



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:05 PM GMT

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
<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-20026982
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-20026982

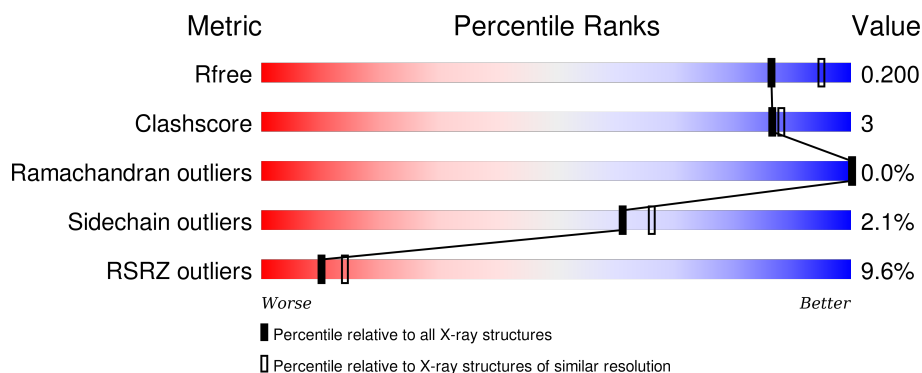
1 Overall quality at a glance

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 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	277	<div> <div>3%</div> <div>92%</div> <div>6% •</div> </div>
1	B	277	<div> <div>9%</div> <div>92%</div> <div>6% •</div> </div>
1	C	277	<div> <div>6%</div> <div>91%</div> <div>5% • •</div> </div>
1	D	277	<div> <div>15%</div> <div>90%</div> <div>7% •</div> </div>
1	E	277	<div> <div>5%</div> <div>90%</div> <div>7% • •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	277	
1	G	277	
1	H	277	
1	I	277	
1	J	277	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PRO	B	301	-	-	-	X
2	PRO	F	301	-	-	-	X
2	PRO	G	301	-	-	-	X

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:

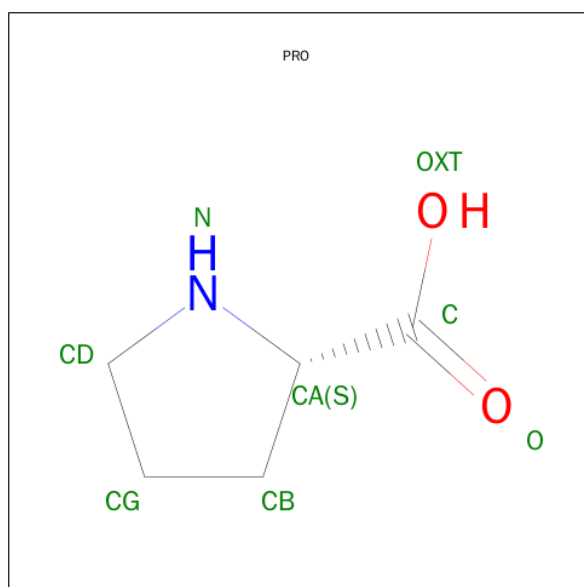
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP G7KRM5
A	-1	ASN	-	expression tag	UNP G7KRM5
A	0	ALA	-	expression tag	UNP G7KRM5
B	-2	SER	-	expression tag	UNP G7KRM5
B	-1	ASN	-	expression tag	UNP G7KRM5
B	0	ALA	-	expression tag	UNP G7KRM5
C	-2	SER	-	expression tag	UNP G7KRM5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

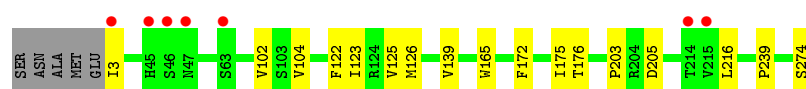
- Molecule 3 is water.

