



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:51 pm BST

PDB ID : 3AN1  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

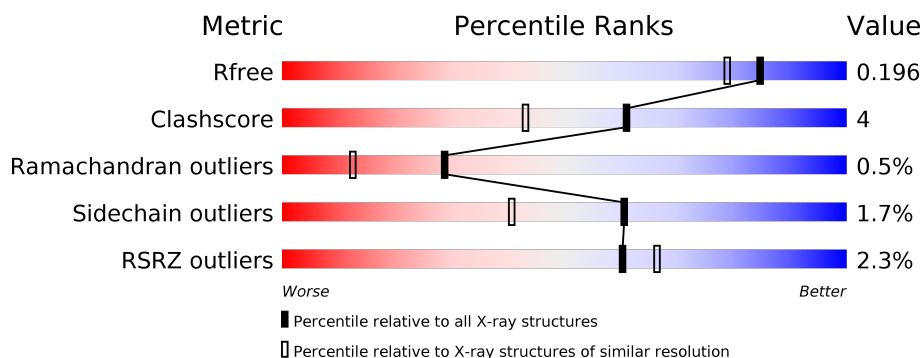
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>••</div> </div> </div>
1	B	1331	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>••</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	URC	A	1333	-	X	-	-
5	URC	B	1332	-	X	-	-
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.

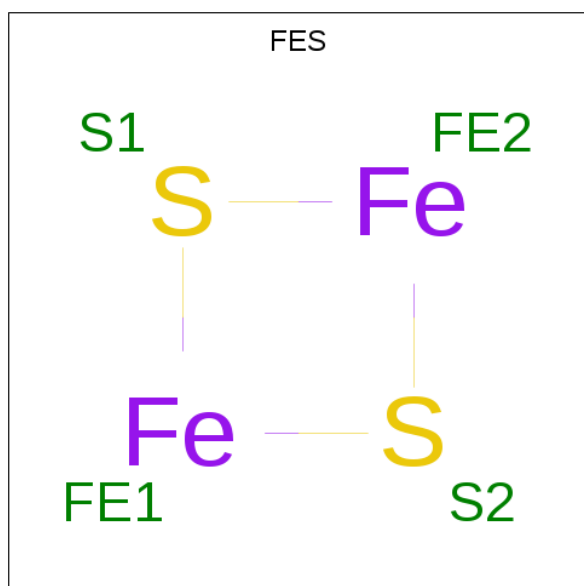
- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

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 (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

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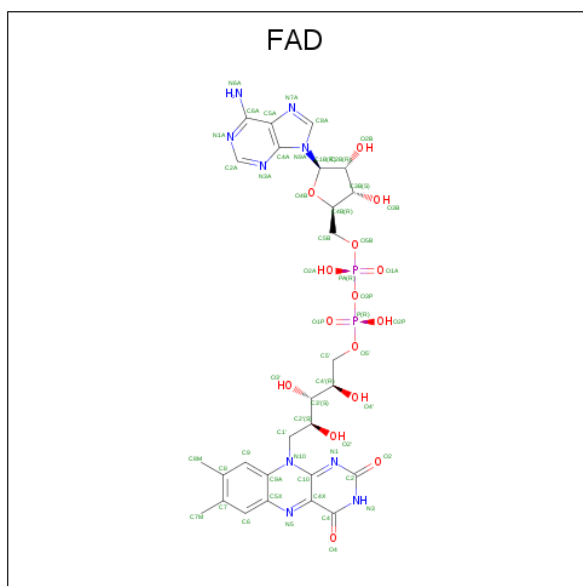
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

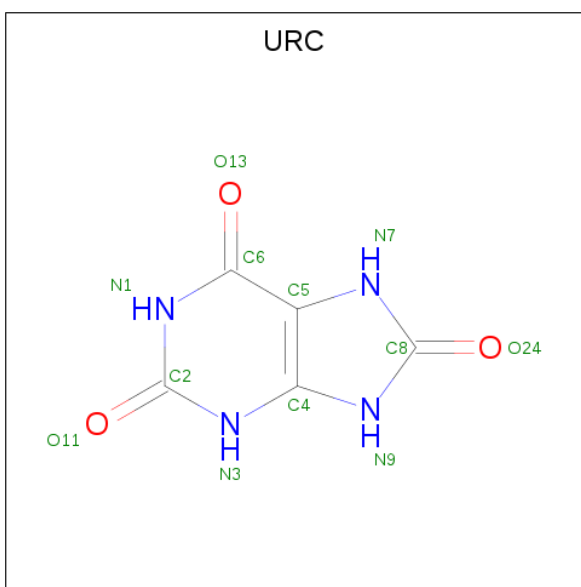
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



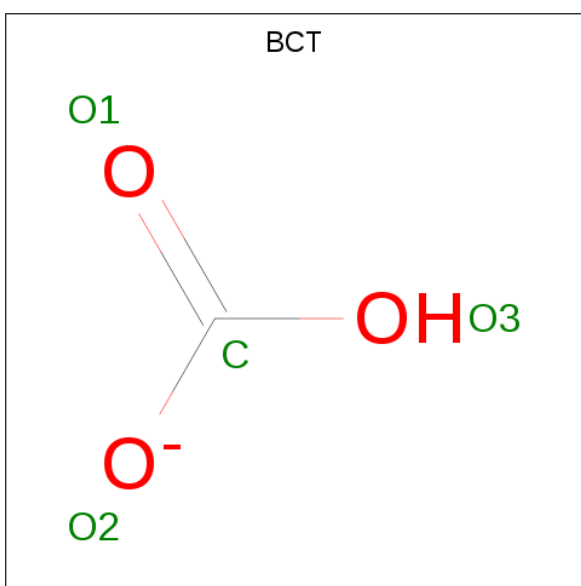
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0
			53	27	9	15	2	0
4	B	1	Total	C	N	O	P	0
			53	27	9	15	2	0

- Molecule 5 is URIC ACID (three-letter code: URC) (formula: C<sub>5</sub>H<sub>4</sub>N<sub>4</sub>O<sub>3</sub>).



