



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:07 am GMT

PDB ID : 3AX9
Title : Bovine xanthine oxidase, protease cleaved form
Authors : Ishikita, H.; Eger, B.T.; Pai, E.F.; Okamoto, K.; Nishino, T.
Deposited on : 2011-03-31
Resolution : 2.30 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28683
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

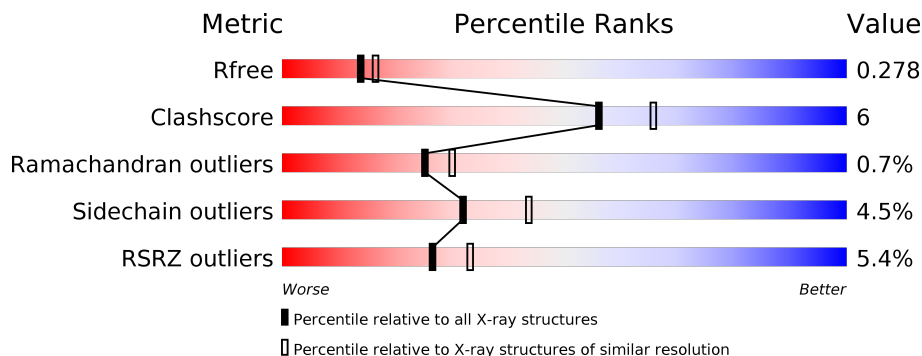
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1332	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>8%</div> </div> </div>
1	B	1332	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	A	1338	-	-	-	X
7	GOL	B	1338	-	-	-	X
8	SAL	A	1341	-	-	-	X
8	SAL	B	1340	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 19797 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.

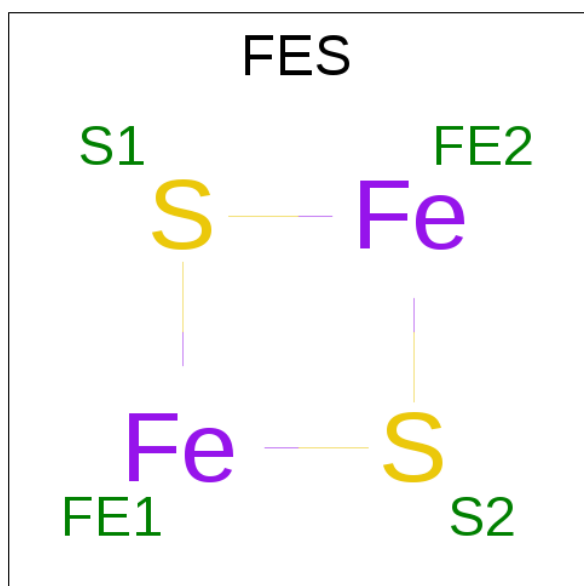
- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1225	Total	C	N	O	S	0	0	0
			9476	6013	1632	1771	60			
1	B	1218	Total	C	N	O	S	0	0	0
			9433	5988	1623	1763	59			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	HIS	ASP	CONFLICT	UNP P80457
B	552	HIS	ASP	CONFLICT	UNP P80457

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



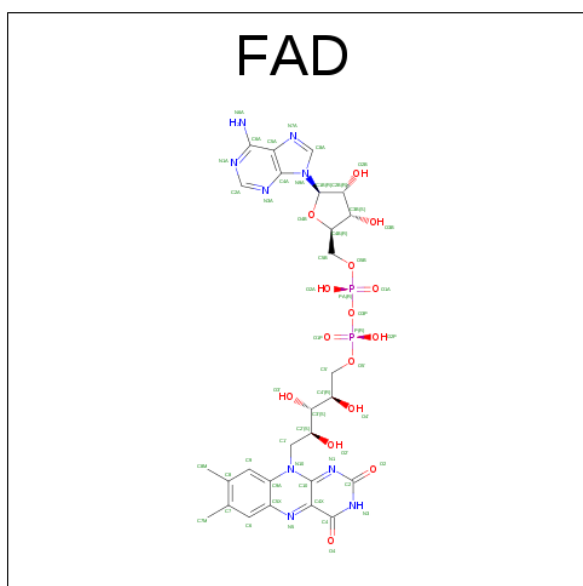
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		

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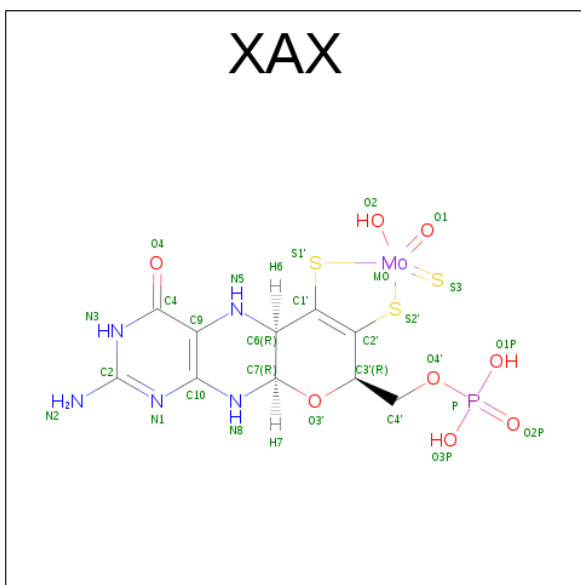
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is {[(5AR,8R,9AR)-2-AMINO-4-OXO-6,7-DI(SULFANYL-KAPPAS)-3,5,5A,8,9A,10-HEXAHYDRO-4H-PYRANO[3,2-G]PTERIDIN-8-YL] METHYL DIHYDROGENATO(2-) PHOSPHATE}(HYDROXY)OXO(THIOXO)MOLYBDENUM (three-letter code: XAX) (formula: $C_{10}H_{13}MoN_5O_8PS_3$).

