



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:14 AM UTC

PDB ID : 5K3G / pdb_00005k3g
Title : Crystals structure of Acyl-CoA oxidase-1 in Caenorhabditis elegans, Apo form-I
Authors : Zhang, X.; Li, K.; Jones, R.A.; Bruner, S.D.; Butcher, R.A.
Deposited on : 2016-05-19
Resolution : 2.86 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

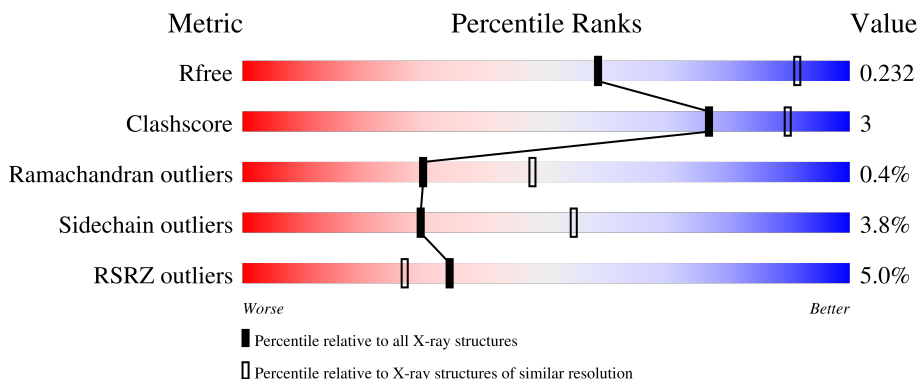
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

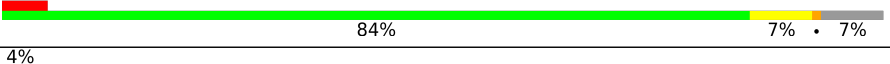
The reported resolution of this entry is 2.86 Å.

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	684	
1	B	684	
1	C	684	
1	D	684	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20012 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 Acyl-coenzyme A oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	629	Total	C	N	O	S	0	0	0
			4998	3173	879	923	23			
1	B	633	Total	C	N	O	S	0	0	0
			5031	3196	884	927	24			
1	C	630	Total	C	N	O	S	0	0	0
			5005	3180	881	921	23			
1	D	626	Total	C	N	O	S	0	0	0
			4978	3163	876	916	23			

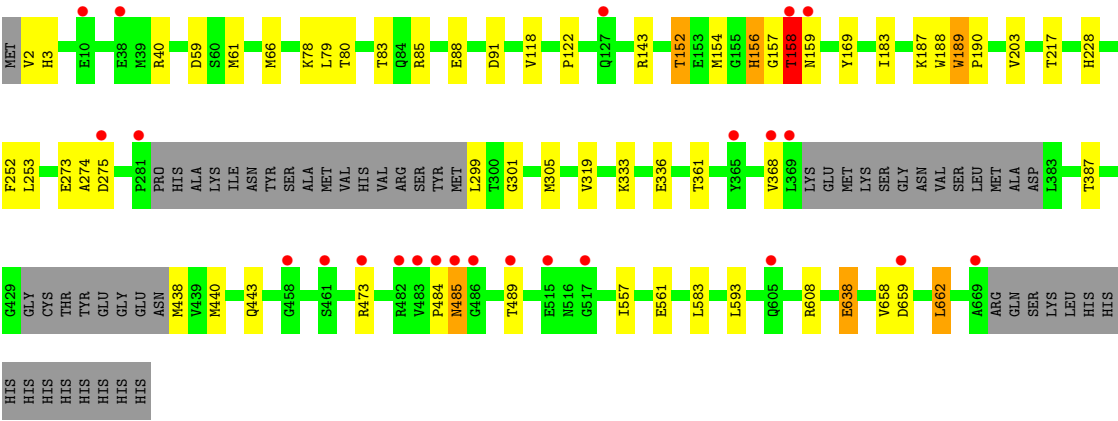
There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	675	HIS	-	expression tag	UNP O62140
A	676	HIS	-	expression tag	UNP O62140
A	677	HIS	-	expression tag	UNP O62140
A	678	HIS	-	expression tag	UNP O62140
A	679	HIS	-	expression tag	UNP O62140
A	680	HIS	-	expression tag	UNP O62140
A	681	HIS	-	expression tag	UNP O62140
A	682	HIS	-	expression tag	UNP O62140
A	683	HIS	-	expression tag	UNP O62140
A	684	HIS	-	expression tag	UNP O62140
B	675	HIS	-	expression tag	UNP O62140
B	676	HIS	-	expression tag	UNP O62140
B	677	HIS	-	expression tag	UNP O62140
B	678	HIS	-	expression tag	UNP O62140
B	679	HIS	-	expression tag	UNP O62140
B	680	HIS	-	expression tag	UNP O62140
B	681	HIS	-	expression tag	UNP O62140
B	682	HIS	-	expression tag	UNP O62140
B	683	HIS	-	expression tag	UNP O62140
B	684	HIS	-	expression tag	UNP O62140
C	675	HIS	-	expression tag	UNP O62140

