



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:59 PM UTC

PDB ID : 6ADJ / pdb_00006adj
Title : Rat Xanthine oxidoreductase, D428E variant
Authors : Okamoto, K.; Kawaguchi, Y.
Deposited on : 2018-08-01
Resolution : 2.18 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

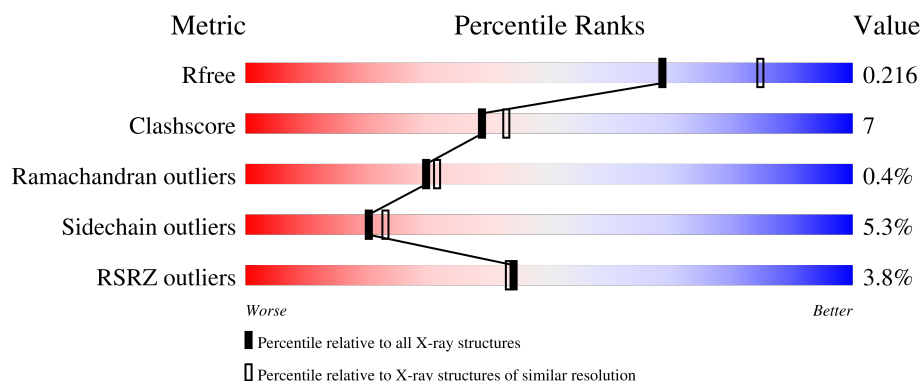
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	5% 82% 13% ...
1	B	1331	3% 80% 13% ...

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 21477 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.

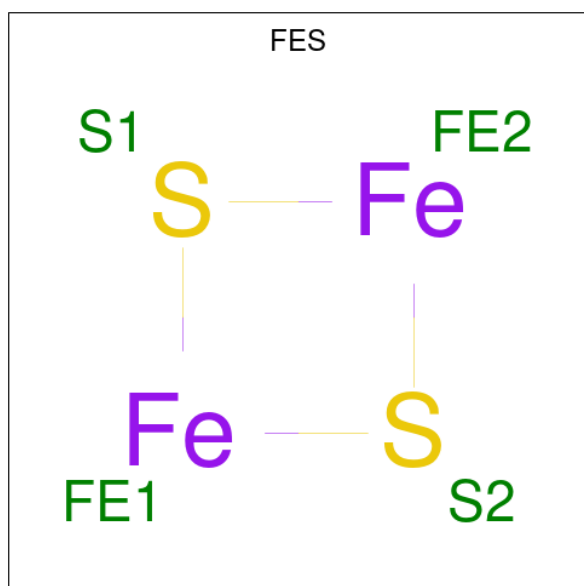
- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1297	Total	C	N	O	S	0	0	0
			10030	6357	1727	1881	65			
1	B	1286	Total	C	N	O	S	0	0	0
			9938	6301	1709	1864	64			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	428	GLU	ASP	see sequence details	UNP P22985
B	428	GLU	ASP	see sequence details	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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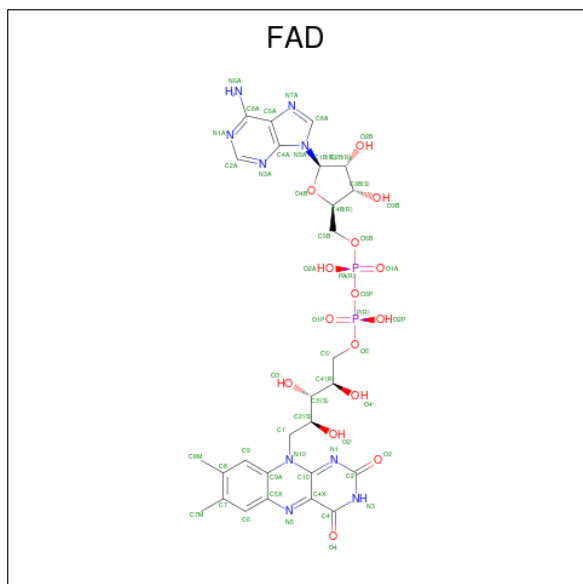
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

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

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

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



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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	623	Total 623	O 623	0	0
5	B	762	Total 762	O 762	0	0

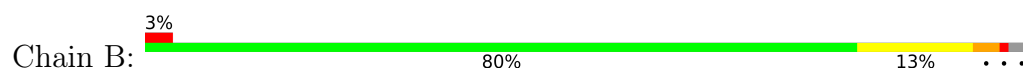
3 Residue-property plots [i](#)

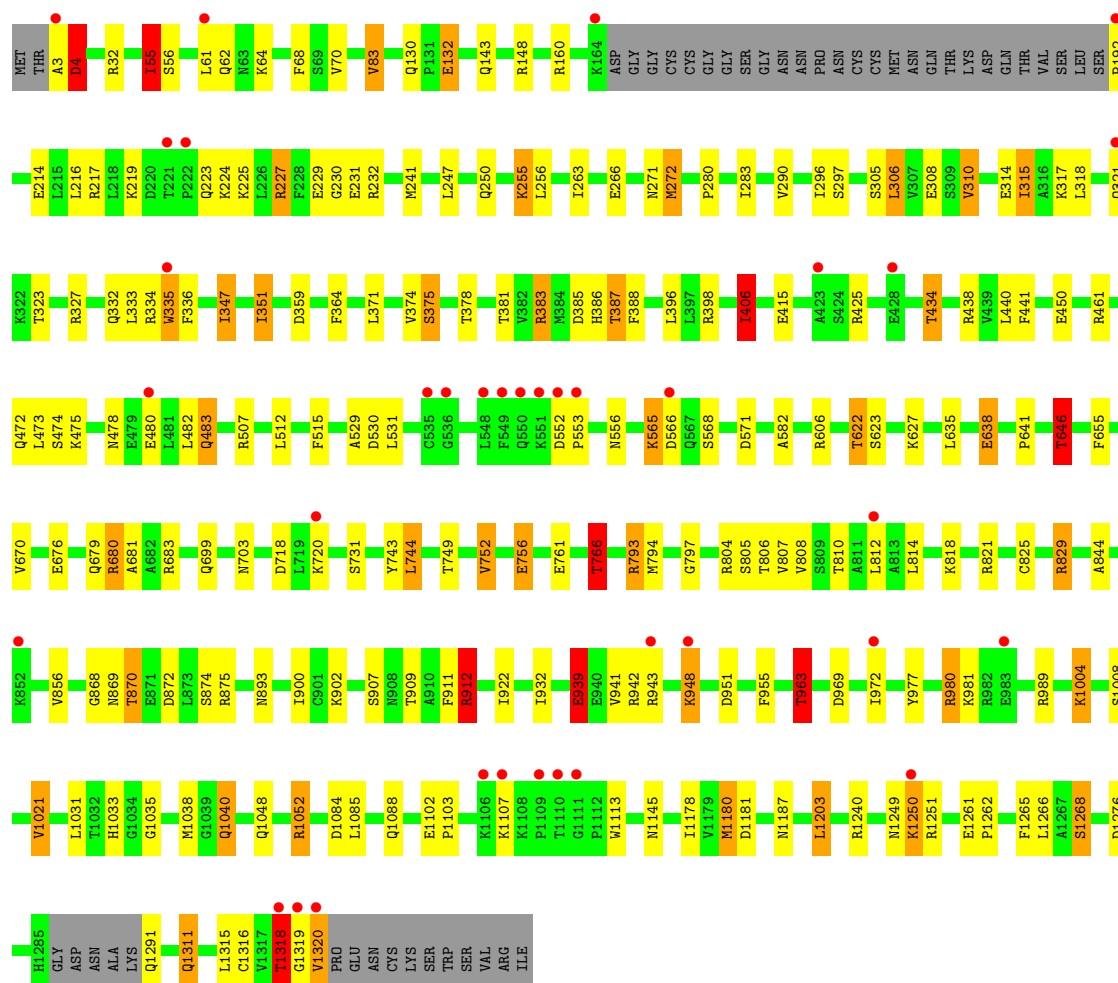
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Xanthine dehydrogenase/oxidase



