



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:43 PM UTC

PDB ID : 4Y TZ / pdb_00004ytz
Title : Rat xanthine oxidoreductase, C-terminal deletion protein variant, crystal grown without dithiothreitol
Authors : Nishino, T.; Okamoto, K.; Kawaguchi, Y.; Matsumura, T.; Eger, B.T.; Pai, E.F.; Nishino, T.
Deposited on : 2015-03-18
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

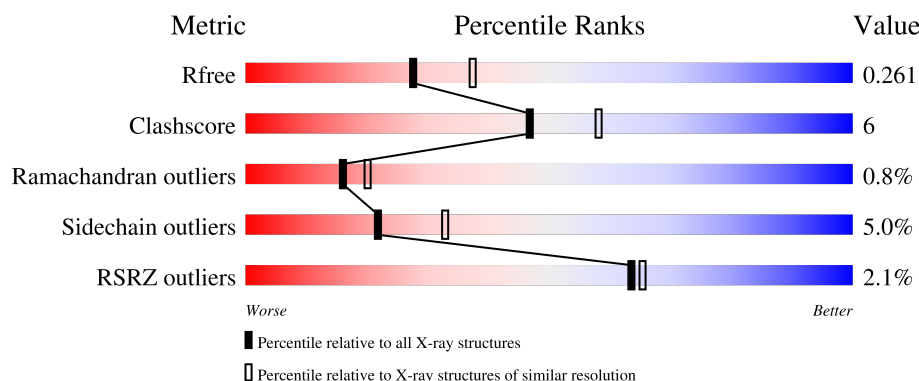
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

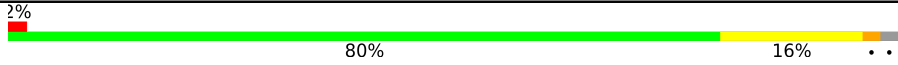
The reported resolution of this entry is 2.30 Å.

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	1315	
1	B	1315	

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
4	URC	A	1404	-	X	-	-

2 Entry composition [i](#)

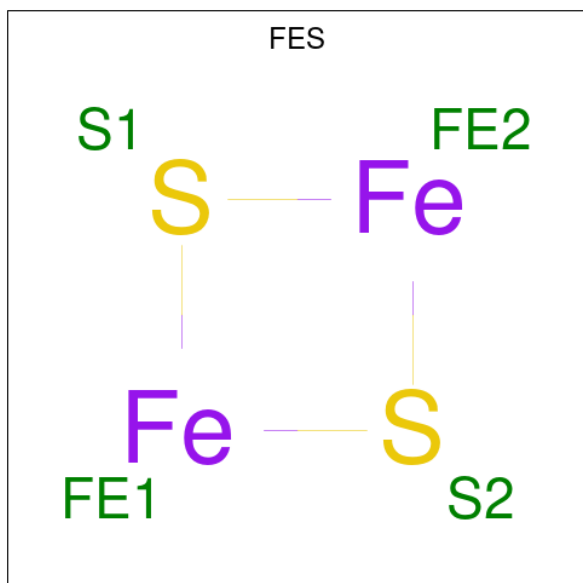
There are 7 unique types of molecules in this entry. The entry contains 20067 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

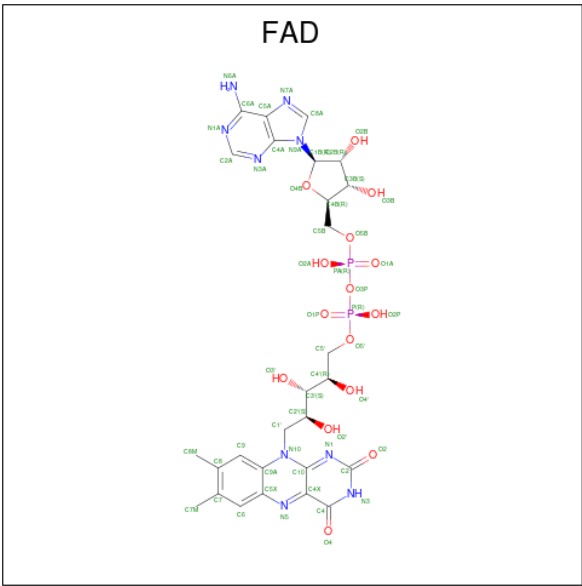
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1289	Total	C	N	O	S	0	0	0
			9964	6314	1714	1873	63			
1	B	1273	Total	C	N	O	S	0	0	0
			9840	6232	1696	1849	63			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



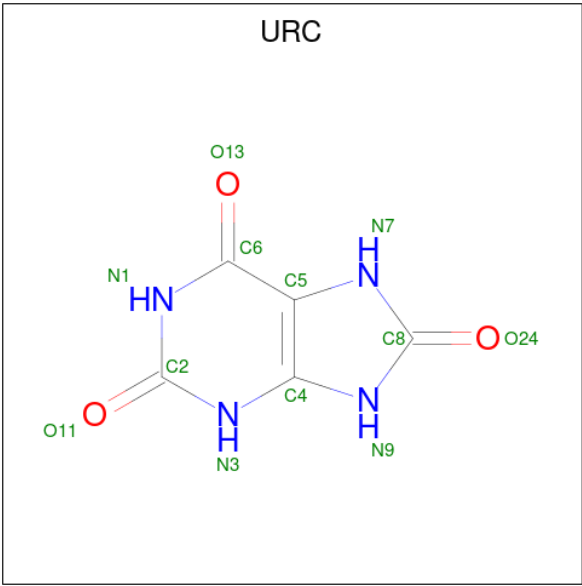
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	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 URIC ACID (CCD ID: URC) (formula: C₅H₄N₄O₃).



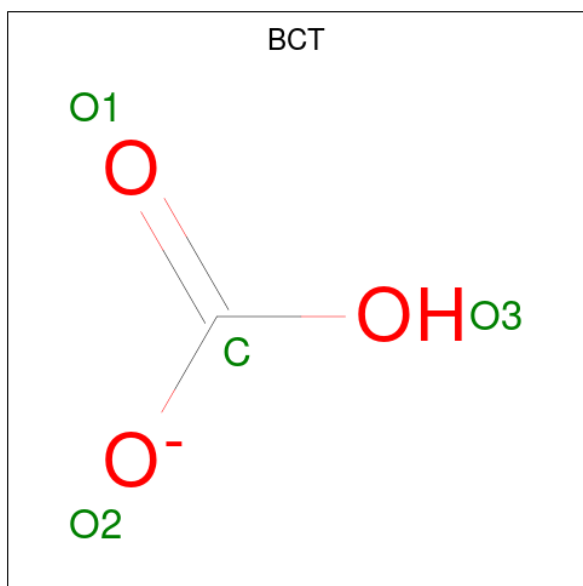
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	5	4	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			12	5	4	3		

- Molecule 5 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Ca	0	0
			2	2		
6	B	2	Total	Ca	0	0
			2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	40	Total	O	0	0
			40	40		
7	B	65	Total	O	0	0
			65	65		

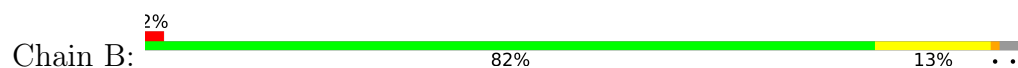
3 Residue-property plots [i](#)

