



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 06:55 PM EDT

PDB ID : 5K3H
Title : Crystals structure of Acyl-CoA oxidase-1 in *Caenorhabditis elegans*, Apo form-II
Authors : Zhang, X.; Li, K.; Jones, R.A.; Bruner, S.D.; Butcher, R.A.
Deposited on : 2016-05-19
Resolution : 2.48 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

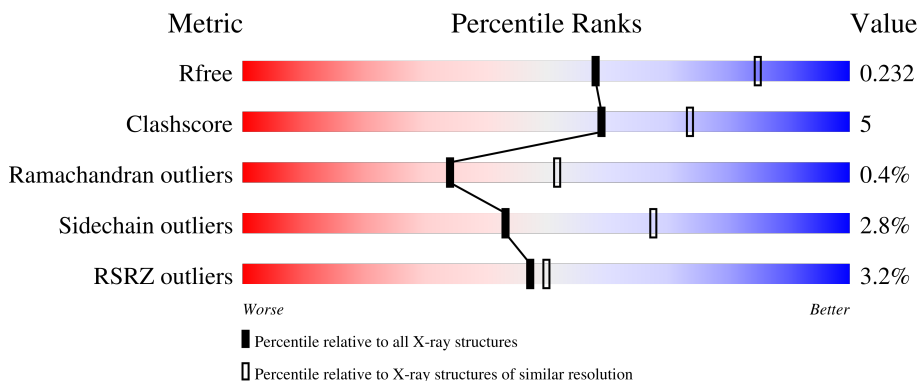
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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.



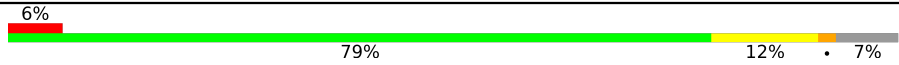

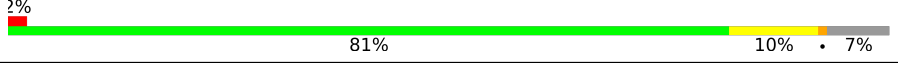
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	 4% 79% 12% • 7%
1	B	684	 2% 82% 10% • 7%
1	C	684	 3% 81% 11% 7%
1	D	684	 % 83% 8% • 7%
1	E	684	 2% 81% 11% • 7%

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Mol	Chain	Length	Quality of chain
1	F	684	 6% 79% 12% 7%
1	G	684	 3% 82% 11% 7%
1	H	684	 2% 81% 10% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41742 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
			Total	C	N	O	S			
1	A	634	5036	3199	885	928	24	0	0	0
1	B	635	5039	3198	887	931	23	0	0	0
1	C	633	5023	3190	885	925	23	0	0	0
1	D	634	5035	3196	886	930	23	0	0	0
1	E	635	5036	3197	887	929	23	0	0	0
1	F	633	5030	3193	885	929	23	0	0	0
1	G	634	5032	3195	886	928	23	0	0	0
1	H	634	5035	3196	886	930	23	0	0	0

There are 80 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

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

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

- Molecule 2 is water.

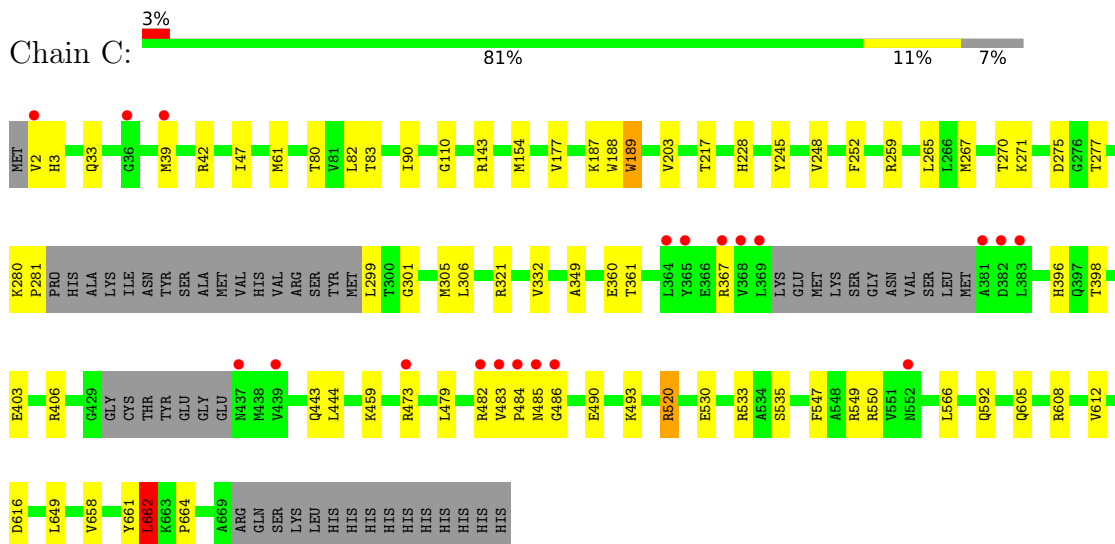
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	150	Total 150	O 150	0	0
2	B	180	Total 180	O 180	0	0
2	C	199	Total 199	O 199	0	0
2	D	215	Total 215	O 215	0	0
2	E	188	Total 188	O 188	0	0
2	F	156	Total 156	O 156	0	0
2	G	203	Total 203	O 203	0	0

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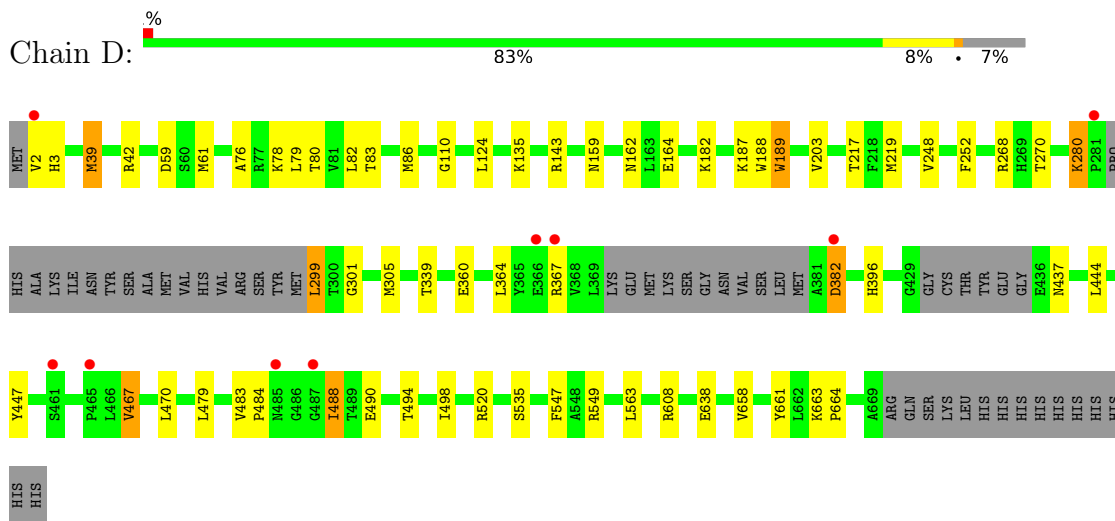
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	185	Total 185	O 185	0	0

