



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:55 PM UTC

PDB ID : 3R8K / pdb_00003r8k
Title : Crystal structure of human SOUL protein (hexagonal form)
Authors : Ambrosi, E.K.; Capaldi, S.; Bovi, M.; Saccomani, G.; Perduca, M.; Monaco, H.L.
Deposited on : 2011-03-24
Resolution : 2.85 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

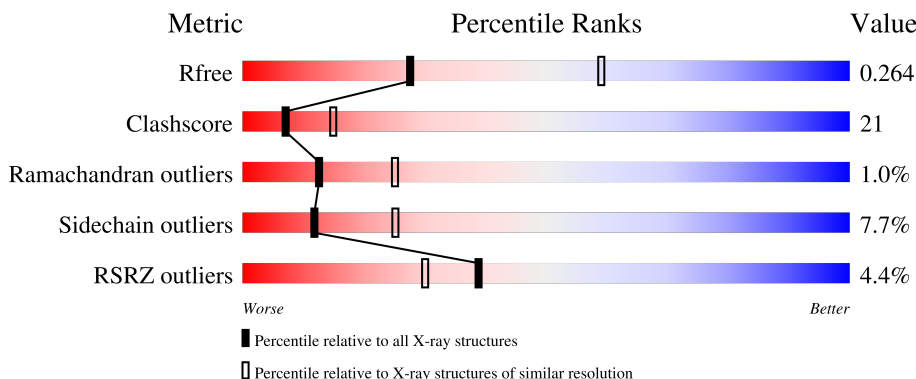
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	212	2% 48% 33% • 15%
1	B	212	• 58% 22% 5% 15%
1	C	212	6% 46% 30% • 19%
1	D	212	6% 48% 32% • 18%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5631 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 Heme-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1431	910	233	284	4			
1	B	180	Total	C	N	O	S	0	0	0
			1431	910	233	284	4			
1	C	172	Total	C	N	O	S	0	0	0
			1378	879	224	271	4			
1	D	174	Total	C	N	O	S	0	0	0
			1391	886	226	275	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP Q9Y5Z4
A	-1	ARG	-	expression tag	UNP Q9Y5Z4
A	0	GLY	-	expression tag	UNP Q9Y5Z4
A	1	SER	-	expression tag	UNP Q9Y5Z4
A	206	LEU	-	expression tag	UNP Q9Y5Z4
A	207	VAL	-	expression tag	UNP Q9Y5Z4
A	208	PRO	-	expression tag	UNP Q9Y5Z4
A	209	ARG	-	expression tag	UNP Q9Y5Z4
B	-2	MET	-	expression tag	UNP Q9Y5Z4
B	-1	ARG	-	expression tag	UNP Q9Y5Z4
B	0	GLY	-	expression tag	UNP Q9Y5Z4
B	1	SER	-	expression tag	UNP Q9Y5Z4
B	206	LEU	-	expression tag	UNP Q9Y5Z4
B	207	VAL	-	expression tag	UNP Q9Y5Z4
B	208	PRO	-	expression tag	UNP Q9Y5Z4
B	209	ARG	-	expression tag	UNP Q9Y5Z4
C	-2	MET	-	expression tag	UNP Q9Y5Z4
C	-1	ARG	-	expression tag	UNP Q9Y5Z4
C	0	GLY	-	expression tag	UNP Q9Y5Z4
C	1	SER	-	expression tag	UNP Q9Y5Z4
C	206	LEU	-	expression tag	UNP Q9Y5Z4

