Full wwPDB X-ray Structure Validation Report (i)

Sep 19, 2023 – 12:14 AM EDT

PDB ID	:	5BSH
Title	:	Crystal structure of Medicago truncatula (delta)1-Pyrroline-5-Carboxylate Reductase (MtP5CR) in complex with L-Proline
Authors	:	Ruszkowski, M.; Nocek, B.; Forlani, G.; Dauter, Z.
Deposited on	:	2015-06-02
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

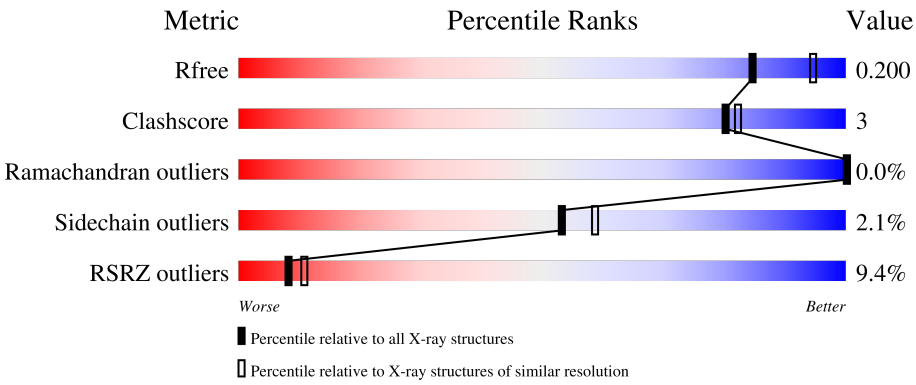
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	277	3% 92% 6% •
1	B	277	10% 92% 6% •
1	C	277	6% 91% 5% • •
1	D	277	16% 90% 7% •
1	E	277	5% 90% 7% • •

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Mol	Chain	Length	Quality of chain
1	F	277	3% 93% 5%
1	G	277	25% 91% 5%
1	H	277	9% 91% 6%
1	I	277	6% 92% 5%
1	J	277	11% 88% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20686 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 Pyrroline-5-carboxylate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	272	2012	1270	350	385	7	0	3	0
1	B	272	2018	1272	351	389	6	0	4	0
1	C	268	1969	1241	342	379	7	0	2	0
1	D	268	1970	1241	343	380	6	0	2	0
1	E	272	2020	1274	351	388	7	0	4	0
1	F	272	2020	1274	351	388	7	0	4	0
1	G	263	1925	1213	335	371	6	0	1	0
1	H	272	2003	1265	348	383	7	0	2	0
1	I	270	1979	1248	345	380	6	0	1	0
1	J	271	1995	1258	347	384	6	0	2	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP G7KRM5
A	-1	ASN	-	expression tag	UNP G7KRM5
A	0	ALA	-	expression tag	UNP G7KRM5
B	-2	SER	-	expression tag	UNP G7KRM5
B	-1	ASN	-	expression tag	UNP G7KRM5
B	0	ALA	-	expression tag	UNP G7KRM5
C	-2	SER	-	expression tag	UNP G7KRM5
C	-1	ASN	-	expression tag	UNP G7KRM5
C	0	ALA	-	expression tag	UNP G7KRM5

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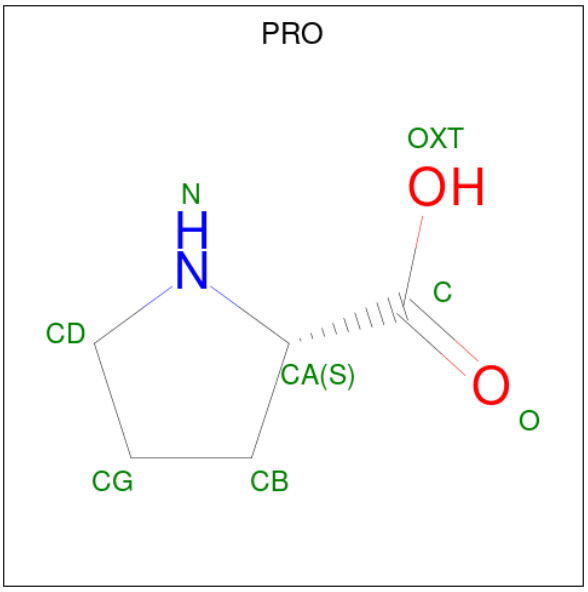
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP G7KRM5
D	-1	ASN	-	expression tag	UNP G7KRM5
D	0	ALA	-	expression tag	UNP G7KRM5
E	-2	SER	-	expression tag	UNP G7KRM5
E	-1	ASN	-	expression tag	UNP G7KRM5
E	0	ALA	-	expression tag	UNP G7KRM5
F	-2	SER	-	expression tag	UNP G7KRM5
F	-1	ASN	-	expression tag	UNP G7KRM5
F	0	ALA	-	expression tag	UNP G7KRM5
G	-2	SER	-	expression tag	UNP G7KRM5
G	-1	ASN	-	expression tag	UNP G7KRM5
G	0	ALA	-	expression tag	UNP G7KRM5
H	-2	SER	-	expression tag	UNP G7KRM5
H	-1	ASN	-	expression tag	UNP G7KRM5
H	0	ALA	-	expression tag	UNP G7KRM5
I	-2	SER	-	expression tag	UNP G7KRM5
I	-1	ASN	-	expression tag	UNP G7KRM5
I	0	ALA	-	expression tag	UNP G7KRM5
J	-2	SER	-	expression tag	UNP G7KRM5
J	-1	ASN	-	expression tag	UNP G7KRM5
J	0	ALA	-	expression tag	UNP G7KRM5

- Molecule 2 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	8	5	1	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	8	5	1	2	0	0
2	C	1	8	5	1	2	0	0
2	D	1	8	5	1	2	0	0
2	E	1	8	5	1	2	0	0
2	F	1	8	5	1	2	0	0
2	G	1	8	5	1	2	0	0
2	H	1	8	5	1	2	0	0
2	I	1	8	5	1	2	0	0
2	J	1	8	5	1	2	0	0

- Molecule 3 is water.