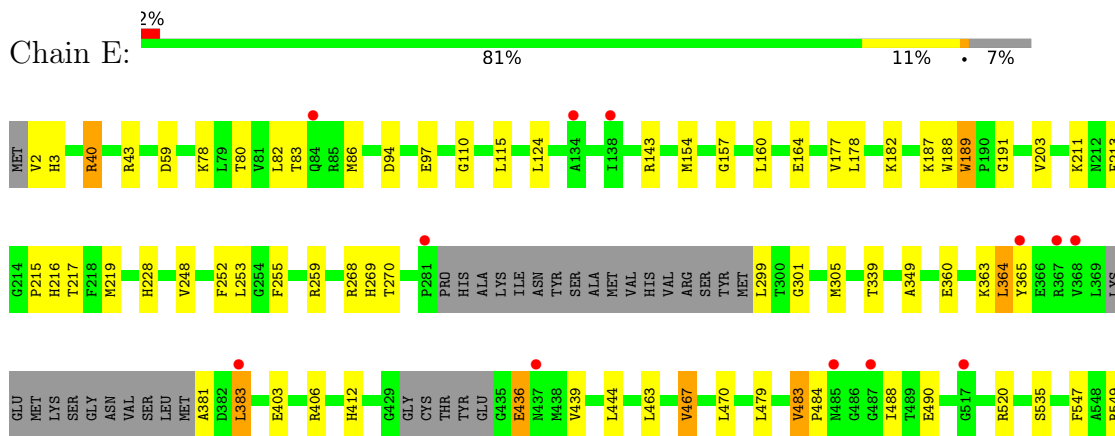
- Molecule 1: Acyl-coenzyme A oxidase

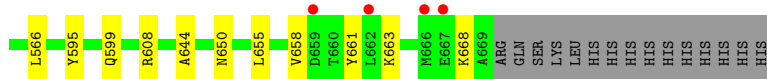


- Molecule 1: Acyl-coenzyme A oxidase

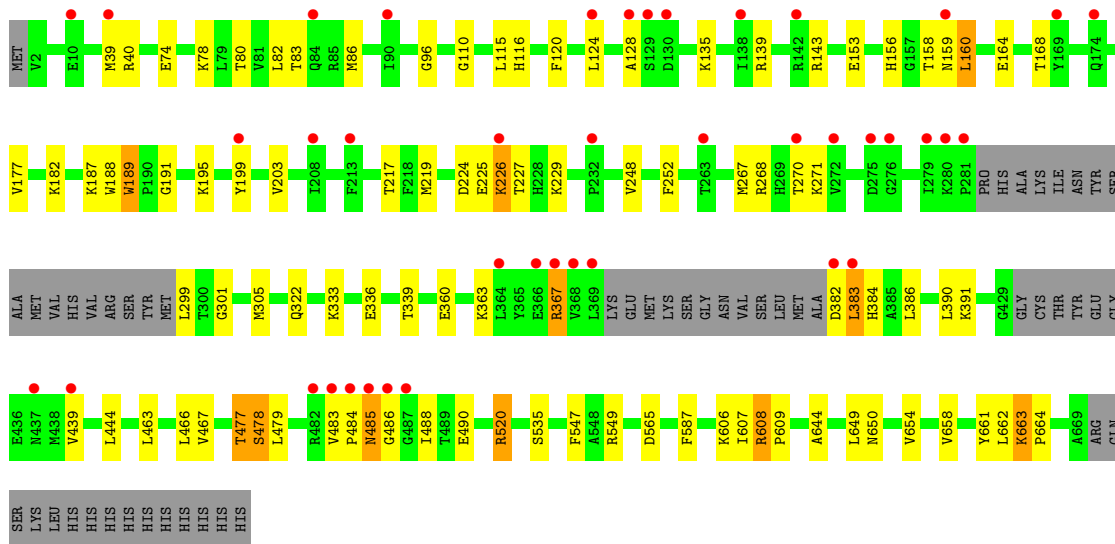
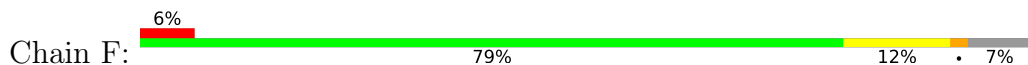


- Molecule 1: Acyl-coenzyme A oxidase

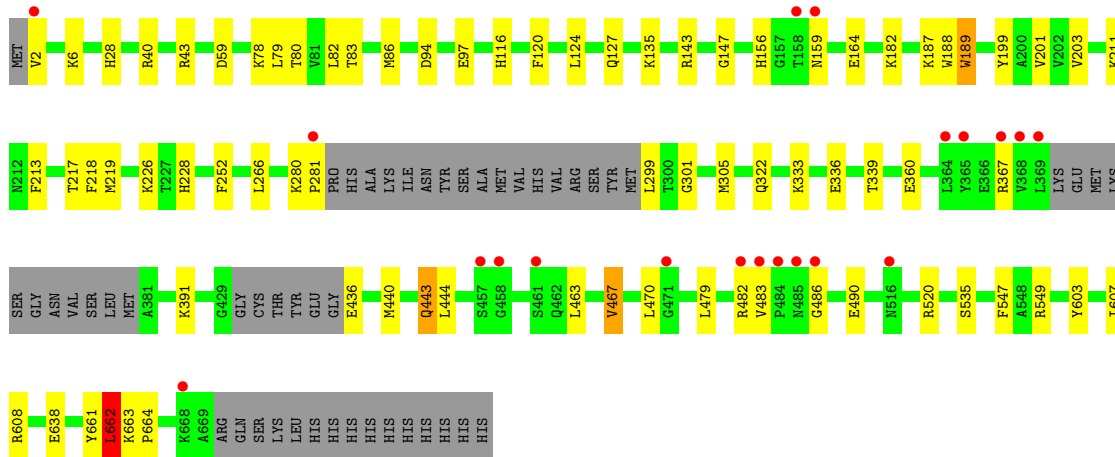
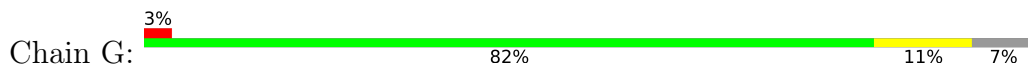




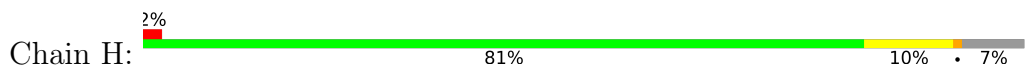
- Molecule 1: Acyl-coenzyme A oxidase



- Molecule 1: Acyl-coenzyme A oxidase



- Molecule 1: Acyl-coenzyme A oxidase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	153.07Å 140.79Å 154.93Å 90.00° 117.20° 90.00°	Depositor
Resolution (Å)	49.24 – 2.48 49.24 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.24-2.48) 99.7 (49.24-2.48)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 2.48Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.191 , 0.232 0.193 , 0.232	Depositor DCC
R_{free} test set	10075 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtrriage
Anisotropy	0.331	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.074 for l,-k,h	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	41742	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.36 % 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 3.1995e-05. 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	0.44	0/5137	0.61	0/6943
1	B	0.45	0/5140	0.62	0/6949
1	C	0.46	0/5124	0.60	0/6928
1	D	0.48	0/5136	0.62	0/6944
1	E	0.45	0/5137	0.64	0/6945
1	F	0.44	0/5131	0.60	0/6937
1	G	0.47	0/5133	0.62	0/6940
1	H	0.46	0/5136	0.62	0/6944
All	All	0.45	0/41074	0.62	0/55530

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	5036	0	5056	57	0
1	B	5039	0	5058	45	0
1	C	5023	0	5047	44	0
1	D	5035	0	5055	37	0
1	E	5036	0	5056	49	0
1	F	5030	0	5050	73	0
1	G	5032	0	5053	46	0
1	H	5035	0	5055	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	150	0	0	5	0
2	B	180	0	0	2	0
2	C	199	0	0	3	0
2	D	215	0	0	2	0
2	E	188	0	0	1	0
2	F	156	0	0	2	0
2	G	203	0	0	1	0
2	H	185	0	0	6	0
All	All	41742	0	40430	376	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 5.