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		

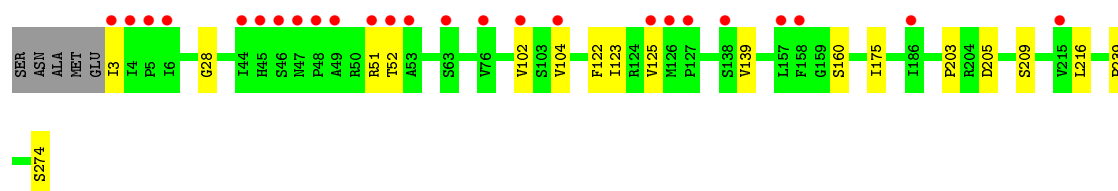
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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.

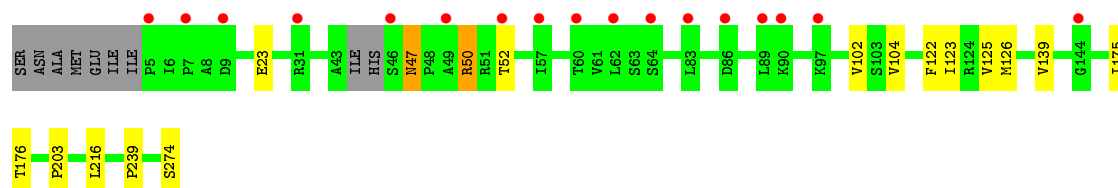
- Molecule 1: Pyrroline-5-carboxylate reductase



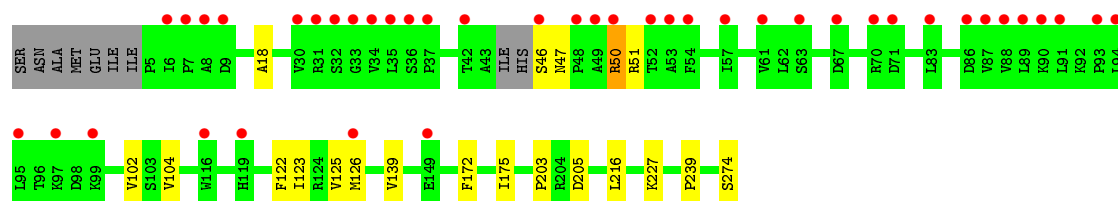
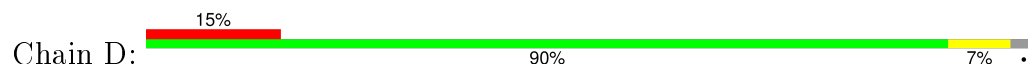
- Molecule 1: Pyrroline-5-carboxylate reductase



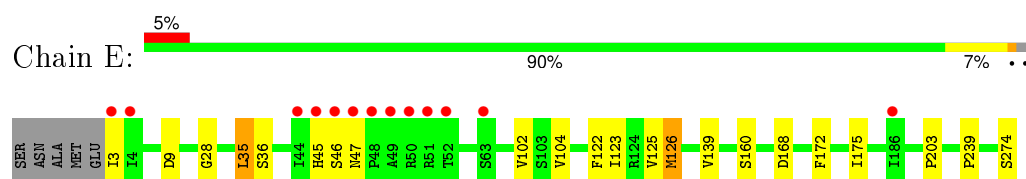
- Molecule 1: Pyrroline-5-carboxylate reductase



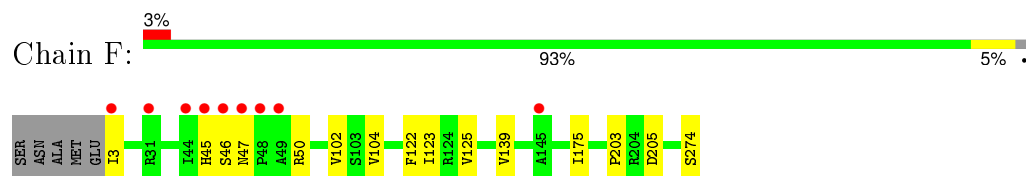
- Molecule 1: Pyrroline-5-carboxylate reductase