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 (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



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 (three-letter code: 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		

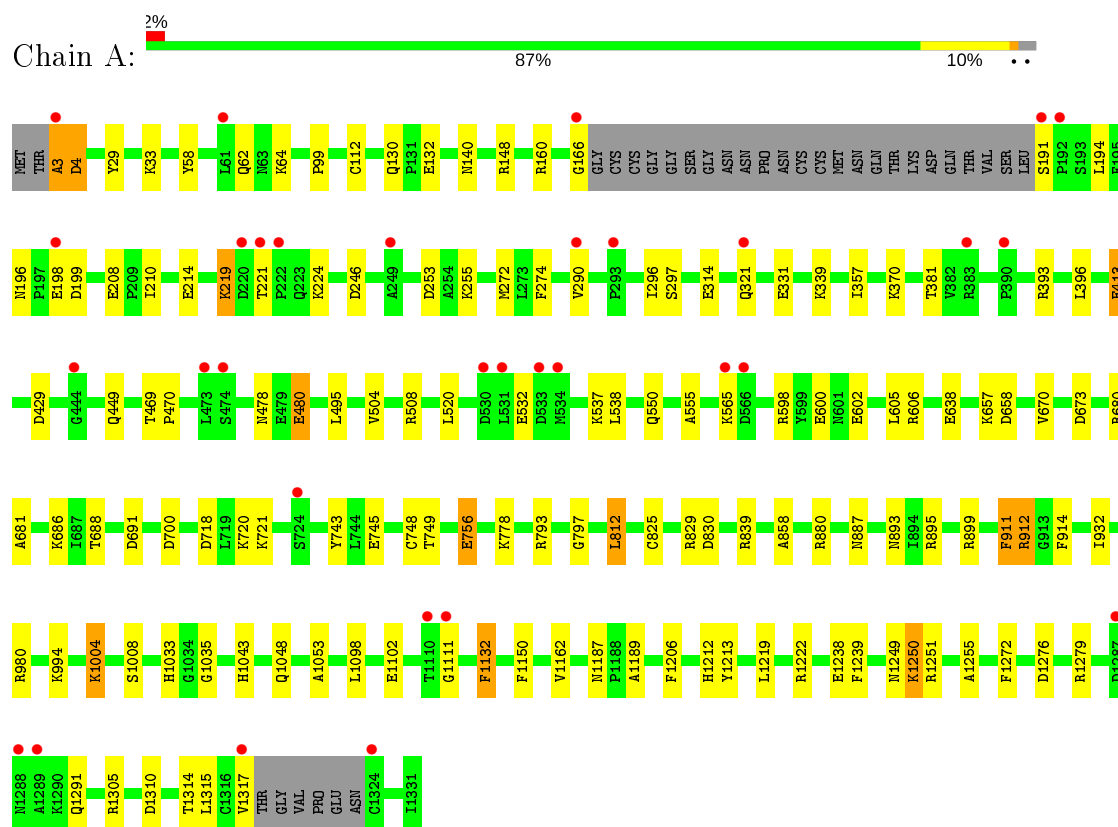
- Molecule 8 is water.

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

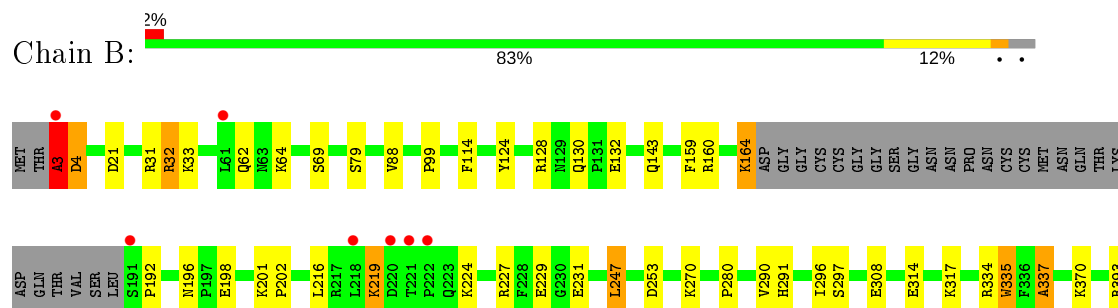
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

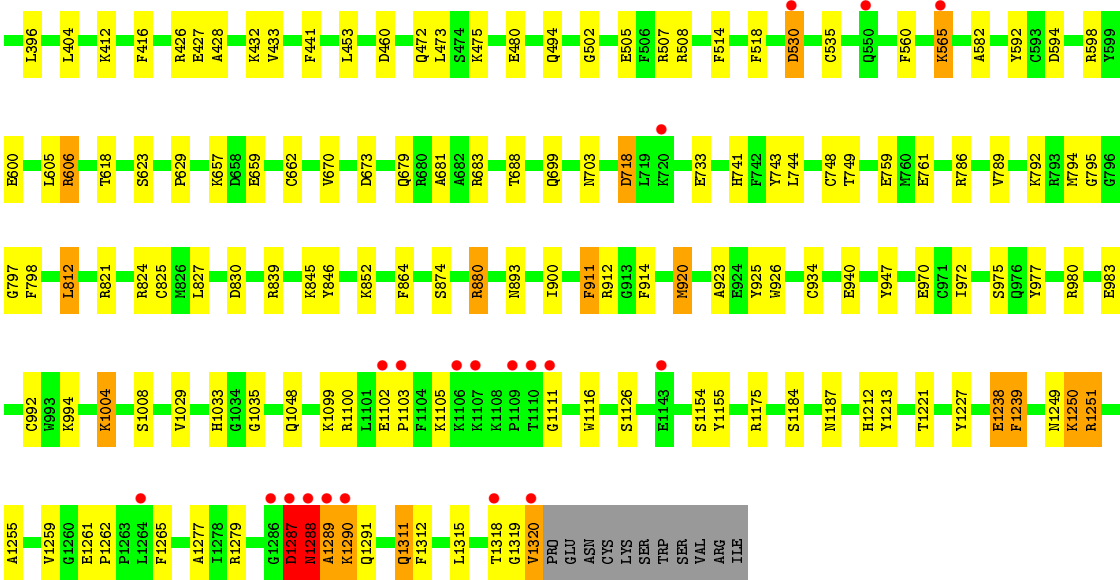
#### • Molecule 1: Xanthine dehydrogenase/oxidase



#### • 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (2.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	22752	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, URC, CA, FES, BCT, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.27	19/10248 (0.2%)	1.11	33/13865 (0.2%)
1	B	1.47	58/10185 (0.6%)	1.27	51/13784 (0.4%)
All	All	1.37	77/20433 (0.4%)	1.19	84/27649 (0.3%)

