



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:23 AM UTC

PDB ID : 3AX9 / pdb_00003ax9
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

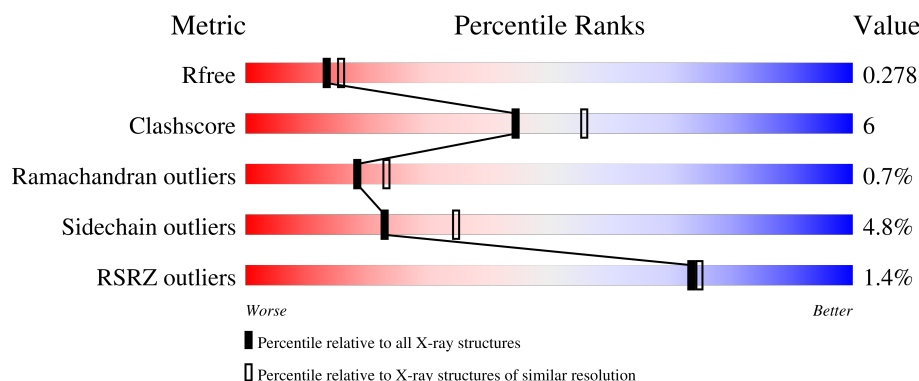
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	1332	% 77% 14% • 8%
1	B	1332	% 76% 14% • 9%

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.

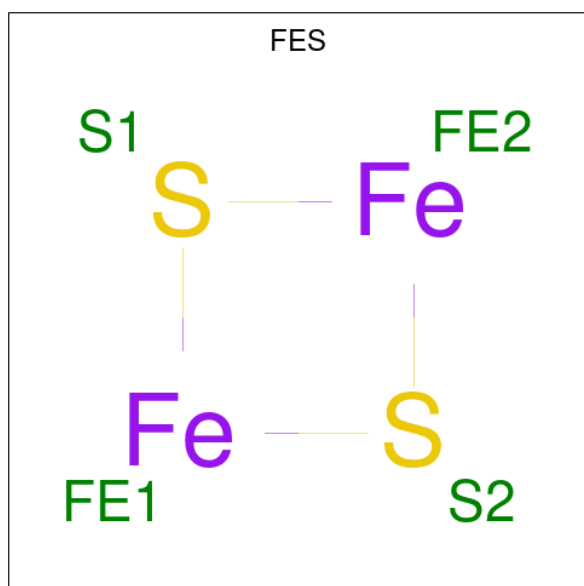
- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

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 (CCD ID: FES) (formula: Fe₂S₂).



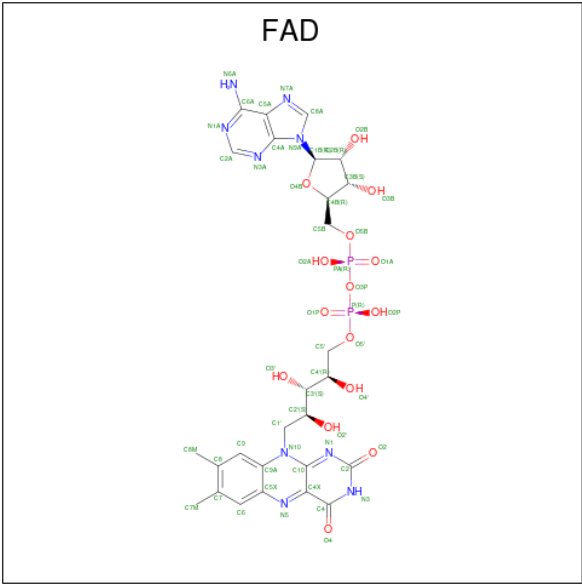
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		

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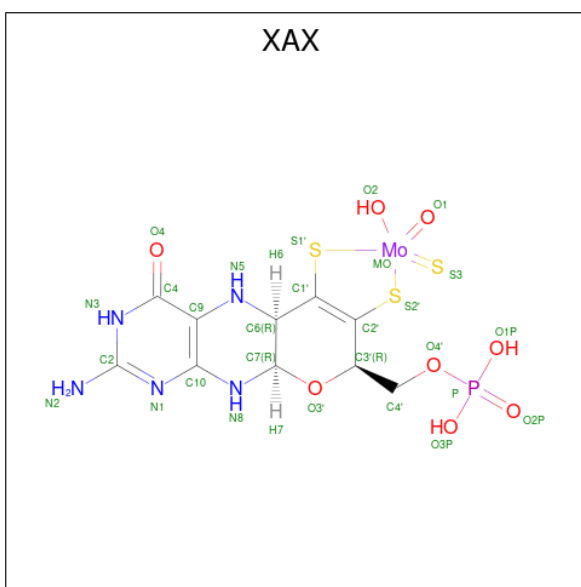
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- 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 (CCD ID: XAX) (formula: C₁₀H₁₃MoN₅O₈PS₃).

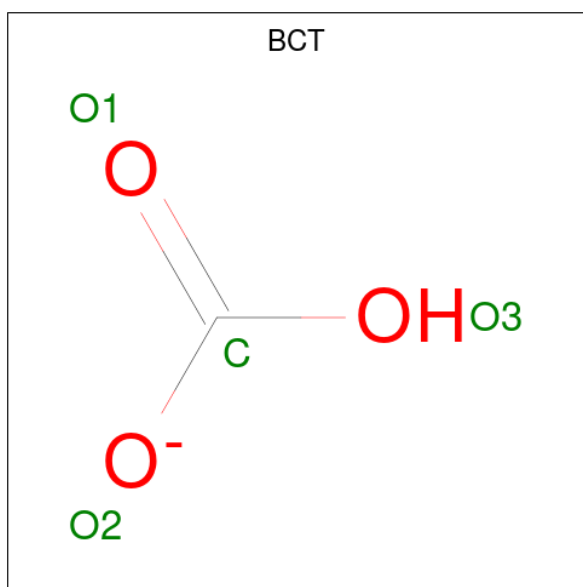


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total 28	C 10	Mo 1	N 5	O 8	P 1	S 3	0	0
4	B	1	Total 28	C 10	Mo 1	N 5	O 8	P 1	S 3	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

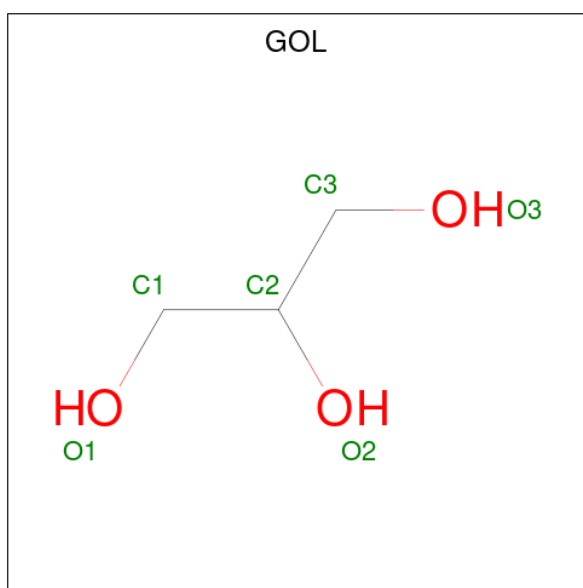
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0

- Molecule 6 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



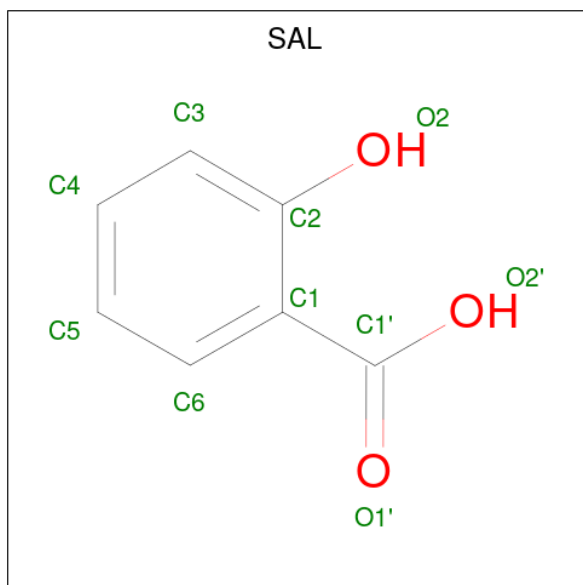
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

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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 (CCD ID: SAL) (formula: C₇H₆O₃).