All (376) 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:658:VAL:HA	1:A:662:LEU:HB2	1.30	1.13
1:G:661:TYR:O	1:G:664:PRO:HD2	1.56	1.04
1:H:658:VAL:HA	1:H:662:LEU:HB2	1.36	1.03
1:F:658:VAL:HG22	1:F:662:LEU:HD12	1.44	0.99
1:F:658:VAL:HA	1:F:662:LEU:HB2	1.44	0.97
1:F:663:LYS:HB3	1:F:664:PRO:HD3	1.46	0.95
1:F:40:ARG:HH22	1:F:96:GLY:HA3	1.33	0.94
1:C:661:TYR:HB3	1:D:80:THR:HG21	1.50	0.94
1:A:382:ASP:N	1:A:447:TYR:HH	1.65	0.93
1:H:658:VAL:HG22	1:H:662:LEU:HD23	1.49	0.92
1:H:663:LYS:HB3	1:H:664:PRO:HD3	1.52	0.91
1:A:83:THR:HG22	1:A:143:ARG:HH11	1.35	0.88
1:B:83:THR:HG22	1:B:143:ARG:HH11	1.38	0.86
1:E:157:GLY:H	1:F:322:GLN:HE22	1.18	0.86
1:H:177:VAL:HG22	1:H:259:ARG:HG2	1.60	0.83
1:H:483:VAL:HG23	1:H:485:ASN:HB2	1.61	0.83
1:E:80:THR:HG21	1:F:661:TYR:HB3	1.63	0.80
1:F:227:THR:HG23	1:F:229:LYS:H	1.47	0.80
1:A:360:GLU:OE2	1:A:549:ARG:HD2	1.83	0.78
1:F:565:ASP:HB3	1:F:607:ILE:HD11	1.68	0.76
1:C:360:GLU:OE2	1:C:549:ARG:HD2	1.86	0.75
1:C:83:THR:HG22	1:C:143:ARG:NH1	2.03	0.74
1:B:83:THR:HG22	1:B:143:ARG:NH1	2.03	0.73
1:C:661:TYR:HB3	1:D:80:THR:CG2	2.18	0.73
1:A:339:THR:HG21	1:B:438:MET:HG2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:661:TYR:O	1:C:664:PRO:HD2	1.90	0.72
1:E:360:GLU:OE2	1:E:549:ARG:HD2	1.90	0.72
1:C:267:MET:HB3	1:C:271:LYS:HD3	1.72	0.71
1:E:83:THR:HG22	1:E:143:ARG:HH11	1.55	0.71
1:A:663:LYS:HB3	1:A:664:PRO:HD3	1.72	0.70
1:F:40:ARG:NH2	1:F:96:GLY:HA3	2.06	0.70
1:D:83:THR:HG22	1:D:143:ARG:NH1	2.07	0.69
1:E:157:GLY:N	1:F:322:GLN:HE22	1.91	0.68
1:G:661:TYR:O	1:G:664:PRO:CD	2.36	0.68
1:F:83:THR:HG22	1:F:143:ARG:HH11	1.57	0.68
1:A:177:VAL:HG22	1:A:259:ARG:HG2	1.74	0.67
1:B:203:VAL:HG22	1:B:217:THR:HG22	1.77	0.66
1:F:159:ASN:O	1:F:160:LEU:HB2	1.96	0.66
1:B:360:GLU:OE2	1:B:549:ARG:HD2	1.94	0.66
1:D:83:THR:HG22	1:D:143:ARG:HH11	1.60	0.66
1:A:83:THR:HG22	1:A:143:ARG:NH1	2.07	0.66
1:H:663:LYS:HB3	1:H:664:PRO:CD	2.26	0.65
1:F:224:ASP:HB3	1:F:227:THR:HG22	1.79	0.64
1:C:203:VAL:HG22	1:C:217:THR:HG22	1.79	0.64
1:G:80:THR:HG21	1:H:661:TYR:HB3	1.79	0.64
1:G:83:THR:HG22	1:G:143:ARG:NH1	2.12	0.64
1:H:83:THR:HG22	1:H:143:ARG:HH11	1.63	0.64
1:F:565:ASP:HB3	1:F:607:ILE:CD1	2.28	0.64
1:B:463:LEU:HD22	1:B:467:VAL:HG13	1.81	0.63
1:A:403:GLU:OE2	1:A:406:ARG:NH2	2.31	0.63
1:C:270:THR:HG22	1:C:281:PRO:HD3	1.81	0.62
1:D:159:ASN:ND2	1:D:162:ASN:OD1	2.32	0.62
1:G:333:LYS:O	1:G:336:GLU:HB2	2.00	0.62
1:F:115:LEU:HD13	1:F:191:GLY:HA3	1.81	0.62
1:D:2:VAL:HG13	1:D:3:HIS:H	1.63	0.61
1:D:164:GLU:OE2	1:D:182:LYS:HE3	2.00	0.61
1:H:164:GLU:OE2	1:H:182:LYS:HE3	2.00	0.61
1:G:203:VAL:HG22	1:G:217:THR:HG22	1.81	0.61
1:A:403:GLU:OE2	1:A:406:ARG:NE	2.33	0.61
1:B:156:HIS:NE2	1:B:164:GLU:OE2	2.30	0.61
1:B:488:ILE:HD12	1:B:571:VAL:HG21	1.82	0.61
1:H:268:ARG:HG2	1:H:269:HIS:CD2	2.36	0.61
1:A:228:HIS:CD2	1:B:658:VAL:HG11	2.36	0.61
1:A:663:LYS:CB	1:A:664:PRO:HD3	2.30	0.61
1:A:661:TYR:O	1:A:664:PRO:HD2	2.00	0.61
1:H:658:VAL:HA	1:H:662:LEU:CB	2.23	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HD2	1:A:46:GLU:OE2	2.00	0.60
1:E:83:THR:HG22	1:E:143:ARG:NH1	2.16	0.60
1:F:661:TYR:O	1:F:664:PRO:HD2	2.00	0.60
1:E:463:LEU:HD22	1:E:467:VAL:HG13	1.84	0.60
1:F:663:LYS:HB3	1:F:664:PRO:CD	2.27	0.59
1:H:142:ARG:NH1	1:H:144:GLU:OE2	2.35	0.59
1:C:403:GLU:OE2	1:C:406:ARG:NH2	2.32	0.59
1:A:533:ARG:NH2	2:A:704:HOH:O	2.35	0.59
1:F:565:ASP:CB	1:F:607:ILE:HD11	2.32	0.59
1:E:164:GLU:OE2	1:E:182:LYS:HE3	2.02	0.58
1:C:349:ALA:HB2	1:C:566:LEU:HD22	1.86	0.58
1:E:203:VAL:HG22	1:E:217:THR:HG22	1.85	0.58
1:C:42:ARG:NH1	2:C:701:HOH:O	2.34	0.58
1:D:299:LEU:N	2:D:704:HOH:O	2.37	0.58
1:C:484:PRO:O	1:C:485:ASN:HB2	2.04	0.58
1:F:360:GLU:OE2	1:F:549:ARG:HD2	2.04	0.58
1:E:444:LEU:HD23	1:E:535:SER:HB3	1.86	0.57
1:C:42:ARG:HD2	2:C:701:HOH:O	2.03	0.57
1:F:363:LYS:NZ	2:F:705:HOH:O	2.37	0.57
1:A:339:THR:CG2	1:B:438:MET:HG2	2.32	0.57
1:A:662:LEU:HD12	1:B:146:ILE:HD11	1.87	0.56
1:C:188:TRP:O	1:C:189:TRP:HB2	2.06	0.56
1:G:187:LYS:O	1:G:252:PHE:HA	2.05	0.56
1:D:270:THR:HG22	1:D:280:LYS:HD3	1.86	0.56
1:H:360:GLU:OE2	1:H:549:ARG:HD2	2.05	0.56
1:B:227:THR:HG23	1:B:229:LYS:H	1.70	0.56
1:H:83:THR:HG22	1:H:143:ARG:NH1	2.19	0.56
1:F:444:LEU:HD23	1:F:535:SER:HB3	1.87	0.55
1:G:116:HIS:O	1:G:120:PHE:HB3	2.07	0.55