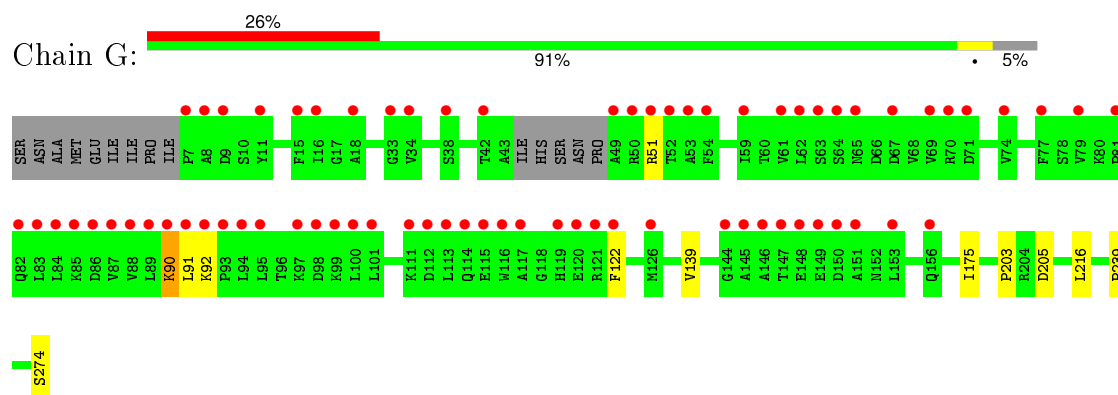
- Molecule 1: Pyrroline-5-carboxylate reductase



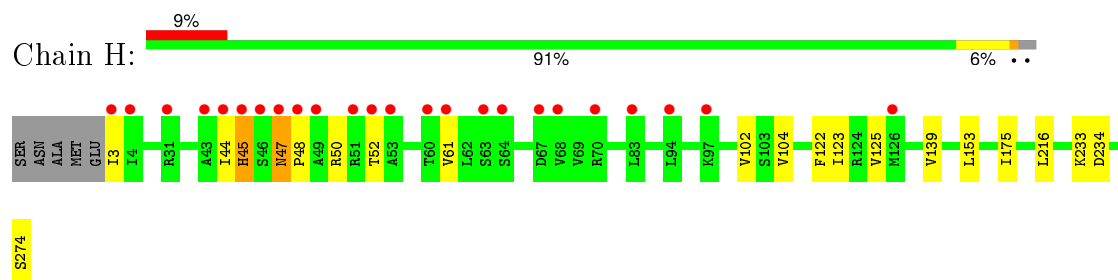
- Molecule 1: Pyrroline-5-carboxylate reductase



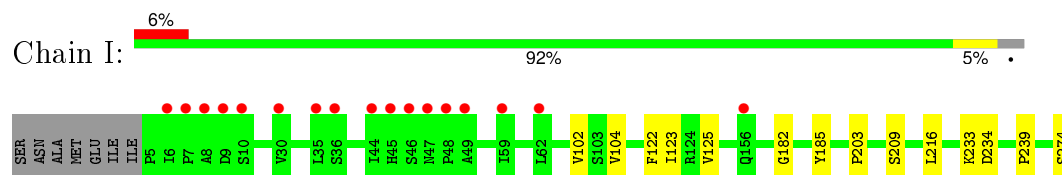
- Molecule 1: Pyrroline-5-carboxylate reductase



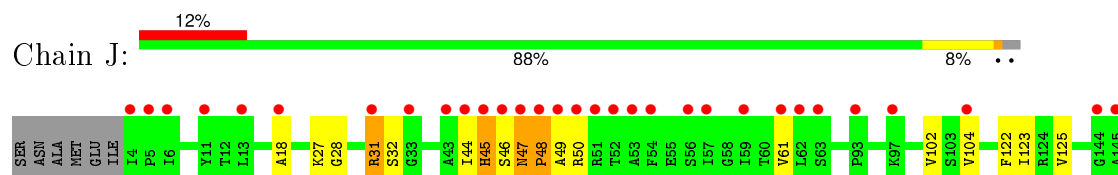
- Molecule 1: Pyrroline-5-carboxylate reductase

