



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:46 PM EDT

PDB ID : 4YRW / pdb_00004yrw
Title : rat xanthine oxidoreductase, C-terminal deletion protein variant
Authors : Okamoto, K.
Deposited on : 2015-03-16
Resolution : 1.99 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

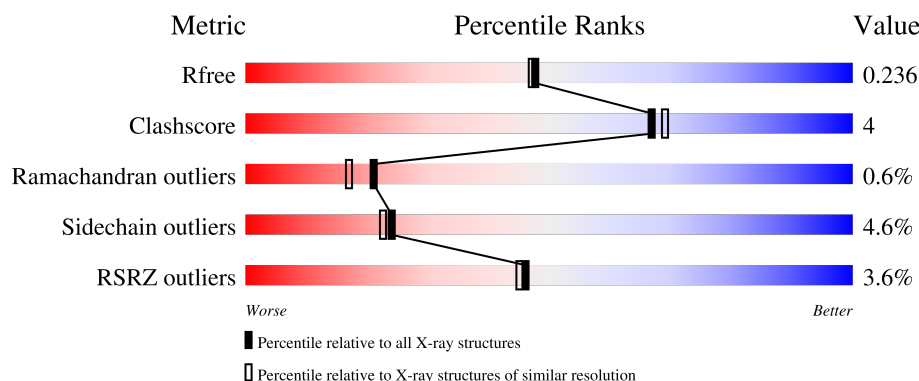
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	4% 84% 11% ...
1	B	1315	3% 85% 11% ..

2 Entry composition [i](#)

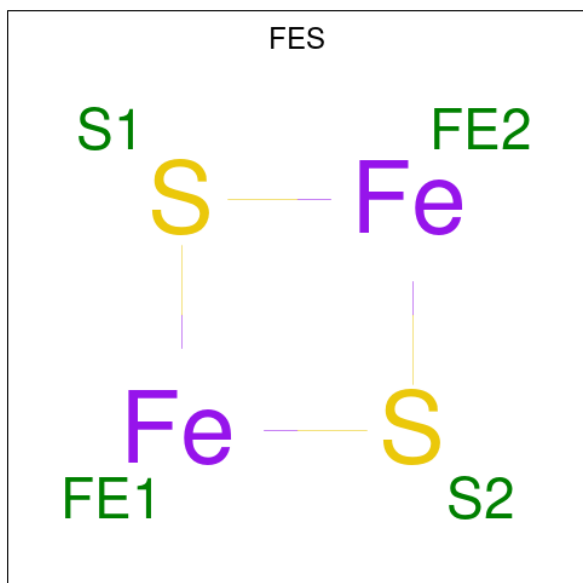
There are 8 unique types of molecules in this entry. The entry contains 20715 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

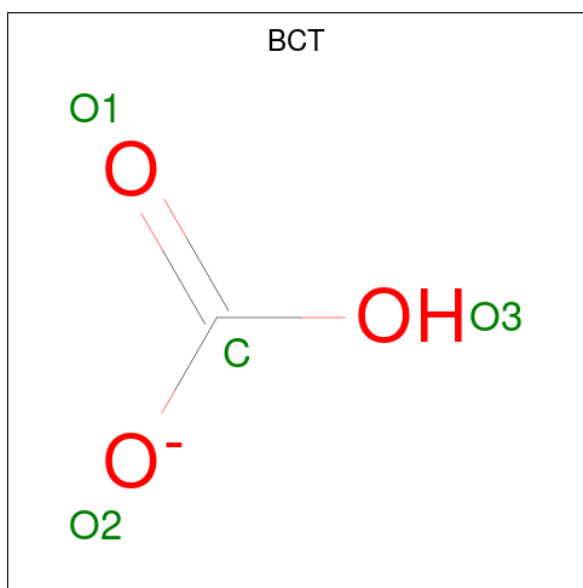
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1289	Total	C	N	O	S	0	0	0
			9964	6314	1714	1873	63			
1	B	1286	Total	C	N	O	S	0	0	0
			9939	6298	1711	1867	63			

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



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

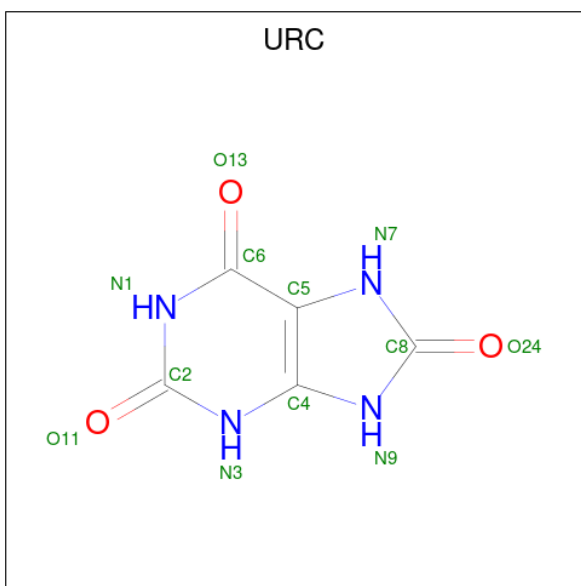
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

- Molecule 6 is URIC ACID (CCD ID: URC) (formula: $C_5H_4N_4O_3$).



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

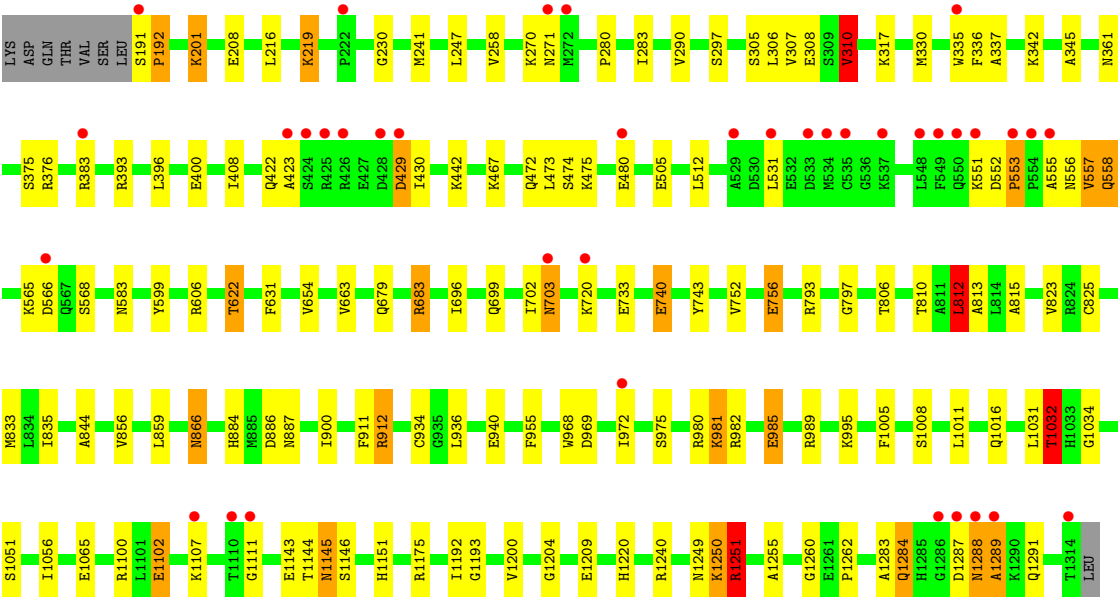
- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	250	Total	O	0	0
			250	250		
8	B	388	Total	O	0	0
			388	388		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.50Å 138.47Å 222.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.33 – 1.99 43.33 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.33-1.99) 99.7 (43.33-1.99)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.79 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.186 , 0.229 0.194 , 0.236	Depositor DCC
R_{free} test set	10396 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20715	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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, URC, GOL, FAD, BCT, 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	1.27	22/10174 (0.2%)	1.21	40/13767 (0.3%)
1	B	1.40	46/10149 (0.5%)	1.22	40/13734 (0.3%)
All	All	1.34	68/20323 (0.3%)	1.21	80/27501 (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	B	0	1