1:G:59:ASP:OD1	1:G:78:LYS:NZ	2.39	0.55
1:G:479:LEU:HB3	1:G:483:VAL:HG13	1.88	0.55
1:A:115:LEU:HD13	1:A:191:GLY:HA3	1.87	0.55
1:F:83:THR:HG22	1:F:143:ARG:NH1	2.22	0.55
1:F:663:LYS:CB	1:F:664:PRO:HD3	2.29	0.55
1:H:533:ARG:NH2	2:H:705:HOH:O	2.40	0.55
1:G:360:GLU:OE2	1:G:549:ARG:HD2	2.07	0.55
1:E:403:GLU:OE2	1:E:406:ARG:NE	2.32	0.54
1:H:203:VAL:HG22	1:H:217:THR:HG22	1.89	0.54
1:H:658:VAL:HG22	1:H:662:LEU:CD2	2.30	0.54
1:E:484:PRO:O	1:H:520:ARG:NH2	2.41	0.54
1:B:483:VAL:HG13	1:C:520:ARG:NH2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:GLU:OE2	1:D:549:ARG:HD2	2.07	0.53
1:A:382:ASP:N	2:A:707:HOH:O	2.40	0.53
1:F:139:ARG:NH2	2:F:711:HOH:O	2.42	0.53
1:A:280:LYS:HD2	1:A:281:PRO:HD2	1.91	0.53
1:F:363:LYS:O	1:F:367:ARG:HB2	2.09	0.53
1:F:382:ASP:CG	1:F:383:LEU:H	2.12	0.53
1:G:164:GLU:OE2	1:G:182:LYS:HE3	2.09	0.53
1:C:80:THR:HG21	1:D:661:TYR:HB3	1.89	0.53
1:B:301:GLY:O	1:B:305:MET:HG2	2.09	0.52
1:E:80:THR:CG2	1:F:661:TYR:HB3	2.37	0.52
1:F:188:TRP:O	1:F:189:TRP:HB2	2.08	0.52
1:F:383:LEU:HD13	1:F:384:HIS:N	2.24	0.52
1:H:188:TRP:O	1:H:189:TRP:HB2	2.09	0.52
1:H:80:THR:O	1:H:84:GLN:HG2	2.09	0.52
1:C:301:GLY:O	1:C:305:MET:HG2	2.09	0.52
1:F:608:ARG:HB3	1:F:609:PRO:HD3	1.91	0.52
1:G:80:THR:CG2	1:H:661:TYR:HB3	2.40	0.52
1:A:444:LEU:HD23	1:A:535:SER:HB3	1.92	0.52
1:F:382:ASP:OD1	1:F:382:ASP:N	2.43	0.52
1:E:40:ARG:NH2	1:E:94:ASP:OD1	2.43	0.52
1:G:40:ARG:NH2	1:G:94:ASP:OD2	2.36	0.52
1:C:661:TYR:O	1:C:664:PRO:CD	2.58	0.51
1:D:467:VAL:HG22	1:D:470:LEU:HD12	1.92	0.51
1:F:156:HIS:NE2	1:F:164:GLU:OE1	2.33	0.51
1:B:62:PRO:HA	2:B:763:HOH:O	2.11	0.51
1:B:187:LYS:HB2	1:B:253:LEU:HB3	1.93	0.51
1:C:658:VAL:HA	1:C:662:LEU:HB2	1.91	0.51
1:D:484:PRO:O	1:F:520:ARG:NH2	2.44	0.51
1:E:110:GLY:HA3	1:E:248:VAL:HG23	1.93	0.51
1:E:381:ALA:N	2:E:709:HOH:O	2.42	0.51
1:C:110:GLY:HA3	1:C:248:VAL:HG23	1.93	0.51
1:D:444:LEU:HD23	1:D:535:SER:HB3	1.93	0.50
1:H:654:VAL:HA	2:H:774:HOH:O	2.10	0.50
1:D:82:LEU:O	1:D:86:MET:HB2	2.10	0.50
1:B:188:TRP:O	1:B:189:TRP:HB2	2.12	0.50
1:F:226:LYS:HG3	1:F:227:THR:N	2.27	0.50
1:G:661:TYR:O	1:G:663:LYS:N	2.44	0.50
1:A:188:TRP:O	1:A:189:TRP:HB2	2.10	0.50
1:E:2:VAL:HG13	1:E:3:HIS:H	1.76	0.50
1:F:479:LEU:HB2	1:F:490:GLU:OE2	2.12	0.50
1:E:479:LEU:HB2	1:E:490:GLU:OE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:483:VAL:HG23	1:F:486:GLY:CA	2.43	0.49
1:F:607:ILE:O	1:F:607:ILE:HG22	2.11	0.49
1:B:110:GLY:HA3	1:B:248:VAL:HG23	1.94	0.49
1:E:187:LYS:HB2	1:E:253:LEU:HB3	1.94	0.49
1:E:154:MET:HE1	1:E:188:TRP:CZ3	2.48	0.49
1:A:59:ASP:OD1	1:A:78:LYS:NZ	2.46	0.49
1:H:128:ALA:O	1:H:268:ARG:NH1	2.41	0.49
1:D:188:TRP:O	1:D:189:TRP:HB2	2.12	0.49
1:G:663:LYS:HB3	1:G:664:PRO:HD3	1.95	0.48
1:H:383:LEU:HD12	1:H:466:LEU:HD11	1.96	0.48
1:G:43:ARG:NH2	1:G:97:GLU:OE1	2.36	0.48
1:H:187:LYS:O	1:H:252:PHE:HA	2.12	0.48
1:H:658:VAL:O	1:H:663:LYS:HB2	2.13	0.48
1:A:663:LYS:CB	1:A:664:PRO:CD	2.91	0.48
1:C:479:LEU:HB2	1:C:490:GLU:OE2	2.12	0.48
1:E:599:GLN:OE1	1:H:459:LYS:NZ	2.35	0.48
1:E:115:LEU:HD13	1:E:191:GLY:HA3	1.96	0.48
1:C:33:GLN:OE1	1:C:550:ARG:HD2	2.13	0.48
1:D:203:VAL:HG22	1:D:217:THR:HG22	1.94	0.48
1:H:40:ARG:HG3	2:H:740:HOH:O	2.14	0.48
1:H:396:HIS:HB2	2:H:733:HOH:O	2.14	0.48
1:E:483:VAL:HG13	1:H:520:ARG:NH2	2.29	0.48
1:B:602:PHE:CE2	1:C:459:LYS:HG2	2.49	0.48
1:A:382:ASP:N	1:A:447:TYR:OH	2.39	0.47
1:E:187:LYS:O	1:E:252:PHE:HA	2.13	0.47
1:F:477:THR:OG1	1:F:478:SER:N	2.45	0.47
1:H:381:ALA:N	1:H:384:HIS:HB3	2.28	0.47
1:E:595:TYR:O	1:E:599:GLN:HG2	2.14	0.47
1:G:156:HIS:NE2	1:G:164:GLU:OE1	2.34	0.47
1:H:82:LEU:O	1:H:86:MET:HB2	2.14	0.47
1:F:187:LYS:O	1:F:252:PHE:HA	2.14	0.47
1:A:203:VAL:HG22	1:A:217:THR:HG22	1.95	0.47
1:E:364:LEU:HB3	1:E:383:LEU:HD11	1.96	0.47
1:G:479:LEU:HB2	1:G:490:GLU:OE1	2.15	0.47
1:C:265:LEU:O	1:C:267:MET:HG3	2.15	0.47
2:G:743:HOH:O	1:H:649:LEU:HB2	2.14	0.47
1:E:211:LYS:HD2	1:E:213:PHE:CZ	2.49	0.47
1:F:128:ALA:O	1:F:268:ARG:NH1	2.48	0.47
1:G:662:LEU:HD13	1:G:662:LEU:H	1.80	0.47
1:A:463:LEU:HD22	1:A:467:VAL:HG13	1.95	0.47
1:E:188:TRP:O	1:E:189:TRP:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:GLU:OE2	1:F:182:LYS:HD2	2.14	0.47
1:G:124:LEU:HD21	1:G:219:MET:HE1	1.95	0.47
1:A:362:VAL:HA	1:A:365:TYR:HB2	1.95	0.47
1:C:80:THR:CG2	1:D:661:TYR:HB3	2.44	0.47
