



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2016 – 01:59 PM EST

PDB ID : 5FT8
Title : Structure of a Cysteine Desulfurase-Sulfur Acceptor Complex from Escherichia coli at 2.50 Angstrom resolution
Authors : Fernandez, F.J.; Arda, A.; Lopez-Esteva, M.; Aranda, J.; Penya-Soler, E.; Garces, F.; Round, A.; Campos-Oliva, R.; Bruix, M.; Coll, M.; Tunon, I.; Jimenez-Barbero, J.; Vega, M.C.
Deposited on : 2016-01-11
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

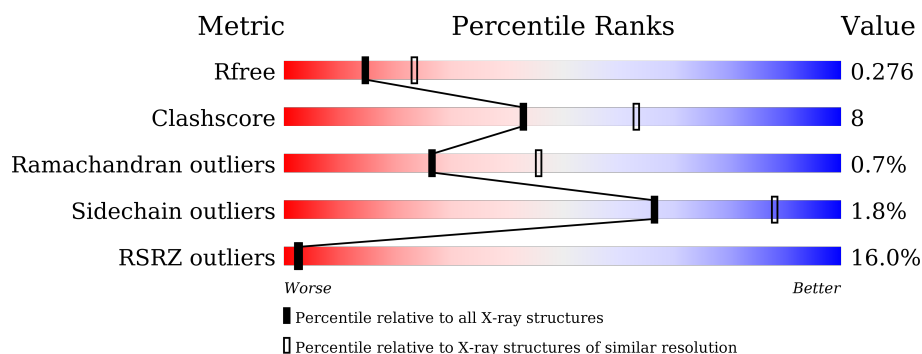
1 Overall quality at a glance

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 $\leq 5\%$. 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	403	
1	C	403	
1	E	403	
1	G	403	
1	I	403	
1	K	403	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	403	
1	O	403	
2	B	154	
2	D	154	
2	F	154	
2	H	154	
2	J	154	
2	L	154	
2	N	154	
2	P	154	

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
4	CSS	D	1152	-	-	X	-
5	PEG	A	1405	-	-	-	X
5	PEG	I	1404	-	-	-	X
6	GOL	C	1409	-	-	-	X
6	GOL	C	1411	-	-	-	X
6	GOL	G	1406	-	-	-	X
6	GOL	I	1407	-	-	-	X
6	GOL	I	1408	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 34325 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 CYSTEINE DESULFURASE CSDA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	2	0
			3051	1934	531	574	12			
1	C	400	Total	C	N	O	S	0	0	0
			3040	1927	528	573	12			
1	E	400	Total	C	N	O	S	0	2	0
			3058	1937	532	577	12			
1	G	400	Total	C	N	O	S	0	2	0
			3052	1934	529	577	12			
1	I	400	Total	C	N	O	S	0	2	0
			3052	1933	530	577	12			
1	K	400	Total	C	N	O	S	0	1	0
			3050	1933	531	574	12			
1	M	398	Total	C	N	O	S	0	1	0
			3027	1920	525	570	12			
1	O	398	Total	C	N	O	S	0	0	0
			3024	1918	525	570	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q46925
A	0	ALA	-	EXPRESSION TAG	UNP Q46925
C	-1	GLY	-	EXPRESSION TAG	UNP Q46925
C	0	ALA	-	EXPRESSION TAG	UNP Q46925
E	-1	GLY	-	EXPRESSION TAG	UNP Q46925
E	0	ALA	-	EXPRESSION TAG	UNP Q46925
G	-1	GLY	-	EXPRESSION TAG	UNP Q46925
G	0	ALA	-	EXPRESSION TAG	UNP Q46925
I	-1	GLY	-	EXPRESSION TAG	UNP Q46925
I	0	ALA	-	EXPRESSION TAG	UNP Q46925
K	-1	GLY	-	EXPRESSION TAG	UNP Q46925
K	0	ALA	-	EXPRESSION TAG	UNP Q46925
M	-1	GLY	-	EXPRESSION TAG	UNP Q46925

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	0	ALA	-	EXPRESSION TAG	UNP Q46925
O	-1	GLY	-	EXPRESSION TAG	UNP Q46925
O	0	ALA	-	EXPRESSION TAG	UNP Q46925

- Molecule 2 is a protein called SULFUR ACCEPTOR PROTEIN CSDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	147	Total	C	N	O	S	0	0	0
			1131	718	202	209	2			
2	D	143	Total	C	N	O	S	0	0	0
			1099	696	197	204	2			
2	F	135	Total	C	N	O	S	0	0	0
			1031	654	180	195	2			
2	H	144	Total	C	N	O	S	0	2	0
			1122	712	201	207	2			
2	J	141	Total	C	N	O	S	0	0	0
			1076	684	188	202	2			
2	L	139	Total	C	N	O	S	0	0	0
			1060	672	186	200	2			
2	N	139	Total	C	N	O	S	0	0	0
			1060	672	186	200	2			
2	P	97	Total	C	N	O	S	0	0	0
			728	458	128	141	1			

There are 56 discrepancies between the modelled and reference sequences:

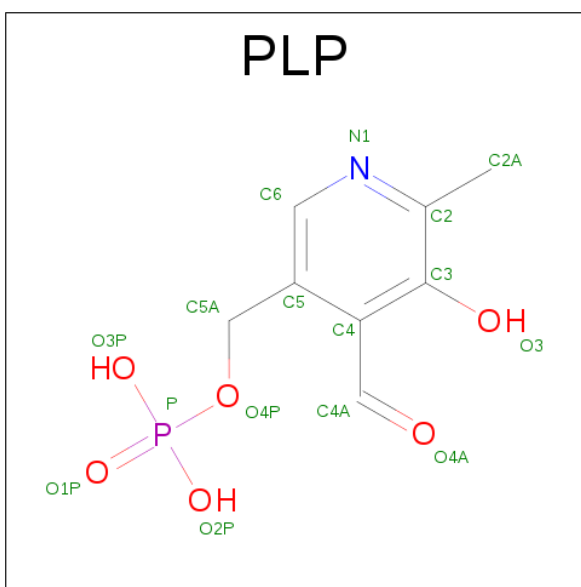
Chain	Residue	Modelled	Actual	Comment	Reference
B	148	LYS	-	EXPRESSION TAG	UNP P0AGF2
B	149	HIS	-	EXPRESSION TAG	UNP P0AGF2
B	150	HIS	-	EXPRESSION TAG	UNP P0AGF2
B	151	HIS	-	EXPRESSION TAG	UNP P0AGF2
B	152	HIS	-	EXPRESSION TAG	UNP P0AGF2
B	153	HIS	-	EXPRESSION TAG	UNP P0AGF2
B	154	HIS	-	EXPRESSION TAG	UNP P0AGF2
D	148	LYS	-	EXPRESSION TAG	UNP P0AGF2
D	149	HIS	-	EXPRESSION TAG	UNP P0AGF2
D	150	HIS	-	EXPRESSION TAG	UNP P0AGF2
D	151	HIS	-	EXPRESSION TAG	UNP P0AGF2
D	152	HIS	-	EXPRESSION TAG	UNP P0AGF2
D	153	HIS	-	EXPRESSION TAG	UNP P0AGF2
D	154	HIS	-	EXPRESSION TAG	UNP P0AGF2
F	148	LYS	-	EXPRESSION TAG	UNP P0AGF2

Continued on next page...

Continued from previous page...

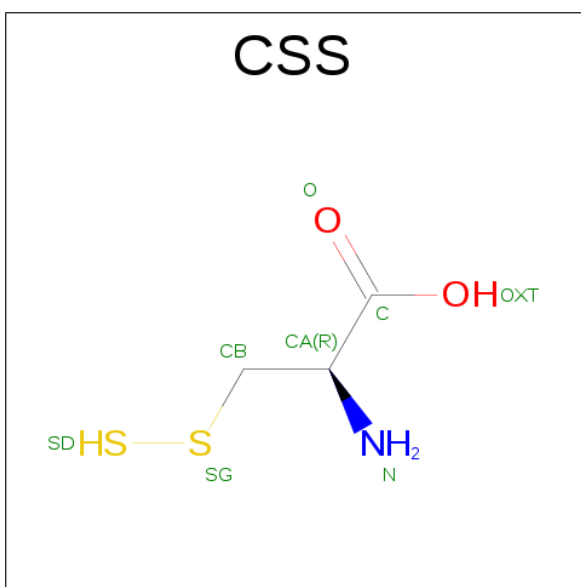
Chain	Residue	Modelled	Actual	Comment	Reference
F	149	HIS	-	EXPRESSION TAG	UNP P0AGF2
F	150	HIS	-	EXPRESSION TAG	UNP P0AGF2
F	151	HIS	-	EXPRESSION TAG	UNP P0AGF2
F	152	HIS	-	EXPRESSION TAG	UNP P0AGF2
F	153	HIS	-	EXPRESSION TAG	UNP P0AGF2
F	154	HIS	-	EXPRESSION TAG	UNP P0AGF2
H	148	LYS	-	EXPRESSION TAG	UNP P0AGF2
H	149	HIS	-	EXPRESSION TAG	UNP P0AGF2
H	150	HIS	-	EXPRESSION TAG	UNP P0AGF2
H	151	HIS	-	EXPRESSION TAG	UNP P0AGF2
H	152	HIS	-	EXPRESSION TAG	UNP P0AGF2
H	153	HIS	-	EXPRESSION TAG	UNP P0AGF2
H	154	HIS	-	EXPRESSION TAG	UNP P0AGF2
J	148	LYS	-	EXPRESSION TAG	UNP P0AGF2
J	149	HIS	-	EXPRESSION TAG	UNP P0AGF2
J	150	HIS	-	EXPRESSION TAG	UNP P0AGF2
J	151	HIS	-	EXPRESSION TAG	UNP P0AGF2
J	152	HIS	-	EXPRESSION TAG	UNP P0AGF2
J	153	HIS	-	EXPRESSION TAG	UNP P0AGF2
J	154	HIS	-	EXPRESSION TAG	UNP P0AGF2
L	148	LYS	-	EXPRESSION TAG	UNP P0AGF2
L	149	HIS	-	EXPRESSION TAG	UNP P0AGF2
L	150	HIS	-	EXPRESSION TAG	UNP P0AGF2
L	151	HIS	-	EXPRESSION TAG	UNP P0AGF2
L	152	HIS	-	EXPRESSION TAG	UNP P0AGF2
L	153	HIS	-	EXPRESSION TAG	UNP P0AGF2
L	154	HIS	-	EXPRESSION TAG	UNP P0AGF2
N	148	LYS	-	EXPRESSION TAG	UNP P0AGF2
N	149	HIS	-	EXPRESSION TAG	UNP P0AGF2
N	150	HIS	-	EXPRESSION TAG	UNP P0AGF2
N	151	HIS	-	EXPRESSION TAG	UNP P0AGF2
N	152	HIS	-	EXPRESSION TAG	UNP P0AGF2
N	153	HIS	-	EXPRESSION TAG	UNP P0AGF2
N	154	HIS	-	EXPRESSION TAG	UNP P0AGF2
P	148	LYS	-	EXPRESSION TAG	UNP P0AGF2
P	149	HIS	-	EXPRESSION TAG	UNP P0AGF2
P	150	HIS	-	EXPRESSION TAG	UNP P0AGF2
P	151	HIS	-	EXPRESSION TAG	UNP P0AGF2
P	152	HIS	-	EXPRESSION TAG	UNP P0AGF2
P	153	HIS	-	EXPRESSION TAG	UNP P0AGF2
P	154	HIS	-	EXPRESSION TAG	UNP P0AGF2

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	I	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	K	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	M	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	O	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is S-MERCAPTOCYSTEINE (three-letter code: CSS) (formula: C₃H₇NO₂S₂).



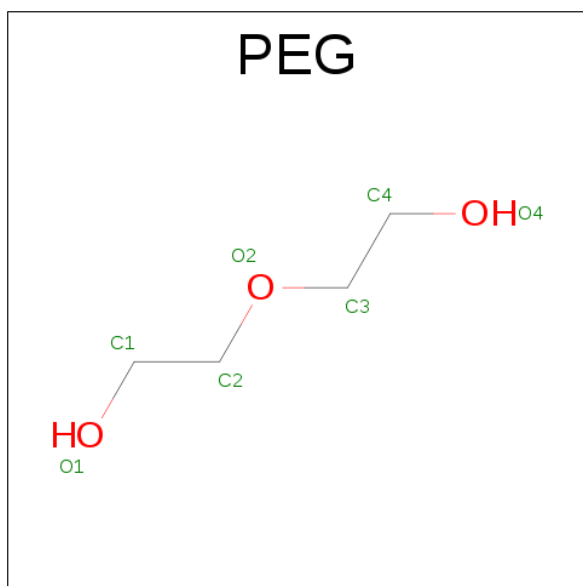
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 7	C 3	N 1	O 1	S 2	0	0
4	B	1	Total 7	C 3	N 1	O 1	S 2	0	0
4	C	1	Total 7	C 3	N 1	O 1	S 2	0	0
4	D	1	Total 7	C 3	N 1	O 1	S 2	0	0
4	E	1	Total 7	C 3	N 1	O 1	S 2	0	0
4	F	1	Total 7	C 3	N 1	O 1	S 2	0	0
4	G	1	Total 7	C 3	N 1	O 1	S 2	0	0
4	H	1	Total 7	C 3	N 1	O 1	S 2	0	0
4	I	1	Total 7	C 3	N 1	O 1	S 2	0	0
4	J	1	Total 7	C 3	N 1	O 1	S 2	0	0
4	K	1	Total 7	C 3	N 1	O 1	S 2	0	0
4	L	1	Total 7	C 3	N 1	O 1	S 2	0	0
4	M	1	Total 7	C 3	N 1	O 1	S 2	0	0
4	N	1	Total 7	C 3	N 1	O 1	S 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	O	1	Total	C	N	O	S	0	0
			7	3	1	1	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



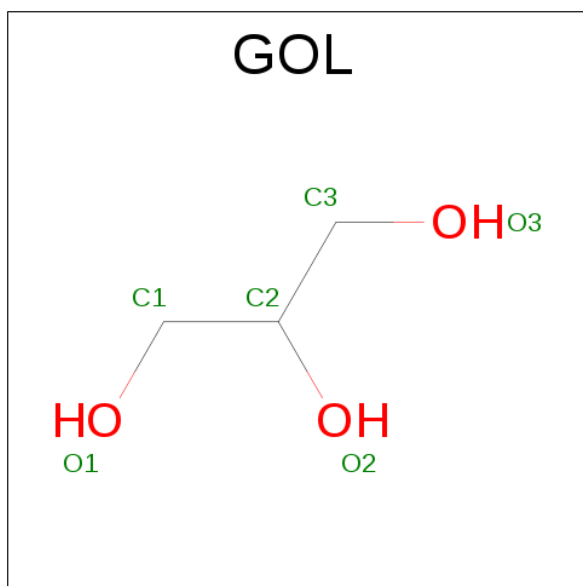
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		
5	H	1	Total	C	O	0	0
			7	4	3		
5	I	1	Total	C	O	0	0
			7	4	3		
5	K	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 6	C 3	O 3	0	0
6	A	1	Total 6	C 3	O 3	0	0
6	A	1	Total 6	C 3	O 3	0	0
6	A	1	Total 6	C 3	O 3	0	0
6	A	1	Total 6	C 3	O 3	0	0
6	A	1	Total 6	C 3	O 3	0	0
6	B	1	Total 6	C 3	O 3	0	0
6	B	1	Total 6	C 3	O 3	0	0
6	B	1	Total 6	C 3	O 3	0	0
6	C	1	Total 6	C 3	O 3	0	0
6	C	1	Total 6	C 3	O 3	0	0
6	C	1	Total 6	C 3	O 3	0	0
6	C	1	Total 6	C 3	O 3	0	0
6	C	1	Total 6	C 3	O 3	0	0
6	C	1	Total 6	C 3	O 3	0	0
6	C	1	Total 6	C 3	O 3	0	0
6	C	1	Total 6	C 3	O 3	0	0
6	C	1	Total 6	C 3	O 3	0	0
6	C	1	Total 6	C 3	O 3	0	0
6	C	1	Total 6	C 3	O 3	0	0
6	D	1	Total 6	C 3	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	I	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	M	1	Total	C	O	0	0
			6	3	3		

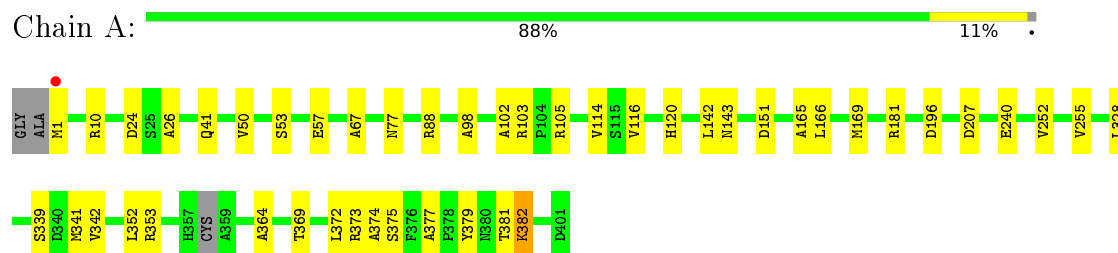
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	197	Total	O	0	0
			197	197		
7	B	57	Total	O	0	0
			57	57		
7	C	132	Total	O	0	0
			132	132		
7	D	34	Total	O	0	0
			34	34		
7	E	180	Total	O	0	0
			180	180		
7	F	15	Total	O	0	0
			15	15		
7	G	169	Total	O	0	0
			169	169		
7	H	38	Total	O	0	0
			38	38		
7	I	127	Total	O	0	0
			127	127		
7	J	14	Total	O	0	0
			14	14		
7	K	38	Total	O	0	0
			38	38		
7	L	3	Total	O	0	0
			3	3		
7	M	13	Total	O	0	0
			13	13		
7	N	2	Total	O	0	0
			2	2		
7	O	2	Total	O	0	0
			2	2		

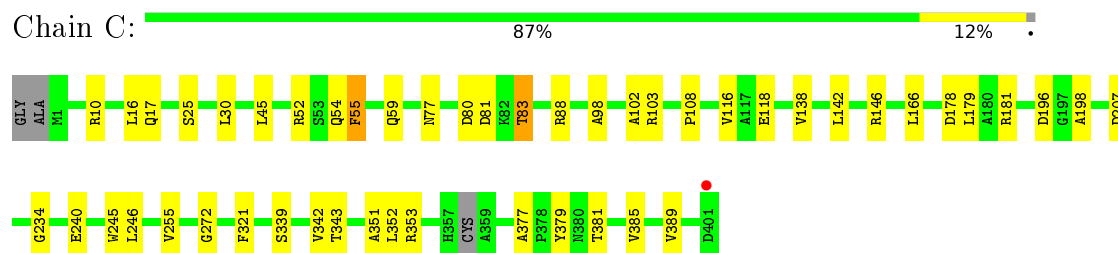
3 Residue-property plots

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.

