



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:25 PM UTC

PDB ID : 3AN1 / pdb_00003an1
Title : Crystal structure of rat D428A mutant, urate bound form
Authors : Okamoto, K.; Kawaguchi, Y.; Eger, B.T.; Pai, E.F.; Nishino, T.
Deposited on : 2010-08-27
Resolution : 1.73 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

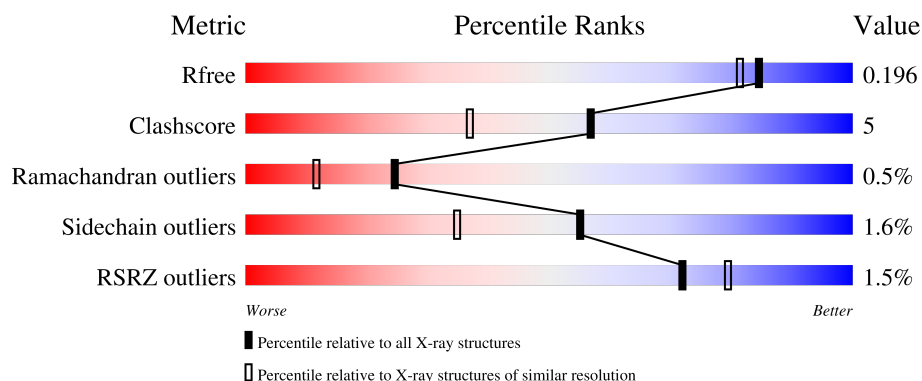
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	1331	% 85% 11% ..
1	B	1331	% 82% 14% ..

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	B	1334	-	X	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 22752 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.

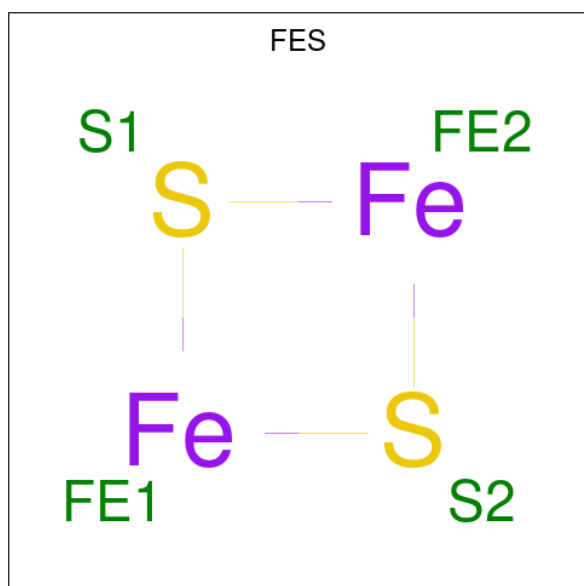
- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1299	Total	C	N	O	S	0	0	0
			10037	6360	1729	1883	65			
1	B	1292	Total	C	N	O	S	0	0	0
			9975	6322	1717	1872	64			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	428	ALA	ASP	engineered mutation	UNP P22985
B	428	ALA	ASP	engineered mutation	UNP P22985

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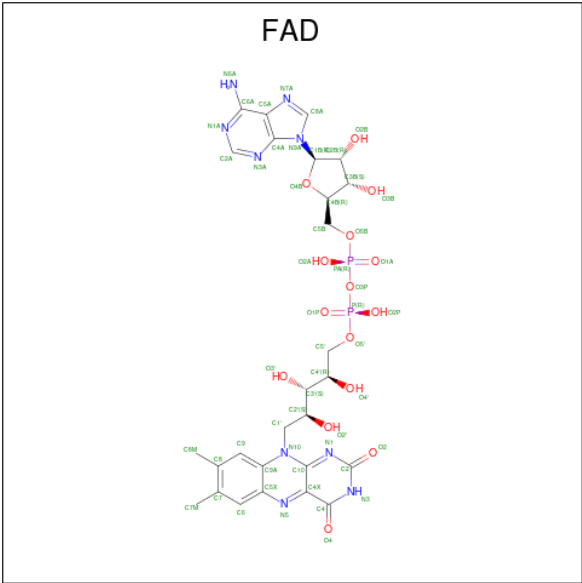
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

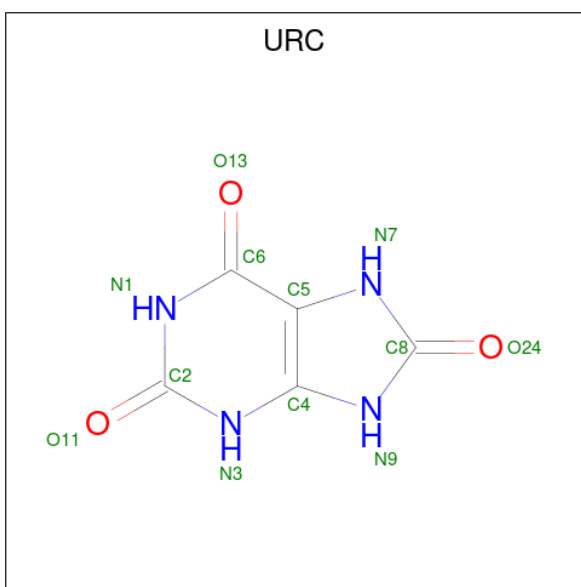
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



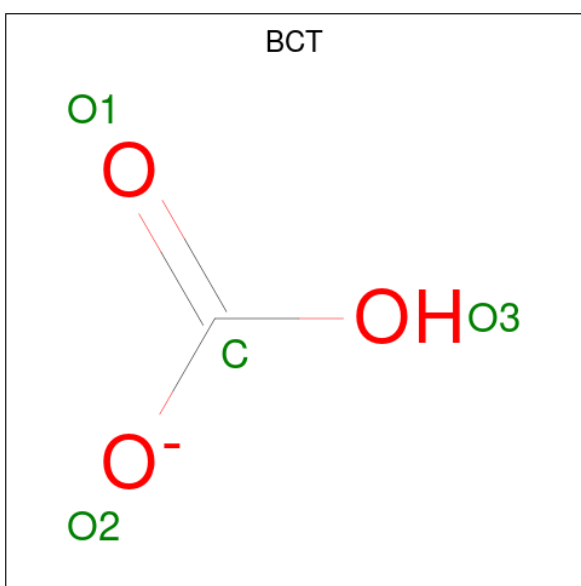
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is URIC ACID (CCD ID: URC) (formula: C₅H₄N₄O₃).



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

- 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	B	1	Total	C	O	0	0
			6	3	3		

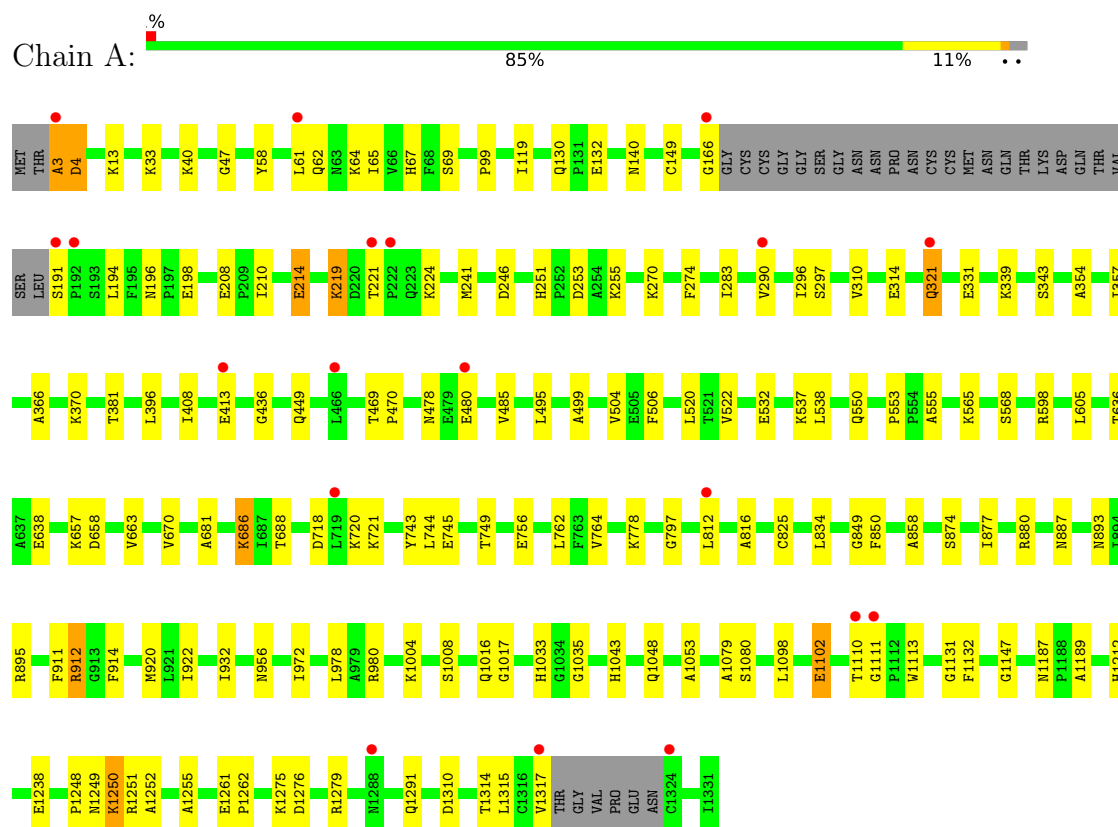
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1272	Total	O	0	0
			1272	1272		
8	B	1298	Total	O	0	0
			1298	1298		