1:D:479:LEU:HB2	1:D:490:GLU:OE2	2.14	0.47
1:B:124:LEU:HD21	1:B:219:MET:CE	2.44	0.47
1:B:488:ILE:HG22	1:B:492:ILE:HG13	1.97	0.47
1:C:228:HIS:CD2	1:D:658:VAL:HG11	2.50	0.47
1:E:655:LEU:O	1:E:658:VAL:HG22	2.15	0.46
1:F:224:ASP:OD2	1:F:227:THR:HG22	2.15	0.46
1:G:79:LEU:O	1:G:83:THR:HG23	2.15	0.46
1:G:188:TRP:O	1:G:189:TRP:HB2	2.15	0.46
1:G:301:GLY:O	1:G:305:MET:HG2	2.14	0.46
1:A:226:LYS:HA	1:A:226:LYS:HD3	1.63	0.46
1:A:634:GLY:HA2	2:A:791:HOH:O	2.15	0.46
1:A:224:ASP:O	1:A:228:HIS:N	2.48	0.46
1:E:216:HIS:HD2	1:E:270:THR:HG21	1.80	0.46
1:H:479:LEU:O	1:H:483:VAL:HG22	2.15	0.46
1:A:25:PHE:HB2	1:A:559:ILE:HD13	1.96	0.46
1:A:40:ARG:NH2	1:A:94:ASP:OD1	2.48	0.46
1:A:207:TYR:CE2	1:A:212:ASN:HB2	2.49	0.46
1:D:382:ASP:HB2	1:D:447:TYR:CE1	2.51	0.46
1:G:226:LYS:HA	1:G:226:LYS:HD3	1.70	0.46
1:A:349:ALA:HB2	1:A:566:LEU:HD22	1.96	0.46
1:B:475:GLU:OE1	1:B:493:LYS:NZ	2.49	0.46
1:F:463:LEU:HD22	1:F:467:VAL:HG13	1.98	0.46
1:C:39:MET:SD	1:C:42:ARG:NH1	2.89	0.46
1:C:306:LEU:HB2	1:C:398:THR:HG23	1.98	0.46
1:G:467:VAL:HG22	1:G:470:LEU:HD12	1.98	0.45
1:H:59:ASP:OD1	1:H:78:LYS:NZ	2.49	0.45
1:F:203:VAL:HG22	1:F:217:THR:HG22	1.98	0.45
1:D:661:TYR:O	1:D:663:LYS:N	2.49	0.45
1:F:124:LEU:HD21	1:F:219:MET:CE	2.46	0.45
1:C:177:VAL:HG22	1:C:259:ARG:HG2	1.98	0.45
1:F:153:GLU:HG2	1:F:187:LYS:HD3	1.97	0.45
1:F:484:PRO:O	1:F:485:ASN:HB2	2.15	0.45
1:G:391:LYS:HD2	1:G:440:MET:SD	2.55	0.45
1:B:467:VAL:HG22	1:B:470:LEU:HD12	1.99	0.45
1:E:160:LEU:HB3	1:E:215:PRO:HG3	1.99	0.45
1:E:301:GLY:O	1:E:305:MET:HG2	2.17	0.45
1:B:224:ASP:HB3	1:B:227:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:TRP:CE3	1:F:252:PHE:HB3	2.52	0.45
1:F:658:VAL:CG2	1:F:662:LEU:HD12	2.31	0.45
1:G:83:THR:HG22	1:G:143:ARG:HH11	1.81	0.45
1:G:443:GLN:HE21	1:G:443:GLN:HB2	1.59	0.45
1:H:187:LYS:HB2	1:H:253:LEU:HB3	1.98	0.45
1:A:450:LYS:NZ	2:A:714:HOH:O	2.46	0.45
1:F:267:MET:HB3	1:F:271:LYS:HD3	1.99	0.45
1:E:436:GLU:O	1:E:439:VAL:HG12	2.16	0.45
1:A:265:LEU:O	1:A:267:MET:HG3	2.17	0.44
1:B:187:LYS:O	1:B:252:PHE:HA	2.17	0.44
1:D:663:LYS:HB3	1:D:664:PRO:HD3	1.99	0.44
1:C:530:GLU:OE2	1:C:533:ARG:NH1	2.50	0.44
1:F:477:THR:O	1:F:587:PHE:O	2.35	0.44
1:B:382:ASP:OD2	1:B:447:TYR:OH	2.33	0.44
1:C:245:TYR:CE2	1:C:248:VAL:HG21	2.53	0.44
1:C:396:HIS:HB2	2:C:705:HOH:O	2.17	0.44
1:G:6:LYS:HG3	1:G:28:HIS:CD2	2.52	0.44
1:B:82:LEU:O	1:B:86:MET:HB2	2.18	0.44
1:D:301:GLY:O	1:D:305:MET:HG2	2.16	0.44
1:E:668:LYS:HE3	1:E:668:LYS:HB2	1.80	0.44
1:D:2:VAL:HG13	1:D:3:HIS:N	2.33	0.44
1:G:211:LYS:HE3	1:G:213:PHE:CE2	2.52	0.44
1:A:665:MET:HB2	1:B:80:THR:HG22	1.99	0.44
1:F:565:ASP:C	1:F:607:ILE:HD11	2.37	0.44
1:H:444:LEU:HD23	1:H:535:SER:HB3	2.00	0.44
1:F:158:THR:HG21	1:F:439:VAL:HG11	2.00	0.43
1:F:168:THR:O	1:F:177:VAL:HG12	2.17	0.43
1:A:124:LEU:HD21	1:A:219:MET:HE1	2.00	0.43
1:C:493:LYS:HB2	1:C:493:LYS:HE3	1.90	0.43
1:F:267:MET:HG2	1:F:270:THR:O	2.18	0.43
1:H:349:ALA:HB2	1:H:566:LEU:HD22	2.00	0.43
1:A:195:LYS:HE3	1:B:649:LEU:O	2.18	0.43
1:D:164:GLU:OE2	1:D:182:LYS:CE	2.66	0.43
1:G:147:GLY:HA2	1:G:199:TYR:O	2.18	0.43
1:A:82:LEU:O	1:A:86:MET:HB2	2.18	0.43
1:E:661:TYR:HB3	1:F:80:THR:HG21	2.00	0.43
1:F:82:LEU:O	1:F:86:MET:HB2	2.18	0.43
1:F:135:LYS:O	1:F:139:ARG:HG3	2.18	0.43
1:H:271:LYS:NZ	2:H:711:HOH:O	2.52	0.43
1:D:110:GLY:HA3	1:D:248:VAL:HG23	2.00	0.43
1:E:228:HIS:CD2	1:F:658:VAL:HG11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:GLU:HG3	1:F:78:LYS:HE2	2.01	0.43
1:F:301:GLY:O	1:F:305:MET:HG2	2.17	0.43
1:B:124:LEU:HD21	1:B:219:MET:HE1	2.01	0.43
1:B:224:ASP:OD1	1:B:227:THR:HG22	2.18	0.43
1:A:2:VAL:HG13	1:A:3:HIS:H	1.83	0.43
1:B:242:LYS:HB2	1:B:242:LYS:HE3	1.83	0.43
1:C:482:ARG:HD2	1:C:592:GLN:NE2	2.33	0.43
1:G:86:MET:CE	1:G:143:ARG:HH12	2.31	0.43
1:F:116:HIS:O	1:F:120:PHE:HB3	2.19	0.43
1:B:235:THR:O	1:B:253:LEU:HA	2.18	0.43
1:D:396:HIS:HB2	2:D:889:HOH:O	2.19	0.43
1:B:154:MET:HG2	1:B:184:THR:HA	2.01	0.42
1:A:236:ILE:HD12	1:A:253:LEU:HD13	2.00	0.42
1:B:661:TYR:O	1:B:663:LYS:N	2.52	0.42
1:D:124:LEU:HD21	1:D:219:MET:CE	2.48	0.42
1:E:43:ARG:NE	1:E:97:GLU:OE2	2.41	0.42
1:H:160:LEU:HD23	1:H:163:LEU:HD11	1.99	0.42
1:H:663:LYS:CB	1:H:664:PRO:HD3	2.34	0.42
1:A:333:LYS:O	1:A:336:GLU:HB2	2.19	0.42
1:A:583:LEU:HD21	1:A:593:LEU:HD22	2.01	0.42