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1056	ILE	C-O	-7.14	1.18	1.24
1	B	812	LEU	CB-CG	-6.98	1.39	1.53
1	B	555	ALA	CA-C	6.85	1.57	1.52
1	B	1193	GLY	N-CA	6.42	1.54	1.45
1	B	1016	GLN	N-CA	-6.32	1.38	1.45
1	B	258	VAL	C-O	-6.17	1.16	1.24
1	B	583	ASN	C-O	-6.17	1.17	1.24
1	B	989	ARG	C-O	-6.11	1.17	1.24
1	B	568	SER	C-O	6.11	1.30	1.23
1	B	553	PRO	CA-C	6.07	1.56	1.52
1	A	336	PHE	CA-C	6.00	1.57	1.52
1	B	192	PRO	N-CA	5.95	1.53	1.47
1	A	190	LEU	CA-C	5.95	1.65	1.52
1	B	408	ILE	N-CA	5.91	1.50	1.46
1	B	1102	GLU	C-O	-5.89	1.18	1.24
1	A	756	GLU	CA-C	-5.87	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307	VAL	C-O	5.80	1.30	1.24
1	B	558	GLN	C-O	-5.75	1.17	1.24
1	B	703	ASN	N-CA	-5.72	1.38	1.46
1	B	442	LYS	N-CA	5.70	1.52	1.45
1	B	740	GLU	CD-OE1	5.69	1.36	1.25
1	A	1111	GLY	N-CA	5.67	1.52	1.44
1	A	86	THR	C-O	-5.66	1.17	1.24
1	A	577	LEU	CA-C	5.65	1.59	1.52
1	B	1005	PHE	N-CA	5.62	1.52	1.46
1	A	465	ALA	CA-C	5.61	1.59	1.53
1	B	230	GLY	N-CA	5.56	1.50	1.44
1	B	940	GLU	CA-C	-5.56	1.45	1.52
1	B	208	GLU	C-O	-5.55	1.16	1.23
1	A	422	GLN	CA-C	-5.54	1.45	1.52
1	B	480	GLU	N-CA	-5.52	1.39	1.46
1	A	756	GLU	N-CA	5.48	1.52	1.46
1	B	1220	HIS	N-CA	5.47	1.53	1.46
1	B	102	GLU	N-CA	-5.45	1.39	1.46
1	A	949	GLU	C-O	-5.41	1.17	1.23
1	B	631	PHE	C-O	-5.39	1.17	1.23
1	B	124	TYR	CA-C	-5.37	1.45	1.52
1	B	740	GLU	CD-OE2	5.35	1.35	1.25
1	A	240	THR	CB-CG2	-5.34	1.34	1.52
1	A	792	LYS	C-O	-5.33	1.17	1.24
1	B	565	LYS	C-O	-5.33	1.17	1.24
1	A	776	VAL	CA-C	5.32	1.59	1.52
1	B	1260	GLY	N-CA	5.31	1.52	1.45
1	B	1111	GLY	N-CA	5.26	1.51	1.44
1	A	4	ASP	C-O	-5.25	1.17	1.24
1	B	815	ALA	C-O	5.22	1.30	1.24
1	A	278	VAL	C-O	-5.21	1.18	1.24
1	A	749	THR	N-CA	5.19	1.52	1.46
1	B	793	ARG	CZ-NH1	5.17	1.40	1.32
1	A	596	ILE	C-O	-5.16	1.18	1.25
1	B	1284	GLN	CD-NE2	-5.15	1.22	1.33
1	B	663	VAL	N-CA	-5.14	1.40	1.46
1	B	884	HIS	CA-CB	5.14	1.60	1.53
1	B	84	ALA	N-CA	-5.12	1.40	1.46
1	B	859	LEU	CA-C	-5.12	1.46	1.52
1	A	161	THR	C-O	-5.11	1.17	1.24
1	B	361	ASN	C-O	-5.11	1.19	1.24
1	B	423	ALA	CA-C	5.09	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1175	ARG	N-CA	-5.09	1.40	1.46
1	A	345	ALA	N-CA	5.09	1.52	1.46
1	B	1200	VAL	N-CA	5.08	1.52	1.46
1	B	230	GLY	C-O	-5.08	1.19	1.23
1	B	305	SER	C-O	-5.06	1.17	1.24
1	B	813	ALA	CA-CB	-5.06	1.45	1.53
1	A	162	PHE	C-O	-5.04	1.17	1.24
1	B	505	GLU	CA-C	5.04	1.59	1.52
1	A	818	LYS	C-O	-5.02	1.18	1.24
1	A	1071	VAL	N-CA	5.01	1.49	1.45