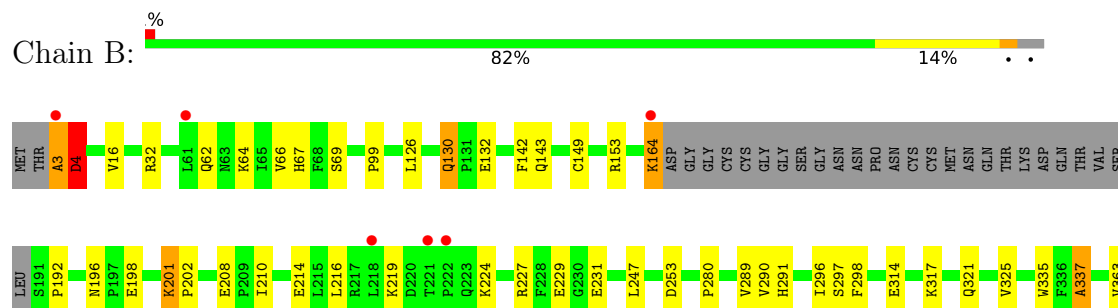
3 Residue-property plots

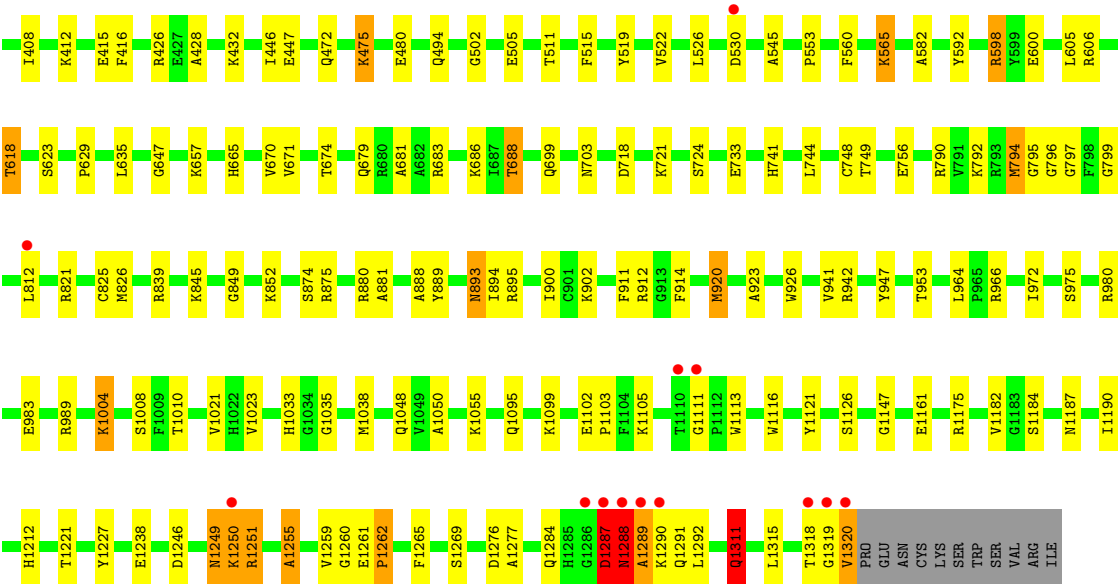
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	98.54Å 138.24Å 222.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.35 – 1.73 42.35 – 1.73	Depositor EDS
% Data completeness (in resolution range)	95.5 (42.35-1.73) 95.5 (42.35-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.160 , 0.198 0.159 , 0.196	Depositor DCC
R_{free} test set	6032 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22752	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: URC, FES, GOL, CA, 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	1.48	40/10248 (0.4%)	1.29	28/13865 (0.2%)
1	B	1.73	85/10185 (0.8%)	1.47	34/13784 (0.2%)
All	All	1.61	125/20433 (0.6%)	1.38	62/27649 (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	A	0	1
1	B	0	2
All	All	0	3

