



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:41 AM UTC

PDB ID : 5BSH / pdb_00005bsh
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

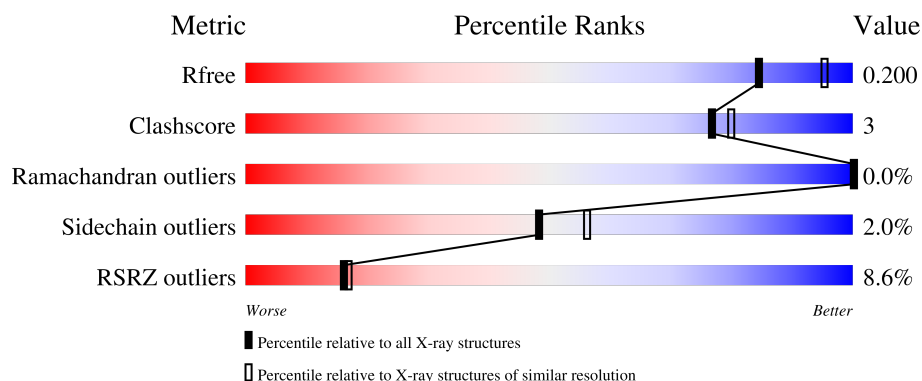
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	277	3% 90% 8% .
1	B	277	7% 91% 7% .
1	C	277	5% 88% 8% ..
1	D	277	16% 87% 9% .
1	E	277	5% 90% 7% ..

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Mol	Chain	Length	Quality of chain
1	F	277	3% 92% 6%
1	G	277	23% 90% 5% 5%
1	H	277	5% 90% 7%
1	I	277	7% 92% 5%
1	J	277	10% 87% 8%

2 Entry composition

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

There are 30 discrepancies between the modelled and reference sequences:

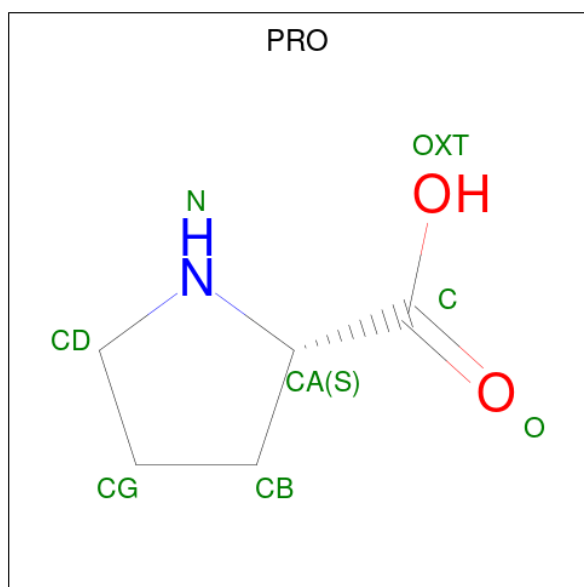
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP G7KRM5
A	-1	ASN	-	expression tag	UNP G7KRM5
A	0	ALA	-	expression tag	UNP G7KRM5
B	-2	SER	-	expression tag	UNP G7KRM5
B	-1	ASN	-	expression tag	UNP G7KRM5
B	0	ALA	-	expression tag	UNP G7KRM5
C	-2	SER	-	expression tag	UNP G7KRM5
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 (CCD ID: PRO) (formula: C₅H₉NO₂).



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

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

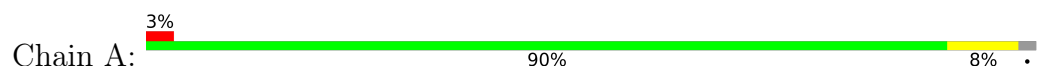
- Molecule 3 is water.

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

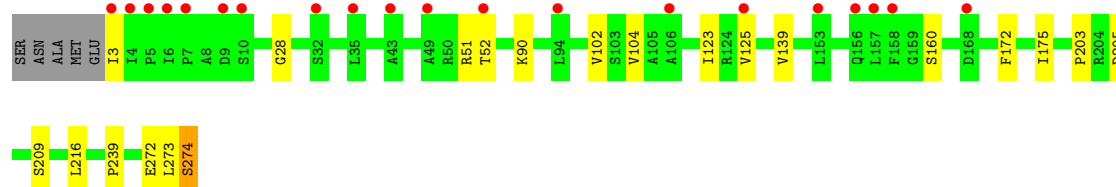
3 Residue-property plots [i](#)

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.

