



## Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 04:40 PM BST

PDB ID : 4A34  
Title : Crystal structure of the fucose mutarotase in complex with L-fucose from *Streptococcus pneumoniae*  
Authors : Higgins, M.A.; Boraston, A.B.  
Deposited on : 2011-09-29  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

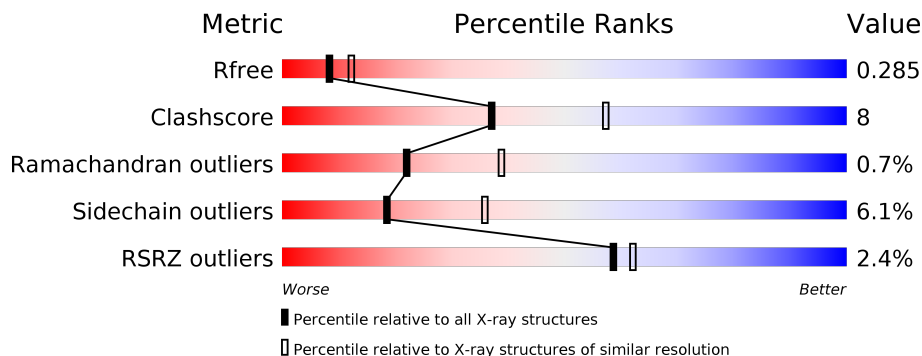
# 1 Overall quality at a glance i

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . 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	147	
1	B	147	
1	C	147	
1	D	147	
1	E	147	
1	F	147	

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Mol	Chain	Length	Quality of chain
1	G	147	<p>3% 69% 21% 5% 5%</p>
1	H	147	<p>% 82% 10% 5%</p>
1	I	147	<p>3% 80% 14% . .</p>
1	J	147	<p>3% 78% 16% 5%</p>
1	K	147	<p>% 77% 15% 5%</p>
1	L	147	<p>2% 78% 15% 5%</p>
1	M	147	<p>3% 78% 16% 5%</p>
1	N	147	<p>3% 80% 15% 5%</p>
1	O	147	<p>3% 75% 17% 5%</p>
1	P	147	<p>% 80% 14% 5%</p>
1	Q	147	<p>3% 67% 24% 5%</p>
1	R	147	<p>3% 80% 13% 5%</p>
1	S	147	<p>2% 79% 12% 5%</p>
1	T	147	<p>3% 78% 14% 5%</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 22775 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 RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	140	1087	694	178	208	7	0	0	0
1	B	140	1080	690	178	205	7	0	0	0
1	C	140	1073	685	177	204	7	0	0	0
1	D	140	1095	699	178	211	7	0	1	0
1	E	139	1075	685	175	208	7	0	0	0
1	F	140	1073	686	176	204	7	0	0	0
1	G	140	1098	702	180	209	7	0	0	0
1	H	140	1089	696	178	208	7	0	0	0
1	I	142	1100	702	180	211	7	0	0	0
1	J	140	1076	687	177	205	7	0	0	0
1	K	140	1086	693	177	209	7	0	0	0
1	L	140	1098	702	180	209	7	0	0	0
1	M	140	1094	699	179	209	7	0	0	0
1	N	140	1075	689	174	205	7	0	0	0
1	O	140	1079	689	177	206	7	0	0	0
1	P	140	1080	689	177	207	7	0	0	0

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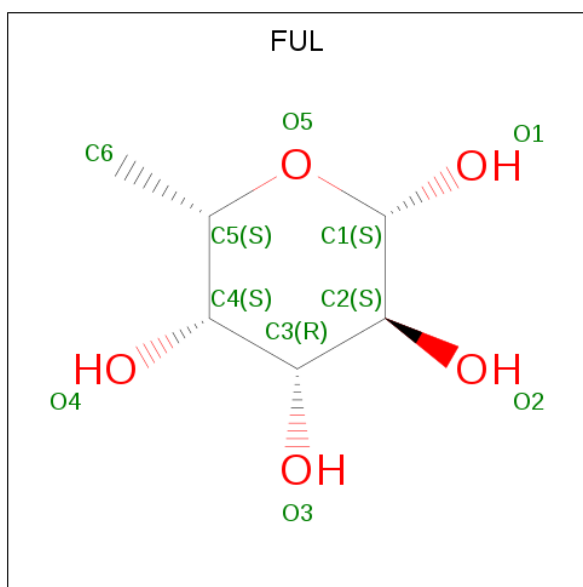
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	140	1084	692	177	208	7	0	0	0
1	R	140	1080	691	175	207	7	0	0	0
1	S	140	1094	702	180	205	7	0	0	0
1	T	140	1079	690	177	205	7	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	GLN	-	expression tag	UNP Q04I09
B	147	GLN	-	expression tag	UNP Q04I09
C	147	GLN	-	expression tag	UNP Q04I09
D	147	GLN	-	expression tag	UNP Q04I09
E	147	GLN	-	expression tag	UNP Q04I09
F	147	GLN	-	expression tag	UNP Q04I09
G	147	GLN	-	expression tag	UNP Q04I09
H	147	GLN	-	expression tag	UNP Q04I09
I	147	GLN	-	expression tag	UNP Q04I09
J	147	GLN	-	expression tag	UNP Q04I09
K	147	GLN	-	expression tag	UNP Q04I09
L	147	GLN	-	expression tag	UNP Q04I09
M	147	GLN	-	expression tag	UNP Q04I09
N	147	GLN	-	expression tag	UNP Q04I09
O	147	GLN	-	expression tag	UNP Q04I09
P	147	GLN	-	expression tag	UNP Q04I09
Q	147	GLN	-	expression tag	UNP Q04I09
R	147	GLN	-	expression tag	UNP Q04I09
S	147	GLN	-	expression tag	UNP Q04I09
T	147	GLN	-	expression tag	UNP Q04I09

- Molecule 2 is beta-L-fucopyranose (three-letter code: FUL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	C	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		
2	E	1	Total	C	O	0	0
			11	6	5		
2	F	1	Total	C	O	0	0
			11	6	5		
2	G	1	Total	C	O	0	0
			11	6	5		
2	H	1	Total	C	O	0	0
			11	6	5		
2	I	1	Total	C	O	0	0
			11	6	5		
2	J	1	Total	C	O	0	0
			11	6	5		
2	K	1	Total	C	O	0	0
			11	6	5		
2	L	1	Total	C	O	0	0
			11	6	5		
2	M	1	Total	C	O	0	0
			11	6	5		
2	N	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	C	O	0	0
			11	6	5		
2	P	1	Total	C	O	0	0
			11	6	5		
2	Q	1	Total	C	O	0	0
			11	6	5		
2	R	1	Total	C	O	0	0
			11	6	5		
2	S	1	Total	C	O	0	0
			11	6	5		
2	T	1	Total	C	O	0	0
			11	6	5		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	1	Total	K	0	0
			1	1		
3	Q	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		
3	K	1	Total	K	0	0
			1	1		
3	E	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		
3	N	1	Total	K	0	0
			1	1		
3	L	1	Total	K	0	0
			1	1		
3	S	1	Total	K	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	49	Total O 49 49	0	0
4	C	46	Total O 46 46	0	0
4	D	38	Total O 38 38	0	0
4	E	58	Total O 58 58	0	0
4	F	44	Total O 44 44	0	0
4	G	28	Total O 28 28	0	0
4	H	41	Total O 41 41	0	0
4	I	30	Total O 30 30	0	0
4	J	22	Total O 22 22	0	0
4	K	56	Total O 56 56	0	0
4	L	31	Total O 31 31	0	0
4	M	46	Total O 46 46	0	0
4	N	50	Total O 50 50	0	0
4	O	44	Total O 44 44	0	0
4	P	55	Total O 55 55	0	0
4	Q	27	Total O 27 27	0	0
4	R	34	Total O 34 34	0	0
4	S	48	Total O 48 48	0	0
4	T	45	Total O 45 45	0	0



### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

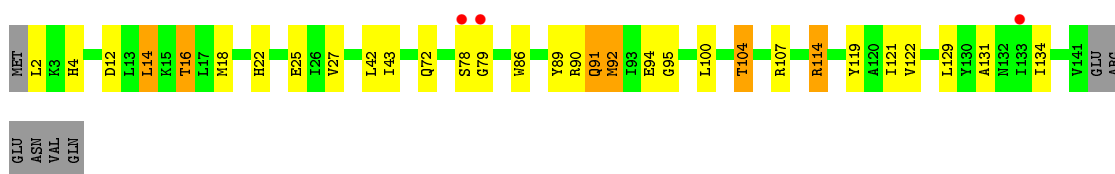
- Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain A: 




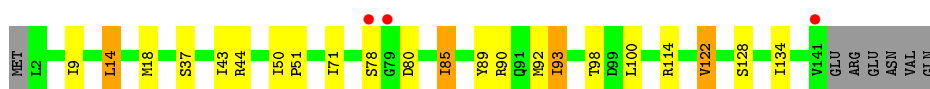
- Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain B: 




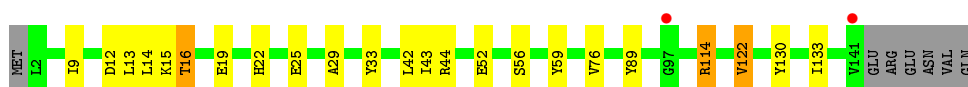
- Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain C: 



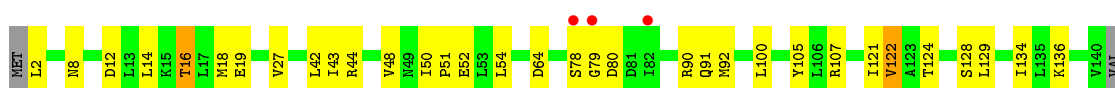
- Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain D: 



- Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

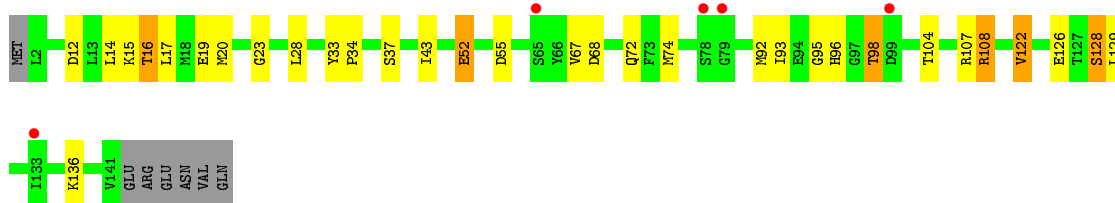
Chain E: 



GLU  
ARG  
GLU  
ASN  
VAL  
GLN

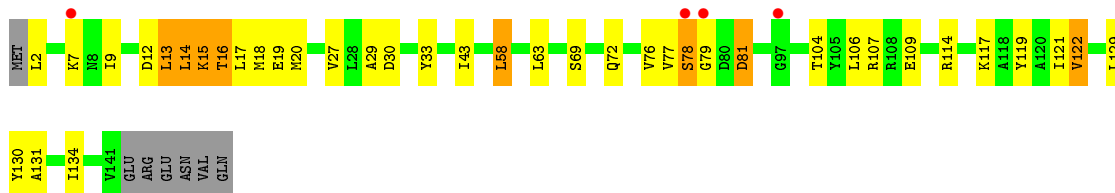
• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain F: 




• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain G: 




• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain H: 




• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain I: 




• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

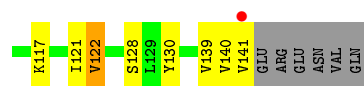
Chain J: 



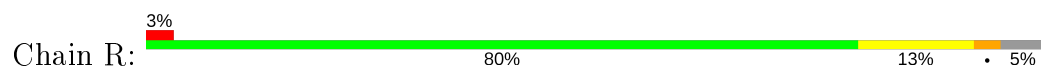
• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain K: 

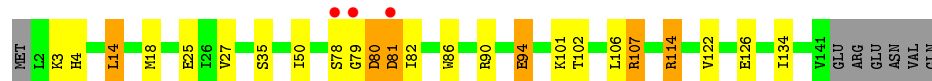
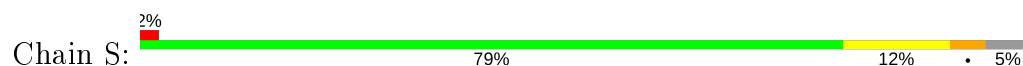




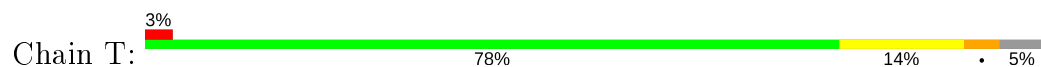
- Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN



- Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN



- Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.32Å 144.16Å 165.46Å 90.00° 97.51° 90.00°	Depositor
Resolution (Å)	19.97 – 2.50 19.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.97-2.50) 99.6 (19.97-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.50Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.225 , 0.292 0.220 , 0.285	Depositor DCC
$R_{free}$ test set	5139 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.5	Xtrriage
Anisotropy	0.042	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22775	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: K, FUL

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	0.42	0/1107	0.59	0/1502
1	B	0.42	0/1100	0.59	0/1492
1	C	0.43	0/1093	0.57	0/1485
1	D	0.41	0/1115	0.58	0/1513
1	E	0.42	0/1095	0.58	0/1488
1	F	0.41	0/1093	0.57	0/1485
1	G	0.43	0/1118	0.62	0/1514
1	H	0.40	0/1109	0.59	0/1505
1	I	0.41	0/1120	0.57	0/1520
1	J	0.43	0/1096	0.60	0/1489
1	K	0.40	0/1106	0.61	0/1502
1	L	0.41	0/1118	0.57	0/1514
1	M	0.43	0/1114	0.59	0/1510
1	N	0.43	0/1095	0.63	0/1488
1	O	0.41	0/1099	0.61	0/1493
1	P	0.42	0/1100	0.59	0/1494
1	Q	0.40	0/1104	0.59	0/1498
1	R	0.40	0/1100	0.58	0/1494
1	S	0.44	0/1114	0.63	0/1506
1	T	0.43	0/1099	0.61	0/1493
All	All	0.42	0/22095	0.59	0/29985

There are no bond length outliers.

There are no bond angle outliers.

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	1087	0	1084	11	0
1	B	1080	0	1076	20	0
1	C	1073	0	1058	17	0
1	D	1095	0	1093	16	0
1	E	1075	0	1063	22	0
1	F	1073	0	1064	23	0
1	G	1098	0	1116	29	0
1	H	1089	0	1091	14	0
1	I	1100	0	1098	17	0
1	J	1076	0	1068	18	0
1	K	1086	0	1083	18	0
1	L	1098	0	1116	16	0
1	M	1094	0	1105	14	0
1	N	1075	0	1070	15	0
1	O	1079	0	1069	26	0
1	P	1080	0	1072	24	0
1	Q	1084	0	1081	24	0
1	R	1080	0	1079	12	0
1	S	1094	0	1116	16	0
1	T	1079	0	1077	20	0
2	A	11	0	12	0	0
2	B	11	0	12	0	0
2	C	11	0	12	1	0
2	D	11	0	12	0	0
2	E	11	0	12	1	0
2	F	11	0	12	2	0
2	G	11	0	12	0	0
2	H	11	0	12	0	0
2	I	11	0	12	2	0
2	J	11	0	12	0	0
2	K	11	0	12	0	0
2	L	11	0	12	0	0
2	M	11	0	12	0	0
2	N	11	0	12	0	0
2	O	11	0	12	0	0
2	P	11	0	12	0	0
2	Q	11	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	11	0	12	0	0
2	S	11	0	12	0	0
2	T	11	0	12	1	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	N	1	0	0	0	0
3	Q	1	0	0	0	0
3	S	1	0	0	0	0
4	A	58	0	0	0	0
4	B	49	0	0	3	0
4	C	46	0	0	2	0
4	D	38	0	0	1	0
4	E	58	0	0	1	0
4	F	44	0	0	1	0
4	G	28	0	0	1	0
4	H	41	0	0	0	0
4	I	30	0	0	1	0
4	J	22	0	0	0	0
4	K	56	0	0	0	0
4	L	31	0	0	2	0
4	M	46	0	0	0	0
4	N	50	0	0	0	0
4	O	44	0	0	5	0
4	P	55	0	0	0	0
4	Q	27	0	0	1	0
4	R	34	0	0	0	0
4	S	48	0	0	0	0
4	T	45	0	0	0	0
All	All	22775	0	21919	343	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 8.