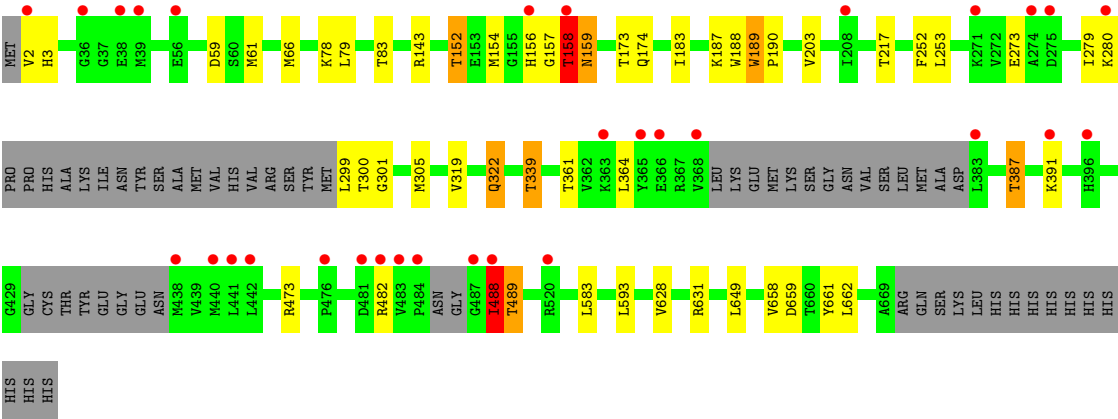
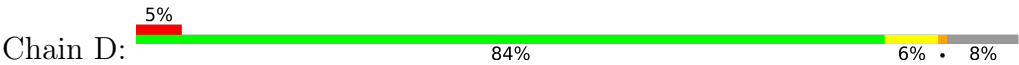
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Chain	Residue	Modelled	Actual	Comment	Reference
C	676	HIS	-	expression tag	UNP O62140
C	677	HIS	-	expression tag	UNP O62140
C	678	HIS	-	expression tag	UNP O62140
C	679	HIS	-	expression tag	UNP O62140
C	680	HIS	-	expression tag	UNP O62140
C	681	HIS	-	expression tag	UNP O62140
C	682	HIS	-	expression tag	UNP O62140
C	683	HIS	-	expression tag	UNP O62140
C	684	HIS	-	expression tag	UNP O62140
D	675	HIS	-	expression tag	UNP O62140
D	676	HIS	-	expression tag	UNP O62140
D	677	HIS	-	expression tag	UNP O62140
D	678	HIS	-	expression tag	UNP O62140
D	679	HIS	-	expression tag	UNP O62140
D	680	HIS	-	expression tag	UNP O62140
D	681	HIS	-	expression tag	UNP O62140
D	682	HIS	-	expression tag	UNP O62140
D	683	HIS	-	expression tag	UNP O62140
D	684	HIS	-	expression tag	UNP O62140