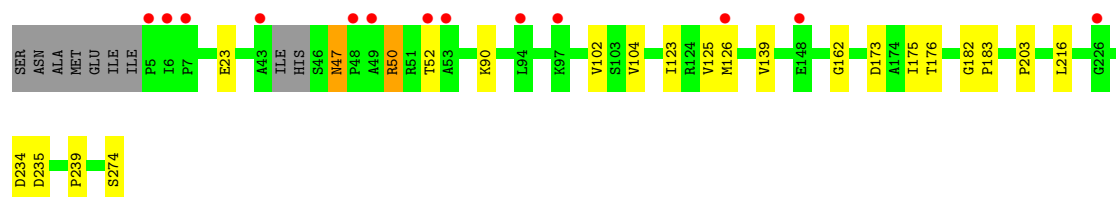
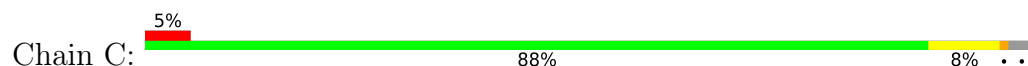
- Molecule 1: Pyrroline-5-carboxylate reductase



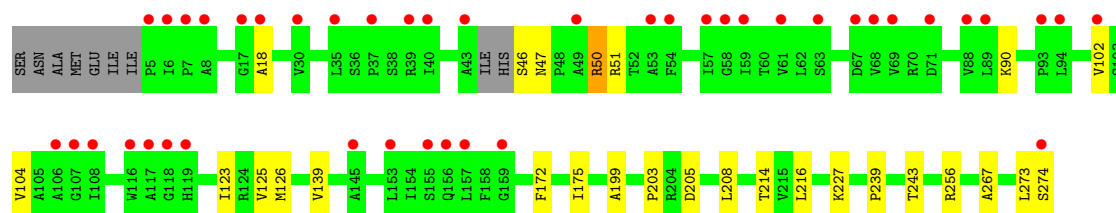
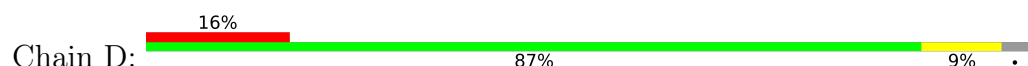
- Molecule 1: Pyrroline-5-carboxylate reductase



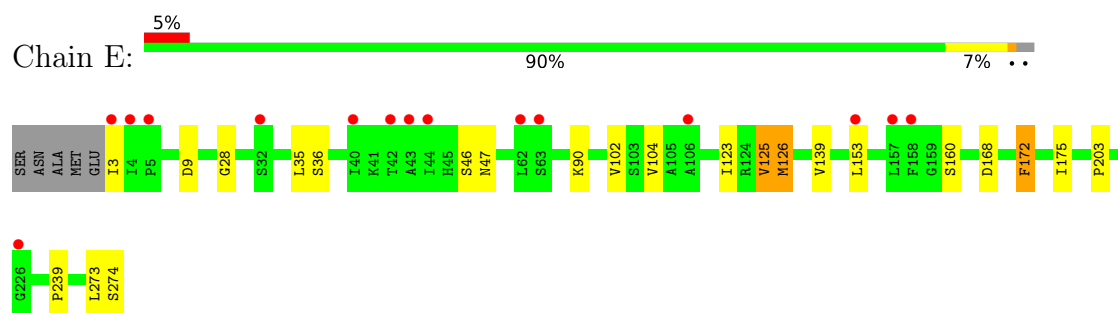
- Molecule 1: Pyrroline-5-carboxylate reductase