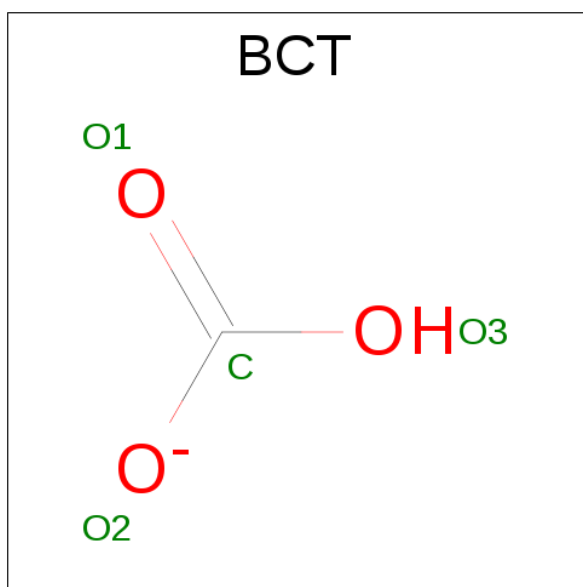


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
4	B	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

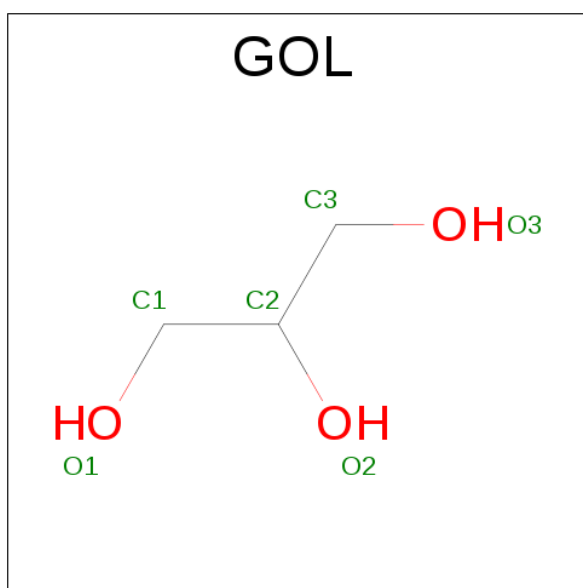
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		
6	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



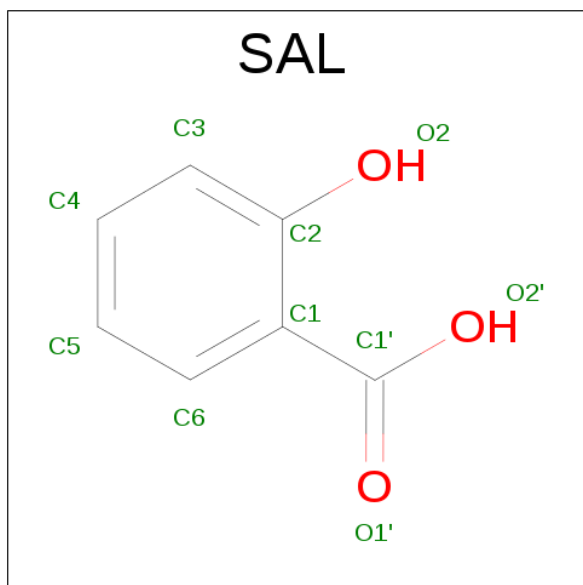
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

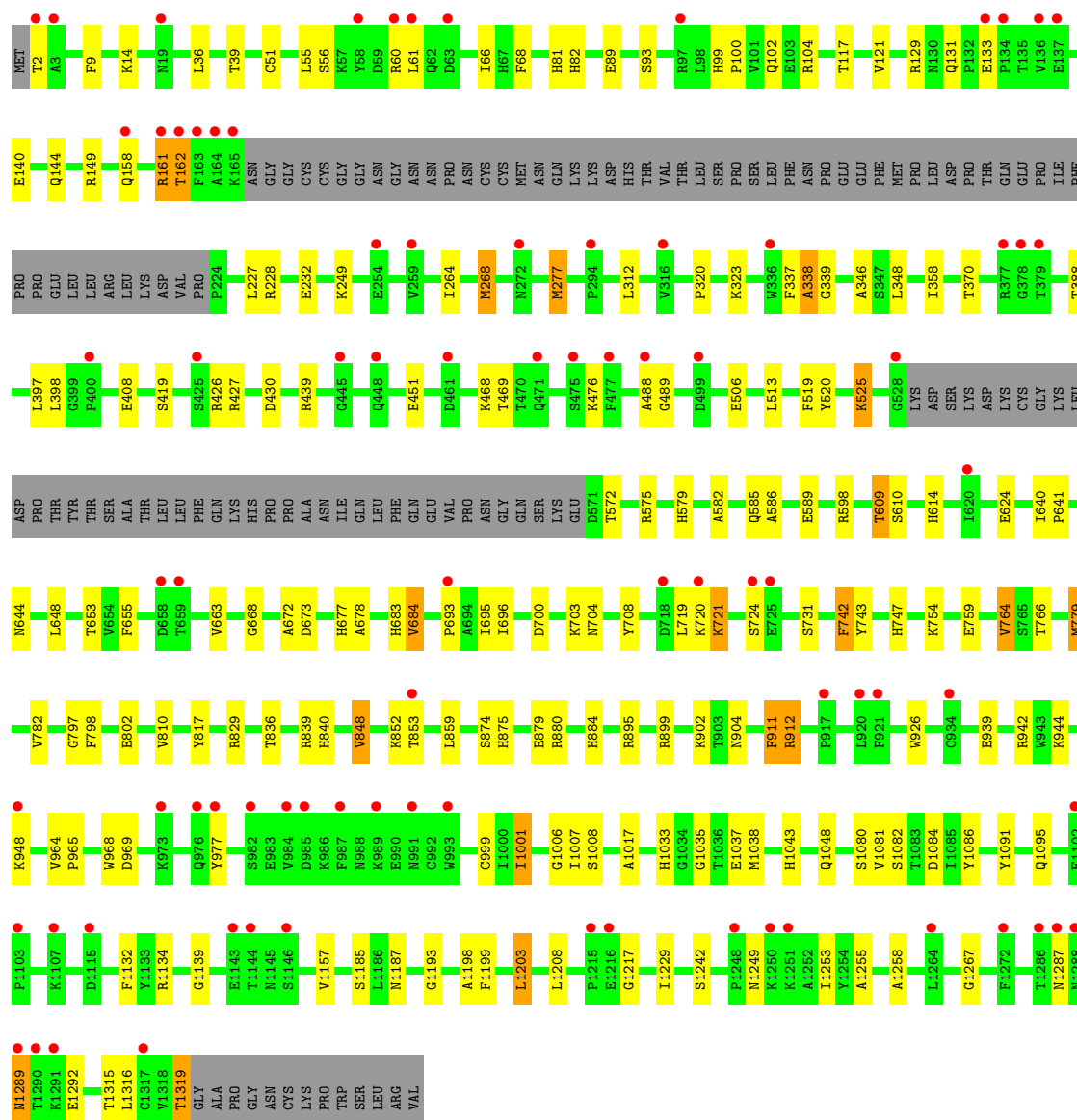
- Molecule 8 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: $C_7H_6O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	7	3		
8	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	367	Total	O	0	0
			367	367		
9	B	283	Total	O	0	0
			283	283		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.20Å 72.97Å 142.26Å 90.00° 98.84° 90.00°	Depositor
Resolution (Å)	38.13 – 2.30 38.14 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.13-2.30) 99.3 (38.14-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.215 , 0.279 0.216 , 0.278	Depositor DCC
R_{free} test set	5953 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.1	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	19797	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XAX, GOL, SAL, CA, FES, BCT, FAD