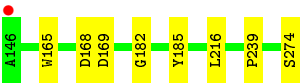


- Molecule 1: Pyrroline-5-carboxylate reductase



- 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 33.49 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.0 (40.00-2.10) 85.5 (33.49-2.09)	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	Depositor
R, R_{free}	0.180 , 0.197 0.185 , 0.200	Depositor DCC
R_{free} test set	1928 reflections (1.06%)	DCC
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 183948 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	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(°)	Ideal(°)
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 ⓘ

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:CD2	1:H:45:HIS:H	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:HG2	1:D:50:ARG:HH11	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:N	1:H:45:HIS:CD2	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:J:31:ARG:HG3	1:J:32:SER:N	2.26	0.51
1:D:239:PRO:HG3	1:F:203:PRO:HA	1.92	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:I:216:LEU:CD1	1:J:216:LEU:CD1	2.91	0.48
1:E:104:VAL:HA	1:E:125:VAL:O	2.13	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:J:45:HIS:HD2	1:J:46:SER:N	2.14	0.46
1:E:203:PRO:HA	1:G:239:PRO:HG3	1.97	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:J:44:ILE:HG12	1:J:61:VAL:HG13	1.97	0.45
1:F:3:ILE:HG22	1:F:3:ILE:O	2.16	0.45
1:B:3:ILE:HG22	1:B:3:ILE:O	2.17	0.45
1:H:3:ILE:HG22	1:H:3:ILE:O	2.17	0.45
1:A:3:ILE:O	1:A:3:ILE:HG22	2.17	0.45
1:J:28:GLY:O	1:J:31:ARG:CG	2.61	0.44
1:A:216:LEU:CD1	1:B:216:LEU:CD1	2.95	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:J:48:PRO:CD	1:J:49:ALA:N	2.80	0.44
1:C:216:LEU:CD1	1:D:216:LEU:CD1	2.96	0.44
1:A:104:VAL:HA	1:A:125:VAL:O	2.18	0.44
1:B:102:VAL:HA	1:B:123:ILE:O	2.18	0.43
1:A:102:VAL:HA	1:A: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:HD23	1:H:153:LEU:C	2.38	0.42
1:H:233:LYS:HE2	1:H:234:ASP:OD1	2.20	0.42
1:D:50:ARG:CG	1:D:50:ARG:HH11	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:I:102:VAL:HA	1:I:123:ILE:O	2.20	0.41
1:D:102:VAL:HA	1:D: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:F:50:ARG:HA	1:F:50:ARG:HD2	1.73	0.41
1:E:139:VAL:HG23	1:E:172:PHE:CZ	2.56	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%)	39	37
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%)	84	89
1	B	212/212 (100%)	208 (98%)	4 (2%)	65	70
1	C	206/212 (97%)	202 (98%)	4 (2%)	65	70
1	D	206/212 (97%)	201 (98%)	5 (2%)	57	61
1	E	212/212 (100%)	202 (95%)	10 (5%)	32	30
1	F	212/212 (100%)	208 (98%)	4 (2%)	65	70
1	G	200/212 (94%)	194 (97%)	6 (3%)	48	51
1	H	210/212 (99%)	206 (98%)	4 (2%)	65	70
1	I	207/212 (98%)	205 (99%)	2 (1%)	82	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	209/212 (99%)	205 (98%)	4 (2%)	65	70
All	All	2085/2120 (98%)	2040 (98%)	45 (2%)	61	64