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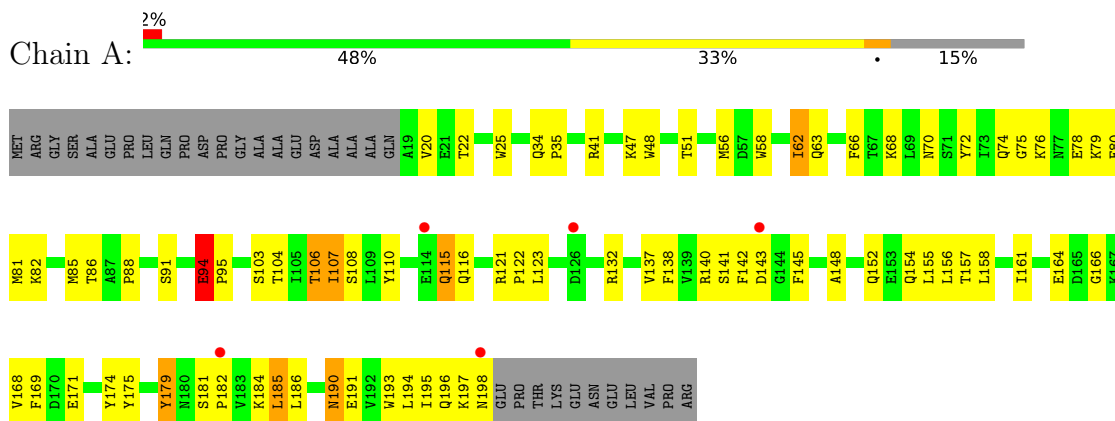
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Chain	Residue	Modelled	Actual	Comment	Reference
C	207	VAL	-	expression tag	UNP Q9Y5Z4
C	208	PRO	-	expression tag	UNP Q9Y5Z4
C	209	ARG	-	expression tag	UNP Q9Y5Z4
D	-2	MET	-	expression tag	UNP Q9Y5Z4
D	-1	ARG	-	expression tag	UNP Q9Y5Z4
D	0	GLY	-	expression tag	UNP Q9Y5Z4
D	1	SER	-	expression tag	UNP Q9Y5Z4
D	206	LEU	-	expression tag	UNP Q9Y5Z4
D	207	VAL	-	expression tag	UNP Q9Y5Z4
D	208	PRO	-	expression tag	UNP Q9Y5Z4
D	209	ARG	-	expression tag	UNP Q9Y5Z4

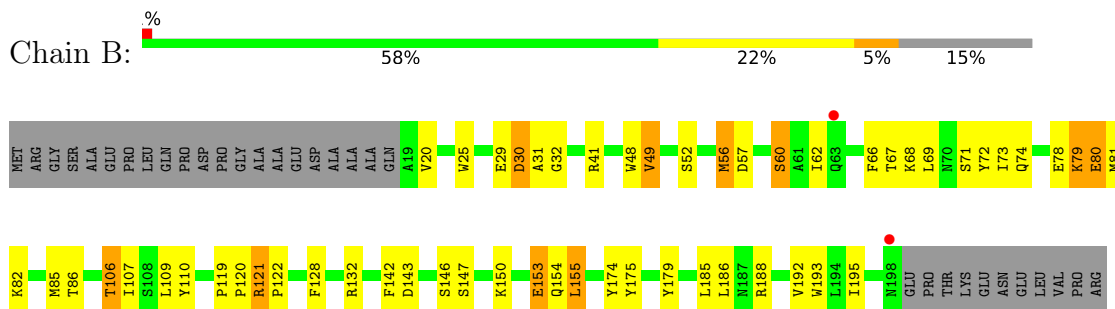
3 Residue-property plots [i](#)

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.