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 (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	600	GLU	CD-OE2	12.88	1.39	1.25
1	B	983	GLU	CG-CD	9.54	1.66	1.51
1	B	947	TYR	CE2-CZ	9.29	1.50	1.38
1	B	992	CYS	CB-SG	-8.51	1.67	1.82
1	A	600	GLU	CD-OE2	7.97	1.34	1.25
1	B	3	ALA	CA-CB	7.86	1.69	1.52
1	B	535	CYS	CB-SG	-7.50	1.69	1.82
1	B	748	CYS	CB-SG	7.15	1.94	1.82
1	B	934	CYS	CB-SG	-6.82	1.70	1.82
1	B	795	GLY	N-CA	6.80	1.56	1.46
1	B	1320	VAL	CA-CB	6.72	1.68	1.54
1	B	789	VAL	CB-CG1	6.70	1.67	1.52
1	B	441	PHE	CD1-CE1	6.63	1.52	1.39
1	A	413	GLU	CG-CD	6.57	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	846	TYR	CG-CD2	6.48	1.47	1.39
1	B	600	GLU	CG-CD	6.43	1.61	1.51
1	B	983	GLU	CD-OE1	6.43	1.32	1.25
1	B	983	GLU	CD-OE2	6.38	1.32	1.25
1	B	335	TRP	CB-CG	6.36	1.61	1.50
1	A	756	GLU	CD-OE1	6.26	1.32	1.25
1	A	339	LYS	CE-NZ	6.23	1.64	1.49
1	B	1111	GLY	N-CA	6.21	1.55	1.46
1	B	1251	ARG	CG-CD	-6.18	1.36	1.51
1	B	920	MET	SD-CE	-6.14	1.43	1.77
1	B	1239	PHE	CD1-CE1	6.03	1.51	1.39
1	A	1272	PHE	CE2-CZ	5.94	1.48	1.37
1	A	748	CYS	CB-SG	5.87	1.92	1.82
1	B	1239	PHE	CG-CD2	5.75	1.47	1.38
1	B	623	SER	CB-OG	-5.75	1.34	1.42
1	B	308	GLU	CB-CG	-5.72	1.41	1.52
1	B	970	GLU	CD-OE2	5.71	1.31	1.25
1	A	208	GLU	CD-OE2	5.68	1.31	1.25
1	B	839	ARG	CZ-NH1	5.67	1.40	1.33
1	B	1277	ALA	CA-CB	5.67	1.64	1.52
1	B	925	TYR	CD2-CE2	5.62	1.47	1.39
1	A	1111	GLY	N-CA	5.62	1.54	1.46
1	B	794	MET	C-O	5.61	1.34	1.23
1	B	427	GLU	CD-OE2	5.57	1.31	1.25
1	A	1150	PHE	CE1-CZ	5.53	1.47	1.37
1	B	983	GLU	CB-CG	5.51	1.62	1.52
1	B	518	PHE	CD1-CE1	5.50	1.50	1.39
1	B	761	GLU	CD-OE2	-5.49	1.19	1.25
1	A	1239	PHE	CD1-CE1	5.46	1.50	1.39
1	A	1132	PHE	CE2-CZ	5.41	1.47	1.37
1	B	970	GLU	CD-OE1	5.41	1.31	1.25
1	A	745	GLU	CB-CG	5.38	1.62	1.52
1	B	88	VAL	CB-CG1	5.37	1.64	1.52
1	A	1213	TYR	CD2-CE2	5.35	1.47	1.39
1	B	846	TYR	CE1-CZ	5.34	1.45	1.38
1	B	337	ALA	CA-CB	5.34	1.63	1.52
1	B	69	SER	N-CA	5.33	1.57	1.46
1	B	433	VAL	CB-CG2	5.33	1.64	1.52
1	B	308	GLU	CD-OE1	-5.32	1.19	1.25
1	B	1213	TYR	CE2-CZ	5.29	1.45	1.38
1	B	79	SER	CB-OG	5.28	1.49	1.42
1	B	582	ALA	CA-CB	5.28	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	972	ILE	CB-CG2	5.26	1.69	1.52
1	B	977	TYR	CB-CG	-5.25	1.43	1.51
1	A	1206	PHE	CE2-CZ	5.24	1.47	1.37
1	A	480	GLU	CG-CD	5.23	1.59	1.51
1	B	270	LYS	CD-CE	5.23	1.64	1.51
1	A	1162	VAL	CB-CG1	5.21	1.63	1.52
1	A	600	GLU	CD-OE1	5.21	1.31	1.25
1	B	798	PHE	CD2-CE2	5.21	1.49	1.39
1	A	29	TYR	CD2-CE2	5.19	1.47	1.39
1	B	662	CYS	CB-SG	5.19	1.91	1.82
1	B	659	GLU	CB-CG	-5.19	1.42	1.52
1	B	480	GLU	CD-OE1	5.17	1.31	1.25
1	B	1029	VAL	CB-CG2	5.13	1.63	1.52
1	B	114	PHE	CD2-CE2	5.10	1.49	1.39
1	A	602	GLU	CD-OE1	5.09	1.31	1.25
1	B	1155	TYR	CD2-CE2	5.07	1.47	1.39
1	B	940	GLU	CD-OE2	5.07	1.31	1.25
1	B	1312	PHE	CE1-CZ	5.04	1.47	1.37
1	B	1238	GLU	CD-OE2	5.03	1.31	1.25
1	B	994	LYS	CB-CG	5.02	1.66	1.52
1	B	480	GLU	N-CA	-5.01	1.36	1.46