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

Some 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 carbohydrates 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	-	4,8,8	0.56	0	5,10,10	1.10	0
2	PRO	B	301	-	4,8,8	0.49	0	5,10,10	1.06	0
2	PRO	C	301	-	4,8,8	0.54	0	5,10,10	1.09	0
2	PRO	D	301	-	4,8,8	0.56	0	5,10,10	1.10	1 (20%)
2	PRO	E	301	-	4,8,8	0.53	0	5,10,10	1.10	1 (20%)
2	PRO	F	301	-	4,8,8	0.50	0	5,10,10	1.11	0
2	PRO	G	301	-	4,8,8	0.54	0	5,10,10	1.06	0
2	PRO	H	301	-	4,8,8	0.51	0	5,10,10	1.12	1 (20%)
2	PRO	I	301	-	4,8,8	0.50	0	5,10,10	1.07	0
2	PRO	J	301	-	4,8,8	0.53	0	5,10,10	1.07	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	-	-	0/0/11/11	0/1/1/1
2	PRO	B	301	-	-	0/0/11/11	0/1/1/1
2	PRO	C	301	-	-	0/0/11/11	0/1/1/1
2	PRO	D	301	-	-	0/0/11/11	0/1/1/1
2	PRO	E	301	-	-	0/0/11/11	0/1/1/1
2	PRO	F	301	-	-	0/0/11/11	0/1/1/1
2	PRO	G	301	-	-	0/0/11/11	0/1/1/1
2	PRO	H	301	-	-	0/0/11/11	0/1/1/1
2	PRO	I	301	-	-	0/0/11/11	0/1/1/1
2	PRO	J	301	-	-	0/0/11/11	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	PRO	CD-N-CA	2.02	112.08	107.07
2	D	301	PRO	CD-N-CA	2.11	112.30	107.07
2	E	301	PRO	CD-N-CA	2.12	112.33	107.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.05	7 (2%) 59 66	37, 55, 85, 125	0
1	B	272/277 (98%)	0.36	25 (9%) 11 15	38, 67, 109, 142	0
1	C	268/277 (96%)	0.18	17 (6%) 23 31	37, 65, 111, 146	0
1	D	268/277 (96%)	0.60	42 (15%) 3 4	38, 84, 145, 157	0
1	E	272/277 (98%)	0.04	13 (4%) 34 43	39, 55, 89, 115	0
1	F	272/277 (98%)	-0.09	9 (3%) 50 59	39, 59, 95, 132	0
1	G	263/277 (94%)	1.26	72 (27%) 1 1	41, 93, 175, 246	0
1	H	272/277 (98%)	0.26	24 (8%) 12 17	44, 66, 112, 167	0
1	I	270/277 (97%)	0.28	17 (6%) 23 31	41, 76, 129, 155	0
1	J	271/277 (97%)	0.61	32 (11%) 6 8	41, 80, 130, 163	0
All	All	2700/2770 (97%)	0.34	258 (9%) 10 14	37, 65, 134, 246	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	94	LEU	16.7
1	G	18	ALA	10.7
1	H	3	ILE	10.6
1	G	113	LEU	8.5
1	G	8	ALA	7.9
1	G	87	VAL	7.9
1	C	46	SER	7.8
1	G	89	LEU	7.8
1	G	119	HIS	7.7
1	G	34	VAL	7.4
1	G	88	VAL	7.4
1	B	3	ILE	7.3
1	G	63	SER	7.2

