



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:13 AM UTC

PDB ID : 3U5T / pdb_00003u5t
Title : The crystal structure of 3-oxoacyl-[acyl-carrier-protein] reductase from *Sinorhizobium meliloti*
Authors : Zhang, Z.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : 2011-10-11
Resolution : 2.40 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
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

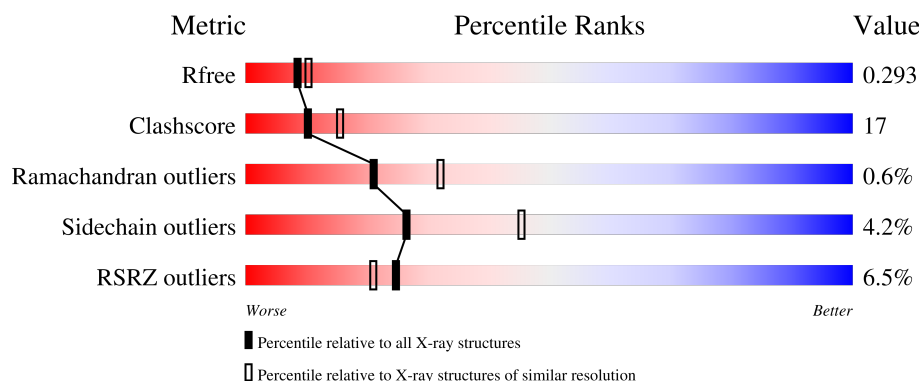
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	267	2% 61% 24% • 14%
1	B	267	2% 61% 24% • 13%
1	C	267	15% 46% 32% • 20%
1	D	267	3% 68% 17% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6619 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 3-oxoacyl-[acyl-carrier-protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	Se	0	0	0
			1649	1034	303	309	3			
1	B	233	Total	C	N	O	Se	0	0	0
			1672	1048	306	315	3			
1	C	214	Total	C	N	O	Se	0	0	0
			1534	965	278	288	3			
1	D	228	Total	C	N	O	Se	0	0	0
			1636	1027	300	306	3			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	expression tag	UNP Q92W70
A	-21	HIS	-	expression tag	UNP Q92W70
A	-20	HIS	-	expression tag	UNP Q92W70
A	-19	HIS	-	expression tag	UNP Q92W70
A	-18	HIS	-	expression tag	UNP Q92W70
A	-17	HIS	-	expression tag	UNP Q92W70
A	-16	HIS	-	expression tag	UNP Q92W70
A	-15	SER	-	expression tag	UNP Q92W70
A	-14	SER	-	expression tag	UNP Q92W70
A	-13	GLY	-	expression tag	UNP Q92W70
A	-12	VAL	-	expression tag	UNP Q92W70
A	-11	ASP	-	expression tag	UNP Q92W70
A	-10	LEU	-	expression tag	UNP Q92W70
A	-9	GLY	-	expression tag	UNP Q92W70
A	-8	THR	-	expression tag	UNP Q92W70
A	-7	GLU	-	expression tag	UNP Q92W70
A	-6	ASN	-	expression tag	UNP Q92W70
A	-5	LEU	-	expression tag	UNP Q92W70
A	-4	TYR	-	expression tag	UNP Q92W70
A	-3	PHE	-	expression tag	UNP Q92W70
A	-2	GLN	-	expression tag	UNP Q92W70

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q92W70
A	0	MSE	-	expression tag	UNP Q92W70
B	-22	MSE	-	expression tag	UNP Q92W70
B	-21	HIS	-	expression tag	UNP Q92W70
B	-20	HIS	-	expression tag	UNP Q92W70
B	-19	HIS	-	expression tag	UNP Q92W70
B	-18	HIS	-	expression tag	UNP Q92W70
B	-17	HIS	-	expression tag	UNP Q92W70
B	-16	HIS	-	expression tag	UNP Q92W70
B	-15	SER	-	expression tag	UNP Q92W70
B	-14	SER	-	expression tag	UNP Q92W70