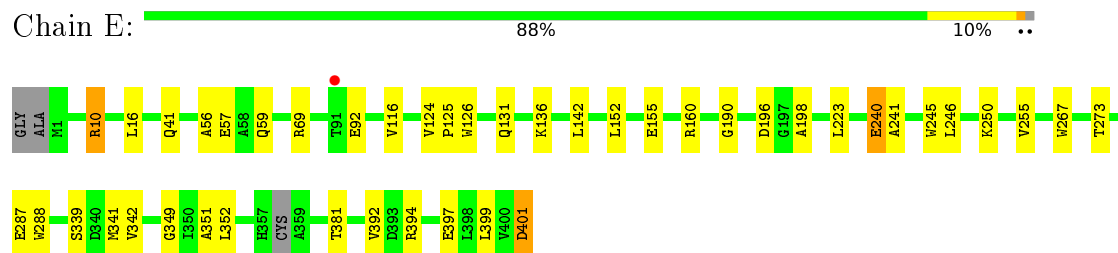
• Molecule 1: CYSTEINE DESULFURASE CSDA



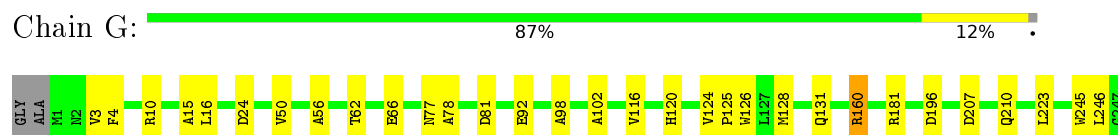
• Molecule 1: CYSTEINE DESULFURASE CSDA



• Molecule 1: CYSTEINE DESULFURASE CSDA

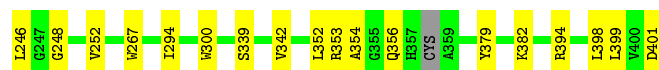
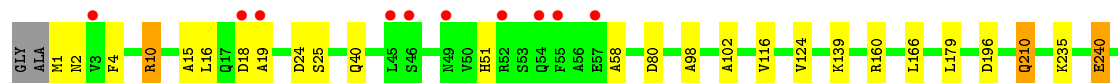
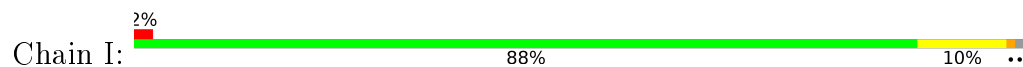


• Molecule 1: CYSTEINE DESULFURASE CSDA

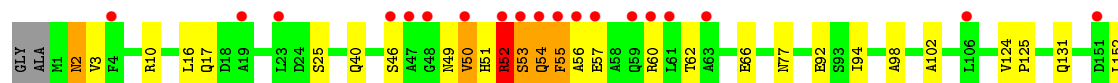
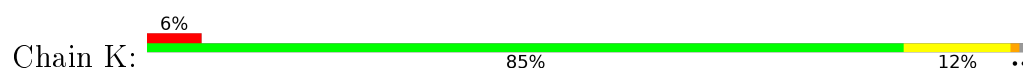




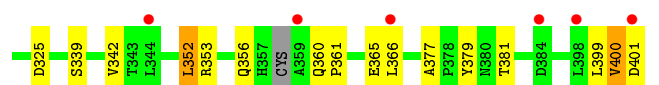
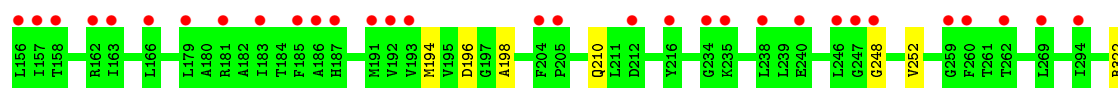
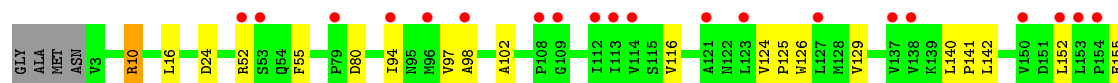
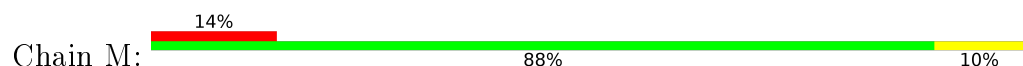
• Molecule 1: CYSTEINE DESULFURASE CSDA



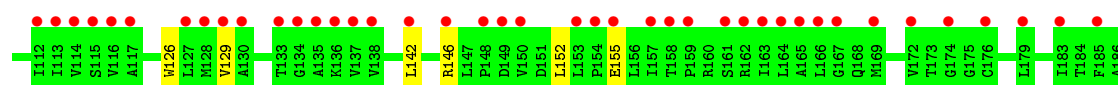
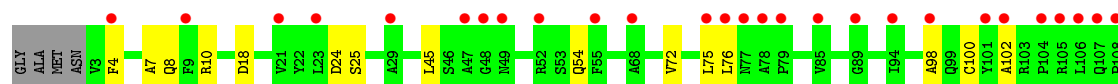
• Molecule 1: CYSTEINE DESULFURASE CSDA

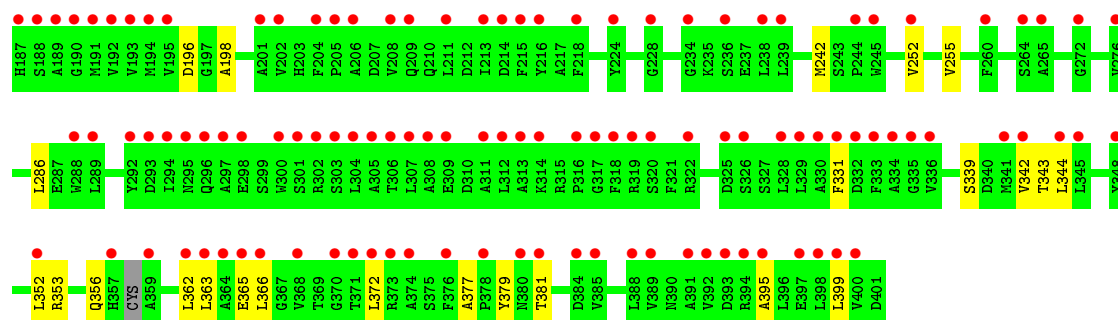


• Molecule 1: CYSTEINE DESULFURASE CSDA

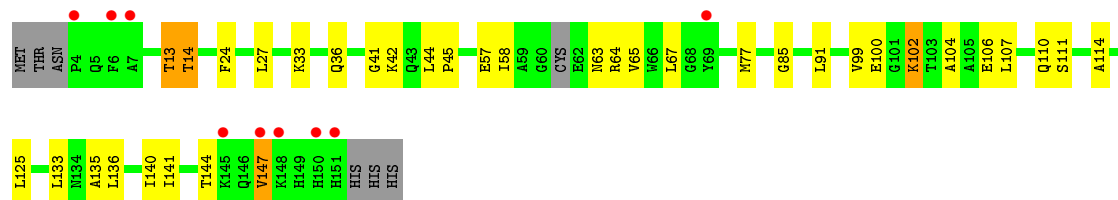


• Molecule 1: CYSTEINE DESULFURASE CSDA

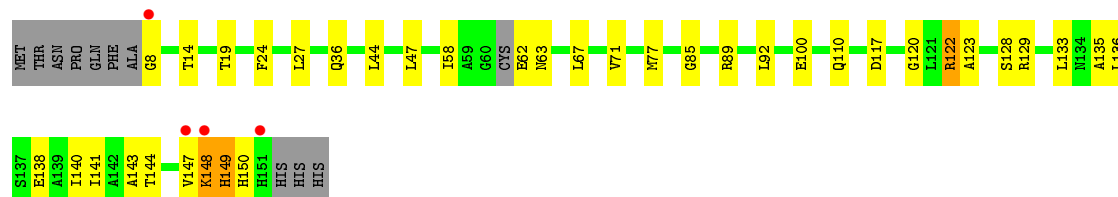




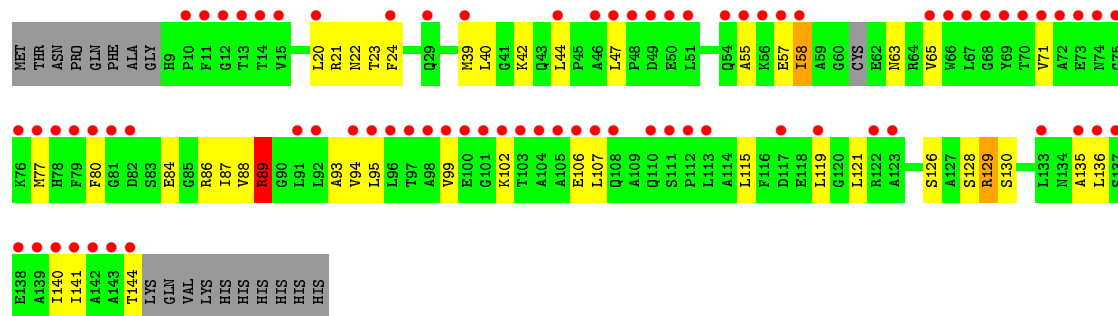
• Molecule 2: SULFUR ACCEPTOR PROTEIN CSDE



• Molecule 2: SULFUR ACCEPTOR PROTEIN CSDE



• Molecule 2: SULFUR ACCEPTOR PROTEIN CSDE

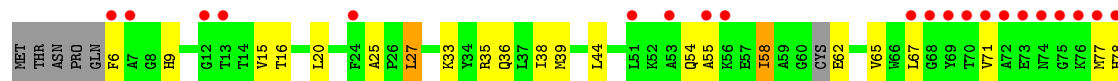


• Molecule 2: SULFUR ACCEPTOR PROTEIN CSDE

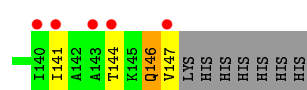
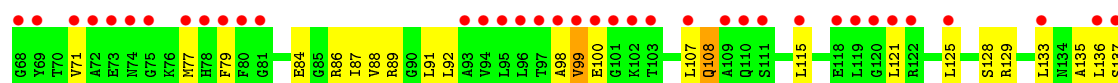
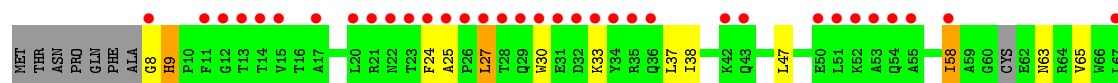




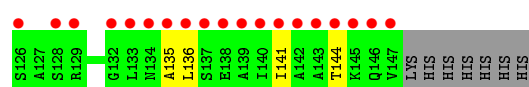
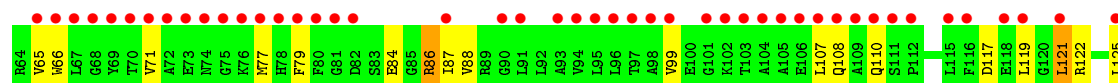
• Molecule 2: SULFUR ACCEPTOR PROTEIN CSDE



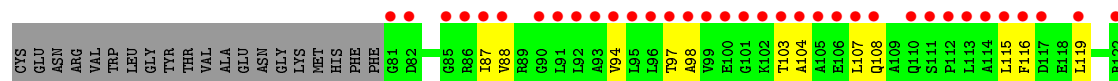
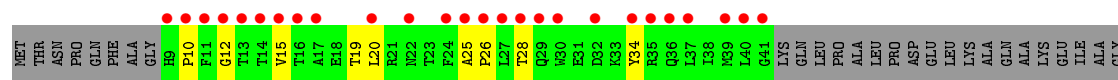
• Molecule 2: SULFUR ACCEPTOR PROTEIN CSDE

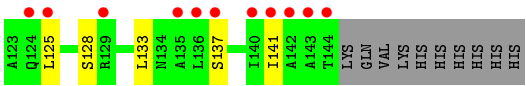


• Molecule 2: SULFUR ACCEPTOR PROTEIN CSDE



• Molecule 2: SULFUR ACCEPTOR PROTEIN CSDE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.86Å 115.14Å 604.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 2.50 48.30 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.30-2.50) 97.8 (48.30-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.254 , 0.279 0.252 , 0.276	Depositor DCC
R_{free} test set	1999 reflections (1.13%)	DCC
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	34325	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, PEG, CSS, PLP