All (343) 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:S:80:ASP:CB	1:S:81:ASP:HA	1.71	1.19
1:S:80:ASP:HB3	1:S:81:ASP:HA	1.20	1.18
1:O:79:GLY:HA2	1:O:80:ASP:HB2	1.22	1.11
1:J:96:HIS:H	1:J:97:GLY:CA	1.63	1.10
1:J:96:HIS:N	1:J:97:GLY:HA2	1.65	1.09
1:K:17:LEU:HA	1:K:20:MET:HE2	1.41	1.01
1:J:96:HIS:H	1:J:97:GLY:HA2	0.82	0.95
1:S:80:ASP:HB3	1:S:81:ASP:CA	2.01	0.89
1:B:16:THR:HG21	1:B:43:ILE:HD11	1.55	0.88
1:I:16:THR:HG21	1:I:43:ILE:HD11	1.56	0.87
1:P:12:ASP:O	1:P:16:THR:HG22	1.76	0.85
1:O:79:GLY:CA	1:O:80:ASP:HB2	2.07	0.84
1:O:69:SER:OG	1:O:104:THR:HG22	1.76	0.84
1:O:79:GLY:HA2	1:O:80:ASP:CB	2.04	0.83
1:C:71:ILE:HD12	1:C:93:ILE:HD13	1.57	0.83
1:P:79:GLY:HA3	1:P:80:ASP:HB2	1.62	0.81
1:K:79:GLY:HA2	1:K:80:ASP:O	1.80	0.81
1:F:17:LEU:HA	1:F:20:MET:HE3	1.60	0.81
1:D:16:THR:HG21	1:D:43:ILE:HD11	1.63	0.81
1:S:80:ASP:HB2	1:S:81:ASP:HA	1.64	0.80
1:J:16:THR:HG21	1:J:43:ILE:HD11	1.63	0.80
1:B:2:LEU:HD22	1:G:18:MET:HG2	1.62	0.80
1:P:78:SER:H	1:P:79:GLY:HA2	1.47	0.79
1:O:14:LEU:HD13	1:T:14:LEU:HD13	1.64	0.78
1:N:17:LEU:HD23	1:N:20:MET:HE1	1.65	0.77
1:J:12:ASP:O	1:J:16:THR:HG22	1.85	0.76
1:G:12:ASP:O	1:G:16:THR:HG23	1.85	0.76
1:N:79:GLY:HA2	1:N:80:ASP:HB2	1.68	0.75
1:E:12:ASP:O	1:E:16:THR:HG23	1.87	0.74
1:Q:94:GLU:HB2	1:Q:100:LEU:HD13	1.69	0.73
1:O:16:THR:HG21	1:O:43:ILE:HD11	1.69	0.72
1:P:79:GLY:CA	1:P:80:ASP:HB2	2.19	0.72
1:F:12:ASP:O	1:F:16:THR:HG22	1.90	0.71
1:G:17:LEU:HA	1:G:20:MET:HE3	1.71	0.71
1:B:12:ASP:O	1:B:16:THR:HG23	1.91	0.70
1:O:12:ASP:O	1:O:16:THR:CG2	2.40	0.70
1:H:141:VAL:O	1:H:141:VAL:HG12	1.90	0.70
1:M:12:ASP:O	1:M:16:THR:HG23	1.90	0.70
1:L:14:LEU:HD12	1:Q:18:MET:SD	2.32	0.70
1:O:58:LEU:HD22	1:O:63:LEU:HD11	1.74	0.70
1:Q:27:VAL:HG13	1:Q:121:ILE:HG12	1.74	0.68
1:B:27:VAL:HG22	1:B:134:ILE:HG12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:GLN:HG3	1:F:104:THR:HG22	1.75	0.68
1:F:17:LEU:HA	1:F:20:MET:CE	2.24	0.68
1:A:72:GLN:HG3	1:A:104:THR:CG2	2.24	0.67
1:S:80:ASP:CB	1:S:81:ASP:CA	2.56	0.67
1:H:78:SER:CB	1:H:79:GLY:CA	2.72	0.67
1:P:16:THR:HB	1:P:41:LYS:NZ	2.10	0.66
1:O:12:ASP:O	1:O:16:THR:HG22	1.94	0.66
1:R:12:ASP:O	1:R:16:THR:HG22	1.95	0.66
1:H:76:VAL:HA	1:H:130:TYR:CE1	2.31	0.66
1:E:18:MET:SD	1:J:14:LEU:HD23	2.36	0.65
1:F:52:GLU:HG3	4:F:2024:HOH:O	1.96	0.65
1:T:80:ASP:C	1:T:82:ILE:H	1.98	0.65
1:J:96:HIS:N	1:J:97:GLY:CA	2.39	0.65
1:K:77:VAL:O	1:K:80:ASP:HB2	1.96	0.65
1:A:69:SER:OG	1:A:104:THR:HG22	1.97	0.64
1:B:72:GLN:HG3	1:B:104:THR:HG22	1.78	0.64
1:C:14:LEU:HD12	1:H:18:MET:SD	2.36	0.64
1:G:72:GLN:HG3	1:G:104:THR:CG2	2.28	0.64
1:I:12:ASP:O	1:I:16:THR:HG22	1.97	0.64
1:A:9:ILE:HD11	1:A:14:LEU:HB2	1.79	0.64
1:P:25:GLU:OE2	1:P:136:LYS:HE2	1.97	0.64
1:K:25:GLU:OE1	1:K:114:ARG:HD3	1.98	0.63
1:G:17:LEU:HA	1:G:20:MET:CE	2.28	0.63
1:C:14:LEU:HD13	1:H:14:LEU:HD13	1.81	0.63
1:L:13:LEU:O	1:L:17:LEU:HG	1.99	0.63
1:H:78:SER:CB	1:H:79:GLY:HA3	2.29	0.63
1:S:86:TRP:O	1:S:90:ARG:HG3	1.99	0.62
1:P:78:SER:N	1:P:79:GLY:HA2	2.10	0.62
1:A:72:GLN:HG3	1:A:104:THR:HG23	1.81	0.62
1:G:117:LYS:HG3	4:G:2026:HOH:O	2.00	0.62
1:E:16:THR:HG21	1:E:43:ILE:HD11	1.80	0.62
1:K:12:ASP:O	1:K:16:THR:CG2	2.49	0.61
1:N:22:HIS:HE1	1:O:108:ARG:HH22	1.49	0.61
1:P:43:ILE:O	1:P:122:VAL:HA	2.01	0.61
1:F:12:ASP:O	1:F:16:THR:CG2	2.49	0.60
1:M:16:THR:HG21	1:M:43:ILE:HD11	1.82	0.60
1:S:25:GLU:OE1	1:S:114:ARG:HD3	2.02	0.60
1:C:80:ASP:O	4:C:2036:HOH:O	2.16	0.59
1:H:49:ASN:HB2	1:H:52:GLU:OE2	2.02	0.59
1:J:16:THR:HG21	1:J:43:ILE:CD1	2.32	0.59
1:B:4:HIS:ND1	1:S:94:GLU:HG3	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:12:ASP:O	1:R:16:THR:CG2	2.50	0.59
1:J:93:ILE:HG23	1:J:98:THR:HG22	1.84	0.58
1:J:27:VAL:HG22	1:J:134:ILE:HG12	1.86	0.58
1:T:78:SER:H	1:T:79:GLY:HA3	1.67	0.58
1:P:79:GLY:HA3	1:P:80:ASP:O	2.04	0.57
1:Q:140:VAL:O	1:Q:141:VAL:HB	2.04	0.57
1:G:72:GLN:HG3	1:G:104:THR:HG23	1.86	0.57
1:E:54:LEU:HD23	1:E:92:MET:HE3	1.87	0.57
1:Q:76:VAL:HG13	1:Q:80:ASP:HB3	1.86	0.57
1:E:27:VAL:HG22	1:E:134:ILE:HG12	1.87	0.57
1:N:22:HIS:CE1	1:O:108:ARG:HH12	2.22	0.56
1:P:16:THR:HG21	1:P:43:ILE:HD11	1.88	0.56
1:B:91:GLN:H	1:B:94:GLU:H	1.51	0.56
1:O:14:LEU:CD1	1:T:14:LEU:HD13	2.35	0.56
4:O:2031:HOH:O	1:T:4:HIS:HE1	1.88	0.56
1:F:95:GLY:O	1:F:96:HIS:HB2	2.05	0.56
1:L:27:VAL:HG22	1:L:134:ILE:HG12	1.87	0.56
1:Q:82:ILE:HD12	1:Q:82:ILE:H	1.70	0.56
1:D:25:GLU:OE1	1:D:114:ARG:HD3	2.06	0.56
1:D:15:LYS:HD2	1:I:15:LYS:HD2	1.88	0.55
1:N:77:VAL:O	1:N:80:ASP:HB2	2.06	0.55
1:E:14:LEU:O	1:E:18:MET:HG3	2.06	0.55
1:O:27:VAL:HG13	1:O:121:ILE:HG12	1.87	0.55
1:F:67:VAL:HG22	1:F:68:ASP:H	1.72	0.55
1:M:25:GLU:OE2	1:M:136:LYS:HE2	2.08	0.55
1:Q:29:ALA:HB1	1:Q:33:TYR:HB3	1.89	0.55
1:O:91:GLN:O	1:O:94:GLU:O	2.24	0.54
1:N:67:VAL:HG22	1:N:68:ASP:H	1.73	0.54
1:F:126:GLU:OE2	1:F:128:SER:HB3	2.07	0.54
1:O:20:MET:HE3	1:O:26:ILE:HD12	1.89	0.54
1:C:18:MET:SD	1:H:14:LEU:HD12	2.48	0.54
1:K:17:LEU:HD23	1:K:20:MET:HE1	1.89	0.54
1:T:27:VAL:HG22	1:T:134:ILE:HG12	1.90	0.54
1:D:12:ASP:O	1:D:16:THR:HG22	2.08	0.53
1:E:51:PRO:O	1:E:92:MET:HE1	2.08	0.53
1:N:72:GLN:HG2	1:N:106:LEU:CD2	2.39	0.53
1:P:12:ASP:O	1:P:16:THR:CG2	2.53	0.53
1:C:89:TYR:O	1:C:93:ILE:HG23	2.08	0.53
1:L:43:ILE:O	1:L:122:VAL:HA	2.07	0.53
1:M:14:LEU:HD12	1:R:18:MET:SD	2.49	0.53
1:O:16:THR:HA	1:O:19:GLU:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:ILE:O	1:H:122:VAL:HA	2.09	0.52
1:D:16:THR:HG21	1:D:43:ILE:CD1	2.36	0.52
1:F:93:ILE:O	1:F:98:THR:HG23	2.10	0.52
1:I:25:GLU:OE1	1:I:114:ARG:HD3	2.09	0.52
1:F:72:GLN:HG3	1:F:104:THR:CG2	2.38	0.52
4:C:2014:HOH:O	1:D:44:ARG:NH2	2.42	0.52
1:R:16:THR:HA	1:R:19:GLU:HG2	1.92	0.52
1:I:63:LEU:CD1	1:I:71:ILE:HD11	2.40	0.52
1:G:81:ASP:N	1:G:81:ASP:OD1	2.36	0.51
1:E:64:ASP:OD2	1:E:136:LYS:HD3	2.10	0.51
1:F:43:ILE:O	1:F:122:VAL:HA	2.10	0.51
1:N:72:GLN:HG2	1:N:106:LEU:HD21	1.92	0.51
1:O:16:THR:HG21	1:O:43:ILE:CD1	2.40	0.51
1:T:76:VAL:HG12	1:T:79:GLY:HA3	1.92	0.51
1:K:44:ARG:HG2	1:K:46:ASP:OD2	2.11	0.51
1:D:29:ALA:HB1	1:D:33:TYR:HB3	1.92	0.51
1:G:43:ILE:O	1:G:122:VAL:HA	2.11	0.51
1:L:81:ASP:O	1:L:82:ILE:HB	2.10	0.51
1:K:18:MET:HG2	1:P:2:LEU:HD12	1.92	0.51
1:P:79:GLY:HA3	1:P:80:ASP:CB	2.31	0.51
1:O:2:LEU:N	4:O:2001:HOH:O	2.44	0.51
1:T:78:SER:N	1:T:79:GLY:HA3	2.25	0.51
1:T:78:SER:OG	1:T:79:GLY:HA2	2.10	0.51
1:I:16:THR:HA	1:I:19:GLU:HG2	1.92	0.50
1:K:76:VAL:HA	1:K:130:TYR:CE1	2.46	0.50
1:K:12:ASP:O	1:K:16:THR:HG23	2.11	0.50
1:F:28:LEU:HD23	1:F:122:VAL:HG13	1.94	0.50
1:G:14:LEU:O	1:G:18:MET:HG3	2.12	0.50
1:I:64:ASP:OD2	1:I:136:LYS:HD3	2.12	0.50
1:R:133:ILE:HG22	1:R:135:LEU:HD12	1.92	0.50
1:I:27:VAL:HG22	1:I:134:ILE:HG12	1.94	0.50
1:A:27:VAL:HB	1:A:121:ILE:HG12	1.95	0.49
1:K:16:THR:HG21	1:K:43:ILE:HD11	1.93	0.49
1:P:16:THR:HB	1:P:41:LYS:HZ1	1.77	0.49
1:M:16:THR:HA	1:M:19:GLU:HG2	1.94	0.49
1:L:5:ILE:CD1	1:Q:60:LEU:HD22	2.42	0.49
1:H:25:GLU:OE1	1:H:114:ARG:HD3	2.13	0.49
1:N:76:VAL:HA	1:N:130:TYR:CE1	2.48	0.49
1:N:14:LEU:HG	1:S:14:LEU:HD13	1.93	0.49
1:B:25:GLU:OE2	1:B:114:ARG:NH1	2.46	0.49
1:K:12:ASP:O	1:K:16:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:52:GLU:CD	1:L:52:GLU:H	2.16	0.49
1:N:18:MET:SD	1:S:14:LEU:HD12	2.53	0.49
1:E:43:ILE:O	1:E:122:VAL:HA	2.13	0.49
1:G:30:ASP:HB3	1:G:131:ALA:HB3	1.94	0.48
1:L:99:ASP:OD2	1:L:101:LYS:HB3	2.13	0.48
1:O:12:ASP:O	1:O:16:THR:HG23	2.13	0.48
1:L:2:LEU:HD12	1:Q:18:MET:HG2	1.96	0.48
1:A:109:GLU:H	1:A:109:GLU:CD	2.17	0.48
1:C:71:ILE:CD1	1:C:93:ILE:HD13	2.36	0.48
1:C:9:ILE:HG21	1:C:14:LEU:HG	1.96	0.48
1:P:16:THR:HG21	1:P:43:ILE:CD1	2.44	0.48
4:O:2031:HOH:O	1:T:3:LYS:HE2	2.14	0.48
1:T:80:ASP:C	1:T:82:ILE:N	2.67	0.48
1:L:78:SER:HA	1:L:79:GLY:HA2	1.63	0.48
1:M:17:LEU:HD23	1:M:20:MET:HE1	1.95	0.48
1:M:27:VAL:HG21	1:M:115:SER:HB2	1.96	0.48
1:G:69:SER:OG	1:G:104:THR:HG22	2.14	0.48
1:G:12:ASP:O	1:G:16:THR:CG2	2.60	0.47
1:C:90:ARG:HG2	1:C:100:LEU:HD22	1.95	0.47
