



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:17 PM EDT

PDB ID : 6LHM / pdb_00006lhm
Title : Structure of human PYCR2
Authors : Baburajendran, N.
Deposited on : 2019-12-09
Resolution : 3.40 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
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

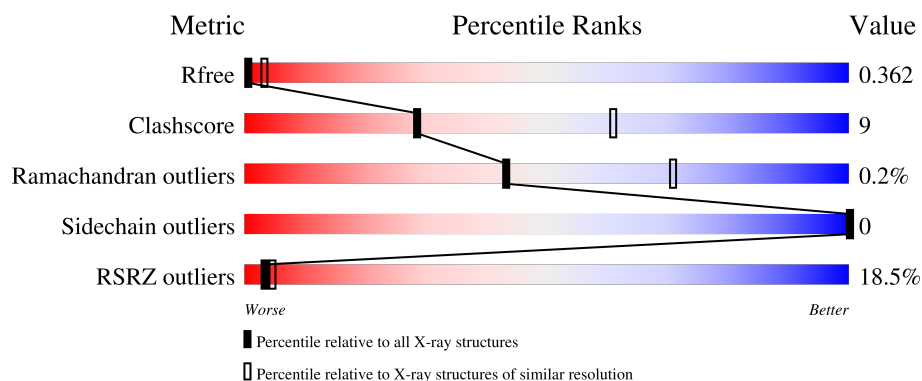
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	301	12% 70% 19% 11%
1	B	301	17% 73% 16% 11%
1	C	301	18% 67% 19% 14%
1	D	301	14% 72% 18% 9%
1	E	301	21% 69% 14% 17%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9211 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			1884	1192	319	359	14			
1	B	269	Total	C	N	O	S	0	0	0
			1893	1196	326	358	13			
1	C	258	Total	C	N	O	S	0	0	0
			1789	1131	306	340	12			
1	D	273	Total	C	N	O	S	0	0	0
			1934	1216	333	373	12			
1	E	249	Total	C	N	O	S	0	0	0
			1711	1076	287	336	12			

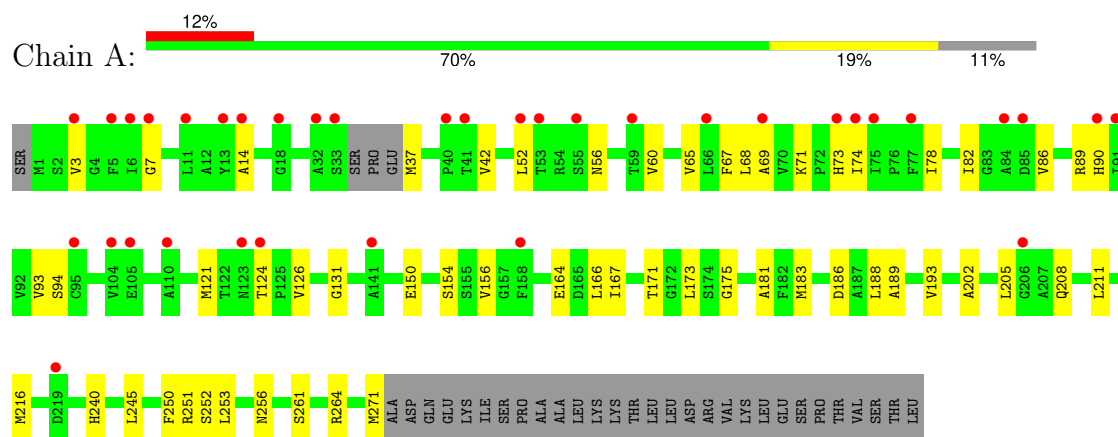
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q96C36
A	239	THR	ILE	conflict	UNP Q96C36
B	0	SER	-	expression tag	UNP Q96C36
B	239	THR	ILE	conflict	UNP Q96C36
C	0	SER	-	expression tag	UNP Q96C36
C	239	THR	ILE	conflict	UNP Q96C36
D	0	SER	-	expression tag	UNP Q96C36
D	239	THR	ILE	conflict	UNP Q96C36
E	0	SER	-	expression tag	UNP Q96C36
E	239	THR	ILE	conflict	UNP Q96C36