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	0.52	0/3123	0.64	0/4251
1	C	0.52	1/3106 (0.0%)	0.65	3/4229 (0.1%)
1	E	0.54	3/3124 (0.1%)	0.64	2/4253 (0.0%)
1	G	0.55	3/3121 (0.1%)	0.67	3/4249 (0.1%)
1	I	0.53	2/3118 (0.1%)	0.66	2/4245 (0.0%)
1	K	0.50	1/3117 (0.0%)	0.66	2/4244 (0.0%)
1	M	0.48	0/3096	0.58	2/4217 (0.0%)
1	O	0.46	0/3090	0.56	0/4208
2	B	0.57	0/1152	0.66	0/1557
2	D	0.55	0/1118	0.71	2/1511 (0.1%)
2	F	0.55	0/1047	0.69	1/1417 (0.1%)
2	H	0.53	0/1144	0.66	0/1545
2	J	0.52	0/1093	0.66	0/1478
2	L	0.55	1/1076 (0.1%)	0.67	1/1455 (0.1%)
2	N	0.50	0/1076	0.61	0/1455
2	P	0.41	0/736	0.51	0/997
All	All	0.52	11/33337 (0.0%)	0.64	18/45311 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	126	TRP	CD2-CE2	5.68	1.48	1.41
1	E	267	TRP	CD2-CE2	5.48	1.48	1.41
1	C	245	TRP	CD2-CE2	5.47	1.48	1.41
1	G	267	TRP	CD2-CE2	5.37	1.47	1.41
1	E	126	TRP	CD2-CE2	5.34	1.47	1.41
1	I	267	TRP	CD2-CE2	5.27	1.47	1.41
1	K	267	TRP	CD2-CE2	5.21	1.47	1.41
2	L	30	TRP	CD2-CE2	5.15	1.47	1.41
1	G	245	TRP	CD2-CE2	5.08	1.47	1.41
1	I	300	TRP	CD2-CE2	5.08	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	245	TRP	CD2-CE2	5.05	1.47	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	160	ARG	NE-CZ-NH2	-14.29	113.16	120.30
1	K	160	ARG	NE-CZ-NH1	11.31	125.96	120.30
1	C	103	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	M	10	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	I	160	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	G	181	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	E	10	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	G	160	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	I	10	ARG	NE-CZ-NH1	7.10	123.85	120.30
2	D	122	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	M	10	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	L	27	LEU	CA-CB-CG	6.60	130.49	115.30
1	C	103	ARG	CB-CG-CD	6.56	128.65	111.60
1	C	103	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	G	78	ALA	C-N-CD	5.66	140.29	128.40
2	D	100	GLU	N-CA-CB	-5.48	100.74	110.60
1	E	10	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	F	89	ARG	NE-CZ-NH1	5.10	122.85	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	3051	0	3017	41	0
1	C	3040	0	2999	35	0
1	E	3058	0	3013	42	0
1	G	3052	0	3009	40	0
1	I	3052	0	3007	37	0
1	K	3050	0	3005	58	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	3027	0	2986	42	0
1	O	3024	0	2981	38	0
2	B	1131	0	1141	28	0
2	D	1099	0	1111	31	0
2	F	1031	0	1044	46	0
2	H	1122	0	1138	25	0
2	J	1076	0	1091	33	0
2	L	1060	0	1077	36	0
2	N	1060	0	1077	30	0
2	P	728	0	742	21	0
3	A	15	0	7	1	0
3	C	15	0	6	2	0
3	E	15	0	6	2	0
3	G	15	0	7	1	0
3	I	15	0	6	1	0
3	K	15	0	6	2	0
3	M	15	0	6	2	0
3	O	15	0	7	2	0
4	A	7	0	4	1	0
4	B	7	0	5	0	0
4	C	7	0	4	0	0
4	D	7	0	5	5	0
4	E	7	0	4	0	0
4	F	7	0	5	0	0
4	G	7	0	4	0	0
4	H	7	0	5	0	0
4	I	7	0	4	0	0
4	J	7	0	5	1	0
4	K	7	0	4	0	0
4	L	7	0	5	1	0
4	M	7	0	4	0	0
4	N	7	0	5	0	0
4	O	7	0	4	0	0
5	A	21	0	30	3	0
5	B	7	0	10	0	0
5	C	28	0	40	1	0
5	E	28	0	40	0	0
5	G	7	0	10	0	0
5	H	7	0	10	0	0
5	I	7	0	10	0	0
5	K	7	0	10	1	0
6	A	66	0	88	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	18	0	24	0	0
6	C	66	0	88	2	0
6	D	6	0	8	1	0
6	E	66	0	88	1	0
6	G	42	0	56	2	0
6	H	6	0	8	0	0
6	I	30	0	40	3	0
6	M	6	0	8	0	0
7	A	197	0	0	9	0
7	B	57	0	0	5	0
7	C	132	0	0	3	0
7	D	34	0	0	2	0
7	E	180	0	0	5	0
7	F	15	0	0	1	0
7	G	169	0	0	11	0
7	H	38	0	0	1	0
7	I	127	0	0	2	0
7	J	14	0	0	5	0
7	K	38	0	0	1	0
7	L	3	0	0	0	0
7	M	13	0	0	0	0
7	N	2	0	0	0	0
7	O	2	0	0	0	0
All	All	34325	0	33124	542	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 (542) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:25:ALA:O	2:J:27:LEU:HD23	1.48	1.14
1:G:62:THR:HG23	7:G:2044:HOH:O	1.50	1.12
2:P:98:ALA:HB2	2:P:115:LEU:HD22	1.22	1.12
1:A:252:VAL:HG21	1:A:255:VAL:HG22	1.38	1.06
1:O:344:LEU:HD12	1:O:399:LEU:HD21	1.43	0.99
2:B:91:LEU:HD13	2:B:133:LEU:HD11	1.43	0.97
1:E:241:ALA:HB2	6:E:1409:GOL:H12	1.46	0.95
2:J:67:LEU:HD21	2:J:140:ILE:CD1	1.96	0.95
2:N:27:LEU:HD22	2:N:33:LYS:HE3	1.47	0.95
2:L:91:LEU:HD13	2:L:133:LEU:HD11	1.48	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:95:LEU:HD21	2:F:140:ILE:HD11	1.51	0.90
1:K:50:VAL:HG22	1:K:51:HIS:H	1.36	0.89
2:H:35[A]:ARG:HH11	2:H:35[A]:ARG:HG3	1.37	0.89
1:I:18:ASP:O	1:K:52:ARG:HG2	1.74	0.88
2:L:58:ILE:HG21	2:L:135:ALA:HB1	1.56	0.88
1:O:252:VAL:HG21	1:O:255:VAL:HG22	1.53	0.88
2:J:16:THR:O	2:J:20:LEU:HD13	1.74	0.87
4:A:1403:CSS:SD	7:A:2189:HOH:O	2.31	0.87
2:F:126:SER:O	2:F:129:ARG:HG3	1.75	0.86
1:E:131[B]:GLN:O	1:E:131[B]:GLN:NE2	2.08	0.86
2:D:58:ILE:HG21	2:D:135:ALA:HB1	1.56	0.85
1:M:94:ILE:HG23	1:M:194:MET:HE3	1.57	0.85
2:N:77:MET:HE2	2:N:107:LEU:HD22	1.57	0.85
2:B:77:MET:CE	2:B:107:LEU:HD12	2.07	0.83
2:F:39:MET:O	2:F:42:LYS:HG2	1.79	0.83
1:M:116:VAL:HG21	1:M:365:GLU:HG3	1.61	0.82
2:D:62:GLU:HG2	4:D:1152:CSS:SD	2.19	0.82
1:K:51:HIS:O	1:K:52:ARG:HB2	1.77	0.82
2:F:95:LEU:HD21	2:F:140:ILE:CD1	2.09	0.80
2:B:58:ILE:HG21	2:B:135:ALA:HB1	1.65	0.79
2:N:27:LEU:CD2	2:N:33:LYS:HE3	2.11	0.79
2:H:35[A]:ARG:NH1	2:H:35[A]:ARG:HG3	1.90	0.79
2:F:39:MET:O	2:F:42:LYS:CG	2.32	0.78
2:H:58:ILE:HG21	2:H:135:ALA:HB1	1.63	0.78
1:A:252:VAL:HG21	1:A:255:VAL:CG2	2.12	0.78
1:C:108:PRO:HB2	6:C:1414:GOL:H11	1.63	0.78
2:B:102:LYS:NZ	2:B:110:GLN:OE1	2.18	0.77
2:H:72:ALA:HB3	2:H:74:ASN:OD1	1.82	0.77
1:M:400:VAL:HG13	1:M:401:ASP:H	1.51	0.76
2:J:67:LEU:HD21	2:J:140:ILE:HD12	1.69	0.75
1:M:400:VAL:HG13	1:M:401:ASP:OD1	1.87	0.75
1:E:131[B]:GLN:C	1:E:131[B]:GLN:NE2	2.41	0.75
1:C:52:ARG:NH2	7:C:2026:HOH:O	2.18	0.74
1:C:339:SER:O	1:C:342:VAL:HG12	1.87	0.74
2:J:15:VAL:HG12	2:J:20:LEU:HD11	1.69	0.74
1:A:328:LEU:HD22	1:A:373:ARG:HD2	1.69	0.74
1:K:399:LEU:O	2:L:86:ARG:NH2	2.21	0.73
1:E:397:GLU:HG3	7:E:2172:HOH:O	1.88	0.73
1:M:10:ARG:NH2	1:M:381:THR:HG22	2.04	0.73
1:M:400:VAL:HG13	1:M:401:ASP:N	2.04	0.73
1:G:116:VAL:HG21	1:G:365:GLU:HG3	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:94:ILE:HA	1:M:194:MET:CE	2.18	0.73
1:O:352:LEU:CD2	1:O:372:LEU:HD21	2.18	0.73
2:N:77:MET:HE2	2:N:107:LEU:CD2	2.19	0.72
2:F:40:LEU:HD22	2:F:93:ALA:HB3	1.72	0.72
1:G:210:GLN:OE1	7:G:2107:HOH:O	2.05	0.72
2:B:77:MET:HE2	2:B:107:LEU:HD12	1.71	0.71
1:E:10:ARG:HG3	1:E:16:LEU:CD2	2.19	0.71
2:D:147:VAL:O	2:D:147:VAL:HG12	1.91	0.71
1:K:49:ASN:O	1:K:50:VAL:HG12	1.90	0.71
2:D:58:ILE:HG21	2:D:135:ALA:CB	2.20	0.71
2:B:77:MET:HE3	2:B:107:LEU:HD12	1.73	0.71
1:E:288:TRP:CD1	7:E:2140:HOH:O	2.44	0.70
2:N:77:MET:CE	2:N:107:LEU:CD2	2.68	0.70
1:O:352:LEU:HD22	1:O:372:LEU:HD21	1.72	0.70
2:F:40:LEU:HD22	2:F:93:ALA:CB	2.21	0.70
2:N:58:ILE:HG21	2:N:135:ALA:HB1	1.73	0.70
1:C:178:ASP:OD2	1:C:181:ARG:CZ	2.40	0.69
1:I:248:GLY:O	1:I:252:VAL:HG13	1.91	0.69
1:K:248:GLY:O	1:K:252:VAL:HG13	1.92	0.69
1:K:56:ALA:O	1:K:60:ARG:HG3	1.92	0.69
2:L:92:LEU:HD13	2:L:136:LEU:HD13	1.74	0.69
2:F:129:ARG:HH11	2:F:130:SER:H	1.39	0.69
2:F:21:ARG:HD2	2:F:21:ARG:C	2.14	0.69
2:H:35[A]:ARG:CG	2:H:35[A]:ARG:HH11	2.04	0.68
2:F:58:ILE:HG21	2:F:135:ALA:HB1	1.75	0.68
1:A:364:ALA:HB3	7:A:2172:HOH:O	1.94	0.68
2:D:143:ALA:O	2:D:147:VAL:HG23	1.94	0.68
2:N:108:GLN:HE22	2:N:141:ILE:HG23	1.58	0.68
1:O:252:VAL:HG21	1:O:255:VAL:CG2	2.23	0.68
1:A:67:ALA:HB2	5:A:1405:PEG:H12	1.76	0.67
1:I:342:VAL:HG23	1:I:352:LEU:HD12	1.75	0.67
2:F:102:LYS:HB3	2:F:107:LEU:CD1	2.24	0.67
1:O:146:ARG:HE	1:O:366:LEU:HD22	1.59	0.67
2:D:62:GLU:HG2	4:D:1152:CSS:HD	1.56	0.67
2:F:44:LEU:HD23	2:F:89:ARG:HD2	1.77	0.67
2:F:115:LEU:HD13	2:F:115:LEU:O	1.93	0.67
1:O:344:LEU:CD1	1:O:399:LEU:HD21	2.23	0.67
1:A:67:ALA:HB2	5:A:1405:PEG:C1	2.26	0.66
2:J:58:ILE:HG21	2:J:135:ALA:HB1	1.77	0.66
1:K:62:THR:CG2	1:K:66:GLU:OE2	2.43	0.66
2:L:99:VAL:HG22	2:L:100:GLU:H	1.61	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ARG:NH1	1:C:321:PHE:HA	2.10	0.65
2:B:102:LYS:HG3	2:B:106:GLU:OE1	1.96	0.65
2:H:141:ILE:O	2:H:144:THR:HG22	1.97	0.65
1:E:131[B]:GLN:C	1:E:131[B]:GLN:HE21	1.99	0.65
1:K:51:HIS:CE1	1:K:55:PHE:HB3	2.32	0.64
1:K:356:GLN:HB2	4:L:1148:CSS:SD	2.37	0.64
2:D:62:GLU:N	4:D:1152:CSS:HD	1.96	0.64
2:D:123:ALA:HB1	1:E:160:ARG:HD3	1.80	0.64
1:M:94:ILE:HA	1:M:194:MET:HE1	1.79	0.64
2:B:141:ILE:O	2:B:144:THR:HG22	1.97	0.64
1:G:15:ALA:HB3	7:G:2018:HOH:O	1.97	0.64
1:E:401:ASP:HB2	2:F:86:ARG:HH22	1.62	0.63
2:J:9:HIS:CD2	7:J:2001:HOH:O	2.51	0.63
1:E:351:ALA:HB2	1:G:50:VAL:HG12	1.81	0.63
2:N:77:MET:HE3	2:N:79:PHE:CE2	2.34	0.62
1:O:344:LEU:HD12	1:O:399:LEU:CD2	2.22	0.62
2:J:78:HIS:CE1	7:J:2001:HOH:O	2.53	0.62
1:I:294:ILE:HG22	7:I:2093:HOH:O	1.99	0.62
1:M:10:ARG:HG3	1:M:16:LEU:CD2	2.30	0.62
2:N:141:ILE:O	2:N:144:THR:HG22	2.00	0.61
2:D:141:ILE:O	2:D:144:THR:HG22	2.01	0.61
2:J:25:ALA:O	2:J:27:LEU:CD2	2.36	0.61
1:G:339:SER:O	1:G:342:VAL:HG12	2.01	0.61
2:H:65:VAL:CG1	2:H:136:LEU:HD21	2.31	0.61
2:B:65:VAL:CG1	2:B:136:LEU:HD21	2.31	0.60
2:J:71:VAL:HG22	2:J:77:MET:HG2	1.84	0.60
1:M:94:ILE:HA	1:M:194:MET:HE3	1.82	0.60
2:B:91:LEU:HD13	2:B:133:LEU:CD1	2.25	0.60
1:M:339:SER:O	1:M:342:VAL:HG12	2.01	0.60
1:I:51:HIS:CE1	1:I:58:ALA:HB1	2.37	0.59
1:I:15:ALA:O	1:I:19:ALA:HB2	2.02	0.59
1:O:395:ALA:O	1:O:399:LEU:HD23	2.02	0.59
1:K:10:ARG:NH1	1:K:381:THR:HG22	2.17	0.59
1:C:80:ASP:O	1:C:83:THR:HG22	2.01	0.59
2:N:86:ARG:HB3	2:N:86:ARG:HH11	1.68	0.59
1:A:53:SER:OG	7:A:2037:HOH:O	2.17	0.59
1:K:345:LEU:HD13	1:K:352:LEU:HD21	1.84	0.59
2:P:15:VAL:HG13	2:P:19:THR:CG2	2.33	0.59
1:O:72:VAL:O	1:O:75:LEU:HG	2.03	0.59
1:E:250:LYS:NZ	1:E:273:THR:HA	2.18	0.58
2:L:141:ILE:O	2:L:144:THR:HG22	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:141:ILE:O	2:J:144:THR:HG22	2.03	0.58
2:L:91:LEU:HD13	2:L:133:LEU:CD1	2.28	0.58
2:N:108:GLN:NE2	2:N:141:ILE:HG23	2.19	0.58
2:J:39:MET:CE	7:J:2007:HOH:O	2.51	0.58
1:M:97:VAL:HB	1:M:194:MET:CE	2.33	0.58
1:M:399:LEU:O	1:M:400:VAL:HG12	2.02	0.58
1:A:252:VAL:CG2	1:A:255:VAL:HG22	2.25	0.58
2:B:41:GLY:HA3	7:B:2015:HOH:O	2.02	0.58
1:O:352:LEU:HD22	1:O:372:LEU:CD2	2.33	0.58
1:A:328:LEU:CD2	1:A:373:ARG:HD2	2.34	0.58
1:E:351:ALA:HB2	1:G:50:VAL:CG1	2.33	0.58
1:O:10:ARG:NH1	1:O:381:THR:HG22	2.19	0.58
1:C:353:ARG:HD3	7:C:2116:HOH:O	2.03	0.57
1:E:41:GLN:OE1	1:E:57:GLU:HG2	2.04	0.57
2:J:67:LEU:HD21	2:J:140:ILE:HD13	1.83	0.57
2:B:13:THR:OG1	2:B:14:THR:N	2.35	0.57
2:F:102:LYS:HG3	2:F:106:GLU:OE1	2.03	0.57
1:A:10:ARG:NH1	1:A:381:THR:HG22	2.20	0.57
2:F:21:ARG:HD2	2:F:22:ASN:N	2.20	0.57
1:K:50:VAL:HG22	1:K:51:HIS:N	2.13	0.57
2:D:14:THR:O	7:D:2001:HOH:O	2.18	0.57
2:F:39:MET:O	2:F:42:LYS:HG3	2.04	0.57
2:J:71:VAL:HG21	2:J:147:VAL:CG1	2.34	0.57
2:B:33:LYS:NZ	7:B:2012:HOH:O	2.34	0.57
1:O:342:VAL:HG23	1:O:352:LEU:HD12	1.85	0.57
2:L:98:ALA:HB2	2:L:115:LEU:HD22	1.87	0.57
2:P:104:ALA:HA	2:P:107:LEU:HD22	1.87	0.57
2:P:20:LEU:HB3	2:P:119:LEU:HD21	1.86	0.57
2:B:125:LEU:CD1	2:B:133:LEU:HD13	2.35	0.56
1:K:62:THR:HG22	1:K:66:GLU:OE2	2.04	0.56
1:E:250:LYS:HZ3	1:E:273:THR:HA	1.70	0.56
1:C:138:VAL:HG22	5:C:1405:PEG:O4	2.06	0.56
1:E:10:ARG:NH1	1:E:381:THR:HG22	2.21	0.56
2:P:12:GLY:HA2	2:P:97:THR:HG23	1.88	0.56
2:N:71:VAL:HG12	2:N:77:MET:HG2	1.87	0.56
1:A:339:SER:O	1:A:342:VAL:HG12	2.05	0.56
2:J:15:VAL:CG1	2:J:20:LEU:HD11	2.35	0.56
1:I:354:ALA:C	2:J:62:GLU:OE2	2.44	0.56
2:B:67:LEU:HD21	2:B:140:ILE:HG13	1.87	0.56
1:G:399:LEU:O	2:H:86:ARG:NH2	2.25	0.56
1:K:3:VAL:HG13	1:K:3:VAL:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:ALA:CB	7:G:2018:HOH:O	2.54	0.55
2:D:123:ALA:HB1	1:E:160:ARG:CD	2.36	0.55
1:A:114:VAL:HG22	1:A:165:ALA:HB3	1.87	0.55
1:E:152:LEU:HD12	1:E:155:GLU:OE1	2.06	0.55
1:I:16:LEU:HD11	1:I:379:TYR:HB2	1.88	0.55
1:I:10:ARG:HG3	1:I:16:LEU:HD13	1.88	0.55
2:J:15:VAL:HG12	2:J:20:LEU:CD1	2.36	0.55
1:A:105:ARG:NH1	7:A:2068:HOH:O	2.33	0.55
2:B:77:MET:HE1	2:B:104:ALA:HA	1.89	0.55
1:C:17:GLN:HA	1:C:17:GLN:NE2	2.21	0.55
2:F:40:LEU:CD2	2:F:93:ALA:CB	2.83	0.55
2:P:98:ALA:HB2	2:P:115:LEU:CD2	2.16	0.55
1:A:369:THR:HG21	7:A:2176:HOH:O	2.04	0.55
2:D:150:HIS:NE2	1:I:210:GLN:O	2.40	0.55
1:A:151:ASP:OD1	1:A:181[B]:ARG:NH1	2.40	0.55
2:D:8:GLY:N	2:L:108:GLN:HB3	2.22	0.55
2:P:15:VAL:HG13	2:P:19:THR:HG21	1.88	0.55
1:E:401:ASP:CB	2:F:86:ARG:HH22	2.20	0.55
2:F:40:LEU:CD2	2:F:93:ALA:HB1	2.37	0.55
1:K:400:VAL:O	1:K:400:VAL:HG13	2.07	0.55
2:L:58:ILE:HG21	2:L:135:ALA:CB	2.34	0.55
1:M:342:VAL:HG23	1:M:352:LEU:HD12	1.88	0.54
1:M:356:GLN:OE1	1:M:360:GLN:HB2	2.06	0.54
1:K:399:LEU:HD23	2:L:38:ILE:HD13	1.88	0.54
2:N:119:LEU:O	2:N:121:LEU:HD13	2.07	0.54
1:A:50:VAL:HG23	1:C:351:ALA:HB2	1.89	0.54
2:D:44:LEU:HD23	2:D:89:ARG:HD2	1.90	0.54
2:F:22:ASN:HB3	7:F:2004:HOH:O	2.06	0.54
2:J:65:VAL:CG1	2:J:136:LEU:HD21	2.38	0.54
1:K:166:LEU:HD23	1:K:179:LEU:CD1	2.38	0.54
2:D:117:ASP:OD1	2:D:122:ARG:CG	2.56	0.54
1:O:152:LEU:HD12	1:O:155:GLU:OE1	2.08	0.53
2:B:42:LYS:HD3	7:B:2016:HOH:O	2.07	0.53
2:D:77:MET:CE	2:D:147:VAL:HG21	2.39	0.53
2:N:77:MET:CE	2:N:107:LEU:HD22	2.30	0.53
1:O:339:SER:O	1:O:342:VAL:HG12	2.08	0.53
2:B:114:ALA:HB3	7:B:2040:HOH:O	2.07	0.53
1:C:83:THR:OG1	1:C:234:GLY:O	2.26	0.53
1:C:10:ARG:NH1	1:C:381:THR:HG22	2.24	0.53
1:C:80:ASP:OD1	1:C:81:ASP:N	2.42	0.53
1:M:400:VAL:HG22	1:M:401:ASP:H	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:LEU:CD1	2:B:133:LEU:HD11	2.27	0.53
1:G:347:GLU:HB3	2:H:30:TRP:CZ3	2.43	0.53
6:C:1416:GOL:O1	6:C:1416:GOL:O3	2.27	0.53
2:L:125:LEU:HD12	2:L:133:LEU:HD13	1.91	0.53
1:K:50:VAL:HG13	1:K:51:HIS:N	2.24	0.52
2:N:117:ASP:OD1	2:N:122:ARG:CG	2.57	0.52
2:F:102:LYS:HB3	2:F:107:LEU:HD13	1.90	0.52
2:F:71:VAL:HG12	2:F:77:MET:HG2	1.90	0.52
1:M:322:ARG:HE	1:M:325:ASP:HA	1.74	0.52
2:N:27:LEU:HD13	2:N:33:LYS:NZ	2.24	0.52
2:L:71:VAL:HG12	2:L:77:MET:HG2	1.92	0.52
1:M:152:LEU:HD12	1:M:155:GLU:OE1	2.10	0.52
1:M:97:VAL:HB	1:M:194:MET:HE1	1.92	0.52
2:P:103:THR:O	2:P:107:LEU:HD13	2.09	0.52
1:G:334:ALA:HA	7:G:2069:HOH:O	2.09	0.52
2:L:125:LEU:CD1	2:L:133:LEU:HD13	2.39	0.52
2:P:108:GLN:OE1	2:P:141:ILE:HG23	2.09	0.52
1:E:255:VAL:HG11	1:G:120:HIS:NE2	2.25	0.51
1:K:152:LEU:HD12	1:K:155:GLU:OE1	2.11	0.51
1:M:400:VAL:HG22	1:M:401:ASP:N	2.25	0.51
2:P:88:VAL:HG13	2:P:133:LEU:HD11	1.91	0.51
2:F:119:LEU:HB3	2:F:121:LEU:HD13	1.93	0.51
1:I:25:SER:HG	1:I:379:TYR:HH	1.59	0.51