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	980	ARG	NE-CZ-NH2	-18.71	110.95	120.30
1	A	980	ARG	NE-CZ-NH1	15.31	127.96	120.30
1	B	32	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	B	160	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	B	514	PHE	CB-CG-CD2	-8.88	114.58	120.80
1	B	1111	GLY	N-CA-C	-8.58	91.65	113.10
1	B	160	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	B	508	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	B	880	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	B	460	ASP	CB-CG-OD2	8.04	125.54	118.30
1	B	426	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	B	1004	LYS	CD-CE-NZ	7.93	129.94	111.70
1	B	748	CYS	CA-CB-SG	-7.66	100.22	114.00
1	A	1305	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	A	429	ASP	CB-CG-OD1	7.36	124.93	118.30
1	B	507	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	B	786	ARG	NE-CZ-NH1	-7.19	116.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	A	980	ARG	CG-CD-NE	-7.06	96.97	111.80
1	B	1279	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	B	1100	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	B	830	ASP	CB-CG-OD2	6.66	124.29	118.30
1	B	824	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	A	899	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	B	128	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	160	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	980	ARG	CD-NE-CZ	6.33	132.46	123.60
1	A	812	LEU	CB-CG-CD1	-6.12	100.59	111.00
1	B	718	ASP	CB-CG-OD1	6.07	123.77	118.30
1	B	370	LYS	CD-CE-NZ	-6.00	97.89	111.70
1	A	606	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	B	673	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	160	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	B	1318	THR	CA-C-N	5.96	128.12	116.20
1	B	606	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	393	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	164	LYS	CD-CE-NZ	5.92	125.31	111.70
1	A	1276	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	B	404	LEU	CB-CG-CD2	-5.91	100.96	111.00
1	B	21	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	416	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	A	680	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	700	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	1222	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	B	1318	THR	N-CA-C	5.69	126.37	111.00
1	B	1318	THR	C-N-CA	5.68	134.23	122.30
1	A	839	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	B	830	ASP	CB-CG-OD1	-5.65	113.22	118.30
1	A	508	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	793	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	429	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	B	473	LEU	CB-CG-CD2	5.51	120.37	111.00
1	A	148	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	1102	GLU	CA-CB-CG	5.41	125.30	113.40
1	A	1004	LYS	CD-CE-NZ	5.39	124.10	111.70
1	B	1239	PHE	CB-CG-CD2	-5.37	117.04	120.80
1	A	812	LEU	CA-CB-CG	-5.36	102.97	115.30
1	A	748	CYS	CA-CB-SG	-5.34	104.40	114.00
1	A	830	ASP	CB-CG-OD2	5.33	123.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	TYR	CZ-CE2-CD2	-5.31	115.02	119.80
1	B	864	PHE	CB-CG-CD2	-5.31	117.08	120.80
1	A	1305	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	B	33	LYS	CD-CE-NZ	-5.29	99.54	111.70
1	B	453	LEU	CB-CG-CD1	-5.28	102.02	111.00
1	A	994	LYS	CD-CE-NZ	5.27	123.82	111.70
1	B	594	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	518	PHE	CB-CG-CD2	-5.24	117.13	120.80
1	A	829	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	1317	VAL	CB-CA-C	-5.22	101.48	111.40
1	B	759	GLU	OE1-CD-OE2	-5.21	117.05	123.30
1	B	159	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	B	334	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	B	508	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	393	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	1219	LEU	CB-CG-CD2	-5.12	102.30	111.00
1	B	31	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	994	LYS	CD-CE-NZ	5.10	123.44	111.70
1	B	812	LEU	CA-CB-CG	-5.10	103.57	115.30
1	B	247	LEU	CB-CG-CD1	5.09	119.65	111.00
1	A	691	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	673	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	592	TYR	CZ-CE2-CD2	-5.06	115.25	119.80
1	B	827	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	B	1154	SER	N-CA-CB	-5.01	102.99	110.50

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	80	0
1	B	9975	0	9986	103	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
8	B	1298	0	0	21	0
All	All	22752	0	20116	181	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 4.

All (181) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1310:ASP:O	1:A:1314:THR:HG23	1.85	0.77
1:A:214:GLU:HG3	8:A:2004:HOH:O	1.83	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
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:NE2	1:B:1311:GLN:H	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:CD	1:B:565:LYS:H	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: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:321:GLN:HG2	1:A:413:GLU:CD	2.20	0.62
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:3:ALA:CA	1:A:4:ASP:CB	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:191:SER:CA	8:A:2315:HOH:O	2.50	0.59
1:A:3:ALA:CA	1:A:4:ASP:HB2	2.32	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
1:B:920:MET:HE3	1:B:1265:PHE:CG	2.39	0.57
1:B:565:LYS:HD3	1:B:565:LYS:H	1.69	0.57
1:B:812:LEU:HD11	1:B:825:CYS:CB	2.23	0.56
1:A:196:ASN:OD1	1:A:198:GLU:OE1	2.24	0.56
1:A:62:GLN:OE1	1:A:64:LYS:HE2	2.06	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:1250:LYS:HD3	1:A:1251:ARG:N	2.23	0.54
1:A:255:LYS:HE2	1:A:274:PHE:CE2	2.43	0.54
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:331:GLU:HG3	8:A:2422:HOH:O	2.10	0.51
1:A:1048:GLN:NE2	1:A:1187:ASN:HD22	2.08	0.51
1:A:296:ILE:HD11	1:A:314:GLU:HG3	1.91	0.51
1:B:812:LEU:HD21	1:B:825:CYS:HB2	1.92	0.51
1:A:272:MET:HE3	8:A:2328:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ILE:CD1	1:A:314:GLU:HG3	2.41	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: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
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:B:1259:VAL:O	1:B:1259:VAL:HG22	2.14	0.47
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.14	0.47
1:B:618:THR:OG1	1:B:688:THR:OG1	2.30	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:A:812:LEU:HA	1:A:812:LEU:HD23	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:B:699:GLN:HE21	1:B:703:ASN:CG	2.15	0.46
1:A:520:LEU:HD22	1:A:538:LEU:HD11	1.99	0.45
1:B:1175:ARG:HA	1:B:1238:GLU:O	2.17	0.45
1:B:605:LEU:HB3	1:B:812:LEU:HD21	1.98	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:143:GLN:CD	1:B:337:ALA:O	2.54	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:618:THR:HG1	1:B:688:THR:HG1	1.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.80	0.44
1:B:923:ALA:HA	1:B:926:TRP:NE1	2.32	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:1048:GLN:NE2	1:B:1187:ASN:HD22	2.15	0.43
1:B:412:LYS:CE	8:B:1831:HOH:O	2.66	0.43
1:B:1287:ASP:OD1	1:B:1289:ALA:HB3	2.18	0.43
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: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:A:911:PHE:O	1:A:912:ARG:C	2.58	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:1221:THR:HG22	1:B:1227:TYR:HB2	2.00	0.41
1:B:472:GLN:HE22	1:B:475:LYS:NZ	2.17	0.41
1:B:1212:HIS:CD2	8:B:2178:HOH:O	2.26	0.41
1:A:357:ILE:HD12	1:A:357:ILE:C	2.40	0.41
1:B:164:LYS:HB2	1:B:164:LYS:HE2	1.66	0.41
1:B:741:HIS:HA	1:B:911:PHE:CE1	2.56	0.41
1:A:1033:HIS:HE1	1:A:1043:HIS:ND1	2.19	0.41
1:A:686:LYS:HE3	1:A:686:LYS:HB3	1.46	0.41
1:A:1132:PHE:CG	1:B:1126:SER:HB2	2.56	0.41
1:B:606:ARG:HD2	1:B:606:ARG:HH11	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%)	34	17
1	B	1288/1331 (97%)	1245 (97%)	36 (3%)	7 (0%)	29	12
All	All	2581/2662 (97%)	2495 (97%)	74 (3%)	12 (0%)	29	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%)	1079 (98%)	17 (2%)	62	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1089/1123 (97%)	1069 (98%)	20 (2%)	59	38
All	All	2185/2246 (97%)	2148 (98%)	37 (2%)	60	41