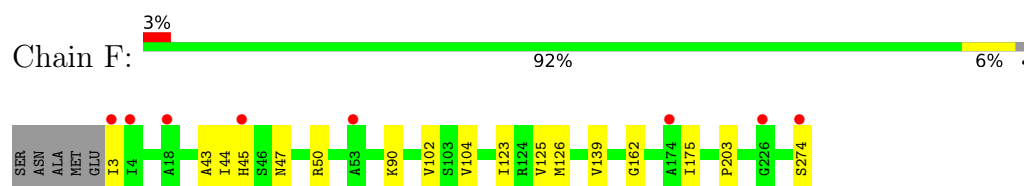
- Molecule 1: Pyrroline-5-carboxylate reductase



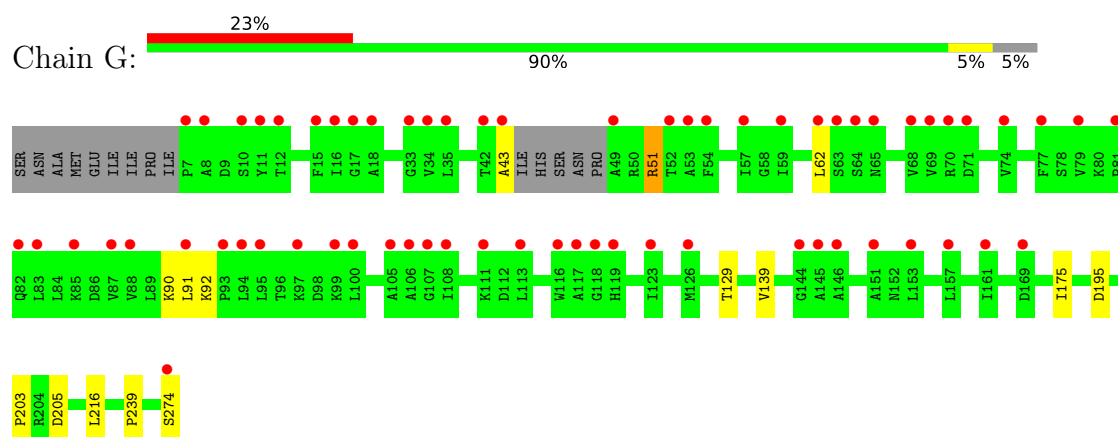
● Molecule 1: Pyrroline-5-carboxylate reductase



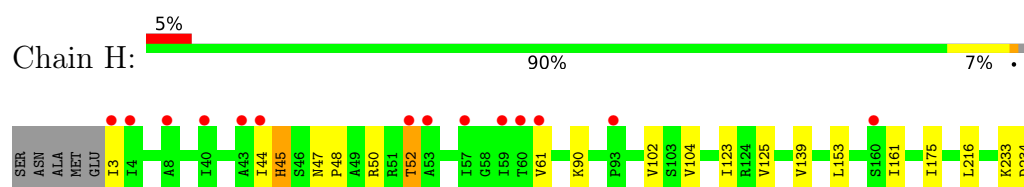
● Molecule 1: Pyrroline-5-carboxylate reductase



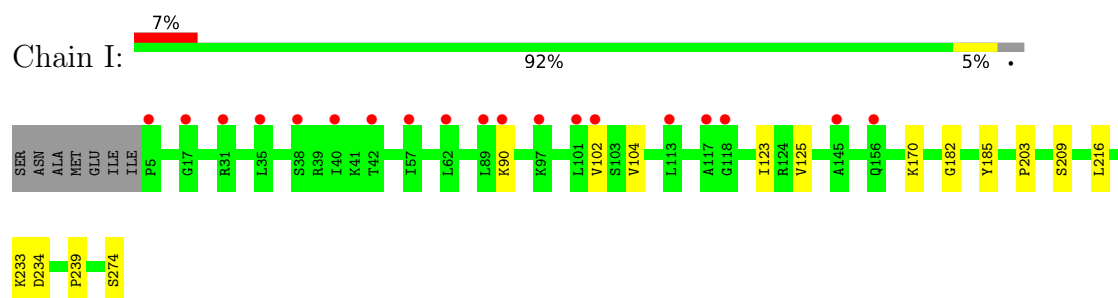
● Molecule 1: Pyrroline-5-carboxylate reductase