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	920	MET	SD-CE	-14.43	1.43	1.79
1	B	553	PRO	CA-C	10.34	1.57	1.51
1	B	69	SER	N-CA	9.51	1.57	1.45
1	A	920	MET	SD-CE	-8.77	1.57	1.79
1	B	480	GLU	N-CA	-8.29	1.36	1.46
1	B	794	MET	C-O	8.29	1.34	1.23
1	B	446	ILE	CA-CB	7.94	1.65	1.54
1	B	1111	GLY	N-CA	7.77	1.55	1.44
1	B	600	GLU	CD-OE2	7.61	1.39	1.25
1	B	795	GLY	N-CA	7.50	1.56	1.45
1	A	1017	GLY	N-CA	7.41	1.53	1.45
1	A	1111	GLY	N-CA	7.13	1.54	1.44
1	B	1276	ASP	N-CA	7.00	1.54	1.46
1	B	1277	ALA	CA-CB	6.97	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1121	TYR	N-CA	6.76	1.54	1.46
1	A	834	LEU	N-CA	6.71	1.54	1.46
1	B	130	GLN	N-CA	6.70	1.52	1.46
1	A	65	ILE	N-CA	6.66	1.54	1.46
1	B	142	PHE	N-CA	6.61	1.53	1.46
1	B	1095	GLN	N-CA	6.59	1.54	1.46
1	B	16	VAL	CA-CB	6.52	1.62	1.53
1	B	363	VAL	N-CA	6.51	1.54	1.46
1	B	582	ALA	CA-CB	6.45	1.63	1.53
1	B	1010	THR	CA-CB	6.40	1.64	1.53
1	A	1016	GLN	C-O	6.36	1.31	1.23
1	B	953	THR	C-O	6.24	1.32	1.23
1	A	1079	ALA	CA-CB	6.08	1.62	1.53
1	B	902	LYS	C-O	6.07	1.31	1.24
1	A	13	LYS	CA-C	-5.96	1.45	1.52
1	B	208	GLU	N-CA	5.95	1.55	1.45
1	A	208	GLU	N-CA	5.95	1.54	1.45
1	B	426	ARG	CD-NE	5.91	1.54	1.46
1	A	553	PRO	CA-C	5.84	1.57	1.52
1	A	69	SER	N-CA	5.83	1.52	1.45
1	B	790	ARG	N-CA	5.81	1.53	1.46
1	B	416	PHE	CA-C	-5.80	1.45	1.52
1	A	1276	ASP	N-CA	5.77	1.53	1.46
1	A	1276	ASP	CG-OD2	5.77	1.36	1.25
1	A	816	ALA	CA-CB	5.76	1.62	1.53
1	B	942	ARG	N-CA	5.75	1.53	1.46
1	B	522	VAL	N-CA	5.74	1.53	1.46
1	B	598	ARG	CD-NE	5.72	1.54	1.46
1	B	1021	VAL	N-CA	5.71	1.52	1.46
1	A	1110	THR	CA-CB	5.71	1.62	1.53
1	B	756	GLU	CA-C	-5.70	1.45	1.52
1	A	354	ALA	CA-CB	5.69	1.61	1.53
1	A	568	SER	N-CA	5.69	1.53	1.46
1	B	1260	GLY	N-CA	5.69	1.52	1.45
1	B	983	GLU	CG-CD	5.68	1.66	1.52
1	B	416	PHE	C-N	5.68	1.41	1.33
1	A	922	ILE	N-CA	5.67	1.53	1.46
1	A	764	VAL	C-O	5.65	1.29	1.23
1	B	337	ALA	CA-CB	5.62	1.63	1.52
1	B	989	ARG	C-O	5.61	1.31	1.24
1	B	671	VAL	CA-CB	-5.61	1.47	1.54
1	B	526	LEU	N-CA	5.60	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	635	LEU	C-O	-5.59	1.17	1.24
1	B	511	THR	N-CA	5.56	1.53	1.46
1	A	1248	PRO	C-O	5.55	1.30	1.23
1	A	636	THR	CA-CB	5.51	1.62	1.53
1	B	665	HIS	N-CA	5.50	1.52	1.46
1	B	839	ARG	CZ-NH1	5.48	1.40	1.32
1	B	1246	ASP	CA-C	-5.47	1.47	1.53
1	B	447	GLU	N-CA	-5.45	1.39	1.46
1	B	446	ILE	N-CA	5.42	1.53	1.46
1	B	337	ALA	C-O	5.42	1.30	1.24
1	B	724	SER	CA-C	-5.41	1.45	1.52
1	B	1190	ILE	CA-CB	5.41	1.61	1.54
1	B	893	ASN	C-O	5.41	1.30	1.24
1	B	210	ILE	CA-CB	5.40	1.59	1.54
1	A	40	LYS	N-CA	5.40	1.52	1.45
1	A	745	GLU	CA-C	5.38	1.59	1.52
1	B	545	ALA	CA-CB	5.37	1.62	1.53
1	B	826	MET	C-O	5.36	1.30	1.24
1	B	325	VAL	N-CA	5.36	1.52	1.46
1	A	119	ILE	N-CA	5.35	1.52	1.46
1	B	1320	VAL	CA-CB	5.34	1.68	1.54
1	A	47	GLY	N-CA	5.33	1.53	1.45
1	B	1251	ARG	CG-CD	-5.31	1.36	1.52
1	A	1080	SER	N-CA	5.31	1.52	1.46
1	B	674	THR	CA-CB	5.29	1.60	1.54
1	B	688	THR	N-CA	5.28	1.52	1.46
1	A	1252	ALA	N-CA	5.28	1.52	1.45
1	B	519	TYR	N-CA	5.27	1.52	1.46
1	A	485	VAL	CA-CB	-5.27	1.48	1.54
1	A	849	GLY	N-CA	5.27	1.53	1.46
1	B	647	GLY	C-O	5.27	1.29	1.23
1	B	796	GLY	C-O	5.26	1.30	1.24
1	B	1311	GLN	N-CA	5.25	1.53	1.46
1	B	126	LEU	C-O	5.24	1.30	1.24
1	A	850	PHE	N-CA	-5.23	1.40	1.46
1	B	875	ARG	CD-NE	5.22	1.53	1.46
1	B	849	GLY	N-CA	5.20	1.52	1.46
1	A	1275	LYS	N-CA	5.18	1.52	1.46
1	A	762	LEU	N-CA	5.18	1.52	1.46
1	B	964	LEU	N-CA	5.18	1.51	1.46
1	B	214	GLU	N-CA	5.18	1.52	1.46
1	B	1161	GLU	N-CA	5.18	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	888	ALA	CA-C	5.17	1.60	1.52
1	B	298	PHE	C-O	-5.16	1.17	1.24
1	B	553	PRO	C-O	-5.16	1.20	1.25
1	B	947	TYR	CE2-CZ	5.16	1.50	1.38
1	B	1055	LYS	C-O	5.15	1.30	1.23
1	B	1182	VAL	N-CA	5.15	1.52	1.46
1	B	1050	ALA	N-CA	5.14	1.52	1.46
1	A	522	VAL	CA-CB	-5.13	1.48	1.54
1	A	1131	GLY	N-CA	5.11	1.50	1.45
1	B	941	VAL	CA-C	5.11	1.59	1.52
1	B	894	ILE	CA-CB	5.11	1.61	1.54
1	A	310	VAL	C-O	5.10	1.29	1.24
1	A	339	LYS	CE-NZ	5.09	1.64	1.49
1	B	1023	VAL	CA-CB	5.09	1.60	1.54
1	B	415	GLU	N-CA	5.09	1.52	1.46
1	A	67	HIS	N-CA	5.08	1.52	1.46
1	B	1249	ASN	C-O	-5.07	1.18	1.23
1	A	1110	THR	CA-C	5.05	1.58	1.52
1	B	475	LYS	C-O	5.04	1.30	1.23
1	B	1255	ALA	CA-CB	5.03	1.60	1.53
1	B	972	ILE	CB-CG2	5.03	1.69	1.52
1	A	321	GLN	CD-NE2	5.03	1.43	1.33
1	A	506	PHE	N-CA	5.02	1.52	1.46
1	B	647	GLY	N-CA	5.02	1.50	1.45
1	B	67	HIS	N-CA	5.02	1.52	1.46
1	B	966	ARG	N-CA	-5.02	1.40	1.46
1	B	1269	SER	N-CA	5.02	1.52	1.46

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1111	GLY	N-CA-C	-10.14	91.65	112.34
1	B	1318	THR	N-CA-C	10.01	126.37	112.45
1	A	980	ARG	NE-CZ-NH2	-9.17	110.95	119.20
1	A	1262	PRO	N-CA-C	8.03	120.50	110.70
1	A	978	LEU	N-CA-C	7.48	119.07	111.07
1	B	1292	LEU	N-CA-C	7.19	120.40	109.62
1	B	1318	THR	CA-C-N	6.96	134.23	121.70
1	B	1318	THR	C-N-CA	6.96	134.23	121.70
1	A	499	ALA	CA-C-N	-6.84	112.71	119.76
1	A	499	ALA	C-N-CA	-6.84	112.71	119.76
1	A	980	ARG	CG-CD-NE	-6.83	96.97	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	980	ARG	NE-CZ-NH1	6.46	127.96	121.50
1	B	1262	PRO	N-CA-C	6.33	118.43	110.70
1	B	748	CYS	CA-CB-SG	-6.17	100.22	114.40
1	A	663	VAL	N-CA-C	-6.07	100.83	108.84
1	B	1284	GLN	N-CA-C	-6.03	104.83	111.82
1	B	130	GLN	CA-C-N	6.01	125.69	119.56
1	B	130	GLN	C-N-CA	6.01	125.69	119.56
1	B	201	LYS	CA-C-N	5.97	125.88	119.85
1	B	201	LYS	C-N-CA	5.97	125.88	119.85
1	A	343	SER	CA-CB-OG	-5.94	99.21	111.10
1	B	4	ASP	N-CA-C	5.88	123.31	110.80
1	A	1147	GLY	N-CA-C	-5.86	105.30	112.68
1	A	980	ARG	CD-NE-CZ	5.76	132.46	124.40
1	A	119	ILE	N-CA-C	-5.74	104.92	110.72
1	A	366	ALA	N-CA-C	5.72	118.28	111.71
1	B	289	VAL	CA-C-N	-5.70	115.07	122.99
1	B	289	VAL	C-N-CA	-5.70	115.07	122.99
1	A	408	ILE	CA-C-N	-5.67	113.37	120.51
1	A	408	ILE	C-N-CA	-5.67	113.37	120.51
1	B	1111	GLY	CA-C-N	-5.66	114.78	120.21
1	B	1111	GLY	C-N-CA	-5.66	114.78	120.21
1	B	1004	LYS	CD-CE-NZ	5.64	129.94	111.90
1	A	1102	GLU	CA-CB-CG	5.60	125.30	114.10
1	A	972	ILE	CB-CA-C	5.60	121.33	112.26
1	A	1113	TRP	N-CA-C	-5.40	105.40	111.28
1	B	881	ALA	N-CA-C	-5.37	105.43	111.28
1	A	149	CYS	CB-CA-C	-5.37	100.71	109.56
1	B	515	PHE	CA-CB-CG	-5.35	108.45	113.80
1	B	214	GLU	N-CA-C	5.35	117.80	111.33
1	B	889	TYR	N-CA-C	5.30	118.03	109.40
1	B	799	GLY	N-CA-C	-5.28	107.71	114.37
1	B	321	GLN	N-CA-C	5.28	118.51	111.75
1	A	956	ASN	N-CA-C	5.23	118.96	112.58
1	A	436	GLY	N-CA-C	-5.22	100.80	113.18
1	A	1317	VAL	CB-CA-C	-5.22	101.48	111.40
1	B	1147	GLY	N-CA-C	-5.22	106.17	112.48
1	B	895	ARG	CA-C-N	-5.20	118.54	122.33
1	B	895	ARG	C-N-CA	-5.20	118.54	122.33
1	B	149	CYS	CB-CA-C	-5.16	101.05	109.56
1	A	874	SER	N-CA-C	5.15	116.89	111.28
1	B	66	VAL	O-C-N	5.13	128.46	122.97
1	A	1261	GLU	CA-C-N	-5.11	115.11	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1261	GLU	C-N-CA	-5.11	115.11	120.38
1	A	251	HIS	CA-C-N	-5.11	114.40	119.56
1	A	251	HIS	C-N-CA	-5.11	114.40	119.56
1	B	408	ILE	O-C-N	5.10	126.01	121.57
1	B	1113	TRP	CA-C-O	-5.09	115.13	120.63
1	A	877	ILE	N-CA-C	-5.09	105.54	110.42
1	B	618	THR	OG1-CB-CG2	-5.09	99.13	109.30
1	B	623	SER	CB-CA-C	-5.06	102.94	110.88
1	B	592	TYR	N-CA-C	-5.00	102.78	110.14