2:N:8:GLY:O	2:N:9:HIS:CD2	2.63	0.51
2:D:62:GLU:N	4:D:1152:CSS:SD	2.83	0.51
2:F:115:LEU:HD13	2:F:115:LEU:C	2.31	0.51
1:O:7:ALA:O	1:O:8:GLN:C	2.49	0.51
1:C:166:LEU:HD23	1:C:179:LEU:CD1	2.40	0.51
1:K:396:LEU:O	1:K:400:VAL:HB	2.10	0.51
2:L:25:ALA:O	2:L:27:LEU:CD1	2.58	0.51
1:C:118:GLU:OE1	7:C:2054:HOH:O	2.19	0.51
2:F:94:VAL:HG13	2:F:115:LEU:HD12	1.93	0.51
2:H:147:VAL:O	2:H:147:VAL:HG13	2.10	0.51
1:E:69:ARG:HB2	7:E:2055:HOH:O	2.11	0.51
2:J:39:MET:HE1	7:J:2007:HOH:O	2.10	0.51
1:K:3:VAL:HG23	1:M:55:PHE:CD1	2.45	0.51
1:O:100:CYS:HB2	1:O:242:MET:HE3	1.93	0.51
2:D:138:GLU:OE1	2:D:138:GLU:HA	2.10	0.51
2:J:98:ALA:HB2	2:J:115:LEU:CD2	2.40	0.51
1:M:94:ILE:CG2	1:M:194:MET:HE3	2.35	0.51
1:K:98:ALA:O	1:K:102:ALA:HB3	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:79:PHE:CE2	2:L:99:VAL:HG21	2.46	0.51
1:A:151:ASP:OD1	1:A:181[B]:ARG:CZ	2.59	0.50
1:A:181[B]:ARG:NH2	7:A:2101:HOH:O	2.44	0.50
2:F:55:ALA:HB2	2:F:80:PHE:HE1	1.76	0.50
2:H:92:LEU:HD13	2:H:136:LEU:HD13	1.92	0.50
1:I:1:MET:O	1:I:2:ASN:CG	2.50	0.50
2:L:27:LEU:HG	2:L:33:LYS:HE3	1.92	0.50
2:D:147:VAL:O	2:D:147:VAL:CG1	2.58	0.50
2:J:39:MET:HE2	7:J:2007:HOH:O	2.12	0.50
7:A:2037:HOH:O	1:C:17:GLN:HG3	2.09	0.50
2:H:58:ILE:HG21	2:H:135:ALA:CB	2.38	0.50
1:A:352:LEU:N	7:A:2166:HOH:O	2.41	0.50
2:N:87:ILE:HD12	2:N:88:VAL:N	2.27	0.50
2:B:125:LEU:HD12	2:B:133:LEU:HD13	1.93	0.49
1:M:342:VAL:HG11	2:N:62:GLU:OE1	2.11	0.49
1:O:356:GLN:HA	1:O:363:LEU:HD11	1.93	0.49
2:F:20:LEU:O	2:F:23:THR:HG23	2.12	0.49
1:K:339:SER:O	1:K:342:VAL:HG12	2.12	0.49
1:E:124:VAL:HG21	1:G:252:VAL:HG11	1.93	0.49
2:L:98:ALA:HB2	2:L:115:LEU:CD2	2.42	0.49
1:E:287:GLU:HB3	7:E:2052:HOH:O	2.12	0.49
1:I:1:MET:O	1:I:2:ASN:ND2	2.45	0.49
1:K:131:GLN:HG2	7:K:2009:HOH:O	2.11	0.49
1:K:51:HIS:O	1:K:52:ARG:CB	2.57	0.49
1:K:54:GLN:HG2	1:K:57:GLU:CD	2.32	0.49
1:E:116:VAL:HG11	1:E:142:LEU:HG	1.95	0.49
1:I:4:PHE:HA	6:I:1405:GOL:H32	1.95	0.49
1:O:25:SER:HG	1:O:379:TYR:HH	1.61	0.49
1:I:4:PHE:HA	6:I:1405:GOL:O2	2.13	0.49
4:D:1152:CSS:C	4:D:1152:CSS:SD	3.01	0.49
2:F:95:LEU:O	2:F:99:VAL:HG22	2.12	0.49
1:E:10:ARG:HG3	1:E:16:LEU:HD21	1.94	0.48
2:L:8:GLY:O	2:L:9:HIS:ND1	2.45	0.48
2:P:108:GLN:NE2	2:P:141:ILE:HD13	2.27	0.48
2:J:71:VAL:HG21	2:J:147:VAL:HG11	1.94	0.48
2:L:146:GLN:NE2	2:L:147:VAL:HG12	2.28	0.48
1:C:146:ARG:HH12	1:C:321:PHE:HA	1.78	0.48
2:N:65:VAL:CG1	2:N:136:LEU:HD21	2.44	0.48
1:O:45:LEU:HD21	1:O:54:GLN:OE1	2.14	0.48
2:J:98:ALA:HB2	2:J:115:LEU:HD22	1.94	0.48
1:E:339:SER:O	1:E:342:VAL:HG12	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:GLU:HG3	1:G:246:LEU:HD11	1.96	0.48
2:B:44:LEU:HD12	2:B:45:PRO:HD2	1.96	0.48
1:A:196:ASP:OD2	3:A:1402:PLP:N1	2.47	0.48
1:A:116:VAL:HG11	1:A:142:LEU:HG	1.94	0.48
1:A:26:ALA:CB	1:A:328:LEU:HD21	2.44	0.48
1:I:246:LEU:HD11	1:K:92:GLU:HG3	1.96	0.48
1:K:287:GLU:HG3	2:P:28:THR:HG21	1.96	0.48
2:P:20:LEU:CD2	2:P:94:VAL:HG13	2.44	0.48
2:B:24:PHE:HA	2:B:27:LEU:HD12	1.96	0.47
2:D:92:LEU:HD13	2:D:136:LEU:HD13	1.95	0.47
2:F:65:VAL:CG1	2:F:136:LEU:HD21	2.44	0.47
1:O:7:ALA:O	1:O:10:ARG:N	2.47	0.47
1:E:349:GLY:HA2	1:G:50:VAL:HG23	1.95	0.47
1:K:16:LEU:HD11	1:K:379:TYR:HB2	1.95	0.47
2:P:25:ALA:N	2:P:26:PRO:CD	2.78	0.47
1:O:343:THR:HG21	2:P:87:ILE:HD13	1.97	0.47
2:F:87:ILE:HD13	2:F:128:SER:OG	2.13	0.47
2:B:77:MET:HE1	2:B:104:ALA:CA	2.44	0.47
2:L:99:VAL:HG23	2:L:107:LEU:HD11	1.95	0.47
2:L:37:LEU:HD21	2:L:121:LEU:HD22	1.96	0.47
1:K:62:THR:HG22	1:K:66:GLU:CD	2.35	0.47
2:N:58:ILE:HG21	2:N:135:ALA:CB	2.42	0.47
2:J:44:LEU:HD23	2:J:89:ARG:HD2	1.96	0.47
1:K:340:ASP:OD1	2:L:87:ILE:HG13	2.14	0.47
2:D:24:PHE:HA	2:D:27:LEU:HD22	1.97	0.47
2:F:20:LEU:O	2:F:23:THR:CG2	2.63	0.47
2:L:91:LEU:CD1	2:L:133:LEU:HD11	2.34	0.47
2:L:24:PHE:O	2:L:27:LEU:HD12	2.15	0.47
1:A:143:ASN:HD22	6:A:1411:GOL:H12	1.79	0.46
1:E:341:MET:CE	1:E:392:VAL:HG13	2.46	0.46
1:K:51:HIS:CG	1:K:52:ARG:H	2.34	0.46
1:E:56:ALA:O	1:E:59:GLN:HG2	2.14	0.46
1:I:196:ASP:OD2	3:I:1402:PLP:N1	2.49	0.46
1:K:399:LEU:HD23	2:L:38:ILE:CD1	2.46	0.46
1:C:16:LEU:HD12	1:C:30:LEU:CD1	2.45	0.46
2:H:134:ASN:ND2	7:H:2036:HOH:O	2.47	0.46
1:I:19:ALA:O	1:K:52:ARG:HD3	2.16	0.46
1:M:97:VAL:HB	1:M:194:MET:HE2	1.97	0.46
1:O:395:ALA:O	1:O:399:LEU:CD2	2.64	0.46
2:D:71:VAL:O	2:D:71:VAL:HG23	2.16	0.46
1:K:2:ASN:O	1:K:296:GLN:NE2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:342:VAL:HG23	1:K:352:LEU:HD12	1.98	0.46
1:M:10:ARG:HG3	1:M:16:LEU:HD21	1.98	0.46
2:D:120:GLY:HA3	6:D:1153:GOL:H2	1.97	0.46
1:E:131[B]:GLN:CA	1:E:131[B]:GLN:HE21	2.29	0.46
1:G:294:ILE:HG22	7:G:2126:HOH:O	2.16	0.46
2:J:15:VAL:CG1	2:J:20:LEU:CD1	2.93	0.46
2:L:25:ALA:O	2:L:27:LEU:HD12	2.14	0.46
1:O:331:PHE:CZ	1:O:372:LEU:HD22	2.51	0.46
1:K:25:SER:HG	1:K:379:TYR:HH	1.64	0.46
1:M:360:GLN:HB3	1:M:361:PRO:HD3	1.98	0.45
2:F:87:ILE:HD12	2:F:88:VAL:N	2.32	0.45
2:D:123:ALA:CB	1:E:160:ARG:HD3	2.45	0.45
2:F:57:GLU:O	2:F:65:VAL:O	2.35	0.45
1:I:124:VAL:HG21	1:K:252:VAL:HG11	1.99	0.45
1:K:55:PHE:N	1:K:55:PHE:CD1	2.73	0.45
2:N:119:LEU:C	2:N:121:LEU:HD13	2.36	0.45
1:A:169:MET:HE3	1:A:328:LEU:HD12	1.99	0.45
2:D:128:SER:O	2:D:133:LEU:HD23	2.16	0.45
1:G:4:PHE:HA	7:G:2008:HOH:O	2.16	0.45
1:G:62:THR:HG22	1:G:66:GLU:OE1	2.17	0.45
7:A:2060:HOH:O	1:C:272:GLY:HA2	2.16	0.45
1:I:10:ARG:HG3	1:I:16:LEU:CD1	2.47	0.45
2:B:147:VAL:O	2:B:147:VAL:HG12	2.17	0.45
1:G:248:GLY:O	1:G:252:VAL:HG13	2.16	0.45
1:K:198:ALA:HB3	3:K:1402:PLP:C2	2.47	0.45
1:A:352:LEU:HD11	1:A:374:ALA:HA	1.99	0.45
2:F:94:VAL:CG1	2:F:115:LEU:HD12	2.46	0.45
2:H:146[B]:GLN:NE2	2:H:146[B]:GLN:CA	2.80	0.45
1:M:116:VAL:HG11	1:M:142:LEU:HG	1.99	0.45
1:M:248:GLY:O	1:M:252:VAL:HG13	2.16	0.45
2:N:48:PRO:HD2	2:N:51:LEU:HD12	1.99	0.45
1:E:124:VAL:N	1:E:125:PRO:CD	2.80	0.45
1:I:339:SER:O	1:I:342:VAL:HG12	2.17	0.45
1:K:53:SER:O	1:K:55:PHE:CD1	2.70	0.45
2:J:27:LEU:HG	2:J:27:LEU:O	2.17	0.44
1:K:196:ASP:OD2	3:K:1402:PLP:N1	2.49	0.44
1:M:400:VAL:CG1	1:M:401:ASP:H	2.20	0.44
2:L:141:ILE:HA	2:L:144:THR:HG22	1.99	0.44
1:O:75:LEU:HD12	1:O:76:LEU:HD23	1.99	0.44
2:L:87:ILE:HD12	2:L:88:VAL:N	2.32	0.44
1:C:178:ASP:OD2	1:C:181:ARG:NH2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:ALA:HB3	1:C:379:TYR:CE1	2.53	0.44
6:G:1408:GOL:H2	7:G:2034:HOH:O	2.15	0.44
2:J:107:LEU:HD21	2:J:140:ILE:HG23	1.98	0.44
1:O:142:LEU:HD11	1:O:362:LEU:CD1	2.48	0.44
1:A:88:ARG:HD3	1:C:88:ARG:HB3	1.99	0.44
1:K:400:VAL:O	1:K:400:VAL:CG1	2.65	0.44
1:A:57:GLU:HG3	6:A:1409:GOL:O3	2.17	0.44
1:C:25:SER:HG	1:C:379:TYR:HH	1.65	0.44
1:M:140:LEU:HD12	1:M:141:PRO:HD2	1.98	0.44
2:B:58:ILE:HG21	2:B:135:ALA:CB	2.42	0.44
2:P:20:LEU:HD23	2:P:94:VAL:HG13	1.99	0.44
2:B:63:ASN:HD21	2:B:85:GLY:H	1.66	0.44
1:G:128:MET:O	1:G:131:GLN:HG3	2.18	0.44
1:I:342:VAL:HG23	1:I:352:LEU:CD1	2.44	0.44
2:L:65:VAL:CG1	2:L:136:LEU:HD21	2.48	0.44
1:E:255:VAL:HG11	1:G:120:HIS:CD2	2.53	0.44
2:H:63:ASN:HD21	2:H:85:GLY:H	1.65	0.44
1:C:246:LEU:HD23	1:C:246:LEU:N	2.32	0.43
1:G:377:ALA:HB3	1:G:379:TYR:CE1	2.53	0.43
1:K:53:SER:O	1:K:55:PHE:CE1	2.70	0.43
2:F:129:ARG:HD2	2:F:130:SER:H	1.82	0.43
1:A:382:LYS:HZ1	2:H:53:ALA:HB1	1.83	0.43
2:F:63:ASN:HD21	2:F:84:GLU:HB2	1.83	0.43
1:I:116:VAL:HG13	1:I:139:LYS:CG	2.48	0.43
1:I:116:VAL:HG13	1:I:139:LYS:HG3	2.01	0.43
1:K:62:THR:HG23	1:K:66:GLU:OE2	2.17	0.43
1:E:246:LEU:HD11	1:G:92:GLU:HG3	2.00	0.43
1:I:240:GLU:HA	1:I:240:GLU:OE1	2.19	0.43
1:O:252:VAL:CG2	1:O:255:VAL:HG22	2.37	0.43
2:P:116:PHE:CZ	2:P:125:LEU:HD13	2.53	0.43
1:A:41:GLN:HE22	1:A:57:GLU:HG2	1.83	0.43
1:M:322:ARG:NH2	1:M:325:ASP:OD1	2.49	0.43
1:A:120:HIS:CD2	1:C:255:VAL:HG11	2.54	0.43
1:A:328:LEU:HD23	1:A:375:SER:HB3	2.00	0.43
2:L:99:VAL:CG2	2:L:107:LEU:HD21	2.48	0.43
2:H:35[B]:ARG:HH11	2:H:35[B]:ARG:HD2	1.67	0.43
1:M:52:ARG:HB2	1:O:18:ASP:HA	2.00	0.43
1:E:342:VAL:HG23	1:E:352:LEU:HD12	2.01	0.43
2:J:129:ARG:HH12	2:J:134:ASN:HD21	1.64	0.43
1:C:116:VAL:HG21	1:C:142:LEU:HG	2.01	0.43
2:N:57:GLU:HG2	2:N:66:TRP:NE1	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:344:LEU:HD21	2:P:34:TYR:CD1	2.53	0.43
1:K:295:ASN:OD1	1:M:52:ARG:HD2	2.19	0.42
2:N:63:ASN:HD21	2:N:84:GLU:HB2	1.84	0.42
1:O:98:ALA:O	1:O:102:ALA:HB3	2.19	0.42
1:O:142:LEU:HD12	1:O:365:GLU:OE1	2.19	0.42
2:B:42:LYS:NZ	7:B:2017:HOH:O	2.52	0.42
2:B:57:GLU:OE2	2:B:64:ARG:NH1	2.45	0.42
1:C:342:VAL:HG13	1:C:343:THR:N	2.33	0.42
1:C:342:VAL:HG23	1:C:352:LEU:HD12	2.01	0.42
1:G:347:GLU:HB3	2:H:30:TRP:CH2	2.54	0.42
1:K:166:LEU:HD23	1:K:179:LEU:HD12	2.02	0.42
1:M:98:ALA:O	1:M:102:ALA:HB3	2.19	0.42
1:O:126:TRP:HA	1:O:129:VAL:HG12	2.01	0.42
1:E:136:LYS:HG2	7:E:2076:HOH:O	2.18	0.42
2:F:102:LYS:CB	2:F:107:LEU:CD1	2.95	0.42
1:G:196:ASP:OD2	3:G:1402:PLP:N1	2.51	0.42
2:J:141:ILE:HA	2:J:144:THR:HG22	2.01	0.42
2:P:98:ALA:CB	2:P:115:LEU:HD22	2.16	0.42
1:O:377:ALA:HB3	1:O:379:TYR:CE1	2.54	0.42
1:C:45:LEU:HD21	1:C:54:GLN:OE1	2.18	0.42
2:D:117:ASP:OD1	2:D:122:ARG:HG3	2.20	0.42
2:D:63:ASN:HD21	2:D:85:GLY:H	1.66	0.42
1:E:240:GLU:OE1	1:E:240:GLU:HA	2.19	0.42
2:H:65:VAL:HG11	2:H:136:LEU:HD21	2.01	0.42
1:I:398:LEU:HD23	2:J:35:ARG:HD2	2.02	0.42
1:K:94:ILE:HG12	1:K:194:MET:CE	2.50	0.42
1:M:198:ALA:HB3	3:M:1402:PLP:C2	2.49	0.42
1:I:235:LYS:HZ3	6:I:1408:GOL:H2	1.85	0.42
1:K:124:VAL:N	1:K:125:PRO:CD	2.83	0.42
1:K:2:ASN:N	1:K:2:ASN:ND2	2.67	0.42
2:F:63:ASN:ND2	2:F:84:GLU:HB2	2.35	0.42
1:G:357:HIS:HE1	1:G:371:THR:HG23	1.85	0.42
2:L:99:VAL:HG13	2:L:100:GLU:N	2.35	0.42
1:O:75:LEU:HD12	1:O:76:LEU:CD2	2.50	0.42
1:A:98:ALA:O	1:A:102:ALA:HB3	2.20	0.42
1:C:55:PHE:CE1	1:C:59:GLN:HG2	2.54	0.42
1:C:77:ASN:HD22	1:C:207:ASP:CG	2.22	0.42
1:I:40:GLN:OE1	1:K:40:GLN:OE1	2.37	0.42
2:L:63:ASN:HD21	2:L:84:GLU:HB2	1.85	0.42
1:M:196:ASP:OD2	3:M:1402:PLP:N1	2.53	0.42
1:C:385:VAL:O	1:C:389:VAL:HG23	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:399:LEU:O	2:F:86:ARG:NH2	2.53	0.42
2:F:115:LEU:HD13	2:F:119:LEU:HD13	2.01	0.42
2:H:71:VAL:HG12	2:H:77:MET:HG2	2.02	0.42
2:L:146:GLN:HE22	2:L:147:VAL:HG12	1.83	0.42
2:L:87:ILE:HD13	2:L:128:SER:OG	2.19	0.42
1:O:196:ASP:OD2	3:O:1402:PLP:N1	2.52	0.42
2:D:67:LEU:HD21	2:D:140:ILE:HG13	2.01	0.42
1:I:10:ARG:NH2	7:I:2006:HOH:O	2.53	0.42
1:C:196:ASP:OD2	3:C:1402:PLP:N1	2.53	0.41
1:C:198:ALA:HB3	3:C:1402:PLP:C2	2.50	0.41
1:E:196:ASP:OD2	3:E:1402:PLP:N1	2.52	0.41
2:F:141:ILE:HA	2:F:144:THR:HG22	2.02	0.41
2:H:67:LEU:HD21	2:H:140:ILE:HG13	2.02	0.41
1:K:77:ASN:HD22	1:K:207:ASP:CG	2.24	0.41
2:P:133:LEU:O	2:P:137:SER:N	2.53	0.41
2:F:23:THR:HG23	2:F:24:PHE:CD2	2.55	0.41
1:I:166:LEU:HD23	1:I:179:LEU:CD1	2.50	0.41
2:N:117:ASP:OD1	2:N:122:ARG:HG2	2.21	0.41
2:N:122:ARG:NH1	2:N:125:LEU:HD23	2.35	0.41
1:E:223:LEU:HD12	1:E:223:LEU:HA	1.86	0.41
1:I:252:VAL:HG11	1:K:124:VAL:HG21	2.02	0.41
1:A:166:LEU:HD12	1:A:166:LEU:HA	1.86	0.41
1:G:337:HIS:HE2	2:H:63:ASN:HD22	1.68	0.41
1:K:55:PHE:H	1:K:55:PHE:HD1	1.58	0.41
2:P:128:SER:O	2:P:133:LEU:HD13	2.19	0.41
1:A:103:ARG:HD3	5:A:1404:PEG:O1	2.21	0.41
1:G:98:ALA:O	1:G:102:ALA:HB3	2.21	0.41
1:I:51:HIS:CE1	1:I:58:ALA:CB	3.03	0.41
1:K:267:TRP:CD1	5:K:1404:PEG:C4	3.03	0.41
2:D:129:ARG:HG2	7:D:2028:HOH:O	2.20	0.41
1:G:10:ARG:HE	1:G:16:LEU:HD13	1.85	0.41
1:G:223:LEU:HD12	1:G:223:LEU:HA	1.80	0.41
1:G:347:GLU:CB	2:H:30:TRP:CZ3	3.03	0.41
1:I:399:LEU:HD23	2:J:38:ILE:HD13	2.03	0.41
1:A:24:ASP:OD2	1:A:353:ARG:NH1	2.54	0.41
2:F:129:ARG:HD2	2:F:130:SER:N	2.35	0.41
1:O:75:LEU:HD23	1:O:286:LEU:HD22	2.02	0.41
1:A:41:GLN:NE2	6:A:1409:GOL:O2	2.45	0.41
1:G:196:ASP:C	1:G:196:ASP:OD1	2.58	0.41
1:G:56:ALA:HB1	7:G:2039:HOH:O	2.19	0.41
2:J:71:VAL:HG21	2:J:147:VAL:CG2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:10:ARG:HH21	1:M:381:THR:HG22	1.80	0.41
2:N:63:ASN:ND2	2:N:84:GLU:HB2	2.35	0.41
1:A:77:ASN:HD22	1:A:207:ASP:CG	2.24	0.41
1:C:98:ALA:O	1:C:102:ALA:HB3	2.21	0.41
2:D:117:ASP:OD1	2:D:122:ARG:HG2	2.20	0.41
2:F:102:LYS:CG	2:F:106:GLU:OE1	2.67	0.41
2:H:98:ALA:HB2	2:H:115:LEU:HD23	2.01	0.41
1:I:98:ALA:O	1:I:102:ALA:HB3	2.21	0.41
1:O:198:ALA:HB3	3:O:1402:PLP:C2	2.50	0.41
1:G:24:ASP:OD2	1:G:353:ARG:NH1	2.54	0.41
1:K:240:GLU:HA	1:K:240:GLU:OE1	2.21	0.41
1:A:377:ALA:HB3	1:A:379:TYR:CE1	2.55	0.40
1:G:62:THR:CG2	7:G:2044:HOH:O	2.31	0.40
1:I:24:ASP:OD2	1:I:353:ARG:NH1	2.54	0.40
1:K:51:HIS:CG	1:K:52:ARG:N	2.88	0.40
2:N:117:ASP:OD1	2:N:122:ARG:HG3	2.21	0.40
1:A:53:SER:HA	1:E:190:GLY:HA3	2.03	0.40
1:E:198:ALA:HB3	3:E:1402:PLP:C2	2.51	0.40
2:F:87:ILE:HD12	2:F:88:VAL:HG23	2.02	0.40
1:I:356:GLN:HB2	4:J:1148:CSS:SD	2.61	0.40
2:J:27:LEU:HD12	2:J:33:LYS:HZ2	1.85	0.40
1:O:24:ASP:OD2	1:O:353:ARG:NH1	2.54	0.40
1:A:341:MET:HG2	1:A:372:LEU:HD11	2.02	0.40
1:G:357:HIS:CE1	1:G:371:THR:HG23	2.56	0.40
1:G:400:VAL:O	1:G:401:ASP:CG	2.60	0.40
2:L:63:ASN:ND2	2:L:84:GLU:HB2	2.36	0.40
1:M:126:TRP:HA	1:M:129:VAL:HG12	2.04	0.40
2:N:141:ILE:HA	2:N:144:THR:HG22	2.02	0.40
2:D:148:LYS:C	2:D:149:HIS:ND1	2.74	0.40
1:G:124:VAL:N	1:G:125:PRO:CD	2.84	0.40
1:G:160:ARG:HG3	7:G:2093:HOH:O	2.21	0.40
1:M:124:VAL:N	1:M:125:PRO:CD	2.84	0.40
1:M:342:VAL:HG23	1:M:352:LEU:CD1	2.51	0.40
1:A:240:GLU:OE1	1:A:240:GLU:HA	2.22	0.40
1:G:77:ASN:HD22	1:G:207:ASP:CG	2.25	0.40
2:H:148:LYS:HD2	2:H:148:LYS:HA	1.89	0.40
1:I:196:ASP:OD1	1:I:196:ASP:C	2.59	0.40
1:M:24:ASP:OD2	1:M:353:ARG:NH1	2.54	0.40
1:M:377:ALA:HB3	1:M:379:TYR:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	398/403 (99%)	386 (97%)	12 (3%)	0	100	100
1	C	396/403 (98%)	385 (97%)	11 (3%)	0	100	100
1	E	398/403 (99%)	386 (97%)	12 (3%)	0	100	100
1	G	398/403 (99%)	386 (97%)	11 (3%)	1 (0%)	46	68
1	I	398/403 (99%)	386 (97%)	12 (3%)	0	100	100
1	K	397/403 (98%)	385 (97%)	9 (2%)	3 (1%)	24	41
1	M	395/403 (98%)	384 (97%)	10 (2%)	1 (0%)	46	68
1	O	394/403 (98%)	380 (96%)	13 (3%)	1 (0%)	46	68
2	B	143/154 (93%)	136 (95%)	4 (3%)	3 (2%)	9	14
2	D	139/154 (90%)	135 (97%)	2 (1%)	2 (1%)	14	24
2	F	131/154 (85%)	128 (98%)	1 (1%)	2 (2%)	13	22
2	H	142/154 (92%)	134 (94%)	5 (4%)	3 (2%)	9	14
2	J	137/154 (89%)	130 (95%)	3 (2%)	4 (3%)	6	8
2	L	135/154 (88%)	127 (94%)	4 (3%)	4 (3%)	5	7
2	N	135/154 (88%)	128 (95%)	3 (2%)	4 (3%)	5	7
2	P	93/154 (60%)	84 (90%)	8 (9%)	1 (1%)	17	31
All	All	4229/4456 (95%)	4080 (96%)	120 (3%)	29 (1%)	26	46