● Molecule 1: Acyl-coenzyme A oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.43Å 140.55Å 131.34Å 90.00° 91.18° 90.00°	Depositor
Resolution (Å)	48.85 – 2.86 48.85 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.85-2.86) 99.8 (48.85-2.86)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.216 , 0.226 0.220 , 0.232	Depositor DCC
R_{free} test set	3598 reflections (5.33%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.056 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	20012	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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	0.20	0/5099	0.48	0/6893
1	B	0.20	0/5132	0.47	0/6937
1	C	0.20	0/5106	0.46	0/6903
1	D	0.20	0/5077	0.47	0/6861
All	All	0.20	0/20414	0.47	0/27594

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	4998	0	5010	41	0
1	B	5031	0	5054	30	0
1	C	5005	0	5034	34	0
1	D	4978	0	5006	26	0
All	All	20012	0	20104	117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:HG2	1:A:321:ARG:HH21	1.61	0.63
1:B:227:THR:HG23	1:B:229:LYS:H	1.65	0.61
1:B:224:ASP:HB3	1:B:227:THR:HG22	1.84	0.60
1:A:458:GLY:HA2	1:C:561:GLU:HG2	1.86	0.58
1:A:339:THR:HG21	1:B:438:MET:HG2	1.88	0.56
1:A:440:MET:HE2	1:A:440:MET:HA	1.88	0.56
1:D:79:LEU:O	1:D:83:THR:HG23	2.07	0.54
1:B:173:THR:O	1:B:175:GLU:HG3	2.08	0.54
1:C:156:HIS:HA	1:D:322:GLN:HE22	1.73	0.54
1:D:188:TRP:O	1:D:189:TRP:HB2	2.08	0.53
1:B:79:LEU:O	1:B:83:THR:HG23	2.08	0.53
1:B:583:LEU:HD11	1:B:593:LEU:HD22	1.90	0.53
1:A:188:TRP:O	1:A:189:TRP:HB2	2.09	0.53
1:C:188:TRP:O	1:C:189:TRP:HB2	2.08	0.52
1:A:79:LEU:O	1:A:83:THR:HG23	2.08	0.52
1:A:367:ARG:HB3	1:A:367:ARG:NH1	2.25	0.52
1:C:583:LEU:HD11	1:C:593:LEU:HD22	1.92	0.52
1:C:79:LEU:O	1:C:83:THR:HG23	2.09	0.51
1:B:187:LYS:HB2	1:B:253:LEU:HB3	1.91	0.51
1:B:382:ASP:OD1	1:B:464:GLY:HA3	2.11	0.51
1:B:188:TRP:O	1:B:189:TRP:HB2	2.10	0.51
1:C:187:LYS:HB2	1:C:253:LEU:HB3	1.92	0.51
1:C:85:ARG:O	1:C:88:GLU:HG2	2.10	0.50
1:A:85:ARG:O	1:A:88:GLU:HG2	2.11	0.50
1:A:458:GLY:CA	1:C:561:GLU:HG2	2.42	0.50
1:B:164:GLU:OE1	1:B:182:LYS:HE3	2.12	0.50