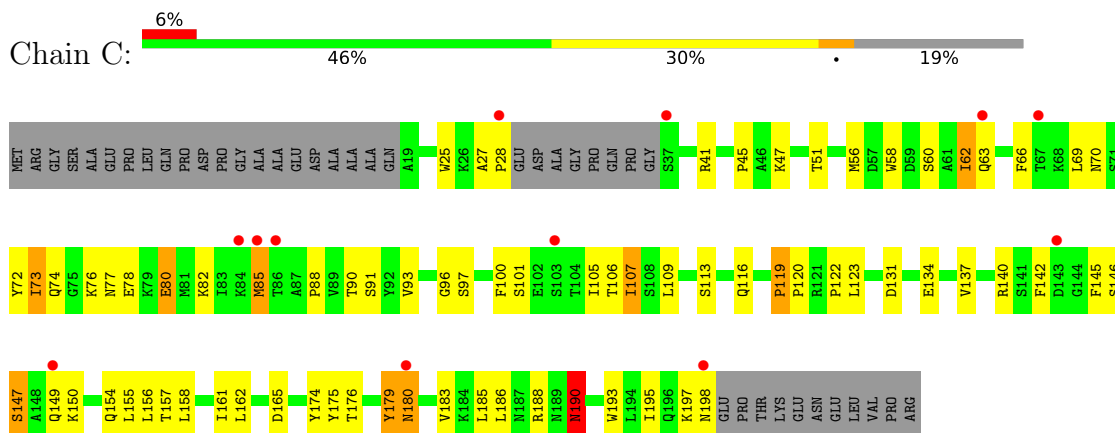
- Molecule 1: Heme-binding protein 2



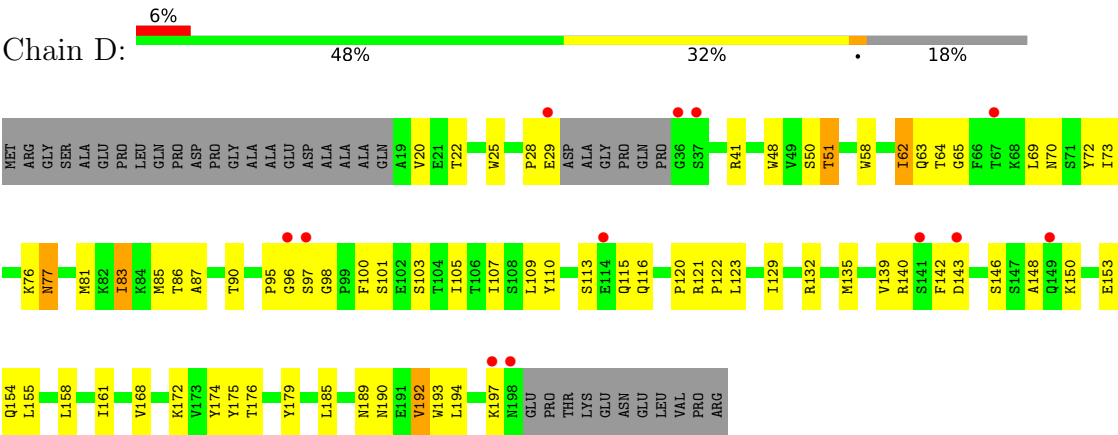
- Molecule 1: Heme-binding protein 2



- Molecule 1: Heme-binding protein 2



● Molecule 1: Heme-binding protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	143.92Å 143.92Å 242.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.40 – 2.85 55.40 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (55.40-2.85) 99.8 (55.40-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.64 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.235 , 0.268 0.228 , 0.264	Depositor DCC
R_{free} test set	1763 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	71.6	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5631	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7355e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.52	0/1468	0.90	3/1994 (0.2%)
1	B	0.52	0/1468	0.92	5/1994 (0.3%)
1	C	0.50	0/1412	0.89	4/1915 (0.2%)
1	D	0.43	0/1425	0.86	1/1932 (0.1%)
All	All	0.50	0/5773	0.89	13/7835 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	MET	N-CA-C	-7.04	102.06	113.19
1	B	32	GLY	CA-C-N	6.64	126.60	119.76
1	B	32	GLY	C-N-CA	6.64	126.60	119.76
1	A	94	GLU	CA-C-N	6.56	126.52	119.76
1	A	94	GLU	C-N-CA	6.56	126.52	119.76
1	A	56	MET	N-CA-C	-6.18	105.53	114.12
1	B	121	ARG	CA-C-N	5.80	126.29	120.14
1	B	121	ARG	C-N-CA	5.80	126.29	120.14
1	C	56	MET	N-CA-C	-5.64	104.28	113.19
1	C	119	PRO	CA-C-N	5.47	125.74	119.83
1	C	119	PRO	C-N-CA	5.47	125.74	119.83
1	D	50	SER	N-CA-C	5.29	116.44	108.46
1	C	165	ASP	N-CA-C	-5.24	105.55	112.94

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	1431	0	1381	67	0
1	B	1431	0	1381	45	0
1	C	1378	0	1337	64	0
1	D	1391	0	1346	61	0
All	All	5631	0	5445	231	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 21.