B	-13	GLY	-	expression tag	UNP Q92W70
B	-12	VAL	-	expression tag	UNP Q92W70
B	-11	ASP	-	expression tag	UNP Q92W70
B	-10	LEU	-	expression tag	UNP Q92W70
B	-9	GLY	-	expression tag	UNP Q92W70
B	-8	THR	-	expression tag	UNP Q92W70
B	-7	GLU	-	expression tag	UNP Q92W70
B	-6	ASN	-	expression tag	UNP Q92W70
B	-5	LEU	-	expression tag	UNP Q92W70
B	-4	TYR	-	expression tag	UNP Q92W70
B	-3	PHE	-	expression tag	UNP Q92W70
B	-2	GLN	-	expression tag	UNP Q92W70
B	-1	SER	-	expression tag	UNP Q92W70
B	0	MSE	-	expression tag	UNP Q92W70
C	-22	MSE	-	expression tag	UNP Q92W70
C	-21	HIS	-	expression tag	UNP Q92W70
C	-20	HIS	-	expression tag	UNP Q92W70
C	-19	HIS	-	expression tag	UNP Q92W70
C	-18	HIS	-	expression tag	UNP Q92W70
C	-17	HIS	-	expression tag	UNP Q92W70
C	-16	HIS	-	expression tag	UNP Q92W70
C	-15	SER	-	expression tag	UNP Q92W70
C	-14	SER	-	expression tag	UNP Q92W70
C	-13	GLY	-	expression tag	UNP Q92W70
C	-12	VAL	-	expression tag	UNP Q92W70
C	-11	ASP	-	expression tag	UNP Q92W70
C	-10	LEU	-	expression tag	UNP Q92W70
C	-9	GLY	-	expression tag	UNP Q92W70
C	-8	THR	-	expression tag	UNP Q92W70
C	-7	GLU	-	expression tag	UNP Q92W70
C	-6	ASN	-	expression tag	UNP Q92W70

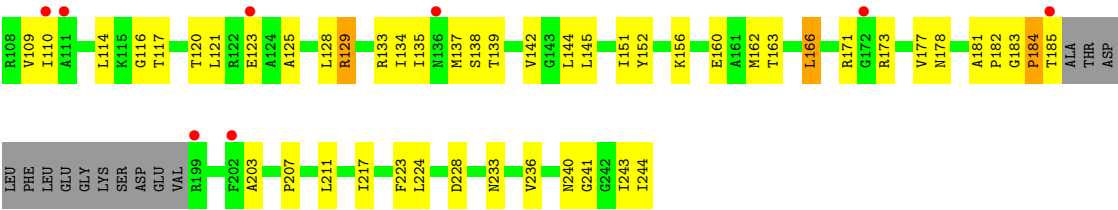
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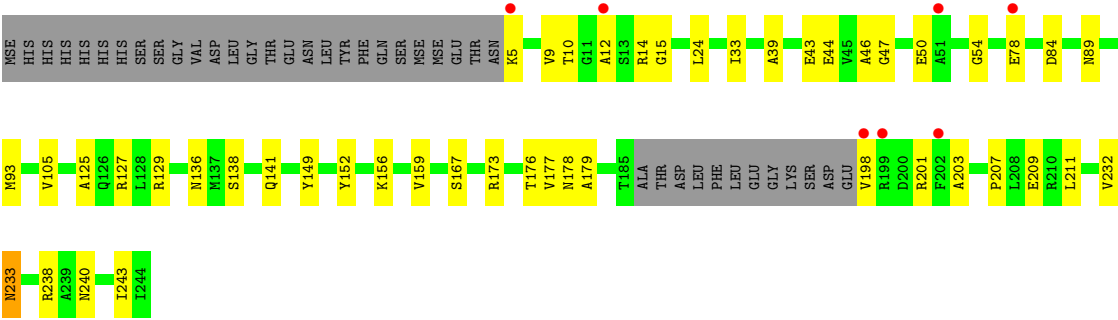
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	LEU	-	expression tag	UNP Q92W70
C	-4	TYR	-	expression tag	UNP Q92W70
C	-3	PHE	-	expression tag	UNP Q92W70
C	-2	GLN	-	expression tag	UNP Q92W70
C	-1	SER	-	expression tag	UNP Q92W70
C	0	MSE	-	expression tag	UNP Q92W70
D	-22	MSE	-	expression tag	UNP Q92W70
D	-21	HIS	-	expression tag	UNP Q92W70
D	-20	HIS	-	expression tag	UNP Q92W70
D	-19	HIS	-	expression tag	UNP Q92W70
D	-18	HIS	-	expression tag	UNP Q92W70
D	-17	HIS	-	expression tag	UNP Q92W70
D	-16	HIS	-	expression tag	UNP Q92W70
D	-15	SER	-	expression tag	UNP Q92W70
D	-14	SER	-	expression tag	UNP Q92W70
D	-13	GLY	-	expression tag	UNP Q92W70
D	-12	VAL	-	expression tag	UNP Q92W70
D	-11	ASP	-	expression tag	UNP Q92W70
D	-10	LEU	-	expression tag	UNP Q92W70
D	-9	GLY	-	expression tag	UNP Q92W70
D	-8	THR	-	expression tag	UNP Q92W70
D	-7	GLU	-	expression tag	UNP Q92W70
D	-6	ASN	-	expression tag	UNP Q92W70