1:D:583:LEU:HD11	1:D:593:LEU:HD22	1.94	0.50
1:C:438:MET:HE3	1:D:339:THR:HG23	1.93	0.49
1:A:208:ILE:O	1:A:209:LYS:HD3	2.11	0.49
1:A:187:LYS:O	1:A:252:PHE:HA	2.12	0.49
1:B:12:ASP:O	1:B:13:ASN:C	2.55	0.49
1:B:187:LYS:O	1:B:252:PHE:HA	2.13	0.49
1:A:154:MET:HE3	1:A:183:ILE:HG12	1.93	0.49
1:A:83:THR:HG22	1:A:143:ARG:NH1	2.28	0.48
1:C:187:LYS:O	1:C:252:PHE:HA	2.13	0.48
1:C:557:ILE:O	1:C:561:GLU:HG3	2.13	0.48
1:D:83:THR:HG22	1:D:143:ARG:NH1	2.28	0.48
1:D:273:GLU:OE2	1:D:279:ILE:HD11	2.13	0.48
1:A:339:THR:HG23	1:B:438:MET:HE3	1.94	0.48
1:D:2:VAL:HG13	1:D:3:HIS:H	1.77	0.48
1:D:61:MET:HG2	1:D:66:MET:HE2	1.96	0.48
1:C:203:VAL:HG22	1:C:217:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:VAL:HG13	1:C:3:HIS:H	1.79	0.47
1:D:203:VAL:HG22	1:D:217:THR:HG22	1.96	0.47
1:A:203:VAL:HG22	1:A:217:THR:HG22	1.96	0.47
1:A:583:LEU:HD11	1:A:593:LEU:HD22	1.95	0.47
1:D:488:ILE:HG13	1:D:489:THR:N	2.28	0.47
1:A:85:ARG:HE	1:A:88:GLU:CD	2.23	0.47
1:A:61:MET:HG2	1:A:66:MET:HE2	1.96	0.47
1:D:187:LYS:O	1:D:252:PHE:HA	2.15	0.47
1:D:387:THR:O	1:D:391:LYS:HG2	2.15	0.47
1:C:83:THR:HG22	1:C:143:ARG:NH1	2.31	0.46
1:C:273:GLU:C	1:C:275:ASP:N	2.73	0.46
1:D:187:LYS:HB2	1:D:253:LEU:HB3	1.96	0.46
1:B:83:THR:HG22	1:B:143:ARG:NH1	2.30	0.46
1:D:301:GLY:O	1:D:305:MET:HG2	2.15	0.46
1:C:368:VAL:HG23	1:C:368:VAL:O	2.14	0.46
1:B:301:GLY:O	1:B:305:MET:HG2	2.16	0.46
1:C:61:MET:HG2	1:C:66:MET:HE2	1.97	0.46
1:C:158:THR:HB	1:C:159:ASN:H	1.53	0.46
1:A:187:LYS:HB2	1:A:253:LEU:HB3	1.97	0.46
1:A:169:TYR:OH	1:A:274:ALA:HA	2.16	0.45
1:C:301:GLY:O	1:C:305:MET:HG2	2.17	0.45
1:B:61:MET:HG2	1:B:66:MET:HE2	1.98	0.45
1:A:321:ARG:HH21	1:A:321:ARG:CG	2.25	0.45
1:D:154:MET:HE3	1:D:183:ILE:HG12	1.99	0.45
1:A:501:ARG:O	1:A:505:LYS:HB2	2.16	0.45
1:A:529:VAL:HG23	1:B:338:GLN:HG2	1.97	0.45
1:A:557:ILE:O	1:A:561:GLU:HG3	2.17	0.45
1:A:183:ILE:CD1	1:B:638:GLU:HA	2.47	0.45
1:C:154:MET:HE3	1:C:183:ILE:HG12	1.98	0.44
1:D:159:ASN:OD1	1:D:159:ASN:N	2.45	0.44
1:A:339:THR:HG21	1:B:438:MET:CG	2.47	0.44
1:A:388:SER:HB3	1:A:440:MET:O	2.18	0.44
1:B:382:ASP:OD2	1:B:466:LEU:HB2	2.18	0.44