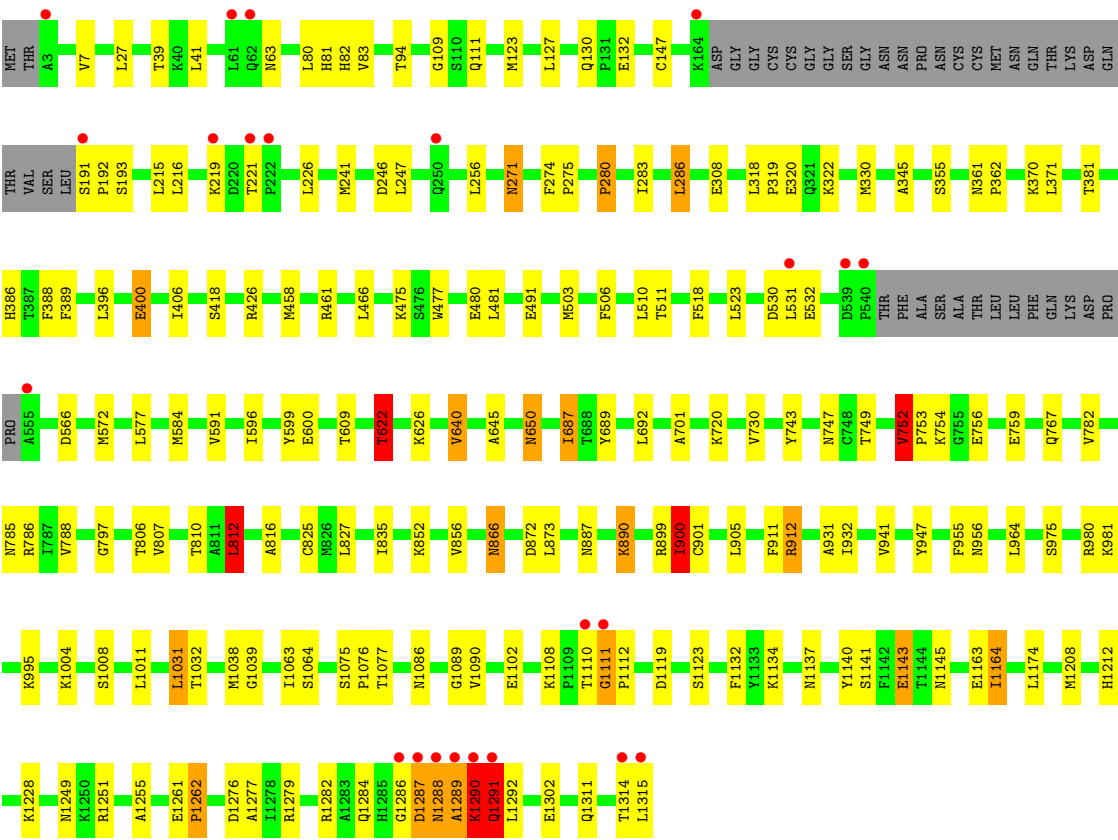
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.17Å 139.12Å 223.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.30 29.87 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.87-2.30) 96.8 (29.87-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.207 , 0.265 0.206 , 0.261	Depositor DCC
R_{free} test set	5404 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 21.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20067	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.14	8/10174 (0.1%)	1.14	29/13767 (0.2%)
1	B	1.22	15/10045 (0.1%)	1.18	19/13588 (0.1%)
All	All	1.18	23/20219 (0.1%)	1.16	48/27355 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	905	LEU	CA-C	7.04	1.59	1.52
1	A	310	VAL	CA-CB	6.48	1.62	1.54
1	B	1064	SER	CA-C	6.38	1.60	1.52
1	B	355	SER	C-O	-5.89	1.16	1.24
1	A	446	ILE	CA-CB	5.78	1.61	1.54
1	B	812	LEU	N-CA	-5.75	1.39	1.46
1	B	1032	THR	CA-CB	5.73	1.64	1.53
1	B	1276	ASP	CA-C	5.70	1.60	1.52
1	B	39	THR	CA-C	5.59	1.60	1.52
1	B	591	VAL	N-CA	5.54	1.52	1.46
1	A	1071	VAL	CA-CB	5.52	1.58	1.54
1	A	752	VAL	CA-CB	5.34	1.61	1.54
1	A	553	PRO	CA-C	5.34	1.57	1.52
1	B	596	ILE	CA-CB	5.31	1.62	1.54
1	A	855	THR	CA-CB	5.30	1.59	1.53
1	B	7	VAL	CA-CB	5.28	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	730	VAL	CA-CB	5.28	1.61	1.54
1	A	1289	ALA	CA-CB	5.20	1.62	1.53
1	B	280	PRO	N-CA	-5.16	1.44	1.47
1	B	1110	THR	CA-CB	5.13	1.62	1.54
1	B	147	CYS	C-O	-5.12	1.18	1.24
1	A	788	VAL	CA-CB	5.09	1.60	1.54
1	B	1111	GLY	N-CA	5.05	1.51	1.44

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	ASN	N-CA-C	8.25	122.65	112.58
1	B	1291	GLN	N-CA-C	-7.98	93.79	110.80
1	A	812	LEU	CA-CB-CG	-7.77	89.11	116.30
1	A	1111	GLY	CA-C-N	-7.42	112.68	120.03
1	A	1111	GLY	C-N-CA	-7.42	112.68	120.03
1	B	752	VAL	CB-CA-C	7.16	119.42	111.18
1	B	752	VAL	N-CA-C	6.96	115.04	107.60
1	A	1148	ASN	CA-C-N	-6.91	111.20	119.84
1	A	1148	ASN	C-N-CA	-6.91	111.20	119.84
1	A	499	ALA	CA-C-N	-6.45	113.31	119.76
1	A	499	ALA	C-N-CA	-6.45	113.31	119.76
1	B	812	LEU	CA-CB-CG	-6.44	93.75	116.30
1	B	531	LEU	CA-CB-CG	6.44	138.83	116.30
1	B	640	VAL	N-CA-CB	6.28	115.92	110.08
1	B	1262	PRO	N-CA-C	6.18	118.24	110.70
1	A	353	THR	N-CA-C	-6.10	104.69	111.71
1	B	1064	SER	CB-CA-C	6.10	118.79	109.34
1	A	809	SER	N-CA-C	6.01	118.32	111.11
1	B	692	LEU	CA-C-N	-5.95	113.63	119.76
1	B	692	LEU	C-N-CA	-5.95	113.63	119.76
1	A	421	LYS	N-CA-C	5.91	118.86	108.75
1	A	1089	GLY	N-CA-C	-5.91	105.65	112.50
1	B	80	LEU	N-CA-C	5.85	120.12	112.92
1	A	1262	PRO	CA-C-N	-5.82	113.77	119.64
1	A	1262	PRO	C-N-CA	-5.82	113.77	119.64
1	A	577	LEU	CA-C-N	-5.70	114.09	119.85
1	A	577	LEU	C-N-CA	-5.70	114.09	119.85
1	A	466	LEU	N-CA-C	5.66	118.99	111.75
1	A	1262	PRO	N-CA-C	5.61	117.54	110.70
1	B	900	ILE	CB-CA-C	5.60	118.65	110.98
1	A	1049	VAL	N-CA-C	5.60	116.24	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	971	CYS	N-CA-C	5.50	117.35	111.36
1	A	468	THR	N-CA-C	5.49	116.94	111.07
1	B	622	THR	N-CA-CB	-5.39	102.47	110.61
1	B	1089	GLY	N-CA-C	-5.33	106.19	112.64
1	A	874	SER	N-CA-C	5.30	117.75	111.33
1	A	801	LYS	N-CA-C	-5.29	105.54	112.41
1	B	1112	PRO	N-CA-C	5.22	118.91	111.13
1	B	1137	ASN	N-CA-C	5.15	118.82	111.92
1	B	109	GLY	N-CA-C	-5.13	106.67	115.61
1	A	283	ILE	CA-C-N	5.09	125.12	119.32
1	A	283	ILE	C-N-CA	5.09	125.12	119.32
1	A	486	CYS	N-CA-C	5.08	116.51	111.07
1	B	956	ASN	N-CA-C	5.07	118.73	112.24
1	A	726	ALA	N-CA-C	5.06	117.63	110.10
1	A	596	ILE	CA-C-N	5.03	125.03	119.90
1	A	596	ILE	C-N-CA	5.03	125.03	119.90
1	A	988	ASN	N-CA-C	5.03	116.76	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1111	GLY	Peptide