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	640	VAL	N-CA-CB	9.58	118.99	110.08
1	B	812	LEU	CA-CB-CG	-9.13	84.34	116.30
1	A	900	ILE	CB-CA-C	8.97	124.05	110.96
1	A	347	ILE	CB-CA-C	-8.45	100.74	112.14
1	B	1111	GLY	CA-C-N	-8.29	112.26	120.21
1	B	1111	GLY	C-N-CA	-8.29	112.26	120.21
1	A	433	VAL	N-CA-C	8.19	119.54	109.30
1	B	812	LEU	CD1-CG-CD2	8.14	128.70	110.80
1	A	1286	GLY	N-CA-C	8.13	122.48	112.73
1	A	406	ILE	CB-CA-C	-8.00	98.66	110.33
1	B	1288	ASN	N-CA-C	7.79	120.14	108.31
1	B	703	ASN	N-CA-CB	-7.53	98.70	110.30
1	B	1111	GLY	N-CA-C	-7.33	97.39	112.34
1	B	429	ASP	N-CA-CB	-7.28	100.84	110.88
1	B	430	ILE	N-CA-C	7.15	119.02	108.65
1	A	1032	THR	CB-CA-C	-7.09	94.99	111.09
1	B	297	SER	CB-CA-C	6.98	121.50	110.19
1	A	1052	ARG	NE-CZ-NH2	-6.91	112.98	119.20
1	B	1032	THR	CB-CA-C	-6.91	95.60	110.45
1	B	654	VAL	N-CA-C	-6.86	104.08	110.53
1	B	622	THR	N-CA-CB	-6.78	100.23	110.73
1	B	696	ILE	CB-CA-C	-6.67	106.04	111.71
1	B	1034	GLY	N-CA-C	6.67	121.97	113.24
1	A	344	VAL	CB-CA-C	-6.65	104.13	110.65
1	B	201	LYS	CA-CB-CG	6.53	127.16	114.10
1	B	1032	THR	OG1-CB-CG2	6.36	122.02	109.30
1	B	1251	ARG	N-CA-C	6.31	124.23	110.80
1	A	310	VAL	N-CA-CB	6.26	118.58	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	SER	CA-C-N	-6.25	112.03	119.84
1	A	191	SER	C-N-CA	-6.25	112.03	119.84
1	A	70	VAL	N-CA-CB	-6.19	100.91	112.36
1	A	593	CYS	N-CA-C	6.04	118.39	111.02
1	A	1148	ASN	CA-C-N	-6.01	113.57	119.64
1	A	1148	ASN	C-N-CA	-6.01	113.57	119.64
1	A	340	GLN	CB-CA-C	-6.00	101.47	110.88
1	B	756	GLU	CB-CA-C	-5.95	98.93	109.70
1	B	1032	THR	N-CA-CB	5.93	121.57	111.66
1	A	1135	THR	CA-C-N	-5.84	114.30	120.66
1	A	1135	THR	C-N-CA	-5.84	114.30	120.66
1	A	94	THR	N-CA-CB	-5.81	100.45	110.32
1	A	812	LEU	CB-CA-C	-5.78	101.20	110.79
1	B	812	LEU	N-CA-C	5.77	117.24	111.07
1	B	1250	LYS	CA-C-N	5.74	132.51	121.54
1	B	1250	LYS	C-N-CA	5.74	132.51	121.54
1	A	163	ALA	N-CA-C	5.74	118.17	109.63
1	B	70	VAL	CG1-CB-CG2	5.72	123.38	110.80
1	B	1100	ARG	N-CA-C	5.65	117.44	111.28
1	A	83	VAL	N-CA-CB	-5.57	103.08	112.44
1	B	835	ILE	CA-C-N	-5.53	113.81	122.65
1	B	835	ILE	C-N-CA	-5.53	113.81	122.65
1	A	396	LEU	N-CA-C	5.51	119.48	112.87
1	A	1262	PRO	N-CA-C	5.51	117.42	110.70
1	A	1032	THR	CA-CB-OG1	5.46	117.80	109.60
1	B	310	VAL	N-CA-CB	5.44	118.74	110.58
1	A	149	CYS	N-CA-C	5.41	119.89	113.12
1	B	702	ILE	CA-C-O	5.38	126.65	121.05
1	B	342	LYS	N-CA-C	5.35	117.87	111.71
1	B	553	PRO	CA-C-N	-5.33	114.75	120.03
1	B	553	PRO	C-N-CA	-5.33	114.75	120.03
1	A	94	THR	OG1-CB-CG2	5.33	119.96	109.30
1	A	869	ASN	N-CA-C	5.31	119.45	112.92
1	B	98	HIS	N-CA-C	-5.29	102.78	110.08
1	B	1032	THR	CA-CB-OG1	5.27	117.50	109.60
1	A	163	ALA	CA-C-N	5.22	129.82	122.46
1	A	163	ALA	C-N-CA	5.22	129.82	122.46
1	B	1005	PHE	CA-C-N	5.21	125.67	120.98
1	B	1005	PHE	C-N-CA	5.21	125.67	120.98
1	B	1251	ARG	N-CA-CB	-5.20	101.70	110.49
1	B	812	LEU	N-CA-CB	-5.19	102.48	110.01
1	A	70	VAL	CG1-CB-CG2	5.18	122.19	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	422	GLN	N-CA-C	5.14	117.80	110.24
1	A	338	GLY	N-CA-C	5.13	120.97	112.66
1	B	40	LYS	N-CA-C	5.12	118.08	110.14
1	A	1052	ARG	NE-CZ-NH1	5.11	126.61	121.50
1	A	782	VAL	CA-C-N	-5.07	115.01	120.03
1	A	782	VAL	C-N-CA	-5.07	115.01	120.03
1	A	337	ALA	N-CA-C	-5.07	101.55	108.24
1	A	688	THR	CB-CA-C	5.07	118.99	109.71
1	A	442	LYS	CA-C-N	-5.06	114.74	119.85
1	A	442	LYS	C-N-CA	-5.06	114.74	119.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	886	ASP	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	9967	85	0
1	B	9939	0	9942	65	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	53	0	31	1	0
5	B	53	0	31	2	0
6	A	12	0	4	0	0
6	B	12	0	4	0	0
7	A	6	0	8	0	0
7	B	12	0	16	0	0
8	A	250	0	0	1	0
8	B	388	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20715	0	20003	148	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 (148) 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:982:ARG:NH1	8:B:4101:HOH:O	1.56	1.21
1:B:192:PRO:HD2	8:B:4376:HOH:O	1.55	1.04
1:B:740:GLU:HG2	1:B:833:MET:SD	1.99	1.02
1:A:423:ALA:O	1:A:424:SER:HB3	1.69	0.92
1:A:618:THR:OG1	1:A:688:THR:HG22	1.71	0.89
1:B:982:ARG:CZ	8:B:4101:HOH:O	2.06	0.87
1:A:565:LYS:H	1:A:565:LYS:HD3	1.45	0.81
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.45	0.81
1:A:231:GLU:OE2	1:A:680:ARG:NH2	2.13	0.81
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.46	0.78
1:A:565:LYS:HD3	1:A:565:LYS:N	1.98	0.78
1:B:982:ARG:NH2	8:B:4101:HOH:O	2.13	0.78
1:A:426:ARG:HH11	1:A:426:ARG:HB3	1.51	0.75
1:A:709:GLY:O	1:A:899:ARG:NH2	2.20	0.74
1:B:130:GLN:HE21	1:B:132:GLU:H	1.34	0.74
1:B:472:GLN:HA	1:B:475:LYS:HD3	1.70	0.73
1:A:130:GLN:HE21	1:A:132:GLU:H	1.33	0.73
1:A:446:ILE:HD12	1:A:534:MET:HB2	1.70	0.72
1:A:423:ALA:O	1:A:424:SER:CB	2.37	0.72
1:A:446:ILE:HD12	1:A:534:MET:CB	2.21	0.70
1:B:271:ASN:HB2	1:B:683:ARG:NH1	2.05	0.70
1:A:388:PHE:HA	1:A:396:LEU:HG	1.75	0.69
1:B:981:LYS:O	1:B:985:GLU:HG2	1.93	0.69
1:A:812:LEU:HD11	1:A:825:CYS:CB	2.24	0.68
1:B:241:MET:HE2	1:B:283:ILE:HG21	1.74	0.68
1:B:699:GLN:O	1:B:703:ASN:HB2	1.94	0.68
1:A:618:THR:OG1	1:A:688:THR:CG2	2.42	0.67
1:A:740:GLU:HG3	1:A:833:MET:HE3	1.75	0.67
1:B:1283:ALA:HA	1:B:1288:ASN:HD21	1.59	0.67
1:A:371:LEU:CD2	1:A:406:ILE:HG23	2.26	0.66
1:A:421:LYS:HD2	8:A:3146:HOH:O	1.97	0.64
1:B:191:SER:OG	1:B:192:PRO:HD3	1.98	0.64
1:A:565:LYS:N	1:A:565:LYS:CD	2.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:LEU:HD11	1:A:825:CYS:HB3	1.81	0.62