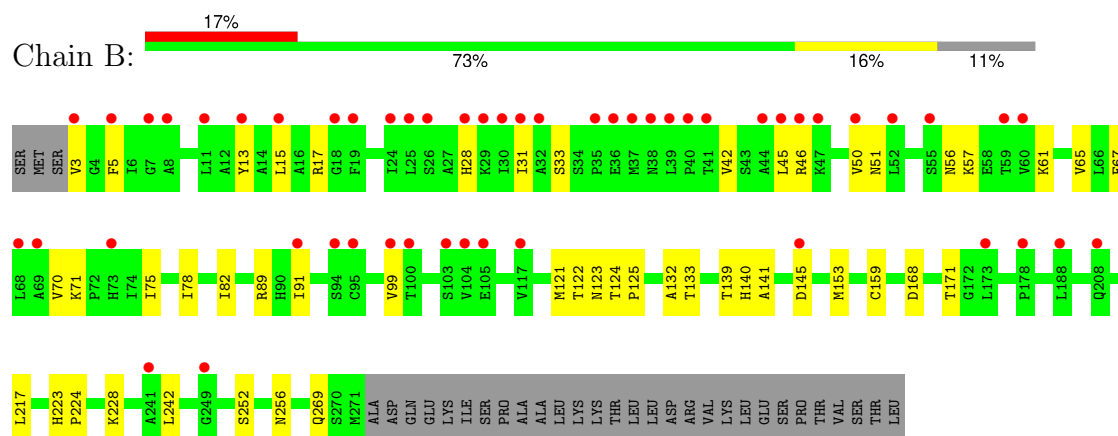
3 Residue-property plots [i](#)

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.

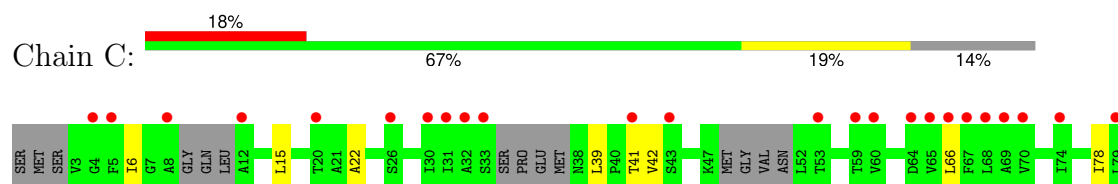
• Molecule 1: Pyrroline-5-carboxylate reductase 2