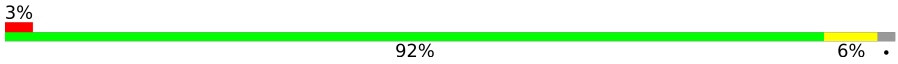
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	112	112	112	0	0
3	B	74	74	74	0	0
3	C	66	67	67	0	1
3	D	58	58	58	0	0
3	E	97	97	97	0	0
3	F	81	81	81	0	0
3	G	50	50	50	0	0
3	H	60	60	60	0	0
3	I	54	54	54	0	0
3	J	42	42	42	0	0

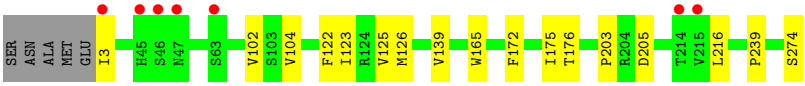
3 Residue-property plots (i)

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: Pyrroline-5-carboxylate reductase

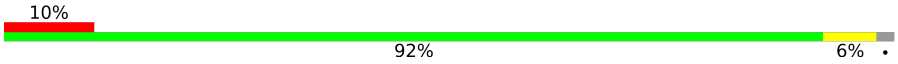
Chain A:

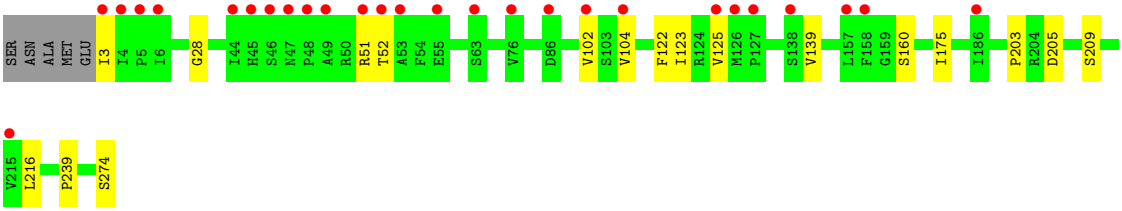




• Molecule 1: Pyrroline-5-carboxylate reductase

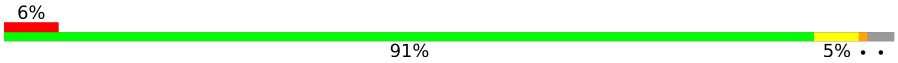
Chain B:

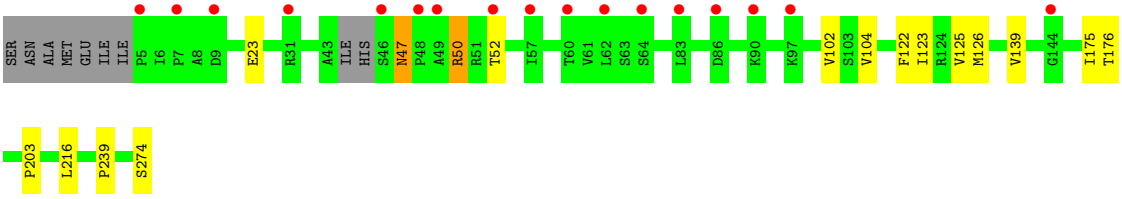




• Molecule 1: Pyrroline-5-carboxylate reductase

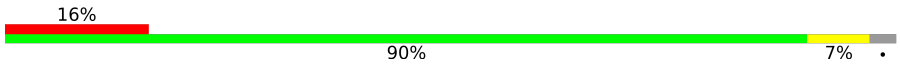
Chain C:

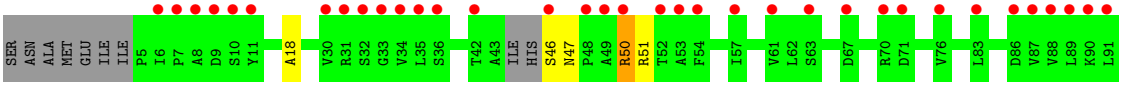


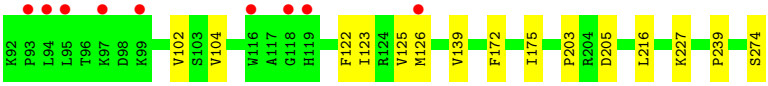


• Molecule 1: Pyrroline-5-carboxylate reductase

Chain D:

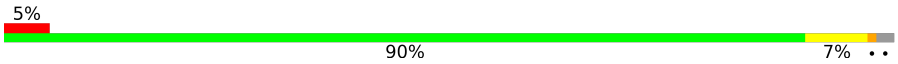


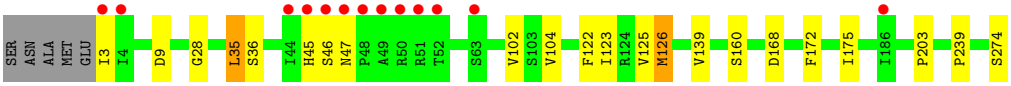




• Molecule 1: Pyrroline-5-carboxylate reductase

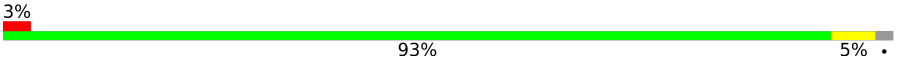
Chain E:





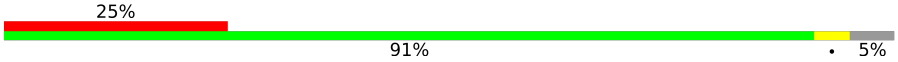
• Molecule 1: Pyrroline-5-carboxylate reductase

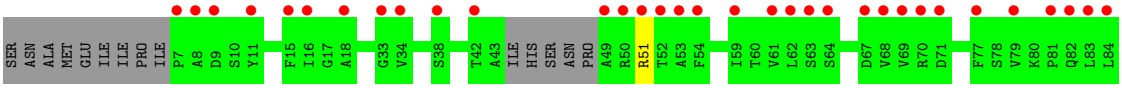
Chain F:

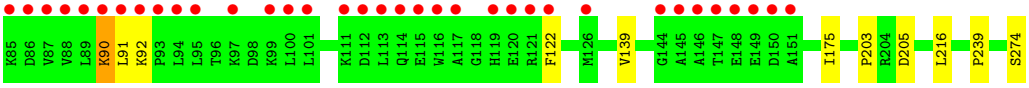


• Molecule 1: Pyrroline-5-carboxylate reductase

Chain G:

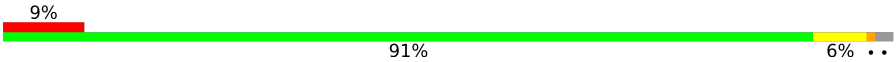


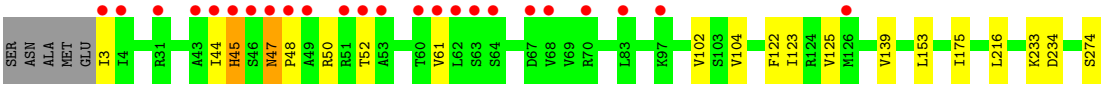




• Molecule 1: Pyrroline-5-carboxylate reductase

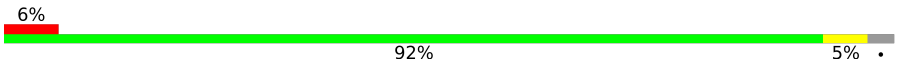
Chain H:

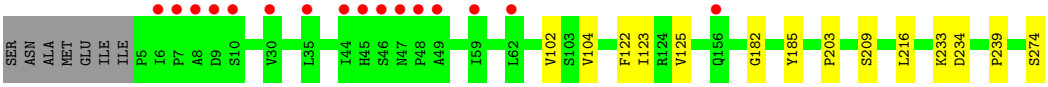




• Molecule 1: Pyrroline-5-carboxylate reductase

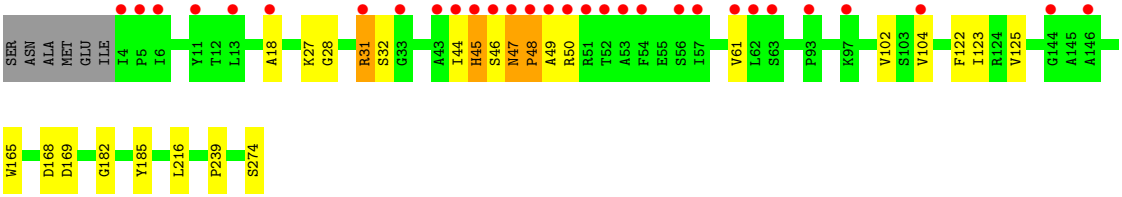
Chain I:





• Molecule 1: Pyrroline-5-carboxylate reductase

Chain J:


SER
ASN
ALA
MET
GLU
ILE
I4
P5
I6
Y11
T12
L13
A18
K27
G28
R31
S32
G33
A43
I44
H45
S46
N47
P48
A49
R50
R51
T52
A53
F54
E55
S56
I57
V61
L62
S63
P93
K97
V102
S103
V104
F122
I123
R124
V125
G144
A145
A146