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	9964	0	9968	118	0
1	B	9840	0	9841	118	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	53	0	31	2	0
3	B	53	0	31	2	0
4	A	12	0	4	0	0
4	B	12	0	4	0	0
5	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	4	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	40	0	0	0	0
7	B	65	0	0	0	0
All	All	20067	0	19879	228	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 (228) 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:B:1291:GLN:O	1:B:1291:GLN:HG3	1.64	0.96
1:B:1282:ARG:HE	1:B:1290:LYS:CB	1.76	0.96
1:B:1282:ARG:HE	1:B:1290:LYS:HB3	1.30	0.96
1:A:191:SER:HB2	1:A:560:PHE:O	1.71	0.90
1:A:461:ARG:HG3	1:A:461:ARG:HH11	1.38	0.88
1:B:1290:LYS:O	1:B:1291:GLN:O	1.91	0.87
1:A:1265:PHE:O	1:A:1268:SER:HB2	1.75	0.86
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.42	0.85
1:A:710:SER:HA	1:A:899:ARG:NH2	1.91	0.85
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.43	0.81
1:A:710:SER:HA	1:A:899:ARG:HH21	1.48	0.79
1:B:1164:ILE:HD13	1:B:1277:ALA:HB1	1.67	0.76
1:A:753:PRO:HD3	1:A:816:ALA:HB1	1.67	0.75
1:B:216:LEU:O	1:B:219:LYS:HG2	1.86	0.75
1:B:1164:ILE:HD13	1:B:1277:ALA:CB	2.20	0.72
1:B:1282:ARG:HE	1:B:1290:LYS:HB2	1.54	0.71
1:B:687:ILE:HG12	1:B:689:TYR:CZ	2.26	0.71
1:A:1289:ALA:HB1	1:A:1290:LYS:HA	1.72	0.70
1:B:388:PHE:CD1	1:B:396:LEU:CD2	2.77	0.68
1:B:752:VAL:HG22	1:B:754:LYS:HE2	1.74	0.68
1:B:1290:LYS:O	1:B:1291:GLN:C	2.37	0.68
1:A:242:GLU:O	1:A:246:ASP:HB2	1.94	0.67
1:A:710:SER:O	1:A:875:ARG:NH2	2.27	0.67
1:A:55:ILE:HG23	1:A:83:VAL:HG13	1.78	0.66
1:A:467:LYS:O	1:A:470:PRO:HD2	1.96	0.66
1:B:1141:SER:OG	1:B:1143:GLU:HG2	1.95	0.66
1:A:606:ARG:HD3	1:A:679:GLN:HA	1.79	0.65
1:A:432:LYS:O	1:A:457:GLY:HA3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:GLU:HB3	1:B:584:MET:SD	2.37	0.65
1:A:58:TYR:CE2	1:A:219:LYS:HD3	2.32	0.64
1:B:900:ILE:C	1:B:900:ILE:HD12	2.23	0.62
1:B:1291:GLN:O	1:B:1291:GLN:CG	2.44	0.62
1:B:1289:ALA:H	1:B:1290:LYS:HZ3	1.46	0.62
1:A:920:MET:HE3	1:A:1265:PHE:CG	2.36	0.61
1:A:598:ARG:O	1:B:600:GLU:HG2	2.00	0.61
1:A:920:MET:HE3	1:A:1265:PHE:CD2	2.36	0.61
1:B:1286:GLY:O	1:B:1287:ASP:HB2	2.01	0.60
1:B:749:THR:HG22	1:B:812:LEU:HD22	1.81	0.60
1:B:1290:LYS:HD2	1:B:1290:LYS:C	2.27	0.60
1:A:324:GLU:HB2	1:A:411:SER:HB3	1.83	0.59
1:A:216:LEU:O	1:A:219:LYS:HG2	2.02	0.59
1:B:1282:ARG:NE	1:B:1290:LYS:CB	2.59	0.58
1:A:216:LEU:O	1:A:219:LYS:CG	2.52	0.58
1:B:318:LEU:HB3	1:B:319:PRO:HD2	1.84	0.58
1:B:1289:ALA:N	1:B:1290:LYS:HZ3	2.00	0.58
1:B:1290:LYS:HZ3	1:B:1290:LYS:H	1.52	0.57
1:A:794:MET:HE3	1:A:1038:MET:HB3	1.86	0.57
1:A:932:ILE:HG12	1:A:1279:ARG:NE	2.19	0.57
1:A:1102:GLU:HG3	1:A:1106:LYS:HE2	1.85	0.57
1:B:1279:ARG:HH12	1:B:1291:GLN:N	2.03	0.57
1:B:1287:ASP:HA	1:B:1288:ASN:O	2.04	0.57
1:B:389:PHE:O	1:B:461:ARG:NH1	2.36	0.57
1:A:708:TYR:CD2	1:A:900:ILE:HD11	2.39	0.57
1:B:388:PHE:CD1	1:B:396:LEU:HD22	2.39	0.56
1:A:812:LEU:HD11	1:A:825:CYS:HB3	1.87	0.56
1:B:458:MET:HE2	1:B:511:THR:HG21	1.87	0.56
1:B:318:LEU:HB3	1:B:319:PRO:CD	2.36	0.56
1:B:191:SER:HB2	1:B:192:PRO:CD	2.36	0.56
1:B:1140:TYR:OH	1:B:1145:ASN:ND2	2.39	0.56
1:B:111:GLN:HB3	1:B:1039:GLY:O	2.07	0.55
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.06	0.55
1:B:426:ARG:HD3	1:B:1212:HIS:CG	2.42	0.55
1:A:461:ARG:HG3	1:A:461:ARG:NH1	2.15	0.54
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	2.05	0.54
1:A:995:LYS:HZ1	1:A:1284:GLN:HE21	1.55	0.54
1:B:1291:GLN:HA	1:B:1292:LEU:HD23	1.90	0.54
1:A:948:LYS:HG2	1:A:951:ASP:OD2	2.08	0.54
1:B:1086:ASN:O	1:B:1090:VAL:HG23	2.07	0.53
1:B:400:GLU:CD	1:B:400:GLU:H	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:955:PHE:HA	1:B:1145:ASN:ND2	2.19	0.53
1:A:263:ILE:HG22	1:A:267:MET:HE2	1.90	0.53
1:B:1282:ARG:NE	1:B:1290:LYS:HB2	2.20	0.53
1:A:132:GLU:HB3	1:A:165:ASP:HB2	1.89	0.53
1:A:483:GLN:HE22	1:A:1311:GLN:HE22	1.55	0.53
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	2.07	0.53
1:A:521:THR:HG22	1:A:525:LYS:HD2	1.91	0.52
1:B:191:SER:CB	1:B:192:PRO:CD	2.88	0.52
1:B:1287:ASP:OD2	1:B:1290:LYS:NZ	2.43	0.52
1:A:812:LEU:HD11	1:A:825:CYS:CB	2.40	0.52
1:B:645:ALA:HB1	1:B:650:ASN:ND2	2.24	0.52
1:B:812:LEU:HD11	1:B:825:CYS:HB3	1.91	0.52
1:A:812:LEU:CD1	1:A:825:CYS:HB3	2.40	0.52
1:B:753:PRO:HD3	1:B:816:ALA:HB1	1.91	0.52
1:B:1038:MET:HE3	1:B:1077:THR:CG2	2.40	0.52
1:B:1279:ARG:HH12	1:B:1291:GLN:CA	2.23	0.51
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.92	0.51
1:A:911:PHE:O	1:A:912:ARG:C	2.52	0.51
1:A:157:GLN:HE22	1:A:558:GLN:HE22	1.58	0.51
1:A:880:ARG:HD2	1:A:914:PHE:O	2.11	0.51
1:B:388:PHE:CD1	1:B:396:LEU:HD21	2.46	0.51
1:B:503:MET:HG2	1:B:1302:GLU:CD	2.36	0.50
1:B:747:ASN:HB2	1:B:827:LEU:HD12	1.93	0.50
1:B:866:ASN:C	1:B:866:ASN:HD22	2.19	0.50
1:B:975:SER:O	1:B:980:ARG:HD3	2.11	0.50
1:B:1119:ASP:O	1:B:1123:SER:HB3	2.12	0.50
1:A:1158:ALA:HA	1:A:1177:ASP:O	2.11	0.50
1:B:1286:GLY:O	1:B:1287:ASP:CB	2.60	0.50
1:B:806:THR:O	1:B:810:THR:HG23	2.12	0.50
1:B:1163:GLU:HB2	1:B:1174:LEU:HD11	1.94	0.49
1:A:241:MET:HE2	1:A:283:ILE:HG21	1.93	0.49
1:A:995:LYS:NZ	1:A:1284:GLN:NE2	2.61	0.49
1:A:290:VAL:HG13	1:A:297:SER:HB2	1.93	0.49
1:A:793:ARG:NH1	1:B:756:GLU:OE2	2.35	0.49
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.28	0.49
1:B:1279:ARG:NH1	1:B:1291:GLN:HB3	2.27	0.49
1:B:911:PHE:O	1:B:912:ARG:C	2.55	0.49
1:A:132:GLU:HB3	1:A:165:ASP:CB	2.43	0.48
1:A:599:TYR:HA	1:B:599:TYR:HA	1.94	0.48
1:B:27:LEU:HD21	1:B:41:LEU:HB2	1.95	0.48