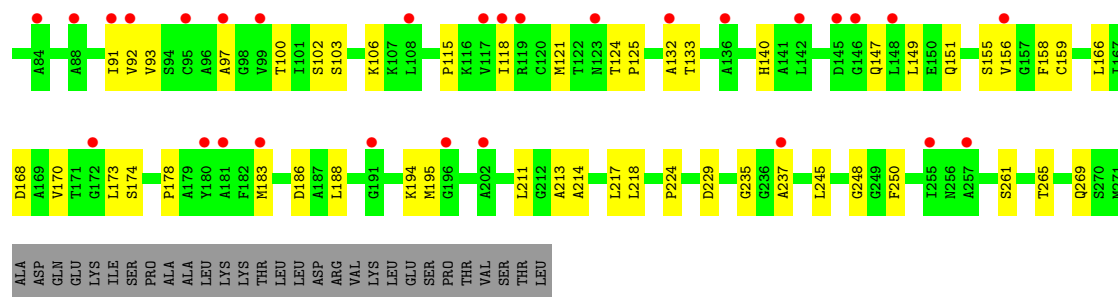


• Molecule 1: Pyrroline-5-carboxylate reductase 2

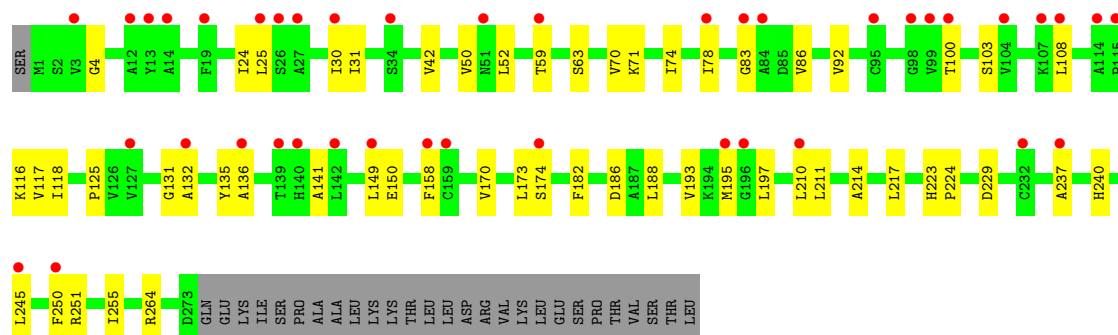


• Molecule 1: Pyrroline-5-carboxylate reductase 2

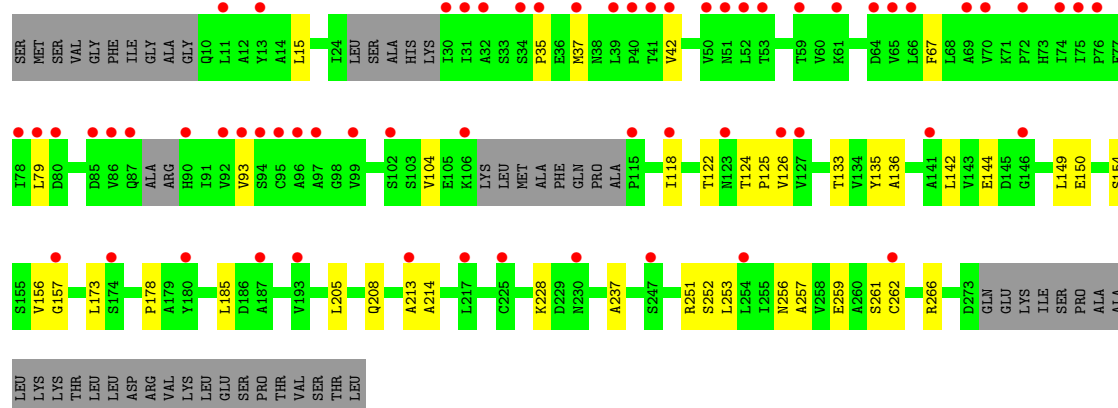




• Molecule 1: Pyrroline-5-carboxylate reductase 2



• Molecule 1: Pyrroline-5-carboxylate reductase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	101.90Å 110.31Å 155.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.90 – 3.40 46.90 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (46.90-3.40) 97.7 (46.90-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.329 , 0.360 0.331 , 0.362	Depositor DCC
R_{free} test set	2006 reflections (8.10%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	9211	wwPDB-VP
Average B, all atoms (Å ²)	76.0	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 [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	0.11	0/1910	0.29	0/2601
1	B	0.10	0/1921	0.29	0/2617
1	C	0.09	0/1812	0.27	0/2464
1	D	0.11	0/1963	0.30	0/2677
1	E	0.09	0/1729	0.26	0/2356
All	All	0.10	0/9335	0.28	0/12715

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	1884	0	1845	48	0
1	B	1893	0	1871	35	0
1	C	1789	0	1737	40	0
1	D	1934	0	1907	44	0
1	E	1711	0	1644	29	0
All	All	9211	0	9004	160	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 9.