W165
D168
D169
G182
Y185
L216
P239
S274

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	87.49Å 100.93Å 101.92Å 67.65° 85.46° 89.44°	Depositor
Resolution (Å)	40.00 – 2.10 33.49 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.0 (40.00-2.10) 97.0 (33.49-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.180 , 0.197 0.185 , 0.200	Depositor DCC
R_{free} test set	1941 reflections (1.06%)	wwPDB-VP
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	20686	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.89	0/2041	0.81	0/2761
1	B	0.83	0/2047	0.80	0/2769
1	C	0.79	0/1996	0.79	0/2697
1	D	0.79	0/1997	0.77	0/2698
1	E	0.87	0/2049	0.84	1/2772 (0.0%)
1	F	0.79	0/2049	0.78	0/2772
1	G	0.77	0/1950	0.80	1/2632 (0.0%)
1	H	0.77	1/2032 (0.0%)	0.78	1/2749 (0.0%)
1	I	0.78	0/2008	0.78	0/2715
1	J	0.79	0/2024	0.79	1/2738 (0.0%)
All	All	0.81	1/20193 (0.0%)	0.79	4/27303 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	48	PRO	N-CD	5.17	1.55	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	47	ASN	C-N-CD	6.23	141.48	128.40
1	E	35	LEU	CA-CB-CG	5.80	128.65	115.30
1	H	47	ASN	C-N-CD	5.65	140.26	128.40
1	G	90	LYS	CD-CE-NZ	5.44	124.20	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2012	0	2080	11	0
1	B	2018	0	2078	10	0
1	C	1969	0	2033	10	0
1	D	1970	0	2031	16	0
1	E	2020	0	2083	12	0
1	F	2020	0	2083	8	0
1	G	1925	0	1988	5	0
1	H	2003	0	2073	17	0
1	I	1979	0	2043	8	0
1	J	1995	0	2056	28	0
2	A	8	0	7	0	0
2	B	8	0	7	0	0
2	C	8	0	7	0	0
2	D	8	0	7	0	0
2	E	8	0	7	0	0
2	F	8	0	7	0	0
2	G	8	0	7	0	0
2	H	8	0	7	0	0
2	I	8	0	7	0	0
2	J	8	0	7	0	0
3	A	112	0	0	1	0
3	B	74	0	0	1	0
3	C	67	0	0	1	0
3	D	58	0	0	2	0
3	E	97	0	0	2	0
3	F	81	0	0	1	0
3	G	50	0	0	1	0
3	H	60	0	0	0	0
3	I	54	0	0	0	0
3	J	42	0	0	2	0
All	All	20686	0	20618	111	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 3.