1:F:74:MET:CE	2:F:1142:FUL:H3	2.45	0.47
1:O:14:LEU:HD12	1:T:18:MET:SD	2.54	0.47
1:S:82:ILE:H	1:S:82:ILE:HD12	1.79	0.47
1:B:18:MET:HG3	1:G:2:LEU:HD12	1.96	0.47
1:B:22:HIS:ND1	2:C:1142:FUL:O5	2.45	0.47
1:R:30:ASP:HB3	1:R:131:ALA:HB3	1.95	0.47
1:M:94:GLU:HG2	1:M:100:LEU:HD11	1.97	0.47
1:R:27:VAL:HB	1:R:121:ILE:HG12	1.97	0.47
1:C:50:ILE:N	1:C:51:PRO:HD2	2.29	0.47
1:F:23:GLY:HA2	1:F:136:LYS:HE3	1.96	0.47
1:H:141:VAL:O	1:H:141:VAL:CG1	2.59	0.47
1:I:63:LEU:HD13	1:I:71:ILE:HD11	1.97	0.47
1:R:27:VAL:HG22	1:R:134:ILE:HG12	1.97	0.47
1:E:2:LEU:N	4:E:2001:HOH:O	2.46	0.47
1:F:55:ASP:OD1	1:F:96:HIS:HE1	1.98	0.47
1:G:15:LYS:HD3	1:G:19:GLU:OE1	2.14	0.47
1:S:50:ILE:HG13	1:S:126:GLU:HB2	1.95	0.47
1:B:91:GLN:HA	1:B:92:MET:C	2.36	0.47
1:E:90:ARG:NH2	1:E:105:TYR:OH	2.48	0.47
1:M:50:ILE:N	1:M:51:PRO:HD2	2.30	0.47
1:B:27:VAL:HB	1:B:121:ILE:HG12	1.96	0.46
1:D:12:ASP:O	1:D:16:THR:CG2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:89:TYR:OH	1:P:131:ALA:HB1	2.15	0.46
1:G:29:ALA:HB1	1:G:33:TYR:HB3	1.96	0.46
1:B:14:LEU:HD12	1:G:18:MET:SD	2.56	0.46
1:L:49:ASN:HB2	1:L:52:GLU:OE2	2.15	0.46
1:J:107:ARG:HB2	1:J:110:ASP:OD2	2.16	0.46
2:I:1144:FUL:H63	1:J:139:VAL:HG21	1.97	0.46
1:E:27:VAL:HB	1:E:121:ILE:HG12	1.99	0.45
1:F:67:VAL:HG22	1:F:68:ASP:N	2.30	0.45
1:H:25:GLU:OE2	1:H:136:LYS:HE2	2.16	0.45
1:T:25:GLU:OE1	1:T:114:ARG:HD3	2.17	0.45
1:T:67:VAL:HG21	1:T:136:LYS:HD3	1.99	0.45
2:I:1144:FUL:O5	1:J:22:HIS:ND1	2.40	0.45
1:L:41:LYS:NZ	4:L:2006:HOH:O	2.37	0.45
1:N:79:GLY:HA2	1:N:80:ASP:CB	2.42	0.45
1:T:86:TRP:O	1:T:90:ARG:HG2	2.16	0.45
1:M:17:LEU:HA	1:M:20:MET:HE3	1.97	0.45
1:O:72:GLN:HG3	1:O:104:THR:CG2	2.47	0.45
4:B:2048:HOH:O	1:G:2:LEU:N	2.48	0.45
1:K:27:VAL:HG22	1:K:134:ILE:HG12	1.98	0.45
1:L:69:SER:N	4:L:2025:HOH:O	2.48	0.45
1:Q:104:THR:HG22	1:Q:105:TYR:N	2.32	0.45
1:O:29:ALA:HB1	1:O:33:TYR:HB3	1.97	0.45
1:D:89:TYR:CZ	1:D:133:ILE:HD11	2.51	0.45
1:E:51:PRO:HA	1:E:92:MET:HE1	1.99	0.45
1:F:74:MET:HE1	2:F:1142:FUL:H3	1.99	0.45
1:I:7:LYS:NZ	4:I:2001:HOH:O	2.50	0.45
1:O:83:PRO:HG2	1:O:86:TRP:CE2	2.52	0.45
1:P:16:THR:HB	1:P:41:LYS:HZ2	1.82	0.45
1:J:12:ASP:O	1:J:16:THR:CG2	2.61	0.44
1:Q:78:SER:HA	1:Q:79:GLY:HA2	1.64	0.44
1:C:43:ILE:O	1:C:122:VAL:HA	2.16	0.44
1:D:59:TYR:O	1:I:3:LYS:HE3	2.17	0.44
1:K:15:LYS:HD2	1:P:12:ASP:HA	1.99	0.44
1:Q:63:LEU:HD12	1:Q:98:THR:HG21	1.99	0.44
1:E:78:SER:HA	1:E:79:GLY:HA2	1.74	0.44
1:G:77:VAL:O	1:G:79:GLY:N	2.50	0.44
1:D:76:VAL:HA	1:D:130:TYR:CE1	2.52	0.44
1:B:78:SER:HA	1:B:79:GLY:HA2	1.73	0.44
1:F:33:TYR:CG	1:F:34:PRO:HD2	2.52	0.44
1:G:16:THR:HA	1:G:19:GLU:HG2	2.00	0.44
1:O:107:ARG:HG2	4:O:2040:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:3:LYS:HB3	1:S:4:HIS:CD2	2.53	0.44
1:T:76:VAL:CG1	1:T:77:VAL:N	2.81	0.44
1:D:16:THR:HA	1:D:19:GLU:HG2	2.00	0.44
1:I:33:TYR:CD1	1:I:34:PRO:HD2	2.53	0.44
1:J:91:GLN:O	1:J:94:GLU:O	2.36	0.44
1:L:14:LEU:HD13	1:Q:14:LEU:CD2	2.47	0.44
1:D:43:ILE:O	1:D:122:VAL:HA	2.17	0.44
1:I:43:ILE:O	1:I:122:VAL:HA	2.17	0.44
1:K:30:ASP:HB3	1:K:131:ALA:HB3	1.98	0.44
1:Q:89:TYR:O	1:Q:92:MET:HB3	2.18	0.44
1:Q:94:GLU:HB2	1:Q:100:LEU:CD1	2.42	0.43
1:S:79:GLY:O	1:S:80:ASP:O	2.36	0.43
1:I:74:MET:SD	1:I:108:ARG:HG3	2.58	0.43
4:B:2011:HOH:O	1:C:44:ARG:NH2	2.49	0.43
1:K:14:LEU:HD23	1:P:18:MET:SD	2.59	0.43
1:P:64:ASP:OD2	1:P:136:LYS:HD3	2.18	0.43
1:S:27:VAL:HG22	1:S:134:ILE:HG12	1.99	0.43
1:J:50:ILE:HG13	1:J:126:GLU:HB2	2.01	0.43
1:A:19:GLU:OE2	1:A:119:TYR:OH	2.29	0.43
1:B:2:LEU:N	4:B:2001:HOH:O	2.51	0.43
1:F:15:LYS:O	1:F:19:GLU:HG3	2.17	0.43
1:P:13:LEU:HA	1:P:16:THR:HG23	2.00	0.43
1:R:77:VAL:O	1:R:80:ASP:HB2	2.18	0.43
1:T:27:VAL:HB	1:T:121:ILE:HG12	1.99	0.43
1:T:82:ILE:HA	1:T:83:PRO:HD3	1.94	0.43
1:O:30:ASP:HB3	1:O:131:ALA:HB3	2.00	0.43
1:T:130:TYR:CZ	2:T:1142:FUL:H62	2.54	0.43
1:A:69:SER:OG	1:A:104:THR:CG2	2.65	0.43
1:A:78:SER:HA	1:A:79:GLY:HA2	1.68	0.43
1:G:107:ARG:HG2	1:G:109:GLU:OE2	2.18	0.43
1:G:27:VAL:HG22	1:G:134:ILE:HG12	2.00	0.43
1:I:107:ARG:O	1:I:108:ARG:C	2.57	0.43
1:G:76:VAL:HA	1:G:130:TYR:CE1	2.54	0.43
1:M:89:TYR:CE2	1:M:133:ILE:HD11	2.54	0.43
1:P:27:VAL:HG22	1:P:134:ILE:HG12	2.00	0.43
1:Q:117:LYS:O	4:Q:2024:HOH:O	2.21	0.43
1:N:25:GLU:CG	1:N:136:LYS:HG3	2.49	0.43
1:B:119:TYR:CD1	1:C:37:SER:HB3	2.54	0.43
1:E:48:VAL:O	1:E:124:THR:HB	2.19	0.43
1:O:41:LYS:NZ	4:O:2010:HOH:O	2.51	0.43
1:P:14:LEU:O	1:P:18:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:25:GLU:OE1	1:Q:114:ARG:HD3	2.18	0.43
1:T:78:SER:N	1:T:79:GLY:CA	2.82	0.42
1:D:29:ALA:HB1	1:D:33:TYR:CB	2.48	0.42
1:H:6:PRO:CB	1:H:56:SER:HB2	2.49	0.42
1:I:12:ASP:O	1:I:16:THR:CG2	2.67	0.42
1:R:43:ILE:O	1:R:122:VAL:HA	2.19	0.42
1:J:61:MET:HA	1:J:62:PRO:HD2	1.89	0.42
1:Q:27:VAL:CG1	1:Q:121:ILE:HG12	2.46	0.42
1:R:83:PRO:HG3	1:R:130:TYR:HB2	2.01	0.42
1:G:17:LEU:HD23	1:G:20:MET:CE	2.49	0.42
1:K:17:LEU:HD23	1:K:20:MET:CE	2.49	0.42
1:Q:55:ASP:OD1	1:Q:96:HIS:HE1	2.03	0.42
1:P:79:GLY:CA	1:P:80:ASP:CB	2.89	0.42
1:H:76:VAL:HG12	1:H:130:TYR:CD2	2.55	0.42
1:N:27:VAL:HG22	1:N:134:ILE:HG12	2.00	0.42
1:C:93:ILE:HD12	1:C:98:THR:HB	2.00	0.42
1:Q:48:VAL:HG11	1:Q:53:LEU:HD13	2.01	0.42
1:C:114:ARG:HG2	1:C:134:ILE:HD13	2.01	0.42
1:E:16:THR:HA	1:E:19:GLU:HG2	2.00	0.42
1:S:107:ARG:HH11	1:S:107:ARG:HG3	1.84	0.42
1:B:91:GLN:HA	1:B:95:GLY:H	1.85	0.41
1:F:107:ARG:O	1:F:108:ARG:C	2.57	0.41
1:G:9:ILE:HG23	1:G:13:LEU:HB3	2.01	0.41
1:C:14:LEU:O	1:C:18:MET:HG3	2.19	0.41
1:B:94:GLU:HG3	1:B:100:LEU:HG	2.02	0.41
1:D:9:ILE:HD11	1:D:56:SER:HB3	2.02	0.41
1:M:33:TYR:CG	1:M:34:PRO:HD2	2.56	0.41
1:L:29:ALA:HB1	1:L:33:TYR:HB3	2.01	0.41
1:M:94:GLU:HG3	1:M:94:GLU:O	2.20	0.41
1:Q:43:ILE:O	1:Q:122:VAL:HA	2.20	0.41
1:Q:83:PRO:HG3	1:Q:130:TYR:HB2	2.03	0.41
1:C:85:ILE:HD13	1:C:128:SER:OG	2.21	0.41
1:E:90:ARG:HG3	1:E:100:LEU:HD22	2.02	0.41
1:G:58:LEU:HD12	1:G:58:LEU:HA	1.91	0.41
1:A:9:ILE:HD11	1:A:14:LEU:CB	2.48	0.41
1:K:77:VAL:O	1:K:78:SER:C	2.59	0.41
1:F:37:SER:HB3	1:G:119:TYR:CD1	2.56	0.41
1:G:27:VAL:HB	1:G:121:ILE:HG12	2.03	0.41
1:L:3:LYS:HD3	1:Q:62:PRO:HG3	2.03	0.41
1:E:54:LEU:HD23	1:E:92:MET:CE	2.51	0.41
1:E:8:ASN:ND2	1:E:52:GLU:HG2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:LEU:HD23	1:F:20:MET:CE	2.51	0.41
1:R:44:ARG:HD3	1:R:46:ASP:OD2	2.21	0.41
1:E:50:ILE:N	1:E:51:PRO:HD2	2.35	0.40
1:B:89:TYR:OH	1:B:131:ALA:HB1	2.21	0.40
1:B:86:TRP:O	1:B:90:ARG:HG3	2.21	0.40
1:D:22:HIS:ND1	2:E:1141:FUL:O5	2.45	0.40
1:I:16:THR:HG21	1:I:43:ILE:CD1	2.37	0.40
1:G:16:THR:HG21	1:G:43:ILE:HD11	2.04	0.40
1:M:30:ASP:HB3	1:M:131:ALA:HB3	2.03	0.40
1:N:89:TYR:OH	1:N:131:ALA:HB1	2.20	0.40
1:Q:104:THR:CG2	1:Q:105:TYR:N	2.84	0.40
1:E:18:MET:HG2	1:J:2:LEU:HD12	2.03	0.40
1:A:29:ALA:HB1	1:A:33:TYR:HB3	2.04	0.40
4:D:2005:HOH:O	1:E:44:ARG:NH2	2.54	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	138/147 (94%)	134 (97%)	4 (3%)	0	100	100
1	B	138/147 (94%)	131 (95%)	6 (4%)	1 (1%)	22	39
1	C	138/147 (94%)	134 (97%)	3 (2%)	1 (1%)	22	39
1	D	139/147 (95%)	131 (94%)	8 (6%)	0	100	100
1	E	137/147 (93%)	131 (96%)	6 (4%)	0	100	100
1	F	138/147 (94%)	131 (95%)	6 (4%)	1 (1%)	22	39
1	G	138/147 (94%)	130 (94%)	7 (5%)	1 (1%)	22	39
1	H	138/147 (94%)	133 (96%)	5 (4%)	0	100	100
1	I	140/147 (95%)	137 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	138/147 (94%)	125 (91%)	11 (8%)	2 (1%)	11	20
1	K	138/147 (94%)	132 (96%)	3 (2%)	3 (2%)	6	10
1	L	138/147 (94%)	135 (98%)	2 (1%)	1 (1%)	22	39
1	M	138/147 (94%)	135 (98%)	3 (2%)	0	100	100
1	N	138/147 (94%)	133 (96%)	5 (4%)	0	100	100
1	O	138/147 (94%)	131 (95%)	5 (4%)	2 (1%)	11	20
1	P	138/147 (94%)	131 (95%)	6 (4%)	1 (1%)	22	39
1	Q	138/147 (94%)	132 (96%)	6 (4%)	0	100	100
1	R	138/147 (94%)	133 (96%)	4 (3%)	1 (1%)	22	39
1	S	138/147 (94%)	130 (94%)	6 (4%)	2 (1%)	11	20
1	T	138/147 (94%)	130 (94%)	4 (3%)	4 (3%)	4	6
All	All	2762/2940 (94%)	2639 (96%)	103 (4%)	20 (1%)	22	39