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	ALA	Peptide
1	B	1287	ASP	Peptide
1	B	3	ALA	Peptide

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	10037	0	10044	81	0
1	B	9975	0	9986	105	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	53	0	31	0	0
4	B	53	0	31	0	0
5	A	12	0	4	0	0
5	B	12	0	4	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	6	0	8	0	0
7	B	6	0	8	1	0
8	A	1272	0	0	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	1298	0	0	21	0
All	All	22752	0	20116	184	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (184) 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:3:ALA:HB3	1:B:4:ASP:CB	1.60	1.29
1:B:1250:LYS:HD2	8:B:2231:HOH:O	1.32	1.21
1:A:253:ASP:HB3	8:A:2533:HOH:O	1.39	1.20
1:B:3:ALA:CB	1:B:4:ASP:HB3	1.76	1.15
1:B:1212:HIS:HD2	8:B:2178:HOH:O	1.34	1.11
1:B:3:ALA:CB	1:B:4:ASP:CB	2.29	1.08
1:B:812:LEU:HD11	1:B:825:CYS:HB3	1.33	1.06
1:B:1311:GLN:HE21	1:B:1311:GLN:H	1.08	0.97
1:B:703:ASN:HB3	8:B:2223:HOH:O	1.64	0.96
1:A:749:THR:HB	1:A:812:LEU:HD12	1.48	0.95
1:A:1238:GLU:OE2	8:A:2232:HOH:O	1.84	0.93
1:B:1319:GLY:O	1:B:1320:VAL:HG23	1.67	0.92
1:B:821:ARG:CZ	8:B:1446:HOH:O	2.15	0.92
1:A:1238:GLU:OE1	8:A:2224:HOH:O	1.87	0.92
1:A:331:GLU:OE1	8:A:2217:HOH:O	1.89	0.89
1:B:3:ALA:CB	1:B:4:ASP:HB2	2.03	0.89
1:B:852:LYS:HD3	8:B:2479:HOH:O	1.74	0.87
1:B:143:GLN:HE21	1:B:428:ALA:H	1.22	0.87
1:B:3:ALA:HB3	1:B:4:ASP:HB3	0.85	0.85
1:B:749:THR:HB	1:B:812:LEU:HD12	1.58	0.85
1:A:3:ALA:HA	1:A:4:ASP:CB	2.07	0.83
1:A:778:LYS:HE3	8:A:1724:HOH:O	1.81	0.81
1:A:812:LEU:HD11	1:A:825:CYS:HB3	1.63	0.80
1:B:821:ARG:NH1	8:B:1446:HOH:O	2.14	0.79
1:B:1319:GLY:O	1:B:1320:VAL:CG2	2.29	0.79
1:A:718:ASP:H	1:A:893:ASN:HD22	1.28	0.79
1:B:718:ASP:H	1:B:893:ASN:HD22	1.32	0.78
1:A:214:GLU:HG3	8:A:2004:HOH:O	1.83	0.77
1:A:1310:ASP:O	1:A:1314:THR:HG23	1.85	0.77
1:B:216:LEU:O	1:B:219:LYS:HG3	1.83	0.77
1:B:679:GLN:HG2	1:B:683:ARG:NH1	2.00	0.76
1:A:58:TYR:CE2	1:A:219:LYS:HD3	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LYS:HE2	1:A:381:THR:HG21	1.69	0.74
1:B:130:GLN:HE21	1:B:132:GLU:H	1.35	0.73
1:B:505:GLU:OE1	8:B:2356:HOH:O	2.07	0.72
1:B:1311:GLN:H	1:B:1311:GLN:NE2	1.86	0.71
1:B:290:VAL:HG22	1:B:297:SER:HB2	1.73	0.71
1:B:688:THR:HG23	8:B:1562:HOH:O	1.90	0.70
1:A:3:ALA:HA	1:A:4:ASP:HB3	1.73	0.70
1:B:1315:LEU:HD13	1:B:1320:VAL:HB	1.74	0.69
1:A:532:GLU:OE2	1:A:537:LYS:HG2	1.91	0.69
1:B:565:LYS:H	1:B:565:LYS:CD	2.06	0.69
1:B:699:GLN:NE2	1:B:703:ASN:OD1	2.26	0.69
1:B:143:GLN:HE21	1:B:428:ALA:N	1.90	0.68
1:B:1033:HIS:HD2	1:B:1035:GLY:H	1.41	0.68
1:A:321:GLN:HG2	1:A:413:GLU:CD	2.20	0.67
1:B:3:ALA:HB1	1:B:4:ASP:HB2	1.75	0.66
1:A:1033:HIS:HD2	1:A:1035:GLY:H	1.44	0.65
1:A:605:LEU:HD13	1:A:812:LEU:HD23	1.79	0.65
1:A:812:LEU:HD21	1:A:825:CYS:HB2	1.79	0.65
1:A:718:ASP:H	1:A:893:ASN:ND2	1.95	0.65
1:A:1212:HIS:HE1	8:A:2256:HOH:O	1.79	0.64
1:A:932:ILE:HD13	1:A:1279:ARG:NH2	2.12	0.64
1:B:605:LEU:HD13	1:B:812:LEU:HD23	1.79	0.63
1:B:679:GLN:HG2	1:B:683:ARG:HH12	1.64	0.63
1:A:33:LYS:NZ	8:A:1904:HOH:O	2.19	0.62
1:A:688:THR:HG23	8:A:1952:HOH:O	2.00	0.62
1:A:130:GLN:HE21	1:A:132:GLU:H	1.46	0.62
1:A:778:LYS:HD3	8:A:1359:HOH:O	2.00	0.61
1:A:191:SER:N	8:A:2315:HOH:O	2.33	0.60
1:A:1212:HIS:HD2	8:A:2001:HOH:O	1.84	0.60
1:B:1033:HIS:CD2	1:B:1035:GLY:H	2.20	0.59
1:A:290:VAL:CG2	1:A:297:SER:HB2	2.32	0.59
1:B:565:LYS:H	1:B:565:LYS:CE	2.15	0.59
1:B:432:LYS:HE2	8:B:1802:HOH:O	2.02	0.59
1:B:718:ASP:H	1:B:893:ASN:ND2	2.00	0.59
1:A:1033:HIS:CD2	1:A:1035:GLY:H	2.21	0.59
1:B:227:ARG:NH1	1:B:229:GLU:OE2	2.34	0.59
1:A:3:ALA:CA	1:A:4:ASP:HB2	2.32	0.59
1:A:191:SER:CA	8:A:2315:HOH:O	2.50	0.59
1:B:62:GLN:OE1	1:B:64:LYS:HE2	2.03	0.59
1:B:196:ASN:OD1	1:B:198:GLU:HG2	2.04	0.58
1:B:606:ARG:HD3	1:B:679:GLN:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:LYS:H	1:B:565:LYS:HD3	1.69	0.57
1:B:812:LEU:HD11	1:B:825:CYS:CB	2.23	0.56
1:A:62:GLN:OE1	1:A:64:LYS:HE2	2.06	0.56
1:A:196:ASN:OD1	1:A:198:GLU:OE1	2.24	0.56
1:B:1251:ARG:HG2	8:B:2231:HOH:O	2.06	0.56
1:A:290:VAL:HG22	1:A:297:SER:HB2	1.88	0.56
1:A:495:LEU:HB2	1:A:504:VAL:HG13	1.87	0.55
1:B:143:GLN:HG2	1:B:428:ALA:HB2	1.89	0.55
1:A:749:THR:HB	1:A:812:LEU:CD1	2.32	0.54
1:A:191:SER:HA	8:A:2315:HOH:O	2.08	0.54
1:B:530:ASP:HA	8:B:1954:HOH:O	2.07	0.54
1:B:296:ILE:CD1	1:B:314:GLU:HG3	2.38	0.54
1:A:255:LYS:HE2	1:A:274:PHE:CE2	2.43	0.54
1:A:1250:LYS:HD3	1:A:1251:ARG:N	2.23	0.54
1:A:3:ALA:CA	1:A:4:ASP:CB	2.78	0.53
1:B:143:GLN:HE22	1:B:335:TRP:HA	1.72	0.53
1:B:1048:GLN:HE22	1:B:1187:ASN:HD22	1.55	0.53
1:A:1048:GLN:HE22	1:A:1187:ASN:HD22	1.57	0.53
1:A:1291:GLN:HG3	8:A:2169:HOH:O	2.08	0.52
1:B:1099:LYS:O	1:B:1102:GLU:HG2	2.09	0.52
1:B:618:THR:HG21	8:B:2381:HOH:O	2.09	0.52
1:A:270:LYS:NZ	8:A:2524:HOH:O	2.40	0.52
1:A:331:GLU:HG3	8:A:2422:HOH:O	2.10	0.51
1:A:241:MET:HE2	1:A:283:ILE:HG21	1.91	0.51
1:A:296:ILE:HD11	1:A:314:GLU:HG3	1.91	0.51
1:A:1048:GLN:NE2	1:A:1187:ASN:HD22	2.08	0.51
1:B:812:LEU:HD21	1:B:825:CYS:HB2	1.92	0.51
1:A:296:ILE:CD1	1:A:314:GLU:HG3	2.41	0.51
1:B:699:GLN:HE21	1:B:703:ASN:CG	2.15	0.51
1:A:555:ALA:O	1:A:1238:GLU:HA	2.12	0.50
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.94	0.50
1:B:143:GLN:CD	1:B:337:ALA:O	2.54	0.50
1:B:1212:HIS:HE1	8:B:2469:HOH:O	1.94	0.50
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.94	0.49
1:A:321:GLN:HG2	1:A:413:GLU:OE2	2.12	0.49
1:B:62:GLN:HB2	1:B:64:LYS:HG2	1.94	0.49
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.94	0.49
1:A:480:GLU:HG2	8:A:1729:HOH:O	2.12	0.49
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.12	0.49
1:A:638:GLU:HG3	8:A:2486:HOH:O	2.13	0.49
1:B:192:PRO:HG2	1:B:560:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:ARG:NH2	8:A:2230:HOH:O	2.46	0.48
1:A:932:ILE:HD11	8:A:1397:HOH:O	2.13	0.48
1:B:143:GLN:NE2	1:B:428:ALA:H	2.02	0.48
1:B:657:LYS:HD2	8:B:1694:HOH:O	2.12	0.48
1:B:565:LYS:HD3	1:B:565:LYS:N	2.29	0.48
1:B:1250:LYS:CD	8:B:2231:HOH:O	2.16	0.47
1:A:449:GLN:NE2	8:A:2002:HOH:O	2.46	0.47
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.14	0.47
1:B:1259:VAL:HG22	1:B:1259:VAL:O	2.14	0.47
1:A:357:ILE:HD12	1:A:357:ILE:C	2.40	0.47
1:A:911:PHE:O	1:A:912:ARG:C	2.58	0.47
1:B:812:LEU:HD23	1:B:812:LEU:HA	1.50	0.47
1:B:733:GLU:HG2	1:B:845:LYS:HG2	1.98	0.46
1:B:920:MET:HE3	1:B:1265:PHE:CG	2.50	0.46
1:A:812:LEU:HD23	1:A:812:LEU:HA	1.67	0.46
1:B:1184:SER:HA	7:B:1334:GOL:H12	1.97	0.46
1:B:1102:GLU:HG2	1:B:1103:PRO:HD3	1.98	0.46
1:B:1288:ASN:HD21	1:B:1291:GLN:HE21	1.64	0.46
1:A:520:LEU:HD22	1:A:538:LEU:HD11	1.99	0.45
1:B:605:LEU:HB3	1:B:812:LEU:HD21	1.98	0.45
1:B:1175:ARG:HA	1:B:1238:GLU:O	2.17	0.45
1:B:412:LYS:HE3	8:B:1831:HOH:O	2.14	0.45
1:A:166:GLY:HA3	8:A:2277:HOH:O	2.16	0.45
1:A:605:LEU:HB3	1:A:812:LEU:HD21	1.97	0.45
1:B:291:HIS:HE1	1:B:314:GLU:OE2	1.98	0.45
1:A:210:ILE:HD13	1:A:210:ILE:HG21	1.72	0.45
1:B:618:THR:OG1	1:B:688:THR:OG1	2.30	0.45
1:B:62:GLN:CD	1:B:64:LYS:HE2	2.42	0.45
1:B:1105:LYS:HG3	1:B:1116:TRP:CZ2	2.52	0.45
1:A:721:LYS:HE3	8:A:2367:HOH:O	2.16	0.45
1:B:923:ALA:HA	1:B:926:TRP:NE1	2.32	0.44
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.80	0.44
1:A:469:THR:N	1:A:470:PRO:CD	2.81	0.44
1:A:756:GLU:OE1	1:B:792:LYS:HE3	2.17	0.44
1:A:657:LYS:O	1:A:658:ASP:HB2	2.19	0.43
1:A:370:LYS:HG2	1:A:381:THR:HG23	2.01	0.43
1:B:296:ILE:HD11	1:B:314:GLU:HG3	2.00	0.43
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.18	0.43
1:B:412:LYS:CE	8:B:1831:HOH:O	2.66	0.43
1:B:1048:GLN:NE2	1:B:1187:ASN:HD22	2.15	0.43
1:B:1287:ASP:OD1	1:B:1289:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ARG:NH1	8:A:2079:HOH:O	2.45	0.43
1:B:432:LYS:HG3	8:B:1840:HOH:O	2.19	0.43
1:B:502:GLY:HA2	8:B:1340:HOH:O	2.18	0.43
1:B:201:LYS:HA	1:B:202:PRO:HD3	1.90	0.42
1:B:975:SER:O	1:B:980:ARG:HD3	2.19	0.42
1:B:231:GLU:OE2	1:B:629:PRO:HG2	2.18	0.42
1:B:794:MET:HE3	1:B:1038:MET:HB3	2.02	0.42
1:A:1250:LYS:HD3	1:A:1251:ARG:H	1.84	0.42
1:A:194:LEU:HD22	1:A:1189:ALA:HA	2.01	0.42
1:B:565:LYS:CD	1:B:565:LYS:N	2.77	0.42
1:B:1289:ALA:HA	1:B:1290:LYS:HA	1.86	0.42
1:B:1288:ASN:ND2	1:B:1291:GLN:HE21	2.17	0.42
1:A:858:ALA:HA	1:A:893:ASN:O	2.20	0.42
1:B:32:ARG:NH2	1:B:598:ARG:HD2	2.35	0.42
1:B:472:GLN:HE22	1:B:475:LYS:NZ	2.17	0.41
1:B:1221:THR:HG22	1:B:1227:TYR:HB2	2.00	0.41
1:B:1212:HIS:CD2	8:B:2178:HOH:O	2.26	0.41
1:B:153:ARG:C	1:B:153:ARG:HD2	2.46	0.41
1:B:164:LYS:HE2	1:B:164:LYS:HB2	1.66	0.41
1:B:741:HIS:HA	1:B:911:PHE:CE1	2.56	0.41
1:A:686:LYS:HE3	1:A:686:LYS:HB3	1.46	0.41
1:A:1033:HIS:HE1	1:A:1043:HIS:ND1	2.19	0.41
1:A:1132:PHE:CG	1:B:1126:SER:HB2	2.56	0.41
1:B:606:ARG:HH11	1:B:606:ARG:HD2	1.64	0.41
1:B:880:ARG:HD2	1:B:914:PHE:HB3	2.03	0.41
1:A:478:ASN:OD1	1:A:480:GLU:HG2	2.21	0.40
1:A:932:ILE:HD13	1:A:1279:ARG:CZ	2.50	0.40
1:B:874:SER:HB3	1:B:900:ILE:HG21	2.03	0.40
1:B:852:LYS:HD2	8:B:2096:HOH:O	2.22	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	1293/1331 (97%)	1250 (97%)	38 (3%)	5 (0%)	30	16
1	B	1288/1331 (97%)	1245 (97%)	36 (3%)	7 (0%)	24	12
All	All	2581/2662 (97%)	2495 (97%)	74 (3%)	12 (0%)	24	12

