400	R5P	P-O3P	-2.10	1.47	1.54
2	C	400	R5P	P-O2P	-2.10	1.47	1.54
2	F	400	R5P	P-O3P	-2.09	1.47	1.54
2	I	400	R5P	P-O3P	-2.08	1.47	1.54
2	L	400	R5P	P-O3P	-2.06	1.47	1.54
2	P	400	R5P	P-O3P	-2.05	1.47	1.54
2	I	400	R5P	P-O2P	-2.04	1.47	1.54
2	R	400	R5P	P-O3P	-2.01	1.47	1.54
2	Q	400	R5P	P-O3P	-2.01	1.47	1.54
2	O	400	R5P	P-O5	2.01	1.67	1.60
2	J	400	R5P	C5-C4	2.01	1.54	1.51
2	M	400	R5P	C5-C4	2.04	1.54	1.51
2	I	400	R5P	C5-C4	2.04	1.54	1.51
2	R	400	R5P	P-O5	2.05	1.67	1.60
2	D	400	R5P	C5-C4	2.07	1.54	1.51
2	S	400	R5P	P-O5	2.07	1.67	1.60
2	R	400	R5P	C5-C4	2.09	1.54	1.51
2	G	400	R5P	P-O5	2.10	1.67	1.60
2	N	400	R5P	P-O5	2.12	1.67	1.60
2	K	400	R5P	C5-C4	2.12	1.54	1.51
2	L	400	R5P	C5-C4	2.13	1.54	1.51
2	N	400	R5P	C5-C4	2.14	1.54	1.51
2	C	400	R5P	P-O5	2.15	1.67	1.60
2	K	400	R5P	P-O5	2.15	1.67	1.60
2	B	400	R5P	C2-C1	2.19	1.54	1.50
2	A	400	R5P	P-O5	2.21	1.67	1.60
2	O	400	R5P	C5-C4	2.21	1.55	1.51
2	P	400	R5P	P-O5	2.22	1.67	1.60
2	C	400	R5P	C5-C4	2.26	1.55	1.51
2	N	400	R5P	C2-C1	2.29	1.54	1.50
2	J	400	R5P	P-O5	2.32	1.68	1.60
2	D	400	R5P	P-O5	2.33	1.68	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	400	R5P	C2-C1	2.40	1.54	1.50
2	L	400	R5P	P-O5	2.41	1.68	1.60
2	H	400	R5P	C2-C1	2.42	1.54	1.50
2	R	400	R5P	C2-C1	2.54	1.54	1.50
2	F	400	R5P	C2-C1	2.56	1.54	1.50
2	I	400	R5P	C2-C1	2.57	1.54	1.50
2	O	400	R5P	C2-C1	2.63	1.54	1.50
2	S	400	R5P	C2-C1	2.64	1.54	1.50
2	D	400	R5P	C2-C1	2.70	1.55	1.50
2	Q	400	R5P	C2-C1	2.71	1.55	1.50
2	K	400	R5P	C2-C1	2.74	1.55	1.50
2	T	400	R5P	C2-C1	2.79	1.55	1.50
2	J	400	R5P	C2-C1	2.83	1.55	1.50
2	L	400	R5P	C2-C1	2.85	1.55	1.50
2	P	400	R5P	C2-C1	2.86	1.55	1.50
2	A	400	R5P	C2-C1	2.89	1.55	1.50
2	E	400	R5P	C2-C1	2.90	1.55	1.50
2	C	400	R5P	C2-C1	3.04	1.55	1.50
2	G	400	R5P	C2-C1	3.06	1.55	1.50
2	O	400	R5P	O1-C1	4.47	1.40	1.19
2	H	400	R5P	O1-C1	4.49	1.40	1.19
2	I	400	R5P	O1-C1	4.52	1.40	1.19
2	B	400	R5P	O1-C1	4.54	1.40	1.19
2	M	400	R5P	O1-C1	4.56	1.40	1.19
2	N	400	R5P	O1-C1	4.56	1.40	1.19
2	Q	400	R5P	O1-C1	4.57	1.40	1.19
2	R	400	R5P	O1-C1	4.59	1.41	1.19
2	S	400	R5P	O1-C1	4.60	1.41	1.19
2	L	400	R5P	O1-C1	4.60	1.41	1.19
2	F	400	R5P	O1-C1	4.61	1.41	1.19
2	G	400	R5P	O1-C1	4.62	1.41	1.19
2	J	400	R5P	O1-C1	4.63	1.41	1.19
2	E	400	R5P	O1-C1	4.64	1.41	1.19
2	D	400	R5P	O1-C1	4.64	1.41	1.19
2	P	400	R5P	O1-C1	4.66	1.41	1.19
2	T	400	R5P	O1-C1	4.68	1.41	1.19
2	A	400	R5P	O1-C1	4.73	1.41	1.19
2	K	400	R5P	O1-C1	4.73	1.41	1.19
2	C	400	R5P	O1-C1	4.75	1.41	1.19

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	400	R5P	O1-C1-C2	-5.18	110.49	125.60
2	I	400	R5P	O1-C1-C2	-5.06	110.85	125.60
2	N	400	R5P	O1-C1-C2	-5.05	110.89	125.60