1:C:321:ARG:HA	1:C:332:VAL:O	2.19	0.42
1:G:201:VAL:HA	1:G:218:PHE:O	2.19	0.42
1:A:500:LYS:HB3	1:A:500:LYS:HE2	1.85	0.42
1:B:333:LYS:O	1:B:336:GLU:HB2	2.19	0.42
1:D:187:LYS:O	1:D:252:PHE:HA	2.19	0.42
1:F:110:GLY:HA3	1:F:248:VAL:HG23	2.00	0.42
1:F:135:LYS:HE3	1:F:135:LYS:HB2	1.88	0.42
1:A:23:ALA:HB2	1:A:613:SER:OG	2.20	0.42
1:A:51:LEU:HD11	1:A:101:LEU:HD12	2.01	0.42
1:B:660:THR:O	1:B:664:PRO:HG2	2.19	0.42
1:H:242:LYS:HB2	1:H:242:LYS:HE3	1.90	0.42
1:H:267:MET:HG2	1:H:270:THR:O	2.19	0.42
1:C:275:ASP:HB3	1:C:277:THR:OG1	2.20	0.42
1:E:59:ASP:OD1	1:E:78:LYS:NZ	2.53	0.42
1:E:349:ALA:HB2	1:E:566:LEU:HD22	2.02	0.42
1:H:483:VAL:O	1:H:485:ASN:HB3	2.19	0.42
1:H:486:GLY:HA3	1:H:487:GLY:HA2	1.82	0.42
1:C:187:LYS:O	1:C:252:PHE:HA	2.19	0.42
1:C:444:LEU:HD23	1:C:535:SER:HB3	2.02	0.42
1:D:39:MET:CE	1:D:42:ARG:NH2	2.82	0.42
1:E:178:LEU:HD23	1:E:255:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:644:ALA:O	1:E:650:ASN:ND2	2.52	0.42
1:C:612:VAL:HG12	1:C:616:ASP:OD2	2.19	0.42
1:E:177:VAL:HG22	1:E:259:ARG:HG2	2.01	0.42
1:F:386:LEU:HD22	1:F:466:LEU:HD13	2.02	0.42
1:F:565:ASP:OD2	1:F:606:LYS:NZ	2.52	0.42
1:G:228:HIS:CD2	1:H:658:VAL:HG11	2.55	0.42
1:H:37:GLY:HA3	2:H:740:HOH:O	2.20	0.42
1:A:85:ARG:O	1:A:88:GLU:HG2	2.19	0.42
1:C:188:TRP:HD1	1:C:189:TRP:CD1	2.38	0.42
1:C:483:VAL:HG23	1:C:486:GLY:HA3	2.01	0.42
1:D:76:ALA:O	1:D:80:THR:HG23	2.19	0.42
1:E:216:HIS:CD2	1:E:270:THR:HG21	2.55	0.41
1:F:333:LYS:O	1:F:336:GLU:HB2	2.20	0.41
1:H:593:LEU:HD12	1:H:593:LEU:HA	1.89	0.41
1:B:56:GLU:CD	1:B:56:GLU:H	2.24	0.41
1:C:2:VAL:HG13	1:C:3:HIS:H	1.84	0.41
1:G:444:LEU:HD23	1:G:535:SER:HB3	2.01	0.41
1:G:661:TYR:HB3	1:H:80:THR:CG2	2.50	0.41
1:A:245:TYR:CE2	1:A:248:VAL:HG21	2.55	0.41
1:A:403:GLU:OE2	1:A:406:ARG:CZ	2.68	0.41
1:B:299:LEU:HD22	1:B:299:LEU:HA	1.94	0.41
1:G:483:VAL:HG21	1:G:486:GLY:HA3	2.01	0.41
1:E:412:HIS:CD2	1:F:189:TRP:HE1	2.39	0.41
1:G:603:TYR:O	1:G:607:ILE:HG12	2.21	0.41
1:A:603:TYR:HA	1:A:606:LYS:HB3	2.01	0.41
1:E:82:LEU:O	1:E:86:MET:HB2	2.21	0.41
1:A:402:ILE:HD13	1:A:423:ILE:HG22	2.02	0.41
1:B:118:VAL:O	1:B:122:PRO:HG2	2.19	0.41
1:B:306:LEU:HB2	1:B:398:THR:HG23	2.03	0.41
1:B:595:TYR:O	1:B:599:GLN:HG2	2.20	0.41
1:D:483:VAL:HB	1:F:520:ARG:NH2	2.36	0.41
1:G:483:VAL:HG21	1:G:490:GLU:HG3	2.02	0.41
1:H:160:LEU:HB3	1:H:215:PRO:HG3	2.03	0.41
1:A:383:LEU:HA	1:A:383:LEU:HD12	1.79	0.41
1:G:661:TYR:HB3	1:H:80:THR:HG21	2.03	0.41
1:H:79:LEU:HD21	1:H:113:MET:HG3	2.02	0.41
1:A:124:LEU:HD21	1:A:219:MET:CE	2.50	0.41
1:A:164:GLU:HB2	1:A:185:ALA:HB2	2.02	0.41
1:B:164:GLU:OE1	1:B:182:LYS:HE3	2.21	0.41
1:B:177:VAL:HG22	1:B:259:ARG:HG2	2.03	0.41
1:E:661:TYR:O	1:E:663:LYS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:LYS:HA	1:F:195:LYS:HD3	1.92	0.41
1:G:127:GLN:O	1:G:266:LEU:HB3	2.20	0.41
1:G:280:LYS:HA	1:G:281:PRO:HA	1.90	0.41
1:A:437:ASN:N	2:A:723:HOH:O	2.53	0.41
1:D:59:ASP:OD1	1:D:78:LYS:NZ	2.54	0.41
1:E:467:VAL:HG22	1:E:470:LEU:HD12	2.03	0.41
1:D:494:THR:O	1:D:498:ILE:HG23	2.22	0.40
1:D:563:LEU:HD23	1:D:563:LEU:HA	1.91	0.40
1:F:299:LEU:HD21	1:F:390:LEU:HD13	2.03	0.40
1:G:82:LEU:HD23	1:G:82:LEU:HA	1.93	0.40
1:C:82:LEU:HD23	1:C:82:LEU:HA	1.92	0.40
1:F:199:TYR:OH	1:F:225:GLU:OE2	2.33	0.40
1:H:336:GLU:OE2	1:H:608:ARG:NH2	2.53	0.40
1:E:124:LEU:HD21	1:E:219:MET:CE	2.51	0.40
1:E:268:ARG:HG2	1:E:269:HIS:CD2	2.56	0.40
1:F:644:ALA:O	1:F:650:ASN:ND2	2.54	0.40
1:G:463:LEU:HD22	1:G:467:VAL:HG13	2.03	0.40
1:H:189:TRP:N	1:H:190:PRO:CD	2.85	0.40
1:H:388:SER:OG	1:H:443:GLN:NE2	2.53	0.40
1:B:623:ARG:HD3	2:B:774:HOH:O	2.20	0.40
1:C:47:ILE:HG12	1:C:90:ILE:HG22	2.04	0.40
1:D:79:LEU:O	1:D:83:THR:HG23	2.22	0.40
1:G:662:LEU:H	1:G:662:LEU:CD1	2.34	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	624/684 (91%)	610 (98%)	13 (2%)	1 (0%)	47 66
1	B	627/684 (92%)	613 (98%)	12 (2%)	2 (0%)	41 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	625/684 (91%)	609 (97%)	14 (2%)	2 (0%)	41	59
1	D	626/684 (92%)	613 (98%)	10 (2%)	3 (0%)	29	46
1	E	627/684 (92%)	614 (98%)	11 (2%)	2 (0%)	41	59
1	F	625/684 (91%)	607 (97%)	15 (2%)	3 (0%)	29	46
1	G	626/684 (92%)	617 (99%)	7 (1%)	2 (0%)	41	59
1	H	626/684 (92%)	609 (97%)	14 (2%)	3 (0%)	29	46
All	All	5006/5472 (92%)	4892 (98%)	96 (2%)	18 (0%)	34	52