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	149	HIS
2	J	55	ALA
1	K	17	GLN
1	K	50	VAL
1	K	52	ARG
2	L	9	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	9	HIS
1	O	4	PHE
2	H	8	GLY
2	J	58	ILE
2	L	58	ILE
2	N	58	ILE
2	P	10	PRO
2	F	58	ILE
2	J	54	GLN
2	D	47	LEU
2	F	47	LEU
2	H	47	LEU
2	L	47	LEU
1	M	400	VAL
2	N	47	LEU
1	G	3	VAL
2	B	99	VAL
2	B	100	GLU
2	H	99	VAL
2	J	99	VAL
2	L	99	VAL
2	N	99	VAL
2	B	147	VAL

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	316/315 (100%)	314 (99%)	2 (1%)	90	97
1	C	314/315 (100%)	311 (99%)	3 (1%)	82	95
1	E	316/315 (100%)	313 (99%)	3 (1%)	84	95
1	G	316/315 (100%)	315 (100%)	1 (0%)	94	99
1	I	316/315 (100%)	310 (98%)	6 (2%)	65	87
1	K	315/315 (100%)	307 (98%)	8 (2%)	55	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	313/315 (99%)	309 (99%)	4 (1%)	76	92
1	O	312/315 (99%)	312 (100%)	0	100	100
2	B	115/122 (94%)	110 (96%)	5 (4%)	35	61
2	D	112/122 (92%)	108 (96%)	4 (4%)	42	69
2	F	105/122 (86%)	103 (98%)	2 (2%)	65	87
2	H	114/122 (93%)	108 (95%)	6 (5%)	28	50
2	J	109/122 (89%)	101 (93%)	8 (7%)	17	32
2	L	108/122 (88%)	103 (95%)	5 (5%)	33	57
2	N	108/122 (88%)	104 (96%)	4 (4%)	41	68
2	P	75/122 (62%)	75 (100%)	0	100	100
All	All	3364/3496 (96%)	3303 (98%)	61 (2%)	66	88