1:A:240:THR:HG22	1:A:243:GLU:H	1.64	0.62
1:B:552:ASP:HB3	1:B:553:PRO:HD2	1.83	0.61
1:B:58:TYR:CE2	1:B:219:LYS:HD3	2.36	0.60
1:B:606:ARG:HD3	1:B:679:GLN:HA	1.82	0.60
1:A:371:LEU:HD23	1:A:406:ILE:HG23	1.84	0.59
1:B:1250:LYS:HG3	1:B:1251:ARG:H	1.67	0.59
1:A:138:ILE:HD12	1:A:163:ALA:HB2	1.83	0.58
1:A:812:LEU:HD11	1:A:825:CYS:HB2	1.87	0.57
1:B:336:PHE:O	1:B:336:PHE:HD1	1.88	0.56
1:A:63:ASN:O	1:A:64:LYS:HB3	2.05	0.56
1:A:1286:GLY:O	1:A:1287:ASP:HB3	2.05	0.56
1:B:157:GLN:HE22	1:B:558:GLN:HE22	1.53	0.56
1:A:539:ASP:OD1	1:A:540:PRO:HD2	2.05	0.56
1:B:1032:THR:HG21	8:B:4364:HOH:O	2.06	0.55
1:B:1032:THR:CG2	1:B:1065:GLU:O	2.55	0.55
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	2.04	0.55
1:B:1288:ASN:O	1:B:1289:ALA:CB	2.55	0.55
1:A:532:GLU:OE1	1:A:537:LYS:HG2	2.07	0.54
1:A:812:LEU:HD21	1:A:825:CYS:N	2.22	0.54
1:B:271:ASN:HB2	1:B:683:ARG:CZ	2.37	0.54
1:A:446:ILE:O	1:A:446:ILE:CG2	2.55	0.54
1:A:866:ASN:C	1:A:866:ASN:HD22	2.16	0.54
1:B:1288:ASN:O	1:B:1289:ALA:HB3	2.07	0.54
1:B:271:ASN:O	1:B:271:ASN:ND2	2.40	0.54
1:A:870:THR:HG22	1:A:907:SER:OG	2.08	0.53
1:A:1032:THR:CG2	1:A:1065:GLU:O	2.58	0.52
1:A:280:PRO:HB2	1:A:286:LEU:HD23	1.91	0.51
1:A:852:LYS:CE	1:A:852:LYS:HA	2.41	0.51
1:A:1032:THR:HG23	1:A:1065:GLU:O	2.11	0.51
1:A:392:TYR:OH	1:A:429:ASP:OD2	2.25	0.50
1:B:911:PHE:O	1:B:912:ARG:C	2.53	0.50
1:B:472:GLN:HE22	1:B:475:LYS:NZ	2.09	0.50
1:A:240:THR:CG2	1:A:242:GLU:HB2	2.41	0.50
1:B:552:ASP:HB3	1:B:553:PRO:CD	2.41	0.50
1:B:969:ASP:HA	1:B:972:ILE:CG1	2.42	0.49
1:A:426:ARG:HH11	1:A:426:ARG:CB	2.24	0.49
1:A:555:ALA:O	1:A:1238:GLU:HA	2.13	0.48
1:A:255:LYS:HE2	1:A:274:PHE:CE1	2.48	0.48
1:A:721:LYS:O	1:A:725:GLU:HG3	2.13	0.48
1:A:164:LYS:C	1:A:165:ASP:OD1	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:900:ILE:HD12	1:A:900:ILE:C	2.39	0.48
1:A:1080:SER:O	1:A:1258:ALA:HB1	2.14	0.47
1:B:1032:THR:HG23	1:B:1065:GLU:O	2.14	0.47
1:A:764:VAL:O	1:A:791:VAL:HG22	2.14	0.47
1:A:64:LYS:HE3	1:A:66:VAL:HG12	1.96	0.47
1:A:792:LYS:HE3	1:B:756:GLU:OE1	2.15	0.47
1:A:565:LYS:H	1:A:565:LYS:CD	2.13	0.47
1:B:975:SER:O	1:B:980:ARG:HD3	2.14	0.47
1:B:306:LEU:O	1:B:310:VAL:HG13	2.15	0.46
1:A:361:ASN:N	1:A:362:PRO:CD	2.79	0.46
1:A:190:LEU:HD13	1:A:191:SER:H	1.80	0.46
1:A:571:ASP:CG	1:A:1052:ARG:HD3	2.41	0.46
1:A:571:ASP:OD1	1:A:1052:ARG:HD3	2.15	0.46
1:B:900:ILE:HD12	1:B:900:ILE:N	2.31	0.46
1:A:446:ILE:HD12	1:A:534:MET:HB3	1.94	0.46
1:A:995:LYS:HZ3	1:A:1284:GLN:HE21	1.64	0.46
1:B:337:ALA:HB2	5:B:4004:FAD:C6	2.46	0.46
1:B:557:VAL:HG13	1:B:1240:ARG:HG2	1.97	0.46
1:B:335:TRP:CE3	1:B:335:TRP:HA	2.50	0.46
1:A:863:HIS:O	1:A:898:GLY:HA2	2.16	0.45
1:B:1151:HIS:NE2	1:B:1251:ARG:HG3	2.31	0.45
1:A:749:THR:O	1:A:812:LEU:HD22	2.15	0.45
1:A:153:ARG:HD2	1:A:153:ARG:C	2.42	0.45
1:B:336:PHE:O	1:B:336:PHE:CD1	2.67	0.45
1:B:866:ASN:C	1:B:866:ASN:HD22	2.24	0.45
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.17	0.45
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	1.99	0.45
1:A:387:THR:O	1:A:396:LEU:HD21	2.16	0.45
1:A:740:GLU:HG2	1:A:1211:LEU:HD21	1.98	0.44
1:A:321:GLN:HG2	1:A:413:GLU:CD	2.42	0.44
1:B:336:PHE:CD1	1:B:336:PHE:C	2.96	0.44
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.17	0.44
1:A:1203:LEU:C	1:A:1203:LEU:HD23	2.43	0.44
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.17	0.44
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.33	0.43
1:B:1144:THR:OG1	1:B:1146:SER:OG	2.24	0.43
1:A:345:ALA:HB1	5:A:3005:FAD:H4'	2.00	0.43
1:A:302:CYS:HB2	1:A:347:ILE:HD11	2.01	0.43
1:B:812:LEU:HD21	1:B:823:VAL:O	2.19	0.43
1:A:99:PRO:O	1:A:103:ARG:HG3	2.19	0.43
1:A:679:GLN:HE21	1:A:683:ARG:NH2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:PRO:HD2	1:A:429:ASP:OD1	2.19	0.42
1:A:617:ILE:HG23	1:A:687:ILE:CD1	2.49	0.42
1:B:812:LEU:HD11	1:B:825:CYS:CB	2.50	0.42
1:A:749:THR:O	1:A:812:LEU:CD2	2.68	0.42
1:B:375:SER:O	1:B:376:ARG:C	2.63	0.42
1:B:473:LEU:O	1:B:474:SER:HB2	2.20	0.42
1:B:308:GLU:HG2	1:B:330:MET:HE1	2.02	0.41
1:B:123:MET:HE3	1:B:127:LEU:HG	2.02	0.41
1:B:393:ARG:NH2	1:B:429:ASP:OD1	2.45	0.41
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	2.18	0.41
1:B:968:TRP:O	1:B:972:ILE:HG12	2.21	0.41
1:B:934:CYS:HB3	1:B:936:LEU:HD12	2.02	0.41
1:B:1151:HIS:O	1:B:1251:ARG:HD3	2.21	0.41
1:A:498:ASP:O	1:A:499:ALA:C	2.62	0.41
1:A:1102:GLU:HB3	1:A:1103:PRO:HD3	2.02	0.41
1:B:969:ASP:HA	1:B:972:ILE:HG12	2.02	0.41
1:B:1204:GLY:HA3	1:B:1209:GLU:OE2	2.21	0.41
1:A:794:MET:HE3	1:A:1038:MET:HB3	2.03	0.41
1:A:670:VAL:HG11	1:A:681:ALA:HB3	2.03	0.41
1:A:740:GLU:HG3	1:A:833:MET:CE	2.47	0.41
1:A:446:ILE:O	1:A:446:ILE:HG22	2.19	0.41
1:A:599:TYR:HA	1:B:599:TYR:HA	2.03	0.41
1:A:975:SER:O	1:A:980:ARG:HD3	2.21	0.41
1:B:806:THR:O	1:B:810:THR:HG23	2.21	0.41
1:A:911:PHE:O	1:A:912:ARG:C	2.64	0.41
1:A:1013:PHE:CD1	1:A:1013:PHE:C	2.99	0.41
1:B:99:PRO:O	1:B:103:ARG:HG3	2.22	0.40
1:B:134:THR:OG1	1:B:137:GLU:HG3	2.22	0.40
1:B:396:LEU:HD12	1:B:396:LEU:C	2.46	0.40
1:A:241:MET:CE	1:A:245:LEU:HD11	2.51	0.40
1:A:447:GLU:HA	1:A:475:LYS:O	2.21	0.40
1:B:345:ALA:HB1	5:B:4004:FAD:H4'	2.04	0.40
1:B:733:GLU:HA	1:B:844:ALA:O	2.22	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%)	1239 (96%)	38 (3%)	8 (1%)	21	17
1	B	1282/1315 (98%)	1242 (97%)	32 (2%)	8 (1%)	21	17
All	All	2567/2630 (98%)	2481 (97%)	70 (3%)	16 (1%)	21	17