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	78	SER
1	K	79	GLY
1	K	80	ASP
1	O	80	ASP
1	S	78	SER
1	S	80	ASP
1	B	91	GLN
1	C	78	SER
1	F	108	ARG
1	K	78	SER
1	T	78	SER
1	T	81	ASP
1	O	78	SER
1	T	79	GLY
1	G	78	SER
1	J	81	ASP
1	L	82	ILE
1	P	80	ASP
1	R	80	ASP
1	T	77	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	119/130 (92%)	115 (97%)	4 (3%)	37 63
1	B	117/130 (90%)	108 (92%)	9 (8%)	13 25
1	C	115/130 (88%)	110 (96%)	5 (4%)	29 53
1	D	121/130 (93%)	113 (93%)	8 (7%)	16 32
1	E	118/130 (91%)	110 (93%)	8 (7%)	16 30
1	F	116/130 (89%)	108 (93%)	8 (7%)	15 30
1	G	123/130 (95%)	110 (89%)	13 (11%)	6 13
1	H	120/130 (92%)	113 (94%)	7 (6%)	20 38
1	I	121/130 (93%)	115 (95%)	6 (5%)	24 46
1	J	117/130 (90%)	111 (95%)	6 (5%)	24 45
1	K	120/130 (92%)	113 (94%)	7 (6%)	20 38
1	L	123/130 (95%)	118 (96%)	5 (4%)	30 55
1	M	122/130 (94%)	116 (95%)	6 (5%)	25 47
1	N	117/130 (90%)	113 (97%)	4 (3%)	37 63
1	O	117/130 (90%)	112 (96%)	5 (4%)	29 53
1	P	118/130 (91%)	112 (95%)	6 (5%)	24 45
1	Q	119/130 (92%)	105 (88%)	14 (12%)	5 10
1	R	119/130 (92%)	112 (94%)	7 (6%)	19 37
1	S	123/130 (95%)	112 (91%)	11 (9%)	9 19
1	T	118/130 (91%)	111 (94%)	7 (6%)	19 37
All	All	2383/2600 (92%)	2237 (94%)	146 (6%)	18 36