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	0.71	0/9675	0.75	3/13085 (0.0%)
1	B	0.67	0/9631	0.73	6/13026 (0.0%)
All	All	0.69	0/19306	0.74	9/26111 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	839	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	B	839	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	513	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	398	LEU	CA-CB-CG	5.65	128.29	115.30
1	B	1203	LEU	CA-CB-CG	5.54	128.05	115.30
1	B	398	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	942	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	1325	CYS	N-CA-C	5.05	124.63	111.00
1	A	942	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	9476	0	9483	112	0
1	B	9433	0	9440	113	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	53	0	31	1	0
3	B	53	0	31	2	0
4	A	28	0	10	1	0
4	B	28	0	10	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	18	0	24	1	0
7	B	12	0	16	0	0
8	A	10	0	5	0	0
8	B	10	0	4	1	0
9	A	367	0	0	5	0
9	B	283	0	0	5	0
All	All	19797	0	19054	222	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 6.

All (222) 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:884:HIS:HE1	1:A:1006:GLY:H	1.17	0.92
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	1.68	0.92
1:A:995:LYS:HZ1	1:A:1284:GLN:HE21	1.20	0.89
1:A:131:GLN:HE21	1:A:133:GLU:H	1.18	0.89
1:A:695:ILE:H	1:A:904:ASN:HD22	1.21	0.88
1:B:884:HIS:HE1	1:B:1006:GLY:H	1.25	0.84
1:B:720:LYS:O	1:B:721:LYS:HB2	1.77	0.84
1:B:764:VAL:HG22	1:B:766:THR:HG22	1.66	0.76
1:B:764:VAL:CG2	1:B:766:THR:HG22	2.16	0.76
1:A:995:LYS:HZ1	1:A:1284:GLN:NE2	1.84	0.74
1:A:131:GLN:NE2	1:A:133:GLU:H	1.83	0.74
1:B:36:LEU:HD22	1:B:89:GLU:HG3	1.69	0.74
1:A:571:ASP:N	9:A:1440:HOH:O	2.20	0.73
1:B:884:HIS:CE1	1:B:1006:GLY:H	2.05	0.73
1:A:131:GLN:HE21	1:A:133:GLU:N	1.88	0.71
1:A:673:ASP:OD2	1:A:677:HIS:HD2	1.74	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:ILE:H	1:B:904:ASN:HD22	1.39	0.71
1:A:601:ASN:O	1:A:821:HIS:HD2	1.74	0.71
1:B:939:GLU:HG2	1:B:977:TYR:CE2	2.27	0.70
1:B:609:THR:HG22	9:B:1398:HOH:O	1.92	0.69
1:A:427:ARG:O	1:A:427:ARG:HG2	1.94	0.68
1:A:1143:GLU:H	1:A:1143:GLU:CD	1.96	0.68
1:A:1033:HIS:CD2	1:A:1035:GLY:H	2.11	0.68
1:A:1033:HIS:HD2	1:A:1035:GLY:H	1.41	0.67
1:A:995:LYS:NZ	1:A:1284:GLN:NE2	2.41	0.66
1:A:1287:ASN:ND2	1:A:1289:ASN:H	1.94	0.65
1:B:853:THR:HG23	1:B:944:LYS:NZ	2.11	0.65
1:A:1324:ASN:ND2	1:A:1324:ASN:N	2.44	0.65
1:B:610:SER:O	1:B:663:VAL:O	2.14	0.64
1:B:60:ARG:HB3	1:B:60:ARG:HH11	1.63	0.64
1:B:1249:ASN:O	1:B:1255:ALA:HA	1.98	0.64
1:A:58:TYR:HD1	1:A:65:ILE:HG13	1.62	0.63
1:A:884:HIS:CE1	1:A:1006:GLY:H	2.08	0.62
1:B:427:ARG:O	1:B:427:ARG:HG2	1.97	0.62
1:A:880:ARG:O	1:A:884:HIS:HD2	1.80	0.62
1:B:640:ILE:HG12	1:B:779:MET:HE1	1.82	0.62
1:B:880:ARG:O	1:B:884:HIS:HD2	1.82	0.62
1:B:1048:GLN:HE22	1:B:1187:ASN:HD22	1.48	0.61
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.35	0.61
1:B:673:ASP:OD2	1:B:677:HIS:HD2	1.84	0.61
1:A:623:SER:HA	1:A:626:GLN:HE21	1.66	0.60
1:A:850:PHE:CD1	1:A:930:VAL:HG13	2.37	0.60
1:A:61:LEU:O	1:A:62:GLN:HB3	2.01	0.60
1:B:232:GLU:OE1	1:B:677:HIS:HE1	1.85	0.60
1:A:765:SER:O	1:A:801:LYS:HD3	2.02	0.60
1:A:1287:ASN:HD22	1:A:1287:ASN:C	2.05	0.59
1:A:1324:ASN:HD22	1:A:1324:ASN:H	1.49	0.59
1:A:439:ARG:NH2	1:A:451:GLU:OE1	2.35	0.59
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.38	0.58
1:A:695:ILE:H	1:A:904:ASN:ND2	1.96	0.58
1:B:488:ALA:HA	1:B:1319:THR:OG1	2.03	0.58
1:A:1207:THR:OG1	1:A:1208:LEU:HD13	2.03	0.57
1:B:1185:SER:HA	9:B:1486:HOH:O	2.03	0.57
1:A:1324:ASN:O	1:A:1325:CYS:HB3	2.02	0.57
1:A:1325:CYS:O	1:A:1326:LYS:C	2.42	0.57
1:B:572:THR:HA	1:B:575:ARG:HD3	1.85	0.57
1:A:1088:GLN:HG2	1:A:1133:TYR:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ILE:O	1:B:268:MET:HG2	2.05	0.56