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	1008	SER
1	B	1251	ARG
1	B	1287	ASP
1	B	1289	ALA
1	A	424	SER
1	B	912	ARG
1	A	797	GLY
1	A	912	ARG
1	A	1287	ASP
1	B	797	GLY
1	B	887	ASN
1	A	474	SER
1	A	552	ASP
1	A	887	ASN
1	B	556	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%)	1028 (94%)	60 (6%)	19	17
1	B	1085/1109 (98%)	1044 (96%)	41 (4%)	29	29
All	All	2173/2218 (98%)	2072 (95%)	101 (5%)	24	22

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	61	LEU
1	A	64	LYS
1	A	70	VAL
1	A	83	VAL
1	A	94	THR
1	A	96	LYS
1	A	164	LYS
1	A	190	LEU
1	A	221	THR
1	A	240	THR
1	A	242	GLU
1	A	247	LEU
1	A	286	LEU
1	A	290	VAL
1	A	297	SER
1	A	306	LEU
1	A	310	VAL
1	A	313	GLU
1	A	347	ILE
1	A	383	ARG
1	A	394	LYS
1	A	396	LEU
1	A	404	LEU
1	A	406	ILE
1	A	424	SER
1	A	426	ARG
1	A	446	ILE
1	A	447	GLU
1	A	483	GLN
1	A	494	GLN
1	A	512	LEU
1	A	557	VAL
1	A	565	LYS
1	A	626	LYS

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Mol	Chain	Res	Type
1	A	640	VAL
1	A	683	ARG
1	A	686	LYS
1	A	687	ILE
1	A	688	THR
1	A	744	LEU
1	A	752	VAL
1	A	807	VAL
1	A	818	LYS
1	A	852	LYS
1	A	856	VAL
1	A	870	THR
1	A	900	ILE
1	A	932	ILE
1	A	983	GLU
1	A	1011	LEU
1	A	1031	LEU
1	A	1032	THR
1	A	1052	ARG
1	A	1085	LEU
1	A	1106	LYS
1	A	1108	LYS
1	A	1134	LYS
1	A	1288	ASN
1	A	1315	LEU
1	B	28	VAL
1	B	61	LEU
1	B	62	GLN
1	B	70	VAL
1	B	201	LYS
1	B	216	LEU
1	B	219	LYS
1	B	247	LEU
1	B	270	LYS
1	B	280	PRO
1	B	290	VAL
1	B	310	VAL
1	B	317	LYS
1	B	383	ARG
1	B	400	GLU
1	B	467	LYS
1	B	512	LEU

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Mol	Chain	Res	Type
1	B	531	LEU
1	B	551	LYS
1	B	557	VAL
1	B	566	ASP
1	B	622	THR
1	B	683	ARG
1	B	720	LYS
1	B	743	TYR
1	B	752	VAL
1	B	812	LEU
1	B	856	VAL
1	B	866	ASN
1	B	981	LYS
1	B	985	GLU
1	B	1011	LEU
1	B	1031	LEU
1	B	1032	THR
1	B	1051	SER
1	B	1102	GLU
1	B	1107	LYS
1	B	1143	GLU
1	B	1145	ASN
1	B	1262	PRO
1	B	1291	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	207	GLN
1	A	250	GLN
1	A	271	ASN
1	A	386	HIS
1	A	556	ASN
1	A	679	GLN
1	A	705	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

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Mol	Chain	Res	Type
1	A	1288	ASN
1	A	1291	GLN
1	B	130	GLN
1	B	157	GLN
1	B	207	GLN
1	B	223	GLN
1	B	271	ASN
1	B	291	HIS
1	B	350	ASN
1	B	449	GLN
1	B	472	GLN
1	B	550	GLN
1	B	703	ASN
1	B	866	ASN
1	B	869	ASN
1	B	1145	ASN
1	B	1284	GLN
1	B	1285	HIS
1	B	1288	ASN
1	B	1306	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	FAD	B	4004	-	58,58,58	1.91	17 (29%)	85,89,89	1.74	17 (20%)
6	URC	B	4006	-	13,13,13	2.64	5 (38%)	17,19,19	2.88	8 (47%)
3	BCT	A	3003	-	3,3,3	0.62	0	2,3,3	1.40	0
7	GOL	B	4008	-	5,5,5	0.52	0	5,5,5	0.40	0
2	FES	B	4001	1	0,4,4	-	-	-	-	-
2	FES	A	3002	1	0,4,4	-	-	-	-	-
7	GOL	A	3007	-	5,5,5	0.71	0	5,5,5	0.73	0
3	BCT	B	4005	-	3,3,3	0.56	0	2,3,3	1.34	0
2	FES	B	4002	1	0,4,4	-	-	-	-	-
5	FAD	A	3005	-	58,58,58	1.64	14 (24%)	85,89,89	1.80	22 (25%)
7	GOL	B	4007	-	5,5,5	0.62	0	5,5,5	0.42	0
6	URC	A	3006	-	13,13,13	2.54	5 (38%)	17,19,19	2.44	6 (35%)
2	FES	A	3001	1	0,4,4	-	-	-	-	-

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
5	FAD	B	4004	-	-	0/34/50/50	0/6/6/6
6	URC	A	3006	-	-	-	0/2/2/2
6	URC	B	4006	-	-	-	0/2/2/2
2	FES	B	4001	1	-	-	0/1/1/1
2	FES	A	3002	1	-	-	0/1/1/1
7	GOL	A	3007	-	-	0/4/4/4	-
5	FAD	A	3005	-	-	0/34/50/50	0/6/6/6
2	FES	B	4002	1	-	-	0/1/1/1
7	GOL	B	4008	-	-	0/4/4/4	-
2	FES	A	3001	1	-	-	0/1/1/1
7	GOL	B	4007	-	-	0/4/4/4	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	4006	URC	C5-C4	7.30	1.51	1.37
6	A	3006	URC	C5-C4	5.79	1.48	1.37
5	A	3005	FAD	C9A-C5X	4.82	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4004	FAD	C5A-N7A	-4.48	1.30	1.39
5	B	4004	FAD	C9A-C5X	4.16	1.47	1.41
5	B	4004	FAD	C8A-N9A	-4.12	1.30	1.37
5	B	4004	FAD	C5X-N5	-4.02	1.32	1.39
5	A	3005	FAD	C5A-C4A	3.83	1.45	1.39
6	A	3006	URC	O24-C8	3.76	1.31	1.23
6	B	4006	URC	O24-C8	3.61	1.31	1.23
6	A	3006	URC	O13-C6	3.58	1.30	1.23
5	B	4004	FAD	C5A-C4A	3.52	1.45	1.39
5	B	4004	FAD	PA-O2A	-3.30	1.40	1.55
5	B	4004	FAD	C4A-N9A	-3.20	1.31	1.37
5	B	4004	FAD	C4-N3	-3.16	1.32	1.38
6	A	3006	URC	C2-N3	-3.09	1.32	1.37
5	B	4004	FAD	P-O1P	-2.97	1.40	1.50
6	B	4006	URC	O11-C2	2.73	1.29	1.23
5	B	4004	FAD	C1'-N10	-2.71	1.41	1.47
5	A	3005	FAD	C8-C7	2.70	1.47	1.40
5	B	4004	FAD	C2-N3	-2.68	1.33	1.39
5	A	3005	FAD	C5A-N7A	-2.68	1.34	1.39
5	B	4004	FAD	C8-C7	2.59	1.47	1.40
5	B	4004	FAD	PA-O1A	-2.59	1.41	1.50
5	B	4004	FAD	P-O2P	-2.53	1.43	1.55
5	A	3005	FAD	C2'-C3'	-2.51	1.49	1.53
6	B	4006	URC	C5-C6	2.44	1.49	1.41
5	A	3005	FAD	C9-C8	2.44	1.42	1.39
5	B	4004	FAD	C2'-C3'	-2.39	1.49	1.53
5	A	3005	FAD	O2-C2	2.35	1.29	1.24
5	A	3005	FAD	C4-N3	-2.33	1.34	1.38
5	A	3005	FAD	C2B-C3B	-2.32	1.47	1.53
5	A	3005	FAD	C5A-C6A	2.28	1.47	1.41
5	A	3005	FAD	C5X-N5	-2.28	1.35	1.39
5	A	3005	FAD	O2'-C2'	2.24	1.48	1.43
5	A	3005	FAD	C4A-N9A	-2.22	1.33	1.37
6	B	4006	URC	O13-C6	2.20	1.27	1.23
5	A	3005	FAD	C4X-N5	2.18	1.35	1.30
6	A	3006	URC	C5-C6	2.13	1.48	1.41
5	B	4004	FAD	O4B-C4B	-2.12	1.40	1.45
5	B	4004	FAD	P-O3P	-2.07	1.57	1.59