2	H	400	R5P	O1-C1-C2	-4.89	111.34	125.60
2	B	400	R5P	O1-C1-C2	-4.88	111.38	125.60
2	Q	400	R5P	O1-C1-C2	-4.84	111.50	125.60
2	S	400	R5P	O1-C1-C2	-4.82	111.55	125.60
2	R	400	R5P	O1-C1-C2	-4.62	112.13	125.60
2	T	400	R5P	O1-C1-C2	-4.58	112.24	125.60
2	O	400	R5P	O1-C1-C2	-4.57	112.28	125.60
2	J	400	R5P	O1-C1-C2	-4.56	112.30	125.60
2	K	400	R5P	O1-C1-C2	-4.50	112.50	125.60
2	D	400	R5P	O1-C1-C2	-4.49	112.52	125.60
2	C	400	R5P	O1-C1-C2	-4.47	112.58	125.60
2	E	400	R5P	O1-C1-C2	-4.42	112.72	125.60
2	F	400	R5P	O1-C1-C2	-4.40	112.78	125.60
2	G	400	R5P	O1-C1-C2	-4.29	113.09	125.60
2	L	400	R5P	O1-C1-C2	-4.26	113.17	125.60
2	P	400	R5P	O1-C1-C2	-4.26	113.18	125.60
2	A	400	R5P	O1-C1-C2	-4.17	113.45	125.60
2	G	400	R5P	O3-C3-C2	2.08	112.60	108.93
2	I	400	R5P	O3P-P-O5	2.32	113.23	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	R5P	2	0
2	B	400	R5P	2	0
2	C	400	R5P	2	0
2	D	400	R5P	2	0
2	E	400	R5P	1	0
2	F	400	R5P	2	0
2	G	400	R5P	2	0
2	H	400	R5P	2	0
2	I	400	R5P	1	0
2	J	400	R5P	2	0
2	K	400	R5P	1	0
2	L	400	R5P	2	0
2	M	400	R5P	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	400	R5P	2	0
2	O	400	R5P	2	0
2	P	400	R5P	2	0
2	Q	400	R5P	3	0
2	R	400	R5P	2	0
2	S	400	R5P	2	0
2	T	400	R5P	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	276/295 (93%)	-0.12	3 (1%)	82	84	19, 32, 59, 78	0
1	B	276/295 (93%)	-0.16	5 (1%)	71	75	19, 32, 59, 78	0
1	C	276/295 (93%)	-0.15	6 (2%)	65	69	19, 32, 59, 78	0
1	D	276/295 (93%)	-0.10	3 (1%)	82	84	19, 32, 59, 78	0
1	E	276/295 (93%)	-0.18	1 (0%)	93	93	19, 32, 59, 78	0
1	F	276/295 (93%)	-0.12	5 (1%)	71	75	19, 32, 59, 78	0
1	G	276/295 (93%)	-0.19	1 (0%)	93	93	19, 32, 59, 78	0
1	H	276/295 (93%)	-0.07	4 (1%)	78	80	19, 32, 59, 78	0
1	I	276/295 (93%)	-0.12	6 (2%)	65	69	19, 32, 59, 78	0
1	J	276/295 (93%)	-0.10	10 (3%)	46	51	19, 32, 59, 78	0
1	K	276/295 (93%)	-0.21	4 (1%)	78	80	19, 32, 59, 78	0
1	L	276/295 (93%)	-0.12	8 (2%)	55	60	19, 32, 59, 78	0
1	M	276/295 (93%)	-0.17	6 (2%)	65	69	19, 32, 59, 78	0
1	N	276/295 (93%)	-0.08	5 (1%)	71	75	19, 32, 59, 78	0
1	O	276/295 (93%)	-0.13	4 (1%)	78	80	19, 32, 59, 78	0
1	P	276/295 (93%)	-0.10	8 (2%)	55	60	19, 32, 59, 78	0
1	Q	276/295 (93%)	-0.11	5 (1%)	71	75	19, 32, 59, 78	0
1	R	276/295 (93%)	-0.10	2 (0%)	89	90	19, 32, 59, 78	0
1	S	276/295 (93%)	-0.08	6 (2%)	65	69	19, 32, 59, 78	0
1	T	276/295 (93%)	-0.11	7 (2%)	61	65	19, 32, 59, 78	0
All	All	5520/5900 (93%)	-0.13	99 (1%)	71	75	19, 32, 60, 78	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	10	GLY	12.4
1	H	181	VAL	7.3
1	N	10	GLY	7.2
1	S	10	GLY	6.8
1	L	10	GLY	6.5
1	O	10	GLY	6.5
1	E	10	GLY	6.0
1	C	10	GLY	5.6
1	L	288	SER	5.0
1	H	10	GLY	4.8
1	N	181	VAL	4.5