All (231) 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:A:140:ARG:HB2	1:A:158:LEU:HD12	1.33	1.07
1:C:85:MET:HG2	1:C:185:LEU:HD21	1.42	1.01
1:D:140:ARG:HB2	1:D:158:LEU:HD13	1.40	1.01
1:D:155:LEU:HD21	1:D:192:VAL:HB	1.45	0.96
1:D:28:PRO:O	1:D:29:GLU:HB3	1.78	0.81
1:A:140:ARG:CB	1:A:158:LEU:HD12	2.11	0.80
1:D:153:GLU:HG3	1:D:154:GLN:N	1.97	0.80
1:D:155:LEU:CD2	1:D:192:VAL:HB	2.13	0.78
1:A:197:LYS:O	1:A:198:ASN:HB2	1.80	0.78
1:A:107:ILE:N	1:A:107:ILE:HD12	2.00	0.76
1:C:60:SER:O	1:C:63:GLN:HG2	1.86	0.76
1:D:51:THR:HG22	1:D:69:LEU:HD21	1.69	0.74
1:A:142:PHE:CD2	1:A:154:GLN:HG3	2.23	0.74
1:C:147:SER:HB2	1:C:150:LYS:H	1.52	0.73
1:A:34:GLN:HG2	1:A:35:PRO:HD2	1.71	0.71
1:C:197:LYS:O	1:C:198:ASN:HB2	1.90	0.70
1:D:142:PHE:O	1:D:189:ASN:HB3	1.92	0.70
1:B:85:MET:HG2	1:B:185:LEU:HD21	1.75	0.68
1:C:45:PRO:HD3	1:C:134:GLU:HB3	1.74	0.68
1:C:74:GLN:O	1:C:82:LYS:HG2	1.92	0.68
1:C:140:ARG:HD3	1:C:154:GLN:OE1	1.94	0.68
1:B:49:VAL:HG22	1:B:69:LEU:HD22	1.76	0.67
1:C:70:ASN:HA	1:C:73:ILE:HG22	1.76	0.67
1:D:69:LEU:HB3	1:D:109:LEU:HD12	1.77	0.67
1:A:107:ILE:HD12	1:A:107:ILE:H	1.58	0.66
1:B:142:PHE:CD2	1:B:154:GLN:HG3	2.31	0.66
1:B:72:TYR:CD2	1:B:122:PRO:HB3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:TYR:H	1:C:179:TYR:HD2	1.44	0.65
1:A:48:TRP:CZ3	1:A:110:TYR:HB2	2.31	0.65
1:C:51:THR:HG22	1:C:69:LEU:HD21	1.78	0.64
1:D:140:ARG:HB2	1:D:158:LEU:CD1	2.21	0.64
1:C:107:ILE:HD12	1:C:107:ILE:N	2.13	0.64
1:B:107:ILE:HD12	1:B:107:ILE:N	2.13	0.63
1:B:107:ILE:HD12	1:B:107:ILE:H	1.63	0.63
1:C:183:VAL:CG1	1:C:185:LEU:HG	2.28	0.63
1:B:48:TRP:CZ3	1:B:110:TYR:HB2	2.33	0.62
1:A:95:PRO:HA	1:A:103:SER:HB3	1.81	0.62
1:D:48:TRP:CZ3	1:D:110:TYR:HB2	2.34	0.62
1:D:158:LEU:HD23	1:D:194:LEU:HD12	1.80	0.62
1:A:85:MET:HG3	1:A:185:LEU:HD22	1.82	0.62
1:D:76:LYS:HG2	1:D:123:LEU:HB2	1.82	0.62
1:D:48:TRP:CH2	1:D:110:TYR:HB2	2.35	0.62
1:D:58:TRP:O	1:D:62:ILE:HG22	2.00	0.62
1:B:179:TYR:CE2	1:B:188:ARG:NH1	2.68	0.61
1:D:73:ILE:HG22	1:D:83:ILE:HD11	1.81	0.61
1:D:142:PHE:CD2	1:D:154:GLN:HG3	2.36	0.61
1:C:179:TYR:N	1:C:179:TYR:CD2	2.69	0.61
1:C:77:ASN:HB2	1:C:120:PRO:HB2	1.82	0.60
1:B:155:LEU:HD12	1:B:192:VAL:HG21	1.84	0.59
1:D:153:GLU:HG3	1:D:154:GLN:H	1.64	0.59
1:A:78:GLU:C	1:A:80:GLU:H	2.11	0.59
1:B:69:LEU:HB3	1:B:109:LEU:HD13	1.85	0.59
1:A:48:TRP:CH2	1:A:110:TYR:HB2	2.39	0.58
1:A:169:PHE:CD1	1:A:194:LEU:HD13	2.40	0.57
1:C:91:SER:HA	1:C:106:THR:O	2.04	0.57
1:A:107:ILE:H	1:A:107:ILE:CD1	2.17	0.57
1:B:56:MET:HE3	1:C:156:LEU:HD12	1.85	0.57
1:D:90:THR:HA	1:D:176:THR:O	2.04	0.57
1:B:153:GLU:HG2	1:B:154:GLN:N	2.20	0.56
1:B:79:LYS:HE3	1:B:120:PRO:HA	1.88	0.56
1:A:107:ILE:N	1:A:107:ILE:CD1	2.69	0.56
1:A:152:GLN:O	1:A:156:LEU:HD12	2.07	0.55
1:C:62:ILE:HD13	1:C:62:ILE:O	2.06	0.55
1:C:76:LYS:C	1:C:123:LEU:HG	2.32	0.55
1:A:179:TYR:N	1:A:179:TYR:CD2	2.74	0.55
1:C:66:PHE:O	1:C:66:PHE:CG	2.60	0.54
1:D:140:ARG:CB	1:D:158:LEU:HD13	2.26	0.54
1:C:157:THR:O	1:C:161:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:VAL:HG22	1:D:193:TRP:CD1	2.43	0.54
1:D:77:ASN:HB2	1:D:120:PRO:HB2	1.88	0.54
1:A:155:LEU:HD11	1:A:174:TYR:CD2	2.43	0.54
1:B:155:LEU:HD23	1:C:100:PHE:CE1	2.43	0.54
1:C:175:TYR:CE2	1:C:195:ILE:HD11	2.43	0.54
1:D:69:LEU:CB	1:D:109:LEU:HD12	2.37	0.53
1:C:47:LYS:HD2	1:C:119:PRO:HG3	1.89	0.53
1:D:86:THR:HG21	1:D:110:TYR:O	2.08	0.53
1:A:25:TRP:CE3	1:B:41:ARG:HG2	2.43	0.53
1:C:175:TYR:HE2	1:C:195:ILE:HD11	1.72	0.53