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		

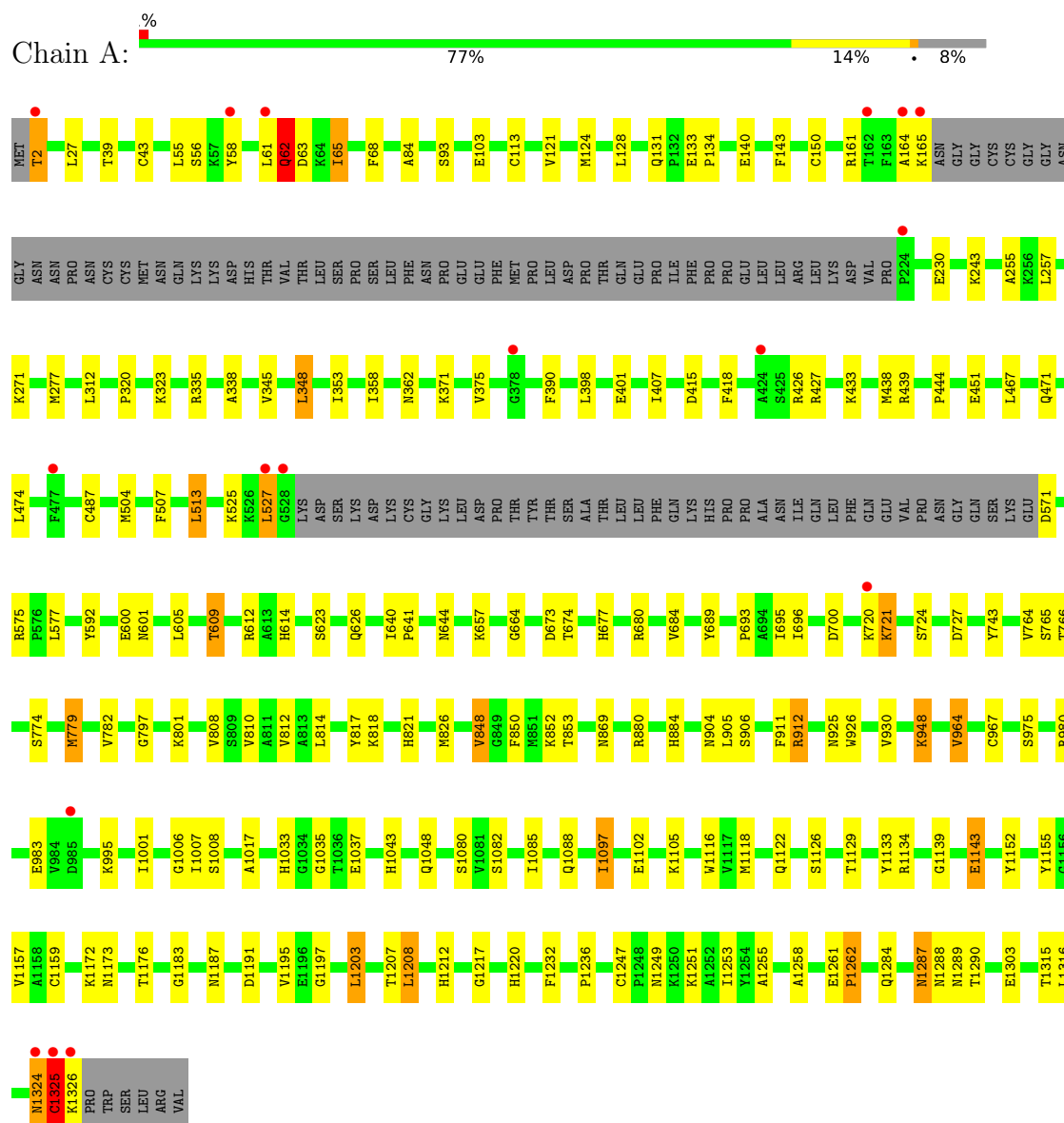
- Molecule 9 is water.

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

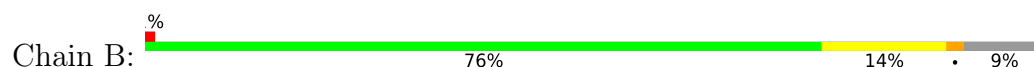
3 Residue-property plots [i](#)

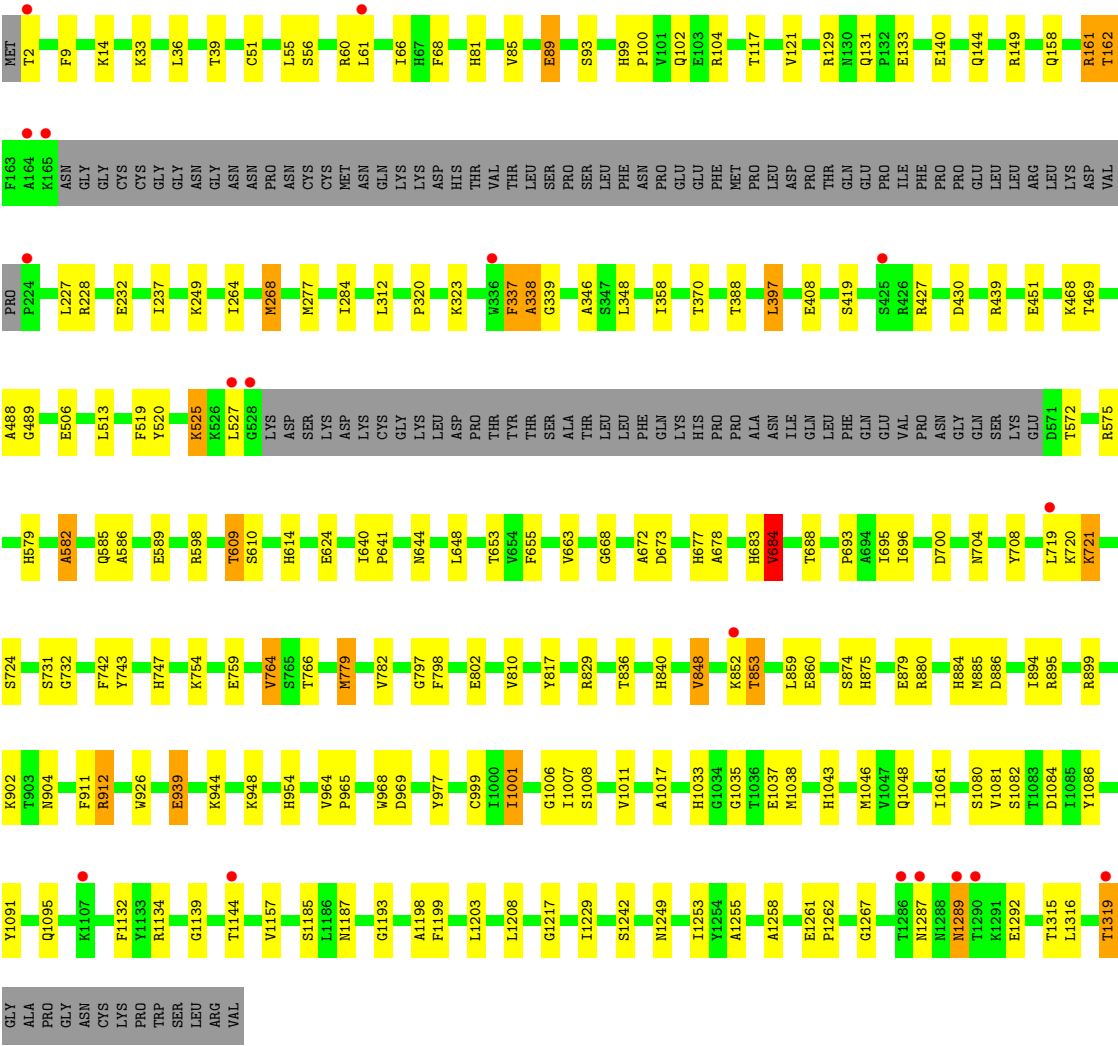
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Xanthine dehydrogenase/oxidase