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	PRO
1	A	112	CYS
1	A	140	ASN
1	A	199	ASP
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	720	LYS
1	A	743	TYR
1	A	911	PHE
1	A	1004	LYS
1	A	1250	LYS
1	A	1315	LEU
1	B	99	PRO
1	B	219	LYS
1	B	224	LYS
1	B	247	LEU
1	B	253	ASP
1	B	280	PRO
1	B	317	LYS
1	B	396	LEU
1	B	494	GLN
1	B	530	ASP
1	B	565	LYS
1	B	743	TYR
1	B	744	LEU
1	B	911	PHE
1	B	1004	LYS
1	B	1239	PHE
1	B	1250	LYS
1	B	1288	ASN
1	B	1290	LYS

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Mol	Chain	Res	Type
1	B	1311	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	145	ASN
1	A	291	HIS
1	A	332	GLN
1	A	449	GLN
1	A	472	GLN
1	A	483	GLN
1	A	585	GLN
1	A	642	ASN
1	A	704	ASN
1	A	893	ASN
1	A	1033	HIS
1	A	1048	GLN
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	291	HIS
1	B	332	GLN
1	B	472	GLN
1	B	585	GLN
1	B	699	GLN
1	B	893	ASN
1	B	1033	HIS
1	B	1048	GLN
1	B	1088	GLN
1	B	1173	ASN
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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	A	1334	-	0,3,3	0.00	-	0,3,3	0.00	-
2	FES	B	4002	1	0,4,4	0.00	-	-		
6	BCT	B	1333	-	0,3,3	0.00	-	0,3,3	0.00	-
2	FES	A	3002	1	0,4,4	0.00	-	-		
2	FES	A	3001	1	0,4,4	0.00	-	-		
7	GOL	A	1335	-	5,5,5	0.39	0	5,5,5	0.60	0
2	FES	B	4001	1	0,4,4	0.00	-	-		
4	FAD	B	4006	-	51,58,58	1.83	9 (17%)	60,89,89	2.02	12 (20%)
5	URC	B	1332	-	13,13,13	3.73	9 (69%)	11,19,19	6.41	7 (63%)
5	URC	A	1333	-	13,13,13	4.19	7 (53%)	11,19,19	6.91	7 (63%)
4	FAD	A	3006	-	51,58,58	1.74	11 (21%)	60,89,89	1.81	11 (18%)
7	GOL	B	1334	-	5,5,5	1.85	1 (20%)	5,5,5	3.08	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	4002	1	-	-	0/1/1/1
2	FES	A	3002	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FES	A	3001	1	-	-	0/1/1/1
5	URC	A	1333	-	-	-	0/2/2/2
2	FES	B	4001	1	-	-	0/1/1/1
4	FAD	B	4006	-	-	5/30/50/50	0/6/6/6
5	URC	B	1332	-	-	-	0/2/2/2
7	GOL	A	1335	-	-	0/4/4/4	-
4	FAD	A	3006	-	-	5/30/50/50	0/6/6/6
7	GOL	B	1334	-	-	3/4/4/4	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1333	URC	C4-N3	-8.72	1.35	1.46
5	B	1332	URC	C5-C6	-7.49	1.39	1.52
5	A	1333	URC	C5-C6	-6.96	1.40	1.52
5	A	1333	URC	O13-C6	6.36	1.36	1.23
5	B	1332	URC	C4-N3	-5.99	1.38	1.46
4	B	4006	FAD	C10-N1	5.28	1.40	1.33
4	B	4006	FAD	O4B-C1B	5.15	1.48	1.41
5	B	1332	URC	O13-C6	4.84	1.33	1.23
4	A	3006	FAD	C4X-N5	4.74	1.40	1.33
5	A	1333	URC	O24-C8	4.72	1.33	1.23
5	B	1332	URC	O24-C8	4.53	1.32	1.23
4	A	3006	FAD	C4-N3	4.32	1.40	1.33
4	B	4006	FAD	C1'-N10	4.28	1.52	1.48
4	B	4006	FAD	C4-N3	3.92	1.39	1.33
4	B	4006	FAD	C4X-N5	3.89	1.38	1.33
7	B	1334	GOL	O2-C2	3.84	1.54	1.43
4	A	3006	FAD	C10-N1	3.79	1.38	1.33
4	A	3006	FAD	C9A-N10	3.49	1.43	1.38
5	A	1333	URC	C4-N9	-3.44	1.40	1.44
4	B	4006	FAD	C9A-N10	3.28	1.42	1.38
4	A	3006	FAD	C2A-N3A	3.21	1.37	1.32
5	B	1332	URC	C2-N3	3.19	1.41	1.34
4	B	4006	FAD	C2A-N3A	3.15	1.37	1.32
5	A	1333	URC	C5-N7	-3.12	1.39	1.45
5	B	1332	URC	C5-N7	-3.10	1.39	1.45
5	B	1332	URC	O11-C2	3.08	1.29	1.23
4	A	3006	FAD	O4B-C1B	3.04	1.45	1.41
4	A	3006	FAD	C1'-N10	2.97	1.51	1.48
5	B	1332	URC	C2-N1	2.68	1.42	1.37
4	A	3006	FAD	C2B-C1B	-2.56	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4006	FAD	C4X-C10	2.48	1.41	1.38
5	A	1333	URC	C2-N1	2.39	1.41	1.37
4	A	3006	FAD	C2A-N1A	2.35	1.38	1.33
5	B	1332	URC	C8-N7	2.25	1.39	1.35
4	B	4006	FAD	C5X-N5	2.20	1.39	1.35
4	A	3006	FAD	O4B-C4B	-2.12	1.40	1.45
4	A	3006	FAD	O3B-C3B	2.10	1.47	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1333	URC	C5-C4-N9	16.91	110.47	102.64
5	B	1332	URC	C5-C4-N9	14.50	109.35	102.64
5	B	1332	URC	C4-N9-C8	-13.25	103.89	112.89
5	A	1333	URC	C4-N9-C8	-12.72	104.25	112.89
4	A	3006	FAD	C4-N3-C2	7.60	121.56	115.14
4	B	4006	FAD	N3A-C2A-N1A	-6.85	117.97	128.68
4	B	4006	FAD	C1'-N10-C9A	5.88	122.92	118.29
5	A	1333	URC	N1-C2-N3	5.72	122.14	116.12
4	B	4006	FAD	C10-C4X-N5	-5.27	117.61	121.26
7	B	1334	GOL	C3-C2-C1	-5.06	92.05	111.70
5	B	1332	URC	N7-C8-N9	4.90	113.36	108.76
4	B	4006	FAD	C4-N3-C2	4.68	119.10	115.14
5	B	1332	URC	N1-C2-N3	4.64	121.01	116.12
5	A	1333	URC	N7-C8-N9	4.59	113.07	108.76
4	B	4006	FAD	C2A-N1A-C6A	4.52	126.49	118.75
4	A	3006	FAD	C4X-C4-N3	-4.11	117.81	123.43
4	B	4006	FAD	C4X-N5-C5X	4.03	120.80	116.77
4	A	3006	FAD	C7-C6-C5X	-3.68	116.01	121.22
4	A	3006	FAD	O4'-C4'-C3'	-3.32	101.04	109.10
7	B	1334	GOL	O1-C1-C2	-3.20	94.86	110.20
4	B	4006	FAD	C4X-C4-N3	-3.18	119.08	123.43
4	A	3006	FAD	C5A-C6A-N6A	3.13	125.10	120.35
4	A	3006	FAD	N3A-C2A-N1A	-2.84	124.25	128.68
5	B	1332	URC	O13-C6-N1	2.69	125.79	121.01
7	B	1334	GOL	O3-C3-C2	2.63	122.83	110.20
4	B	4006	FAD	O4B-C1B-C2B	-2.63	103.08	106.93
5	A	1333	URC	O24-C8-N7	-2.62	122.18	125.94
4	A	3006	FAD	C1'-N10-C9A	2.58	120.32	118.29
5	B	1332	URC	O24-C8-N9	-2.30	122.64	125.94
5	A	1333	URC	O11-C2-N1	-2.29	117.50	121.82
4	B	4006	FAD	C4-C4X-C10	2.20	121.41	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3006	FAD	C4X-N5-C5X	2.19	118.96	116.77
5	B	1332	URC	O11-C2-N3	-2.19	118.56	122.92
4	A	3006	FAD	C4A-C5A-N7A	-2.16	107.15	109.40
5	A	1333	URC	C6-N1-C2	-2.08	123.46	126.25
7	B	1334	GOL	O2-C2-C1	-2.07	100.02	109.12
4	A	3006	FAD	O5'-C5'-C4'	-2.06	103.85	109.36
4	B	4006	FAD	C5A-C6A-N1A	-2.03	115.76	120.35
4	A	3006	FAD	O3'-C3'-C4'	2.02	113.70	108.81
4	B	4006	FAD	C4X-C10-N10	2.01	122.37	120.30
4	B	4006	FAD	C9A-N10-C10	-2.01	119.28	121.91