1:B:147:SER:OG	1:B:150:LYS:HB2	2.08	0.53
1:C:76:LYS:HG3	1:C:123:LEU:HD12	1.89	0.53
1:C:66:PHE:C	1:C:66:PHE:CD2	2.86	0.53
1:B:175:TYR:CD2	1:B:195:ILE:HD11	2.44	0.52
1:C:107:ILE:HD12	1:C:107:ILE:H	1.75	0.52
1:A:66:PHE:C	1:A:66:PHE:CD2	2.88	0.52
1:B:81:MET:CG	1:B:120:PRO:HG2	2.40	0.52
1:C:76:LYS:HG2	1:C:123:LEU:HB2	1.91	0.51
1:C:70:ASN:O	1:C:73:ILE:HG22	2.09	0.51
1:A:121:ARG:HG3	1:A:122:PRO:HD2	1.92	0.51
1:C:90:THR:HA	1:C:176:THR:O	2.11	0.51
1:D:51:THR:HG22	1:D:69:LEU:CD2	2.38	0.51
1:C:73:ILE:HD11	1:C:85:MET:HA	1.93	0.51
1:A:20:VAL:HB	1:B:186:LEU:HD21	1.93	0.51
1:A:175:TYR:HE2	1:A:195:ILE:HD11	1.76	0.51
1:C:66:PHE:O	1:C:66:PHE:CD2	2.64	0.50
1:A:51:THR:HG21	1:A:68:LYS:HD2	1.94	0.50
1:A:169:PHE:CE1	1:A:194:LEU:HD13	2.46	0.50
1:D:143:ASP:O	1:D:150:LYS:HE2	2.12	0.50
1:D:175:TYR:HB2	1:D:193:TRP:HB2	1.93	0.49
1:D:25:TRP:CZ3	1:D:41:ARG:HG2	2.47	0.49
1:B:66:PHE:C	1:B:66:PHE:CD2	2.91	0.49
1:C:179:TYR:CE1	1:C:188:ARG:CZ	2.95	0.49
1:A:85:MET:CG	1:A:185:LEU:CD2	2.91	0.49
1:C:72:TYR:CD1	1:C:72:TYR:C	2.91	0.49
1:D:70:ASN:OD1	1:D:73:ILE:HD11	2.12	0.49
1:C:93:VAL:HG22	1:C:105:ILE:HG12	1.94	0.49
1:D:65:GLY:O	1:D:69:LEU:HG	2.13	0.49
1:B:175:TYR:HD2	1:B:195:ILE:HD11	1.77	0.48
1:C:88:PRO:HB3	1:C:179:TYR:CE2	2.49	0.48
1:A:74:GLN:HA	1:A:74:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PHE:CZ	1:A:196:GLN:HG3	2.47	0.48
1:B:175:TYR:HB2	1:B:193:TRP:HB2	1.94	0.48
1:A:175:TYR:HB2	1:A:193:TRP:HB2	1.95	0.48
1:A:191:GLU:HG3	1:A:193:TRP:HE1	1.78	0.48
1:B:48:TRP:CE2	1:B:132:ARG:NH1	2.81	0.48
1:C:145:PHE:CD2	1:C:146:SER:O	2.66	0.48
1:A:164:GLU:C	1:A:166:GLY:H	2.22	0.48
1:D:63:GLN:HG3	1:D:64:THR:N	2.28	0.48
1:C:179:TYR:HD2	1:C:179:TYR:N	2.09	0.48
1:C:180:ASN:HB3	1:C:190:ASN:OD1	2.14	0.48
1:D:28:PRO:O	1:D:29:GLU:CB	2.57	0.47
1:A:74:GLN:C	1:A:82:LYS:HD3	2.40	0.47
1:A:179:TYR:H	1:A:190:ASN:HD22	1.63	0.47
1:B:78:GLU:C	1:B:80:GLU:H	2.22	0.47
1:A:157:THR:O	1:A:161:ILE:HG13	2.15	0.46
1:C:58:TRP:CD2	1:C:58:TRP:O	2.68	0.46
1:A:76:LYS:O	1:A:76:LYS:HG2	2.14	0.46
1:A:175:TYR:CE2	1:A:195:ILE:HD11	2.50	0.46
1:C:183:VAL:HG12	1:C:185:LEU:HG	1.98	0.46
1:D:142:PHE:CE1	1:D:190:ASN:HB2	2.50	0.46
1:B:68:LYS:O	1:B:71:SER:HB2	2.16	0.46
1:A:158:LEU:C	1:A:158:LEU:HD23	2.41	0.46
1:C:72:TYR:CD1	1:C:73:ILE:N	2.84	0.46
1:B:81:MET:SD	1:B:120:PRO:HG2	2.55	0.46
1:D:179:TYR:CD1	1:D:179:TYR:N	2.83	0.46
1:A:179:TYR:H	1:A:190:ASN:ND2	2.14	0.46
1:C:88:PRO:HB3	1:C:179:TYR:CD2	2.51	0.46
1:A:62:ILE:CD1	1:A:182:PRO:HG3	2.46	0.45
1:D:25:TRP:CE3	1:D:41:ARG:HG2	2.51	0.45
1:A:75:GLY:HA2	1:A:81:MET:O	2.16	0.45
1:A:51:THR:O	1:A:106:THR:HA	2.15	0.45
1:A:78:GLU:C	1:A:80:GLU:N	2.74	0.45
1:D:96:GLY:HA3	1:D:101:SER:HB2	1.97	0.45
1:B:121:ARG:HG3	1:B:122:PRO:HD2	1.98	0.45
1:C:142:PHE:CD2	1:C:154:GLN:HG3	2.52	0.45
1:C:72:TYR:CE2	1:C:122:PRO:HB3	2.51	0.45
1:D:86:THR:O	1:D:185:LEU:HD13	2.17	0.45
1:D:158:LEU:HD23	1:D:194:LEU:CD1	2.47	0.45
1:A:184:LYS:O	1:A:184:LYS:HG3	2.17	0.45
1:A:197:LYS:O	1:A:198:ASN:CB	2.57	0.45
1:A:41:ARG:HG2	1:B:25:TRP:CZ3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:ILE:HG12	1:C:73:ILE:O	2.17	0.45
1:A:72:TYR:CD1	1:A:72:TYR:C	2.95	0.45
1:C:78:GLU:C	1:C:80:GLU:H	2.25	0.45
1:D:48:TRP:CE2	1:D:132:ARG:NH1	2.85	0.45
1:D:121:ARG:HG3	1:D:122:PRO:HD2	1.99	0.45
1:C:142:PHE:CD1	1:C:142:PHE:C	2.95	0.44
1:C:155:LEU:HD11	1:C:174:TYR:CD2	2.53	0.44
1:D:95:PRO:HD3	1:D:172:LYS:O	2.17	0.44
1:B:57:ASP:OD1	1:B:60:SER:HB3	2.17	0.44