• Molecule 1: Xanthine dehydrogenase/oxidase





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 38.13 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.13-2.30) 99.3 (38.13-2.30)	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 (4.98%)	wwPDB-VP
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 , 40.6	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: FES, BCT, XAX, CA, FAD, GOL, SAL

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	0.87	2/9675 (0.0%)	1.03	15/13085 (0.1%)
1	B	0.82	0/9631	1.00	11/13026 (0.1%)
All	All	0.85	2/19306 (0.0%)	1.02	26/26111 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	964	VAL	CA-CB	7.16	1.58	1.53
1	A	121	VAL	CA-CB	6.36	1.62	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1011	VAL	CA-C-N	8.40	127.97	119.24
1	B	1011	VAL	C-N-CA	8.40	127.97	119.24
1	A	1262	PRO	CA-C-N	-7.91	111.32	120.89
1	A	1262	PRO	C-N-CA	-7.91	111.32	120.89
1	A	1325	CYS	N-CA-C	6.49	124.63	110.80
1	B	1261	GLU	CA-C-N	-5.55	114.66	120.38
1	B	1261	GLU	C-N-CA	-5.55	114.66	120.38
1	A	925	ASN	N-CA-C	5.46	117.69	111.02
1	A	362	ASN	CA-C-N	-5.35	113.39	119.28
1	A	362	ASN	C-N-CA	-5.35	113.39	119.28
1	B	732	GLY	N-CA-C	5.34	118.33	110.80
1	B	284	ILE	CA-C-N	5.33	124.78	119.24
1	B	284	ILE	C-N-CA	5.33	124.78	119.24
1	B	684	VAL	CB-CA-C	5.27	117.73	111.20
1	A	467	LEU	N-CA-C	5.25	116.69	110.97
1	A	766	THR	N-CA-C	5.22	117.33	109.23
1	A	674	THR	CA-C-N	-5.17	113.71	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	674	THR	C-N-CA	-5.17	113.71	119.19
1	B	85	VAL	CB-CA-C	-5.11	103.77	110.98
1	A	774	SER	CB-CA-C	-5.09	102.67	110.81
1	A	1102	GLU	CA-C-N	-5.08	114.38	119.56
1	A	1102	GLU	C-N-CA	-5.08	114.38	119.56
1	B	582	ALA	N-CA-C	5.03	117.42	111.33
1	A	1007	ILE	N-CA-C	5.03	115.00	107.51
1	B	1262	PRO	N-CA-C	5.02	116.83	110.70
1	A	869	ASN	N-CA-C	5.02	119.04	113.02

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	115	0
1	B	9433	0	9440	117	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	230	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 (230) 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:A:1143:GLU:CD	1:A:1143:GLU:H	1.96	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
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:B:640:ILE:HG12	1:B:779:MET:HE1	1.75	0.69
1:A:427:ARG:O	1:A:427:ARG:HG2	1.94	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:N	1:A:1324:ASN:ND2	2.44	0.65
1:A:1287:ASN:HD22	1:A:1287:ASN:C	2.05	0.64
1:B:610:SER:O	1:B:663:VAL:O	2.14	0.64
1:B:60:ARG:HH11	1:B:60:ARG:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1325:CYS:O	1:A:1326:LYS:C	2.42	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:1324:ASN:H	1:A:1324:ASN:HD22	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:B:572:THR:HA	1:B:575:ARG:HD3	1.85	0.57
1:A:1203:LEU:C	1:A:1203:LEU:HD12	2.29	0.57
1:A:1088:GLN:HG2	1:A:1133:TYR:CE1	2.40	0.56
1:B:264:ILE:O	1:B:268:MET:HG2	2.05	0.56
1:B:853:THR:HG23	1:B:944:LYS:HZ2	1.71	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:N	1:A:1324:ASN:HD22	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:A:640:ILE:HG12	1:A:779:MET:HE1	1.91	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: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:B:1315:THR:O	1:B:1316:LEU:HB2	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1126:SER:HB2	1:B:1132:PHE:CD1	2.44	0.52
1:A:1159:CYS:O	1:A:1176:THR:HA	2.09	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:1033:HIS:HD2	1:B:1035:GLY:H	1.58	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:B:885:MET:HE2	1:B:894:ILE:HD11	1.91	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:62:GLN:O	1:A:62:GLN:NE2	2.35	0.50
1:A:471:GLN:NE2	1:A:474:LEU:CD1	2.73	0.50
1:B:624:GLU:HB3	1:B:684:VAL:HG13	1.94	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:B:1038:MET:HG3	4:B:3003:XAX:C4	2.41	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
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:A:131:GLN:HE21	1:A:133:GLU:C	2.21	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:B:911:PHE:O	1:B:912:ARG:C	2.57	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:27:LEU:HD13	1:A:39:THR:HG22	1.95	0.47
1:A:1315:THR:O	1:A:1316:LEU:HB2	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:779:MET:HE2	1:B:779:MET:HB2	1.44	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:B:1081:VAL:O	1:B:1084:ASP:HB2	2.13	0.47
1:A:1326:LYS:O	1:A:1326:LYS:CG	2.63	0.47
1:A:911:PHE:O	1:A:912:ARG:C	2.56	0.47
1:A:612:ARG:HG3	1:A:689:TYR:CG	2.49	0.46
1:A:600:GLU:CD	1:B:598:ARG:HG2	2.41	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:419:SER:HB2	1:B:519:PHE:CD1	2.51	0.46
1:B:1289:ASN:HB2	1:B:1292:GLU:HB2	1.97	0.46
1:A:1143:GLU:CD	1:A:1143:GLU:N	2.68	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:641:PRO:HG3	1:B:817:TYR:CE2	2.51	0.45
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.51	0.45
1:A:353:ILE:O	1:A:353:ILE:HG22	2.15	0.45
1:A:1037:GLU:HB2	1:A:1043:HIS:CD2	2.52	0.45
1:B:853:THR:HG23	1:B:944:LYS:HZ3	1.81	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:912:ARG:NH2	1:B:1198:ALA:HB2	2.32	0.45
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.52	0.45
1:A:56:SER:HB2	1:A:84:ALA:HB3	1.99	0.45
1:B:131:GLN:HE21	1:B:133:GLU:C	2.25	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
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:HD22	1:B:1289:ASN:H	1.65	0.44
1:A:905:LEU:O	1:A:906:SER:C	2.57	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:886:ASP:CG	1:B:954:HIS:CE1	2.96	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:605:LEU:HD23	1:A:605:LEU:C	2.42	0.44
1:A:1097:ILE:CD1	1:A:1129:THR:HG22	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:779:MET:HG2	1:B:810:VAL:HG13	2.00	0.44
1:B:1082:SER:HB2	4:B:3003:XAX:O3P	2.17	0.44
1:A:507:PHE:CD1	1:A:1303:GLU:HA	2.53	0.44
1:B:1046:MET:HE2	1:B:1046:MET:HA	2.00	0.43
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:A:427:ARG:HD3	1:A:1212:HIS:CD2	2.53	0.43
1:B:388:THR:O	1:B:397:LEU:HD13	2.18	0.43
1:B:1007:ILE:HD12	1:B:1258:ALA:HB3	2.00	0.43
1:B:1080:SER:O	1:B:1258:ALA:HB1	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:A:779:MET:HE1	1:A:814:LEU:HD13	2.01	0.42
1:B:104:ARG:HD2	1:B:104:ARG:HA	1.89	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:9:PHE:CE2	1:B:14:LYS:HB2	2.54	0.42
1:B:337:PHE:C	1:B:337:PHE:CD2	2.96	0.42
1:B:912:ARG:CZ	1:B:1198:ALA:HB2	2.50	0.42
1:B:999:CYS:SG	1:B:1001:ILE:HD12	2.58	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:338:ALA:HB2	3:B:1335:FAD:C6	2.50	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: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
1:A:1287:ASN:ND2	1:A:1287:ASN:C	2.72	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:721:LYS:O	1:A:724:SER:HB2	2.20	0.41
1:A:1082:SER:HB2	4:A:3003:XAX:O3P	2.21	0.41
1:B:721:LYS:CA	1:B:724:SER:HB2	2.50	0.41
1:B:798:PHE:HA	4:B:3003:XAX:HN5	1.84	0.41
1:B:525:LYS:HD2	1:B:525:LYS:HA	1.86	0.41
1:B:1091:TYR:O	1:B:1095:GLN:HG2	2.19	0.41
1:B:104:ARG:CZ	1:B:162:THR:HG21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1289:ASN:H	1:B:1289:ASN:ND2	2.19	0.41
1:A:55:LEU:HD12	1:A:68:PHE:CE1	2.55	0.41
1:A:471:GLN:HE21	1:A:474:LEU:HD12	1.85	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:A:124:MET:HE3	1:A:128:LEU:HD11	2.03	0.41
1:A:1173:ASN:O	1:A:1236:PRO:HA	2.20	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:B:968:TRP:HA	1:B:1157:VAL:HG11	2.03	0.41
1:A:1183:GLY:HA2	1:A:1247:CYS:O	2.21	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:1199:PHE:CE1	1:B:1267:GLY:HA2	2.55	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:113:CYS:O	1:A:592:TYR:OH	2.36	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:B:158:GLN:O	1:B:161:ARG:HB2	2.21	0.40
1:B:525:LYS:C	1:B:527:LEU:H	2.29	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	1219/1332 (92%)	1162 (95%)	46 (4%)	11 (1%)	14	17
1	B	1212/1332 (91%)	1147 (95%)	58 (5%)	7 (1%)	21	27
All	All	2431/2664 (91%)	2309 (95%)	104 (4%)	18 (1%)	18	23