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	4006	FAD	N10-C1'-C2'-O2'
4	B	4006	FAD	N10-C1'-C2'-C3'
4	A	3006	FAD	N10-C1'-C2'-O2'
4	A	3006	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'

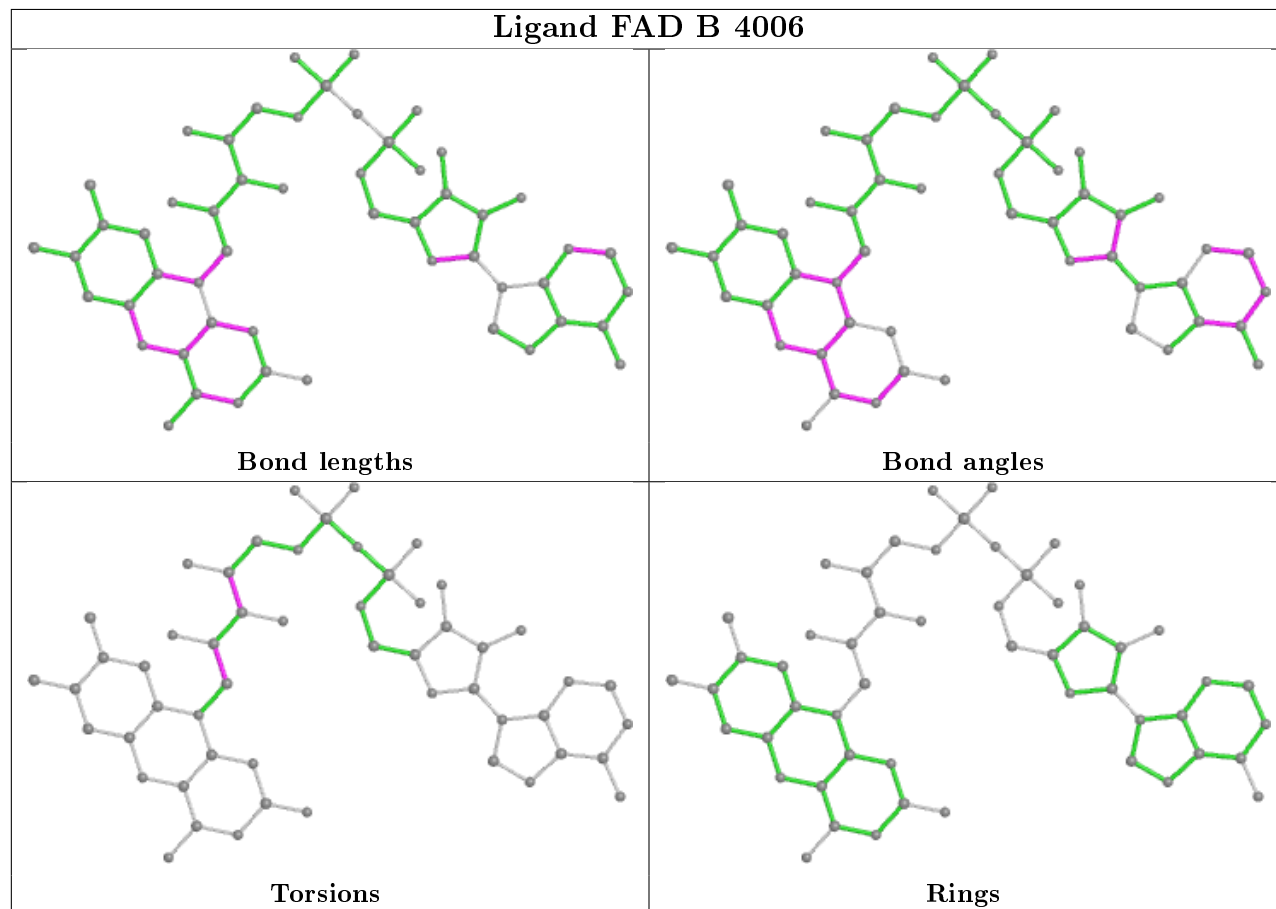
There are no ring outliers.