All (111) 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:F:205[B]:ASP:OD1	3:F:402:HOH:O	1.55	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:ASP:HB3	3:E:453:HOH:O	1.56	1.03
1:E:160:SER:HB3	3:E:443:HOH:O	1.56	1.02
1:D:205:ASP:HB2	3:D:446:HOH:O	1.59	1.02
1:H:44:ILE:HG12	1:H:61:VAL:HG13	1.46	0.94
1:J:168[B]:ASP:OD2	3:J:401:HOH:O	1.91	0.87
1:H:44:ILE:HG12	1:H:61:VAL:CG1	2.12	0.79
1:H:47:ASN:ND2	1:H:50:ARG:HG2	1.98	0.78
1:H:45:HIS:H	1:H:45:HIS:CD2	2.00	0.76
1:J:28:GLY:HA2	1:J:31:ARG:HG2	1.68	0.75
1:C:52:THR:HG22	3:C:454:HOH:O	1.87	0.75
1:J:168[B]:ASP:OD1	3:J:401:HOH:O	2.06	0.73
1:D:18:ALA:O	1:D:50:ARG:NE	2.22	0.72
1:J:28:GLY:O	1:J:31:ARG:HG3	1.91	0.71
1:C:126[B]:MET:HE1	1:C:176:THR:HA	1.74	0.70
1:H:44:ILE:CG1	1:H:61:VAL:CG1	2.71	0.68
1:D:126:MET:HE2	1:D:172:PHE:HD2	1.60	0.67
1:B:205:ASP:HB2	3:B:452:HOH:O	1.95	0.66
1:J:48:PRO:HD2	1:J:49:ALA:H	1.60	0.66
1:D:126:MET:CE	1:D:172:PHE:CD2	2.79	0.66
1:A:205:ASP:HB2	3:A:477:HOH:O	1.98	0.63
1:D:50:ARG:HH11	1:D:50:ARG:HG2	1.64	0.62
1:D:126:MET:HE2	1:D:172:PHE:CD2	2.33	0.62
1:E:28:GLY:HA3	1:E:160:SER:OG	1.99	0.62
1:H:44:ILE:CG1	1:H:61:VAL:HG13	2.26	0.61
1:J:47:ASN:ND2	1:J:50:ARG:HG2	2.14	0.61
1:J:45:HIS:CD2	1:J:46:SER:HB3	2.36	0.61
1:H:44:ILE:HG13	1:H:61:VAL:HG11	1.83	0.60
1:H:44:ILE:CG1	1:H:61:VAL:HG11	2.32	0.59
1:A:239:PRO:HG3	1:I:203:PRO:HA	1.86	0.57
1:D:50:ARG:HG2	1:D:50:ARG:NH1	2.17	0.57
1:B:28:GLY:HA3	1:B:160[B]:SER:OG	2.07	0.55
1:F:139:VAL:HG21	1:F:175:ILE:HD13	1.88	0.55
1:A:139:VAL:HG21	1:A:175:ILE:HD13	1.86	0.55
1:C:139:VAL:HG21	1:C:175:ILE:HD13	1.89	0.55
1:B:139:VAL:HG21	1:B:175:ILE:HD13	1.89	0.55
1:C:203:PRO:HA	1:E:239:PRO:HG3	1.89	0.55
1:G:139:VAL:HG21	1:G:175:ILE:HD13	1.91	0.53
1:H:45:HIS:CD2	1:H:45:HIS:N	2.73	0.53
1:J:168[B]:ASP:OD1	1:J:169:ASP:N	2.42	0.53
1:J:48:PRO:CD	1:J:49:ALA:H	2.22	0.52
1:H:139:VAL:HG21	1:H:175:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:PRO:HG3	1:F:203:PRO:HA	1.92	0.51
1:J:31:ARG:HG3	1:J:32:SER:N	2.26	0.51
1:G:203:PRO:HA	1:I:239:PRO:HG3	1.92	0.51
1:D:139:VAL:HG21	1:D:175:ILE:HD13	1.93	0.51
1:J:28:GLY:CA	1:J:31:ARG:HG2	2.37	0.50
1:J:28:GLY:HA2	1:J:31:ARG:CG	2.41	0.50
1:C:23:GLU:OE1	1:C:50:ARG:NH2	2.45	0.49
1:C:47:ASN:OD1	1:C:47:ASN:N	2.46	0.49
1:J:45:HIS:CD2	1:J:45:HIS:C	2.85	0.49
1:E:104:VAL:HA	1:E:125:VAL:O	2.13	0.48
1:I:216:LEU:CD1	1:J:216:LEU:CD1	2.91	0.48
1:G:216:LEU:CD1	1:H:216:LEU:CD1	2.92	0.48
1:D:227:LYS:NZ	3:D:403:HOH:O	2.39	0.47
1:F:47:ASN:OD1	1:F:50:ARG:N	2.34	0.47
1:B:104:VAL:HA	1:B:125:VAL:O	2.14	0.47
1:E:139:VAL:HG21	1:E:175:ILE:HD13	1.95	0.47
1:B:203:PRO:HA	1:J:239:PRO:HG3	1.97	0.46
1:H:104:VAL:HA	1:H:125:VAL:O	2.16	0.46
1:E:203:PRO:HA	1:G:239:PRO:HG3	1.97	0.46