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
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%)	980 (95%)	50 (5%)	22	34
1	B	1026/1128 (91%)	977 (95%)	49 (5%)	23	35
All	All	2056/2256 (91%)	1957 (95%)	99 (5%)	23	35

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	62	GLN
1	A	63	ASP
1	A	65	ILE
1	A	93	SER
1	A	103	GLU
1	A	140	GLU
1	A	161	ARG
1	A	165	LYS
1	A	243	LYS
1	A	257	LEU
1	A	271	LYS
1	A	312	LEU
1	A	345	VAL
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	513	LEU
1	A	525	LYS
1	A	527	LEU
1	A	575	ARG
1	A	577	LEU
1	A	609	THR
1	A	657	LYS
1	A	680	ARG
1	A	684	VAL
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	853	THR
1	A	948	LYS
1	A	983	GLU
1	A	1001	ILE
1	A	1097	ILE
1	A	1134	ARG

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Mol	Chain	Res	Type
1	A	1143	GLU
1	A	1203	LEU
1	A	1208	LEU
1	A	1220	HIS
1	A	1287	ASN
1	A	1290	THR
1	A	1324	ASN
1	B	33	LYS
1	B	61	LEU
1	B	89	GLU
1	B	129	ARG
1	B	140	GLU
1	B	161	ARG
1	B	162	THR
1	B	237	ILE
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	397	LEU
1	B	468	LYS
1	B	506	GLU
1	B	513	LEU
1	B	525	LYS
1	B	609	THR
1	B	648	LEU
1	B	684	VAL
1	B	688	THR
1	B	719	LEU
1	B	731	SER
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	853	THR
1	B	860	GLU
1	B	895	ARG
1	B	899	ARG

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Mol	Chain	Res	Type
1	B	939	GLU
1	B	948	LYS
1	B	969	ASP
1	B	1001	ILE
1	B	1061	ILE
1	B	1134	ARG
1	B	1144	THR
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	131	GLN
1	A	146	ASN
1	A	272	ASN
1	A	387	HIS
1	A	448	GLN
1	A	471	GLN
1	A	473	GLN
1	A	614	HIS
1	A	626	GLN
1	A	677	HIS
1	A	683	HIS
1	A	821	HIS
1	A	840	HIS
1	A	884	HIS
1	A	904	ASN
1	A	925	ASN
1	A	1033	HIS
1	A	1048	GLN
1	A	1212	HIS
1	A	1284	GLN
1	A	1285	HIS
1	A	1287	ASN
1	A	1324	ASN

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Mol	Chain	Res	Type
1	B	131	GLN
1	B	146	ASN
1	B	261	ASN
1	B	292	HIS
1	B	387	HIS
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	1016	GLN
1	B	1033	HIS
1	B	1048	GLN
1	B	1088	GLN
1	B	1108	ASN
1	B	1284	GLN
1	B	1288	ASN
1	B	1289	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	FAD	A	1335	-	58,58,58	1.12	3 (5%)	85,89,89	1.62	17 (20%)
2	FES	A	1333	1	0,4,4	-	-	-	-	-
2	FES	B	1333	1	0,4,4	-	-	-	-	-
2	FES	B	1334	1	0,4,4	-	-	-	-	-
6	BCT	B	1337	-	3,3,3	0.56	0	2,3,3	0.36	0
7	GOL	A	1339	-	5,5,5	0.49	0	5,5,5	0.88	0
7	GOL	A	1340	-	5,5,5	0.27	0	5,5,5	1.03	0
8	SAL	A	1341	-	10,10,10	2.09	1 (10%)	13,13,13	1.55	1 (7%)
3	FAD	B	1335	-	58,58,58	1.15	5 (8%)	85,89,89	1.71	18 (21%)
8	SAL	B	1340	-	10,10,10	1.89	1 (10%)	13,13,13	1.48	2 (15%)
7	GOL	A	1338	-	5,5,5	0.47	0	5,5,5	0.81	0
4	XAX	B	3003	-	21,31,31	2.25	4 (19%)	22,52,52	2.50	8 (36%)
2	FES	A	1334	1	0,4,4	-	-	-	-	-
7	GOL	B	1339	-	5,5,5	0.22	0	5,5,5	0.28	0
7	GOL	B	1338	-	5,5,5	0.42	0	5,5,5	0.57	0
6	BCT	A	1337	-	3,3,3	0.63	0	2,3,3	0.85	0
4	XAX	A	3003	-	21,31,31	2.53	4 (19%)	22,52,52	2.61	12 (54%)