• Molecule 1: Xanthine dehydrogenase/oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.84Å 138.66Å 222.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.40 – 2.18 42.40 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.40-2.18) 99.4 (42.40-2.18)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.98 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.167 , 0.210 0.175 , 0.216	Depositor DCC
R_{free} test set	1635 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.7	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	0.95	EDS
Total number of atoms	21477	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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: CA, FES, 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	0.96	12/10241 (0.1%)	1.10	22/13855 (0.2%)
1	B	1.01	9/10147 (0.1%)	1.15	40/13730 (0.3%)
All	All	0.99	21/20388 (0.1%)	1.12	62/27585 (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	13
1	B	0	22
All	All	0	35

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	230	GLY	C-O	-6.80	1.18	1.24
1	A	90	GLY	C-O	-6.41	1.16	1.24
1	A	870	THR	C-O	-5.85	1.16	1.23
1	A	1021	VAL	C-O	-5.74	1.18	1.24
1	A	108	HIS	CE1-NE2	5.72	1.38	1.32
1	B	829	ARG	CD-NE	-5.72	1.38	1.46
1	B	902	LYS	N-CA	-5.65	1.39	1.46
1	A	1111	GLY	N-CA	5.60	1.52	1.44
1	B	305	SER	C-O	-5.58	1.17	1.24
1	B	582	ALA	N-CA	5.48	1.52	1.46
1	B	941	VAL	N-CA	-5.46	1.40	1.46
1	B	623	SER	N-CA	5.44	1.52	1.46
1	B	641	PRO	C-O	-5.37	1.17	1.24
1	A	71	ASN	C-O	-5.28	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1180	MET	C-O	-5.23	1.18	1.24
1	A	125	THR	C-O	-5.22	1.18	1.24
1	A	227	ARG	C-O	-5.22	1.18	1.23
1	A	1222	ARG	N-CA	5.19	1.51	1.46
1	A	879	GLU	N-CA	-5.03	1.40	1.46
1	A	1117	VAL	C-O	-5.02	1.18	1.24
1	A	1102	GLU	N-CA	5.01	1.51	1.46

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	868	GLY	CA-C-N	10.01	135.00	120.38
1	A	868	GLY	C-N-CA	10.01	135.00	120.38
1	B	347	ILE	CB-CA-C	-9.42	99.92	111.97
1	B	766	THR	CB-CA-C	-8.82	89.97	109.56
1	A	766	THR	CB-CA-C	-8.28	91.18	109.56
1	B	1318	THR	N-CA-C	-8.07	99.66	110.55
1	B	868	GLY	CA-C-N	7.93	132.37	120.31
1	B	868	GLY	C-N-CA	7.93	132.37	120.31
1	B	869	ASN	CA-CB-CG	-7.60	105.00	112.60
1	B	646	THR	CB-CA-C	-7.49	95.51	110.42
1	B	766	THR	CA-CB-OG1	7.25	120.48	109.60
1	A	646	THR	CB-CA-C	-6.96	97.12	114.11
1	A	944	LYS	CB-CA-C	-6.93	98.90	110.68
1	B	638	GLU	CB-CA-C	-6.90	97.87	110.63
1	B	1318	THR	CB-CA-C	6.83	123.35	109.76
1	A	963	THR	N-CA-CB	-6.72	100.52	110.53
1	B	565	LYS	CA-C-N	6.66	129.87	120.28
1	B	565	LYS	C-N-CA	6.66	129.87	120.28
1	B	4	ASP	CA-CB-CG	6.56	119.16	112.60
1	B	515	PHE	CA-CB-CG	-6.55	107.25	113.80
1	A	1262	PRO	N-CA-C	6.48	118.60	110.70
1	B	963	THR	N-CA-CB	-6.37	101.03	110.53
1	B	869	ASN	CB-CA-C	-6.36	98.46	110.67
1	B	622	THR	CB-CA-C	6.26	121.30	110.72
1	A	766	THR	CA-CB-OG1	6.25	118.97	109.60
1	B	1084	ASP	CA-CB-CG	6.23	118.83	112.60
1	B	374	VAL	CA-C-N	6.08	132.09	122.36
1	B	374	VAL	C-N-CA	6.08	132.09	122.36
1	B	406	ILE	CB-CA-C	-6.00	101.74	110.63
1	B	83	VAL	N-CA-CB	-5.84	102.65	112.47
1	B	55	ILE	CB-CA-C	5.75	119.14	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	PHE	CA-CB-CG	-5.70	108.10	113.80
1	B	321	GLN	CB-CG-CD	5.67	122.24	112.60
1	B	566	ASP	CB-CA-C	-5.64	100.20	110.63
1	B	347	ILE	N-CA-CB	5.58	117.07	110.55
1	A	347	ILE	CB-CA-C	-5.54	104.88	111.97
1	B	829	ARG	CB-CG-CD	-5.53	98.59	111.30
1	A	434	THR	CB-CA-C	-5.49	97.90	109.38
1	B	761	GLU	CB-CA-C	5.48	119.74	109.71
1	A	909	THR	CB-CA-C	-5.48	101.81	114.41
1	B	1088	GLN	CA-C-N	5.47	126.17	119.99
1	B	1088	GLN	C-N-CA	5.47	126.17	119.99
1	B	646	THR	CA-CB-OG1	5.47	117.80	109.60
1	A	497	PRO	N-CA-CB	-5.45	97.53	103.25
1	A	460	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	829	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	B	939	GLU	N-CA-CB	5.33	118.43	110.22
1	B	223	GLN	CB-CA-C	5.27	118.44	109.84
1	B	386	HIS	CA-C-N	5.27	127.87	120.28
1	B	386	HIS	C-N-CA	5.27	127.87	120.28
1	A	564	PRO	CA-C-N	5.17	127.21	120.28
1	A	564	PRO	C-N-CA	5.17	127.21	120.28
1	A	863	HIS	CA-CB-CG	5.17	118.97	113.80
1	B	1113	TRP	CA-C-N	5.12	127.13	120.28
1	B	1113	TRP	C-N-CA	5.12	127.13	120.28
1	A	347	ILE	N-CA-CB	5.10	116.52	110.55
1	A	793	ARG	CD-NE-CZ	5.10	131.54	124.40
1	B	1249	ASN	CA-C-N	5.09	127.81	120.38
1	B	1249	ASN	C-N-CA	5.09	127.81	120.38
1	A	498	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	4	ASP	CA-CB-CG	5.05	117.66	112.60
1	A	870	THR	CA-C-O	-5.04	115.35	120.99