1:B:622:THR:CG2	1:B:626:LYS:HE3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:SER:CB	1:B:192:PRO:HD3	2.44	0.47
1:A:708:TYR:HB2	1:A:900:ILE:HG13	1.96	0.47
1:B:1290:LYS:O	1:B:1290:LYS:HD2	2.14	0.47
1:A:345:ALA:HB1	3:A:1403:FAD:H4'	1.97	0.47
1:B:812:LEU:HD11	1:B:825:CYS:CB	2.45	0.47
1:B:1289:ALA:C	1:B:1290:LYS:O	2.57	0.47
1:B:386:HIS:CG	1:B:466:LEU:HD11	2.49	0.47
1:B:477:TRP:HD1	1:B:523:LEU:HD23	1.79	0.47
1:A:880:ARG:HB3	1:A:914:PHE:O	2.14	0.47
1:B:1075:SER:HB3	1:B:1076:PRO:HD2	1.96	0.47
1:B:1282:ARG:NE	1:B:1290:LYS:HB3	2.13	0.47
1:B:191:SER:HB2	1:B:192:PRO:HD3	1.96	0.47
1:A:99:PRO:HG2	1:A:203:LEU:HD13	1.98	0.46
1:A:322:LYS:HD3	1:A:410:TYR:HB3	1.97	0.46
1:A:884:HIS:HB3	1:A:920:MET:HG3	1.97	0.46
1:A:708:TYR:HD2	1:A:900:ILE:HD11	1.81	0.46
1:B:1290:LYS:HZ3	1:B:1290:LYS:N	2.13	0.46
1:B:418:SER:HB2	1:B:518:PHE:CD1	2.51	0.46
1:B:1141:SER:HG	1:B:1143:GLU:HG2	1.79	0.46
1:A:138:ILE:HD12	1:A:163:ALA:HB2	1.98	0.46
1:A:153:ARG:HG2	1:A:556:ASN:ND2	2.32	0.46
1:A:792:LYS:NZ	1:A:1064:SER:O	2.44	0.46
1:A:1187:ASN:HA	1:A:1188:PRO:HD2	1.81	0.45
1:A:1003:THR:HG22	1:A:1266:LEU:HD21	1.98	0.45
1:A:1151:HIS:NE2	1:A:1251:ARG:O	2.48	0.45
1:B:475:LYS:HA	1:B:475:LYS:HD3	1.73	0.45
1:B:900:ILE:HD12	1:B:901:CYS:N	2.31	0.45
1:B:1290:LYS:O	1:B:1291:GLN:HG3	2.16	0.45
1:A:280:PRO:HB2	1:A:286:LEU:HD23	1.99	0.45
1:A:969:ASP:HA	1:A:972:ILE:HG12	1.97	0.45
1:A:446:ILE:HD11	1:A:535:CYS:HB3	1.99	0.45
1:A:1046:MET:HA	1:A:1046:MET:HE2	1.98	0.45
1:A:241:MET:O	1:A:245:LEU:HG	2.17	0.45
1:A:516:PHE:CE2	1:A:520:LEU:HD11	2.51	0.45
1:A:1034:GLY:HA3	1:A:1074:THR:HG21	1.99	0.45
1:B:361:ASN:N	1:B:362:PRO:CD	2.80	0.45
1:B:572:MET:HE2	1:B:577:LEU:HD13	1.99	0.45
1:B:767:GLN:HG2	1:B:1038:MET:CE	2.46	0.45
1:A:1204:GLY:HA3	1:A:1209:GLU:OE2	2.17	0.45
1:A:58:TYR:CZ	1:A:219:LYS:HD3	2.52	0.44
1:A:549:PHE:CE2	1:A:551:LYS:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:926:TRP:CE3	1:A:927:MET:N	2.85	0.44
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.80	0.44
1:A:51:CYS:SG	1:A:71:ASN:HB3	2.58	0.44
1:A:216:LEU:O	1:A:219:LYS:HG3	2.17	0.44
1:A:336:PHE:O	1:A:337:ALA:O	2.36	0.44
1:B:1287:ASP:HA	1:B:1288:ASN:C	2.42	0.44
1:A:792:LYS:HE3	1:B:756:GLU:OE1	2.17	0.44
1:A:55:ILE:HG23	1:A:83:VAL:CG1	2.46	0.44
1:A:762:LEU:N	1:A:762:LEU:HD12	2.33	0.44
1:B:785:ASN:OD1	1:B:786:ARG:NH1	2.49	0.44
1:A:324:GLU:HB2	1:A:411:SER:CB	2.48	0.43
1:A:812:LEU:HD21	1:A:823:VAL:O	2.18	0.43
1:B:81:HIS:O	1:B:82:HIS:HB2	2.16	0.43
1:B:241:MET:HE2	1:B:283:ILE:HG21	1.98	0.43
1:B:308:GLU:HG2	1:B:330:MET:HE1	2.01	0.43
1:A:652:GLU:HB2	1:A:870:THR:HG21	2.00	0.43
1:A:469:THR:N	1:A:470:PRO:CD	2.81	0.43
1:B:1279:ARG:HH12	1:B:1291:GLN:CB	2.32	0.43
1:A:720:LYS:HA	1:A:720:LYS:HD3	1.57	0.43
1:B:271:ASN:O	1:B:271:ASN:CG	2.62	0.43
1:B:931:ALA:HA	1:B:941:VAL:HG21	2.00	0.43
1:A:1080:SER:OG	1:A:1261:GLU:HG3	2.18	0.43
1:B:1279:ARG:HH12	1:B:1291:GLN:HB3	1.83	0.43
1:B:481:LEU:C	1:B:481:LEU:HD23	2.44	0.43
1:A:646:THR:HG23	1:A:647:GLY:N	2.34	0.42
1:B:701:ALA:CB	1:B:901:CYS:HB3	2.49	0.42
1:A:750:ILE:HG12	1:A:824:ARG:HB2	2.01	0.42
1:A:1124:ALA:HB3	1:B:1134:LYS:HD2	2.00	0.42
1:B:872:ASP:CG	1:B:873:LEU:H	2.27	0.42
1:A:191:SER:CB	1:A:560:PHE:O	2.54	0.42
1:A:516:PHE:CZ	1:A:520:LEU:HD11	2.55	0.42
1:A:640:VAL:HA	1:A:641:PRO:HD3	1.89	0.42
1:B:609:THR:HG21	1:B:835:ILE:HD11	2.01	0.42
1:A:1180:MET:HE2	1:A:1262:PRO:HB2	2.01	0.42
1:B:345:ALA:HB1	3:B:1403:FAD:H4'	2.01	0.42
1:A:315:ILE:HD13	1:A:327:ARG:HG2	2.00	0.42
1:A:792:LYS:NZ	1:B:759:GLU:OE1	2.49	0.42
1:B:995:LYS:HZ1	1:B:1284:GLN:HE21	1.66	0.42
1:B:645:ALA:HB1	1:B:650:ASN:HD22	1.85	0.42
1:A:337:ALA:HB2	3:A:1403:FAD:C6	2.50	0.42
1:A:1086:ASN:O	1:A:1090:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:NE	1:A:1201:GLN:HE21	2.17	0.42
1:A:441:PHE:CE2	1:A:526:LEU:HD21	2.55	0.42
1:A:644:ASN:O	1:A:653:THR:HA	2.20	0.42
1:B:1208:MET:HG2	1:B:1228:LYS:O	2.20	0.42
1:A:1075:SER:HB3	1:A:1076:PRO:HD2	2.02	0.41
1:A:336:PHE:CD1	1:A:336:PHE:C	2.99	0.41
1:A:995:LYS:HZ3	1:A:1284:GLN:NE2	2.18	0.41
1:B:506:PHE:CZ	1:B:510:LEU:HD11	2.55	0.41
1:A:365:MET:HG2	1:A:454:CYS:SG	2.61	0.41
1:A:1021:VAL:HG12	1:A:1093:ALA:HB1	2.03	0.41
1:B:256:LEU:O	3:B:1403:FAD:H2B	2.20	0.41
1:B:899:ARG:HD2	1:B:899:ARG:HA	1.92	0.41
1:A:670:VAL:HG21	1:A:682:ALA:HA	2.02	0.41
1:B:274:PHE:HA	1:B:275:PRO:HD3	1.87	0.41
1:B:1038:MET:HE3	1:B:1077:THR:HG21	2.02	0.41
1:A:900:ILE:HD12	1:A:900:ILE:C	2.46	0.41
1:B:130:GLN:HE21	1:B:132:GLU:H	1.68	0.41
1:A:889:TYR:OH	1:A:924:GLU:OE2	2.36	0.41
1:B:280:PRO:HB2	1:B:286:LEU:HD23	2.03	0.41
1:B:371:LEU:HD12	1:B:388:PHE:CE1	2.55	0.41
1:A:912:ARG:NH2	1:A:1198:ALA:HB2	2.36	0.40
1:A:842:PHE:HA	1:A:864:PHE:O	2.21	0.40
1:A:1185:SER:OG	1:A:1191:ASP:OD2	2.37	0.40
1:A:1228:LYS:HA	1:A:1228:LYS:HD2	1.83	0.40
1:B:123:MET:HE3	1:B:127:LEU:HG	2.03	0.40
1:A:45:GLU:OE2	1:A:1225:SER:HB3	2.21	0.40
1:A:149:CYS:O	1:A:1197:GLY:HA3	2.22	0.40
1:A:628:VAL:HG21	1:A:681:ALA:HA	2.02	0.40
1:A:571:ASP:OD2	1:A:1052:ARG:HD2	2.21	0.40
1:A:1126:SER:HB2	1:B:1132:PHE:CG	2.56	0.40
1:B:81:HIS:CD2	1:B:226:LEU:HD11	2.57	0.40
1:B:215:LEU:HA	1:B:215:LEU:HD23	1.81	0.40
1:B:1031:LEU:HB3	1:B:1063:ILE:HG12	2.03	0.40
1:A:709:GLY:O	1:A:899:ARG:NH2	2.51	0.40
1:A:804:ARG:HG3	1:A:836:THR:O	2.21	0.40
1:B:890:LYS:HE2	1:B:890:LYS:HB3	1.81	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	1285/1315 (98%)	1218 (95%)	59 (5%)	8 (1%)	21	27
1	B	1267/1315 (96%)	1213 (96%)	42 (3%)	12 (1%)	14	17
All	All	2552/2630 (97%)	2431 (95%)	101 (4%)	20 (1%)	16	20