All (160) 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:262:CYS:SG	1:E:266:ARG:NH1	2.55	0.79
1:A:121:MET:HE3	1:A:175:GLY:HA3	1.66	0.77
1:A:126:VAL:HG12	1:A:131:GLY:HA3	1.69	0.74
1:B:70:VAL:HG23	1:B:75:ILE:HG12	1.69	0.73
1:C:217:LEU:HD22	1:E:185:LEU:HD13	1.71	0.73
1:C:229:ASP:OD2	1:D:223:HIS:NE2	2.23	0.71
1:A:126:VAL:HB	1:A:156:VAL:HG13	1.72	0.70
1:A:3:VAL:HG23	1:A:65:VAL:HG13	1.74	0.70
1:C:217:LEU:HD21	1:C:224:PRO:HG3	1.74	0.69
1:A:216:MET:HE2	1:D:125:PRO:HB3	1.75	0.69
1:C:147:GLN:HG2	1:C:151:GLN:HE22	1.57	0.68
1:B:28:HIS:O	1:B:51:ASN:ND2	2.27	0.67
1:A:251:ARG:NH1	1:D:186:ASP:OD2	2.24	0.66
1:D:217:LEU:HD21	1:D:224:PRO:HG3	1.77	0.66
1:A:82:ILE:HG22	1:A:86:VAL:HG23	1.77	0.66
1:A:173:LEU:HD11	1:D:188:LEU:HB3	1.77	0.65
1:B:123:ASN:HB2	1:B:125:PRO:HD2	1.79	0.65
1:C:194:LYS:NZ	1:E:259:GLU:OE2	2.26	0.65
1:C:39:LEU:HD12	1:C:41:THR:HG23	1.79	0.65
1:C:93:VAL:HG21	1:C:149:LEU:HD21	1.78	0.65
1:A:121:MET:HE2	1:A:171:THR:HG23	1.77	0.65
1:A:186:ASP:OD2	1:D:251:ARG:NH1	2.28	0.64
1:B:252:SER:O	1:B:256:ASN:ND2	2.29	0.63
1:C:168:ASP:OD1	1:C:269:GLN:NE2	2.32	0.62
1:D:24:ILE:HG13	1:D:25:LEU:HD23	1.81	0.62
1:B:65:VAL:HG12	1:B:91:ILE:HB	1.82	0.61
1:A:193:VAL:O	1:C:235:GLY:N	2.29	0.61
1:D:83:GLY:O	1:D:86:VAL:HG12	2.01	0.60
1:D:92:VAL:HB	1:D:117:VAL:HG23	1.83	0.59
1:A:78:ILE:HG23	1:A:82:ILE:HD13	1.83	0.59
1:A:181:ALA:HB2	1:D:210:LEU:HD22	1.85	0.59
1:A:52:LEU:H	1:A:52:LEU:HD23	1.67	0.58
1:A:166:LEU:HD23	1:D:197:LEU:HD23	1.85	0.58
1:A:252:SER:O	1:A:256:ASN:ND2	2.37	0.58
1:B:61:LYS:O	1:B:89:ARG:NH2	2.35	0.57
1:A:60:VAL:HG21	1:A:82:ILE:HG23	1.86	0.57
1:C:261:SER:HA	1:E:237:ALA:HB1	1.87	0.56
1:E:15:LEU:HD23	1:E:156:VAL:HG11	1.88	0.55
1:C:186:ASP:OD2	1:E:251:ARG:NH1	2.39	0.55
1:D:135:TYR:OH	1:D:150:GLU:OE2	2.23	0.55
1:A:189:ALA:HA	1:A:202:ALA:HB1	1.89	0.55
1:C:115:PRO:HD2	1:C:140:HIS:ND1	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:TYR:OH	1:B:17:ARG:NH1	2.40	0.54
1:D:25:LEU:HD23	1:D:25:LEU:H	1.71	0.54
1:C:183:MET:HG3	1:E:228:LYS:HE2	1.90	0.54
1:B:228:LYS:HE3	1:B:242:LEU:HD13	1.90	0.53
1:C:188:LEU:HB3	1:E:173:LEU:HD11	1.90	0.53
1:C:237:ALA:HB1	1:E:261:SER:HA	1.91	0.53
1:B:123:ASN:HD21	1:B:132:ALA:HB3	1.73	0.53
1:A:211:LEU:HD13	1:D:214:ALA:HB3	1.89	0.53
1:D:71:LYS:HB2	1:D:74:ILE:HG12	1.90	0.52
1:A:14:ALA:HB1	1:A:126:VAL:HG22	1.92	0.52
1:A:150:GLU:O	1:A:154:SER:N	2.42	0.51
1:A:188:LEU:HB3	1:D:173:LEU:HD11	1.91	0.51
1:A:37:MET:HA	1:A:42:VAL:HG11	1.93	0.51
1:A:89:ARG:HD3	1:A:90:HIS:N	2.25	0.51
1:B:5:PHE:HD1	1:B:67:PHE:HB2	1.75	0.51
1:A:208:GLN:NE2	1:D:131:GLY:O	2.44	0.51