D	-5	LEU	-	expression tag	UNP Q92W70
D	-4	TYR	-	expression tag	UNP Q92W70
D	-3	PHE	-	expression tag	UNP Q92W70
D	-2	GLN	-	expression tag	UNP Q92W70
D	-1	SER	-	expression tag	UNP Q92W70
D	0	MSE	-	expression tag	UNP Q92W70

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	33	Total O 33 33	0	0
2	B	47	Total O 47 47	0	0
2	C	11	Total O 11 11	0	0
2	D	37	Total O 37 37	0	0



● Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.17Å 95.40Å 112.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 2.40 48.22 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.4 (48.22-2.40) 97.3 (48.22-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.244 , 0.285 0.249 , 0.293	Depositor DCC
R_{free} test set	1961 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6619	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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	0.62	0/1666	0.88	0/2256
1	B	0.57	0/1689	0.88	5/2288 (0.2%)
1	C	0.43	0/1546	0.80	0/2088
1	D	0.48	0/1653	0.80	1/2238 (0.0%)
All	All	0.53	0/6554	0.84	6/8870 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	233	ASN	N-CA-C	6.31	118.11	108.07
1	B	226	GLY	CA-C-N	5.23	124.73	119.19
1	B	226	GLY	C-N-CA	5.23	124.73	119.19
1	B	131	GLY	N-CA-C	-5.22	107.04	115.08
1	B	65	ASP	CA-C-N	5.21	125.51	119.47
1	B	65	ASP	C-N-CA	5.21	125.51	119.47

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	1649	0	1692	56	0
1	B	1672	0	1714	58	0
1	C	1534	0	1561	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1636	0	1681	35	0
2	A	33	0	0	2	0
2	B	47	0	0	4	0
2	C	11	0	0	0	0
2	D	37	0	0	0	0
All	All	6619	0	6648	224	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 17.

All (224) 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:C:69:VAL:HG12	1:C:123:GLU:HG3	1.51	0.92
1:A:223:PHE:CE1	1:A:228:ASP:O	2.24	0.91
1:A:176:THR:HB	1:A:233:ASN:HB3	1.56	0.88
1:B:93:MSE:HE3	1:B:152:TYR:CE2	2.12	0.85
1:D:178:ASN:OD1	1:D:233:ASN:HA	1.78	0.83
1:C:8:ILE:HD11	1:C:83:VAL:HG21	1.60	0.82
1:C:10:THR:HG23	1:C:90:ALA:H	1.44	0.81
1:A:223:PHE:HE1	1:A:228:ASP:O	1.61	0.81
1:B:189:LEU:O	1:B:189:LEU:CD1	2.30	0.79
1:C:16:ILE:HD11	1:C:185:THR:HG21	1.65	0.78
1:A:57:LEU:HD13	1:D:105:VAL:HG21	1.65	0.77
1:C:77:GLU:HA	1:C:82:GLY:H	1.50	0.76
1:C:33:ILE:HD12	1:C:33:ILE:H	1.51	0.76
1:C:16:ILE:O	1:C:20:ILE:HG13	1.86	0.76