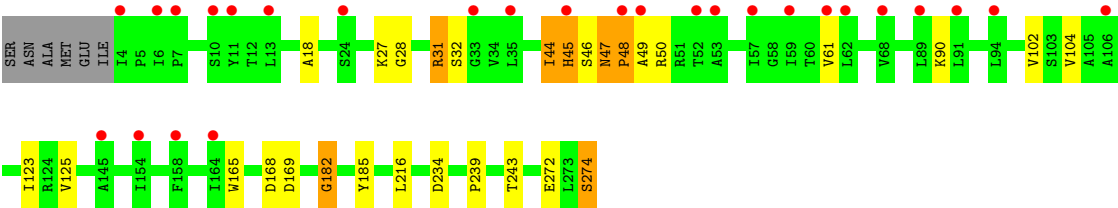
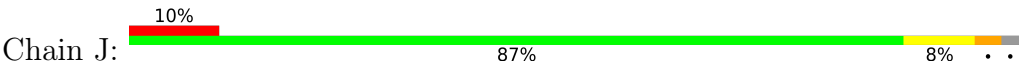
● Molecule 1: Pyrroline-5-carboxylate reductase



● Molecule 1: Pyrroline-5-carboxylate reductase



● Molecule 1: Pyrroline-5-carboxylate reductase



4 Data and refinement statistics

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 40.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.0 (40.00-2.10) 97.6 (40.00-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (1.02%)	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)	0.31 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

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

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	1.25	5/2041 (0.2%)	1.04	2/2761 (0.1%)
1	B	1.17	0/2047	1.01	2/2769 (0.1%)
1	C	1.13	3/1996 (0.2%)	1.00	1/2697 (0.0%)
1	D	1.13	5/1997 (0.3%)	0.98	2/2698 (0.1%)
1	E	1.21	1/2049 (0.0%)	1.05	2/2772 (0.1%)
1	F	1.12	1/2049 (0.0%)	0.99	0/2772
1	G	1.06	0/1950	1.02	3/2632 (0.1%)
1	H	1.09	1/2032 (0.0%)	1.00	3/2749 (0.1%)
1	I	1.10	1/2008 (0.0%)	1.00	0/2715
1	J	1.12	2/2024 (0.1%)	1.01	4/2738 (0.1%)
All	All	1.14	19/20193 (0.1%)	1.01	19/27303 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	162	GLY	C-O	-6.54	1.19	1.23
1	F	162	GLY	C-O	-6.37	1.19	1.23
1	A	174	ALA	N-CA	-6.28	1.38	1.46
1	J	234	ASP	C-O	-6.15	1.17	1.24
1	D	208	LEU	N-CA	-6.13	1.39	1.46
1	A	187	TYR	C-O	-5.95	1.17	1.24
1	A	162	GLY	C-O	-5.70	1.19	1.23
1	C	234	ASP	C-O	-5.69	1.17	1.24
1	D	267	ALA	N-CA	5.59	1.53	1.46
1	A	258	ILE	C-O	-5.57	1.17	1.24
1	C	235	ASP	C-O	-5.41	1.17	1.24
1	I	170	LYS	C-O	-5.40	1.17	1.24
1	E	125	VAL	CA-CB	-5.37	1.47	1.54
1	D	214	THR	N-CA	5.28	1.52	1.46
1	A	49	ALA	CA-C	5.24	1.59	1.52
1	H	48	PRO	N-CD	5.24	1.55	1.47
1	J	243	THR	C-O	5.23	1.30	1.24
1	D	256	ARG	CA-C	-5.08	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	243	THR	C-O	5.08	1.29	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	ARG	N-CA-C	7.06	121.16	112.54
1	C	173	ASP	N-CA-C	6.06	117.56	111.07
1	D	199	ALA	N-CA-C	-5.85	105.03	111.82
1	H	161	ILE	CB-CA-C	-5.78	104.60	111.65
1	H	52	THR	N-CA-CB	5.63	118.18	110.01
1	H	273	LEU	N-CA-C	-5.61	106.41	113.20
1	J	182	GLY	CA-C-N	-5.59	113.13	119.28
1	J	182	GLY	C-N-CA	-5.59	113.13	119.28
1	D	273	LEU	N-CA-C	-5.38	106.70	113.20
1	A	273	LEU	N-CA-C	-5.31	106.78	113.20
1	G	51	ARG	N-CA-CB	5.30	118.01	110.06
1	E	172	PHE	N-CA-C	5.25	117.92	111.82
1	E	273	LEU	N-CA-C	-5.20	106.91	113.20
1	B	273	LEU	N-CA-C	-5.20	106.91	113.20
1	G	129	THR	N-CA-C	5.19	117.68	111.71
1	G	195	ASP	N-CA-C	-5.15	105.66	111.28
1	J	47	ASN	CA-C-N	-5.12	113.45	119.84
1	J	47	ASN	C-N-CA	-5.12	113.45	119.84
1	B	172	PHE	N-CA-C	5.04	117.66	111.82