1:B:31:ILE:HA	1:B:51:ASN:HB2	1.92	0.51
1:C:245:LEU:HD11	1:E:257:ALA:HB2	1.93	0.50
1:A:211:LEU:HG	1:D:211:LEU:HD12	1.93	0.50
1:B:56:ASN:ND2	1:B:78:ILE:HD13	2.27	0.50
1:A:164:GLU:HA	1:A:167:ILE:HG13	1.93	0.50
1:D:116:LYS:HG2	1:D:141:ALA:HA	1.93	0.50
1:B:168:ASP:OD1	1:B:269:GLN:NE2	2.45	0.50
1:B:71:LYS:O	1:B:75:ILE:HG13	2.12	0.50
1:B:56:ASN:OD1	1:B:56:ASN:N	2.43	0.49
1:C:97:ALA:HA	1:C:121:MET:HE1	1.94	0.49
1:B:31:ILE:HG12	1:B:51:ASN:HD22	1.77	0.49
1:D:229:ASP:OD1	1:D:229:ASP:N	2.39	0.49
1:A:216:MET:HE3	1:D:182:PHE:HZ	1.78	0.49
1:C:66:LEU:HD23	1:C:92:VAL:HG13	1.95	0.49
1:B:133:THR:O	1:B:159:CYS:HA	2.12	0.49
1:D:245:LEU:HD13	1:D:250:PHE:CD1	2.48	0.49
1:D:70:VAL:HG21	1:D:78:ILE:HD12	1.96	0.48
1:D:30:ILE:HG13	1:D:50:VAL:HG22	1.96	0.48
1:C:39:LEU:O	1:C:42:VAL:HG23	2.14	0.48
1:D:100:THR:O	1:D:103:SER:OG	2.30	0.48
1:A:183:MET:HG3	1:D:251:ARG:CZ	2.44	0.47
1:C:178:PRO:HB3	1:E:213:ALA:HB2	1.96	0.47
1:A:7:GLY:HA3	1:A:69:ALA:HB3	1.96	0.47
1:A:205:LEU:HD13	1:D:170:VAL:HG13	1.96	0.47
1:A:208:GLN:OE1	1:D:158:PHE:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:VAL:HA	1:B:65:VAL:HG23	1.95	0.47
1:C:173:LEU:HD23	1:E:205:LEU:HB2	1.97	0.47
1:D:86:VAL:HG11	1:D:108:LEU:HD11	1.95	0.47
1:A:250:PHE:HE2	1:D:250:PHE:CE1	2.32	0.47
1:C:166:LEU:O	1:C:170:VAL:HG23	2.14	0.47
1:B:141:ALA:HB1	1:B:145:ASP:HB2	1.96	0.47
1:C:100:THR:O	1:C:103:SER:OG	2.26	0.46
1:B:5:PHE:CD1	1:B:67:PHE:HB2	2.51	0.46
1:B:121:MET:HE3	1:B:171:THR:HG23	1.97	0.46
1:A:68:LEU:HB2	1:A:94:SER:HA	1.97	0.45
1:D:132:ALA:HB3	1:D:174:SER:HB2	1.98	0.45
1:C:6:ILE:HG21	1:C:78:ILE:HD13	1.97	0.45
1:C:248:GLY:HA3	1:E:253:LEU:HD21	1.99	0.45
1:B:124:THR:N	1:B:125:PRO:HD2	2.31	0.45
1:C:213:ALA:HB2	1:E:178:PRO:HB3	1.98	0.45
1:A:261:SER:HA	1:D:237:ALA:HB1	1.98	0.45
1:E:142:LEU:HB2	1:E:144:GLU:OE1	2.16	0.45
1:E:154:SER:HA	1:E:157:GLY:O	2.17	0.45
1:C:22:ALA:HB1	1:C:155:SER:HB2	1.98	0.45
1:C:174:SER:HB3	1:E:205:LEU:HB3	1.99	0.45
1:D:251:ARG:O	1:D:255:ILE:HG13	2.16	0.45
1:E:79:LEU:HD12	1:E:104:VAL:HG12	1.98	0.44
1:E:149:LEU:HD12	1:E:149:LEU:HA	1.81	0.44
1:A:253:LEU:HB3	1:D:245:LEU:HD22	2.00	0.44
1:B:46:ARG:HA	1:B:50:VAL:HG12	1.99	0.44
1:B:13:TYR:HD1	1:B:45:LEU:HG	1.82	0.44
1:A:264:ARG:HD2	1:D:240:HIS:ND1	2.32	0.44
1:D:24:ILE:HD12	1:D:24:ILE:HA	1.85	0.44
1:B:15:LEU:HD22	1:B:153:MET:HE1	1.99	0.44
1:D:118:ILE:HG21	1:D:149:LEU:HD23	1.99	0.43
1:D:42:VAL:HB	1:D:52:LEU:HD21	2.01	0.43
1:E:118:ILE:HG23	1:E:136:ALA:O	2.19	0.43
1:D:59:THR:O	1:D:63:SER:OG	2.23	0.43
1:C:15:LEU:HD23	1:C:156:VAL:HG21	2.00	0.43
1:B:15:LEU:HD21	1:B:122:THR:HG21	2.01	0.43