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	ALA
1	A	1008	SER
1	B	1008	SER
1	B	1287	ASP
1	B	1288	ASN
1	B	1289	ALA
1	B	1290	LYS
1	B	532	GLU
1	B	797	GLY
1	B	912	ARG
1	B	947	TYR
1	A	164	LYS
1	A	912	ARG
1	A	423	ALA
1	A	797	GLY
1	B	530	ASP
1	B	1291	GLN
1	A	390	PRO
1	A	556	ASN
1	B	887	ASN

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	1088/1109 (98%)	1029 (95%)	59 (5%)	20	29
1	B	1074/1109 (97%)	1025 (95%)	49 (5%)	24	36
All	All	2162/2218 (98%)	2054 (95%)	108 (5%)	22	33

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	83	VAL
1	A	99	PRO
1	A	160	ARG
1	A	190	LEU
1	A	203	LEU
1	A	219	LYS
1	A	221	THR
1	A	246	ASP
1	A	253	ASP
1	A	270	LYS
1	A	285	GLU
1	A	286	LEU
1	A	297	SER
1	A	310	VAL
1	A	320	GLU
1	A	343	SER
1	A	396	LEU
1	A	404	LEU
1	A	411	SER
1	A	426	ARG
1	A	445	THR
1	A	446	ILE
1	A	461	ARG
1	A	473	LEU
1	A	494	GLN
1	A	508	ARG
1	A	512	LEU
1	A	531	LEU
1	A	550	GLN
1	A	557	VAL

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Mol	Chain	Res	Type
1	A	565	LYS
1	A	640	VAL
1	A	720	LYS
1	A	743	TYR
1	A	744	LEU
1	A	752	VAL
1	A	788	VAL
1	A	812	LEU
1	A	856	VAL
1	A	866	ASN
1	A	899	ARG
1	A	900	ILE
1	A	932	ILE
1	A	943	ARG
1	A	981	LYS
1	A	983	GLU
1	A	985	GLU
1	A	1004	LYS
1	A	1031	LEU
1	A	1064	SER
1	A	1085	LEU
1	A	1107	LYS
1	A	1143	GLU
1	A	1159	CYS
1	A	1203	LEU
1	A	1221	THR
1	A	1234	SER
1	A	1268	SER
1	B	83	VAL
1	B	94	THR
1	B	193	SER
1	B	221	THR
1	B	246	ASP
1	B	247	LEU
1	B	271	ASN
1	B	286	LEU
1	B	320	GLU
1	B	322	LYS
1	B	370	LYS
1	B	381	THR
1	B	400	GLU
1	B	406	ILE

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Mol	Chain	Res	Type
1	B	480	GLU
1	B	491	GLU
1	B	566	ASP
1	B	622	THR
1	B	640	VAL
1	B	650	ASN
1	B	687	ILE
1	B	720	LYS
1	B	743	TYR
1	B	752	VAL
1	B	782	VAL
1	B	788	VAL
1	B	807	VAL
1	B	812	LEU
1	B	852	LYS
1	B	856	VAL
1	B	866	ASN
1	B	890	LYS
1	B	900	ILE
1	B	932	ILE
1	B	964	LEU
1	B	981	LYS
1	B	1004	LYS
1	B	1011	LEU
1	B	1031	LEU
1	B	1102	GLU
1	B	1108	LYS
1	B	1143	GLU
1	B	1164	ILE
1	B	1251	ARG
1	B	1290	LYS
1	B	1291	GLN
1	B	1311	GLN
1	B	1314	THR
1	B	1315	LEU