1:J:45:HIS:HD2	1:J:46:SER:N	2.14	0.46
1:J:182:GLY:HA2	1:J:185:TYR:CD2	2.51	0.46
1:G:205:ASP:HB2	3:G:434:HOH:O	2.16	0.45
1:F:3:ILE:O	1:F:3:ILE:HG22	2.16	0.45
1:J:44:ILE:HG12	1:J:61:VAL:HG13	1.97	0.45
1:B:3:ILE:O	1:B:3:ILE:HG22	2.17	0.45
1:H:3:ILE:HG22	1:H:3:ILE:O	2.17	0.45
1:A:3:ILE:HG22	1:A:3:ILE:O	2.17	0.45
1:A:216:LEU:CD1	1:B:216:LEU:CD1	2.95	0.44
1:J:28:GLY:O	1:J:31:ARG:CG	2.61	0.44
1:J:27:LYS:O	1:J:31:ARG:HG2	2.18	0.44
1:A:126[B]:MET:HE1	1:A:176:THR:HA	1.99	0.44
1:C:216:LEU:CD1	1:D:216:LEU:CD1	2.96	0.44
1:J:48:PRO:CD	1:J:49:ALA:N	2.80	0.44
1:A:104:VAL:HA	1:A:125:VAL:O	2.18	0.44
1:A:102:VAL:HA	1:A:123:ILE:O	2.18	0.43
1:B:102:VAL:HA	1:B:123:ILE:O	2.18	0.43
1:E:3:ILE:O	1:E:3:ILE:HG22	2.17	0.43
1:F:102:VAL:HA	1:F:123:ILE:O	2.19	0.43
1:J:31:ARG:HG3	1:J:32:SER:H	1.82	0.43
1:C:102:VAL:HA	1:C:123:ILE:O	2.19	0.43
1:J:102:VAL:HA	1:J:123:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:VAL:HA	1:D:125:VAL:O	2.19	0.43
1:H:102:VAL:HA	1:H:123:ILE:O	2.19	0.43
1:J:44:ILE:HG13	1:J:61:VAL:HG11	2.00	0.42
1:A:203:PRO:HA	1:C:239:PRO:HG3	2.01	0.42
1:H:153:LEU:C	1:H:153:LEU:HD23	2.38	0.42
1:H:233:LYS:HE2	1:H:234:ASP:OD1	2.20	0.42
1:D:50:ARG:HH11	1:D:50:ARG:CG	2.32	0.42
1:E:126[B]:MET:HE1	1:E:175:ILE:HG22	2.00	0.42
1:J:104:VAL:HA	1:J:125:VAL:O	2.19	0.42
1:I:104:VAL:HA	1:I:125:VAL:O	2.20	0.42
1:A:139:VAL:HG23	1:A:172:PHE:CZ	2.55	0.42
1:E:126[B]:MET:CE	1:E:175:ILE:HG22	2.49	0.42
1:D:47:ASN:OD1	1:D:50:ARG:N	2.33	0.42
1:J:45:HIS:CD2	1:J:46:SER:N	2.87	0.42
1:F:104:VAL:HA	1:F:125:VAL:O	2.20	0.42
1:D:102:VAL:HA	1:D:123:ILE:O	2.20	0.41
1:I:102:VAL:HA	1:I:123:ILE:O	2.20	0.41
1:I:209:SER:HB3	1:J:165:TRP:CZ2	2.55	0.41
1:C:104:VAL:HA	1:C:125:VAL:O	2.21	0.41
1:I:233:LYS:HE2	1:I:234:ASP:OD1	2.20	0.41
1:B:239:PRO:HG3	1:D:203:PRO:HA	2.03	0.41
1:E:139:VAL:HG23	1:E:172:PHE:CZ	2.56	0.41
1:F:50:ARG:HA	1:F:50:ARG:HD2	1.73	0.41
1:A:165:TRP:CZ2	1:B:209:SER:HB3	2.56	0.40
1:I:182:GLY:HA2	1:I:185:TYR:CD2	2.56	0.40
1:H:44:ILE:HG13	1:H:61:VAL:CG1	2.46	0.40
1:J:18:ALA:CB	1:J:44:ILE:HD13	2.52	0.40
1:E:102:VAL:HA	1:E:123:ILE:O	2.21	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	273/277 (99%)	269 (98%)	4 (2%)	0	100	100
1	B	274/277 (99%)	270 (98%)	4 (2%)	0	100	100
1	C	266/277 (96%)	263 (99%)	3 (1%)	0	100	100
1	D	266/277 (96%)	263 (99%)	3 (1%)	0	100	100
1	E	274/277 (99%)	270 (98%)	4 (2%)	0	100	100
1	F	274/277 (99%)	270 (98%)	4 (2%)	0	100	100
1	G	260/277 (94%)	258 (99%)	2 (1%)	0	100	100
1	H	272/277 (98%)	268 (98%)	4 (2%)	0	100	100
1	I	269/277 (97%)	266 (99%)	3 (1%)	0	100	100
1	J	271/277 (98%)	266 (98%)	4 (2%)	1 (0%)	34	32
All	All	2699/2770 (97%)	2663 (99%)	35 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	48	PRO