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	1008	SER
1	B	4	ASP
1	B	1008	SER
1	B	1288	ASN
1	B	912	ARG
1	A	912	ARG
1	B	797	GLY
1	B	1287	ASP
1	A	797	GLY
1	B	1289	ALA
1	A	887	ASN

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	1096/1123 (98%)	1077 (98%)	19 (2%)	53	32
1	B	1089/1123 (97%)	1073 (98%)	16 (2%)	57	38
All	All	2185/2246 (97%)	2150 (98%)	35 (2%)	55	35

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	99	PRO
1	A	140	ASN
1	A	214	GLU

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Mol	Chain	Res	Type
1	A	219	LYS
1	A	221	THR
1	A	224	LYS
1	A	246	ASP
1	A	396	LEU
1	A	550	GLN
1	A	565	LYS
1	A	686	LYS
1	A	720	LYS
1	A	743	TYR
1	A	744	LEU
1	A	1004	LYS
1	A	1102	GLU
1	A	1250	LYS
1	A	1315	LEU
1	B	99	PRO
1	B	164	LYS
1	B	224	LYS
1	B	247	LEU
1	B	253	ASP
1	B	280	PRO
1	B	317	LYS
1	B	494	GLN
1	B	565	LYS
1	B	686	LYS
1	B	721	LYS
1	B	744	LEU
1	B	1004	LYS
1	B	1250	LYS
1	B	1288	ASN
1	B	1311	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	145	ASN
1	A	207	GLN
1	A	291	HIS
1	A	332	GLN
1	A	386	HIS
1	A	556	ASN