1:B:853:THR:HG23	1:B:944:LYS:HZ3	1.70	0.56
1:A:964:VAL:HG23	1:A:1155:TYR:CD2	2.41	0.55
1:A:826:MET:HB3	7:A:1338:GOL:H32	1.87	0.55
1:B:346:ALA:HB1	3:B:1335:FAD:H4'	1.87	0.55
1:A:1324:ASN:HD22	1:A:1324:ASN:N	2.02	0.55
1:B:579:HIS:HB3	1:B:582:ALA:HB2	1.88	0.54
1:B:614:HIS:HD2	1:B:693:PRO:O	1.90	0.54
1:B:848:VAL:HG21	1:B:926:TRP:HB2	1.89	0.54
1:A:1172:LYS:HG3	9:A:1696:HOH:O	2.08	0.53
1:B:655:PHE:CD2	1:B:668:GLY:HA2	2.43	0.53
1:B:721:LYS:HA	1:B:724:SER:HB2	1.89	0.53
1:A:1105:LYS:HE2	1:A:1116:TRP:CZ3	2.43	0.53
1:B:1315:THR:O	1:B:1316:LEU:HB2	2.08	0.53
1:A:58:TYR:CD1	1:A:65:ILE:HG13	2.44	0.53
1:A:601:ASN:O	1:A:821:HIS:CD2	2.58	0.53
1:A:720:LYS:O	1:A:721:LYS:HB2	2.10	0.52
1:A:134:PRO:O	1:A:164:ALA:HA	2.09	0.52
1:B:764:VAL:CG2	1:B:766:THR:CG2	2.86	0.52
1:A:1126:SER:HB2	1:B:1132:PHE:CD1	2.44	0.52
1:A:1203:LEU:C	1:A:1203:LEU:HD12	2.29	0.52
1:A:1159:CYS:O	1:A:1176:THR:HA	2.09	0.52
1:B:1033:HIS:HD2	1:B:1035:GLY:H	1.58	0.52
1:B:144:GLN:HB3	1:B:339:GLY:HA2	1.92	0.52
1:B:840:HIS:HE1	1:B:874:SER:OG	1.93	0.52
1:B:469:THR:HG23	1:B:489:GLY:HA3	1.92	0.51
1:A:644:ASN:HB2	9:A:1687:HOH:O	2.10	0.51
1:A:609:THR:HG23	1:A:664:GLY:HA2	1.92	0.51
1:A:779:MET:HG2	1:A:810:VAL:HG13	1.93	0.50
1:B:131:GLN:HE21	1:B:133:GLU:H	1.59	0.50
1:A:471:GLN:NE2	1:A:474:LEU:CD1	2.73	0.50
1:A:62:GLN:O	1:A:62:GLN:NE2	2.35	0.50
1:B:624:GLU:HB3	1:B:684:VAL:HG13	1.94	0.50
1:B:1038:MET:HG3	4:B:3003:XAX:C4	2.41	0.50
1:B:884:HIS:HE1	1:B:1006:GLY:N	2.02	0.50
1:B:911:PHE:HD2	1:B:912:ARG:N	2.09	0.50
1:A:1324:ASN:O	1:A:1325:CYS:CB	2.60	0.50
1:B:848:VAL:HG13	1:B:859:LEU:HD13	1.92	0.50
1:A:1088:GLN:CG	1:A:1133:TYR:CD1	2.95	0.50
1:A:1287:ASN:HD22	1:A:1288:ASN:N	2.09	0.50
1:B:149:ARG:HD3	1:B:1229:ILE:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:802:GLU:OE1	8:B:1340:SAL:H4	2.11	0.49
1:B:439:ARG:NH2	1:B:451:GLU:OE1	2.45	0.49
1:B:93:SER:HB2	1:B:589:GLU:OE1	2.13	0.49
1:A:848:VAL:HG21	1:A:926:TRP:HB2	1.95	0.49
1:B:696:ILE:HD12	1:B:1217:GLY:HA3	1.94	0.49
1:B:875:HIS:HD2	1:B:879:GLU:OE2	1.94	0.49
1:A:1048:GLN:HE22	1:A:1187:ASN:HD22	1.59	0.48
1:B:55:LEU:HD12	1:B:68:PHE:CE1	2.48	0.48
1:A:747:HIS:HD1	1:A:805:SER:HA	1.76	0.48
1:A:727:ASP:HB3	1:A:852:LYS:HD2	1.94	0.48
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.14	0.47
1:A:1315:THR:O	1:A:1316:LEU:HB2	2.15	0.47
1:A:27:LEU:HD13	1:A:39:THR:HG22	1.95	0.47
1:A:320:PRO:HG2	1:A:323:LYS:HG3	1.94	0.47
1:A:338:ALA:HB2	3:A:1335:FAD:C6	2.44	0.47
1:A:348:LEU:HD13	1:A:407:ILE:HD13	1.96	0.47
1:A:696:ILE:HD12	1:A:1217:GLY:HA3	1.96	0.47
1:A:1017:ALA:HB2	1:A:1085:ILE:HD12	1.96	0.47
1:B:1081:VAL:O	1:B:1084:ASP:HB2	2.13	0.47
1:A:1080:SER:HB3	1:A:1258:ALA:HB1	1.96	0.47
1:B:39:THR:HG22	1:B:51:CYS:HA	1.97	0.47
1:A:1326:LYS:CG	1:A:1326:LYS:O	2.63	0.47
1:A:353:ILE:HG22	1:A:353:ILE:O	2.15	0.47
1:A:612:ARG:HG3	1:A:689:TYR:CG	2.49	0.46
1:B:358:ILE:CD1	1:B:430:ASP:HA	2.45	0.46
1:A:1324:ASN:ND2	9:A:1632:HOH:O	2.48	0.46
1:B:1289:ASN:HB2	1:B:1292:GLU:HB2	1.97	0.46
1:B:419:SER:HB2	1:B:519:PHE:CD1	2.51	0.46
1:B:964:VAL:N	1:B:965:PRO:HD2	2.31	0.46
1:A:1191:ASP:O	1:A:1195:VAL:HG23	2.15	0.46
1:B:358:ILE:HD11	1:B:430:ASP:HA	1.98	0.46
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.51	0.45
1:B:641:PRO:HG3	1:B:817:TYR:CE2	2.51	0.45
1:A:1037:GLU:HB2	1:A:1043:HIS:CD2	2.52	0.45
1:A:808:VAL:O	1:A:812:VAL:HG23	2.17	0.45
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.80	0.45
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.52	0.45
1:B:912:ARG:NH2	1:B:1198:ALA:HB2	2.32	0.45
1:A:56:SER:HB2	1:A:84:ALA:HB3	1.99	0.45
1:B:320:PRO:HD2	1:B:323:LYS:HD3	1.99	0.45
1:A:2:THR:CG2	1:A:230:GLU:OE2	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:CD1	1:A:39:THR:HG22	2.47	0.44
1:A:487:CYS:HB3	1:A:513:LEU:HD13	1.99	0.44