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	211/212 (100%)	209 (99%)	2 (1%)	78	84
1	B	212/212 (100%)	208 (98%)	4 (2%)	57	63
1	C	206/212 (97%)	202 (98%)	4 (2%)	57	63
1	D	206/212 (97%)	201 (98%)	5 (2%)	49	53
1	E	212/212 (100%)	202 (95%)	10 (5%)	26	25
1	F	212/212 (100%)	208 (98%)	4 (2%)	57	63
1	G	200/212 (94%)	194 (97%)	6 (3%)	41	44
1	H	210/212 (99%)	206 (98%)	4 (2%)	57	63
1	I	207/212 (98%)	205 (99%)	2 (1%)	76	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	209/212 (99%)	205 (98%)	4 (2%)	57	63
All	All	2085/2120 (98%)	2040 (98%)	45 (2%)	53	57

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	PHE
1	A	274	SER
1	B	51	ARG
1	B	52	THR
1	B	122	PHE
1	B	274	SER
1	C	47	ASN
1	C	50	ARG
1	C	122	PHE
1	C	274	SER
1	D	46	SER
1	D	50	ARG
1	D	51	ARG
1	D	122	PHE
1	D	274	SER
1	E	9	ASP
1	E	35	LEU
1	E	36	SER
1	E	45	HIS
1	E	46	SER
1	E	47	ASN
1	E	122	PHE
1	E	126[A]	MET
1	E	126[B]	MET
1	E	274	SER
1	F	45	HIS
1	F	46	SER
1	F	122	PHE
1	F	274	SER
1	G	51	ARG
1	G	90	LYS
1	G	91	LEU
1	G	92	LYS
1	G	122	PHE
1	G	274	SER
1	H	45	HIS

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Mol	Chain	Res	Type
1	H	52	THR
1	H	122	PHE
1	H	274	SER
1	I	122	PHE
1	I	274	SER
1	J	31	ARG
1	J	45	HIS
1	J	122	PHE
1	J	274	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	H	45	HIS
1	J	45	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 (i)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PRO	I	301	-	8,8,8	0.78	0	10,10,10	1.06	0
2	PRO	G	301	-	8,8,8	0.76	0	10,10,10	1.07	0
2	PRO	J	301	-	8,8,8	0.90	1 (12%)	10,10,10	1.13	0
2	PRO	D	301	-	8,8,8	0.76	0	10,10,10	1.14	0
2	PRO	H	301	-	8,8,8	0.78	0	10,10,10	1.08	0
2	PRO	B	301	-	8,8,8	0.91	1 (12%)	10,10,10	1.19	0
2	PRO	E	301	-	8,8,8	0.93	1 (12%)	10,10,10	1.06	0
2	PRO	C	301	-	8,8,8	0.89	0	10,10,10	1.10	0
2	PRO	F	301	-	8,8,8	0.71	0	10,10,10	1.09	0
2	PRO	A	301	-	8,8,8	0.91	0	10,10,10	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
2	PRO	I	301	-	-	0/4/11/11	0/1/1/1
2	PRO	G	301	-	-	0/4/11/11	0/1/1/1
2	PRO	J	301	-	-	2/4/11/11	0/1/1/1
2	PRO	D	301	-	-	0/4/11/11	0/1/1/1
2	PRO	H	301	-	-	0/4/11/11	0/1/1/1
2	PRO	B	301	-	-	2/4/11/11	0/1/1/1
2	PRO	E	301	-	-	2/4/11/11	0/1/1/1
2	PRO	C	301	-	-	2/4/11/11	0/1/1/1
2	PRO	F	301	-	-	0/4/11/11	0/1/1/1
2	PRO	A	301	-	-	4/4/11/11	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	PRO	O-C	2.09	1.28	1.22
2	B	301	PRO	O-C	2.09	1.28	1.22
2	J	301	PRO	O-C	2.02	1.28	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	301	PRO	O-C-CA-CB
2	B	301	PRO	O-C-CA-CB
2	B	301	PRO	OXT-C-CA-CB
2	A	301	PRO	OXT-C-CA-N
2	A	301	PRO	O-C-CA-CB
2	A	301	PRO	OXT-C-CA-CB
2	C	301	PRO	OXT-C-CA-CB
2	J	301	PRO	OXT-C-CA-CB
2	A	301	PRO	O-C-CA-N
2	C	301	PRO	O-C-CA-CB
2	E	301	PRO	O-C-CA-CB
2	E	301	PRO	OXT-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	272/277 (98%)	-0.07	7 (2%)	56	61	37, 55, 85, 125	0
1	B	272/277 (98%)	0.36	27 (9%)	7	9	38, 67, 109, 142	0
1	C	268/277 (96%)	0.17	17 (6%)	20	24	37, 65, 111, 146	0
1	D	268/277 (96%)	0.61	44 (16%)	1	2	38, 84, 145, 157	0
1	E	272/277 (98%)	0.02	13 (4%)	30	36	39, 55, 89, 115	0
1	F	272/277 (98%)	-0.10	9 (3%)	46	53	39, 59, 95, 132	0
1	G	263/277 (94%)	1.26	68 (25%)	0	0	41, 93, 175, 246	0
1	H	272/277 (98%)	0.25	24 (8%)	10	12	44, 66, 112, 167	0
1	I	270/277 (97%)	0.26	16 (5%)	22	27	41, 76, 129, 154	0
1	J	271/277 (97%)	0.59	30 (11%)	5	7	41, 80, 130, 163	0
All	All	2700/2770 (97%)	0.33	255 (9%)	8	11	37, 65, 134, 246	0