All (18) 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	D	488	ILE
1	E	189	TRP
1	E	488	ILE
1	F	160	LEU
1	F	189	TRP
1	F	478	SER
1	G	189	TRP
1	G	662	LEU
1	H	189	TRP
1	C	662	LEU
1	D	437	ASN
1	H	487	GLY
1	B	368	VAL
1	H	486	GLY

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	534/579 (92%)	516 (97%)	18 (3%)	37	61
1	B	534/579 (92%)	521 (98%)	13 (2%)	49	72
1	C	532/579 (92%)	518 (97%)	14 (3%)	46	70
1	D	534/579 (92%)	518 (97%)	16 (3%)	41	65
1	E	533/579 (92%)	520 (98%)	13 (2%)	49	72
1	F	534/579 (92%)	519 (97%)	15 (3%)	43	67
1	G	533/579 (92%)	517 (97%)	16 (3%)	41	65
1	H	534/579 (92%)	520 (97%)	14 (3%)	46	70
All	All	4268/4632 (92%)	4149 (97%)	119 (3%)	43	67

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	MET
1	A	42	ARG
1	A	61	MET
1	A	135	LYS
1	A	158	THR
1	A	280	LYS
1	A	298	MET
1	A	299	LEU
1	A	339	THR
1	A	365	TYR
1	A	439	VAL
1	A	467	VAL
1	A	482	ARG
1	A	520	ARG
1	A	547	PHE
1	A	608	ARG
1	A	662	LEU
1	A	663	LYS
1	B	56	GLU
1	B	299	LEU
1	B	339	THR
1	B	361	THR
1	B	382	ASP
1	B	436	GLU
1	B	438	MET
1	B	467	VAL
1	B	483	VAL