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ARG	Sidechain
1	A	227	ARG	Sidechain
1	A	232	ARG	Sidechain
1	A	327	ARG	Sidechain
1	A	438	ARG	Sidechain
1	A	461	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	612	ARG	Sidechain
1	A	680	ARG	Sidechain
1	A	683	ARG	Sidechain
1	A	786	ARG	Sidechain
1	A	804	ARG	Sidechain
1	A	821	ARG	Sidechain
1	A	980	ARG	Sidechain
1	B	1240	ARG	Sidechain
1	B	1318	THR	Peptide
1	B	148	ARG	Sidechain
1	B	160	ARG	Sidechain
1	B	227	ARG	Sidechain
1	B	3	ALA	Peptide
1	B	334	ARG	Sidechain
1	B	335	TRP	Peptide
1	B	383	ARG	Sidechain
1	B	425	ARG	Sidechain
1	B	461	ARG	Sidechain
1	B	507	ARG	Sidechain
1	B	680	ARG	Sidechain
1	B	793	ARG	Sidechain
1	B	821	ARG	Sidechain
1	B	829	ARG	Sidechain
1	B	875	ARG	Sidechain
1	B	912	ARG	Sidechain
1	B	942	ARG	Sidechain
1	B	943	ARG	Sidechain
1	B	980	ARG	Sidechain
1	B	989	ARG	Sidechain

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	10030	0	10041	121	0
1	B	9938	0	9948	155	0
2	A	8	0	0	1	0
2	B	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	0	31	2	0
4	B	53	0	31	0	0
5	A	623	0	0	17	0
5	B	762	0	0	36	0
All	All	21477	0	20051	274	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 7.