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

Mol	Chain	Res	Type
1	A	71	ASN
1	A	130	GLN
1	A	207	GLN

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Mol	Chain	Res	Type
1	A	223	GLN
1	A	260	ASN
1	A	321	GLN
1	A	478	ASN
1	A	483	GLN
1	A	524	GLN
1	A	558	GLN
1	A	650	ASN
1	A	866	ASN
1	A	1088	GLN
1	A	1145	ASN
1	A	1220	HIS
1	A	1284	GLN
1	A	1285	HIS
1	A	1288	ASN
1	B	71	ASN
1	B	130	GLN
1	B	140	ASN
1	B	143	GLN
1	B	157	GLN
1	B	207	GLN
1	B	223	GLN
1	B	260	ASN
1	B	271	ASN
1	B	350	ASN
1	B	650	ASN
1	B	705	ASN
1	B	866	ASN
1	B	1088	GLN
1	B	1095	GLN
1	B	1145	ASN
1	B	1194	GLN
1	B	1284	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	$\# Z > 2$
5	BCT	A	1405	-	3,3,3	1.72	1 (33%)	2,3,3	0.52	0
2	FES	B	1401	1	0,4,4	-	-	-		
2	FES	B	1402	1	0,4,4	-	-	-		
3	FAD	B	1403	-	58,58,58	1.26	5 (8%)	85,89,89	1.87	25 (29%)
4	URC	B	1404	-	13,13,13	4.38	5 (38%)	17,19,19	2.61	6 (35%)
2	FES	A	1401	1	0,4,4	-	-	-		
4	URC	A	1404	-	13,13,13	4.40	5 (38%)	17,19,19	2.81	9 (52%)
2	FES	A	1402	1	0,4,4	-	-	-		
3	FAD	A	1403	-	58,58,58	1.15	5 (8%)	85,89,89	1.58	16 (18%)
5	BCT	B	1405	-	3,3,3	0.83	0	2,3,3	1.34	0

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	B	1401	1	-	-	0/1/1/1
2	FES	B	1402	1	-	-	0/1/1/1
3	FAD	B	1403	-	-	2/34/50/50	0/6/6/6
4	URC	B	1404	-	-	-	0/2/2/2
2	FES	A	1401	1	-	-	0/1/1/1
4	URC	A	1404	-	-	-	0/2/2/2
2	FES	A	1402	1	-	-	0/1/1/1
3	FAD	A	1403	-	-	0/34/50/50	0/6/6/6

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1404	URC	O24-C8	11.61	1.48	1.23
4	A	1404	URC	O24-C8	11.49	1.47	1.23
4	A	1404	URC	O13-C6	8.41	1.39	1.23
4	B	1404	URC	O13-C6	7.53	1.37	1.23
4	B	1404	URC	O11-C2	6.14	1.36	1.23
4	A	1404	URC	O11-C2	5.43	1.34	1.23
3	B	1403	FAD	C4X-N5	3.68	1.38	1.30
3	B	1403	FAD	C2A-N1A	3.19	1.39	1.33
3	A	1403	FAD	C10-N1	3.16	1.39	1.33
3	B	1403	FAD	C8A-N7A	3.04	1.37	1.31
4	A	1404	URC	C5-C4	2.89	1.42	1.37
3	A	1403	FAD	C2A-N1A	2.82	1.38	1.33
4	A	1404	URC	C5-C6	2.75	1.50	1.41
5	A	1405	BCT	O1-C	2.71	1.35	1.25
3	A	1403	FAD	C4X-N5	2.71	1.36	1.30
3	A	1403	FAD	C5A-N7A	-2.64	1.34	1.39
4	B	1404	URC	C5-C6	2.34	1.48	1.41
3	B	1403	FAD	C4-N3	-2.17	1.34	1.38
3	A	1403	FAD	C2A-N3A	2.12	1.37	1.33
3	B	1403	FAD	C2-N3	-2.10	1.34	1.39
4	B	1404	URC	C6-N1	-2.10	1.34	1.38

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1404	URC	N7-C8-N9	6.70	116.71	107.22
3	B	1403	FAD	N3A-C2A-N1A	-6.14	119.28	128.58
4	B	1404	URC	N7-C8-N9	5.69	115.28	107.22
4	A	1404	URC	N3-C2-N1	5.25	123.99	115.74
4	B	1404	URC	N3-C2-N1	4.96	123.54	115.74
3	A	1403	FAD	N3A-C2A-N1A	-4.90	121.17	128.58
4	A	1404	URC	C5-N7-C8	-4.06	103.59	108.82
3	B	1403	FAD	C5X-C9A-N10	3.88	121.48	117.97
3	B	1403	FAD	C5A-N7A-C8A	3.86	109.51	103.45
3	B	1403	FAD	N9A-C8A-N7A	-3.85	108.48	113.94
3	A	1403	FAD	C5A-N7A-C8A	3.78	109.39	103.45
3	B	1403	FAD	C5A-C4A-N3A	-3.76	121.54	126.72
3	A	1403	FAD	O2P-P-O3P	3.70	117.28	107.27
3	B	1403	FAD	C9A-C5X-N5	-3.69	118.54	122.45
3	A	1403	FAD	N9A-C8A-N7A	-3.68	108.71	113.94
4	B	1404	URC	C6-N1-C2	-3.58	121.44	126.37
4	B	1404	URC	C5-N7-C8	-3.51	104.30	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1403	FAD	C4X-C10-N10	3.50	121.48	116.48
3	A	1403	FAD	C5A-C4A-N3A	-3.44	121.99	126.72
3	A	1403	FAD	C4A-C5A-N7A	-3.37	106.73	110.58
3	B	1403	FAD	C4-N3-C2	-3.35	119.69	125.64
4	A	1404	URC	C6-N1-C2	-3.26	121.88	126.37
3	B	1403	FAD	C2A-N3A-C4A	3.13	119.48	111.83
3	B	1403	FAD	C4A-C5A-N7A	-3.01	107.14	110.58
4	A	1404	URC	O24-C8-N7	-3.01	120.10	125.56
4	B	1404	URC	O13-C6-C5	-3.01	120.01	127.26
3	A	1403	FAD	O3'-C3'-C2'	-3.01	102.10	108.93
3	B	1403	FAD	C4X-C4-N3	2.88	120.60	113.25
3	B	1403	FAD	O4-C4-N3	-2.71	115.01	120.11
3	A	1403	FAD	C2A-N3A-C4A	2.66	118.34	111.83
3	B	1403	FAD	C6-C5X-C9A	2.66	122.70	119.05
3	B	1403	FAD	O2A-PA-O3P	2.58	114.24	107.27
3	B	1403	FAD	O3'-C3'-C2'	-2.48	103.30	108.93
3	B	1403	FAD	C4X-C10-N1	-2.47	118.53	124.59
3	A	1403	FAD	C4-N3-C2	-2.46	121.27	125.64
3	B	1403	FAD	C5'-C4'-C3'	-2.39	107.72	112.22
3	B	1403	FAD	C2A-N1A-C6A	2.33	122.56	118.73
3	A	1403	FAD	C4X-C10-N10	2.31	119.78	116.48
3	A	1403	FAD	C6-C5X-C9A	2.30	122.21	119.05
3	A	1403	FAD	C5A-C4A-N9A	2.28	108.30	105.81
4	A	1404	URC	O11-C2-N1	-2.27	117.83	121.86
3	B	1403	FAD	C8M-C8-C9	-2.26	115.59	119.57
3	A	1403	FAD	C4-C4X-C10	2.26	120.81	116.93
3	A	1403	FAD	C1'-C2'-C3'	-2.24	103.58	109.66
3	A	1403	FAD	O4-C4-C4X	-2.20	120.72	126.53
4	B	1404	URC	O11-C2-N1	-2.18	118.00	121.86
3	B	1403	FAD	C9A-N10-C10	-2.17	117.44	120.75
3	A	1403	FAD	C2B-C1B-N9A	2.15	118.65	113.30
4	A	1404	URC	O13-C6-C5	-2.10	122.20	127.26
3	B	1403	FAD	C10-N1-C2	2.09	121.37	116.85
3	B	1403	FAD	C9-C8-C7	2.08	122.74	119.69
4	A	1404	URC	O11-C2-N3	-2.08	118.17	121.86
3	B	1403	FAD	O4'-C4'-C3'	2.07	114.10	109.25
3	B	1403	FAD	O3B-C3B-C4B	-2.04	105.21	111.08
3	B	1403	FAD	N3A-C4A-N9A	2.01	130.58	127.17
4	A	1404	URC	C5-C4-N9	2.00	111.13	108.31

There are no chirality outliers.