1:C:228:HIS:CD2	1:D:658:VAL:HG11	2.53	0.44
1:A:584:GLU:O	1:B:590:SER:HB2	2.18	0.44
1:C:169:TYR:OH	1:C:274:ALA:HA	2.17	0.43
1:A:321:ARG:CG	1:A:321:ARG:NH2	2.82	0.43
1:B:61:MET:HE2	1:B:65:TYR:HD2	1.83	0.43
1:C:59:ASP:OD1	1:C:78:LYS:NZ	2.52	0.43
1:A:301:GLY:O	1:A:305:MET:HG2	2.19	0.43
1:C:152:THR:HB	1:C:157:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:VAL:HA	1:C:662:LEU:HB2	1.99	0.43
1:A:428:ILE:C	1:A:430:GLY:H	2.27	0.43
1:B:118:VAL:O	1:B:122:PRO:HG2	2.19	0.43
1:A:189:TRP:N	1:A:190:PRO:CD	2.82	0.42
1:B:154:MET:HE3	1:B:183:ILE:HG12	2.01	0.42
1:B:203:VAL:HG22	1:B:217:THR:HG22	2.00	0.42
1:A:83:THR:HG22	1:A:143:ARG:HH11	1.84	0.42
1:A:658:VAL:HA	1:A:662:LEU:HB2	2.02	0.42
1:C:484:PRO:O	1:C:485:ASN:CB	2.67	0.42
1:D:59:ASP:OD1	1:D:78:LYS:NZ	2.53	0.42
1:D:158:THR:HB	1:D:159:ASN:H	1.61	0.42
1:A:59:ASP:OD1	1:A:78:LYS:NZ	2.53	0.41
1:C:91:ASP:OD1	1:C:91:ASP:C	2.63	0.41
1:D:152:THR:HB	1:D:157:GLY:HA2	2.02	0.41
1:D:189:TRP:N	1:D:190:PRO:CD	2.84	0.41
1:A:118:VAL:O	1:A:122:PRO:HG2	2.21	0.41
1:C:593:LEU:HD12	1:C:593:LEU:HA	1.93	0.41
1:B:152:THR:HB	1:B:157:GLY:HA2	2.02	0.41
1:C:80:THR:HG21	1:D:661:TYR:HB3	2.02	0.41
1:A:115:LEU:HD13	1:A:191:GLY:HA3	2.01	0.41
1:A:658:VAL:HG11	1:B:228:HIS:CD2	2.56	0.41
1:B:382:ASP:HB3	1:B:466:LEU:HD12	2.03	0.41
1:C:189:TRP:N	1:C:190:PRO:CD	2.83	0.41
1:C:638:GLU:HA	1:D:183:ILE:CD1	2.51	0.41
1:A:61:MET:HE2	1:A:65:TYR:HD2	1.86	0.41
1:B:189:TRP:N	1:B:190:PRO:CD	2.84	0.41
1:C:608:ARG:HD3	1:C:608:ARG:C	2.46	0.41
1:A:333:LYS:O	1:A:336:GLU:HB2	2.21	0.41
1:C:118:VAL:O	1:C:122:PRO:HG2	2.21	0.41
1:A:367:ARG:HB3	1:A:367:ARG:CZ	2.51	0.40
1:C:333:LYS:O	1:C:336:GLU:HB2	2.21	0.40
1:B:156:HIS:NE2	1:B:164:GLU:OE2	2.54	0.40
1:D:628:VAL:O	1:D:631:ARG:HG3	2.21	0.40
1:D:83:THR:HG22	1:D:143:ARG:HH11	1.86	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	621/684 (91%)	601 (97%)	18 (3%)	2 (0%)	36	54
1	B	625/684 (91%)	606 (97%)	17 (3%)	2 (0%)	36	54
1	C	622/684 (91%)	607 (98%)	12 (2%)	3 (0%)	24	42
1	D	616/684 (90%)	600 (97%)	13 (2%)	3 (0%)	24	42
All	All	2484/2736 (91%)	2414 (97%)	60 (2%)	10 (0%)	30	48