All (274) 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:1316:CYS:HB2	5:B:4770:HOH:O	1.19	1.30
1:B:752:VAL:HB	5:B:4649:HOH:O	1.20	1.27
1:B:812:LEU:HB3	5:B:4421:HOH:O	1.06	1.19
1:B:909:THR:HB	5:B:4245:HOH:O	0.89	1.06
1:B:398:ARG:HD2	5:B:4120:HOH:O	1.61	1.01
1:B:323:THR:OG1	1:B:327:ARG:NH1	1.94	1.00
1:A:812:LEU:HD21	1:A:825:CYS:HB2	1.41	0.99
1:B:752:VAL:CB	5:B:4649:HOH:O	1.86	0.97
1:B:939:GLU:HG3	5:B:4101:HOH:O	1.65	0.95
1:B:718:ASP:H	1:B:893:ASN:HD22	1.04	0.93
1:B:752:VAL:CG1	5:B:4649:HOH:O	2.12	0.93
1:B:1040:GLN:H	1:B:1040:GLN:HE21	1.10	0.93
1:A:584:MET:SD	1:B:756:GLU:HB3	2.09	0.93
1:B:812:LEU:HD21	1:B:825:CYS:HB2	1.51	0.93
1:B:271:ASN:OD1	1:B:683:ARG:NH1	2.04	0.90
1:A:1040:GLN:H	1:A:1040:GLN:HE21	1.13	0.89
1:A:872:ASP:OD2	1:A:909:THR:HG23	1.72	0.88
1:A:749:THR:HB	1:A:812:LEU:HD12	1.55	0.88
1:B:646:THR:HG23	5:B:4323:HOH:O	1.74	0.87
1:B:812:LEU:HD11	1:B:825:CYS:HB3	1.57	0.87
1:B:1311:GLN:H	1:B:1311:GLN:HE21	1.18	0.87
1:A:598:ARG:NH1	5:A:3102:HOH:O	2.09	0.85
1:B:793:ARG:HD3	5:B:4636:HOH:O	1.76	0.85
1:B:939:GLU:OE1	5:B:4101:HOH:O	1.96	0.84
1:B:963:THR:HG21	1:B:1181:ASP:OD2	1.78	0.83
1:B:231:GLU:OE2	1:B:680:ARG:NH2	2.11	0.83
1:B:804:ARG:CG	1:B:909:THR:HG21	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:ARG:NE	5:A:3101:HOH:O	1.98	0.82
1:B:939:GLU:CD	5:B:4101:HOH:O	2.23	0.81
1:A:766:THR:HG23	1:A:805:SER:OG	1.80	0.81
1:A:963:THR:HG21	1:A:1181:ASP:OD2	1.79	0.80
1:B:718:ASP:H	1:B:893:ASN:ND2	1.78	0.80
1:A:749:THR:HB	1:A:812:LEU:CD1	2.12	0.80
1:B:385:ASP:OD1	1:B:387:THR:HB	1.83	0.78
1:A:1038:MET:H	1:A:1040:GLN:HE22	1.31	0.78
1:B:351:ILE:HD11	1:B:364:PHE:CE2	2.19	0.78
1:B:55:ILE:HD13	1:B:56:SER:N	1.99	0.77
1:B:351:ILE:HD11	1:B:364:PHE:HE2	1.47	0.77
1:B:1315:LEU:O	1:B:1318:THR:O	2.03	0.77
1:B:1038:MET:H	1:B:1040:GLN:HE22	1.33	0.76
1:B:1265:PHE:O	1:B:1268:SER:HB2	1.85	0.76
1:A:1265:PHE:O	1:A:1268:SER:HB2	1.86	0.75
1:B:872:ASP:OD2	1:B:909:THR:HG22	1.86	0.75
1:B:1040:GLN:HE21	1:B:1040:GLN:N	1.84	0.75
1:A:130:GLN:HE21	1:A:132:GLU:H	1.32	0.75
1:A:359:ASP:OD1	1:A:434:THR:HG21	1.86	0.75
1:B:766:THR:HG23	1:B:805:SER:OG	1.86	0.75
1:B:749:THR:HB	1:B:812:LEU:HD12	1.69	0.75
1:B:812:LEU:HD21	1:B:825:CYS:CB	2.17	0.75
1:B:1180:MET:HE1	1:B:1266:LEU:HD12	1.69	0.74
1:A:359:ASP:OD1	1:A:434:THR:CG2	2.36	0.74
1:A:385:ASP:OD1	1:A:387:THR:HG22	1.87	0.74
1:A:646:THR:HG23	5:A:3181:HOH:O	1.88	0.73
1:A:909:THR:HG22	1:A:910:ALA:H	1.53	0.72
1:A:1040:GLN:HE21	1:A:1040:GLN:N	1.86	0.72
1:A:1180:MET:HE1	1:A:1266:LEU:HD12	1.71	0.72
1:A:812:LEU:HD21	1:A:825:CYS:CB	2.18	0.72
1:A:812:LEU:HD11	1:A:825:CYS:HB3	1.73	0.71
1:B:939:GLU:CG	5:B:4101:HOH:O	2.28	0.69
1:B:130:GLN:HE21	1:B:132:GLU:H	1.41	0.69
1:B:749:THR:HB	1:B:812:LEU:CD1	2.23	0.69
1:A:311:LEU:O	1:A:315:ILE:HG23	1.91	0.69
1:B:241:MET:HE2	1:B:283:ILE:HG21	1.74	0.68
1:A:793:ARG:NH2	5:A:3101:HOH:O	2.27	0.68
1:A:909:THR:HG21	5:A:3433:HOH:O	1.93	0.68
1:B:315:ILE:CD1	5:B:4363:HOH:O	2.42	0.68
1:B:216:LEU:O	1:B:219:LYS:HG3	1.94	0.67
1:B:359:ASP:HA	1:B:434:THR:HG21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:ARG:HG2	1:B:909:THR:HG21	1.76	0.67
1:B:1320:VAL:O	1:B:1320:VAL:CG1	2.43	0.66
1:B:638:GLU:HG3	5:B:4673:HOH:O	1.96	0.66
1:B:55:ILE:CD1	1:B:55:ILE:C	2.69	0.66
1:A:359:ASP:HA	1:A:434:THR:HG21	1.78	0.66
1:B:699:GLN:NE2	1:B:703:ASN:OD1	2.28	0.66
1:B:909:THR:CB	5:B:4245:HOH:O	1.64	0.66
1:A:1048:GLN:HE22	1:A:1187:ASN:HD22	1.44	0.65
1:B:909:THR:CG2	5:B:4245:HOH:O	2.12	0.65
1:B:398:ARG:CD	5:B:4120:HOH:O	2.31	0.65
1:B:315:ILE:HD13	5:B:4363:HOH:O	1.96	0.65
1:B:441:PHE:O	5:B:4103:HOH:O	2.15	0.64
1:B:375:SER:HB2	1:B:378:THR:OG1	1.97	0.64
1:B:680:ARG:NH1	5:B:4102:HOH:O	2.04	0.64
1:B:1040:GLN:H	1:B:1040:GLN:NE2	1.90	0.64
1:B:718:ASP:N	1:B:893:ASN:HD22	1.87	0.64
1:A:376:ARG:HG2	1:A:376:ARG:HH11	1.61	0.63
1:A:943:ARG:HD3	5:A:3118:HOH:O	2.00	0.61
1:A:388:PHE:HA	1:A:396:LEU:HG	1.81	0.61
1:B:306:LEU:O	1:B:310:VAL:HG13	2.01	0.60
1:B:1320:VAL:HG11	5:B:4543:HOH:O	2.00	0.60
1:B:271:ASN:CG	1:B:683:ARG:HD3	2.26	0.60
1:B:70:VAL:HG22	5:B:4621:HOH:O	2.01	0.60
1:B:478:ASN:OD1	1:B:480:GLU:HG3	2.02	0.60
1:A:606:ARG:HD3	1:A:679:GLN:HA	1.83	0.59
1:A:426:ARG:NH2	5:A:3105:HOH:O	2.31	0.59
1:A:1040:GLN:H	1:A:1040:GLN:NE2	1.91	0.59
1:A:646:THR:CG2	5:A:3181:HOH:O	2.49	0.59
1:B:483:GLN:HE21	1:B:483:GLN:HA	1.68	0.59
1:A:256:LEU:HD22	1:A:278:VAL:HG13	1.84	0.58
1:B:192:PRO:HD2	5:B:4646:HOH:O	2.02	0.58
1:A:1203:LEU:HD11	5:A:3389:HOH:O	2.01	0.58
1:B:1320:VAL:O	1:B:1320:VAL:HG12	2.04	0.58
1:B:388:PHE:HA	1:B:396:LEU:HG	1.84	0.58
1:B:335:TRP:CE3	1:B:335:TRP:HA	2.38	0.58
1:A:1038:MET:H	1:A:1040:GLN:NE2	2.02	0.57
1:A:1315:LEU:HD13	5:A:3486:HOH:O	2.04	0.57
1:A:1259:VAL:O	1:A:1259:VAL:HG22	2.06	0.56
1:B:1250:LYS:HD2	1:B:1250:LYS:N	2.21	0.56
1:B:1048:GLN:HE22	1:B:1187:ASN:HD22	1.54	0.55
1:A:662:CYS:SG	1:A:869:ASN:ND2	2.78	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:MET:HE2	1:A:283:ILE:HG21	1.89	0.55
1:A:371:LEU:CD2	1:A:406:ILE:HG23	2.37	0.54
1:A:744:LEU:HD13	2:A:3001:FES:S2	2.47	0.54
1:A:359:ASP:OD1	1:A:434:THR:HG23	2.08	0.54
1:B:62:GLN:HB2	1:B:64:LYS:HG2	1.90	0.54
1:B:939:GLU:HG2	1:B:977:TYR:CE2	2.43	0.54
1:B:1311:GLN:H	1:B:1311:GLN:NE2	1.98	0.54
1:B:804:ARG:HD3	1:B:909:THR:HG21	1.89	0.53
1:B:232:ARG:CZ	1:B:680:ARG:HD3	2.39	0.53
1:B:1033:HIS:HD2	1:B:1035:GLY:H	1.56	0.53
1:B:227:ARG:HD3	1:B:229:GLU:OE2	2.08	0.53
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.89	0.53
1:B:55:ILE:HD13	1:B:55:ILE:C	2.34	0.53
1:A:874:SER:HB3	1:A:900:ILE:HG21	1.91	0.53
1:B:804:ARG:CD	1:B:909:THR:HG21	2.39	0.52
1:A:853:THR:O	1:A:944:LYS:HE3	2.10	0.52
1:B:571:ASP:OD2	1:B:1052:ARG:HD2	2.09	0.52
1:A:296:ILE:CD1	1:A:314:GLU:HG3	2.40	0.52
1:A:900:ILE:N	1:A:900:ILE:HD12	2.24	0.52
1:A:427:GLU:OE2	1:A:1233:GLY:HA3	2.10	0.52
1:A:584:MET:SD	1:B:756:GLU:CB	2.90	0.52
1:B:963:THR:HG21	1:B:1181:ASP:CG	2.34	0.52
1:B:1316:CYS:CB	5:B:4770:HOH:O	2.04	0.52
1:B:371:LEU:CD2	1:B:406:ILE:HG23	2.40	0.51
1:A:296:ILE:HD11	1:A:314:GLU:HG3	1.92	0.51
1:A:290:VAL:CG2	1:A:297:SER:HB2	2.41	0.51
1:B:371:LEU:HD23	1:B:406:ILE:HG23	1.93	0.51
1:A:870:THR:HB	1:A:907:SER:HB2	1.93	0.51
1:A:621:ASP:OD1	1:A:623:SER:OG	2.23	0.51
1:B:806:THR:O	1:B:810:THR:HG23	2.11	0.51
1:A:518:PHE:O	1:A:522:VAL:HG23	2.11	0.50
1:A:571:ASP:OD2	1:A:1052:ARG:HD2	2.11	0.50
1:A:1048:GLN:NE2	1:A:1187:ASN:HD22	2.07	0.50