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Mol	Chain	Res	Type
1	A	567	GLN
1	A	583	ASN
1	A	585	GLN
1	A	817	HIS
1	A	893	ASN
1	A	1033	HIS
1	A	1048	GLN
1	A	1148	ASN
1	A	1173	ASN
1	A	1212	HIS
1	A	1294	GLN
1	B	130	GLN
1	B	143	GLN
1	B	145	ASN
1	B	271	ASN
1	B	287	ASN
1	B	291	HIS
1	B	332	GLN
1	B	350	ASN
1	B	472	GLN
1	B	583	ASN
1	B	585	GLN
1	B	699	GLN
1	B	893	ASN
1	B	1033	HIS
1	B	1048	GLN
1	B	1173	ASN
1	B	1285	HIS
1	B	1288	ASN
1	B	1311	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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
6	BCT	B	1333	-	3,3,3	0.98	0	2,3,3	1.26	0
2	FES	B	4001	1	0,4,4	-	-	-		
7	GOL	A	1335	-	5,5,5	0.41	0	5,5,5	0.66	0
4	FAD	A	3006	-	58,58,58	1.35	5 (8%)	85,89,89	1.66	19 (22%)
5	URC	B	1332	-	13,13,13	2.88	7 (53%)	17,19,19	1.97	5 (29%)
5	URC	A	1333	-	13,13,13	2.85	5 (38%)	17,19,19	2.06	5 (29%)
4	FAD	B	4006	-	58,58,58	1.33	4 (6%)	85,89,89	1.68	15 (17%)
2	FES	B	4002	1	0,4,4	-	-	-		
2	FES	A	3001	1	0,4,4	-	-	-		
2	FES	A	3002	1	0,4,4	-	-	-		
6	BCT	A	1334	-	3,3,3	0.81	0	2,3,3	0.53	0
7	GOL	B	1334	-	5,5,5	1.91	1 (20%)	5,5,5	3.28	4 (80%)

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	4001	1	-	-	0/1/1/1
7	GOL	A	1335	-	-	0/4/4/4	-
4	FAD	A	3006	-	-	6/34/50/50	0/6/6/6
5	URC	B	1332	-	-	-	0/2/2/2
5	URC	A	1333	-	-	-	0/2/2/2
4	FAD	B	4006	-	-	6/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FES	A	3001	1	-	-	0/1/1/1
7	GOL	B	1334	-	-	3/4/4/4	-
2	FES	A	3002	1	-	-	0/1/1/1
2	FES	B	4002	1	-	-	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1333	URC	O13-C6	6.58	1.36	1.23
5	B	1332	URC	C4-N9	5.01	1.44	1.35
5	B	1332	URC	O13-C6	4.98	1.33	1.23
5	A	1333	URC	O24-C8	4.67	1.33	1.23
5	B	1332	URC	O24-C8	4.48	1.32	1.23
4	B	4006	FAD	PA-O3P	4.38	1.64	1.59
4	A	3006	FAD	C4X-N5	4.33	1.40	1.30
5	A	1333	URC	C5-C4	4.30	1.45	1.37
7	B	1334	GOL	O2-C2	3.95	1.54	1.43
4	B	4006	FAD	C4X-N5	3.77	1.38	1.30
4	B	4006	FAD	C10-N1	3.37	1.40	1.33
5	B	1332	URC	O11-C2	3.05	1.29	1.23
5	B	1332	URC	C2-N1	2.80	1.42	1.37
5	A	1333	URC	C4-N9	2.78	1.40	1.35
4	B	4006	FAD	O4B-C1B	2.71	1.48	1.42
5	B	1332	URC	C5-C4	2.66	1.42	1.37
5	A	1333	URC	C2-N1	2.50	1.41	1.37
4	A	3006	FAD	C2A-N1A	2.44	1.38	1.33
4	A	3006	FAD	C10-N1	2.43	1.38	1.33
5	B	1332	URC	C2-N3	2.36	1.41	1.37
4	A	3006	FAD	O4B-C4B	-2.13	1.40	1.45
4	A	3006	FAD	O3B-C3B	2.00	1.47	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4006	FAD	N3A-C2A-N1A	-7.01	117.97	128.58
4	A	3006	FAD	N9A-C8A-N7A	-5.61	105.98	113.94
7	B	1334	GOL	C3-C2-C1	-5.38	92.05	111.80
4	B	4006	FAD	C2A-N1A-C6A	4.73	126.49	118.73
4	A	3006	FAD	C5A-N7A-C8A	4.43	110.41	103.45
5	B	1332	URC	N7-C8-N9	4.33	113.36	107.22
5	A	1333	URC	N7-C8-N9	4.13	113.07	107.22
4	B	4006	FAD	C4X-C10-N10	4.11	122.37	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1333	URC	N3-C2-N1	4.07	122.14	115.74
4	B	4006	FAD	C4-N3-C2	-3.68	119.10	125.64
4	A	3006	FAD	O2A-PA-O3P	3.66	117.17	107.27
4	A	3006	FAD	C4A-N9A-C8A	3.58	109.50	105.74
4	B	4006	FAD	C10-C4X-N5	-3.52	117.61	124.81
4	A	3006	FAD	O4'-C4'-C3'	-3.51	101.04	109.25
4	A	3006	FAD	C2B-C1B-N9A	3.46	121.89	113.30
7	B	1334	GOL	O1-C1-C2	-3.45	94.86	110.38
5	B	1332	URC	N3-C2-N1	3.35	121.01	115.74
4	A	3006	FAD	C4X-C10-N10	3.29	121.19	116.48
5	A	1333	URC	C4-C5-N7	-3.27	103.87	107.36
4	B	4006	FAD	O4B-C1B-N9A	-3.25	101.84	108.09
5	B	1332	URC	O13-C6-N1	3.02	125.79	120.11
4	A	3006	FAD	C4A-C5A-N7A	-3.00	107.15	110.58
5	B	1332	URC	O13-C6-C5	-2.99	120.06	127.26
4	A	3006	FAD	N3A-C2A-N1A	-2.86	124.25	128.58
7	B	1334	GOL	O3-C3-C2	2.77	122.83	110.38
4	B	4006	FAD	C4-C4X-C10	2.61	121.41	116.93
4	A	3006	FAD	C5X-C6-C7	-2.60	116.01	120.83
4	B	4006	FAD	N9A-C8A-N7A	-2.57	110.28	113.94
4	B	4006	FAD	C4X-C10-N1	-2.56	118.31	124.59
4	A	3006	FAD	C4'-C3'-C2'	-2.53	109.37	113.57
5	A	1333	URC	O11-C2-N1	-2.45	117.50	121.86
4	B	4006	FAD	C4'-C3'-C2'	-2.44	109.50	113.57
4	A	3006	FAD	C10-C4X-N5	-2.40	119.91	124.81
4	A	3006	FAD	C4-N3-C2	-2.30	121.56	125.64
4	B	4006	FAD	C4X-C4-N3	2.29	119.08	113.25
4	A	3006	FAD	C4-C4X-C10	2.23	120.75	116.93
4	B	4006	FAD	C5A-N7A-C8A	2.22	106.94	103.45
7	B	1334	GOL	O2-C2-C1	-2.21	100.02	109.18
4	B	4006	FAD	O2A-PA-O3P	2.21	113.25	107.27
4	A	3006	FAD	C6A-C5A-C4A	2.19	120.17	117.18
5	B	1332	URC	C4-N3-C2	-2.13	114.44	120.68
5	A	1333	URC	C6-N1-C2	-2.11	123.46	126.37
4	A	3006	FAD	O3'-C3'-C4'	2.10	113.70	108.93
4	B	4006	FAD	C4A-C5A-N7A	-2.07	108.21	110.58
4	A	3006	FAD	C5A-C4A-N3A	-2.07	123.87	126.72
4	A	3006	FAD	O5'-C5'-C4'	-2.06	103.85	109.36
4	B	4006	FAD	C2A-N3A-C4A	2.06	116.86	111.83
4	A	3006	FAD	C6-C7-C8	2.01	122.63	119.69

There are no chirality outliers.