All (53) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	4006	URC	N7-C8-N9	6.54	116.48	107.22
5	B	4004	FAD	C5A-C4A-N3A	-5.56	119.06	126.72
6	A	3006	URC	N7-C8-N9	5.20	114.58	107.22
5	B	4004	FAD	N3A-C4A-N9A	5.13	135.89	127.17
6	B	4006	URC	N3-C2-N1	4.84	123.35	115.74
5	A	3005	FAD	N3A-C4A-N9A	4.73	135.21	127.17
6	A	3006	URC	N3-C2-N1	4.70	123.13	115.74
5	A	3005	FAD	C5A-C4A-N3A	-4.64	120.33	126.72
6	B	4006	URC	C5-N7-C8	-4.56	102.94	108.82
5	A	3005	FAD	C4A-N9A-C8A	4.37	110.33	105.74
5	A	3005	FAD	O3'-C3'-C2'	-4.27	99.22	108.93
5	B	4004	FAD	O3'-C3'-C2'	-4.14	99.53	108.93
5	B	4004	FAD	C4-C4X-N5	3.56	123.13	118.21
5	B	4004	FAD	C4A-C5A-N7A	-3.56	106.51	110.58
6	A	3006	URC	C5-N7-C8	-3.49	104.32	108.82
5	B	4004	FAD	C2A-N3A-C4A	3.30	119.89	111.83
5	B	4004	FAD	C9A-C5X-N5	-3.25	119.01	122.45
5	A	3005	FAD	C5A-N7A-C8A	3.22	108.50	103.45
5	A	3005	FAD	N9A-C8A-N7A	-3.11	109.53	113.94
5	B	4004	FAD	C4A-N9A-C8A	3.11	109.00	105.74
6	B	4006	URC	O13-C6-C5	-3.09	119.81	127.26
5	B	4004	FAD	C5X-N5-C4X	3.08	123.07	118.09
5	A	3005	FAD	C5'-C4'-C3'	-3.05	106.46	112.22
5	A	3005	FAD	C4A-C5A-N7A	-3.00	107.15	110.58
5	B	4004	FAD	C2B-C1B-N9A	2.98	120.71	113.30
5	A	3005	FAD	O4'-C4'-C3'	2.98	116.22	109.25
5	A	3005	FAD	C9A-C5X-N5	-2.96	119.31	122.45
5	A	3005	FAD	O4-C4-C4X	-2.92	118.81	126.53
5	A	3005	FAD	C2B-C1B-N9A	2.85	120.39	113.30
5	A	3005	FAD	C4-C4X-N5	2.79	122.07	118.21
5	B	4004	FAD	C5A-N7A-C8A	2.79	107.83	103.45
5	B	4004	FAD	O4-C4-C4X	-2.78	119.20	126.53
6	B	4006	URC	O24-C8-N9	-2.55	120.92	125.56
5	A	3005	FAD	C2A-N3A-C4A	2.55	118.06	111.83
5	B	4004	FAD	C10-N1-C2	2.45	122.16	116.85
6	B	4006	URC	N9-C4-N3	2.39	133.96	128.19
6	A	3006	URC	N9-C4-N3	2.39	133.94	128.19
6	A	3006	URC	O13-C6-C5	-2.36	121.57	127.26
5	B	4004	FAD	N3A-C2A-N1A	-2.35	125.02	128.58
6	A	3006	URC	O11-C2-N3	-2.32	117.73	121.86
6	B	4006	URC	O11-C2-N3	-2.30	117.78	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3005	FAD	N6A-C6A-N1A	2.28	123.46	118.38
5	B	4004	FAD	O5B-C5B-C4B	2.24	116.62	108.99
5	B	4004	FAD	C6A-C5A-N7A	2.24	136.40	132.09
5	A	3005	FAD	N3A-C2A-N1A	-2.22	125.22	128.58
6	B	4006	URC	C6-N1-C2	-2.20	123.34	126.37
5	A	3005	FAD	C2B-C3B-C4B	2.15	106.77	102.61
5	A	3005	FAD	C4A-N9A-C1B	-2.09	121.75	126.63
5	A	3005	FAD	O2A-PA-O1A	2.07	122.07	112.44
5	A	3005	FAD	C5X-C9A-N10	2.05	119.82	117.97
5	A	3005	FAD	O2-C2-N1	-2.04	118.41	121.80
5	A	3005	FAD	C8M-C8-C9	-2.02	116.01	119.57
5	B	4004	FAD	C4X-C10-N1	-2.01	119.66	124.59

There are no chirality outliers.

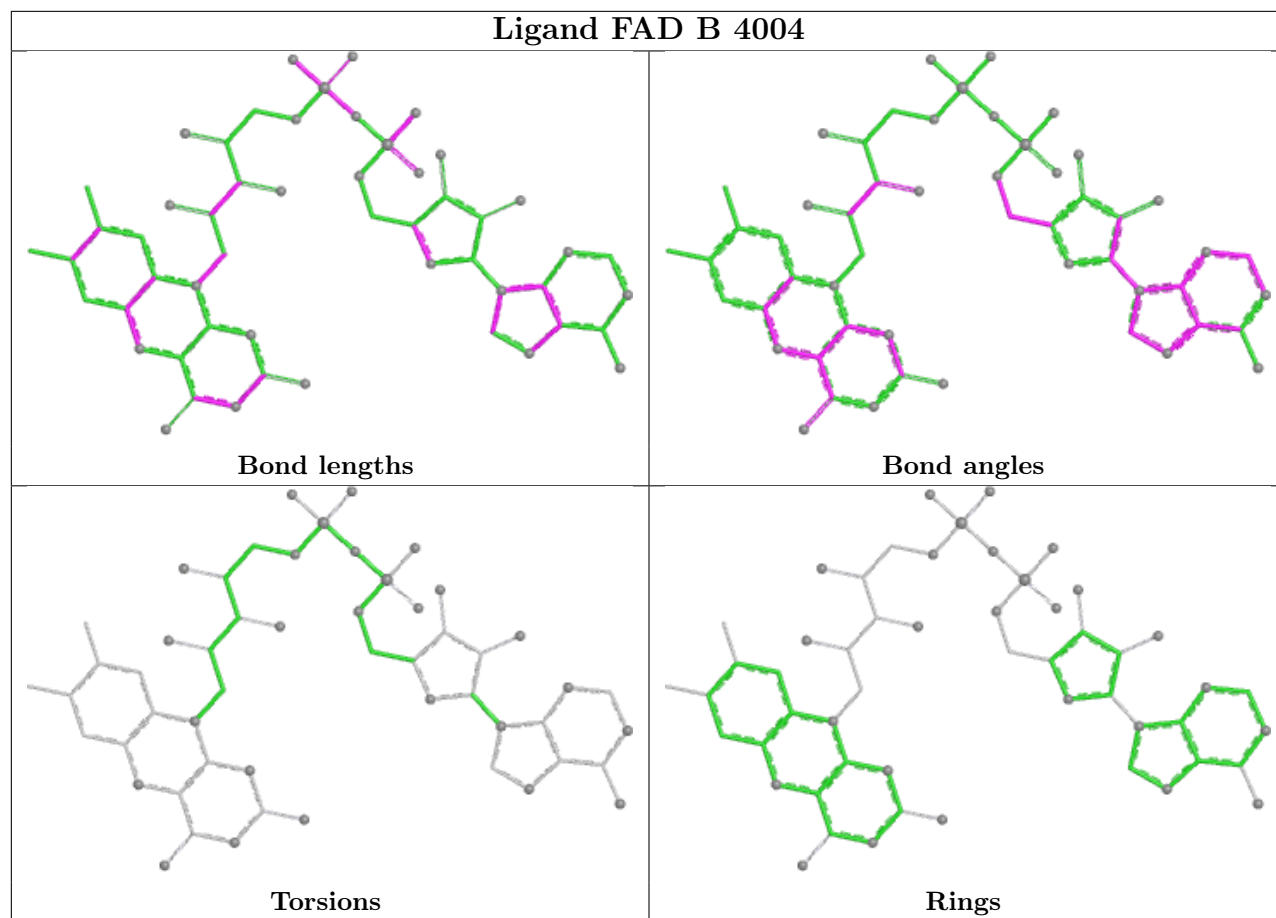
There are no torsion outliers.