1	B	181	VAL	4.4
1	J	10	GLY	4.4
1	M	10	GLY	4.1
1	D	10	GLY	4.0
1	B	11	LYS	3.9
1	P	289	GLU	3.8
1	F	261	HIS	3.7
1	D	181	VAL	3.6
1	I	11	LYS	3.5
1	B	10	GLY	3.5
1	S	286	TYR	3.3
1	Q	284	GLU	3.3
1	Q	234	GLU	3.2
1	C	12	ASP	3.2
1	L	16	ASP	3.2
1	J	288	SER	3.2
1	J	260	ASP	3.2
1	Q	233	ARG	3.1
1	G	282	ALA	3.1
1	T	10	GLY	3.1
1	C	11	LYS	3.1
1	J	285	LEU	3.1
1	P	286	TYR	3.0
1	M	12	ASP	3.0
1	K	181	VAL	2.9
1	J	210	GLY	2.9
1	K	10	GLY	2.9
1	J	286	TYR	2.9
1	S	285	LEU	2.9
1	R	181	VAL	2.8
1	J	16	ASP	2.8
1	A	10	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	P	208	GLU	2.8
1	P	287	LEU	2.8
1	S	11	LYS	2.7
1	K	286	TYR	2.7
1	P	16	ASP	2.7
1	M	181	VAL	2.7
1	Q	208	GLU	2.7
1	A	208	GLU	2.7
1	S	12	ASP	2.6
1	I	289	GLU	2.6
1	D	280	ASP	2.5
1	P	181	VAL	2.5
1	L	287	LEU	2.5
1	M	11	LYS	2.5
1	P	288	SER	2.5
1	T	181	VAL	2.5
1	S	280	ASP	2.5
1	R	288	SER	2.4
1	I	233	ARG	2.4
1	F	285	LEU	2.4
1	A	280	ASP	2.4
1	L	47	LYS	2.3
1	L	281	ARG	2.3
1	J	287	LEU	2.3
1	M	17	GLN	2.3
1	T	283	TYR	2.3
1	T	11	LYS	2.3
1	J	18	PRO	2.3
1	M	14	ARG	2.3
1	I	280	ASP	2.2
1	H	233	ARG	2.2
1	J	231	PRO	2.2
1	C	284	GLU	2.2
1	I	10	GLY	2.1
1	F	284	GLU	2.1
1	B	12	ASP	2.1
1	L	286	TYR	2.1
1	O	286	TYR	2.1
1	P	280	ASP	2.1
1	T	251	ASP	2.1
1	B	74	ASN	2.1
1	C	272	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	286	TYR	2.1
1	F	288	SER	2.1
1	I	181	VAL	2.1
1	Q	235	ALA	2.0
1	N	11	LYS	2.0
1	O	16	ASP	2.0
1	H	182	ARG	2.0
1	L	271	ALA	2.0
1	N	261	HIS	2.0
1	T	261	HIS	2.0
1	K	260	ASP	2.0
1	O	284	GLU	2.0
1	N	288	SER	2.0
1	T	74	ASN	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
2	R5P	A	400	14/14	0.79	0.30	6.01	75,79,82,82	0
2	R5P	C	400	14/14	0.79	0.23	4.99	75,79,82,82	0
2	R5P	K	400	14/14	0.86	0.21	4.46	75,79,82,82	0
2	R5P	M	400	14/14	0.86	0.22	4.29	75,79,82,82	0
2	R5P	N	400	14/14	0.84	0.29	3.90	75,79,82,82	0
2	R5P	J	400	14/14	0.84	0.21	3.78	75,79,82,82	0
2	R5P	D	400	14/14	0.85	0.25	3.66	75,79,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	R5P	I	400	14/14	0.82	0.22	3.56	75,79,82,82	0
2	R5P	P	400	14/14	0.82	0.25	3.52	75,79,82,82	0
2	R5P	G	400	14/14	0.81	0.24	3.44	75,79,82,82	0
2	R5P	H	400	14/14	0.90	0.22	3.27	75,79,82,82	0
2	R5P	B	400	14/14	0.90	0.21	2.56	75,79,82,82	0
2	R5P	E	400	14/14	0.85	0.21	2.45	75,79,82,82	0
2	R5P	O	400	14/14	0.91	0.17	2.03	75,79,82,82	0
2	R5P	R	400	14/14	0.82	0.23	1.96	75,79,82,82	0
2	R5P	L	400	14/14	0.86	0.20	1.83	75,79,82,82	0
2	R5P	T	400	14/14	0.88	0.21	1.60	75,79,82,82	0
2	R5P	Q	400	14/14	0.91	0.17	1.50	75,79,82,82	0
2	R5P	F	400	14/14	0.93	0.16	0.75	75,79,82,82	0
2	R5P	S	400	14/14	0.91	0.15	0.72	75,79,82,82	0

6.5 Other polymers (i)

There are no such residues in this entry.