All (15) torsion outliers are listed below:

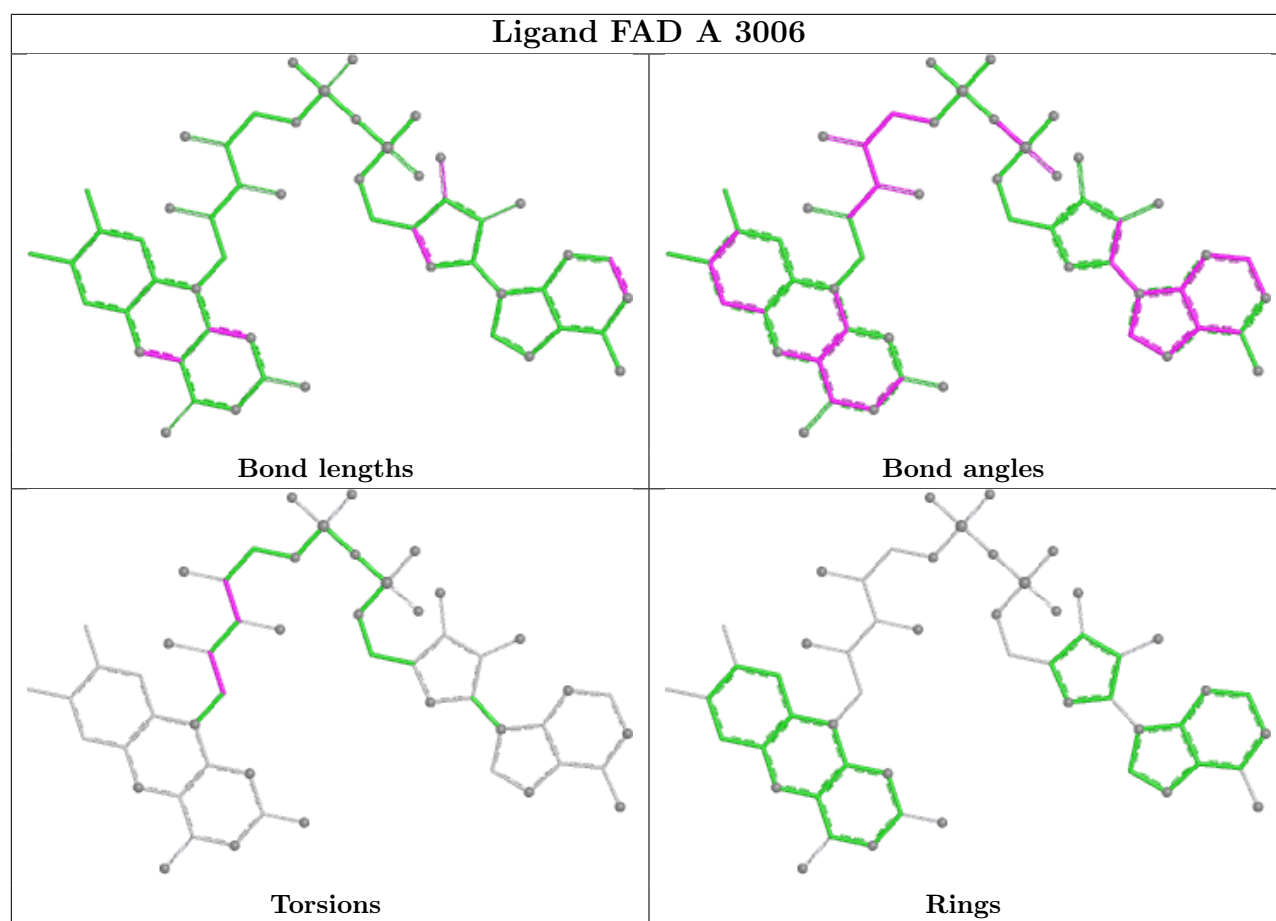
Mol	Chain	Res	Type	Atoms
4	A	3006	FAD	N10-C1'-C2'-O2'
4	A	3006	FAD	N10-C1'-C2'-C3'
4	B	4006	FAD	N10-C1'-C2'-O2'
4	B	4006	FAD	N10-C1'-C2'-C3'
7	B	1334	GOL	O1-C1-C2-O2
7	B	1334	GOL	O1-C1-C2-C3
7	B	1334	GOL	C1-C2-C3-O3
4	A	3006	FAD	C2'-C3'-C4'-O4'
4	A	3006	FAD	C2'-C3'-C4'-C5'
4	B	4006	FAD	C2'-C3'-C4'-C5'
4	A	3006	FAD	O3'-C3'-C4'-O4'
4	B	4006	FAD	O3'-C3'-C4'-O4'
4	B	4006	FAD	C2'-C3'-C4'-O4'
4	B	4006	FAD	O3'-C3'-C4'-C5'
4	A	3006	FAD	O3'-C3'-C4'-C5'

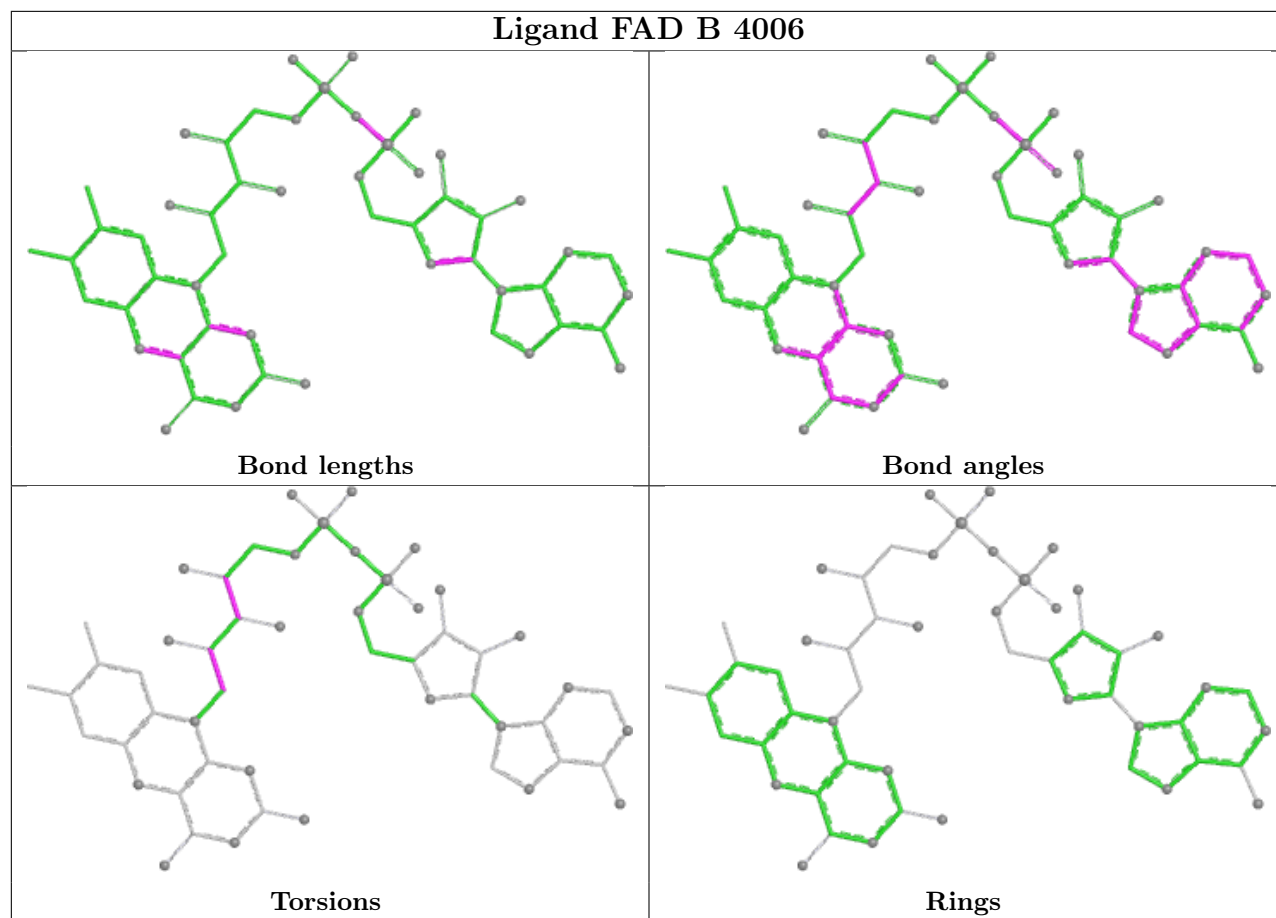
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1334	GOL	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.





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	1299/1331 (97%)	-0.27	19 (1%) 72 79	8, 18, 36, 54	0
1	B	1292/1331 (97%)	-0.41	19 (1%) 72 79	8, 15, 32, 63	0
All	All	2591/2662 (97%)	-0.34	38 (1%) 72 79	8, 16, 34, 63	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1289	ALA	8.9
1	B	1320	VAL	7.5
1	A	1324	CYS	5.1
1	B	1287	ASP	4.9
1	A	61	LEU	4.9
1	A	1317	VAL	4.5
1	B	1288	ASN	4.3
1	B	1318	THR	4.2
1	B	530	ASP	4.1
1	A	1111	GLY	4.1
1	B	1319	GLY	4.1
1	A	1110	THR	4.0
1	B	61	LEU	3.7
1	B	164	LYS	3.7
1	B	221	THR	3.6
1	A	3	ALA	3.6
1	B	1111	GLY	3.6
1	B	3	ALA	3.4
1	B	1110	THR	3.2
1	B	218	LEU	3.1
1	A	192	PRO	3.0
1	B	1286	GLY	3.0
1	A	221	THR	2.8
1	A	222	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	166	GLY	2.5
1	A	466	LEU	2.5
1	B	812	LEU	2.4
1	B	222	PRO	2.3
1	A	191	SER	2.3
1	A	321	GLN	2.3
1	A	812	LEU	2.2
1	A	290	VAL	2.2
1	B	1250	LYS	2.2
1	B	1290	LYS	2.2
1	A	1288	ASN	2.1
1	A	413	GLU	2.1
1	A	719	LEU	2.1
1	A	480	GLU	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.