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
3	FAD	A	1335	-	-	0/34/50/50	0/6/6/6
8	SAL	B	1340	-	-	2/4/4/4	0/1/1/1
2	FES	A	1333	1	-	-	0/1/1/1
2	FES	B	1333	1	-	-	0/1/1/1
2	FES	B	1334	1	-	-	0/1/1/1
7	GOL	A	1340	-	-	2/4/4/4	-
8	SAL	A	1341	-	-	0/4/4/4	0/1/1/1
3	FAD	B	1335	-	-	2/34/50/50	0/6/6/6
7	GOL	A	1338	-	-	0/4/4/4	-
4	XAX	B	3003	-	-	4/6/46/46	0/4/4/4
7	GOL	B	1339	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FES	A	1334	1	-	-	0/1/1/1
7	GOL	B	1338	-	-	2/4/4/4	-
7	GOL	A	1339	-	-	0/4/4/4	-
4	XAX	A	3003	-	-	4/6/46/46	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3003	XAX	O4-C4	7.14	1.37	1.23
4	B	3003	XAX	O4-C4	6.53	1.35	1.23
4	A	3003	XAX	C9-C10	6.49	1.49	1.38
8	A	1341	SAL	C1-C2	6.27	1.50	1.40
4	B	3003	XAX	C9-C10	5.69	1.48	1.38
8	B	1340	SAL	C1-C2	5.47	1.49	1.40
4	A	3003	XAX	C9-N5	4.42	1.48	1.37
4	B	3003	XAX	C9-N5	4.07	1.47	1.37
3	B	1335	FAD	C4X-N5	3.92	1.39	1.30
3	B	1335	FAD	C2A-N3A	3.43	1.40	1.33
3	B	1335	FAD	C2A-N1A	3.10	1.39	1.33
3	A	1335	FAD	C4X-N5	3.09	1.37	1.30
3	A	1335	FAD	C5A-N7A	-3.04	1.33	1.39
4	A	3003	XAX	C9-C4	2.93	1.50	1.41
3	A	1335	FAD	C2A-N1A	2.76	1.38	1.33
4	B	3003	XAX	C9-C4	2.48	1.49	1.41
3	B	1335	FAD	C5A-N7A	-2.36	1.34	1.39
3	B	1335	FAD	C8A-N7A	2.16	1.35	1.31

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3003	XAX	C7-C6-N5	6.05	113.81	107.87
4	A	3003	XAX	C7-C6-N5	5.87	113.63	107.87
4	B	3003	XAX	C2-N1-C10	5.53	123.13	113.36
3	B	1335	FAD	N3A-C2A-N1A	-5.44	120.34	128.58
3	A	1335	FAD	N3A-C2A-N1A	-5.17	120.76	128.58
3	B	1335	FAD	C5A-C4A-N3A	-4.73	120.20	126.72
4	A	3003	XAX	C2-N1-C10	4.17	120.72	113.36
3	A	1335	FAD	C5A-C4A-N3A	-4.16	120.98	126.72
8	A	1341	SAL	C2-C1-C1'	4.15	124.26	120.00
3	B	1335	FAD	N9A-C8A-N7A	-4.07	108.16	113.94
3	B	1335	FAD	C5A-N7A-C8A	3.86	109.51	103.45
4	B	3003	XAX	O4-C4-C9	-3.79	118.11	127.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1335	FAD	C4X-C10-N10	3.67	121.73	116.48
3	B	1335	FAD	C4-N3-C2	-3.64	119.18	125.64
4	B	3003	XAX	C9-C4-N3	3.64	122.12	112.13
4	A	3003	XAX	C2'-C1'-S1'	-3.62	118.09	120.15
3	A	1335	FAD	C4-N3-C2	-3.47	119.47	125.64
3	B	1335	FAD	C4X-C10-N10	3.43	121.39	116.48
3	A	1335	FAD	C5A-N7A-C8A	3.41	108.81	103.45
3	A	1335	FAD	O2-C2-N1	-3.31	116.31	121.80
3	B	1335	FAD	C2A-N3A-C4A	3.29	119.88	111.83
3	B	1335	FAD	N3A-C4A-N9A	3.23	132.66	127.17
3	A	1335	FAD	N9A-C8A-N7A	-3.07	109.58	113.94
4	A	3003	XAX	O3P-P-O4'	-2.96	98.96	106.67
4	A	3003	XAX	O3P-P-O2P	2.96	122.35	110.83
4	A	3003	XAX	C1'-C2'-S2'	-2.90	118.51	120.15
3	A	1335	FAD	C2A-N3A-C4A	2.84	118.77	111.83
4	A	3003	XAX	O4'-P-O2P	-2.81	98.85	106.44
4	A	3003	XAX	C4-C9-N5	2.81	123.92	116.27
4	A	3003	XAX	C9-C4-N3	2.77	119.74	112.13
3	A	1335	FAD	O2A-PA-O3P	2.76	114.74	107.27
3	B	1335	FAD	C4X-C4-N3	2.72	120.18	113.25
4	B	3003	XAX	O4'-P-O2P	-2.71	99.11	106.44
4	A	3003	XAX	O4-C4-C9	-2.68	120.80	127.26
3	B	1335	FAD	C4A-C5A-N7A	-2.65	107.55	110.58
3	B	1335	FAD	C10-C4X-N5	-2.64	119.42	124.81
8	B	1340	SAL	C4-C5-C6	2.63	123.48	120.24
3	A	1335	FAD	C4A-C5A-N7A	-2.62	107.58	110.58
3	A	1335	FAD	C10-C4X-N5	-2.60	119.51	124.81
3	A	1335	FAD	N3A-C4A-N9A	2.59	131.56	127.17
3	B	1335	FAD	O2P-P-O3P	2.54	114.13	107.27
8	B	1340	SAL	C4-C3-C2	-2.54	116.92	120.05
4	B	3003	XAX	C1'-C2'-S2'	-2.53	118.71	120.15
3	A	1335	FAD	C6A-C5A-C4A	2.50	120.60	117.18
3	A	1335	FAD	C4X-C4-N3	2.48	119.58	113.25
4	A	3003	XAX	O3'-C3'-C2'	2.41	112.49	109.09
3	B	1335	FAD	C6A-C5A-C4A	2.39	120.44	117.18
4	B	3003	XAX	O1P-P-O2P	2.35	119.97	110.83
3	A	1335	FAD	C5X-C9A-N10	2.31	120.06	117.97
3	B	1335	FAD	O4-C4-C4X	-2.30	120.45	126.53
3	B	1335	FAD	C4-C4X-N5	2.26	121.32	118.21
3	B	1335	FAD	O2-C2-N1	-2.20	118.14	121.80
4	A	3003	XAX	C2-N3-C4	-2.20	121.13	125.11
3	A	1335	FAD	C2A-N1A-C6A	2.10	122.18	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3003	XAX	C4-C9-N5	2.09	121.96	116.27
3	B	1335	FAD	O4'-C4'-C3'	2.05	114.04	109.25
3	B	1335	FAD	C4X-C10-N1	-2.01	119.66	124.59
3	A	1335	FAD	O4-C4-C4X	-2.00	121.25	126.53

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3003	XAX	C4'-O4'-P-O3P
4	B	3003	XAX	C4'-O4'-P-O1P
4	B	3003	XAX	C4'-O4'-P-O3P
7	B	1338	GOL	O1-C1-C2-C3
4	A	3003	XAX	C4'-O4'-P-O2P
4	B	3003	XAX	C4'-O4'-P-O2P
4	A	3003	XAX	C3'-C4'-O4'-P
4	A	3003	XAX	C4'-O4'-P-O1P
8	B	1340	SAL	C2-C1-C1'-O2'
4	B	3003	XAX	C3'-C4'-O4'-P
7	B	1338	GOL	O1-C1-C2-O2
8	B	1340	SAL	C2-C1-C1'-O1'
3	B	1335	FAD	C3B-C4B-C5B-O5B
3	B	1335	FAD	O4B-C4B-C5B-O5B
7	A	1340	GOL	O2-C2-C3-O3
7	A	1340	GOL	C1-C2-C3-O3