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	382	LYS
2	B	13	THR
2	B	14	THR
2	B	36	GLN
2	B	102	LYS
2	B	111	SER
1	C	55	PHE
1	C	83	THR
1	C	240	GLU
2	D	19	THR
2	D	36	GLN
2	D	110	GLN
2	D	148	LYS
1	E	240	GLU
1	E	394	ARG
1	E	401	ASP
2	F	89	ARG
2	F	129	ARG
1	G	81	ASP
2	H	14	THR
2	H	21	ARG
2	H	35[A]	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	35[B]	ARG
2	H	110	GLN
2	H	138	GLU
1	I	80	ASP
1	I	210	GLN
1	I	240	GLU
1	I	382	LYS
1	I	394	ARG
1	I	401	ASP
2	J	6	PHE
2	J	27	LEU
2	J	36	GLN
2	J	110	GLN
2	J	129	ARG
2	J	134	ASN
2	J	138	GLU
2	J	140	ILE
1	K	2	ASN
1	K	46	SER
1	K	52	ARG
1	K	53	SER
1	K	54	GLN
1	K	55	PHE
1	K	209	GLN
1	K	401	ASP
2	L	89	ARG
2	L	108	GLN
2	L	129	ARG
2	L	137	SER
2	L	146	GLN
1	M	80	ASP
1	M	210	GLN
1	M	352	LEU
1	M	366	LEU
2	N	18	GLU
2	N	86	ARG
2	N	110	GLN
2	N	121	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	41	GLN
1	A	77	ASN
1	A	275	ASN
2	B	22	ASN
2	B	63	ASN
2	B	124	GLN
1	C	131	GLN
1	C	168	GLN
1	C	203	HIS
2	D	63	ASN
1	E	77	ASN
1	E	107	GLN
1	E	168	GLN
1	E	360	GLN
2	F	63	ASN
1	G	131	GLN
1	G	357	HIS
2	H	63	ASN
2	H	108	GLN
2	H	134	ASN
1	I	17	GLN
1	I	51	HIS
1	I	187	HIS
1	I	203	HIS
1	I	210	GLN
1	I	275	ASN
1	I	390	ASN
2	J	22	ASN
2	J	63	ASN
2	J	134	ASN
1	K	2	ASN
1	K	51	HIS
1	K	74	GLN
1	K	131	GLN
1	K	203	HIS
2	L	22	ASN
2	L	63	ASN
2	L	146	GLN
1	M	12	GLN
1	M	131	GLN
1	M	203	HIS
1	M	210	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	390	ASN
2	N	22	ASN
2	N	63	ASN
2	N	124	GLN
1	O	41	GLN
1	O	131	GLN
1	O	203	HIS
2	P	110	GLN
2	P	134	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

90 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	$\# Z > 2$
3	PLP	A	1402	1	15,15,16	4.06	3 (20%)	21,22,23	1.32	2 (9%)
4	CSS	A	1403	1	3,6,7	0.81	0	3,6,8	1.31	0
5	PEG	A	1404	-	6,6,6	0.58	0	5,5,5	0.50	0
5	PEG	A	1405	-	6,6,6	0.63	0	5,5,5	0.32	0
5	PEG	A	1406	-	6,6,6	0.58	0	5,5,5	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	A	1407	-	5,5,5	0.33	0	5,5,5	0.35	0
6	GOL	A	1408	-	5,5,5	0.34	0	5,5,5	0.39	0
6	GOL	A	1409	-	5,5,5	0.47	0	5,5,5	0.37	0
6	GOL	A	1410	-	5,5,5	0.37	0	5,5,5	0.22	0
6	GOL	A	1411	-	5,5,5	0.27	0	5,5,5	0.20	0
6	GOL	A	1412	-	5,5,5	0.25	0	5,5,5	0.35	0
6	GOL	A	1413	-	5,5,5	0.42	0	5,5,5	0.37	0
6	GOL	A	1414	-	5,5,5	0.32	0	5,5,5	0.17	0
6	GOL	A	1415	-	5,5,5	0.48	0	5,5,5	0.37	0
6	GOL	A	1416	-	5,5,5	0.32	0	5,5,5	0.34	0
6	GOL	A	2401	-	5,5,5	0.29	0	5,5,5	0.28	0
4	CSS	B	1152	2	3,6,7	0.85	0	3,6,8	1.91	1 (33%)
5	PEG	B	1153	-	6,6,6	0.55	0	5,5,5	0.29	0
6	GOL	B	1154	-	5,5,5	0.40	0	5,5,5	0.23	0
6	GOL	B	1155	-	5,5,5	0.44	0	5,5,5	0.38	0
6	GOL	B	2401	-	5,5,5	0.30	0	5,5,5	0.18	0
3	PLP	C	1402	1	15,15,16	3.48	3 (20%)	21,22,23	1.28	2 (9%)
4	CSS	C	1403	1	3,6,7	0.90	0	3,6,8	1.14	0
5	PEG	C	1404	-	6,6,6	0.56	0	5,5,5	0.21	0
5	PEG	C	1405	-	6,6,6	0.62	0	5,5,5	0.38	0
5	PEG	C	1406	-	6,6,6	0.58	0	5,5,5	0.30	0
5	PEG	C	1407	-	6,6,6	0.55	0	5,5,5	0.31	0
6	GOL	C	1408	-	5,5,5	0.38	0	5,5,5	0.30	0
6	GOL	C	1409	-	5,5,5	0.35	0	5,5,5	0.28	0
6	GOL	C	1410	-	5,5,5	0.34	0	5,5,5	0.27	0
6	GOL	C	1411	-	5,5,5	0.29	0	5,5,5	0.25	0
6	GOL	C	1412	-	5,5,5	0.29	0	5,5,5	0.19	0
6	GOL	C	1413	-	5,5,5	0.46	0	5,5,5	0.38	0
6	GOL	C	1414	-	5,5,5	0.44	0	5,5,5	0.56	0
6	GOL	C	1415	-	5,5,5	0.42	0	5,5,5	0.31	0
6	GOL	C	1416	-	5,5,5	0.37	0	5,5,5	0.30	0
6	GOL	C	1417	-	5,5,5	0.36	0	5,5,5	0.36	0
6	GOL	C	1418	-	5,5,5	0.32	0	5,5,5	0.19	0
4	CSS	D	1152	2	3,6,7	0.77	0	3,6,8	1.52	0
6	GOL	D	1153	-	5,5,5	0.39	0	5,5,5	0.21	0
3	PLP	E	1402	1	15,15,16	3.51	3 (20%)	21,22,23	1.20	2 (9%)
4	CSS	E	1403	1	3,6,7	0.75	0	3,6,8	1.36	0
5	PEG	E	1404	-	6,6,6	0.60	0	5,5,5	0.34	0
5	PEG	E	1405	-	6,6,6	0.54	0	5,5,5	0.21	0
5	PEG	E	1406	-	6,6,6	0.62	0	5,5,5	0.19	0
5	PEG	E	1407	-	6,6,6	0.57	0	5,5,5	0.34	0
6	GOL	E	1408	-	5,5,5	0.41	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	E	1409	-	5,5,5	0.40	0	5,5,5	0.33	0
6	GOL	E	1410	-	5,5,5	0.34	0	5,5,5	0.50	0
6	GOL	E	1411	-	5,5,5	0.46	0	5,5,5	0.30	0
6	GOL	E	1412	-	5,5,5	0.40	0	5,5,5	0.43	0
6	GOL	E	1413	-	5,5,5	0.45	0	5,5,5	0.31	0
6	GOL	E	1414	-	5,5,5	0.24	0	5,5,5	0.28	0
6	GOL	E	1415	-	5,5,5	0.49	0	5,5,5	0.51	0
6	GOL	E	1416	-	5,5,5	0.36	0	5,5,5	0.30	0
6	GOL	E	1417	-	5,5,5	0.36	0	5,5,5	0.31	0
6	GOL	E	2401	-	5,5,5	0.41	0	5,5,5	0.38	0
4	CSS	F	1145	2	3,6,7	0.79	0	3,6,8	1.39	0
3	PLP	G	1402	1	15,15,16	2.88	3 (20%)	21,22,23	1.92	4 (19%)
4	CSS	G	1403	1	3,6,7	0.78	0	3,6,8	1.27	1 (33%)
5	PEG	G	1404	-	6,6,6	0.58	0	5,5,5	0.37	0
6	GOL	G	1405	-	5,5,5	0.38	0	5,5,5	0.22	0
6	GOL	G	1406	-	5,5,5	0.48	0	5,5,5	0.55	0
6	GOL	G	1407	-	5,5,5	0.44	0	5,5,5	0.25	0
6	GOL	G	1408	-	5,5,5	0.38	0	5,5,5	0.35	0
6	GOL	G	1409	-	5,5,5	0.35	0	5,5,5	0.25	0
6	GOL	G	1410	-	5,5,5	0.39	0	5,5,5	0.43	0
6	GOL	G	1411	-	5,5,5	0.31	0	5,5,5	0.12	0
4	CSS	H	1151	2	3,6,7	0.77	0	3,6,8	1.52	0
5	PEG	H	1152	-	6,6,6	0.56	0	5,5,5	0.35	0
6	GOL	H	1153	-	5,5,5	0.39	0	5,5,5	0.27	0
3	PLP	I	1402	1	15,15,16	3.73	3 (20%)	21,22,23	1.13	2 (9%)
4	CSS	I	1403	1	3,6,7	1.05	0	3,6,8	1.21	1 (33%)
5	PEG	I	1404	-	6,6,6	0.59	0	5,5,5	0.17	0
6	GOL	I	1405	-	5,5,5	0.36	0	5,5,5	0.37	0
6	GOL	I	1406	-	5,5,5	0.32	0	5,5,5	0.16	0
6	GOL	I	1407	-	5,5,5	0.43	0	5,5,5	0.58	0
6	GOL	I	1408	-	5,5,5	0.30	0	5,5,5	0.22	0
6	GOL	I	2401	-	5,5,5	0.43	0	5,5,5	0.45	0
4	CSS	J	1148	2	3,6,7	0.82	0	3,6,8	1.68	1 (33%)
3	PLP	K	1402	1	15,15,16	3.62	3 (20%)	21,22,23	1.09	2 (9%)
4	CSS	K	1403	1	3,6,7	0.95	0	3,6,8	1.36	1 (33%)
5	PEG	K	1404	-	6,6,6	0.64	0	5,5,5	0.42	0
4	CSS	L	1148	2	3,6,7	0.85	0	3,6,8	1.73	1 (33%)
3	PLP	M	1402	1	15,15,16	3.71	3 (20%)	21,22,23	1.22	2 (9%)
4	CSS	M	1403	1	3,6,7	0.77	0	3,6,8	1.24	0
6	GOL	M	1404	-	5,5,5	0.36	0	5,5,5	0.27	0
4	CSS	N	1148	2	3,6,7	0.89	0	3,6,8	1.87	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLP	O	1402	1	15,15,16	3.94	3 (20%)	21,22,23	1.27	2 (9%)
4	CSS	O	1403	1	3,6,7	0.83	0	3,6,8	1.17	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
3	PLP	A	1402	1	-	0/6/6/8	0/1/1/1
4	CSS	A	1403	1	-	0/1/5/7	0/0/0/0
5	PEG	A	1404	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1405	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1406	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1407	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1408	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1409	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1410	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1411	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1412	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1413	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1414	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1415	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1416	-	-	0/4/4/4	0/0/0/0
6	GOL	A	2401	-	-	0/4/4/4	0/0/0/0
4	CSS	B	1152	2	-	0/1/5/7	0/0/0/0
5	PEG	B	1153	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1154	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1155	-	-	0/4/4/4	0/0/0/0
6	GOL	B	2401	-	-	0/4/4/4	0/0/0/0
3	PLP	C	1402	1	-	0/6/6/8	0/1/1/1
4	CSS	C	1403	1	-	0/1/5/7	0/0/0/0
5	PEG	C	1404	-	-	0/4/4/4	0/0/0/0
5	PEG	C	1405	-	-	0/4/4/4	0/0/0/0
5	PEG	C	1406	-	-	0/4/4/4	0/0/0/0
5	PEG	C	1407	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1408	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1409	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1410	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1411	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1412	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1413	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	1414	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1415	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1416	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1417	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1418	-	-	0/4/4/4	0/0/0/0
4	CSS	D	1152	2	-	0/1/5/7	0/0/0/0
6	GOL	D	1153	-	-	0/4/4/4	0/0/0/0
3	PLP	E	1402	1	-	0/6/6/8	0/1/1/1
4	CSS	E	1403	1	-	0/1/5/7	0/0/0/0
5	PEG	E	1404	-	-	0/4/4/4	0/0/0/0
5	PEG	E	1405	-	-	0/4/4/4	0/0/0/0
5	PEG	E	1406	-	-	0/4/4/4	0/0/0/0
5	PEG	E	1407	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1408	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1409	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1410	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1411	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1412	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1413	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1414	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1415	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1416	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1417	-	-	0/4/4/4	0/0/0/0
6	GOL	E	2401	-	-	0/4/4/4	0/0/0/0
4	CSS	F	1145	2	-	0/1/5/7	0/0/0/0
3	PLP	G	1402	1	-	0/6/6/8	0/1/1/1
4	CSS	G	1403	1	-	0/1/5/7	0/0/0/0
5	PEG	G	1404	-	-	0/4/4/4	0/0/0/0
6	GOL	G	1405	-	-	0/4/4/4	0/0/0/0
6	GOL	G	1406	-	-	0/4/4/4	0/0/0/0
6	GOL	G	1407	-	-	0/4/4/4	0/0/0/0
6	GOL	G	1408	-	-	0/4/4/4	0/0/0/0
6	GOL	G	1409	-	-	0/4/4/4	0/0/0/0
6	GOL	G	1410	-	-	0/4/4/4	0/0/0/0
6	GOL	G	1411	-	-	0/4/4/4	0/0/0/0
4	CSS	H	1151	2	-	0/1/5/7	0/0/0/0
5	PEG	H	1152	-	-	0/4/4/4	0/0/0/0
6	GOL	H	1153	-	-	0/4/4/4	0/0/0/0
3	PLP	I	1402	1	-	0/6/6/8	0/1/1/1
4	CSS	I	1403	1	-	0/1/5/7	0/0/0/0
5	PEG	I	1404	-	-	0/4/4/4	0/0/0/0
6	GOL	I	1405	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	I	1406	-	-	0/4/4/4	0/0/0/0
6	GOL	I	1407	-	-	0/4/4/4	0/0/0/0
6	GOL	I	1408	-	-	0/4/4/4	0/0/0/0
6	GOL	I	2401	-	-	0/4/4/4	0/0/0/0
4	CSS	J	1148	2	-	0/1/5/7	0/0/0/0
3	PLP	K	1402	1	-	0/6/6/8	0/1/1/1
4	CSS	K	1403	1	-	0/1/5/7	0/0/0/0
5	PEG	K	1404	-	-	0/4/4/4	0/0/0/0
4	CSS	L	1148	2	-	0/1/5/7	0/0/0/0
3	PLP	M	1402	1	-	0/6/6/8	0/1/1/1
4	CSS	M	1403	1	-	0/1/5/7	0/0/0/0
6	GOL	M	1404	-	-	0/4/4/4	0/0/0/0
4	CSS	N	1148	2	-	0/1/5/7	0/0/0/0
3	PLP	O	1402	1	-	0/6/6/8	0/1/1/1
4	CSS	O	1403	1	-	0/1/5/7	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1402	PLP	C3-C4	3.31	1.47	1.40
3	I	1402	PLP	C3-C4	3.62	1.48	1.40
3	A	1402	PLP	C3-C4	3.72	1.48	1.40
3	C	1402	PLP	C3-C4	3.72	1.48	1.40
3	K	1402	PLP	C3-C4	3.78	1.48	1.40
3	E	1402	PLP	C3-C4	3.81	1.48	1.40
3	M	1402	PLP	C3-C4	3.96	1.49	1.40
3	O	1402	PLP	C3-C4	4.14	1.49	1.40
3	E	1402	PLP	C5-C4	6.06	1.47	1.40
3	G	1402	PLP	C3-C2	7.10	1.45	1.40
3	C	1402	PLP	C5-C4	7.22	1.49	1.40
3	K	1402	PLP	C5-C4	7.24	1.49	1.40
3	I	1402	PLP	C5-C4	7.28	1.49	1.40
3	G	1402	PLP	C5-C4	7.63	1.49	1.40
3	M	1402	PLP	C5-C4	7.71	1.49	1.40
3	O	1402	PLP	C5-C4	7.87	1.49	1.40
3	A	1402	PLP	C5-C4	8.28	1.50	1.40
3	C	1402	PLP	C3-C2	10.46	1.48	1.40
3	K	1402	PLP	C3-C2	11.14	1.48	1.40
3	M	1402	PLP	C3-C2	11.19	1.48	1.40
3	E	1402	PLP	C3-C2	11.32	1.48	1.40
3	I	1402	PLP	C3-C2	11.62	1.49	1.40
3	O	1402	PLP	C3-C2	12.16	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1402	PLP	C3-C2	12.62	1.49	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1402	PLP	C2A-C2-C3	-5.48	115.36	120.90
4	B	1152	CSS	CB-SG-SD	-2.76	98.55	103.94
4	N	1148	CSS	CB-SG-SD	-2.67	98.72	103.94
4	L	1148	CSS	CB-SG-SD	-2.44	99.16	103.94
4	K	1403	CSS	O-C-CA	-2.18	119.88	125.72
3	I	1402	PLP	C3-C4-C5	-2.05	116.27	118.68
4	I	1403	CSS	O-C-CA	-2.03	120.27	125.72
4	G	1403	CSS	O-C-CA	-2.02	120.31	125.72
3	A	1402	PLP	C6-N1-C2	2.02	123.31	119.26
3	E	1402	PLP	O3-C3-C2	2.07	120.57	117.53
3	K	1402	PLP	C6-N1-C2	2.11	123.49	119.26
3	E	1402	PLP	C6-N1-C2	2.11	123.50	119.26
3	M	1402	PLP	O3-C3-C2	2.21	120.76	117.53
4	J	1148	CSS	CB-SG-SD	2.22	108.29	103.94
3	C	1402	PLP	O3-C3-C2	2.24	120.81	117.53
3	K	1402	PLP	O3-C3-C2	2.31	120.92	117.53
3	M	1402	PLP	C6-N1-C2	2.31	123.90	119.26
3	G	1402	PLP	C4A-C4-C5	2.37	123.34	120.90
3	O	1402	PLP	C6-N1-C2	2.64	124.55	119.26
3	G	1402	PLP	C6-N1-C2	2.69	124.67	119.26
3	I	1402	PLP	O3-C3-C2	2.71	121.49	117.53
3	O	1402	PLP	O3-C3-C2	2.75	121.56	117.53
3	C	1402	PLP	C6-N1-C2	2.99	125.26	119.26
3	G	1402	PLP	C2A-C2-N1	3.00	124.57	117.96
3	A	1402	PLP	O3-C3-C2	3.50	122.66	117.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