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Mol	Chain	Res	Type	RSRZ
1	D	35	LEU	7.1
1	J	57	ILE	7.1
1	G	91	LEU	7.0
1	H	44	ILE	6.7
1	G	54	PHE	6.7
1	J	61	VAL	6.5
1	D	49	ALA	6.4
1	E	3	ILE	6.4
1	G	145	ALA	6.4
1	G	64	SER	6.3
1	J	45	HIS	6.3
1	J	63	SER	6.3
1	B	45	HIS	6.3
1	J	4	ILE	6.2
1	D	8	ALA	6.2
1	H	4	ILE	6.2
1	J	44	ILE	6.0
1	G	93	PRO	6.0
1	G	95	LEU	5.9
1	G	99	LYS	5.8
1	I	46	SER	5.8
1	G	116	TRP	5.7
1	G	121	ARG	5.7
1	G	83	LEU	5.7
1	F	46	SER	5.7
1	I	10	SER	5.6
1	B	4	ILE	5.6
1	B	46	SER	5.5
1	H	45	HIS	5.3
1	G	146	ALA	5.3
1	J	46	SER	5.1
1	D	83	LEU	5.1
1	D	32	SER	5.0
1	D	89	LEU	5.0
1	G	53	ALA	5.0
1	I	6	ILE	5.0
1	J	18	ALA	4.9
1	G	49	ALA	4.8
1	D	34	VAL	4.7
1	G	100	LEU	4.6
1	H	46	SER	4.6
1	D	7	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	G	97	LYS	4.5
1	G	52	THR	4.5
1	G	149	GLU	4.5
1	D	48	PRO	4.5
1	I	45	HIS	4.4
1	E	63	SER	4.4
1	B	49	ALA	4.4
1	G	85	LYS	4.4
1	I	48	PRO	4.3
1	E	44	ILE	4.3
1	B	48	PRO	4.3
1	G	111	LYS	4.2
1	J	53	ALA	4.2
1	D	97	LYS	4.2
1	E	4	ILE	4.2
1	G	38	SER	4.1
1	H	63	SER	4.1
1	J	54	PHE	4.1
1	D	53	ALA	4.1
1	G	77	PHE	4.0
1	E	48	PRO	4.0
1	G	50	ARG	4.0
1	D	6	ILE	4.0
1	J	51	ARG	4.0
1	B	125	VAL	3.9
1	G	147	THR	3.9
1	E	46	SER	3.9
1	J	43	ALA	3.8
1	J	144	GLY	3.8
1	J	48	PRO	3.8
1	B	104	VAL	3.7
1	J	47	ASN	3.7
1	D	70	ARG	3.7
1	G	117	ALA	3.7
1	J	93	PRO	3.6
1	D	88	VAL	3.6
1	I	47	ASN	3.6
1	G	51	ARG	3.5
1	D	46	SER	3.5
1	E	49	ALA	3.5
1	D	87	VAL	3.5
1	H	52	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	45	HIS	3.5
1	D	57	ILE	3.5
1	H	48	PRO	3.4
1	G	16	ILE	3.4
1	G	86	ASP	3.4
1	G	61	VAL	3.4
1	B	47	ASN	3.3
1	A	3	ILE	3.3
1	A	46	SER	3.3
1	J	50	ARG	3.3
1	C	83	LEU	3.3
1	D	94	LEU	3.3
1	F	49	ALA	3.3
1	I	35	LEU	3.3
1	G	122	PHE	3.2
1	A	47	ASN	3.2
1	B	158	PHE	3.2
1	C	49	ALA	3.2
1	D	90	LYS	3.2
1	G	62	LEU	3.1
1	D	71	ASP	3.1
1	C	90	LYS	3.1
1	J	5	PRO	3.1
1	D	31	ARG	3.1
1	C	7	PRO	3.1
1	D	30	VAL	3.1
1	C	5	PRO	3.1
1	J	97	LYS	3.1
1	G	11	TYR	3.1
1	H	68	VAL	3.1
1	B	53	ALA	3.0
1	G	71	ASP	3.0
1	G	101	LEU	3.0
1	C	60	THR	3.0
1	D	50	ARG	3.0
1	G	151	ALA	3.0
1	F	44	ILE	3.0
1	G	90	LYS	3.0
1	B	63	SER	3.0
1	F	47	ASN	3.0
1	D	63	SER	2.9
1	G	79	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	9	ASP	2.9
1	C	57	ILE	2.9
1	G	7	PRO	2.9
1	E	52	THR	2.9
1	G	70	ARG	2.9
1	D	9	ASP	2.9
1	J	11	TYR	2.9
1	D	33	GLY	2.9
1	G	148	GLU	2.9
1	J	49	ALA	2.8
1	D	99	LYS	2.8
1	H	126[A]	MET	2.8