All (2) torsion outliers are listed below:

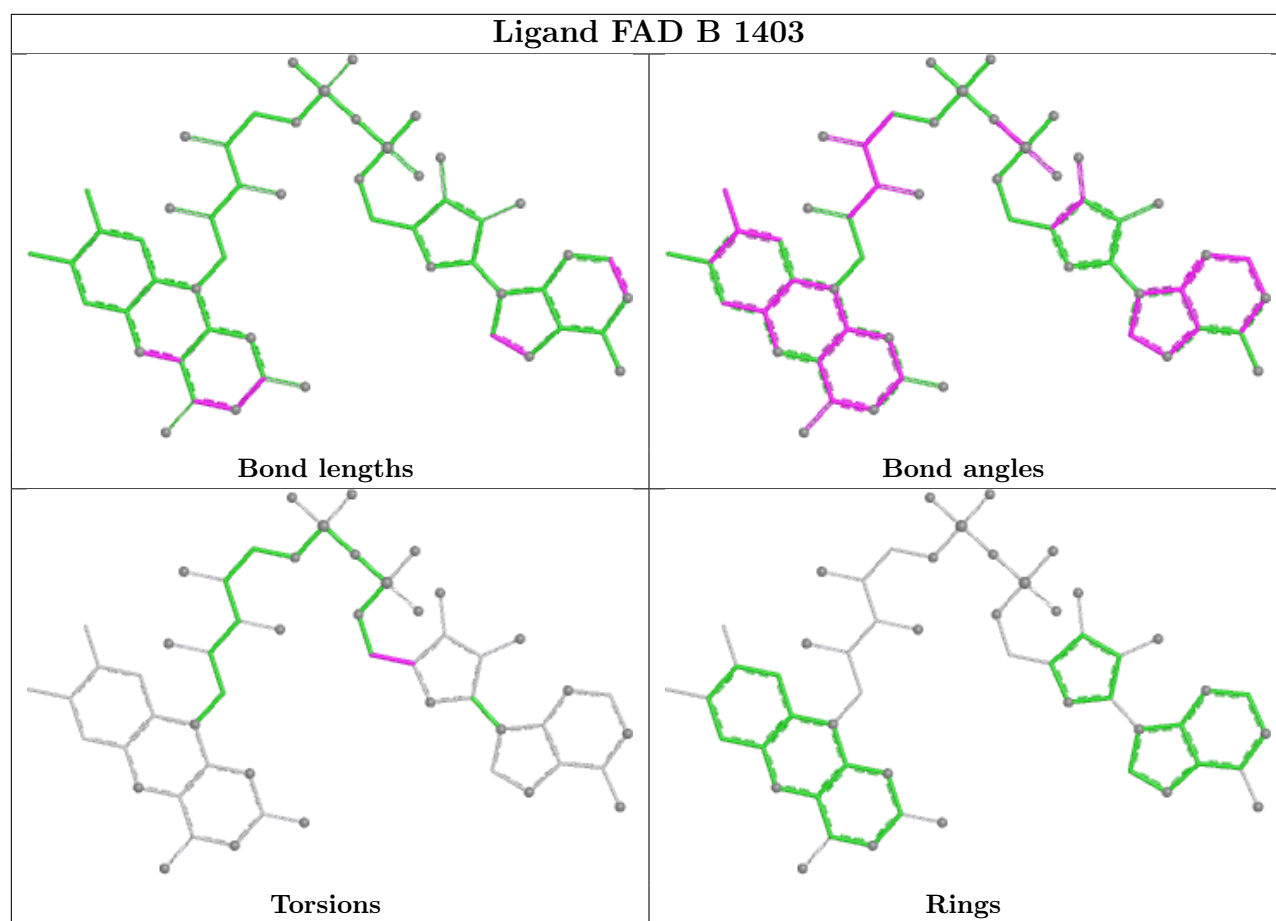
Mol	Chain	Res	Type	Atoms
3	B	1403	FAD	C3B-C4B-C5B-O5B
3	B	1403	FAD	O4B-C4B-C5B-O5B

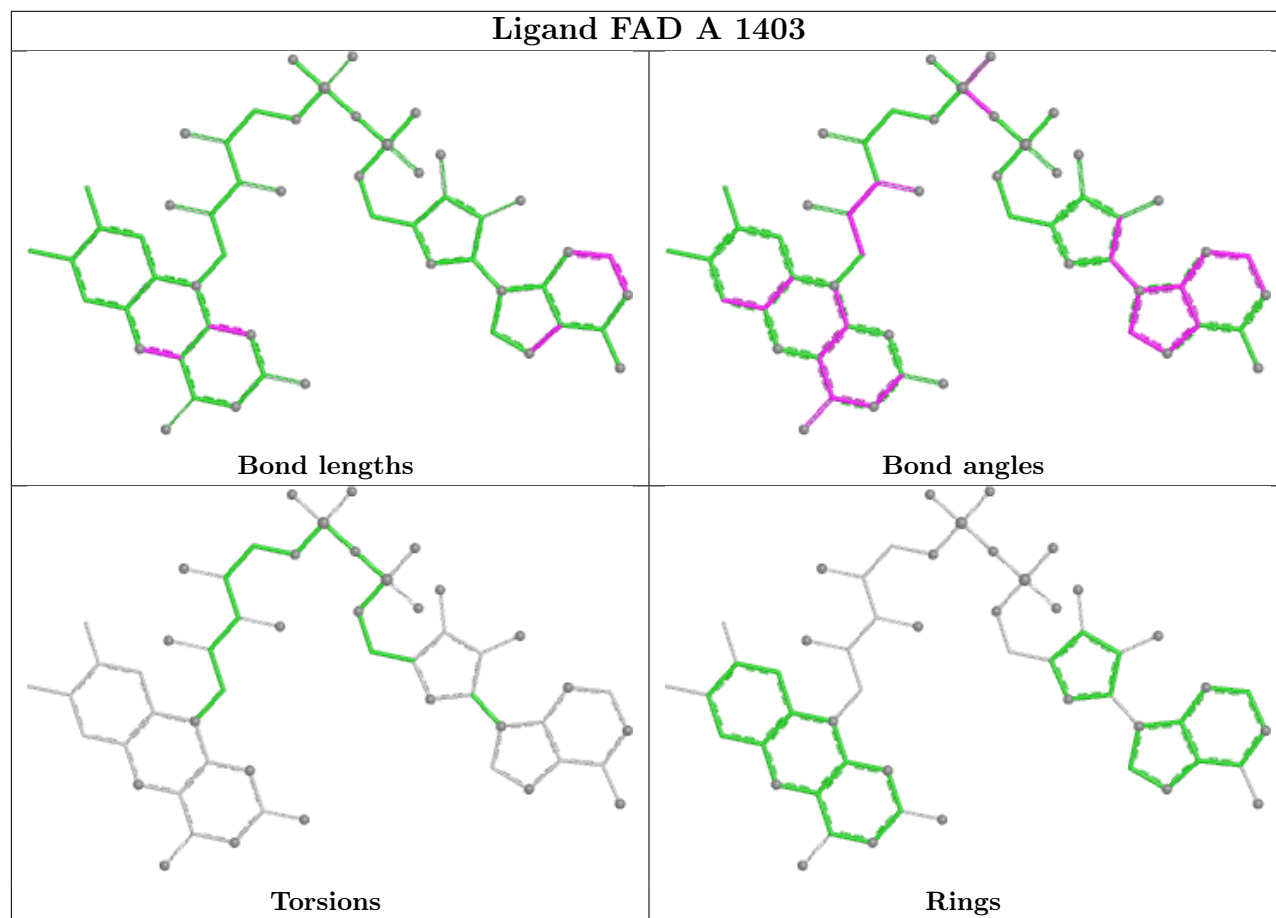
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1403	FAD	2	0
3	A	1403	FAD	2	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.