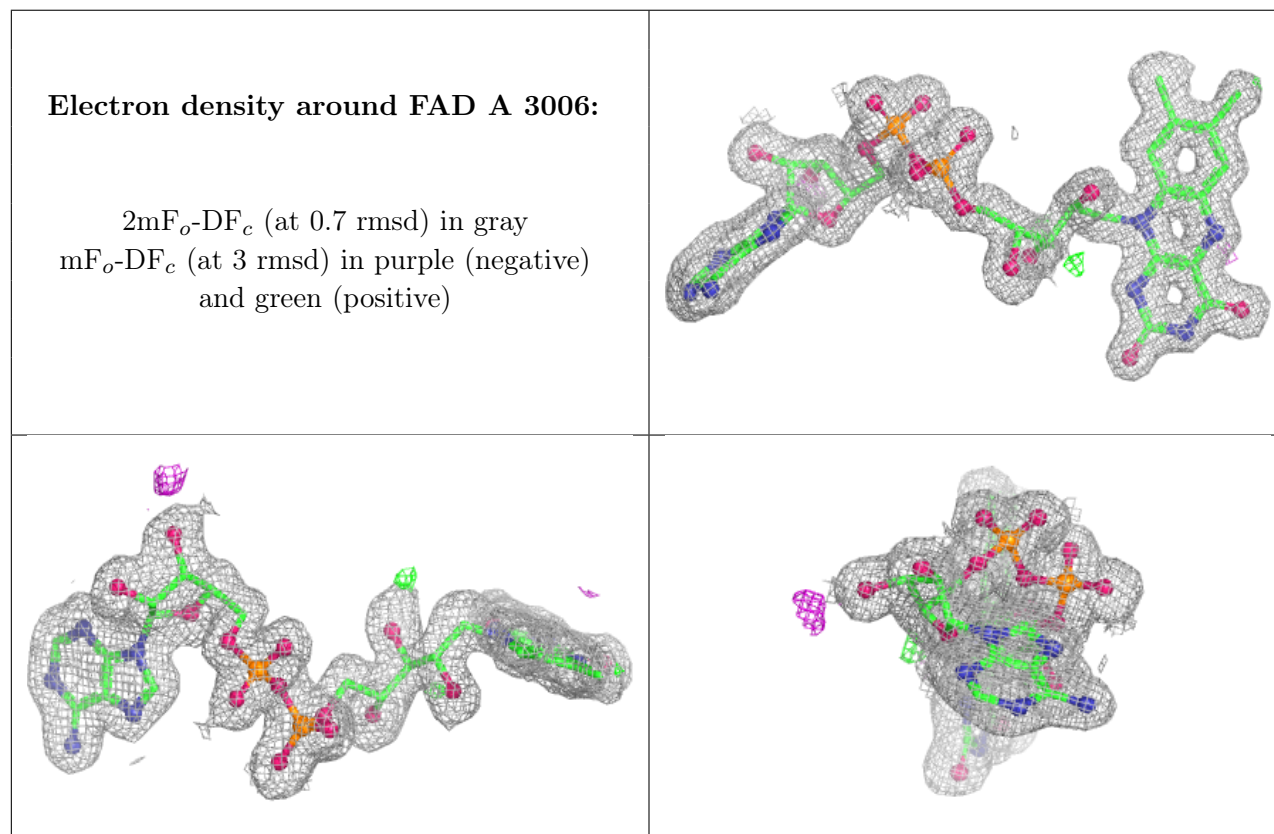
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	B	1334	6/6	0.75	0.18	18,35,37,38	0
5	URC	B	1332	12/12	0.92	0.08	15,20,25,26	0
5	URC	A	1333	12/12	0.93	0.08	18,23,29,31	0
7	GOL	A	1335	6/6	0.96	0.07	20,24,29,29	0
4	FAD	A	3006	53/53	0.98	0.04	13,16,20,21	0
6	BCT	A	1334	4/4	0.98	0.05	15,17,17,17	0
2	FES	B	4001	4/4	0.99	0.05	13,13,14,14	0
3	CA	A	1332	1/1	0.99	0.04	13,13,13,13	0
3	CA	A	4009	1/1	0.99	0.03	15,15,15,15	0

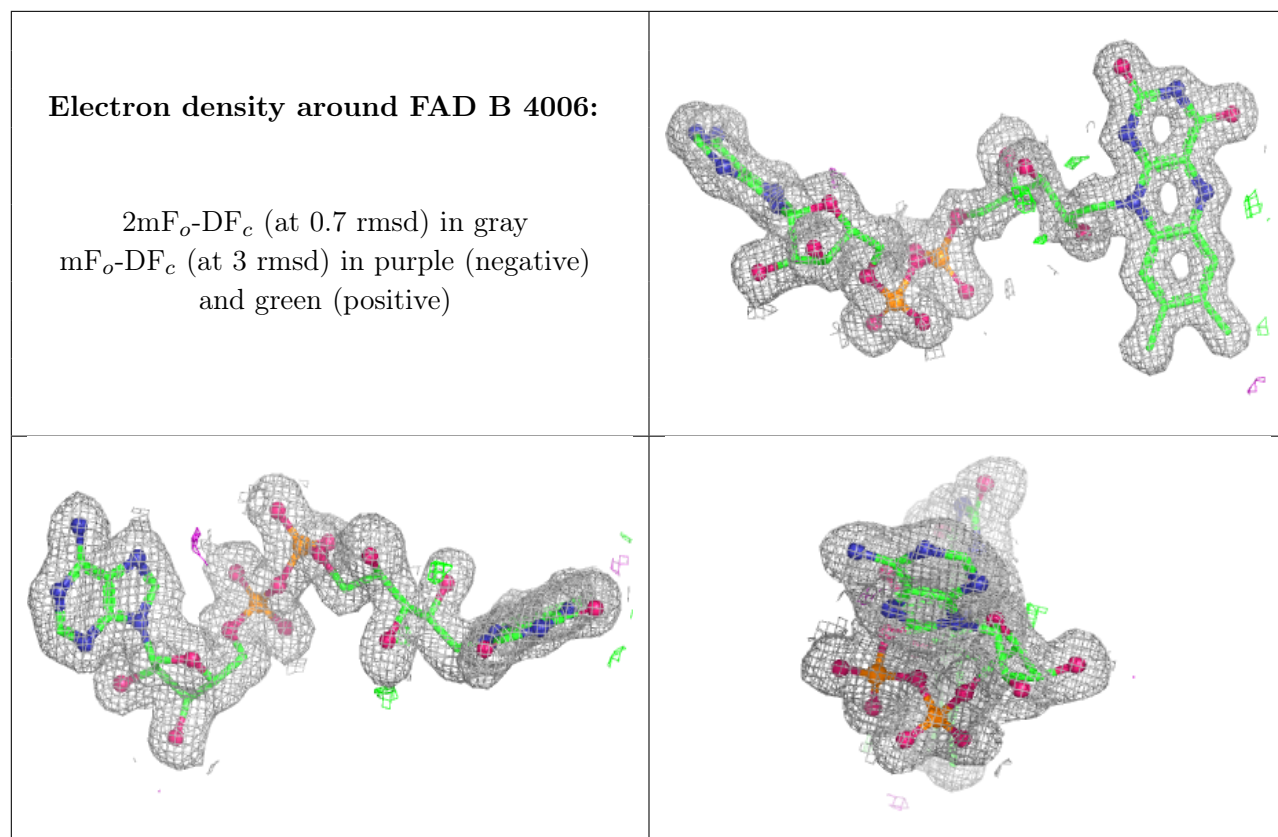
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BCT	B	1333	4/4	0.99	0.04	11,12,13,15	0
2	FES	A	3001	4/4	0.99	0.04	14,14,14,15	0
4	FAD	B	4006	53/53	0.99	0.04	9,12,14,15	0
2	FES	A	3002	4/4	1.00	0.01	11,11,11,12	0
2	FES	B	4002	4/4	1.00	0.01	8,9,9,9	0
3	CA	B	4019	1/1	1.00	0.03	11,11,11,11	0
3	CA	B	1335	1/1	1.00	0.03	11,11,11,11	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.