1	H	49	ALA	2.8
1	J	146	ALA	2.8
1	G	42	THR	2.8
1	I	8	ALA	2.8
1	J	33	GLY	2.8
1	B	157	LEU	2.8
1	H	47	ASN	2.7
1	F	3	ILE	2.7
1	G	144	GLY	2.7
1	G	150	ASP	2.6
1	D	54	PHE	2.6
1	H	51	ARG	2.6
1	H	83	LEU	2.6
1	D	116	TRP	2.6
1	F	45	HIS	2.6
1	F	48	PRO	2.6
1	H	67	ASP	2.6
1	G	82	GLN	2.6
1	G	115	GLU	2.6
1	G	126	MET	2.6
1	H	64	SER	2.5
1	C	144	GLY	2.5
1	J	6	ILE	2.5
1	C	86	ASP	2.5
1	E	47	ASN	2.5
1	G	33	GLY	2.5
1	J	62	LEU	2.5
1	G	59	ILE	2.5
1	D	42	THR	2.4
1	G	114	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	70	ARG	2.4
1	H	43	ALA	2.4
1	C	9	ASP	2.4
1	D	67	ASP	2.4
1	D	93	PRO	2.4
1	D	95	LEU	2.4
1	H	97	LYS	2.4
1	G	9	ASP	2.4
1	G	120	GLU	2.4
1	G	92	LYS	2.4
1	D	86	ASP	2.4
1	A	215	VAL	2.4
1	A	214	THR	2.4
1	D	36	SER	2.4
1	G	67	ASP	2.4
1	B	51	ARG	2.3
1	C	31	ARG	2.3
1	B	6	ILE	2.3
1	G	81	PRO	2.3
1	I	49	ALA	2.3
1	A	45	HIS	2.3
1	B	127	PRO	2.3
1	G	74	VAL	2.3
1	H	61	VAL	2.3
1	D	52	THR	2.3
1	G	112	ASP	2.3
1	I	156	GLN	2.3
1	C	64	SER	2.3
1	I	44	ILE	2.3
1	J	56	SER	2.3
1	I	62	LEU	2.3
1	B	138	SER	2.2
1	C	62	LEU	2.2
1	C	97	LYS	2.2
1	I	7	PRO	2.2
1	C	52	THR	2.2
1	D	119	HIS	2.2
1	E	51	ARG	2.2
1	H	53	ALA	2.2
1	H	60	THR	2.2
1	J	31	ARG	2.2
1	D	91	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	76	VAL	2.2
1	I	30	VAL	2.2
1	B	186	ILE	2.2
1	E	50	ARG	2.2
1	J	13	LEU	2.2
1	G	153	LEU	2.1
1	H	31	ARG	2.1
1	B	5	PRO	2.1
1	F	31	ARG	2.1
1	D	149	GLU	2.1
1	F	145	ALA	2.1
1	E	186	ILE	2.1
1	G	156	GLN	2.1
1	J	59	ILE	2.1
1	G	84	LEU	2.1
1	D	126	MET	2.1
1	D	37	PRO	2.1
1	I	36	SER	2.1
1	B	102	VAL	2.1
1	G	65	ASN	2.1
1	G	69	VAL	2.1
1	J	104	VAL	2.1
1	J	52	THR	2.1
1	G	15	PHE	2.1
1	A	63	SER	2.0
1	C	89	LEU	2.0
1	B	126	MET	2.0
1	I	59	ILE	2.0
1	B	52	THR	2.0
1	B	215	VAL	2.0
1	B	44	ILE	2.0
1	H	94	LEU	2.0
1	J	145	ALA	2.0
1	D	61	VAL	2.0
1	G	98	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(\AA^2)	Q<0.9
2	PRO	F	301	8/8	0.80	0.26	4.18	52,94,106,109	0
2	PRO	B	301	8/8	0.83	0.19	2.44	44,74,87,93	0
2	PRO	G	301	8/8	0.74	0.24	2.24	48,91,93,96	0
2	PRO	E	301	8/8	0.89	0.17	1.78	46,81,90,94	0
2	PRO	C	301	8/8	0.90	0.12	1.41	49,68,74,75	0
2	PRO	J	301	8/8	0.85	0.17	1.41	53,76,85,91	0
2	PRO	H	301	8/8	0.90	0.13	0.47	51,78,82,85	0
2	PRO	I	301	8/8	0.89	0.14	0.46	50,80,88,90	0
2	PRO	D	301	8/8	0.91	0.12	0.39	47,64,66,68	0
2	PRO	A	301	8/8	0.96	0.12	-0.22	49,77,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.