1:B:155:LEU:HD21	1:B:174:TYR:CG	2.53	0.44
1:A:62:ILE:HD13	1:A:62:ILE:O	2.17	0.44
1:A:48:TRP:CE2	1:A:132:ARG:NH1	2.86	0.44
1:A:86:THR:OG1	1:A:110:TYR:O	2.36	0.44
1:A:137:VAL:HB	1:A:193:TRP:HB3	2.00	0.44
1:C:109:LEU:HD23	1:C:109:LEU:HA	1.86	0.44
1:D:98:GLY:C	1:D:100:PHE:H	2.26	0.44
1:C:72:TYR:HD1	1:C:73:ILE:N	2.16	0.43
1:C:96:GLY:HA3	1:C:101:SER:HB2	1.99	0.43
1:A:47:LYS:NZ	1:A:116:GLN:O	2.49	0.43
1:D:142:PHE:HB3	1:D:154:GLN:HG3	2.00	0.43
1:A:115:GLN:OE1	1:A:115:GLN:N	2.50	0.43
1:D:58:TRP:CZ3	1:D:62:ILE:HG21	2.52	0.43
1:D:81:MET:HE3	1:D:81:MET:HB2	1.91	0.43
1:A:66:PHE:CZ	1:A:85:MET:HE1	2.53	0.43
1:B:85:MET:CG	1:B:185:LEU:HD21	2.44	0.43
1:D:142:PHE:CB	1:D:154:GLN:HG3	2.48	0.43
1:C:91:SER:O	1:C:175:TYR:HA	2.18	0.43
1:B:52:SER:OG	1:B:106:THR:HG23	2.19	0.43
1:D:58:TRP:HB3	1:D:148:ALA:HB2	2.01	0.43
1:D:142:PHE:CD1	1:D:142:PHE:C	2.96	0.43
1:B:119:PRO:HA	1:B:120:PRO:HD3	1.89	0.43
1:D:72:TYR:CD1	1:D:72:TYR:C	2.97	0.43
1:D:135:MET:HE1	1:D:175:TYR:HE2	1.84	0.43
1:A:58:TRP:HB3	1:A:148:ALA:HB2	2.01	0.43
1:D:85:MET:HG3	1:D:86:THR:N	2.32	0.43
1:A:94:GLU:HA	1:A:95:PRO:HD3	1.75	0.42
1:C:158:LEU:HD12	1:C:162:LEU:HG	2.00	0.42
1:A:168:VAL:HG12	1:A:197:LYS:HB2	2.01	0.42
1:A:169:PHE:N	1:A:169:PHE:CD2	2.88	0.42
1:B:56:MET:O	1:B:56:MET:HG2	2.19	0.42
1:B:128:PHE:CD2	1:B:128:PHE:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:SER:HA	1:C:116:GLN:HG2	2.00	0.42
1:A:25:TRP:CZ3	1:B:41:ARG:HG2	2.54	0.42
1:A:94:GLU:O	1:A:103:SER:HB2	2.20	0.42
1:B:86:THR:OG1	1:B:110:TYR:O	2.27	0.42
1:D:81:MET:HG2	1:D:120:PRO:HG3	2.01	0.42
1:D:85:MET:HG2	1:D:185:LEU:HD21	2.01	0.42
1:B:29:GLU:C	1:B:31:ALA:H	2.28	0.42
1:C:70:ASN:CA	1:C:73:ILE:HG22	2.46	0.42
1:A:181:SER:HA	1:A:182:PRO:C	2.43	0.42
1:A:179:TYR:HB3	1:A:186:LEU:HB2	2.02	0.42
1:B:72:TYR:CE2	1:B:122:PRO:HB3	2.54	0.42
1:C:76:LYS:O	1:C:123:LEU:HG	2.20	0.42
1:D:161:ILE:H	1:D:161:ILE:HG12	1.63	0.42
1:C:25:TRP:CZ3	1:C:41:ARG:HG2	2.55	0.41
1:D:155:LEU:HD11	1:D:174:TYR:CD2	2.55	0.41
1:B:49:VAL:HG13	1:B:109:LEU:HB2	2.01	0.41
1:D:69:LEU:HD11	1:D:107:ILE:O	2.21	0.41
1:A:123:LEU:HD23	1:A:123:LEU:HA	1.86	0.41
1:D:113:SER:O	1:D:116:GLN:HB2	2.20	0.41
1:B:81:MET:HG2	1:B:120:PRO:HG2	2.02	0.41
1:D:22:THR:HG22	1:D:87:ALA:O	2.21	0.41
1:C:137:VAL:HB	1:C:193:TRP:HB3	2.03	0.41
1:D:103:SER:HB2	1:D:105:ILE:HD11	2.03	0.41
1:B:81:MET:HE3	1:B:81:MET:HB2	1.87	0.41
1:A:70:ASN:O	1:A:74:GLN:HG2	2.21	0.41
1:A:78:GLU:O	1:A:80:GLU:N	2.54	0.41
1:A:88:PRO:HB3	1:A:179:TYR:CZ	2.56	0.41
1:A:107:ILE:HG22	1:A:108:SER:N	2.35	0.41
1:B:74:GLN:O	1:B:82:LYS:HG2	2.21	0.41
1:C:175:TYR:HB2	1:C:193:TRP:HB2	2.02	0.41
1:A:141:SER:HA	1:A:191:GLU:HB3	2.03	0.41
1:C:27:ALA:O	1:C:28:PRO:C	2.63	0.41
1:D:168:VAL:HG11	1:D:197:LYS:HD2	2.01	0.40
1:B:81:MET:SD	1:B:120:PRO:CG	3.10	0.40
1:B:128:PHE:H	1:B:128:PHE:HD2	1.68	0.40
1:D:135:MET:HE1	1:D:175:TYR:CE2	2.57	0.40
1:D:142:PHE:HB3	1:D:154:GLN:OE1	2.22	0.40
1:C:47:LYS:HB2	1:C:116:GLN:OE1	2.21	0.40
1:C:70:ASN:HA	1:C:73:ILE:CG2	2.47	0.40
1:C:190:ASN:OD1	1:C:190:ASN:N	2.55	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	178/212 (84%)	160 (90%)	16 (9%)	2 (1%)	11	24
1	B	178/212 (84%)	160 (90%)	15 (8%)	3 (2%)	7	16
1	C	168/212 (79%)	152 (90%)	14 (8%)	2 (1%)	10	22
1	D	170/212 (80%)	152 (89%)	18 (11%)	0	100	100
All	All	694/848 (82%)	624 (90%)	63 (9%)	7 (1%)	12	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	LYS
1	B	80	GLU
1	C	190	ASN
1	A	190	ASN
1	B	30	ASP
1	B	79	LYS
1	C	80	GLU