26 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1402	PLP	1	0
4	A	1403	CSS	1	0
5	A	1404	PEG	1	0
5	A	1405	PEG	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1409	GOL	2	0
6	A	1411	GOL	1	0
3	C	1402	PLP	2	0
5	C	1405	PEG	1	0
6	C	1414	GOL	1	0
6	C	1416	GOL	1	0
4	D	1152	CSS	5	0
6	D	1153	GOL	1	0
3	E	1402	PLP	2	0
6	E	1409	GOL	1	0
3	G	1402	PLP	1	0
6	G	1406	GOL	1	0
6	G	1408	GOL	1	0
3	I	1402	PLP	1	0
6	I	1405	GOL	2	0
6	I	1408	GOL	1	0
4	J	1148	CSS	1	0
3	K	1402	PLP	2	0
5	K	1404	PEG	1	0
4	L	1148	CSS	1	0
3	M	1402	PLP	2	0
3	O	1402	PLP	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, 95th 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	400/403 (99%)	-0.03	1 (0%) 94 95	28, 40, 54, 74	0
1	C	400/403 (99%)	-0.01	1 (0%) 94 95	27, 41, 60, 88	0
1	E	400/403 (99%)	0.08	1 (0%) 94 95	25, 38, 54, 74	0
1	G	400/403 (99%)	-0.04	1 (0%) 94 95	26, 39, 60, 98	0
1	I	400/403 (99%)	0.16	10 (2%) 61 65	31, 41, 73, 109	0
1	K	400/403 (99%)	0.61	24 (6%) 25 28	47, 67, 90, 116	0
1	M	398/403 (98%)	0.94	57 (14%) 4 3	67, 86, 118, 139	0
1	O	398/403 (98%)	2.14	180 (45%) 0 0	81, 116, 149, 167	0
2	B	147/154 (95%)	0.35	9 (6%) 25 27	29, 50, 82, 116	0
2	D	143/154 (92%)	0.30	4 (2%) 56 61	46, 61, 82, 116	0
2	F	135/154 (87%)	2.99	76 (56%) 0 0	61, 102, 173, 209	0
2	H	144/154 (93%)	0.99	28 (19%) 1 1	40, 66, 113, 155	0
2	J	141/154 (91%)	1.48	36 (25%) 1 1	49, 87, 145, 171	0
2	L	139/154 (90%)	2.74	76 (54%) 0 0	100, 116, 142, 148	0
2	N	139/154 (90%)	4.08	107 (76%) 0 0	122, 142, 161, 178	0
2	P	97/154 (62%)	3.85	72 (74%) 0 0	147, 158, 166, 172	0
All	All	4281/4456 (96%)	0.87	683 (15%) 3 2	25, 56, 146, 209	0