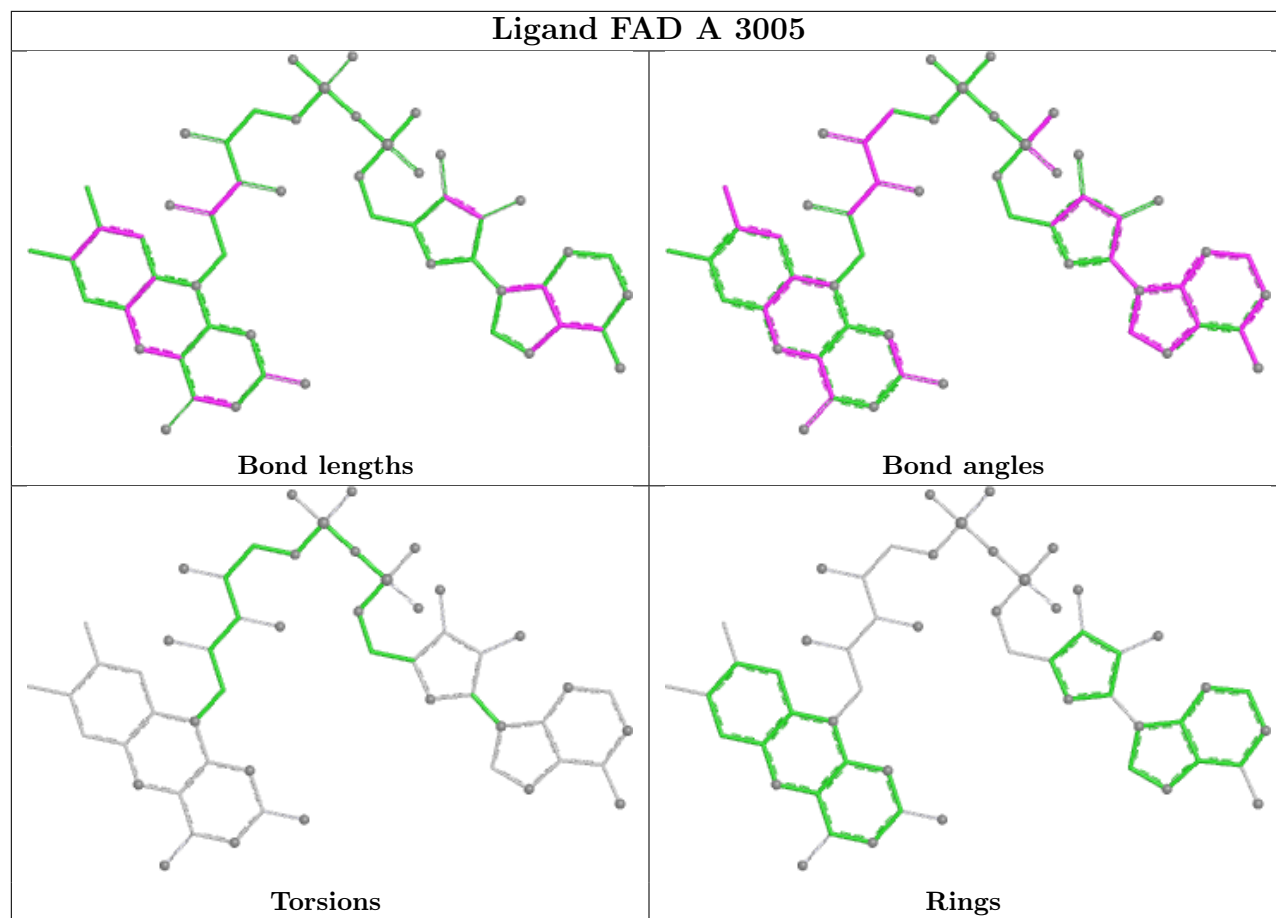
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	4004	FAD	2	0
5	A	3005	FAD	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	1289/1315 (98%)	0.30	51 (3%) 42 41	17, 30, 51, 86	0
1	B	1286/1315 (97%)	-0.00	42 (3%) 49 48	15, 24, 46, 85	0
All	All	2575/2630 (97%)	0.15	93 (3%) 46 45	15, 27, 49, 86	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	423	ALA	7.7
1	A	190	LEU	5.7
1	A	1315	LEU	5.3
1	B	555	ALA	5.3
1	B	1286	GLY	5.0
1	B	191	SER	4.8
1	A	1111	GLY	4.8
1	B	1289	ALA	4.8
1	A	61	LEU	4.7
1	B	1314	THR	4.7
1	A	164	LYS	4.4
1	A	3	ALA	4.2
1	A	396	LEU	4.2
1	A	423	ALA	4.0
1	A	430	ILE	4.0
1	B	164	LYS	4.0
1	A	335	TRP	3.9
1	A	551	LYS	3.9
1	B	428	ASP	3.9
1	B	972	ILE	3.9
1	B	551	LYS	3.9
1	A	165	ASP	3.9
1	B	335	TRP	3.6
1	A	1314	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	466	LEU	3.5
1	B	549	PHE	3.5
1	A	1110	THR	3.4
1	B	1111	GLY	3.3
1	B	535	CYS	3.3
1	B	1288	ASN	3.2
1	B	3	ALA	3.2
1	A	1287	ASP	3.2
1	A	431	ALA	3.1
1	A	550	GLN	3.1
1	A	549	PHE	3.1
1	B	1287	ASP	3.1
1	A	683	ARG	3.1
1	A	290	VAL	3.0
1	B	529	ALA	3.0
1	B	1110	THR	2.9
1	B	720	LYS	2.9
1	A	429	ASP	2.9
1	B	424	SER	2.9
1	B	548	LEU	2.9
1	A	424	SER	2.8
1	A	565	LYS	2.8
1	B	531	LEU	2.8
1	A	443	PRO	2.7
1	A	428	ASP	2.7
1	B	553	PRO	2.7
1	B	271	ASN	2.7
1	A	531	LEU	2.6
1	A	446	ILE	2.6
1	B	32	ARG	2.6
1	B	426	ARG	2.6
1	B	222	PRO	2.5
1	A	377	GLY	2.5
1	A	425	ARG	2.5
1	B	61	LEU	2.4
1	B	383	ARG	2.4
1	A	527	GLY	2.4
1	B	429	ASP	2.4
1	B	550	GLN	2.4
1	B	554	PRO	2.4
1	A	321	GLN	2.3
1	A	422	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	473	LEU	2.3
1	B	534	MET	2.3
1	A	1250	LYS	2.3
1	A	272	MET	2.3
1	B	480	GLU	2.2
1	B	703	ASN	2.2
1	A	33	LYS	2.2
1	B	537	LYS	2.2
1	B	1107	LYS	2.2
1	A	427	GLU	2.2
1	B	566	ASP	2.2
1	A	553	PRO	2.2
1	A	406	ILE	2.2
1	A	721	LYS	2.2
1	A	95	GLN	2.2
1	A	316	ALA	2.2
1	A	247	LEU	2.1
1	B	272	MET	2.1
1	A	249	ALA	2.1
1	A	812	LEU	2.1
1	A	271	ASN	2.1
1	A	992	CYS	2.1
1	B	533	ASP	2.1
1	B	425	ARG	2.1
1	A	370	LYS	2.0
1	A	221	THR	2.0
1	A	719	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