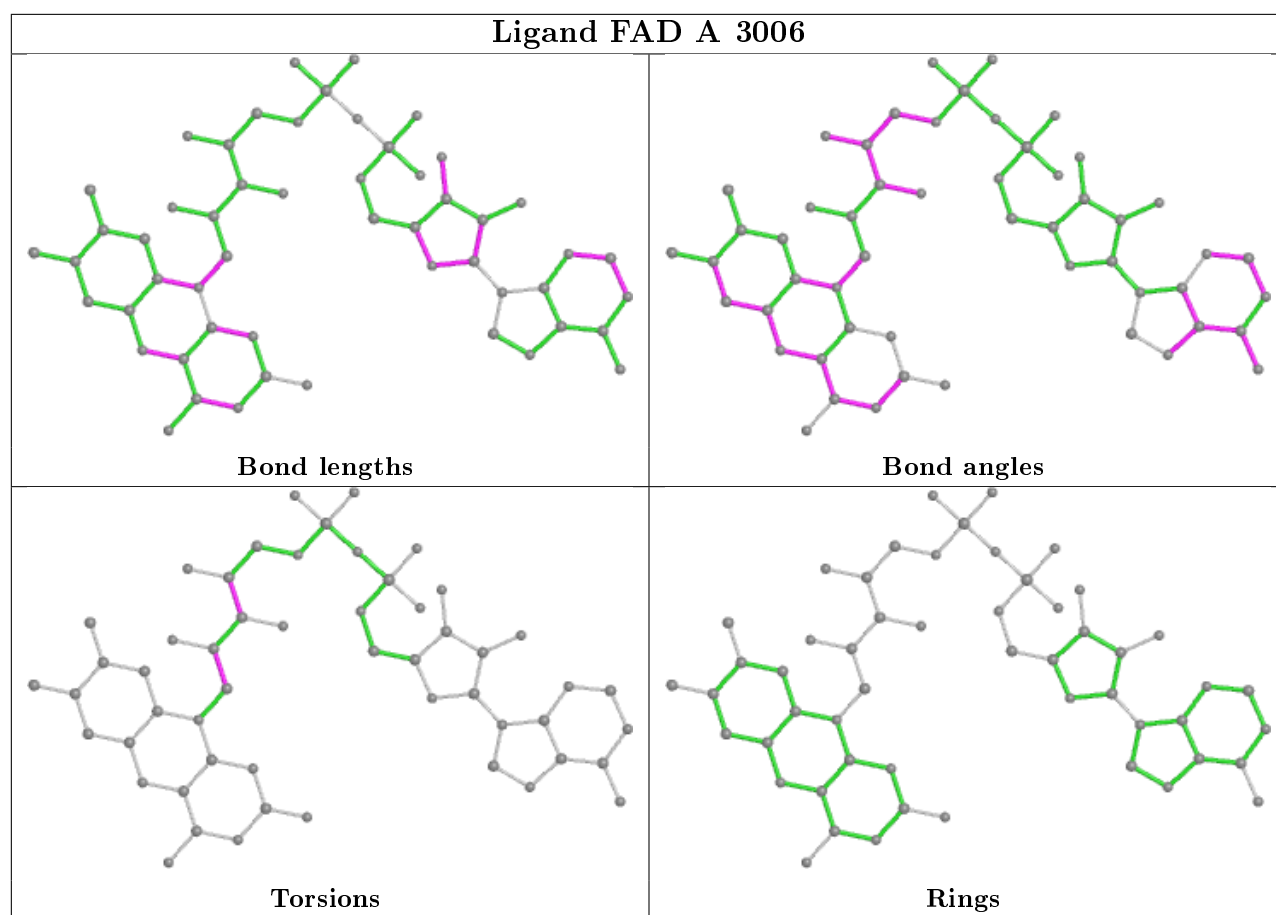
1 monomer is involved in 1 short contact:

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1299/1331 (97%)	-0.02	32 (2%) 57 63	8, 18, 36, 54	0
1	B	1292/1331 (97%)	-0.11	27 (2%) 63 70	8, 15, 32, 63	0
All	All	2591/2662 (97%)	-0.06	59 (2%) 60 66	8, 16, 34, 63	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1289	ALA	10.9
1	A	1324	CYS	7.6
1	B	1287	ASP	7.0
1	A	61	LEU	5.9
1	B	1320	VAL	5.5
1	B	1286	GLY	4.9
1	B	1288	ASN	4.7
1	A	1317	VAL	4.5
1	A	1111	GLY	4.5
1	A	221	THR	4.3
1	B	221	THR	4.3
1	A	1287	ASP	4.2
1	A	3	ALA	4.1
1	B	1111	GLY	4.1
1	B	61	LEU	4.1
1	B	218	LEU	4.1
1	A	1288	ASN	4.0
1	B	1110	THR	3.9
1	A	1110	THR	3.8
1	B	530	ASP	3.8
1	A	191	SER	3.7
1	B	220	ASP	3.5
1	B	1318	THR	3.3
1	B	1106	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	192	PRO	3.2
1	A	220	ASP	3.2
1	A	530	ASP	3.2
1	A	533	ASP	3.1
1	B	3	ALA	2.9
1	A	166	GLY	2.9
1	A	724	SER	2.9
1	A	566	ASP	2.8
1	A	534	MET	2.8
1	B	1107	LYS	2.7
1	A	222	PRO	2.7
1	B	191	SER	2.7
1	A	293	PRO	2.7
1	B	565	LYS	2.5
1	B	1102	GLU	2.5
1	A	565	LYS	2.5
1	A	531	LEU	2.5
1	A	390	PRO	2.4
1	B	1290	LYS	2.4
1	B	222	PRO	2.4
1	A	249	ALA	2.4
1	A	290	VAL	2.3
1	B	720	LYS	2.3
1	A	474	SER	2.2
1	A	473	LEU	2.2
1	B	1264	LEU	2.2
1	A	198	GLU	2.2
1	A	321	GLN	2.2
1	B	1103	PRO	2.1
1	B	1109	PRO	2.1
1	A	1289	ALA	2.1
1	B	1143	GLU	2.1
1	A	444	GLY	2.1
1	A	383	ARG	2.0
1	B	550	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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, 95<sup>th</sup> 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.