1:D:39:ALA:O	1:D:43:GLU:HG2	1.86	0.76
1:C:10:THR:OG1	1:C:90:ALA:HB2	1.87	0.75
1:A:10:THR:CG2	1:A:90:ALA:H	2.00	0.74
1:B:92:ILE:HG12	1:B:94:PRO:HD3	1.69	0.74
1:B:93:MSE:HE2	1:B:149:TYR:CE2	2.22	0.74
1:B:176:THR:HB	1:B:233:ASN:HB3	1.68	0.74
1:B:82:GLY:HA3	1:B:129:ARG:HD2	1.69	0.73
1:C:110:ILE:HG23	1:C:114:LEU:HD23	1.72	0.72
1:B:125:ALA:O	1:B:173:ARG:NH1	2.23	0.69
1:C:10:THR:CG2	1:C:88:ASN:HA	2.22	0.69
1:C:10:THR:HG22	1:C:88:ASN:HA	1.75	0.68
1:A:242:GLY:HA2	1:C:233:ASN:O	1.94	0.68
1:C:31:VAL:O	1:C:33:ILE:HD12	1.94	0.68
1:B:189:LEU:O	1:B:189:LEU:HD13	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:GLY:O	1:C:120:THR:HG23	1.94	0.68
1:D:203:ALA:HA	1:D:211:LEU:HG	1.77	0.67
1:A:10:THR:HG21	2:A:257:HOH:O	1.95	0.67
1:C:182:PRO:HB3	1:C:217:ILE:CG1	2.25	0.67
1:B:123:GLU:HG2	2:B:279:HOH:O	1.96	0.66
1:D:93:MSE:HE2	1:D:149:TYR:CE2	2.31	0.66
1:B:189:LEU:HD12	1:B:189:LEU:C	2.21	0.66
1:C:117:THR:O	1:C:121:LEU:HG	1.95	0.65
1:B:93:MSE:HE3	1:B:152:TYR:CD2	2.30	0.65
1:C:94:PRO:O	1:C:95:LEU:HD23	1.96	0.65
1:D:176:THR:HB	1:D:233:ASN:HB3	1.77	0.65
1:A:178:ASN:OD1	1:A:233:ASN:HA	1.95	0.65
1:D:93:MSE:HE3	1:D:152:TYR:CE2	2.32	0.65
1:C:93:MSE:HE3	1:C:95:LEU:HD21	1.80	0.64
1:C:203:ALA:HA	1:C:211:LEU:HG	1.80	0.64
1:C:93:MSE:HG3	1:C:152:TYR:CD1	2.33	0.64
1:A:10:THR:HG22	1:A:89:ASN:N	2.13	0.62
1:A:57:LEU:HD13	1:D:105:VAL:CG2	2.29	0.62
1:B:189:LEU:O	1:B:189:LEU:HD12	2.00	0.62
1:B:199:ARG:O	1:B:202:PHE:N	2.30	0.62
1:A:240:ASN:HB2	1:A:243:ILE:HG12	1.83	0.61
1:A:44:GLU:HG2	1:A:48:LYS:HE3	1.83	0.60
1:C:77:GLU:HG2	1:C:82:GLY:HA2	1.83	0.60
1:B:93:MSE:HE2	1:B:149:TYR:CD2	2.36	0.60
1:A:82:GLY:HA3	1:A:129:ARG:HH11	1.66	0.60
1:D:93:MSE:HE3	1:D:152:TYR:CD2	2.37	0.60
1:D:198:VAL:HG13	1:D:201:ARG:HH12	1.66	0.60
1:C:117:THR:HG22	1:C:121:LEU:HD11	1.83	0.60
1:A:16:ILE:O	1:A:20:ILE:HG13	2.03	0.59
1:C:135:ILE:HA	1:C:178:ASN:O	2.02	0.59
1:B:10:THR:O	1:B:89:ASN:HB3	2.02	0.59
1:A:10:THR:HG23	1:A:90:ALA:H	1.68	0.58
1:C:117:THR:HG22	1:C:121:LEU:CD1	2.33	0.58
1:A:10:THR:HG22	1:A:89:ASN:H	1.69	0.58
1:C:163:THR:HG23	1:C:177:VAL:HG12	1.86	0.57
1:C:166:LEU:HG	1:C:177:VAL:HG21	1.85	0.57
1:B:77:GLU:OE1	1:B:127:ARG:HG2	2.04	0.57
1:B:189:LEU:CD1	1:B:189:LEU:C	2.77	0.57
1:B:121:LEU:HD22	1:B:166:LEU:HD23	1.87	0.57
1:B:93:MSE:HG3	1:B:152:TYR:CG	2.39	0.56