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	10	0
1	B	2018	0	2078	11	0
1	C	1969	0	2033	13	0
1	D	1970	0	2031	17	0
1	E	2020	0	2083	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2020	0	2083	9	0
1	G	1925	0	1988	6	0
1	H	2003	0	2073	17	0
1	I	1979	0	2043	8	0
1	J	1995	0	2056	27	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	0	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	0	0
All	All	20686	0	20618	117	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 (117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:THR:HG22	3:C:454:HOH:O	1.87	0.75
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:H:44:ILE:CG1	1:H:61:VAL:CG1	2.71	0.68
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:D:126:MET:HE2	1:D:172:PHE:HD2	1.62	0.64
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:C:126[B]:MET:HE1	1:C:176:THR:OG1	1.98	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:D:126:MET:HE2	1:D:172:PHE:CD2	2.36	0.58
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:D:227:LYS:NZ	3:D:403:HOH:O	2.39	0.56
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:E:126[B]:MET:HE1	1:E:175:ILE:HG22	1.88	0.54
1:J:45:HIS:CD2	1:J:45:HIS:C	2.85	0.53
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ASN:OD1	1:C:47:ASN:N	2.46	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:F:47:ASN:OD1	1:F:50:ARG:N	2.34	0.47
1:H:153:LEU:C	1:H:153:LEU:HD23	2.38	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:F:126[B]:MET:HE1	1:F:175:ILE:HG22	1.98	0.45
1:C:126[B]:MET:HE1	1:C:176:THR:HA	1.98	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: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:G:43:ALA:C	1:G:62:LEU:O	2.61	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:B:272:GLU:C	1:B:274:SER:N	2.77	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
1:D:104:VAL:HA	1:D:125:VAL:O	2.19	0.43
1:F:43:ALA:C	1:F:44:ILE:HG13	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126[B]:MET:HE1	1:C:176:THR:CB	2.50	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: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:C:182:GLY:O	1:C:183:PRO:C	2.62	0.41
1:B:239:PRO:HG3	1:D:203:PRO:HA	2.03	0.41
1:E:153:LEU:C	1:E:153:LEU:HD23	2.46	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:D:126:MET:HE3	1:D:172:PHE:CD2	2.57	0.40
1:H:44:ILE:HG13	1:H:61:VAL:CG1	2.46	0.40
1:J:272:GLU:C	1:J:274:SER:N	2.78	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%)	30	28
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 ⓘ

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%)	70	78
1	B	212/212 (100%)	208 (98%)	4 (2%)	50	58
1	C	206/212 (97%)	202 (98%)	4 (2%)	50	58
1	D	206/212 (97%)	201 (98%)	5 (2%)	43	49
1	E	212/212 (100%)	203 (96%)	9 (4%)	26	28
1	F	212/212 (100%)	209 (99%)	3 (1%)	59	67
1	G	200/212 (94%)	195 (98%)	5 (2%)	42	48
1	H	210/212 (99%)	206 (98%)	4 (2%)	50	58
1	I	207/212 (98%)	205 (99%)	2 (1%)	68	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	209/212 (99%)	204 (98%)	5 (2%)	43 49
All	All	2085/2120 (98%)	2042 (98%)	43 (2%)	48 54

All (43) residues with a non-rotameric sidechain are listed below:

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

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Mol	Chain	Res	Type
1	I	90	LYS
1	I	274	SER
1	J	31	ARG
1	J	44	ILE
1	J	45	HIS
1	J	90	LYS
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 oligosaccharides 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	A	301	-	8,8,8	0.95	1 (12%)	10,10,10	1.18	0
2	PRO	G	301	-	8,8,8	0.78	0	10,10,10	1.08	0
2	PRO	D	301	-	8,8,8	0.79	0	10,10,10	1.16	0
2	PRO	B	301	-	8,8,8	0.94	1 (12%)	10,10,10	1.20	0
2	PRO	J	301	-	8,8,8	0.93	1 (12%)	10,10,10	1.14	0
2	PRO	C	301	-	8,8,8	0.92	0	10,10,10	1.11	0
2	PRO	F	301	-	8,8,8	0.73	0	10,10,10	1.10	0
2	PRO	E	301	-	8,8,8	0.96	1 (12%)	10,10,10	1.07	0
2	PRO	I	301	-	8,8,8	0.81	0	10,10,10	1.08	0
2	PRO	H	301	-	8,8,8	0.80	0	10,10,10	1.09	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	A	301	-	-	4/4/11/11	0/1/1/1
2	PRO	G	301	-	-	0/4/11/11	0/1/1/1
2	PRO	D	301	-	-	0/4/11/11	0/1/1/1
2	PRO	B	301	-	-	2/4/11/11	0/1/1/1
2	PRO	J	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	E	301	-	-	2/4/11/11	0/1/1/1
2	PRO	I	301	-	-	0/4/11/11	0/1/1/1
2	PRO	H	301	-	-	0/4/11/11	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	PRO	O-C	2.17	1.28	1.22
2	B	301	PRO	O-C	2.16	1.28	1.22
2	J	301	PRO	O-C	2.09	1.28	1.22
2	A	301	PRO	O-C	2.04	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	B	301	PRO	OXT-C-CA-CB
2	J	301	PRO	O-C-CA-CB
2	A	301	PRO	O-C-CA-CB
2	A	301	PRO	OXT-C-CA-CB
2	B	301	PRO	O-C-CA-CB
2	C	301	PRO	OXT-C-CA-CB
2	J	301	PRO	OXT-C-CA-CB
2	E	301	PRO	OXT-C-CA-CB
2	A	301	PRO	O-C-CA-N
2	A	301	PRO	OXT-C-CA-N
2	C	301	PRO	O-C-CA-CB
2	E	301	PRO	O-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 ⓘ

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	272/277 (98%)	0.19	9 (3%)	49	51	21, 55, 85, 125	3 (1%)
1	B	272/277 (98%)	0.43	20 (7%)	20	22	22, 67, 109, 142	4 (1%)
1	C	268/277 (96%)	0.44	13 (4%)	35	37	22, 65, 111, 146	2 (0%)
1	D	268/277 (96%)	0.77	43 (16%)	5	5	22, 84, 145, 157	2 (0%)
1	E	272/277 (98%)	0.26	15 (5%)	30	32	21, 55, 89, 115	4 (1%)
1	F	272/277 (98%)	0.20	8 (2%)	53	56	22, 59, 95, 132	4 (1%)
1	G	263/277 (94%)	1.09	65 (24%)	2	2	26, 93, 175, 246	1 (0%)
1	H	272/277 (98%)	0.42	14 (5%)	33	35	24, 66, 112, 167	2 (0%)
1	I	270/277 (97%)	0.68	19 (7%)	22	24	23, 76, 129, 154	1 (0%)
1	J	271/277 (97%)	0.78	27 (9%)	12	13	28, 80, 130, 163	2 (0%)
All	All	2700/2770 (97%)	0.52	233 (8%)	16	17	21, 65, 134, 246	25 (0%)