1:B:217:LEU:HD22	1:B:224:PRO:HB3	2.00	0.43
1:C:102:SER:O	1:C:106:LYS:HB2	2.18	0.43
1:C:133:THR:N	1:C:158:PHE:O	2.51	0.43
1:B:139:THR:OG1	1:B:140:HIS:N	2.52	0.43
1:C:195:MET:SD	1:C:195:MET:N	2.91	0.43
1:E:135:TYR:OH	1:E:150:GLU:OE1	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:MET:HG2	1:A:52:LEU:HD13	2.01	0.42
1:A:73:HIS:CE1	1:A:74:ILE:HG13	2.55	0.42
1:C:265:THR:O	1:C:269:GLN:HG3	2.19	0.42
1:E:37:MET:HA	1:E:42:VAL:HG21	2.01	0.42
1:E:122:THR:HB	1:E:133:THR:HG23	2.00	0.42
1:B:13:TYR:HB2	1:B:45:LEU:HD12	2.00	0.42
1:B:123:ASN:ND2	1:B:132:ALA:O	2.53	0.42
1:B:75:ILE:HD12	1:B:99:VAL:HG11	2.02	0.42
1:D:118:ILE:HG23	1:D:136:ALA:O	2.20	0.42
1:A:56:ASN:HB3	1:A:82:ILE:HD11	2.01	0.42
1:C:245:LEU:HD23	1:C:250:PHE:CG	2.55	0.42
1:C:211:LEU:HB2	1:E:214:ALA:HB3	2.01	0.42
1:D:195:MET:HA	1:D:195:MET:HE2	2.01	0.42
1:A:124:THR:C	1:A:126:VAL:H	2.28	0.42
1:B:223:HIS:CG	1:B:224:PRO:HD2	2.56	0.41
1:D:4:GLY:HA2	1:D:30:ILE:O	2.20	0.41
1:B:5:PHE:O	1:B:33:SER:N	2.52	0.41
1:A:271:MET:HE2	1:A:271:MET:HB2	1.83	0.41
1:A:71:LYS:HD2	1:A:73:HIS:NE2	2.36	0.41
1:B:57:LYS:HG3	1:B:82:ILE:HG22	2.01	0.41
1:C:91:ILE:HG23	1:C:118:ILE:HD12	2.02	0.41
1:C:132:ALA:HB2	1:E:208:GLN:HB3	2.02	0.41
1:E:252:SER:O	1:E:256:ASN:ND2	2.30	0.41
1:A:245:LEU:HD13	1:A:250:PHE:CD1	2.56	0.41
1:B:42:VAL:HA	1:B:45:LEU:HB3	2.02	0.41
1:A:240:HIS:CG	1:D:264:ARG:HD3	2.56	0.40
1:E:124:THR:O	1:E:126:VAL:N	2.47	0.40
1:A:73:HIS:ND1	1:A:74:ILE:HG13	2.36	0.40
1:C:133:THR:O	1:C:159:CYS:HA	2.21	0.40
1:A:52:LEU:O	1:A:52:LEU:HG	2.21	0.40
1:E:67:PHE:HA	1:E:93:VAL:O	2.21	0.40
1:E:124:THR:N	1:E:125:PRO:HD2	2.36	0.40
1:A:67:PHE:CD1	1:A:93:VAL:HB	2.57	0.40
1:C:124:THR:N	1:C:125:PRO:HD2	2.35	0.40
1:C:214:ALA:O	1:C:218:LEU:HD12	2.20	0.40
1:D:193:VAL:HA	1:D:197:LEU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	264/301 (88%)	253 (96%)	11 (4%)	0	100	100
1	B	267/301 (89%)	250 (94%)	17 (6%)	0	100	100
1	C	250/301 (83%)	235 (94%)	15 (6%)	0	100	100
1	D	271/301 (90%)	257 (95%)	13 (5%)	1 (0%)	30	59
1	E	241/301 (80%)	229 (95%)	11 (5%)	1 (0%)	30	59
All	All	1293/1505 (86%)	1224 (95%)	67 (5%)	2 (0%)	43	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	31	ILE
1	E	35	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	186/240 (78%)	186 (100%)	0	100	100
1	B	189/240 (79%)	189 (100%)	0	100	100
1	C	173/240 (72%)	173 (100%)	0	100	100
1	D	197/240 (82%)	197 (100%)	0	100	100
1	E	166/240 (69%)	166 (100%)	0	100	100
All	All	911/1200 (76%)	911 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	ASN
1	B	10	GLN
1	B	269	GLN
1	C	151	GLN
1	D	129	GLN
1	E	269	GLN