1:C:110:ILE:O	1:C:114:LEU:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:PHE:HE1	1:C:228:ASP:HB3	1.69	0.56
1:C:34:ASN:ND2	1:C:72:LEU:HD22	2.20	0.56
1:B:93:MSE:HE2	1:B:149:TYR:HE2	1.66	0.56
1:D:93:MSE:HE2	1:D:149:TYR:CD2	2.41	0.56
1:A:93:MSE:HG3	1:A:152:TYR:CD1	2.42	0.55
1:C:182:PRO:HB3	1:C:217:ILE:HG12	1.89	0.55
1:C:77:GLU:HA	1:C:82:GLY:N	2.20	0.55
1:B:109:VAL:HG13	1:B:113:ASN:ND2	2.22	0.55
1:C:78:GLU:HG3	1:C:79:ALA:N	2.21	0.55
1:A:10:THR:HG22	1:A:90:ALA:H	1.73	0.54
1:B:188:ASP:O	1:B:189:LEU:HB3	2.08	0.54
1:C:8:ILE:CD1	1:C:83:VAL:HG11	2.38	0.54
1:A:65:ASP:HB3	1:A:68:ALA:HB3	1.90	0.54
1:B:93:MSE:HG3	1:B:152:TYR:CD1	2.43	0.54
1:B:199:ARG:O	1:B:200:ASP:C	2.51	0.53
1:C:10:THR:HA	1:C:34:ASN:HB3	1.89	0.53
1:A:9:VAL:HG12	1:A:12:ALA:HB2	1.90	0.53
1:B:39:ALA:O	1:B:43:GLU:HG2	2.08	0.53
1:B:178:ASN:OD1	1:B:233:ASN:HA	2.08	0.53
1:C:82:GLY:C	1:C:129:ARG:NH1	2.66	0.53
1:A:44:GLU:O	1:A:48:LYS:HG3	2.08	0.53
1:B:92:ILE:HG12	1:B:94:PRO:CD	2.39	0.53
1:C:50:GLU:HA	1:C:54:GLY:O	2.08	0.53
1:B:141:GLN:HA	1:B:144:LEU:HB2	1.90	0.53
1:C:106:PHE:HD2	1:C:107:ASP:OD1	1.92	0.53
1:C:93:MSE:HG3	1:C:152:TYR:CG	2.44	0.52
1:D:10:THR:O	1:D:89:ASN:HB3	2.09	0.52
1:A:200:ASP:CG	1:A:204:LYS:HE2	2.34	0.52
1:D:84:ASP:OD1	1:D:129:ARG:HD3	2.10	0.52
1:A:20:ILE:HG22	1:A:24:LEU:HD22	1.91	0.52
1:C:44:GLU:O	1:C:48:LYS:HG3	2.09	0.52
1:C:85:VAL:HG22	1:C:133:ARG:HB2	1.90	0.52
1:C:139:THR:HG23	1:C:142:VAL:HG23	1.91	0.52
1:B:213:THR:O	1:B:216:ASP:HB2	2.09	0.51
1:C:69:VAL:CG1	1:C:123:GLU:HG3	2.34	0.51
1:B:15:GLY:HA3	2:B:251:HOH:O	2.09	0.51
1:C:44:GLU:HG3	1:C:48:LYS:HE3	1.91	0.51
1:C:182:PRO:HB3	1:C:217:ILE:HG13	1.91	0.51
1:D:232:VAL:O	1:D:233:ASN:HB3	2.11	0.51
1:A:35:TYR:CZ	1:A:60:GLN:HB2	2.45	0.51
1:D:12:ALA:HB3	1:D:33:ILE:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:PRO:C	1:D:209:GLU:H	2.20	0.50
1:A:229:GLY:O	1:A:231:TRP:N	2.44	0.50
1:C:33:ILE:HD12	1:C:33:ILE:N	2.25	0.50
1:C:84:ASP:OD1	1:C:129:ARG:HB2	2.11	0.50
1:B:10:THR:HA	1:B:34:ASN:HD22	1.77	0.50
1:D:5:LYS:HA	1:D:84:ASP:OD2	2.12	0.50
1:B:109:VAL:HG13	1:B:113:ASN:HD22	1.76	0.49
1:C:93:MSE:HG3	1:C:152:TYR:CE1	2.46	0.49
1:C:207:PRO:HD2	1:C:241:GLY:O	2.12	0.49
1:A:93:MSE:HG3	1:A:152:TYR:CG	2.47	0.49
1:C:114:LEU:HD12	1:C:162:MSE:CE	2.43	0.49
1:B:4:ASN:OD1	1:B:4:ASN:N	2.44	0.49
1:C:133:ARG:HD2	1:C:224:LEU:O	2.12	0.49