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	TRP
1	B	189	TRP
1	C	189	TRP
1	D	189	TRP
1	B	158	THR
1	C	485	ASN
1	D	158	THR
1	C	158	THR
1	D	488	ILE
1	A	325	ILE

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	529/579 (91%)	503 (95%)	26 (5%)	22	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	533/579 (92%)	516 (97%)	17 (3%)	34	59
1	C	531/579 (92%)	516 (97%)	15 (3%)	38	62
1	D	528/579 (91%)	506 (96%)	22 (4%)	26	51
All	All	2121/2316 (92%)	2041 (96%)	80 (4%)	29	54

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	39	MET
1	A	42	ARG
1	A	115	LEU
1	A	152	THR
1	A	209	LYS
1	A	271	LYS
1	A	273	GLU
1	A	277	THR
1	A	298	MET
1	A	299	LEU
1	A	300	THR
1	A	319	VAL
1	A	321	ARG
1	A	339	THR
1	A	361	THR
1	A	387	THR
1	A	440	MET
1	A	442	LEU
1	A	473	ARG
1	A	482	ARG
1	A	485	ASN
1	A	489	THR
1	A	638	GLU
1	A	659	ASP
1	A	662	LEU
1	B	38	GLU
1	B	56	GLU
1	B	152	THR
1	B	156	HIS
1	B	158	THR
1	B	298	MET
1	B	299	LEU

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Mol	Chain	Res	Type
1	B	319	VAL
1	B	322	GLN
1	B	339	THR
1	B	382	ASP
1	B	387	THR
1	B	440	MET
1	B	483	VAL
1	B	489	THR
1	B	659	ASP
1	B	662	LEU
1	C	40	ARG
1	C	152	THR
1	C	156	HIS
1	C	158	THR
1	C	299	LEU
1	C	319	VAL
1	C	361	THR
1	C	387	THR
1	C	440	MET
1	C	443	GLN
1	C	473	ARG
1	C	489	THR
1	C	638	GLU
1	C	659	ASP
1	C	662	LEU
1	D	152	THR
1	D	156	HIS
1	D	158	THR
1	D	159	ASN
1	D	173	THR
1	D	174	GLN
1	D	280	LYS
1	D	299	LEU
1	D	300	THR
1	D	319	VAL
1	D	322	GLN
1	D	339	THR
1	D	361	THR
1	D	364	LEU
1	D	387	THR
1	D	473	ARG
1	D	482	ARG

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Mol	Chain	Res	Type
1	D	488	ILE
1	D	489	THR
1	D	649	LEU
1	D	659	ASP
1	D	662	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	302	GLN
1	A	384	HIS
1	A	443	GLN
1	A	462	GLN
1	A	485	ASN
1	B	162	ASN
1	B	228	HIS
1	B	302	GLN
1	B	397	GLN
1	B	443	GLN
1	C	174	GLN
1	C	302	GLN
1	C	322	GLN
1	C	443	GLN
1	C	639	ASN
1	D	302	GLN
1	D	322	GLN
1	D	328	ASN
1	D	384	HIS
1	D	443	GLN
1	D	568	HIS