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](#)

There are no ligands in this entry.

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	268/301 (89%)	1.18	36 (13%) 7 8	38, 65, 111, 118	0
1	B	269/301 (89%)	1.30	52 (19%) 3 4	35, 76, 116, 122	0
1	C	258/301 (85%)	1.34	53 (20%) 2 4	42, 83, 119, 137	0
1	D	273/301 (90%)	1.13	41 (15%) 5 7	39, 72, 99, 114	0
1	E	249/301 (82%)	1.43	62 (24%) 2 3	41, 79, 139, 145	0
All	All	1317/1505 (87%)	1.27	244 (18%) 3 4	35, 74, 120, 145	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	65	VAL	6.7
1	B	25	LEU	6.3
1	C	32	ALA	5.7
1	E	79	LEU	5.1
1	E	95	CYS	5.0
1	E	75	ILE	4.4
1	C	68	LEU	4.4
1	E	78	ILE	4.4
1	E	74	ILE	4.2
1	E	225	CYS	4.2
1	B	18	GLY	4.1
1	E	34	SER	4.1
1	A	59	THR	4.0
1	A	123	ASN	3.9
1	A	33	SER	3.9
1	E	76	PRO	3.9
1	D	159	CYS	3.8
1	B	40	PRO	3.8
1	E	94	SER	3.8
1	A	18	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	65	VAL	3.8
1	C	64	ASP	3.7
1	B	91	ILE	3.7
1	D	127	VAL	3.6
1	E	59	THR	3.6
1	B	11	LEU	3.6
1	C	99	VAL	3.5
1	B	95	CYS	3.5
1	C	95	CYS	3.5
1	C	118	ILE	3.5
1	A	90	HIS	3.4
1	E	174	SER	3.4
1	C	8	ALA	3.4
1	A	74	ILE	3.4
1	B	45	LEU	3.4
1	E	99	VAL	3.4
1	B	31	ILE	3.4
1	A	75	ILE	3.3
1	A	52	LEU	3.2
1	D	34	SER	3.2
1	E	66	LEU	3.2
1	C	237	ALA	3.2
1	B	173	LEU	3.2
1	B	60	VAL	3.2
1	D	25	LEU	3.1
1	D	83	GLY	3.1
1	C	156	VAL	3.1
1	E	52	LEU	3.1
1	C	117	VAL	3.1
1	E	106	LYS	3.1
1	B	188	LEU	3.0
1	A	53	THR	3.0
1	E	123	ASN	3.0
1	E	87	GLN	3.0
1	A	5	PHE	3.0
1	B	30	ILE	3.0
1	C	12	ALA	2.9
1	E	30	ILE	2.9
1	A	69	ALA	2.9
1	A	84	ALA	2.9
1	A	85	ASP	2.9
1	A	105	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	32	ALA	2.8
1	B	39	LEU	2.8
1	B	26	SER	2.8
1	B	36	GLU	2.8
1	C	20	THR	2.8
1	C	145	ASP	2.8
1	A	32	ALA	2.8
1	A	55	SER	2.8
1	C	257	ALA	2.8
1	E	115	PRO	2.8
1	B	3	VAL	2.8
1	A	158	PHE	2.8
1	E	102	SER	2.8
1	E	118	ILE	2.8
1	D	107	LYS	2.8
1	B	59	THR	2.8
1	B	35	PRO	2.7
1	D	149	LEU	2.7
1	C	255	ILE	2.7
1	C	30	ILE	2.7
1	B	29	LYS	2.7
1	C	69	ALA	2.7
1	E	92	VAL	2.7
1	A	40	PRO	2.7
1	D	232	CYS	2.7
1	A	104	VAL	2.7
1	B	99	VAL	2.7
1	D	210	LEU	2.7
1	D	250	PHE	2.7
1	B	7	GLY	2.7
1	E	51	ASN	2.7
1	C	4	GLY	2.6
1	A	91	ILE	2.6
1	A	141	ALA	2.6
1	C	92	VAL	2.6
1	D	195	MET	2.6
1	B	117	VAL	2.6
1	E	70	VAL	2.6
1	E	35	PRO	2.6
1	C	70	VAL	2.6
1	B	24	ILE	2.6
1	C	26	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	206	GLY	2.6
1	E	64	ASP	2.6
1	E	217	LEU	2.6