1:B:290:VAL:HG22	1:B:297:SER:HB2	1.93	0.50
1:B:55:ILE:HG23	1:B:68:PHE:CE2	2.47	0.50
1:B:359:ASP:OD1	1:B:434:THR:HG21	2.12	0.50
1:B:552:ASP:HB3	1:B:553:PRO:HD2	1.94	0.50
1:B:415:GLU:OE1	1:B:438:ARG:HD2	2.12	0.50
1:A:932:ILE:HD13	1:A:1279:ARG:CZ	2.41	0.50
1:B:70:VAL:CG2	5:B:4621:HOH:O	2.58	0.50
1:A:499:ALA:O	1:A:500:PRO:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1180:MET:HE3	1:A:1263:PRO:HB3	1.94	0.49
1:A:555:ALA:HB3	1:A:1238:GLU:HG2	1.93	0.49
1:A:718:ASP:H	1:A:893:ASN:HD22	1.60	0.49
1:B:1203:LEU:C	1:B:1203:LEU:HD12	2.38	0.49
1:A:972:ILE:HG23	1:A:1000:ILE:HD13	1.95	0.49
1:A:70:VAL:CG2	5:A:3541:HOH:O	2.59	0.49
1:A:1021:VAL:HG22	1:A:1031:LEU:CD1	2.43	0.49
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.93	0.49
1:A:70:VAL:HG22	5:A:3541:HOH:O	2.12	0.49
1:A:496:ALA:O	1:A:499:ALA:N	2.43	0.49
1:B:1048:GLN:NE2	1:B:1187:ASN:HD22	2.11	0.49
1:B:1178:ILE:CG2	1:B:1180:MET:HE2	2.43	0.48
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.28	0.48
1:B:55:ILE:CD1	1:B:56:SER:N	2.74	0.48
1:B:606:ARG:HD3	1:B:679:GLN:HA	1.95	0.48
1:A:256:LEU:HD22	1:A:278:VAL:CG1	2.44	0.48
1:B:308:GLU:HG3	1:B:333:LEU:HD13	1.94	0.48
1:B:804:ARG:HD3	1:B:909:THR:CG2	2.44	0.48
1:B:870:THR:HG22	1:B:907:SER:OG	2.14	0.48
1:A:1033:HIS:CD2	1:A:1035:GLY:H	2.31	0.48
1:B:874:SER:HB3	1:B:900:ILE:HG21	1.96	0.48
1:A:256:LEU:HD13	1:A:280:PRO:HG3	1.95	0.48
1:B:948:LYS:HD3	1:B:951:ASP:OD2	2.13	0.48
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.14	0.47
1:A:539:ASP:OD1	1:A:540:PRO:HD2	2.15	0.47
1:B:900:ILE:N	1:B:900:ILE:HD12	2.30	0.47
1:B:1038:MET:H	1:B:1040:GLN:NE2	2.06	0.47
1:B:1315:LEU:C	1:B:1318:THR:O	2.57	0.47
1:A:963:THR:HG21	1:A:1181:ASP:CG	2.38	0.47
1:A:232:ARG:NH2	1:A:680:ARG:HD3	2.30	0.47
1:A:432:LYS:O	1:A:457:GLY:HA3	2.15	0.47
1:B:351:ILE:HD13	1:B:351:ILE:N	2.29	0.47
1:B:323:THR:HG1	1:B:327:ARG:NH1	2.08	0.46
1:A:232:ARG:HH21	1:A:680:ARG:HD3	1.79	0.46
1:B:232:ARG:NH1	1:B:680:ARG:HD3	2.31	0.46
1:B:336:PHE:HD2	1:B:336:PHE:O	1.98	0.46
1:A:1317:VAL:HG23	1:A:1318:THR:HG23	1.98	0.46
1:A:337:ALA:HA	1:A:428:GLU:HG3	1.98	0.46
1:B:680:ARG:HG2	1:B:683:ARG:NH2	2.30	0.46
1:A:299:GLY:O	1:A:347:ILE:HD11	2.16	0.46
1:B:939:GLU:CG	1:B:977:TYR:CE2	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:LEU:O	1:B:474:SER:HB2	2.16	0.46
1:B:1311:GLN:HE21	1:B:1311:GLN:N	1.99	0.46
1:A:963:THR:HG22	1:A:1155:TYR:CD2	2.51	0.46
1:B:969:ASP:HA	1:B:972:ILE:HG12	1.98	0.46
1:A:371:LEU:HD23	1:A:406:ILE:HG23	1.97	0.45
1:B:296:ILE:CD1	1:B:314:GLU:HG3	2.47	0.45
1:A:290:VAL:HG23	1:A:297:SER:HB2	1.98	0.45
1:B:911:PHE:O	1:B:912:ARG:C	2.59	0.45
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.79	0.45
1:A:153:ARG:HD2	1:A:153:ARG:C	2.41	0.45
1:A:494:GLN:HA	1:A:508:ARG:NH1	2.32	0.45
1:A:58:TYR:CE2	1:A:219:LYS:HD3	2.52	0.45
1:A:555:ALA:HB3	1:A:1238:GLU:CG	2.45	0.45
1:B:55:ILE:C	1:B:55:ILE:HD12	2.41	0.45
1:B:808:VAL:HG12	1:B:812:LEU:CD1	2.47	0.45
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.16	0.45
1:B:255:LYS:HE3	1:B:263:ILE:HD11	1.98	0.45
1:B:398:ARG:NE	5:B:4120:HOH:O	2.50	0.45
1:A:1033:HIS:HE1	1:A:1043:HIS:ND1	2.16	0.44
1:A:870:THR:HG21	5:A:3405:HOH:O	2.18	0.44
1:B:680:ARG:HG2	1:B:683:ARG:HH21	1.83	0.44
1:B:752:VAL:HG12	5:B:4649:HOH:O	1.99	0.44
1:B:794:MET:HE3	1:B:1038:MET:HB3	2.00	0.44
1:A:655:PHE:CD1	1:A:668:GLY:HA2	2.52	0.44
1:B:266:GLU:HB3	1:B:272:MET:HG3	2.00	0.44
1:B:808:VAL:HG12	1:B:812:LEU:HD12	2.00	0.44
1:A:932:ILE:HD11	5:A:3561:HOH:O	2.18	0.44
1:B:32:ARG:NH2	1:B:676:GLU:OE2	2.48	0.43
1:A:962:PHE:CE2	1:A:965:PRO:HD3	2.53	0.43
1:B:635:LEU:HD21	1:B:818:LYS:HD2	2.00	0.43
1:A:357:ILE:C	1:A:357:ILE:HD12	2.43	0.43
1:B:646:THR:HG21	5:B:4603:HOH:O	2.18	0.43
1:B:214:GLU:HG2	1:B:217:ARG:NH2	2.33	0.43
1:B:556:ASN:ND2	5:B:4122:HOH:O	2.50	0.43
1:B:1276:ASP:HB3	5:B:4225:HOH:O	2.19	0.43
1:A:351:ILE:CD1	1:A:406:ILE:HD12	2.48	0.43
1:A:932:ILE:HD13	1:A:1279:ARG:NH2	2.33	0.43
1:B:332:GLN:NE2	5:B:4123:HOH:O	2.51	0.43
1:A:610:SER:OG	1:A:665:HIS:HB3	2.18	0.43
1:A:1033:HIS:HD2	1:A:1035:GLY:H	1.66	0.43
1:B:359:ASP:OD1	1:B:434:THR:CG2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1102:GLU:HG2	1:B:1103:PRO:HD3	2.00	0.43
1:B:955:PHE:HA	1:B:1145:ASN:OD1	2.19	0.43
1:B:315:ILE:HD11	5:B:4795:HOH:O	2.19	0.42
1:A:345:ALA:HB1	4:A:3004:FAD:H4'	2.00	0.42
1:A:794:MET:HE3	1:A:1038:MET:HB3	2.01	0.42
1:A:1311:GLN:HG2	5:A:3534:HOH:O	2.19	0.42
1:B:440:LEU:HB3	1:B:450:GLU:HB2	2.02	0.42
1:A:613:ALA:O	1:A:904:ASN:HB3	2.19	0.42
1:B:336:PHE:C	1:B:336:PHE:CD2	2.98	0.42
1:A:263:ILE:HD11	4:A:3004:FAD:H3B	2.01	0.42
1:A:302:CYS:HB2	1:A:347:ILE:HD11	2.02	0.42
1:A:371:LEU:HD12	1:A:388:PHE:CE1	2.54	0.42
1:B:1004:LYS:NZ	5:B:4125:HOH:O	2.51	0.42
1:A:424:SER:HB3	5:A:3527:HOH:O	2.20	0.41
1:B:335:TRP:HA	1:B:335:TRP:HE3	1.83	0.41
1:A:765:SER:OG	1:A:794:MET:HG2	2.19	0.41
1:B:744:LEU:HD13	2:B:4001:FES:S2	2.60	0.41
1:A:231:GLU:OE2	1:A:680:ARG:NH2	2.54	0.41
1:A:361:ASN:N	1:A:362:PRO:CD	2.84	0.41
1:A:911:PHE:O	1:A:912:ARG:C	2.63	0.41
1:B:472:GLN:NE2	1:B:475:LYS:HD2	2.35	0.41
1:A:806:THR:O	1:A:810:THR:HG23	2.21	0.41
1:B:1021:VAL:HG22	1:B:1031:LEU:CD1	2.51	0.41
1:A:555:ALA:O	1:A:1238:GLU:HA	2.21	0.41
1:A:679:GLN:HE21	1:A:683:ARG:NH1	2.19	0.41
1:A:963:THR:HG22	1:A:1155:TYR:HB2	2.01	0.41
1:B:1319:GLY:O	1:B:1320:VAL:C	2.64	0.41
1:B:1203:LEU:C	1:B:1203:LEU:CD1	2.94	0.41
1:A:457:GLY:O	1:A:507:ARG:NH1	2.49	0.40
1:A:870:THR:HG22	1:A:907:SER:OG	2.21	0.40
1:B:1107:LYS:HE2	1:B:1107:LYS:HB2	1.88	0.40
1:B:1250:LYS:HD2	1:B:1251:ARG:H	1.85	0.40
1:B:655:PHE:HE2	1:B:814:LEU:HD23	1.87	0.40
1:B:844:ALA:HB2	1:B:922:ILE:HD13	2.03	0.40
1:B:55:ILE:HD13	1:B:56:SER:C	2.46	0.40
1:B:699:GLN:HB2	5:B:4814:HOH:O	2.22	0.40
1:A:870:THR:CG2	5:A:3405:HOH:O	2.70	0.40
1:A:1152:TYR:HB3	1:A:1251:ARG:HD2	2.03	0.40
1:A:1264:LEU:C	1:A:1264:LEU:HD23	2.45	0.40
1:B:1250:LYS:HE2	5:B:4598:HOH:O	2.21	0.40
1:A:1180:MET:CE	1:A:1263:PRO:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:ALA:O	1:B:530:ASP:C	2.65	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	1291/1331 (97%)	1235 (96%)	49 (4%)	7 (0%)	24	25
1	B	1280/1331 (96%)	1242 (97%)	34 (3%)	4 (0%)	36	39
All	All	2571/2662 (97%)	2477 (96%)	83 (3%)	11 (0%)	30	31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	4	ASP
1	B	1008	SER
1	A	497	PRO
1	A	912	ARG
1	A	1287	ASP
1	B	912	ARG
1	A	337	ALA
1	A	4	ASP
1	A	797	GLY
1	B	797	GLY