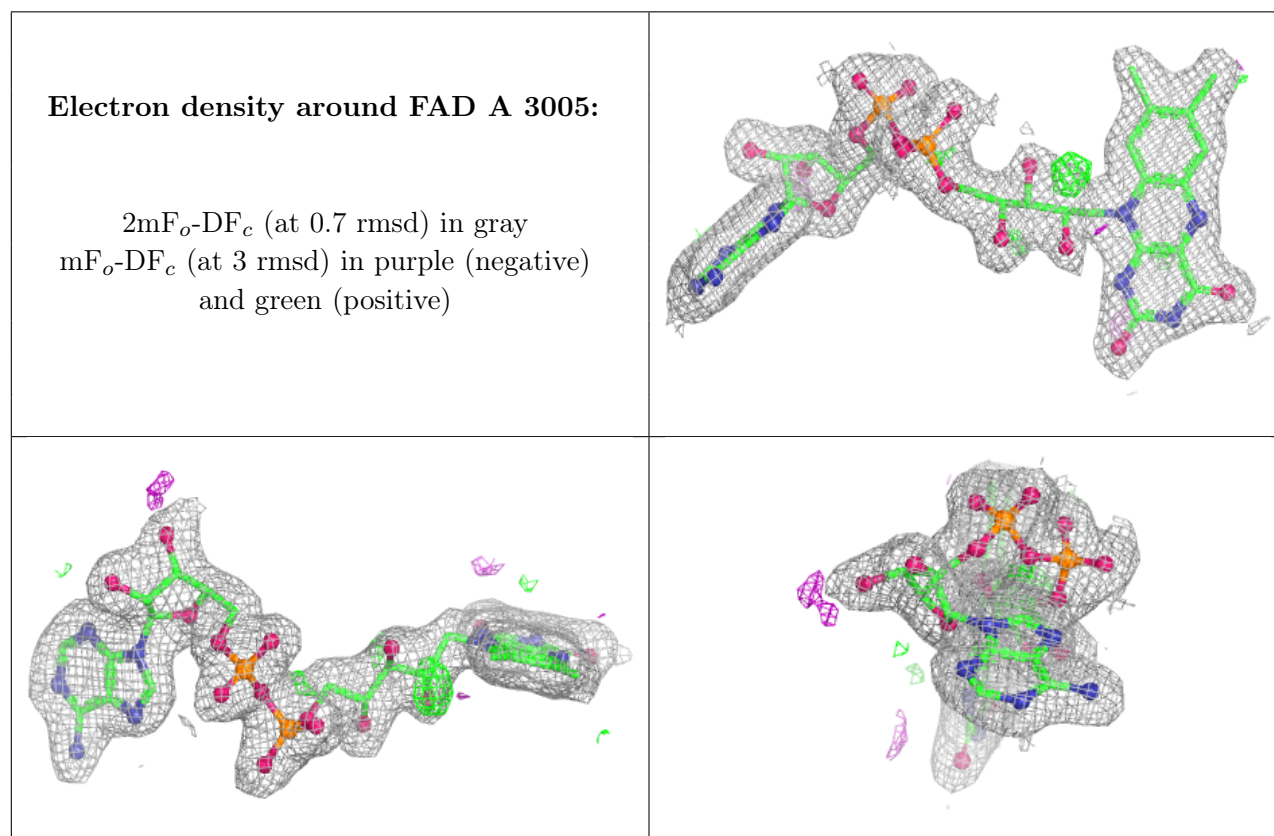
6.4 Ligands [i](#)

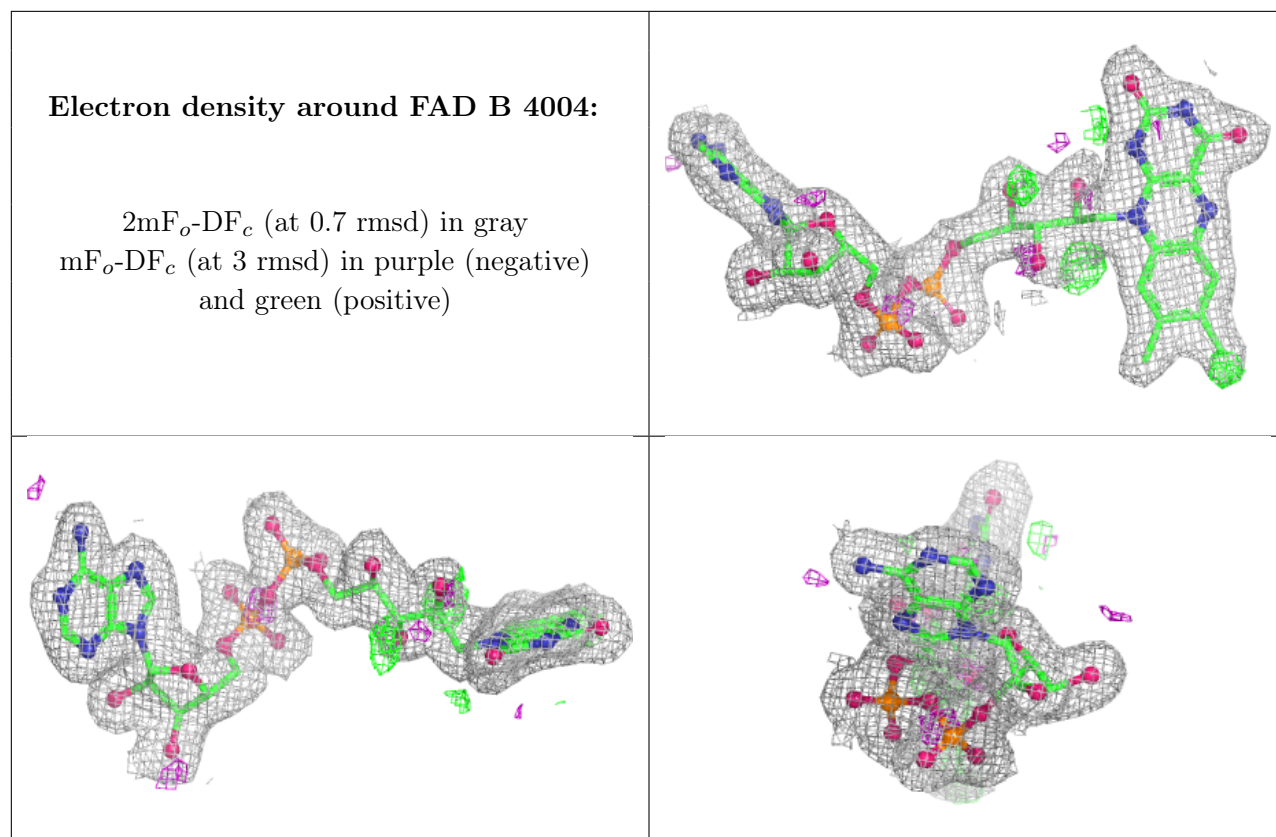
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	A	3007	6/6	0.92	0.12	25,27,28,29	0
7	GOL	B	4007	6/6	0.94	0.08	26,30,31,31	0
7	GOL	B	4008	6/6	0.94	0.09	23,27,28,28	0
6	URC	B	4006	12/12	0.96	0.06	22,24,28,29	0
5	FAD	A	3005	53/53	0.96	0.07	23,30,34,36	0
5	FAD	B	4004	53/53	0.96	0.07	16,21,25,27	0
6	URC	A	3006	12/12	0.96	0.06	24,27,31,31	0
4	CA	A	3004	1/1	0.97	0.10	34,34,34,34	0
3	BCT	A	3003	4/4	0.97	0.07	26,28,28,29	0
3	BCT	B	4005	4/4	0.98	0.04	19,20,21,23	0
2	FES	A	3001	4/4	0.99	0.04	23,23,25,29	0
4	CA	B	4003	1/1	0.99	0.07	24,24,24,24	0
2	FES	A	3002	4/4	0.99	0.02	19,21,24,25	0
2	FES	B	4002	4/4	1.00	0.02	15,15,18,18	0
2	FES	B	4001	4/4	1.00	0.05	20,22,25,25	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.