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	159/183 (87%)	145 (91%)	14 (9%)	9	20
1	B	159/183 (87%)	147 (92%)	12 (8%)	12	26
1	C	154/183 (84%)	142 (92%)	12 (8%)	11	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	155/183 (85%)	145 (94%)	10 (6%)	15	32
All	All	627/732 (86%)	579 (92%)	48 (8%)	12	25

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	62	ILE
1	A	63	GLN
1	A	91	SER
1	A	94	GLU
1	A	104	THR
1	A	106	THR
1	A	107	ILE
1	A	115	GLN
1	A	143	ASP
1	A	145	PHE
1	A	171	GLU
1	A	179	TYR
1	A	185	LEU
1	B	20	VAL
1	B	30	ASP
1	B	49	VAL
1	B	60	SER
1	B	62	ILE
1	B	67	THR
1	B	73	ILE
1	B	106	THR
1	B	143	ASP
1	B	146	SER
1	B	153	GLU
1	B	155	LEU
1	C	62	ILE
1	C	73	ILE
1	C	85	MET
1	C	97	SER
1	C	107	ILE
1	C	131	ASP
1	C	147	SER
1	C	149	GLN
1	C	179	TYR
1	C	180	ASN

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Mol	Chain	Res	Type
1	C	186	LEU
1	C	190	ASN
1	D	20	VAL
1	D	51	THR
1	D	62	ILE
1	D	77	ASN
1	D	83	ILE
1	D	97	SER
1	D	115	GLN
1	D	129	ILE
1	D	146	SER
1	D	192	VAL