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	8	ALA	5.5
1	G	88	VAL	5.5
1	I	5	PRO	5.3
1	G	95	LEU	5.2
1	D	43	ALA	5.1
1	G	93	PRO	5.0
1	G	94	LEU	4.9
1	G	54	PHE	4.8
1	J	59	ILE	4.7
1	J	49	ALA	4.5
1	D	8	ALA	4.5
1	G	7	PRO	4.3
1	G	145	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	49	ALA	4.2
1	D	5	PRO	4.2
1	E	106	ALA	4.2
1	B	158	PHE	4.2
1	B	157	LEU	4.1
1	G	34	VAL	4.1
1	E	4	ILE	4.0
1	G	53	ALA	4.0
1	A	52	THR	4.0
1	J	52	THR	4.0
1	G	43	ALA	3.9
1	G	119	HIS	3.8
1	J	53	ALA	3.8
1	J	4	ILE	3.7
1	G	49	ALA	3.7
1	B	4	ILE	3.7
1	D	145	ALA	3.7
1	G	68	VAL	3.6
1	C	7	PRO	3.6
1	D	53	ALA	3.5
1	G	113	LEU	3.5
1	J	13	LEU	3.5
1	D	89	LEU	3.5
1	G	274	SER	3.5
1	H	4	ILE	3.5
1	G	64	SER	3.5
1	H	52	THR	3.5
1	G	16	ILE	3.4
1	C	5	PRO	3.4
1	G	116	TRP	3.4
1	G	100	LEU	3.4
1	D	7	PRO	3.3
1	C	43	ALA	3.3
1	G	146	ALA	3.3
1	H	60	THR	3.3
1	J	7	PRO	3.3
1	H	53	ALA	3.3
1	I	38	SER	3.2
1	G	81	PRO	3.2
1	J	48	PRO	3.2
1	J	68	VAL	3.2
1	J	164	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	7	PRO	3.2
1	J	10	SER	3.2
1	G	83	LEU	3.1
1	I	145	ALA	3.1
1	C	48	PRO	3.1
1	G	11	TYR	3.0
1	J	11	TYR	3.0
1	G	69	VAL	3.0
1	D	274	SER	3.0
1	F	53	ALA	3.0
1	D	94	LEU	3.0
1	G	87	VAL	3.0
1	G	91	LEU	3.0
1	E	3	ILE	3.0
1	G	107	GLY	3.0
1	D	68	VAL	3.0
1	G	18	ALA	2.9
1	C	6	ILE	2.9
1	G	161	ILE	2.9
1	G	71	ASP	2.9
1	C	52	THR	2.9
1	G	77	PHE	2.9
1	G	117	ALA	2.9
1	I	117	ALA	2.9
1	E	62	LEU	2.9
1	G	62	LEU	2.9
1	G	153	LEU	2.9
1	D	61	VAL	2.8
1	D	108	ILE	2.8
1	G	59	ILE	2.8
1	H	3	ILE	2.8
1	G	105	ALA	2.8
1	D	59	ILE	2.8
1	G	126	MET	2.8
1	I	17	GLY	2.8
1	G	17	GLY	2.8
1	F	4	ILE	2.8
1	H	57	ILE	2.8
1	D	156	GLN	2.7
1	I	97	LYS	2.7
1	D	35	LEU	2.7
1	G	144	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	108	ILE	2.7
1	J	6	ILE	2.7
1	J	57	ILE	2.7
1	I	42	THR	2.6
1	I	57	ILE	2.6
1	I	101	LEU	2.6
1	D	118	GLY	2.6
1	A	53	ALA	2.6
1	H	93	PRO	2.6
1	D	159	GLY	2.6
1	G	97	LYS	2.6
1	D	93	PRO	2.6
1	E	63	SER	2.6
1	E	158	PHE	2.5
1	J	61	VAL	2.5
1	J	154	ILE	2.5
1	A	49	ALA	2.5
1	B	43	ALA	2.5
1	B	52	THR	2.5
1	F	274	SER	2.5
1	B	35	LEU	2.5
1	D	153	LEU	2.5
1	A	44	ILE	2.5
1	G	118	GLY	2.5
1	H	59	ILE	2.5
1	G	99	LYS	2.5
1	D	58	GLY	2.5
1	D	57	ILE	2.5
1	H	40	ILE	2.5
1	I	40	ILE	2.5
1	C	53	ALA	2.5
1	J	145	ALA	2.5
1	A	89	LEU	2.5
1	F	3	ILE	2.5
1	C	148	GLU	2.4