1:B:1289:ASN:H	1:B:1289:ASN:HD22	1.65	0.44
1:B:81:HIS:CD2	1:B:227:LEU:HD11	2.52	0.44
1:A:255:ALA:CB	1:A:277:MET:HG2	2.46	0.44
1:B:640:ILE:HA	1:B:641:PRO:HD3	1.85	0.44
1:B:655:PHE:CE2	1:B:668:GLY:HA2	2.52	0.44
1:A:614:HIS:HD2	1:A:693:PRO:O	2.00	0.44
1:A:1097:ILE:CD1	1:A:1129:THR:HG22	2.47	0.44
1:A:131:GLN:HE21	1:A:133:GLU:C	2.21	0.44
1:A:967:CYS:HB3	1:A:1157:VAL:HG23	2.00	0.44
1:A:471:GLN:NE2	1:A:474:LEU:HD12	2.33	0.44
1:B:1082:SER:HB2	4:B:3003:XAX:O3P	2.17	0.44
1:B:779:MET:HG2	1:B:810:VAL:HG13	2.00	0.44
1:A:507:PHE:CD1	1:A:1303:GLU:HA	2.53	0.44
1:A:695:ILE:HG23	1:A:700:ASP:HB3	2.00	0.43
1:A:143:PHE:HB3	1:A:1232:PHE:CE1	2.53	0.43
1:B:911:PHE:O	1:B:912:ARG:C	2.57	0.43
1:A:427:ARG:HD3	1:A:1212:HIS:CD2	2.53	0.43
1:B:1080:SER:O	1:B:1258:ALA:HB1	2.18	0.43
1:B:1007:ILE:HD12	1:B:1258:ALA:HB3	2.00	0.43
1:B:388:THR:O	1:B:397:LEU:HD13	2.18	0.43
1:B:700:ASP:O	1:B:704:ASN:ND2	2.50	0.43
1:A:150:CYS:O	1:A:1197:GLY:HA3	2.19	0.42
1:A:1152:TYR:HB3	1:A:1251:LYS:HG3	2.01	0.42
1:B:370:THR:HG23	1:B:408:GLU:O	2.19	0.42
1:B:104:ARG:HD2	1:B:104:ARG:HA	1.89	0.42
1:B:277:MET:HA	1:B:277:MET:HE3	2.01	0.42
1:A:427:ARG:NH1	1:A:504:MET:HG3	2.35	0.42
1:A:948:LYS:HB3	1:A:948:LYS:HE2	1.84	0.42
1:B:912:ARG:CZ	1:B:1198:ALA:HB2	2.50	0.42
1:B:9:PHE:CE2	1:B:14:LYS:HB2	2.54	0.42
1:B:999:CYS:SG	1:B:1001:ILE:HD12	2.58	0.42
1:B:338:ALA:HB2	3:B:1335:FAD:C6	2.50	0.42
1:B:2:THR:O	1:B:228:ARG:HD3	2.20	0.42
1:B:232:GLU:OE1	1:B:677:HIS:CE1	2.70	0.42
1:B:672:ALA:HB3	1:B:678:ALA:HB2	2.01	0.42
1:B:683:HIS:HB2	9:B:1620:HOH:O	2.20	0.42
1:A:911:PHE:O	1:A:912:ARG:C	2.56	0.42
1:B:875:HIS:CD2	1:B:879:GLU:OE2	2.72	0.42
1:A:975:SER:HB2	1:A:980:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:GLU:CD	1:A:1143:GLU:N	2.68	0.42
1:A:600:GLU:CD	1:B:598:ARG:HG2	2.41	0.42
1:B:60:ARG:HB3	1:B:60:ARG:NH1	2.32	0.42
1:B:880:ARG:O	1:B:884:HIS:CD2	2.69	0.42
1:A:1082:SER:HB2	4:A:3003:XAX:O3P	2.21	0.41
1:A:721:LYS:O	1:A:724:SER:HB2	2.20	0.41
1:B:798:PHE:HA	4:B:3003:XAX:HN5	1.84	0.41
1:B:721:LYS:CA	1:B:724:SER:HB2	2.50	0.41
1:B:1091:TYR:O	1:B:1095:GLN:HG2	2.19	0.41
1:B:525:LYS:HA	1:B:525:LYS:HD2	1.86	0.41
1:B:104:ARG:CZ	1:B:162:THR:HG21	2.51	0.41
1:B:1289:ASN:H	1:B:1289:ASN:ND2	2.19	0.41
1:A:779:MET:HE1	1:A:814:LEU:HD13	2.01	0.41
1:A:471:GLN:HE21	1:A:474:LEU:HD12	1.85	0.41
1:A:55:LEU:HD12	1:A:68:PHE:CE1	2.55	0.41
1:A:641:PRO:HG3	1:A:817:TYR:CE2	2.56	0.41
1:B:585:GLN:NE2	9:B:1412:HOH:O	2.53	0.41
1:A:1287:ASN:HD22	1:A:1289:ASN:H	1.65	0.41
1:B:853:THR:HG23	1:B:944:LYS:HZ2	1.81	0.41
1:A:1173:ASN:O	1:A:1236:PRO:HA	2.20	0.41
1:B:968:TRP:HA	1:B:1157:VAL:HG11	2.03	0.41
1:B:102:GLN:HG2	1:B:586:ALA:O	2.21	0.41
1:B:644:ASN:O	1:B:653:THR:HA	2.21	0.41
1:A:1062:TYR:OH	1:B:759:GLU:OE2	2.28	0.41
1:A:1183:GLY:HA2	1:A:1247:CYS:O	2.21	0.41
1:B:1199:PHE:CE1	1:B:1267:GLY:HA2	2.55	0.41
1:B:117:THR:O	1:B:121:VAL:HG23	2.21	0.41
1:B:708:TYR:CE2	1:B:902:LYS:HD2	2.56	0.41
1:B:754:LYS:HB2	1:B:759:GLU:HB2	2.02	0.40
1:A:390:PHE:HB3	9:A:1630:HOH:O	2.21	0.40
1:A:415:ASP:OD2	1:A:444:PRO:HA	2.20	0.40
1:A:418:PHE:HA	1:A:438:MET:O	2.21	0.40
1:B:99:HIS:CG	1:B:100:PRO:HD2	2.57	0.40
1:B:1080:SER:HB3	1:B:1258:ALA:HB1	2.03	0.40
1:A:1118:MET:O	1:A:1122:GLN:HG3	2.20	0.40
1:B:1193:GLY:HA2	9:B:1505:HOH:O	2.20	0.40
1:B:56:SER:HA	1:B:66:ILE:O	2.21	0.40
1:B:683:HIS:O	1:B:683:HIS:CG	2.74	0.40
1:B:742:PHE:HA	1:B:829:ARG:NH2	2.37	0.40
1:A:1287:ASN:C	1:A:1287:ASN:ND2	2.72	0.40
1:B:131:GLN:HE21	1:B:133:GLU:C	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:GLN:O	1:B:161:ARG:HB2	2.21	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	1219/1332 (92%)	1162 (95%)	46 (4%)	11 (1%)	20	23
1	B	1212/1332 (91%)	1147 (95%)	58 (5%)	7 (1%)	28	34
All	All	2431/2664 (91%)	2309 (95%)	104 (4%)	18 (1%)	25	30