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	44	ARG
1	A	108	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	122	VAL
1	B	14	LEU
1	B	16	THR
1	B	42	LEU
1	B	92	MET
1	B	104	THR
1	B	107	ARG
1	B	114	ARG
1	B	122	VAL
1	B	129	LEU
1	C	14	LEU
1	C	85	ILE
1	C	92	MET
1	C	93	ILE
1	C	122	VAL
1	D	13	LEU
1	D	14	LEU
1	D	16	THR
1	D	42	LEU
1	D	52[A]	GLU
1	D	52[B]	GLU
1	D	114	ARG
1	D	122	VAL
1	E	16	THR
1	E	42	LEU
1	E	80	ASP
1	E	91	GLN
1	E	107	ARG
1	E	122	VAL
1	E	128	SER
1	E	129	LEU
1	F	14	LEU
1	F	16	THR
1	F	52	GLU
1	F	92	MET
1	F	98	THR
1	F	122	VAL
1	F	128	SER
1	F	129	LEU
1	G	7	LYS
1	G	13	LEU
1	G	14	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	15	LYS
1	G	16	THR
1	G	58	LEU
1	G	63	LEU
1	G	78	SER
1	G	81	ASP
1	G	106	LEU
1	G	114	ARG
1	G	122	VAL
1	G	129	LEU
1	H	14	LEU
1	H	52	GLU
1	H	53	LEU
1	H	98	THR
1	H	100	LEU
1	H	114	ARG
1	H	122	VAL
1	I	16	THR
1	I	35	SER
1	I	92	MET
1	I	114	ARG
1	I	117	LYS
1	I	122	VAL
1	J	16	THR
1	J	28	LEU
1	J	80	ASP
1	J	96	HIS
1	J	98	THR
1	J	114	ARG
1	K	16	THR
1	K	28	LEU
1	K	42	LEU
1	K	44	ARG
1	K	108	ARG
1	K	117	LYS
1	K	136	LYS
1	L	14	LEU
1	L	42	LEU
1	L	102	THR
1	L	114	ARG
1	L	122	VAL
1	M	14	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	M	16	THR
1	M	18	MET
1	M	42	LEU
1	M	80	ASP
1	M	129	LEU
1	N	18	MET
1	N	85	ILE
1	N	92	MET
1	N	129	LEU
1	O	14	LEU
1	O	16	THR
1	O	27	VAL
1	O	82	ILE
1	O	107	ARG
1	P	11	PRO
1	P	16	THR
1	P	28	LEU
1	P	107	ARG
1	P	114	ARG
1	P	122	VAL
1	Q	7	LYS
1	Q	27	VAL
1	Q	28	LEU
1	Q	42	LEU
1	Q	52	GLU
1	Q	82	ILE
1	Q	88	THR
1	Q	94	GLU
1	Q	98	THR
1	Q	100	LEU
1	Q	107	ARG
1	Q	122	VAL
1	Q	128	SER
1	Q	139	VAL
1	R	12	ASP
1	R	16	THR
1	R	42	LEU
1	R	81	ASP
1	R	114	ARG
1	R	122	VAL
1	R	128	SER
1	S	14	LEU