1:A:10:THR:O	1:A:89:ASN:HB3	2.12	0.49
1:B:176:THR:CB	1:B:233:ASN:HB3	2.40	0.49
1:A:180:VAL:O	1:A:182:PRO:HD3	2.13	0.49
1:B:240:ASN:HB2	1:B:243:ILE:HG12	1.92	0.49
1:A:206:ALA:HB1	1:A:241:GLY:O	2.11	0.49
1:C:114:LEU:CD1	1:C:162:MSE:HE2	2.43	0.49
1:A:77:GLU:HG2	1:A:82:GLY:HA2	1.95	0.49
1:A:10:THR:HA	1:A:34:ASN:HD22	1.78	0.49
1:C:89:ASN:HA	1:C:137:MSE:HG3	1.94	0.49
1:D:9:VAL:CG1	1:D:12:ALA:HB2	2.43	0.48
1:C:139:THR:C	1:C:181:ALA:HB1	2.39	0.48
1:B:213:THR:HG21	2:B:287:HOH:O	2.14	0.48
1:B:238:ARG:NH2	2:B:281:HOH:O	2.29	0.48
1:B:23:ARG:HE	1:B:27:ASP:CG	2.21	0.48
1:D:93:MSE:CE	1:D:149:TYR:HE2	2.27	0.48
1:D:240:ASN:HB2	1:D:243:ILE:HG12	1.96	0.48
1:A:62:ASP:OD1	1:A:62:ASP:C	2.57	0.47
1:B:198:VAL:HG12	1:B:199:ARG:N	2.27	0.47
1:C:20:ILE:O	1:C:24:LEU:HD22	2.14	0.47
1:C:34:ASN:HD22	1:C:72:LEU:CD2	2.27	0.47
1:D:156:LYS:O	1:D:159:VAL:HB	2.14	0.47
1:A:200:ASP:OD2	1:A:204:LYS:HE2	2.14	0.47
1:A:64:SER:O	1:A:66:PRO:HD3	2.15	0.47
1:A:229:GLY:O	1:A:230:ALA:C	2.57	0.47
1:B:123:GLU:O	1:B:127:ARG:HB2	2.15	0.47
1:D:125:ALA:O	1:D:173:ARG:NH1	2.43	0.47
1:C:109:VAL:HG11	1:C:151:ILE:HG22	1.97	0.47
1:D:33:ILE:HD12	1:D:46:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:THR:O	1:C:78:GLU:HB3	2.15	0.46
1:A:204:LYS:HA	1:A:209:GLU:HA	1.97	0.46
1:A:23:ARG:HG2	1:A:222:ALA:HB2	1.98	0.46
1:B:9:VAL:CG1	1:B:12:ALA:HB2	2.46	0.46
1:B:38:LYS:H	1:B:38:LYS:HG2	1.53	0.46
1:B:93:MSE:CE	1:B:149:TYR:HE2	2.28	0.46
1:B:207:PRO:HD2	1:B:241:GLY:O	2.15	0.46
1:C:240:ASN:HB2	1:C:243:ILE:HG12	1.97	0.46
1:C:67:ALA:HA	1:C:70:ARG:NH1	2.30	0.46
1:D:138:SER:HA	1:D:156:LYS:HD2	1.98	0.46
1:B:14:ARG:HH22	1:B:187:THR:HB	1.81	0.45
1:C:97:THR:O	1:C:101:THR:OG1	2.33	0.45
1:D:93:MSE:CE	1:D:149:TYR:CE2	2.98	0.45
1:B:163:THR:HG23	1:B:177:VAL:HG12	1.99	0.45
1:A:233:ASN:OD1	1:C:241:GLY:C	2.60	0.45
1:C:25:ALA:HB1	1:C:49:ILE:HG23	1.98	0.45
1:C:183:GLY:O	1:C:184:PRO:C	2.59	0.45
1:D:141:GLN:HG3	1:D:149:TYR:CD2	2.52	0.45
1:A:108:ARG:HA	1:A:108:ARG:HD2	1.85	0.45
1:C:82:GLY:C	1:C:129:ARG:HH11	2.24	0.45
1:B:136:ASN:O	1:B:179:ALA:HA	2.17	0.45
1:A:11:GLY:H	1:A:34:ASN:HD22	1.65	0.44
1:A:114:LEU:HD12	1:A:162:MSE:HE2	1.98	0.44
1:B:65:ASP:OD1	1:B:67:ALA:HB3	2.17	0.44
1:C:203:ALA:CA	1:C:211:LEU:HG	2.46	0.44
1:D:93:MSE:HE2	1:D:149:TYR:HE2	1.78	0.44
1:B:206:ALA:HB1	1:B:241:GLY:O	2.17	0.44