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1325	CYS
1	A	335	ARG
1	A	721	LYS
1	A	912	ARG
1	A	1008	SER
1	B	721	LYS
1	B	1008	SER
1	A	527	LEU
1	A	797	GLY
1	B	912	ARG
1	B	1139	GLY
1	A	43	CYS
1	A	62	GLN
1	B	338	ALA
1	B	797	GLY
1	B	520	TYR
1	A	1139	GLY

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Mol	Chain	Res	Type
1	A	1253	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	1030/1128 (91%)	982 (95%)	48 (5%)	30	41
1	B	1026/1128 (91%)	982 (96%)	44 (4%)	33	45
All	All	2056/2256 (91%)	1964 (96%)	92 (4%)	32	44

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	63	ASP
1	A	93	SER
1	A	103	GLU
1	A	113	CYS
1	A	140	GLU
1	A	161	ARG
1	A	165	LYS
1	A	243	LYS
1	A	271	LYS
1	A	312	LEU
1	A	335	ARG
1	A	337	PHE
1	A	348	LEU
1	A	358	ILE
1	A	371	LYS
1	A	375	VAL
1	A	398	LEU
1	A	401	GLU
1	A	426	ARG
1	A	433	LYS
1	A	501	PRO

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Mol	Chain	Res	Type
1	A	513	LEU
1	A	525	LYS
1	A	609	THR
1	A	657	LYS
1	A	680	ARG
1	A	684	VAL
1	A	719	LEU
1	A	742	PHE
1	A	743	TYR
1	A	764	VAL
1	A	779	MET
1	A	782	VAL
1	A	818	LYS
1	A	848	VAL
1	A	852	LYS
1	A	853	THR
1	A	911	PHE
1	A	939	GLU
1	A	948	LYS
1	A	1001	ILE
1	A	1134	ARG
1	A	1203	LEU
1	A	1220	HIS
1	A	1287	ASN
1	A	1290	THR
1	A	1324	ASN
1	B	61	LEU
1	B	82	HIS
1	B	129	ARG
1	B	140	GLU
1	B	161	ARG
1	B	162	THR
1	B	249	LYS
1	B	268	MET
1	B	277	MET
1	B	312	LEU
1	B	337	PHE
1	B	348	LEU
1	B	426	ARG
1	B	468	LYS
1	B	476	LYS
1	B	506	GLU

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Mol	Chain	Res	Type
1	B	525	LYS
1	B	609	THR
1	B	648	LEU
1	B	684	VAL
1	B	703	LYS
1	B	719	LEU
1	B	731	SER
1	B	742	PHE
1	B	743	TYR
1	B	764	VAL
1	B	779	MET
1	B	782	VAL
1	B	848	VAL
1	B	852	LYS
1	B	895	ARG
1	B	899	ARG
1	B	911	PHE
1	B	948	LYS
1	B	969	ASP
1	B	1001	ILE
1	B	1134	ARG
1	B	1203	LEU
1	B	1208	LEU
1	B	1242	SER
1	B	1253	ILE
1	B	1287	ASN
1	B	1289	ASN
1	B	1319	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	146	ASN
1	A	471	GLN
1	A	614	HIS
1	A	626	GLN
1	A	677	HIS
1	A	821	HIS
1	A	840	HIS
1	A	884	HIS
1	A	904	ASN