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Mol	Chain	Res	Type
1	S	18	MET
1	S	35	SER
1	S	81	ASP
1	S	94	GLU
1	S	101	LYS
1	S	102	THR
1	S	106	LEU
1	S	107	ARG
1	S	114	ARG
1	S	122	VAL
1	T	14	LEU
1	T	81	ASP
1	T	91	GLN
1	T	102	THR
1	T	114	ARG
1	T	122	VAL
1	T	129	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	96	HIS
1	F	96	HIS
1	G	91	GLN
1	J	96	HIS
1	Q	96	HIS
1	S	4	HIS
1	T	4	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FUL	S	1142	-	11,11,11	0.60	0	15,16,16	0.79	0
2	FUL	I	1144	-	11,11,11	0.60	0	15,16,16	1.06	1 (6%)
2	FUL	K	1142	-	11,11,11	0.53	0	15,16,16	0.99	1 (6%)
2	FUL	T	1142	-	11,11,11	0.70	0	15,16,16	0.96	0
2	FUL	Q	1142	-	11,11,11	0.61	0	15,16,16	0.88	0
2	FUL	R	1142	-	11,11,11	0.57	0	15,16,16	1.19	1 (6%)
2	FUL	P	1142	-	11,11,11	0.63	0	15,16,16	0.92	1 (6%)
2	FUL	M	1142	-	11,11,11	0.60	0	15,16,16	0.91	0
2	FUL	E	1141	-	11,11,11	0.63	0	15,16,16	0.96	1 (6%)
2	FUL	C	1142	-	11,11,11	0.53	0	15,16,16	0.99	1 (6%)
2	FUL	L	1142	-	11,11,11	0.55	0	15,16,16	0.88	0
2	FUL	J	1142	-	11,11,11	0.59	0	15,16,16	0.92	1 (6%)
2	FUL	O	1142	-	11,11,11	0.61	0	15,16,16	0.76	0
2	FUL	H	1142	-	11,11,11	0.66	0	15,16,16	0.87	1 (6%)
2	FUL	F	1142	-	11,11,11	0.54	0	15,16,16	0.64	0
2	FUL	D	1142	-	11,11,11	0.60	0	15,16,16	0.79	1 (6%)
2	FUL	A	1142	-	11,11,11	0.61	0	15,16,16	1.16	2 (13%)
2	FUL	B	1142	-	11,11,11	0.66	0	15,16,16	0.75	0
2	FUL	G	1142	-	11,11,11	0.57	0	15,16,16	0.65	0
2	FUL	N	1142	-	11,11,11	0.58	0	15,16,16	0.94	0