1:C:22:ALA:O	1:C:25:ALA:HB3	2.18	0.44
1:A:10:THR:HG23	1:A:90:ALA:CB	2.48	0.44
1:C:160:GLU:OE1	1:C:236:VAL:HG21	2.17	0.44
1:C:33:ILE:H	1:C:33:ILE:CD1	2.25	0.44
1:C:41:ALA:O	1:C:44:GLU:HB3	2.18	0.44
1:A:5:LYS:HB3	1:A:29:PHE:CE1	2.53	0.44
1:C:10:THR:OG1	1:C:90:ALA:CB	2.62	0.44
1:A:207:PRO:O	1:A:209:GLU:HG3	2.17	0.43
1:C:8:ILE:HD12	1:C:83:VAL:HG11	2.00	0.43
1:C:144:LEU:O	1:C:145:LEU:C	2.61	0.43
1:D:14:ARG:HG2	1:D:15:GLY:N	2.32	0.43
1:B:127:ARG:NH1	1:B:127:ARG:HG3	2.33	0.43
1:B:49:ILE:HG21	1:B:56:ALA:HB2	1.99	0.43
1:B:109:VAL:CG1	1:B:113:ASN:HD22	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:THR:HG22	1:C:156:LYS:HG3	1.99	0.43
1:A:82:GLY:CA	1:A:129:ARG:HH11	2.31	0.43
1:D:136:ASN:O	1:D:179:ALA:HA	2.19	0.43
1:D:44:GLU:O	1:D:47:GLY:N	2.51	0.43
1:B:108:ARG:HD2	1:B:108:ARG:HA	1.57	0.43
1:C:125:ALA:O	1:C:173:ARG:NH1	2.26	0.43
1:A:163:THR:HG23	1:A:177:VAL:HG12	2.01	0.43
1:A:5:LYS:HB3	1:A:29:PHE:CD1	2.54	0.43
1:C:134:ILE:C	1:C:135:ILE:HG13	2.43	0.43
1:D:9:VAL:HG12	1:D:12:ALA:HB2	2.01	0.43
1:B:9:VAL:HG12	1:B:12:ALA:HB2	2.01	0.43
1:A:209:GLU:OE2	1:C:171:ARG:HG3	2.18	0.42
1:D:167:SER:HB3	1:D:177:VAL:HB	2.01	0.42
1:D:50:GLU:HA	1:D:54:GLY:O	2.20	0.42
1:B:35:TYR:CZ	1:B:60:GLN:HB2	2.55	0.42
1:C:223:PHE:CE1	1:C:228:ASP:O	2.73	0.42
1:A:24:LEU:HD12	1:A:24:LEU:HA	1.87	0.42
1:A:141:GLN:HG3	1:A:149:TYR:CD2	2.55	0.42
1:B:91:GLY:HA2	1:B:112:VAL:HG12	2.02	0.41
1:C:243:ILE:O	1:C:244:ILE:HB	2.19	0.41
1:A:109:VAL:O	1:A:113:ASN:HB2	2.20	0.41
1:B:235:GLN:OE1	1:D:238:ARG:HB2	2.20	0.41
1:A:136:ASN:O	1:A:179:ALA:HA	2.21	0.41
1:C:138:SER:OG	1:C:139:THR:N	2.54	0.41
1:B:127:ARG:HG3	1:B:127:ARG:HH11	1.85	0.41
1:C:34:ASN:OD1	1:C:34:ASN:C	2.63	0.40
1:C:43:GLU:O	1:C:44:GLU:C	2.64	0.40
1:A:231:TRP:O	1:C:241:GLY:HA2	2.20	0.40
1:D:207:PRO:C	1:D:209:GLU:N	2.78	0.40
1:A:243:ILE:HG13	1:A:244:ILE:HG22	2.03	0.40
1:A:204:LYS:HG2	1:A:209:GLU:HB3	2.04	0.40
1:A:75:THR:HG23	2:A:252:HOH:O	2.21	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	226/267 (85%)	215 (95%)	8 (4%)	3 (1%)	9	14
1	B	229/267 (86%)	215 (94%)	13 (6%)	1 (0%)	30	43
1	C	202/267 (76%)	177 (88%)	24 (12%)	1 (0%)	24	37
1	D	224/267 (84%)	211 (94%)	13 (6%)	0	100	100
All	All	881/1068 (82%)	818 (93%)	58 (7%)	5 (1%)	21	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	ALA
1	A	78	GLU
1	B	200	ASP