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Mol	Chain	Res	Type
1	A	1016	GLN
1	A	1033	HIS
1	A	1048	GLN
1	A	1137	ASN
1	A	1212	HIS
1	A	1284	GLN
1	A	1287	ASN
1	A	1324	ASN
1	B	131	GLN
1	B	144	GLN
1	B	146	ASN
1	B	473	GLN
1	B	614	HIS
1	B	677	HIS
1	B	705	ASN
1	B	821	HIS
1	B	840	HIS
1	B	875	HIS
1	B	884	HIS
1	B	904	ASN
1	B	1033	HIS
1	B	1048	GLN
1	B	1088	GLN
1	B	1108	ASN
1	B	1284	GLN
1	B	1289	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FES	A	1333	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	A	1334	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FAD	A	1335	-	51,58,58	1.24	5 (9%)	54,89,89	1.98	6 (11%)
6	BCT	A	1337	-	0,3,3	0.00	-	0,3,3	0.00	-
7	GOL	A	1338	-	5,5,5	0.47	0	5,5,5	0.70	0
7	GOL	A	1339	-	5,5,5	0.48	0	5,5,5	0.76	0
7	GOL	A	1340	-	5,5,5	0.24	0	5,5,5	0.93	0
8	SAL	A	1341	-	7,10,10	1.40	1 (14%)	9,13,13	1.20	1 (11%)
4	XAX	A	3003	-	23,31,31	2.80	7 (30%)	20,52,52	2.14	7 (35%)
2	FES	B	1333	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	B	1334	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FAD	B	1335	-	51,58,58	1.39	5 (9%)	54,89,89	2.02	9 (16%)
6	BCT	B	1337	-	0,3,3	0.00	-	0,3,3	0.00	-
7	GOL	B	1338	-	5,5,5	0.39	0	5,5,5	0.48	0
7	GOL	B	1339	-	5,5,5	0.21	0	5,5,5	0.24	0
8	SAL	B	1340	-	7,10,10	1.21	1 (14%)	9,13,13	1.45	3 (33%)
4	XAX	B	3003	-	23,31,31	2.58	7 (30%)	20,52,52	2.21	7 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FES	A	1333	1	-	0/0/4/4	0/1/1/1
2	FES	A	1334	1	-	0/0/4/4	0/1/1/1
3	FAD	A	1335	-	-	0/28/50/50	0/6/6/6
6	BCT	A	1337	-	-	0/0/0/0	0/0/0/0
7	GOL	A	1338	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1339	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	1340	-	-	0/4/4/4	0/0/0/0
8	SAL	A	1341	-	-	0/0/4/4	0/1/1/1
4	XAX	A	3003	-	-	0/6/46/46	0/4/4/4
2	FES	B	1333	1	-	0/0/4/4	0/1/1/1
2	FES	B	1334	1	-	0/0/4/4	0/1/1/1
3	FAD	B	1335	-	-	0/28/50/50	0/6/6/6
6	BCT	B	1337	-	-	0/0/0/0	0/0/0/0
7	GOL	B	1338	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1339	-	-	0/4/4/4	0/0/0/0
8	SAL	B	1340	-	-	0/0/4/4	0/1/1/1
4	XAX	B	3003	-	-	0/6/46/46	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3003	XAX	C1'-S1'	-4.87	1.66	1.76
4	A	3003	XAX	C1'-S1'	-4.65	1.67	1.76
4	B	3003	XAX	C2'-S2'	-4.46	1.67	1.76
4	A	3003	XAX	C2'-S2'	-3.62	1.69	1.76
4	A	3003	XAX	C6-N5	2.08	1.48	1.45
4	B	3003	XAX	C4-N3	2.47	1.37	1.33
3	B	1335	FAD	C10-N1	2.48	1.36	1.33
3	A	1335	FAD	C10-N1	2.57	1.36	1.33
3	A	1335	FAD	C2A-N1A	2.63	1.38	1.33
3	A	1335	FAD	C4X-N5	2.85	1.37	1.33
8	B	1340	SAL	C1-C2	2.89	1.49	1.40
3	B	1335	FAD	C2A-N1A	2.95	1.39	1.33
3	A	1335	FAD	C2A-N3A	3.16	1.37	1.32
3	B	1335	FAD	C4-N3	3.20	1.38	1.33
8	A	1341	SAL	C1-C2	3.30	1.50	1.40
3	A	1335	FAD	C1'-N10	3.43	1.51	1.48
4	B	3003	XAX	C9-C10	3.61	1.48	1.41
3	B	1335	FAD	C4X-N5	4.10	1.39	1.33
4	B	3003	XAX	C9-N5	4.31	1.47	1.37
4	A	3003	XAX	C9-C10	4.32	1.49	1.41
4	B	3003	XAX	O4-C4	4.53	1.35	1.24
4	A	3003	XAX	C9-N5	4.68	1.48	1.37
3	B	1335	FAD	C2A-N3A	4.72	1.40	1.32
4	A	3003	XAX	O4-C4	4.99	1.37	1.24
4	B	3003	XAX	C4-C9	6.74	1.49	1.41
4	A	3003	XAX	C4-C9	7.88	1.50	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1335	FAD	N3A-C2A-N1A	-9.78	120.34	128.86
3	A	1335	FAD	N3A-C2A-N1A	-9.29	120.76	128.86
4	B	3003	XAX	C4-C9-C10	-4.06	110.89	114.56
4	A	3003	XAX	C2'-C1'-S1'	-3.62	118.09	120.15
4	B	3003	XAX	N3-C2-N1	-3.25	120.19	125.45
4	A	3003	XAX	O3P-P-O4'	-2.92	98.96	106.73
4	A	3003	XAX	C1'-C2'-S2'	-2.90	118.51	120.15
3	A	1335	FAD	C4X-C4-N3	-2.74	119.58	123.48
4	A	3003	XAX	O4'-P-O2P	-2.72	98.85	106.47
4	B	3003	XAX	O4'-P-O2P	-2.63	99.11	106.47
4	B	3003	XAX	C1'-C2'-S2'	-2.53	118.71	120.15
8	B	1340	SAL	C4-C3-C2	-2.44	116.92	120.05
8	A	1341	SAL	C6-C1-C1'	-2.33	116.65	120.23
3	B	1335	FAD	C4X-C4-N3	-2.32	120.18	123.48
8	B	1340	SAL	C5-C6-C1	-2.04	116.92	120.37
3	B	1335	FAD	C6-C5X-C9A	2.03	121.64	119.00
3	B	1335	FAD	C5X-C9A-N10	2.17	119.27	117.66
3	B	1335	FAD	C4B-O4B-C1B	2.33	112.25	109.77
8	B	1340	SAL	C4-C5-C6	2.38	123.48	120.21
3	B	1335	FAD	C4-C4X-N5	2.41	121.32	118.68
4	B	3003	XAX	O1P-P-O2P	2.42	119.97	110.50
4	A	3003	XAX	C2-N1-C10	2.76	120.72	114.51
3	A	1335	FAD	C4X-N5-C5X	2.94	119.87	116.76
4	A	3003	XAX	O3P-P-O2P	3.03	122.35	110.50
3	A	1335	FAD	C5X-C9A-N10	3.23	120.06	117.66
3	B	1335	FAD	C4X-N5-C5X	3.33	120.28	116.76
4	A	3003	XAX	C4-N3-C2	3.52	121.13	116.06
4	B	3003	XAX	C2-N1-C10	3.83	123.13	114.51
4	B	3003	XAX	C4-N3-C2	3.84	121.59	116.06
3	B	1335	FAD	C4-N3-C2	4.60	119.18	115.16
3	A	1335	FAD	C4-N3-C2	4.93	119.47	115.16
3	B	1335	FAD	C1'-N10-C9A	5.60	123.48	118.35
3	A	1335	FAD	C1'-N10-C9A	6.00	123.85	118.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1335	FAD	1	0
7	A	1338	GOL	1	0
4	A	3003	XAX	1	0
3	B	1335	FAD	2	0
8	B	1340	SAL	1	0
4	B	3003	XAX	3	0