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	FUL	S	1142	-	-	-	0/1/1/1
2	FUL	I	1144	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUL	K	1142	-	-	-	0/1/1/1
2	FUL	T	1142	-	-	-	0/1/1/1
2	FUL	Q	1142	-	-	-	0/1/1/1
2	FUL	R	1142	-	-	-	0/1/1/1
2	FUL	P	1142	-	-	-	0/1/1/1
2	FUL	M	1142	-	-	-	0/1/1/1
2	FUL	E	1141	-	-	-	0/1/1/1
2	FUL	C	1142	-	-	-	0/1/1/1
2	FUL	L	1142	-	-	-	0/1/1/1
2	FUL	J	1142	-	-	-	0/1/1/1
2	FUL	O	1142	-	-	-	0/1/1/1
2	FUL	H	1142	-	-	-	0/1/1/1
2	FUL	F	1142	-	-	-	0/1/1/1
2	FUL	D	1142	-	-	-	0/1/1/1
2	FUL	A	1142	-	-	-	0/1/1/1
2	FUL	B	1142	-	-	-	0/1/1/1
2	FUL	G	1142	-	-	-	0/1/1/1
2	FUL	N	1142	-	-	-	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1142	FUL	O5-C5-C6	2.74	112.61	106.70
2	I	1144	FUL	O5-C5-C6	2.71	112.56	106.70
2	E	1141	FUL	O5-C5-C6	2.48	112.06	106.70
2	R	1142	FUL	O5-C5-C6	2.48	112.06	106.70
2	K	1142	FUL	O5-C5-C6	2.41	111.91	106.70
2	P	1142	FUL	O5-C5-C6	2.39	111.87	106.70
2	A	1142	FUL	O5-C5-C4	-2.20	105.57	109.52
2	C	1142	FUL	C6-C5-C4	-2.13	109.14	113.07
2	H	1142	FUL	O5-C5-C6	2.04	111.11	106.70
2	J	1142	FUL	O5-C5-C6	2.03	111.09	106.70
2	D	1142	FUL	O5-C5-C6	2.01	111.04	106.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1144	FUL	2	0
2	T	1142	FUL	1	0
2	E	1141	FUL	1	0
2	C	1142	FUL	1	0
2	F	1142	FUL	2	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	140/147 (95%)	-0.21	0 <b>100</b> <b>100</b>	26, 35, 46, 52	0
1	B	140/147 (95%)	-0.06	3 (2%) 63 66	27, 36, 54, 59	0
1	C	140/147 (95%)	-0.07	3 (2%) 63 66	28, 37, 57, 59	0
1	D	140/147 (95%)	-0.12	2 (1%) 75 77	27, 35, 51, 55	0
1	E	139/147 (94%)	-0.08	3 (2%) 62 65	24, 33, 49, 57	0
1	F	140/147 (95%)	0.12	5 (3%) 42 46	29, 41, 61, 64	0
1	G	140/147 (95%)	0.06	4 (2%) 51 55	29, 39, 56, 62	0
1	H	140/147 (95%)	0.03	1 (0%) 87 89	25, 40, 56, 58	0
1	I	142/147 (96%)	-0.12	5 (3%) 44 47	28, 36, 51, 55	0
1	J	140/147 (95%)	0.08	5 (3%) 42 46	27, 38, 63, 68	0
1	K	140/147 (95%)	-0.13	2 (1%) 75 77	25, 36, 52, 56	0
1	L	140/147 (95%)	0.10	3 (2%) 63 66	30, 43, 64, 66	0
1	M	140/147 (95%)	-0.07	4 (2%) 51 55	26, 35, 50, 59	0
1	N	140/147 (95%)	-0.13	4 (2%) 51 55	24, 35, 46, 48	0
1	O	140/147 (95%)	0.02	5 (3%) 42 46	27, 37, 58, 60	0
1	P	140/147 (95%)	-0.24	1 (0%) 87 89	25, 34, 44, 48	0
1	Q	140/147 (95%)	0.15	4 (2%) 51 55	30, 41, 66, 70	0
1	R	140/147 (95%)	0.06	5 (3%) 42 46	28, 39, 61, 62	0
1	S	140/147 (95%)	-0.16	3 (2%) 63 66	23, 32, 49, 57	0
1	T	140/147 (95%)	-0.27	4 (2%) 51 55	22, 30, 47, 52	0
All	All	2801/2940 (95%)	-0.05	66 (2%) 59 62	22, 36, 57, 70	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	79	GLY	5.6
1	T	79	GLY	5.2
1	E	79	GLY	5.1
1	C	79	GLY	4.8
1	C	78	SER	4.6
1	O	78	SER	4.3
1	B	79	GLY	4.2
1	J	80	ASP	3.8
1	M	79	GLY	3.7
1	J	81	ASP	3.7
1	O	79	GLY	3.7
1	M	78	SER	3.6
1	O	141	VAL	3.5
1	G	97	GLY	3.4
1	J	78	SER	3.4
1	I	141	VAL	3.2
1	S	79	GLY	3.2
1	B	78	SER	3.2
1	G	78	SER	3.2
1	R	141	VAL	3.2
1	N	141	VAL	3.2
1	D	141	VAL	3.1
1	F	78	SER	3.1
1	Q	94	GLU	3.0
1	F	99	ASP	3.0
1	L	81	ASP	2.9
1	E	78	SER	2.9
1	S	78	SER	2.9
1	K	79	GLY	2.9
1	C	141	VAL	2.8
1	N	78	SER	2.8
1	F	133	ILE	2.8
1	Q	141	VAL	2.8
1	L	101	LYS	2.8
1	L	65	SER	2.7
1	M	141	VAL	2.7
1	I	82	ILE	2.7
1	S	81	ASP	2.6
1	R	91	GLN	2.6
1	R	78	SER	2.6
1	R	95	GLY	2.6
1	T	80	ASP	2.6
1	J	79	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	68	ASP	2.5
1	Q	78	SER	2.4
1	D	97	GLY	2.3
1	O	99	ASP	2.3
1	T	78	SER	2.3
1	I	78	SER	2.3
1	B	133	ILE	2.2
1	Q	79	GLY	2.2
1	O	80	ASP	2.2
1	J	77	VAL	2.2
1	G	79	GLY	2.1
1	H	91	GLN	2.1
1	K	141	VAL	2.1
1	I	79	GLY	2.1
1	R	65	SER	2.1
1	F	65	SER	2.1
1	N	133	ILE	2.1
1	M	81	ASP	2.0
1	E	82	ILE	2.0
1	P	133	ILE	2.0
1	G	7	LYS	2.0
1	I	142	GLU	2.0
1	T	81	ASP	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 monosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FUL	Q	1142	11/11	0.89	0.21	47,49,49,49	0
2	FUL	M	1142	11/11	0.90	0.19	42,44,45,46	0
2	FUL	C	1142	11/11	0.91	0.16	35,38,39,39	0
2	FUL	L	1142	11/11	0.91	0.20	41,44,45,46	0
2	FUL	J	1142	11/11	0.91	0.22	48,49,50,51	0
2	FUL	A	1142	11/11	0.91	0.17	27,29,30,30	0
2	FUL	H	1142	11/11	0.92	0.16	33,36,38,38	0
2	FUL	S	1142	11/11	0.92	0.21	33,35,37,38	0
2	FUL	E	1141	11/11	0.92	0.17	33,34,35,35	0
2	FUL	N	1142	11/11	0.92	0.16	33,35,35,35	0
2	FUL	K	1142	11/11	0.93	0.20	39,40,42,43	0
2	FUL	F	1142	11/11	0.93	0.15	46,46,46,46	0
2	FUL	O	1142	11/11	0.94	0.16	40,40,41,41	0
3	K	S	1143	1/1	0.94	0.07	59,59,59,59	0
2	FUL	G	1142	11/11	0.94	0.13	40,41,41,41	0
2	FUL	I	1144	11/11	0.94	0.18	43,43,44,45	0
2	FUL	R	1142	11/11	0.94	0.15	33,34,36,36	0
3	K	C	1143	1/1	0.94	0.08	58,58,58,58	0
2	FUL	T	1142	11/11	0.95	0.16	37,37,38,40	0
3	K	E	1142	1/1	0.95	0.07	56,56,56,56	0
3	K	K	1143	1/1	0.95	0.05	47,47,47,47	0
2	FUL	D	1142	11/11	0.95	0.16	37,37,38,40	0
2	FUL	P	1142	11/11	0.96	0.14	36,38,39,39	0
3	K	Q	1143	1/1	0.96	0.06	44,44,44,44	0
2	FUL	B	1142	11/11	0.96	0.13	40,41,42,42	0
3	K	B	1143	1/1	0.97	0.09	36,36,36,36	0
3	K	D	1143	1/1	0.97	0.04	43,43,43,43	0
3	K	L	1143	1/1	0.98	0.04	46,46,46,46	0
3	K	N	1143	1/1	0.98	0.05	47,47,47,47	0
3	K	J	1143	1/1	0.98	0.10	47,47,47,47	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.