1	C	136	ALA	2.6
1	E	61	LYS	2.6
1	E	141	ALA	2.6
1	E	39	LEU	2.5
1	B	46	ARG	2.5
1	B	145	ASP	2.5
1	E	53	THR	2.5
1	C	59	THR	2.5
1	B	50	VAL	2.5
1	B	55	SER	2.5
1	E	69	ALA	2.5
1	A	6	ILE	2.5
1	C	148	LEU	2.5
1	D	142	LEU	2.5
1	A	95	CYS	2.4
1	D	174	SER	2.4
1	D	13	TYR	2.4
1	B	103	SER	2.4
1	C	146	GLY	2.4
1	A	14	ALA	2.4
1	C	142	LEU	2.4
1	D	115	PRO	2.4
1	E	127	VAL	2.4
1	B	69	ALA	2.4
1	C	31	ILE	2.4
1	C	88	ALA	2.4
1	E	213	ALA	2.4
1	B	5	PHE	2.4
1	C	91	ILE	2.4
1	D	30	ILE	2.4
1	E	187	ALA	2.4
1	D	19	PHE	2.4
1	C	33	SER	2.4
1	E	126	VAL	2.4
1	B	41	THR	2.3
1	C	53	THR	2.3
1	E	37	MET	2.3
1	B	15	LEU	2.3
1	E	86	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	93	VAL	2.3
1	B	28	HIS	2.3
1	D	14	ALA	2.3
1	B	38	ASN	2.3
1	C	180	TYR	2.3
1	D	51	ASN	2.3
1	E	72	PRO	2.3
1	D	114	ALA	2.3
1	C	108	LEU	2.3
1	B	37	MET	2.3
1	E	13	TYR	2.3
1	E	85	ASP	2.3
1	B	178	PRO	2.3
1	B	32	ALA	2.3
1	C	97	ALA	2.3
1	A	66	LEU	2.3
1	C	41	THR	2.3
1	D	59	THR	2.3
1	C	43	SER	2.3
1	D	158	PHE	2.3
1	E	42	VAL	2.3
1	B	44	ALA	2.2
1	C	196	GLY	2.2
1	B	68	LEU	2.2
1	B	100	THR	2.2
1	B	13	TYR	2.2
1	A	11	LEU	2.2
1	C	191	GLY	2.2
1	A	77	PHE	2.2
1	E	180	TYR	2.2
1	E	247	SER	2.2
1	A	3	VAL	2.2
1	D	78	ILE	2.2
1	B	8	ALA	2.2
1	D	196	GLY	2.2
1	D	245	LEU	2.2
1	E	96	ALA	2.2
1	C	119	ARG	2.2
1	A	41	THR	2.2
1	C	60	VAL	2.2
1	C	74	ILE	2.2
1	C	123	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	7	GLY	2.2
1	B	241	ALA	2.2
1	D	98	GLY	2.2
1	D	100	THR	2.2
1	E	90	HIS	2.2
1	D	104	VAL	2.2
1	C	79	LEU	2.2
1	D	108	LEU	2.2
1	E	254	LEU	2.2
1	D	136	ALA	2.2
1	B	52	LEU	2.1
1	C	66	LEU	2.1
1	E	230	ASN	2.1
1	D	140	HIS	2.1
1	E	193	VAL	2.1
1	B	208	GLN	2.1
1	D	132	ALA	2.1
1	E	97	ALA	2.1
1	B	94	SER	2.1
1	E	157	GLY	2.1
1	C	67	PHE	2.1
1	A	73	HIS	2.1
1	B	47	LYS	2.1
1	A	110	ALA	2.1
1	A	219	ASP	2.1
1	D	95	CYS	2.1
1	E	11	LEU	2.1
1	E	262	CYS	2.1
1	C	183	MET	2.1
1	C	84	ALA	2.1
1	E	31	ILE	2.1
1	B	73	HIS	2.1
1	D	139	THR	2.1
1	E	41	THR	2.1
1	B	249	GLY	2.1
1	E	146	GLY	2.1
1	B	19	PHE	2.1
1	E	40	PRO	2.1
1	B	104	VAL	2.0
1	E	50	VAL	2.0
1	D	84	ALA	2.0
1	D	26	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	13	TYR	2.0
1	A	124	THR	2.0
1	C	132	ALA	2.0
1	C	181	ALA	2.0
1	C	202	ALA	2.0
1	D	12	ALA	2.0
1	D	27	ALA	2.0
1	D	237	ALA	2.0
1	E	80	ASP	2.0
1	C	5	PHE	2.0
1	C	172	GLY	2.0
1	B	105	GLU	2.0
1	D	3	VAL	2.0
1	D	99	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.