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	1096/1124 (98%)	1045 (95%)	51 (5%)	23	28
1	B	1086/1124 (97%)	1022 (94%)	64 (6%)	18	19
All	All	2182/2248 (97%)	2067 (95%)	115 (5%)	20	23

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	83	VAL
1	A	193	SER
1	A	224	LYS
1	A	232	ARG
1	A	247	LEU
1	A	256	LEU
1	A	306	LEU
1	A	310	VAL
1	A	313	GLU
1	A	315	ILE
1	A	347	ILE
1	A	378	THR
1	A	381	THR
1	A	383	ARG
1	A	396	LEU
1	A	398	ARG
1	A	406	ILE
1	A	434	THR
1	A	480	GLU
1	A	482	LEU
1	A	497	PRO
1	A	512	LEU
1	A	550	GLN
1	A	565	LYS
1	A	610	SER
1	A	623	SER
1	A	646	THR
1	A	683	ARG
1	A	686	LYS
1	A	719	LEU
1	A	743	TYR
1	A	744	LEU

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Mol	Chain	Res	Type
1	A	766	THR
1	A	807	VAL
1	A	856	VAL
1	A	870	THR
1	A	909	THR
1	A	939	GLU
1	A	948	LYS
1	A	963	THR
1	A	972	ILE
1	A	981	LYS
1	A	1040	GLN
1	A	1052	ARG
1	A	1085	LEU
1	A	1250	LYS
1	A	1268	SER
1	A	1318	THR
1	A	1325	LYS
1	A	1331	ILE
1	B	4	ASP
1	B	55	ILE
1	B	61	LEU
1	B	83	VAL
1	B	132	GLU
1	B	143	GLN
1	B	224	LYS
1	B	225	LYS
1	B	247	LEU
1	B	250	GLN
1	B	255	LYS
1	B	256	LEU
1	B	272	MET
1	B	280	PRO
1	B	306	LEU
1	B	310	VAL
1	B	315	ILE
1	B	317	LYS
1	B	318	LEU
1	B	347	ILE
1	B	351	ILE
1	B	375	SER
1	B	381	THR
1	B	383	ARG

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Mol	Chain	Res	Type
1	B	387	THR
1	B	406	ILE
1	B	434	THR
1	B	482	LEU
1	B	483	GLN
1	B	512	LEU
1	B	531	LEU
1	B	565	LYS
1	B	568	SER
1	B	622	THR
1	B	627	LYS
1	B	646	THR
1	B	720	LYS
1	B	731	SER
1	B	743	TYR
1	B	744	LEU
1	B	752	VAL
1	B	756	GLU
1	B	766	THR
1	B	807	VAL
1	B	856	VAL
1	B	870	THR
1	B	932	ILE
1	B	939	GLU
1	B	948	LYS
1	B	963	THR
1	B	980	ARG
1	B	981	LYS
1	B	1004	LYS
1	B	1021	VAL
1	B	1040	GLN
1	B	1052	ARG
1	B	1085	LEU
1	B	1203	LEU
1	B	1250	LYS
1	B	1268	SER
1	B	1291	GLN
1	B	1311	GLN
1	B	1318	THR
1	B	1320	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	130	GLN
1	A	145	ASN
1	A	271	ASN
1	A	321	GLN
1	A	472	GLN
1	A	483	GLN
1	A	550	GLN
1	A	585	GLN
1	A	869	ASN
1	A	893	ASN
1	A	1033	HIS
1	A	1040	GLN
1	A	1048	GLN
1	A	1173	ASN
1	A	1194	GLN
1	A	1212	HIS
1	A	1288	ASN
1	A	1294	GLN
1	B	130	GLN
1	B	145	ASN
1	B	332	GLN
1	B	449	GLN
1	B	472	GLN
1	B	483	GLN
1	B	550	GLN
1	B	556	ASN
1	B	567	GLN
1	B	704	ASN
1	B	893	ASN
1	B	1033	HIS
1	B	1040	GLN
1	B	1048	GLN
1	B	1088	GLN
1	B	1173	ASN
1	B	1194	GLN
1	B	1285	HIS
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z > 2$
2	FES	B	4001	1	0,4,4	-	-	-		
4	FAD	B	4004	-	58,58,58	1.76	12 (20%)	85,89,89	1.65	16 (18%)
4	FAD	A	3004	-	58,58,58	1.67	15 (25%)	85,89,89	1.79	20 (23%)
2	FES	A	3001	1	0,4,4	-	-	-		
2	FES	A	3002	1	0,4,4	-	-	-		
2	FES	B	4002	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
2	FES	B	4001	1	-	-	0/1/1/1
4	FAD	B	4004	-	-	0/34/50/50	0/6/6/6
4	FAD	A	3004	-	-	0/34/50/50	0/6/6/6
2	FES	A	3001	1	-	-	0/1/1/1
2	FES	A	3002	1	-	-	0/1/1/1
2	FES	B	4002	1	-	-	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4004	FAD	C9A-C5X	4.59	1.48	1.41
4	B	4004	FAD	C8A-N7A	4.26	1.39	1.31
4	A	3004	FAD	C9A-C5X	4.22	1.48	1.41
4	B	4004	FAD	C5X-N5	-4.10	1.31	1.39
4	B	4004	FAD	PA-O3P	4.06	1.63	1.59
4	B	4004	FAD	C2'-C3'	-3.78	1.46	1.53
4	A	3004	FAD	C5A-C4A	3.53	1.45	1.39
4	A	3004	FAD	PA-O3P	3.52	1.63	1.59
4	B	4004	FAD	C5A-C4A	3.25	1.44	1.39
4	B	4004	FAD	C4-N3	-3.24	1.32	1.38
4	A	3004	FAD	C2-N3	-2.95	1.32	1.39
4	B	4004	FAD	C5A-N7A	-2.78	1.34	1.39
4	B	4004	FAD	C8A-N9A	-2.72	1.32	1.37
4	A	3004	FAD	C5X-N5	-2.72	1.34	1.39
4	A	3004	FAD	C2'-C3'	-2.70	1.48	1.53
4	A	3004	FAD	C8A-N9A	-2.61	1.33	1.37
4	A	3004	FAD	C5A-C6A	2.59	1.48	1.41
4	A	3004	FAD	P-O3P	2.57	1.62	1.59
4	A	3004	FAD	C5A-N7A	-2.53	1.34	1.39
4	A	3004	FAD	C8-C7	2.53	1.47	1.40
4	A	3004	FAD	C1'-C2'	2.46	1.56	1.52
4	A	3004	FAD	C4A-N9A	-2.44	1.32	1.37
4	B	4004	FAD	O2'-C2'	2.41	1.48	1.43
4	B	4004	FAD	C4X-N5	2.33	1.35	1.30
4	B	4004	FAD	C8-C7	2.07	1.45	1.40
4	A	3004	FAD	C4-N3	-2.06	1.35	1.38
4	A	3004	FAD	C6-C5X	-2.06	1.36	1.40