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	190	ASN
1	A	198	ASN
1	B	190	ASN
1	B	196	GLN
1	D	74	GLN
1	D	190	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	180/212 (84%)	0.31	5 (2%) 55 46	38, 68, 102, 118	0
1	B	180/212 (84%)	0.15	2 (1%) 78 73	37, 66, 96, 117	0
1	C	172/212 (81%)	0.49	12 (6%) 22 16	43, 73, 115, 137	0
1	D	174/212 (82%)	0.62	12 (6%) 23 17	47, 79, 116, 130	0
All	All	706/848 (83%)	0.39	31 (4%) 39 30	37, 71, 108, 137	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	149	GLN	3.7
1	D	96	GLY	3.5
1	D	67	THR	3.5
1	C	28	PRO	3.4
1	C	63	GLN	3.3
1	C	143	ASP	3.2
1	D	36	GLY	3.2
1	C	85	MET	3.1
1	D	197	LYS	3.0
1	A	114	GLU	2.9
1	C	37	SER	2.9
1	D	143	ASP	2.9
1	A	126	ASP	2.9
1	D	198	ASN	2.8
1	D	97	SER	2.7
1	D	37	SER	2.7
1	D	29	GLU	2.6
1	C	67	THR	2.5
1	B	198	ASN	2.4
1	C	86	THR	2.4
1	C	180	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	141	SER	2.3
1	A	198	ASN	2.2
1	B	63	GLN	2.2
1	C	198	ASN	2.2
1	C	149	GLN	2.2
1	C	103	SER	2.2
1	A	182	PRO	2.1
1	A	143	ASP	2.1
1	D	114	GLU	2.1
1	C	84	LYS	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.