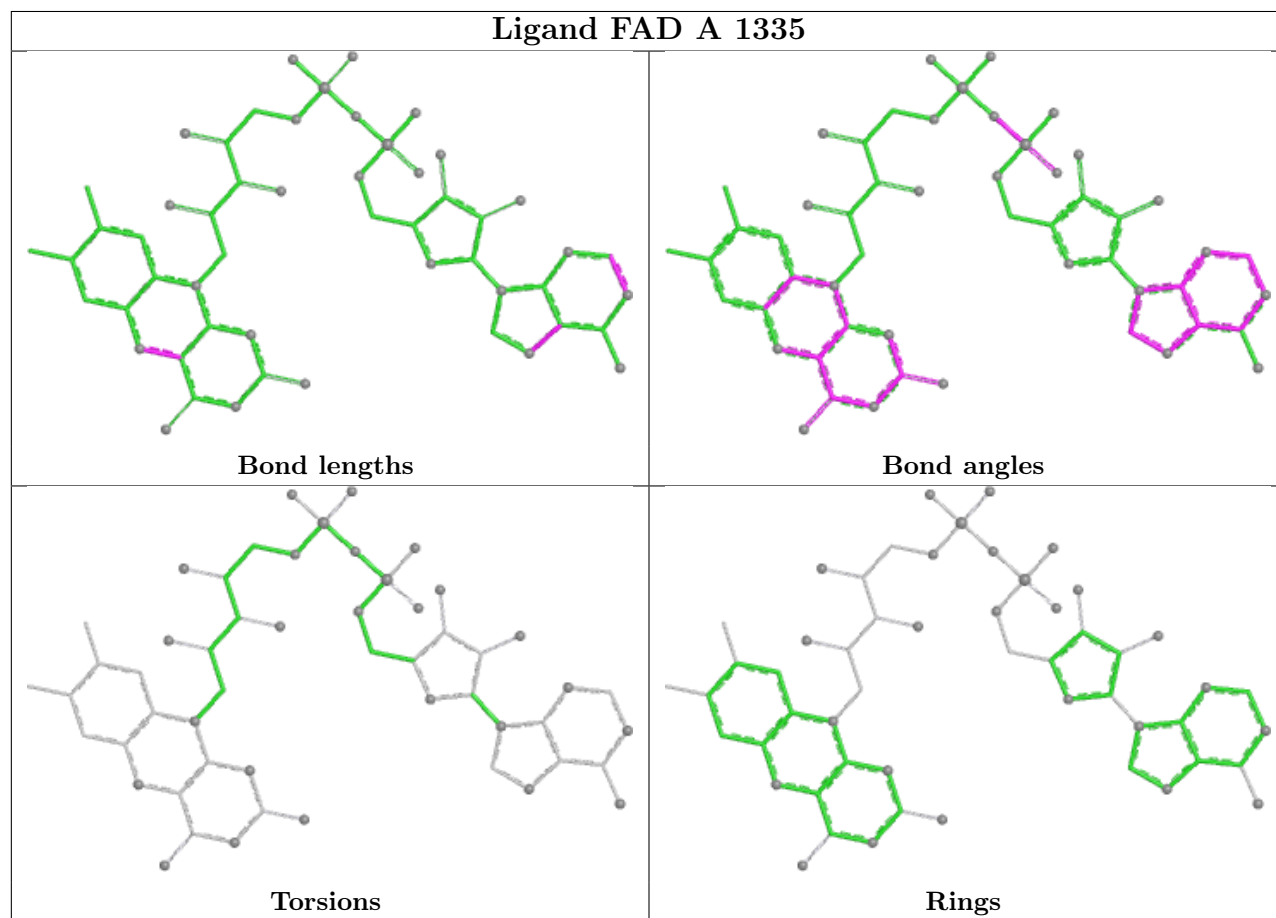
There are no ring outliers.

6 monomers are involved in 9 short contacts:

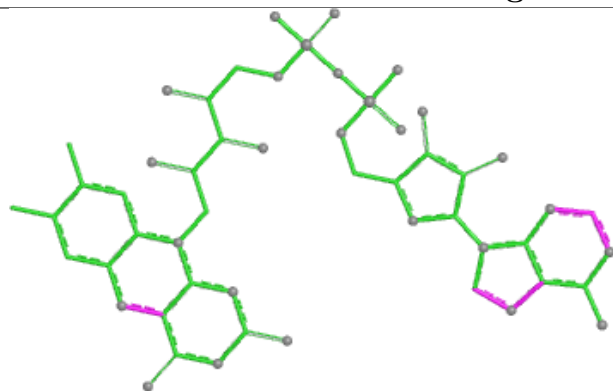
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1335	FAD	1	0
3	B	1335	FAD	2	0
8	B	1340	SAL	1	0
7	A	1338	GOL	1	0
4	B	3003	XAX	3	0
4	A	3003	XAX	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

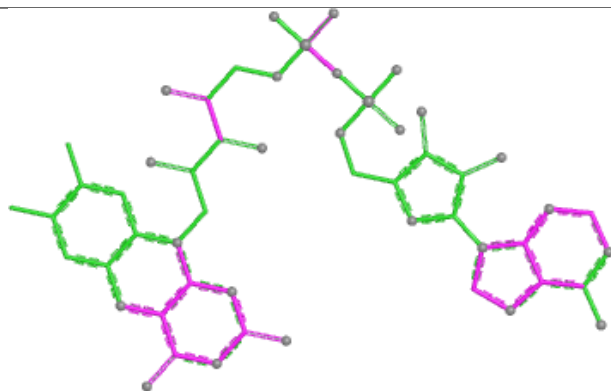
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