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3004	FAD	O3'-C3'-C2'	-5.77	95.82	108.93
4	A	3004	FAD	C5A-C4A-N3A	-5.03	119.79	126.72
4	B	4004	FAD	C5A-C4A-N3A	-4.76	120.17	126.72
4	A	3004	FAD	C4A-C5A-N7A	-4.35	105.61	110.58
4	B	4004	FAD	O2'-C2'-C3'	-4.33	99.13	109.25
4	B	4004	FAD	O3'-C3'-C2'	-4.15	99.50	108.93
4	B	4004	FAD	C9A-C5X-N5	-3.90	118.31	122.45
4	A	3004	FAD	N3A-C4A-N9A	3.80	133.63	127.17
4	A	3004	FAD	O4'-C4'-C3'	3.59	117.64	109.25
4	A	3004	FAD	C4-C4X-N5	3.58	123.15	118.21
4	B	4004	FAD	N3A-C4A-N9A	3.57	133.25	127.17
4	A	3004	FAD	C4A-N9A-C8A	3.17	109.07	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3004	FAD	C5A-N7A-C8A	3.14	108.39	103.45
4	B	4004	FAD	C5'-C4'-C3'	-3.12	106.34	112.22
4	B	4004	FAD	C5X-N5-C4X	2.86	122.72	118.09
4	A	3004	FAD	C2A-N3A-C4A	2.82	118.73	111.83
4	A	3004	FAD	C5'-C4'-C3'	-2.74	107.06	112.22
4	A	3004	FAD	C2B-C3B-C4B	2.70	107.82	102.61
4	B	4004	FAD	C4A-N9A-C8A	2.65	108.52	105.74
4	A	3004	FAD	O2'-C2'-C3'	-2.62	103.12	109.25
4	A	3004	FAD	N9A-C8A-N7A	-2.60	110.25	113.94
4	B	4004	FAD	C4A-C5A-N7A	-2.50	107.72	110.58
4	A	3004	FAD	N3A-C2A-N1A	-2.45	124.87	128.58
4	B	4004	FAD	C2A-N3A-C4A	2.41	117.73	111.83
4	A	3004	FAD	O3P-PA-O1A	-2.40	103.50	110.70
4	B	4004	FAD	N9A-C8A-N7A	-2.34	110.62	113.94
4	B	4004	FAD	C1'-C2'-C3'	-2.25	103.57	109.66
4	A	3004	FAD	O2P-P-O1P	2.21	122.71	112.44
4	A	3004	FAD	C2B-C1B-N9A	2.11	118.54	113.30
4	A	3004	FAD	C6A-C5A-N7A	2.11	136.15	132.09
4	A	3004	FAD	C4X-C10-N10	2.10	119.48	116.48
4	B	4004	FAD	C4-C4X-N5	2.09	121.10	118.21
4	A	3004	FAD	O4-C4-C4X	-2.06	121.09	126.53
4	B	4004	FAD	O4B-C1B-N9A	-2.03	104.20	108.09
4	B	4004	FAD	C5A-N7A-C8A	2.03	106.63	103.45
4	B	4004	FAD	O2P-P-O3P	2.02	112.73	107.27

There are no chirality outliers.

There are no torsion outliers.

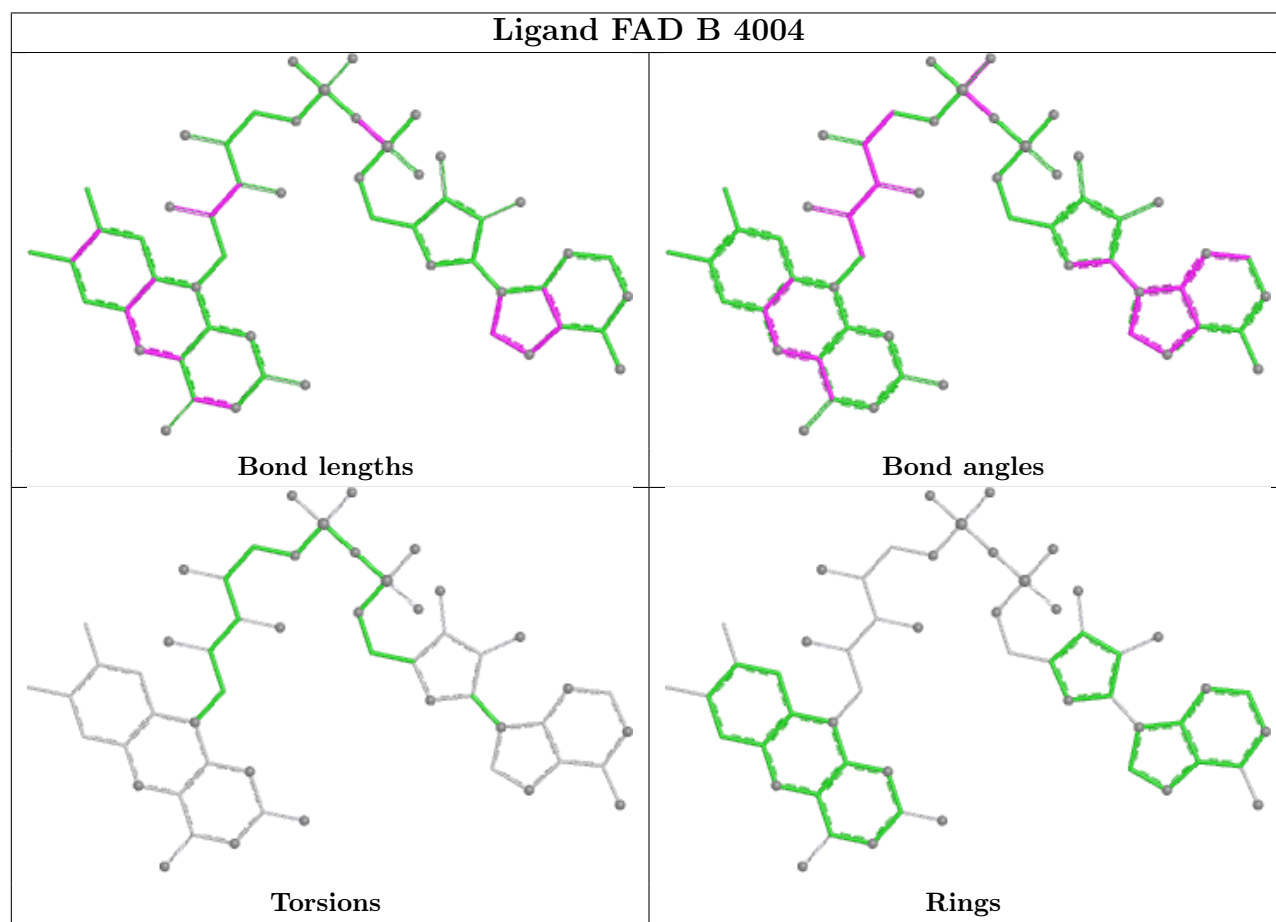
There are no ring outliers.