1	A	61	ALA
1	C	184	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	158/186 (85%)	152 (96%)	6 (4%)	29	49
1	B	161/186 (87%)	152 (94%)	9 (6%)	19	33
1	C	147/186 (79%)	139 (95%)	8 (5%)	20	35
1	D	157/186 (84%)	154 (98%)	3 (2%)	50	71
All	All	623/744 (84%)	597 (96%)	26 (4%)	26	45

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR

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Mol	Chain	Res	Type
1	A	24	LEU
1	A	50	GLU
1	A	117	THR
1	A	205	LEU
1	A	211	LEU
1	B	4	ASN
1	B	5	LYS
1	B	50	GLU
1	B	78	GLU
1	B	127	ARG
1	B	189	LEU
1	B	198	VAL
1	B	204	LYS
1	B	211	LEU
1	C	24	LEU
1	C	64	SER
1	C	78	GLU
1	C	86	LEU
1	C	103	ASP
1	C	128	LEU
1	C	129	ARG
1	C	166	LEU
1	D	24	LEU
1	D	78	GLU
1	D	127	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	88	ASN
1	A	113	ASN
1	B	4	ASN
1	B	34	ASN
1	B	126	GLN
1	C	60	GLN
1	C	136	ASN
1	D	34	ASN
1	D	88	ASN

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	227/267 (85%)	0.21	5 (2%) 62 58	30, 42, 59, 99	0
1	B	230/267 (86%)	0.29	6 (2%) 57 53	24, 42, 56, 65	0
1	C	211/267 (79%)	1.36	40 (18%) 3 2	41, 61, 87, 92	0
1	D	225/267 (84%)	0.39	7 (3%) 51 47	29, 45, 73, 91	0
All	All	893/1068 (83%)	0.55	58 (6%) 25 21	24, 46, 78, 99	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	67	ALA	5.3
1	B	200	ASP	4.3
1	C	63	VAL	4.3
1	B	199	ARG	4.3
1	B	201	ARG	4.2
1	C	36	ALA	3.8
1	B	198	VAL	3.7
1	C	199	ARG	3.7
1	C	6	VAL	3.7
1	A	186	ALA	3.5
1	D	198	VAL	3.5
1	C	15	GLY	3.5
1	C	68	ALA	3.4
1	C	82	GLY	3.3
1	D	202	PHE	3.3
1	C	185	THR	3.2
1	C	11	GLY	3.1
1	C	72	LEU	3.0
1	C	202	PHE	3.0
1	C	34	ASN	3.0
1	C	35	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	172	GLY	2.8
1	A	202	PHE	2.8
1	C	136	ASN	2.7
1	D	12	ALA	2.7
1	C	111	ALA	2.7
1	C	29	PHE	2.7
1	C	55	LYS	2.7
1	C	105	VAL	2.7
1	C	110	ILE	2.6
1	C	41	ALA	2.6
1	C	64	SER	2.6
1	C	61	ALA	2.5
1	C	10	THR	2.5
1	D	78	GLU	2.5
1	B	4	ASN	2.5
1	C	69	VAL	2.5
1	D	199	ARG	2.5
1	C	33	ILE	2.5
1	C	73	PHE	2.5
1	C	45	VAL	2.5
1	C	8	ILE	2.3
1	C	59	ALA	2.3
1	D	51	ALA	2.3
1	C	104	ALA	2.2
1	D	5	LYS	2.2
1	C	43	GLU	2.2
1	A	233	ASN	2.1
1	B	203	ALA	2.1
1	C	75	THR	2.1
1	C	98	ILE	2.1
1	A	211	LEU	2.1
1	C	44	GLU	2.1
1	C	123	GLU	2.1
1	C	42	ALA	2.1
1	A	198	VAL	2.0
1	C	96	THR	2.0
1	C	101	THR	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 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.