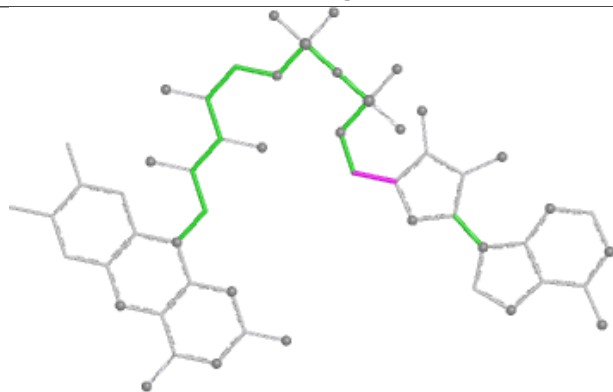
Ligand FAD B 1335



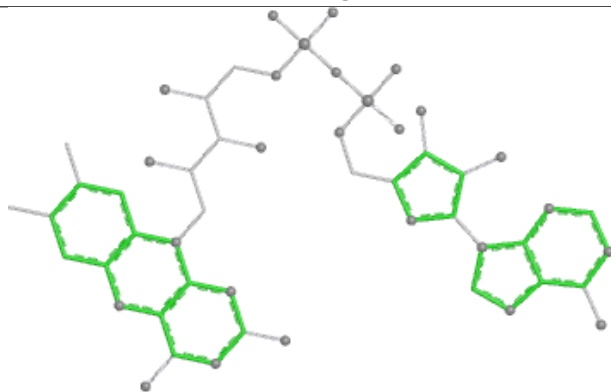
Bond lengths



Bond angles

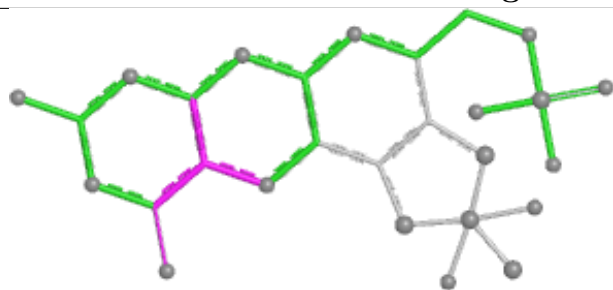


Torsions

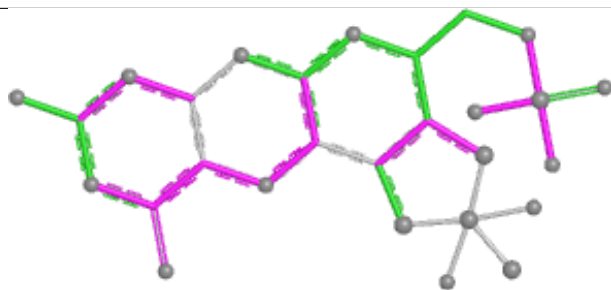


Rings

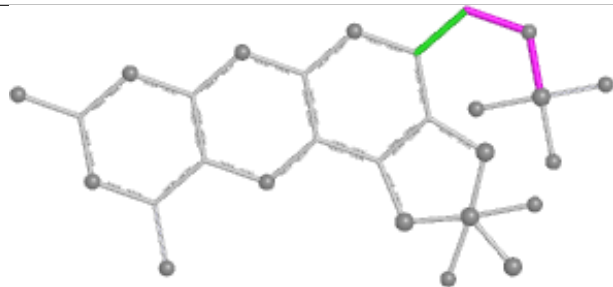
Ligand XAX B 3003



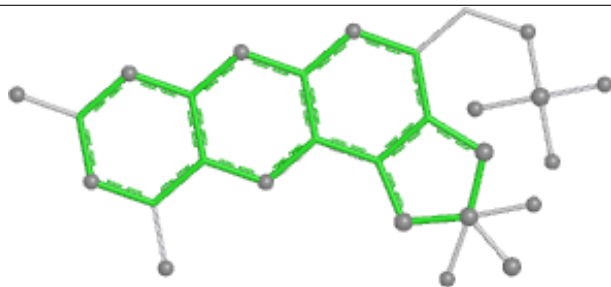
Bond lengths



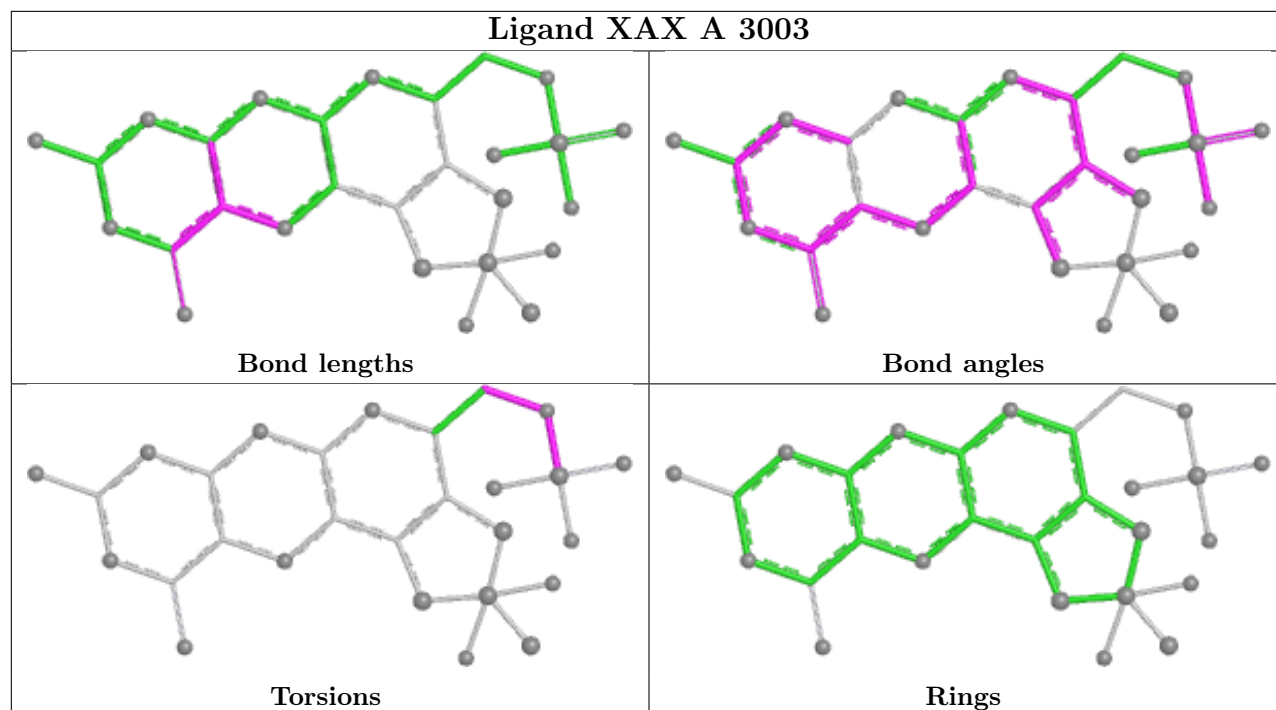
Bond angles



Torsions



Rings



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%)	0.08	17 (1%) 73 75	12, 25, 39, 60	0
1	B	1218/1332 (91%)	0.22	18 (1%) 72 73	17, 29, 45, 63	0
All	All	2443/2664 (91%)	0.15	35 (1%) 73 75	12, 27, 42, 63	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	LEU	4.0
1	B	1287	ASN	3.9
1	A	58	TYR	3.9
1	A	164	ALA	3.7
1	B	528	GLY	3.5
1	A	528	GLY	3.4
1	B	336	TRP	3.1
1	A	424	ALA	2.9
1	A	720	LYS	2.8
1	A	1325	CYS	2.8
1	B	164	ALA	2.8
1	A	378	GLY	2.7
1	A	165	LYS	2.7
1	B	1290	THR	2.6
1	B	224	PRO	2.6
1	B	61	LEU	2.6
1	B	425	SER	2.5
1	B	2	THR	2.5
1	B	1289	ASN	2.5
1	B	165	LYS	2.4
1	A	1326	LYS	2.4
1	B	527	LEU	2.3
1	A	1324	ASN	2.3
1	A	985	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	2	THR	2.3
1	B	852	LYS	2.3
1	A	224	PRO	2.3
1	A	162	THR	2.3
1	A	527	LEU	2.2
1	B	1286	THR	2.2
1	B	1319	THR	2.2
1	B	1107	LYS	2.1
1	A	477	PHE	2.1
1	B	1144	THR	2.1
1	B	719	LEU	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](#)

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	A	1340	6/6	0.79	0.14	33,35,38,39	0
8	SAL	B	1340	10/10	0.84	0.14	37,39,41,44	0
7	GOL	A	1338	6/6	0.89	0.12	22,26,27,28	0
8	SAL	A	1341	10/10	0.90	0.10	22,25,28,29	0
7	GOL	A	1339	6/6	0.93	0.08	27,28,29,30	0
7	GOL	B	1338	6/6	0.94	0.08	20,24,25,26	0
7	GOL	B	1339	6/6	0.95	0.07	21,25,27,30	0
3	FAD	B	1335	53/53	0.96	0.07	19,27,31,33	0
6	BCT	B	1337	4/4	0.96	0.06	24,24,24,24	0
3	FAD	A	1335	53/53	0.96	0.07	14,19,25,28	0
6	BCT	A	1337	4/4	0.97	0.05	14,14,15,17	0
2	FES	B	1334	4/4	0.98	0.04	18,21,21,22	0

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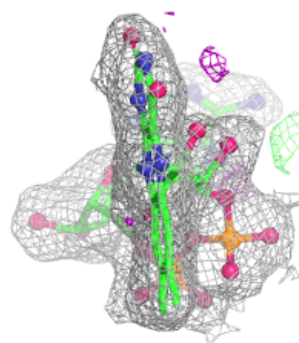
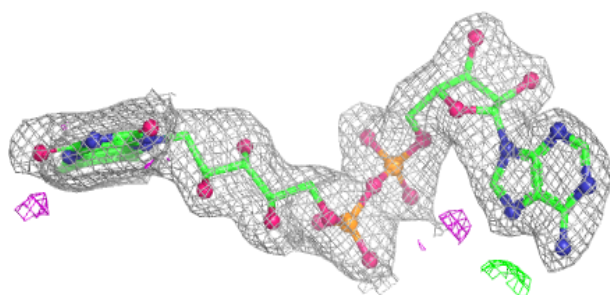
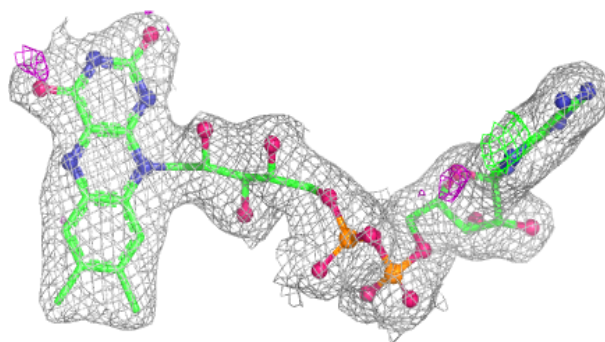
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	XAX	B	3003	28/28	0.98	0.07	20,22,26,33	0
5	CA	A	1336	1/1	0.98	0.03	26,26,26,26	0
5	CA	B	1336	1/1	0.99	0.04	22,22,22,22	0
2	FES	B	1333	4/4	0.99	0.04	20,20,21,22	0
4	XAX	A	3003	28/28	0.99	0.06	16,20,26,33	0
2	FES	A	1333	4/4	0.99	0.03	18,20,21,21	0
2	FES	A	1334	4/4	0.99	0.02	18,18,18,19	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