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Mol	Chain	Res	Type
1	B	520	ARG
1	B	547	PHE
1	B	608	ARG
1	B	654	VAL
1	C	61	MET
1	C	154	MET
1	C	280	LYS
1	C	299	LEU
1	C	361	THR
1	C	367	ARG
1	C	443	GLN
1	C	473	ARG
1	C	520	ARG
1	C	547	PHE
1	C	605	GLN
1	C	608	ARG
1	C	649	LEU
1	C	662	LEU
1	D	39	MET
1	D	61	MET
1	D	135	LYS
1	D	268	ARG
1	D	280	LYS
1	D	299	LEU
1	D	339	THR
1	D	364	LEU
1	D	367	ARG
1	D	382	ASP
1	D	467	VAL
1	D	488	ILE
1	D	520	ARG
1	D	547	PHE
1	D	608	ARG
1	D	638	GLU
1	E	40	ARG
1	E	299	LEU
1	E	339	THR
1	E	363	LYS
1	E	364	LEU
1	E	365	TYR
1	E	383	LEU
1	E	436	GLU

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Mol	Chain	Res	Type
1	E	467	VAL
1	E	483	VAL
1	E	520	ARG
1	E	547	PHE
1	E	608	ARG
1	F	39	MET
1	F	226	LYS
1	F	339	THR
1	F	367	ARG
1	F	383	LEU
1	F	391	LYS
1	F	477	THR
1	F	485	ASN
1	F	488	ILE
1	F	520	ARG
1	F	547	PHE
1	F	608	ARG
1	F	649	LEU
1	F	654	VAL
1	F	663	LYS
1	G	2	VAL
1	G	135	LYS
1	G	159	ASN
1	G	299	LEU
1	G	322	GLN
1	G	339	THR
1	G	367	ARG
1	G	436	GLU
1	G	443	GLN
1	G	467	VAL
1	G	482	ARG
1	G	520	ARG
1	G	547	PHE
1	G	608	ARG
1	G	638	GLU
1	G	662	LEU
1	H	61	MET
1	H	227	THR
1	H	280	LYS
1	H	299	LEU
1	H	339	THR
1	H	365	TYR

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Mol	Chain	Res	Type
1	H	368	VAL
1	H	391	LYS
1	H	436	GLU
1	H	520	ARG
1	H	547	PHE
1	H	608	ARG
1	H	654	VAL
1	H	662	LEU

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	228	HIS
1	D	159	ASN
1	D	162	ASN
1	F	322	GLN
1	G	443	GLN
1	H	269	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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

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	634/684 (92%)	0.22	27 (4%) 35 37	18, 30, 55, 71	0
1	B	635/684 (92%)	0.06	15 (2%) 59 61	15, 26, 46, 67	0
1	C	633/684 (92%)	0.09	20 (3%) 47 50	15, 26, 43, 63	0
1	D	634/684 (92%)	-0.04	9 (1%) 75 77	12, 22, 41, 64	0
1	E	635/684 (92%)	0.09	16 (2%) 57 59	14, 26, 46, 65	0
1	F	633/684 (92%)	0.34	41 (6%) 18 18	18, 30, 58, 71	0
1	G	634/684 (92%)	0.02	20 (3%) 47 50	13, 23, 44, 69	0
1	H	634/684 (92%)	0.07	16 (2%) 57 59	15, 27, 45, 81	0
All	All	5072/5472 (92%)	0.10	164 (3%) 47 50	12, 26, 48, 81	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	VAL	7.7
1	F	486	GLY	7.4
1	F	485	ASN	6.1
1	B	435	GLY	6.0
1	H	368	VAL	5.5
1	C	486	GLY	5.4
1	F	159	ASN	5.4
1	F	484	PRO	5.3
1	H	486	GLY	5.2
1	H	382	ASP	5.2
1	C	382	ASP	4.9
1	H	369	LEU	4.6
1	C	365	TYR	4.6
1	C	364	LEU	4.6
1	H	483	VAL	4.6
1	G	485	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	484	PRO	4.2
1	G	482	ARG	4.1
1	B	487	GLY	4.0
1	F	367	ARG	4.0
1	F	483	VAL	4.0
1	C	437	ASN	4.0
1	B	486	GLY	3.9
1	A	486	GLY	3.6
1	E	365	TYR	3.6
1	B	652	THR	3.6
1	E	134	ALA	3.6
1	F	84	GLN	3.6
1	H	365	TYR	3.6
1	F	142	ARG	3.5
1	D	487	GLY	3.5
1	D	281	PRO	3.5
1	F	39	MET	3.5
1	A	369	LEU	3.5
1	H	381	ALA	3.4
1	B	368	VAL	3.4
1	A	662	LEU	3.4
1	A	484	PRO	3.3
1	C	367	ARG	3.3
1	H	366	GLU	3.3
1	G	483	VAL	3.3
1	C	383	LEU	3.3
1	A	437	ASN	3.2
1	D	367	ARG	3.2
1	E	487	GLY	3.2
1	G	368	VAL	3.1
1	H	367	ARG	3.1
1	H	485	ASN	3.1
1	A	263	THR	3.1
1	A	39	MET	3.0
1	G	471	GLY	3.0
1	H	437	ASN	3.0
1	E	281	PRO	3.0
1	C	369	LEU	3.0
1	C	485	ASN	3.0
1	F	368	VAL	2.9
1	F	281	PRO	2.9
1	A	138	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	169	TYR	2.9
1	A	382	ASP	2.9
1	F	232	PRO	2.9
1	E	383	LEU	2.9
1	F	270	THR	2.9
1	B	365	TYR	2.9
1	F	169	TYR	2.8
1	A	281	PRO	2.8
1	B	382	ASP	2.8
1	F	382	ASP	2.8
1	A	485	ASN	2.8
1	F	487	GLY	2.8
1	E	84	GLN	2.8
1	B	281	PRO	2.8
1	A	366	GLU	2.7
1	C	483	VAL	2.7
1	D	366	GLU	2.7
1	E	138	ILE	2.7
1	C	39	MET	2.7
1	C	484	PRO	2.7
1	F	383	LEU	2.7
1	F	129	SER	2.6
1	G	367	ARG	2.6
1	F	279	ILE	2.6
1	F	174	GLN	2.6
1	F	128	ALA	2.6
1	F	366	GLU	2.6
1	A	552	ASN	2.6
1	E	517	GLY	2.6
1	F	10	GLU	2.6
1	F	130	ASP	2.5
1	E	367	ARG	2.5
1	F	226	LYS	2.5
1	F	263	THR	2.5
1	A	2	VAL	2.5
1	E	368	VAL	2.5
1	D	465	PRO	2.5
1	C	36	GLY	2.4
1	G	159	ASN	2.4
1	H	281	PRO	2.4
1	H	484	PRO	2.4
1	E	666	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	458	GLY	2.4
1	F	124	LEU	2.4
1	A	273	GLU	2.4
1	A	275	ASP	2.4
1	G	486	GLY	2.4
1	B	439	VAL	2.4
1	C	2	VAL	2.4
1	E	437	ASN	2.3
1	F	138	ILE	2.3
1	A	365	TYR	2.3
1	F	199	TYR	2.3
1	F	439	VAL	2.3
1	B	662	LEU	2.3
1	D	382	ASP	2.3
1	C	473	ARG	2.3
1	F	208	ILE	2.3
1	F	276	GLY	2.3
1	B	667	GLU	2.3
1	F	272	VAL	2.3
1	H	555	GLY	2.3
1	F	213	PHE	2.3
1	B	367	ARG	2.2
1	F	482	ARG	2.2
1	G	364	LEU	2.2
1	F	437	ASN	2.2
1	H	429	GLY	2.2
1	B	664	PRO	2.2
1	B	84	GLN	2.2
1	G	365	TYR	2.2
1	A	364	LEU	2.2
1	A	272	VAL	2.2
1	A	87	SER	2.2
1	C	439	VAL	2.2
1	E	667	GLU	2.2
1	F	369	LEU	2.2
1	G	369	LEU	2.2
1	F	364	LEU	2.2
1	F	280	LYS	2.1
1	G	668	LYS	2.1
1	A	557	ILE	2.1
1	E	662	LEU	2.1
1	G	461	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	94	ASP	2.1
1	E	659	ASP	2.1
1	C	552	ASN	2.1
1	D	2	VAL	2.1
1	A	90	ILE	2.1
1	A	482	ARG	2.1
1	C	482	ARG	2.1
1	E	485	ASN	2.1
1	F	90	ILE	2.1
1	F	275	ASP	2.1
1	B	369	LEU	2.1
1	H	363	LYS	2.1
1	G	158	THR	2.1
1	C	368	VAL	2.0
1	G	2	VAL	2.0
1	D	461	SER	2.0
1	G	457	SER	2.0
1	G	516	ASN	2.0
1	G	281	PRO	2.0
1	C	381	ALA	2.0
1	A	227	THR	2.0
1	D	485	ASN	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 monosaccharides 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.