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	1225/1332 (91%)	0.41	49 (4%)	39	46	12, 25, 39, 60	0
1	B	1218/1332 (91%)	0.57	83 (6%)	18	24	17, 29, 45, 63	0
All	All	2443/2664 (91%)	0.49	132 (5%)	26	33	12, 27, 42, 63	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1287	ASN	8.3
1	A	164	ALA	6.5
1	B	165	LYS	6.2
1	A	162	THR	5.6
1	B	2	THR	5.4
1	B	477	PHE	5.0
1	A	58	TYR	4.9
1	B	1144	THR	4.7
1	A	378	GLY	4.3
1	B	162	THR	4.3
1	B	164	ALA	4.3
1	B	1288	ASN	4.2
1	A	498	PRO	4.1
1	A	165	LYS	4.0
1	A	720	LYS	3.9
1	A	1245	ARG	3.8
1	B	1290	THR	3.7
1	B	97	ARG	3.5
1	A	477	PHE	3.5
1	A	161	ARG	3.5
1	A	1288	ASN	3.5
1	A	163	PHE	3.4
1	B	982	SER	3.4
1	B	724	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	499	ASP	3.3
1	B	1264	LEU	3.3
1	A	2	THR	3.2
1	B	1143	GLU	3.2
1	B	985	ASP	3.1
1	A	989	LYS	3.1
1	B	718	ASP	3.1
1	A	397	LEU	3.1
1	A	528	GLY	3.1
1	B	136	VAL	3.1
1	B	445	GLY	3.1
1	A	1246	ASP	3.0
1	B	133	GLU	3.0
1	B	336	TRP	3.0
1	A	61	LEU	3.0
1	B	161	ARG	3.0
1	B	1107	LYS	3.0
1	A	1215	PRO	2.9
1	B	377	ARG	2.9
1	B	659	THR	2.8
1	B	1286	THR	2.8
1	B	1146	SER	2.8
1	B	471	GLN	2.8
1	B	976	GLN	2.8
1	A	97	ARG	2.7
1	B	1248	PRO	2.7
1	B	725	GLU	2.7
1	B	499	ASP	2.7
1	B	1115	ASP	2.7
1	A	983	GLU	2.7
1	A	253	PRO	2.6
1	A	525	LYS	2.6
1	A	60	ARG	2.6
1	B	448	GLN	2.6
1	B	60	ARG	2.6
1	A	252	HIS	2.6
1	B	973	LYS	2.6
1	B	1289	ASN	2.6
1	A	985	ASP	2.5
1	B	989	LYS	2.5
1	B	658	ASP	2.5
1	B	1215	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1325	CYS	2.5
1	B	693	PRO	2.5
1	B	528	GLY	2.5
1	B	991	ASN	2.5
1	B	163	PHE	2.5
1	A	1247	CYS	2.5
1	B	254	GLU	2.5
1	A	799	GLY	2.5
1	B	1250	LYS	2.5
1	B	1317	CYS	2.5
1	B	977	TYR	2.4
1	A	575	ARG	2.4
1	B	378	GLY	2.4
1	B	61	LEU	2.4
1	B	620	ILE	2.4
1	B	720	LYS	2.3
1	A	379	THR	2.3
1	A	523	VAL	2.3
1	B	948	LYS	2.3
1	B	1251	LYS	2.3
1	A	979	ALA	2.3
1	B	134	PRO	2.3
1	B	993	TRP	2.3
1	B	984	VAL	2.3
1	B	1102	GLU	2.3
1	B	1216	GLU	2.3
1	B	461	ASP	2.3
1	B	917	PRO	2.3
1	B	921	PHE	2.2
1	B	63	ASP	2.2
1	B	137	GLU	2.2
1	B	158	GLN	2.2
1	B	58	TYR	2.2
1	A	852	LYS	2.2
1	B	920	LEU	2.2
1	A	1103	PRO	2.2
1	B	1103	PRO	2.2
1	B	379	THR	2.2
1	B	294	PRO	2.2
1	B	400	PRO	2.2
1	A	982	SER	2.2
1	B	425	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1106	LYS	2.1
1	B	316	VAL	2.1
1	A	424	ALA	2.1
1	B	934	CYS	2.1
1	A	1250	LYS	2.1
1	B	272	ASN	2.1
1	A	969	ASP	2.1
1	B	1291	LYS	2.1
1	B	475	SER	2.1
1	A	527	LEU	2.1
1	B	3	ALA	2.1
1	B	1272	PHE	2.1
1	A	973	LYS	2.1
1	A	414	GLU	2.1
1	A	1216	GLU	2.1
1	B	19	ASN	2.1
1	B	259	VAL	2.1
1	B	987	PHE	2.1
1	A	920	LEU	2.0
1	B	853	THR	2.0
1	A	346	ALA	2.0
1	B	488	ALA	2.0
1	A	320	PRO	2.0
1	A	93	SER	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	GOL	A	1338	6/6	0.89	0.21	4.10	22,26,27,28	0
8	SAL	B	1340	10/10	0.89	0.24	3.69	37,39,41,44	0
8	SAL	A	1341	10/10	0.90	0.25	2.88	22,25,28,29	0
7	GOL	B	1338	6/6	0.92	0.21	2.46	20,24,25,26	0
7	GOL	A	1340	6/6	0.84	0.22	1.71	33,35,38,39	0
7	GOL	A	1339	6/6	0.94	0.15	0.35	27,28,29,30	0
6	BCT	A	1337	4/4	0.96	0.18	0.17	14,14,15,17	0
6	BCT	B	1337	4/4	0.98	0.19	0.02	24,24,24,24	0
4	XAX	B	3003	28/28	0.97	0.17	-0.32	20,22,26,33	0
3	FAD	A	1335	53/53	0.96	0.15	-0.82	14,19,25,28	0
5	CA	A	1336	1/1	0.99	0.12	-0.84	26,26,26,26	0
3	FAD	B	1335	53/53	0.95	0.14	-0.94	19,27,31,33	0
7	GOL	B	1339	6/6	0.94	0.12	-1.22	21,25,27,30	0
4	XAX	A	3003	28/28	0.98	0.13	-1.40	16,20,26,33	0
2	FES	B	1333	4/4	0.98	0.11	-1.84	20,20,21,22	0
2	FES	A	1333	4/4	0.98	0.08	-1.85	18,20,21,21	0
2	FES	A	1334	4/4	0.99	0.10	-2.15	18,18,18,19	0
2	FES	B	1334	4/4	0.97	0.11	-2.30	18,21,21,22	0
5	CA	B	1336	1/1	0.99	0.09	-4.19	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.