All (683) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	72	ALA	12.5
2	L	12	GLY	11.9
2	L	24	PHE	11.7
2	N	28	THR	11.4
1	O	114	VAL	11.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	71	VAL	10.8
2	P	9	HIS	10.5
2	F	136	LEU	10.2
1	K	47	ALA	10.2
2	N	142	ALA	10.1
2	N	140	ILE	10.1
2	L	28	THR	10.0
2	F	70	THR	9.9
2	N	73	GLU	9.9
2	P	99	VAL	9.8
2	N	13	THR	9.7
2	F	140	ILE	9.6
2	N	72	ALA	9.6
2	P	34	TYR	9.4
2	L	27	LEU	9.3
2	F	79	PHE	9.3
2	N	14	THR	9.2
2	N	67	LEU	9.2
1	K	46	SER	9.1
2	P	96	LEU	9.0
2	J	72	ALA	9.0
2	P	81	GLY	8.9
2	N	143	ALA	8.8
2	F	67	LEU	8.7
2	N	103	THR	8.6
2	P	116	PHE	8.6
2	P	141	ILE	8.3
1	O	135	ALA	8.3
2	P	100	GLU	8.2
2	P	24	PHE	8.1
2	N	137	SER	8.1
1	O	224	TYR	8.0
2	F	101	GLY	7.9
2	P	11	PHE	7.7
2	N	51	LEU	7.7
2	N	136	LEU	7.6
2	J	70	THR	7.6
2	N	78	HIS	7.6
2	P	95	LEU	7.6
1	K	53	SER	7.6
2	L	80	PHE	7.5
2	F	68	GLY	7.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	48	GLY	7.5
2	P	92	LEU	7.4
2	J	140	ILE	7.4
1	O	234	GLY	7.3
2	N	133	LEU	7.3
2	F	98	ALA	7.3
2	L	69	TYR	7.3
2	F	102	LYS	7.3
2	N	75	GLY	7.2
2	N	53	ALA	7.2
1	O	342	VAL	7.2
1	M	150	VAL	7.2
2	P	82	ASP	7.2
2	L	81	GLY	7.1
2	N	81	GLY	7.1
2	F	69	TYR	7.1
2	P	107	LEU	7.0
2	F	77	MET	7.0
2	F	133	LEU	7.0
1	M	192	VAL	7.0
2	P	97	THR	7.0
2	P	10	PRO	6.9
2	L	95	LEU	6.9
2	F	144	THR	6.9
2	J	76	LYS	6.8
2	N	76	LYS	6.8
2	F	139	ALA	6.7
2	N	112	PRO	6.7
2	N	70	THR	6.7
2	P	94	VAL	6.7
2	F	76	LYS	6.7
1	O	348	TYR	6.7
2	L	53	ALA	6.7
2	F	56	LYS	6.6
2	N	69	TYR	6.6
2	F	80	PHE	6.6
2	L	25	ALA	6.5
2	F	81	GLY	6.4
2	N	116	PHE	6.4
2	F	142	ALA	6.4
2	F	100	GLU	6.3
1	O	193	VAL	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	99	VAL	6.3
2	N	82	ASP	6.3
1	O	333	PHE	6.3
2	L	79	PHE	6.3
2	F	65	VAL	6.2
2	F	137	SER	6.2
2	H	6	PHE	6.2
2	P	91	LEU	6.2
2	N	48	PRO	6.1
2	F	71	VAL	6.1
1	K	52	ARG	6.1
2	F	73	GLU	6.1
1	M	157	ILE	6.1
1	O	312	LEU	6.1
1	O	304	LEU	6.0
2	N	91	LEU	6.0
2	N	107	LEU	6.0
2	P	15	VAL	6.0
2	N	47	LEU	6.0
2	P	103	THR	6.0
1	O	216	TYR	5.9
1	O	134	GLY	5.9
1	O	400	VAL	5.9
2	J	71	VAL	5.9
2	L	110	GLN	5.9
2	L	133	LEU	5.9
2	L	121	LEU	5.8
2	N	24	PHE	5.8
2	N	27	LEU	5.8
1	O	334	ALA	5.8
2	L	103	THR	5.8
2	N	80	PHE	5.8
2	N	45	PRO	5.8
2	N	119	LEU	5.8
2	F	95	LEU	5.7
2	H	98	ALA	5.7
2	N	29	GLN	5.7
1	O	179	LEU	5.7
2	F	111	SER	5.7
1	O	164	LEU	5.7
2	P	16	THR	5.7
2	J	136	LEU	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	7	ALA	5.7
2	N	105	ALA	5.7
1	O	188	SER	5.6
1	I	55	PHE	5.6
2	P	13	THR	5.6
1	O	153	LEU	5.6
1	O	208	VAL	5.6
2	F	143	ALA	5.6
2	N	139	ALA	5.6
2	N	115	LEU	5.6
1	O	328	LEU	5.6
1	M	179	LEU	5.5
1	O	157	ILE	5.5
2	L	13	THR	5.5
2	N	145	LYS	5.5
2	J	144	THR	5.5
1	O	165	ALA	5.5
2	L	115	LEU	5.5
2	N	74	ASN	5.5
2	N	58	ILE	5.5
1	O	150	VAL	5.4
2	L	119	LEU	5.4
2	P	143	ALA	5.4
2	P	115	LEU	5.4
2	H	7	ALA	5.4
2	J	73	GLU	5.4
2	N	110	GLN	5.4
2	J	147	VAL	5.3
2	L	14	THR	5.3
2	N	111	SER	5.3
2	N	23	THR	5.3
1	O	204	PHE	5.3
2	N	104	ALA	5.3
2	L	77	MET	5.3
1	O	206	ALA	5.2
2	P	119	LEU	5.2
2	B	4	PRO	5.2
2	F	12	GLY	5.2
2	P	36	GLN	5.2
1	O	322	ARG	5.2
1	K	348	TYR	5.2
1	O	305	ALA	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	108	PRO	5.2
1	O	185	PHE	5.2
1	O	329	LEU	5.2
2	N	101	GLY	5.2
2	N	79	PHE	5.2
2	L	23	THR	5.1
1	O	399	LEU	5.1
2	P	142	ALA	5.1
1	O	388	LEU	5.1
2	F	108	GLN	5.1
2	N	146	GLN	5.0
2	L	71	VAL	5.0
1	O	215	PHE	5.0
1	O	137	VAL	5.0
1	O	195	VAL	5.0
2	L	58	ILE	5.0
2	F	107	LEU	5.0
1	O	331	PHE	5.0
2	L	29	GLN	5.0
2	N	36	GLN	4.9
1	O	306	THR	4.9
2	J	77	MET	4.9
2	P	104	ALA	4.9
1	O	136	LYS	4.9
2	P	40	LEU	4.9
1	O	317	GLY	4.9
1	O	297	ALA	4.9
2	P	98	ALA	4.9
2	L	50	GLU	4.9
2	F	74	ASN	4.9
2	P	140	ILE	4.9
2	N	98	ALA	4.8
1	O	194	MET	4.8
1	O	371	THR	4.8
1	O	313	ALA	4.8
1	K	61	LEU	4.8
2	F	78	HIS	4.8
1	O	385	VAL	4.8
2	L	120	GLY	4.8
1	O	372	LEU	4.8
2	P	113	LEU	4.8
2	B	147	VAL	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	103	THR	4.8
2	L	26	PRO	4.8
2	P	101	GLY	4.8
1	O	308	ALA	4.8
1	O	146	ARG	4.7
2	J	75	GLY	4.7
1	M	294	ILE	4.7
1	O	9	PHE	4.7
1	O	378	PRO	4.7
2	N	108	GLN	4.7
2	N	26	PRO	4.6
1	M	234	GLY	4.6
2	L	32	ASP	4.6
2	P	90	GLY	4.6
2	F	48	PRO	4.6
1	O	311	ALA	4.6
2	P	37	LEU	4.6
2	N	144	THR	4.5
1	O	189	ALA	4.5
2	F	138	GLU	4.5
1	M	137	VAL	4.5
2	P	144	THR	4.5
2	F	91	LEU	4.5
2	F	11	PHE	4.5
2	L	22	ASN	4.5
2	P	102	LYS	4.5
2	N	118	GLU	4.5
1	M	113	ILE	4.5
2	L	74	ASN	4.4
2	N	102	LYS	4.4
2	P	112	PRO	4.4
2	L	97	THR	4.4
2	F	75	GLY	4.4
2	N	68	GLY	4.4
2	L	78	HIS	4.4
2	F	110	GLN	4.4
1	O	301	SER	4.4
2	N	11	PHE	4.4
2	P	106	GLU	4.4
2	J	107	LEU	4.3
2	N	38	ILE	4.3
1	O	293	ASP	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	148	PRO	4.3
1	M	112	ILE	4.3
2	J	69	TYR	4.3
2	N	87	ILE	4.3
2	N	50	GLU	4.3
1	O	300	TRP	4.3
1	O	384	ASP	4.3
2	P	14	THR	4.2
1	O	102	ALA	4.2
2	J	80	PHE	4.2
1	O	294	ILE	4.2
2	N	138	GLU	4.2
2	L	21	ARG	4.2
1	M	269	LEU	4.2
2	H	149	HIS	4.2
2	F	66	TRP	4.2
2	L	68	GLY	4.2
2	H	74	ASN	4.2
1	O	169	MET	4.2
1	I	54	GLN	4.2
1	O	48	GLY	4.2
1	O	303	SER	4.2
1	O	163	ILE	4.1
1	M	127	LEU	4.1
1	O	395	ALA	4.1
2	N	52	LYS	4.1
1	O	166	LEU	4.1
2	L	20	LEU	4.1
1	C	401	ASP	4.1
2	J	108	GLN	4.1
2	N	121	LEU	4.1
2	F	135	ALA	4.1
2	P	129	ARG	4.1
2	N	141	ILE	4.0
2	L	54	GLN	4.0
2	D	147	VAL	4.0
1	O	292	TYR	4.0
2	P	32	ASP	4.0
1	O	142	LEU	4.0
2	N	95	LEU	4.0
2	N	25	ALA	4.0
2	F	112	PRO	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	96	LEU	3.9
1	O	309	GLU	3.9
2	J	68	GLY	3.9
2	L	111	SER	3.9
2	N	129	ARG	3.9
1	O	374	ALA	3.9
2	H	114	ALA	3.9
1	K	54	GLN	3.9
2	F	94	VAL	3.8
1	O	101	TYR	3.8
1	O	49	ASN	3.8
1	O	129	VAL	3.8
2	N	12	GLY	3.8
2	L	30	TRP	3.8
2	L	33	LYS	3.8
2	J	13	THR	3.8
1	O	78	ALA	3.8
2	L	98	ALA	3.8
2	F	141	ILE	3.8
1	M	185	PHE	3.8
1	M	183	ILE	3.8
1	I	52	ARG	3.8
2	N	106	GLU	3.8
2	F	44	LEU	3.8
1	O	192	VAL	3.7
2	N	66	TRP	3.7
2	N	15	VAL	3.7
1	O	75	LEU	3.7
1	O	363	LEU	3.7
1	O	376	PHE	3.7
1	O	115	SER	3.7
1	O	218	PHE	3.7
1	O	190	GLY	3.7
2	L	99	VAL	3.7
2	P	17	ALA	3.7
2	P	114	ALA	3.7
2	P	124	GLN	3.7
2	L	122	ARG	3.7
1	O	68	ALA	3.7
2	F	46	ALA	3.7
1	I	46	SER	3.6
2	H	150	HIS	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	100	GLU	3.6
2	F	51	LEU	3.6
1	O	116	VAL	3.6
2	L	75	GLY	3.6
1	O	307	LEU	3.6
2	N	99	VAL	3.6
1	O	159	PRO	3.6
2	J	139	ALA	3.6
2	N	77	MET	3.6
2	N	147	VAL	3.6
2	J	51	LEU	3.5
1	O	326	SER	3.5
2	N	43	GLN	3.5
1	M	152	LEU	3.5
2	F	20	LEU	3.5
1	M	79	PRO	3.5
2	P	136	LEU	3.5
2	H	111	SER	3.5
2	J	12	GLY	3.5
2	H	47	LEU	3.5
2	N	40	LEU	3.5
2	L	118	GLU	3.5
2	N	65	VAL	3.5
1	O	112	ILE	3.4
1	O	183	ILE	3.4
2	L	11	PHE	3.4
2	N	16	THR	3.4
2	N	46	ALA	3.4
2	H	107	LEU	3.4
1	O	158	THR	3.4
2	N	94	VAL	3.4
2	L	141	ILE	3.4
2	F	50	GLU	3.4
1	O	79	PRO	3.4
1	O	332	ASP	3.4
1	I	18	ASP	3.4
1	K	23	LEU	3.4
2	H	72	ALA	3.4
2	D	151	HIS	3.4
2	J	101	GLY	3.3
1	O	352	LEU	3.3
2	L	72	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	74	ASN	3.3
1	O	344	LEU	3.3
2	P	25	ALA	3.3
2	B	6	PHE	3.3
2	L	125	LEU	3.3
1	O	4	PHE	3.3
2	J	6	PHE	3.3
2	L	52	LYS	3.3
1	M	216	TYR	3.3
2	L	15	VAL	3.3
2	B	7	ALA	3.3
1	O	176	CYS	3.3
1	O	295	ASN	3.3
2	P	85	GLY	3.3
2	P	27	LEU	3.2
2	L	109	ALA	3.2
2	N	97	THR	3.2
2	P	28	THR	3.2
2	L	17	ALA	3.2
2	J	78	HIS	3.2
2	P	20	LEU	3.2
1	O	205	PRO	3.2
2	F	106	GLU	3.2
2	N	55	ALA	3.2
2	P	125	LEU	3.2
1	O	98	ALA	3.2
2	J	138	GLU	3.2
1	O	209	GLN	3.2
1	K	50	VAL	3.2
1	O	149	ASP	3.1
1	O	318	PHE	3.1
2	H	106	GLU	3.1
1	O	325	ASP	3.1
2	J	79	PHE	3.1
1	K	337[A]	HIS	3.1
1	M	138	VAL	3.1
2	L	136	LEU	3.1
1	M	401	ASP	3.1
2	P	39	MET	3.1
1	O	104	PRO	3.1
2	F	55	ALA	3.1
2	L	144	THR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	12	GLY	3.1
2	N	54	GLN	3.1
1	M	193	VAL	3.1
2	N	96	LEU	3.1
2	F	58	ILE	3.1
2	F	117	ASP	3.1
1	M	156	LEU	3.1
2	F	47	LEU	3.1
2	P	105	ALA	3.1
1	O	244	PRO	3.1
1	M	52	ARG	3.1
1	O	398	LEU	3.1
2	L	143	ALA	3.1
1	O	330	ALA	3.0
2	L	31	GLU	3.0
1	K	63	ALA	3.0
1	O	106	LEU	3.0
1	O	341	MET	3.0
2	F	96	LEU	3.0
2	L	51	LEU	3.0
1	M	191	MET	3.0
2	H	69	TYR	3.0
1	M	246	LEU	3.0
1	O	23	LEU	3.0
2	J	105	ALA	3.0
2	P	41	GLY	3.0
2	L	107	LEU	3.0
1	O	365	GLU	2.9
2	N	8	GLY	2.9
1	M	163	ILE	2.9
2	D	8	GLY	2.9
2	J	53	ALA	2.9
1	O	368	VAL	2.9
2	H	99	VAL	2.9
1	M	259	GLY	2.9
1	O	133	THR	2.9
2	J	67	LEU	2.9
2	J	109	ALA	2.9
2	N	37	LEU	2.9
2	N	109	ALA	2.9
2	L	147	VAL	2.9
1	O	335	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	370	GLY	2.9
2	H	45	PRO	2.9
1	O	392	VAL	2.9
2	P	117	ASP	2.9
2	P	30	TRP	2.9
1	O	202	VAL	2.8
1	O	264	SER	2.8
2	P	108	GLN	2.8
1	O	29	ALA	2.8
2	F	13	THR	2.8
2	L	67	LEU	2.8
1	O	77	ASN	2.8
1	O	364	ALA	2.8
2	H	51	LEU	2.8
1	O	288	TRP	2.8
1	O	314	LYS	2.8
2	F	119	LEU	2.8
1	O	319	ARG	2.8
2	L	101	GLY	2.8
1	O	94	ILE	2.8
1	M	166	LEU	2.8
1	O	336	VAL	2.8
1	K	60	ARG	2.8
1	O	366	LEU	2.8
2	F	57	GLU	2.8
1	O	272	GLY	2.8
1	O	127	LEU	2.8
2	B	145	LYS	2.8
2	L	42	LYS	2.8
2	H	109	ALA	2.7
1	O	296	GLN	2.7
1	M	235	LYS	2.7
2	B	151	HIS	2.7
1	O	21	VAL	2.7
1	M	121	ALA	2.7
1	M	96	MET	2.7
1	O	162	ARG	2.7
2	N	56	LYS	2.7
2	P	135	ALA	2.7
1	O	213	ILE	2.7
2	N	132	GLY	2.7
2	N	49	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	172	VAL	2.6
1	M	262	THR	2.6
1	O	47	ALA	2.6
1	O	201	ALA	2.6
2	P	87	ILE	2.6
1	M	240	GLU	2.6
1	O	373	ARG	2.6
1	I	19	ALA	2.6
2	L	93	ALA	2.6
2	H	108	GLN	2.6
1	M	158	THR	2.6
2	F	104	ALA	2.6
2	N	59	ALA	2.6
1	M	366	LEU	2.6
1	O	76	LEU	2.6
1	O	113	ILE	2.6
1	K	19	ALA	2.6
2	J	103	THR	2.6
2	N	19	THR	2.6
1	M	398	LEU	2.6
1	O	245	TRP	2.6
2	N	20	LEU	2.6
2	L	36	GLN	2.6
2	N	134	ASN	2.6
2	P	110	GLN	2.6
2	F	97	THR	2.6
2	N	135	ALA	2.6
1	M	108	PRO	2.6
1	O	211	LEU	2.6
2	F	54	GLN	2.6
2	B	69	TYR	2.6
2	N	93	ALA	2.5
1	O	238	LEU	2.5
1	O	260	PHE	2.5
1	M	187	HIS	2.5
1	O	359	ALA	2.5
1	K	151	ASP	2.5
2	N	90	GLY	2.5
1	M	114	VAL	2.5
2	D	148	LYS	2.5
2	H	71	VAL	2.5
1	O	316	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	123	LEU	2.5
2	P	22	ASN	2.5
1	M	205	PRO	2.5
1	I	45	LEU	2.5
1	O	394	ARG	2.5
1	I	57	GLU	2.5
1	O	167	GLY	2.5
1	I	3	VAL	2.4
2	P	137	SER	2.4
1	O	55	PHE	2.4
2	H	79	PHE	2.4
2	B	150	HIS	2.4
1	O	320	SER	2.4
1	O	117	ALA	2.4
1	M	53	SER	2.4
1	O	389	VAL	2.4
1	O	397	GLU	2.4
2	B	148	LYS	2.4
2	H	102	LYS	2.4
2	H	77	MET	2.4
2	P	86	ARG	2.4
1	M	247	GLY	2.4
1	O	89	GLY	2.4
2	H	113	LEU	2.4
2	P	88	VAL	2.4
2	F	39	MET	2.4
1	O	154	PRO	2.4
2	F	14	THR	2.4
1	M	153	LEU	2.4
1	K	157	ILE	2.4
1	K	59	GLN	2.4
2	F	29	GLN	2.4
2	H	144	THR	2.4
1	O	191	MET	2.3
1	M	109	GLY	2.3
1	M	162	ARG	2.3
2	P	122	ARG	2.3
2	L	43	GLN	2.3
1	M	186	ALA	2.3
2	L	34	TYR	2.3
2	L	137	SER	2.3
1	O	107	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	252	VAL	2.3
2	F	105	ALA	2.3
2	N	125	LEU	2.3
2	F	49	ASP	2.3
2	F	15	VAL	2.3
2	L	140	ILE	2.3
1	M	260	PHE	2.3
1	O	380	ASN	2.3
2	J	24	PHE	2.3
1	O	155	GLU	2.3
2	N	126	SER	2.3
1	O	128	MET	2.3
2	N	39	MET	2.3
1	M	181	ARG	2.3
2	F	122	ARG	2.3
1	M	238	LEU	2.3
1	O	362	LEU	2.3
2	F	92	LEU	2.3
2	L	73	GLU	2.3
2	H	94	VAL	2.3
1	O	214	ASP	2.3
1	O	138	VAL	2.2
1	O	161	SER	2.2
1	O	357	HIS	2.2
2	N	34	TYR	2.2
1	M	212	ASP	2.2
1	O	393	ASP	2.2
1	O	236	SER	2.2
1	K	166	LEU	2.2
2	F	10	PRO	2.2
1	O	228	GLY	2.2
2	L	94	VAL	2.2
1	O	298	GLU	2.2
2	N	32	ASP	2.2
2	L	102	LYS	2.2
1	O	302	ARG	2.2
2	P	35	ARG	2.2
1	G	294	ILE	2.2
1	M	94	ILE	2.2
1	O	265	ALA	2.2
2	F	123	ALA	2.2
2	L	35	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	57	GLU	2.2
1	K	186	ALA	2.2
1	O	391	ALA	2.2
1	M	344	LEU	2.2
1	O	105	ARG	2.2
2	P	29	GLN	2.2
2	J	55	ALA	2.2
1	I	49	ASN	2.2
1	M	204	PHE	2.2
2	H	8	GLY	2.2
1	O	187	HIS	2.1
1	M	98	ALA	2.1
1	M	248	GLY	2.1
1	O	52	ARG	2.1
2	N	63	ASN	2.1
2	L	55	ALA	2.1
1	E	91	THR	2.1
2	P	26	PRO	2.1
2	F	113	LEU	2.1
2	J	146	GLN	2.1
1	O	174	GLY	2.1
2	H	68	GLY	2.1
1	K	56	ALA	2.1
1	O	276	VAL	2.1
2	P	93	ALA	2.1
2	H	58	ILE	2.1
2	N	10	PRO	2.1
1	O	381	THR	2.1
1	K	4	PHE	2.1
1	M	384	ASP	2.1
1	O	289	LEU	2.1
2	N	35	ARG	2.1
2	L	8	GLY	2.1
1	A	1	MET	2.1
1	K	106	LEU	2.1
2	N	44	LEU	2.1
1	M	359	ALA	2.0
1	K	55	PHE	2.0
2	F	24	PHE	2.0
1	O	130	ALA	2.0
1	O	85	VAL	2.0
1	O	239	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	345	LEU	2.0
2	N	128	SER	2.0
2	P	111	SER	2.0
2	F	82	ASP	2.0
2	J	56	LYS	2.0
1	M	154	PRO	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, 95th 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
6	GOL	I	1407	6/6	0.90	0.39	7.84	42,53,56,69	0
6	GOL	I	1408	6/6	0.72	0.24	4.97	62,71,73,76	0
6	GOL	C	1411	6/6	0.92	0.25	4.23	49,58,74,77	0
6	GOL	C	1409	6/6	0.91	0.24	3.86	55,67,72,73	0
5	PEG	A	1405	7/7	0.86	0.24	3.26	43,51,55,57	0
6	GOL	G	1406	6/6	0.91	0.22	2.61	35,49,53,56	0
5	PEG	I	1404	7/7	0.93	0.16	2.36	36,47,53,55	0
6	GOL	A	1408	6/6	0.89	0.27	1.82	47,62,64,65	0
5	PEG	A	1404	7/7	0.90	0.18	1.80	48,55,57,60	0
6	GOL	E	1413	6/6	0.82	0.20	1.75	50,59,64,64	0
6	GOL	G	1410	6/6	0.84	0.19	1.22	48,52,53,54	0
6	GOL	D	1153	6/6	0.87	0.23	1.18	44,60,64,64	0
6	GOL	C	1417	6/6	0.88	0.20	1.01	43,46,48,52	0
5	PEG	B	1153	7/7	0.84	0.19	0.85	50,58,67,68	0
5	PEG	A	1406	7/7	0.94	0.20	0.82	45,51,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CSS	H	1151	7/8	0.72	0.24	0.80	94,97,107,114	0
3	PLP	C	1402	15/16	0.97	0.18	0.75	29,31,32,33	0
6	GOL	G	1405	6/6	0.88	0.18	0.46	54,60,64,66	0
6	GOL	A	1412	6/6	0.91	0.17	0.34	48,58,59,60	0
4	CSS	D	1152	7/8	0.86	0.15	0.19	86,87,98,101	0
5	PEG	E	1407	7/7	0.91	0.14	-0.08	50,54,59,61	0
3	PLP	E	1402	15/16	0.97	0.18	-0.16	28,29,31,31	0
4	CSS	F	1145	7/8	0.83	0.18	-0.21	97,104,108,115	0
3	PLP	A	1402	15/16	0.98	0.14	-0.23	28,29,30,31	0
3	PLP	O	1402	15/16	0.84	0.22	-0.29	98,103,109,111	0
3	PLP	G	1402	15/16	0.97	0.14	-0.29	28,30,32,37	0
3	PLP	K	1402	15/16	0.96	0.18	-0.34	51,53,55,56	0
4	CSS	G	1403	7/8	0.92	0.15	-0.52	33,34,35,42	0
4	CSS	L	1148	7/8	0.86	0.14	-0.63	105,106,109,110	0
3	PLP	I	1402	15/16	0.97	0.17	-0.71	31,33,38,39	0
4	CSS	I	1403	7/8	0.92	0.14	-0.76	35,38,41,49	0
4	CSS	N	1148	7/8	0.71	0.19	-0.92	141,146,147,148	0
6	GOL	H	1153	6/6	0.85	0.19	-0.97	64,74,75,76	0
6	GOL	C	1418	6/6	0.86	0.15	-1.00	55,56,58,62	0
6	GOL	I	1405	6/6	0.94	0.11	-1.10	37,48,51,53	0
4	CSS	B	1152	7/8	0.89	0.14	-1.12	71,73,83,95	0
4	CSS	E	1403	7/8	0.93	0.15	-1.16	30,32,34,48	0
4	CSS	J	1148	7/8	0.89	0.12	-1.16	87,91,97,104	0
3	PLP	M	1402	15/16	0.93	0.14	-1.18	79,82,85,86	0
4	CSS	C	1403	7/8	0.90	0.13	-1.20	36,39,42,51	0
4	CSS	O	1403	7/8	0.75	0.17	-1.41	113,114,116,116	0
4	CSS	M	1403	7/8	0.79	0.15	-1.55	85,87,88,92	0
4	CSS	K	1403	7/8	0.89	0.14	-1.81	59,61,62,64	0
4	CSS	A	1403	7/8	0.94	0.12	-1.92	35,35,38,46	0
5	PEG	C	1404	7/7	0.91	0.14	-	55,59,72,73	0
5	PEG	C	1407	7/7	0.92	0.24	-	40,57,74,75	0
5	PEG	E	1404	7/7	0.81	0.15	-	50,55,60,64	0
5	PEG	E	1405	7/7	0.90	0.14	-	54,60,65,65	0
6	GOL	A	1409	6/6	0.75	0.25	-	54,59,60,61	0
6	GOL	B	2401	6/6	0.90	0.36	-	54,62,67,71	0
6	GOL	E	1417	6/6	0.90	0.20	-	52,54,56,57	0
6	GOL	A	1410	6/6	0.89	0.17	-	48,57,60,65	0
5	PEG	K	1404	7/7	0.85	0.20	-	57,58,64,65	0
6	GOL	G	1411	6/6	0.86	0.18	-	54,57,67,70	0
6	GOL	C	1416	6/6	0.89	0.19	-	66,71,76,77	0
5	PEG	G	1404	7/7	0.87	0.14	-	54,61,68,70	0
6	GOL	C	1408	6/6	0.81	0.26	-	55,61,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	GOL	I	1406	6/6	0.89	0.21	-	59,65,70,73	0
6	GOL	E	1414	6/6	0.92	0.26	-	58,64,68,71	0
6	GOL	A	1407	6/6	0.82	0.37	-	55,58,60,69	0
6	GOL	M	1404	6/6	0.85	0.21	-	57,62,69,70	0
5	PEG	E	1406	7/7	0.83	0.20	-	45,53,56,57	0
6	GOL	C	1410	6/6	0.92	0.17	-	53,57,58,72	0
6	GOL	E	1412	6/6	0.85	0.29	-	50,59,65,80	0
6	GOL	E	2401	6/6	0.80	0.33	-	44,52,58,62	0
6	GOL	A	1414	6/6	0.88	0.20	-	49,51,53,54	0
6	GOL	E	1410	6/6	0.80	0.16	-	40,43,54,54	0
6	GOL	B	1154	6/6	0.91	0.29	-	47,53,57,58	0
6	GOL	A	1413	6/6	0.86	0.27	-	49,61,64,65	0
6	GOL	C	1414	6/6	0.93	0.45	-	43,45,55,68	0
6	GOL	E	1409	6/6	0.80	0.27	-	50,56,60,60	0
6	GOL	A	1415	6/6	0.83	0.24	-	50,52,55,56	0
5	PEG	C	1405	7/7	0.81	0.26	-	56,64,70,81	0
6	GOL	E	1411	6/6	0.87	0.26	-	46,54,62,63	0
6	GOL	C	1415	6/6	0.84	0.26	-	57,66,69,75	0
6	GOL	A	1411	6/6	0.90	0.12	-	61,63,68,68	0
6	GOL	G	1408	6/6	0.89	0.19	-	51,62,64,67	0
6	GOL	E	1408	6/6	0.90	0.21	-	42,51,53,54	0
5	PEG	H	1152	7/7	0.83	0.27	-	57,58,64,66	0
5	PEG	C	1406	7/7	0.84	0.15	-	48,55,69,69	0
6	GOL	E	1416	6/6	0.81	0.50	-	59,65,72,78	0
6	GOL	B	1155	6/6	0.90	0.14	-	44,52,52,56	0
6	GOL	C	1413	6/6	0.71	0.21	-	52,55,59,66	0
6	GOL	A	2401	6/6	0.90	0.22	-	48,54,63,64	0
6	GOL	G	1409	6/6	0.85	0.20	-	57,61,66,67	0
6	GOL	G	1407	6/6	0.71	0.20	-	57,71,75,75	0
6	GOL	E	1415	6/6	0.81	0.24	-	52,54,59,64	0
6	GOL	A	1416	6/6	0.88	0.24	-	63,70,72,73	0
6	GOL	C	1412	6/6	0.89	0.21	-	48,65,70,73	0
6	GOL	I	2401	6/6	0.73	0.29	-	53,64,68,69	0

6.5 Other polymers ⓘ

There are no such residues in this entry.