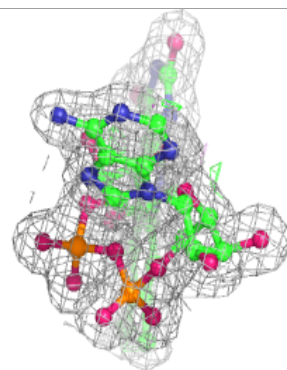
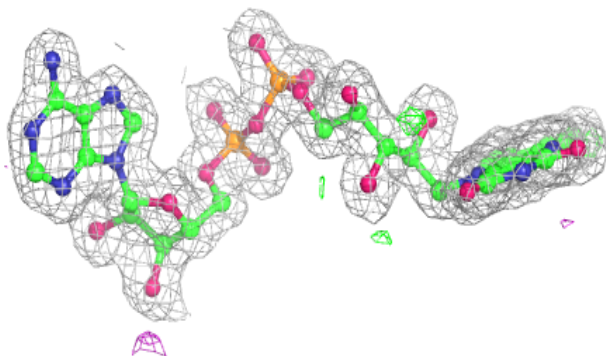
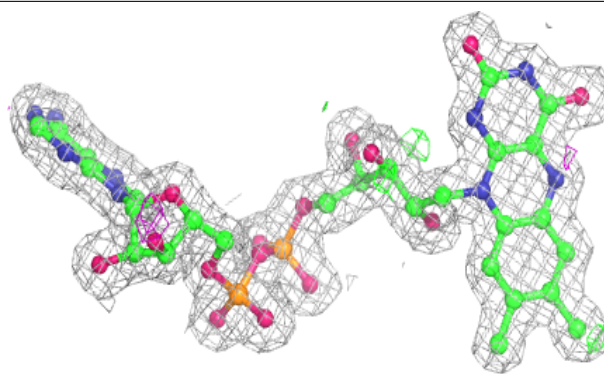
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	B	1334	6/6	0.71	0.19	18,35,37,38	0
5	URC	B	1332	12/12	0.87	0.15	15,20,25,26	0
5	URC	A	1333	12/12	0.89	0.12	18,23,29,31	0
7	GOL	A	1335	6/6	0.97	0.08	20,24,29,29	0
4	FAD	A	3006	53/53	0.98	0.07	13,16,20,21	0
4	FAD	B	4006	53/53	0.98	0.08	9,12,14,15	0
6	BCT	B	1333	4/4	0.99	0.08	11,12,13,15	0
2	FES	A	3001	4/4	0.99	0.05	14,14,14,15	0
6	BCT	A	1334	4/4	0.99	0.09	15,17,17,17	0
2	FES	B	4001	4/4	0.99	0.06	13,13,14,14	0
3	CA	A	4009	1/1	0.99	0.07	15,15,15,15	0
3	CA	B	1335	1/1	1.00	0.06	11,11,11,11	0
2	FES	A	3002	4/4	1.00	0.07	11,11,11,12	0
3	CA	B	4019	1/1	1.00	0.07	11,11,11,11	0
3	CA	A	1332	1/1	1.00	0.06	13,13,13,13	0
2	FES	B	4002	4/4	1.00	0.07	8,9,9,9	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.

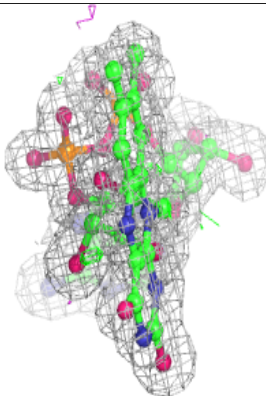
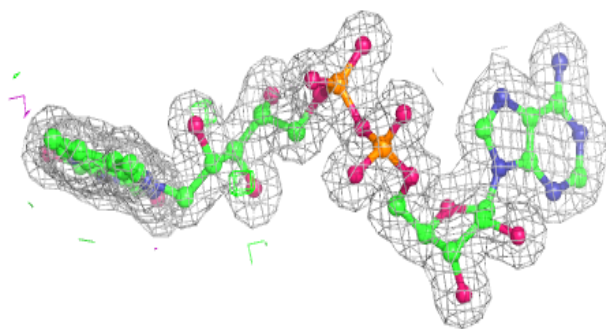
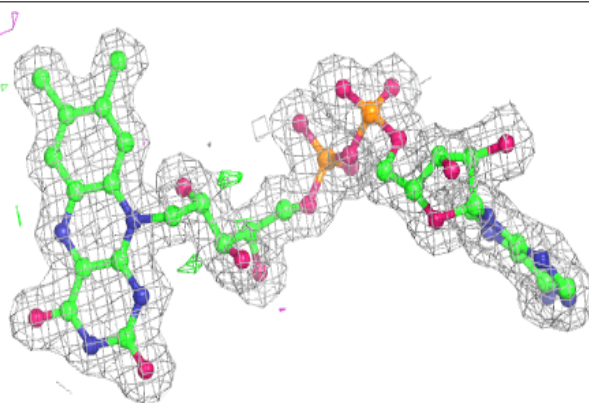


**Electron density around FAD A 3006:**

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

**Electron density around FAD B 4006:**

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



## 6.5 Other polymers

There are no such residues in this entry.