1	G	169	ASP	2.4
1	G	106	ALA	2.4
1	I	35	LEU	2.4
1	J	91	LEU	2.4
1	C	226	GLY	2.4
1	B	6	ILE	2.4
1	D	6	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	74	VAL	2.4
1	G	10	SER	2.4
1	D	37	PRO	2.4
1	G	151	ALA	2.4
1	F	45	HIS	2.4
1	A	47	ASN	2.4
1	H	61	VAL	2.4
1	A	63	SER	2.4
1	H	43	ALA	2.4
1	C	94	LEU	2.4
1	G	65	ASN	2.4
1	E	5	PRO	2.4
1	A	94	LEU	2.3
1	E	40	ILE	2.3
1	E	44	ILE	2.3
1	E	42	THR	2.3
1	D	39	ARG	2.3
1	I	90	LYS	2.3
1	G	12	THR	2.3
1	D	17	GLY	2.3
1	D	116	TRP	2.3
1	G	33	GLY	2.3
1	I	113	LEU	2.3
1	D	54	PHE	2.3
1	D	102	VAL	2.3
1	B	49	ALA	2.3
1	D	18	ALA	2.3
1	H	8	ALA	2.3
1	I	62	LEU	2.3
1	J	62	LEU	2.3
1	A	274	SER	2.2
1	D	155	SER	2.2
1	D	88	VAL	2.2
1	C	97	LYS	2.2
1	G	111	LYS	2.2
1	D	106	ALA	2.2
1	F	18	ALA	2.2
1	G	35	LEU	2.2
1	J	94	LEU	2.2
1	D	119	HIS	2.2
1	D	63	SER	2.2
1	J	158	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	42	THR	2.2
1	G	57	ILE	2.2
1	G	123	ILE	2.2
1	D	30	VAL	2.2
1	D	69	VAL	2.2
1	B	9	ASP	2.2
1	G	157	LEU	2.2
1	I	156	GLN	2.2
1	G	63	SER	2.2
1	G	15	PHE	2.2
1	G	79	VAL	2.2
1	I	118	GLY	2.2
1	J	33	GLY	2.2
1	F	174	ALA	2.2
1	E	153	LEU	2.2
1	B	32	SER	2.2
1	G	52	THR	2.2
1	B	125	VAL	2.1
1	I	102	VAL	2.1
1	F	226	GLY	2.1
1	D	157	LEU	2.1
1	J	35	LEU	2.1
1	E	32	SER	2.1
1	J	24	SER	2.1
1	B	3	ILE	2.1
1	G	82	GLN	2.1
1	H	44	ILE	2.1
1	B	106	ALA	2.1
1	D	49	ALA	2.1
1	E	43	ALA	2.1
1	D	71	ASP	2.1
1	B	5	PRO	2.1
1	B	156	GLN	2.1
1	E	226	GLY	2.1
1	D	117	ALA	2.1
1	J	106	ALA	2.1
1	B	10	SER	2.1
1	J	89	LEU	2.1
1	G	70	ARG	2.1
1	D	107	GLY	2.1
1	D	40	ILE	2.1
1	C	126[A]	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	94	LEU	2.0
1	E	157	LEU	2.0
1	B	168[A]	ASP	2.0
1	I	31	ARG	2.0
1	J	45	HIS	2.0
1	G	85	LYS	2.0
1	H	160	SER	2.0
1	B	153	LEU	2.0
1	I	89	LEU	2.0
1	D	67	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	F	301	8/8	0.73	0.25	52,94,106,109	0
2	PRO	B	301	8/8	0.79	0.21	44,74,87,93	0
2	PRO	G	301	8/8	0.79	0.22	48,91,93,96	0
2	PRO	H	301	8/8	0.84	0.15	51,78,82,85	0
2	PRO	D	301	8/8	0.85	0.14	47,64,66,68	0
2	PRO	I	301	8/8	0.85	0.14	50,80,88,90	0
2	PRO	E	301	8/8	0.86	0.21	46,81,90,94	0
2	PRO	C	301	8/8	0.87	0.13	49,68,74,75	0
2	PRO	A	301	8/8	0.88	0.13	49,77,83,83	0
2	PRO	J	301	8/8	0.88	0.19	53,76,85,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.