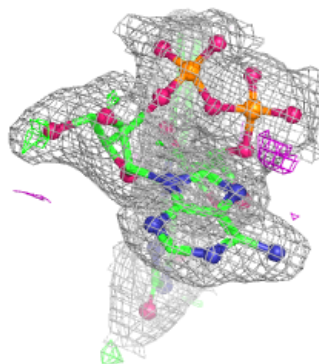
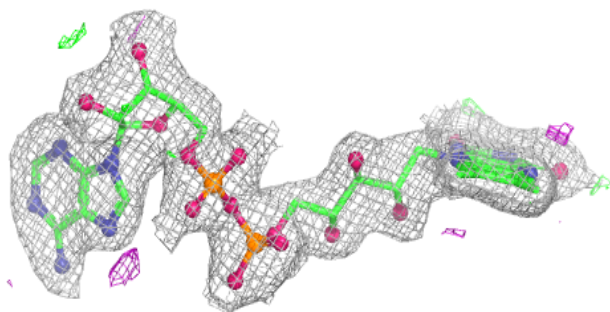
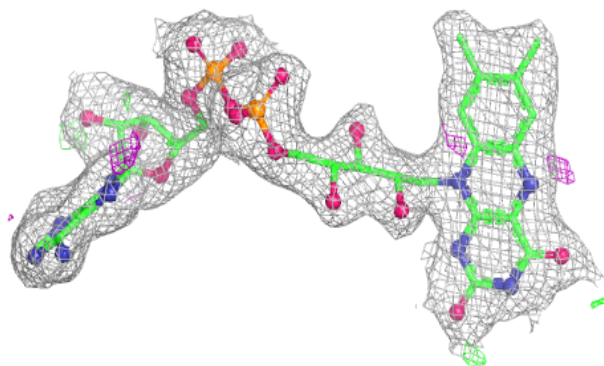
Electron density around FAD B 1335:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



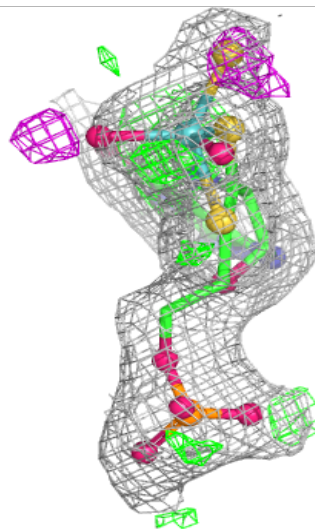
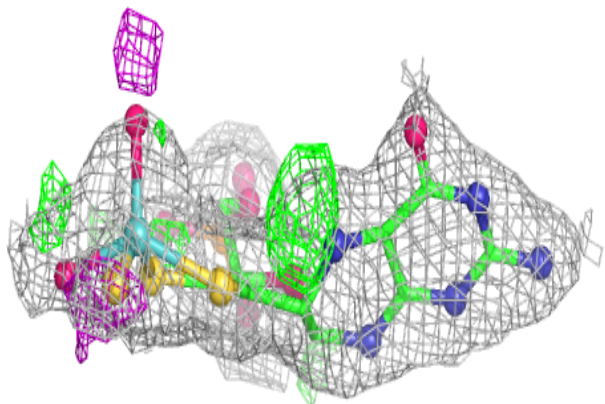
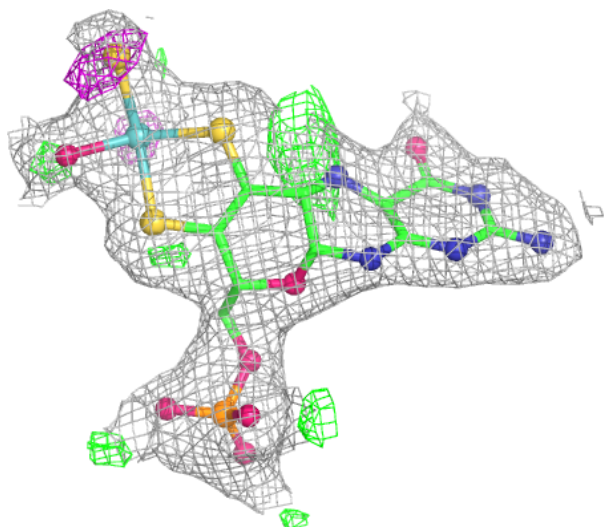
Electron density around FAD A 1335:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



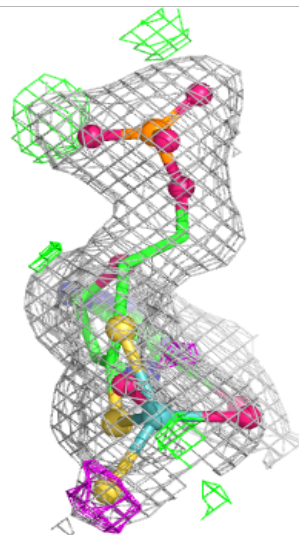
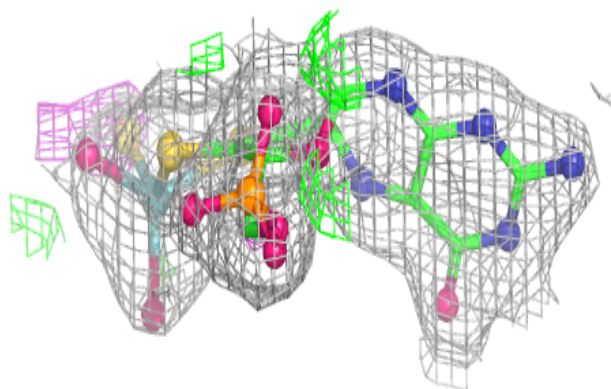
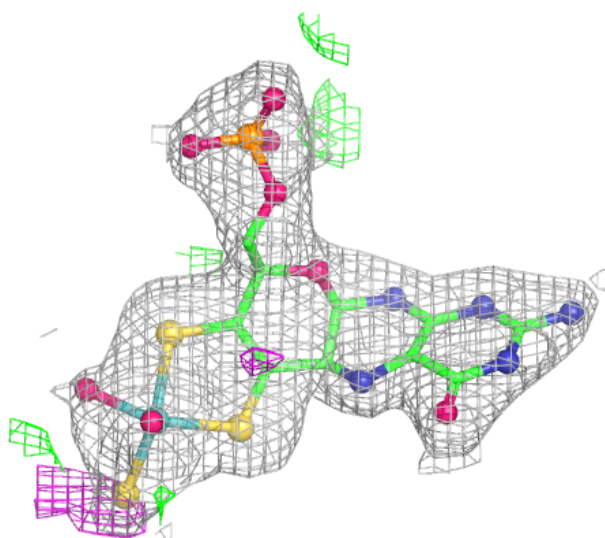
Electron density around XAX B 3003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around XAX A 3003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.