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	1289/1315 (98%)	-0.06	32 (2%) 58 60	20, 35, 59, 94	0
1	B	1273/1315 (96%)	-0.33	23 (1%) 67 69	18, 30, 48, 75	0
All	All	2562/2630 (97%)	-0.19	55 (2%) 63 65	18, 32, 56, 94	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1315	LEU	6.2
1	A	536	GLY	5.5
1	A	1315	LEU	4.8
1	A	1289	ALA	4.6
1	A	534	MET	4.6
1	A	190	LEU	4.3
1	A	423	ALA	4.3
1	A	61	LEU	4.3
1	A	535	CYS	3.8
1	A	165	ASP	3.8
1	B	1314	THR	3.7
1	B	1288	ASN	3.6
1	A	531	LEU	3.6
1	A	553	PRO	3.6
1	B	555	ALA	3.4
1	B	1286	GLY	3.4
1	A	3	ALA	3.3
1	B	531	LEU	3.3
1	B	61	LEU	3.2
1	B	1287	ASP	3.2
1	B	1110	THR	3.1
1	A	551	LYS	3.0
1	B	1289	ALA	2.9
1	A	335	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	537	LYS	2.8
1	A	1111	GLY	2.8
1	B	1111	GLY	2.8
1	B	540	PRO	2.8
1	A	972	ILE	2.7
1	A	555	ALA	2.6
1	A	222	PRO	2.6
1	B	1290	LYS	2.5
1	A	431	ALA	2.4
1	A	529	ALA	2.4
1	A	533	ASP	2.4
1	A	424	SER	2.4
1	A	164	LYS	2.4
1	A	220	ASP	2.3
1	B	222	PRO	2.3
1	B	1291	GLN	2.3
1	B	219	LYS	2.2
1	B	539	ASP	2.2
1	B	62	GLN	2.2
1	B	164	LYS	2.2
1	A	293	PRO	2.2
1	A	1290	LYS	2.1
1	A	1286	GLY	2.1
1	A	1110	THR	2.1
1	B	3	ALA	2.1
1	A	552	ASP	2.1
1	B	191	SER	2.0
1	B	221	THR	2.0
1	A	550	GLN	2.0
1	A	413	GLU	2.0
1	B	250	GLN	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

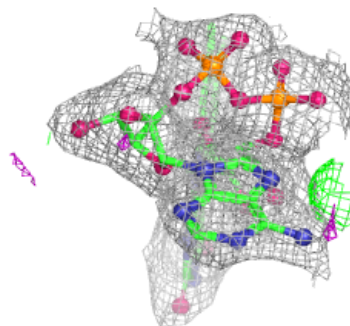
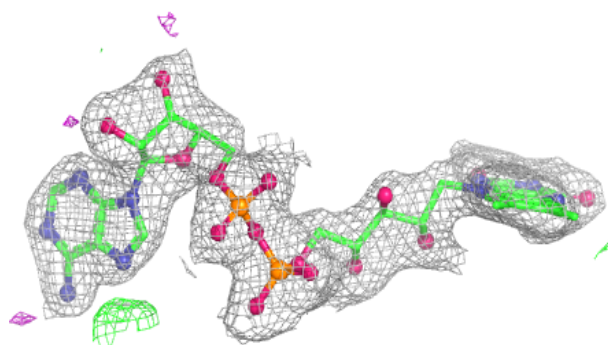
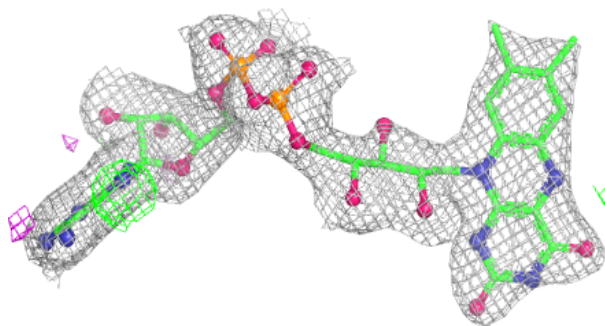
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	URC	A	1404	12/12	0.92	0.08	36,39,41,41	0
4	URC	B	1404	12/12	0.96	0.06	31,34,37,38	0
5	BCT	B	1405	4/4	0.96	0.06	23,24,24,25	0
5	BCT	A	1405	4/4	0.97	0.09	30,33,33,34	0
3	FAD	A	1403	53/53	0.97	0.07	28,35,40,44	0
3	FAD	B	1403	53/53	0.98	0.06	20,25,28,31	0
2	FES	A	1401	4/4	0.99	0.05	31,33,34,35	0
2	FES	A	1402	4/4	0.99	0.03	25,26,26,27	0
2	FES	B	1401	4/4	0.99	0.04	30,31,32,33	0
6	CA	A	1406	1/1	0.99	0.03	31,31,31,31	0
6	CA	A	1407	1/1	0.99	0.03	32,32,32,32	0
6	CA	B	1406	1/1	0.99	0.04	27,27,27,27	0
6	CA	B	1407	1/1	0.99	0.02	29,29,29,29	0
2	FES	B	1402	4/4	1.00	0.02	23,24,25,25	0

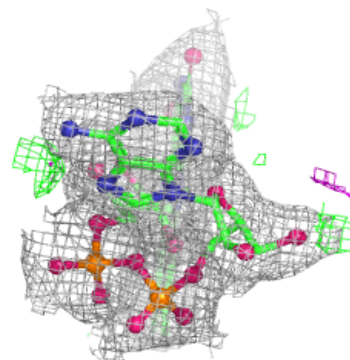
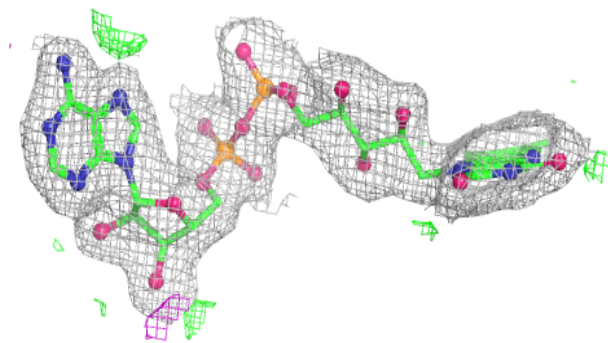
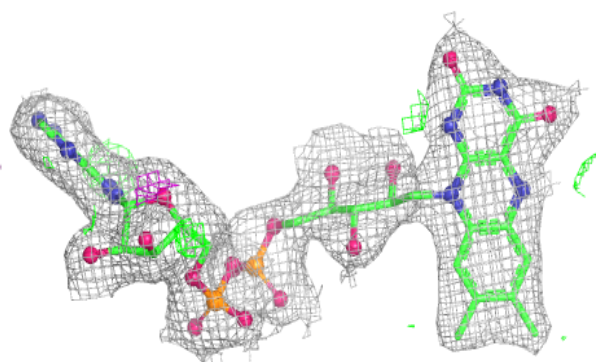
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 1403:

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

**Electron density around FAD B 1403:**

$2mF_o-DF_c$ (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.