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 [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	629/684 (91%)	0.63	38 (6%)	27	20	23, 38, 58, 78	0
1	B	633/684 (92%)	0.38	33 (5%)	33	25	20, 32, 51, 67	0
1	C	630/684 (92%)	0.40	24 (3%)	44	35	19, 32, 51, 75	0
1	D	626/684 (91%)	0.47	31 (4%)	34	27	22, 35, 52, 71	0
All	All	2518/2736 (92%)	0.47	126 (5%)	34	27	19, 34, 54, 78	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	484	PRO	4.7
1	B	487	GLY	4.3
1	D	2	VAL	4.1
1	B	517	GLY	4.0
1	C	484	PRO	3.9
1	B	95	ALA	3.7
1	D	275	ASP	3.7
1	B	381	ALA	3.7
1	A	486	GLY	3.6
1	A	484	PRO	3.6
1	C	127	GLN	3.5
1	A	297	TYR	3.4
1	C	517	GLY	3.4
1	A	38	GLU	3.4
1	B	36	GLY	3.3
1	C	473	ARG	3.3
1	B	39	MET	3.3
1	A	2	VAL	3.2
1	B	439	VAL	3.2
1	C	281	PRO	3.2
1	D	383	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	486	GLY	3.1
1	D	158	THR	3.1
1	C	369	LEU	3.1
1	A	158	THR	3.0
1	C	368	VAL	3.0
1	D	483	VAL	3.0
1	B	369	LEU	3.0
1	A	483	VAL	3.0
1	B	297	TYR	2.9
1	A	172	GLY	2.9
1	D	520	ARG	2.9
1	D	280	LYS	2.9
1	D	442	LEU	2.9
1	B	158	THR	2.8
1	B	442	LEU	2.8
1	A	363	LYS	2.8
1	C	483	VAL	2.8
1	C	275	ASP	2.8
1	D	438	MET	2.8
1	B	438	MET	2.8
1	C	659	ASP	2.8
1	D	363	LYS	2.8
1	B	366	GLU	2.7
1	C	486	GLY	2.7
1	D	487	GLY	2.7
1	A	365	TYR	2.7
1	A	439	VAL	2.7
1	C	485	ASN	2.6
1	A	275	ASP	2.6
1	B	38	GLU	2.6
1	C	38	GLU	2.6
1	B	669	ALA	2.6
1	C	158	THR	2.6
1	A	366	GLU	2.6
1	B	440	MET	2.6
1	D	482	ARG	2.6
1	B	157	GLY	2.6
1	D	440	MET	2.6
1	D	481	ASP	2.6
1	D	156	HIS	2.5
1	A	278	TYR	2.5
1	B	83	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	457	SER	2.5
1	A	485	ASN	2.5
1	B	659	ASP	2.4
1	A	482	ARG	2.4
1	A	489	THR	2.4
1	A	39	MET	2.4
1	D	271	LYS	2.4
1	D	56	GLU	2.4
1	C	365	TYR	2.4
1	A	270	THR	2.4
1	B	172	GLY	2.4
1	B	482	ARG	2.4
1	B	605	GLN	2.4
1	A	300	THR	2.4
1	D	365	TYR	2.4
1	C	669	ALA	2.3
1	C	489	THR	2.3
1	D	36	GLY	2.3
1	A	481	ASP	2.3
1	D	208	ILE	2.3
1	A	169	TYR	2.3
1	A	440	MET	2.3
1	D	274	ALA	2.3
1	A	127	GLN	2.3
1	B	457	SER	2.3
1	B	164	GLU	2.2
1	D	488	ILE	2.2
1	A	157	GLY	2.2
1	A	267	MET	2.2
1	A	475	GLU	2.2
1	B	159	ASN	2.2
1	A	208	ILE	2.2
1	C	458	GLY	2.2
1	A	279	ILE	2.2
1	C	482	ARG	2.2
1	D	396	HIS	2.2
1	A	220	VAL	2.2
1	D	39	MET	2.2
1	B	11	GLY	2.2
1	C	461	SER	2.2
1	B	516	ASN	2.1
1	D	391	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	209	LYS	2.1
1	A	553	GLU	2.1
1	D	366	GLU	2.1
1	A	605	GLN	2.1
1	C	605	GLN	2.1
1	C	159	ASN	2.1
1	B	227	THR	2.1
1	A	273	GLU	2.1
1	A	480	ILE	2.1
1	C	10	GLU	2.1
1	D	38	GLU	2.1
1	A	388	SER	2.1
1	B	489	THR	2.1
1	C	515	GLU	2.1
1	D	368	VAL	2.0
1	B	485	ASN	2.0
1	A	9	GLN	2.0
1	D	476	PRO	2.0
1	D	441	LEU	2.0
1	B	270	THR	2.0
1	B	2	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.