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	94	LEU	18.4
1	H	3	ILE	11.4
1	G	18	ALA	10.1
1	G	113	LEU	9.2
1	G	8	ALA	8.5
1	C	46	SER	8.1
1	D	35	LEU	7.7
1	G	89	LEU	7.6
1	G	34	VAL	7.4
1	G	87	VAL	7.4
1	G	119	HIS	7.4
1	J	57	ILE	7.3
1	G	54	PHE	7.2

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Mol	Chain	Res	Type	RSRZ
1	G	88	VAL	7.2
1	G	63	SER	7.1
1	B	3	ILE	7.1
1	D	49	ALA	6.8
1	E	3	ILE	6.7
1	G	93	PRO	6.7
1	J	63	SER	6.6
1	J	61	VAL	6.6
1	G	91	LEU	6.5
1	D	8	ALA	6.5
1	G	64	SER	6.5
1	H	4	ILE	6.5
1	H	44	ILE	6.5
1	J	4	ILE	6.5
1	J	44	ILE	6.3
1	J	45	HIS	6.2
1	B	45	HIS	6.2
1	G	145	ALA	6.2
1	G	95	LEU	6.1
1	I	10	SER	5.9
1	G	83	LEU	5.9
1	G	116	TRP	5.8
1	I	46	SER	5.8
1	F	46	SER	5.7
1	G	99	LYS	5.5
1	B	4	ILE	5.4
1	G	121	ARG	5.4
1	B	46	SER	5.4
1	I	6	ILE	5.4
1	G	53	ALA	5.3
1	D	32	SER	5.3
1	G	49	ALA	5.2
1	G	146	ALA	5.1
1	J	46	SER	5.1
1	H	45	HIS	5.1
1	D	83	LEU	5.1
1	D	48	PRO	4.9
1	D	34	VAL	4.9
1	D	89	LEU	4.9
1	D	7	PRO	4.9
1	G	52	THR	4.7
1	J	18	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	H	46	SER	4.6
1	I	48	PRO	4.5
1	G	111	LYS	4.5
1	B	49	ALA	4.4
1	G	149	GLU	4.4
1	E	4	ILE	4.4
1	D	53	ALA	4.4
1	G	85	LYS	4.4
1	E	63	SER	4.3
1	G	97	LYS	4.3
1	I	45	HIS	4.3
1	B	48	PRO	4.3
1	J	53	ALA	4.3
1	J	51	ARG	4.2
1	G	50	ARG	4.2
1	G	38	SER	4.2
1	E	44	ILE	4.1
1	G	77	PHE	4.0
1	E	48	PRO	4.0
1	G	100	LEU	4.0
1	J	43	ALA	4.0
1	H	52	THR	3.9
1	B	104	VAL	3.9
1	J	48	PRO	3.9
1	H	63	SER	3.9
1	G	51	ARG	3.8
1	B	125	VAL	3.8
1	D	6	ILE	3.8
1	E	46	SER	3.8
1	J	47	ASN	3.8
1	G	147	THR	3.8
1	J	54	PHE	3.8
1	D	88	VAL	3.8
1	D	70	ARG	3.8
1	G	61	VAL	3.8
1	G	117	ALA	3.7
1	J	144	GLY	3.7
1	I	47	ASN	3.7
1	D	97	LYS	3.7
1	C	83	LEU	3.6
1	D	57	ILE	3.6
1	D	94	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	3	ILE	3.5
1	D	46	SER	3.5
1	C	49	ALA	3.5
1	F	49	ALA	3.5
1	H	48	PRO	3.5
1	A	47	ASN	3.5
1	G	70	ARG	3.4
1	B	53	ALA	3.4
1	B	47	ASN	3.4
1	J	93	PRO	3.4
1	G	86	ASP	3.4
1	E	45	HIS	3.3
1	E	49	ALA	3.3
1	J	5	PRO	3.3
1	D	87	VAL	3.3
1	D	63	SER	3.3
1	J	50	ARG	3.3
1	A	46	SER	3.3
1	J	97	LYS	3.3
1	B	158	PHE	3.3
1	I	35	LEU	3.2
1	G	7	PRO	3.2
1	C	57	ILE	3.2
1	G	16	ILE	3.2
1	G	11	TYR	3.2
1	F	47	ASN	3.2
1	D	31	ARG	3.2
1	I	8	ALA	3.1
1	G	122	PHE	3.1
1	D	71	ASP	3.1
1	D	90	LYS	3.1
1	D	50	ARG	3.1
1	G	71	ASP	3.1
1	I	9	ASP	3.1
1	H	49	ALA	3.1
1	D	30	VAL	3.1
1	G	42	THR	3.0
1	D	9	ASP	3.0
1	G	62	LEU	3.0
1	F	44	ILE	3.0
1	C	60	THR	3.0
1	C	5	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	54	PHE	2.9
1	J	49	ALA	2.9
1	H	68	VAL	2.9
1	F	3	ILE	2.9
1	E	52	THR	2.9
1	D	33	GLY	2.9
1	D	116	TRP	2.9
1	B	63	SER	2.9
1	H	83	LEU	2.9
1	C	90	LYS	2.8
1	B	157	LEU	2.8
1	F	48	PRO	2.8
1	J	33	GLY	2.8
1	J	62	LEU	2.8
1	C	7	PRO	2.8
1	G	59	ILE	2.8
1	G	148	GLU	2.7
1	G	82	GLN	2.7
1	H	47	ASN	2.7
1	G	151	ALA	2.7
1	G	79	VAL	2.7
1	H	126[A]	MET	2.7
1	G	101	LEU	2.7
1	H	51	ARG	2.7
1	G	67	ASP	2.7
1	H	67	ASP	2.7
1	B	51	ARG	2.6
1	J	146	ALA	2.6
1	D	99	LYS	2.6
1	G	144	GLY	2.6
1	I	7	PRO	2.6
1	D	42	THR	2.6
1	G	90	LYS	2.6
1	J	11	TYR	2.6
1	C	86	ASP	2.6
1	G	9	ASP	2.6
1	G	33	GLY	2.6
1	G	115	GLU	2.6
1	C	31	ARG	2.5
1	G	150	ASP	2.5
1	G	126	MET	2.5
1	H	70	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	62	LEU	2.5
1	D	93	PRO	2.5
1	H	53	ALA	2.5
1	G	114	GLN	2.5
1	E	47	ASN	2.5
1	J	6	ILE	2.5
1	C	52	THR	2.4
1	D	52	THR	2.4
1	G	81	PRO	2.4
1	D	67	ASP	2.4
1	H	61	VAL	2.4
1	H	97	LYS	2.4
1	G	92	LYS	2.4
1	J	56	SER	2.4
1	G	112	ASP	2.4
1	B	6	ILE	2.4
1	H	60	THR	2.4
1	B	127	PRO	2.4
1	F	45	HIS	2.4
1	I	44	ILE	2.4
1	B	76	VAL	2.3
1	C	144	GLY	2.3
1	I	49	ALA	2.3
1	I	156	GLN	2.3
1	C	9	ASP	2.3
1	C	97	LYS	2.3
1	H	64	SER	2.3
1	D	95	LEU	2.3
1	A	214	THR	2.3
1	D	61	VAL	2.3
1	C	48	PRO	2.3
1	D	91	LEU	2.2
1	G	84	LEU	2.2
1	D	86	ASP	2.2
1	A	215	VAL	2.2
1	C	62	LEU	2.2
1	J	13	LEU	2.2
1	B	52	THR	2.2
1	J	31	ARG	2.2
1	E	51	ARG	2.2
1	A	45	HIS	2.2
1	B	186	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	138	SER	2.2
1	H	31	ARG	2.2
1	D	36	SER	2.2
1	E	186	ILE	2.2
1	E	50	ARG	2.2
1	G	15	PHE	2.2
1	I	59	ILE	2.1
1	G	69	VAL	2.1
1	F	145	ALA	2.1
1	G	120	GLU	2.1
1	H	62	LEU	2.1
1	A	63	SER	2.1
1	J	52	THR	2.1
1	B	44	ILE	2.1
1	F	31	ARG	2.1
1	D	118	GLY	2.1
1	D	10	SER	2.1
1	D	11	TYR	2.1
1	D	119	HIS	2.1
1	D	76	VAL	2.1
1	J	104	VAL	2.1
1	B	126	MET	2.0
1	D	126	MET	2.0
1	B	102	VAL	2.0
1	I	30	VAL	2.0
1	H	43	ALA	2.0
1	B	215	VAL	2.0
1	B	86	ASP	2.0
1	C	64	SER	2.0
1	B	5	PRO	2.0
1	B	55	GLU	2.0
1	G	68	VAL	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, 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	B-factors(Å^2)	Q<0.9
2	PRO	G	301	8/8	0.76	0.23	48,91,93,96	0
2	PRO	F	301	8/8	0.80	0.26	52,94,106,109	0
2	PRO	B	301	8/8	0.84	0.19	44,74,87,93	0
2	PRO	J	301	8/8	0.86	0.17	53,76,85,91	0
2	PRO	E	301	8/8	0.88	0.17	46,81,90,94	0
2	PRO	I	301	8/8	0.89	0.15	50,80,88,90	0
2	PRO	H	301	8/8	0.90	0.13	51,78,82,85	0
2	PRO	C	301	8/8	0.91	0.12	49,68,74,75	0
2	PRO	D	301	8/8	0.91	0.12	47,64,66,68	0
2	PRO	A	301	8/8	0.96	0.12	49,77,83,83	0

6.5 Other polymers (i)

There are no such residues in this entry.