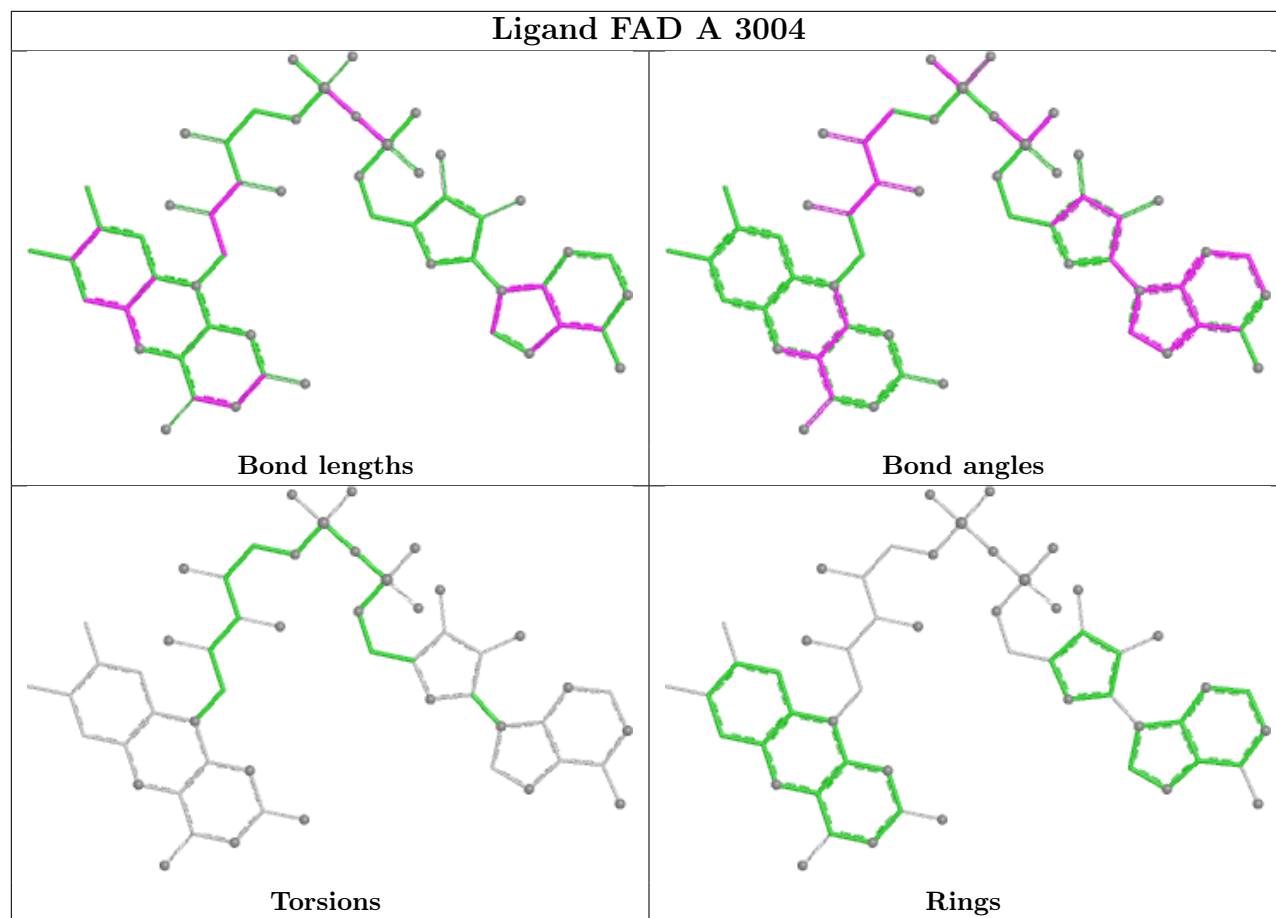
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4001	FES	1	0
4	A	3004	FAD	2	0
2	A	3001	FES	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	1297/1331 (97%)	-0.03	63 (4%) 35 34	13, 25, 53, 108	0
1	B	1286/1331 (96%)	-0.25	36 (2%) 55 54	11, 20, 43, 78	0
All	All	2583/2662 (97%)	-0.14	99 (3%) 44 43	11, 23, 50, 108	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1320	VAL	6.5
1	B	61	LEU	5.8
1	A	1317	VAL	5.8
1	A	1318	THR	5.5
1	A	1315	LEU	5.0
1	A	1325	LYS	4.9
1	A	497	PRO	4.7
1	A	1324	CYS	4.7
1	A	430	ILE	4.7
1	A	500	PRO	4.5
1	B	1111	GLY	4.3
1	A	551	LYS	4.2
1	A	398	ARG	4.2
1	A	496	ALA	4.2
1	B	1110	THR	4.1
1	B	164	LYS	4.1
1	B	335	TRP	4.1
1	B	549	PHE	3.8
1	B	1318	THR	3.8
1	B	222	PRO	3.7
1	B	423	ALA	3.7
1	A	396	LEU	3.6
1	A	3	ALA	3.6
1	A	192	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	869	ASN	3.5
1	A	1111	GLY	3.5
1	B	221	THR	3.4
1	A	1327	TRP	3.4
1	B	3	ALA	3.3
1	A	164	LYS	3.3
1	A	494	GLN	3.3
1	B	548	LEU	3.2
1	A	61	LEU	3.2
1	A	1110	THR	3.2
1	A	466	LEU	3.2
1	A	424	SER	3.2
1	A	427	GLU	3.2
1	B	972	ILE	3.1
1	B	1319	GLY	3.0
1	A	972	ILE	3.0
1	A	222	PRO	3.0
1	A	565	LYS	3.0
1	A	943	ARG	2.9
1	A	432	LYS	2.8
1	A	537	LYS	2.8
1	B	553	PRO	2.8
1	A	534	MET	2.7
1	A	1316	CYS	2.7
1	B	536	GLY	2.7
1	B	948	LYS	2.6
1	B	321	GLN	2.6
1	B	550	GLN	2.6
1	B	428	GLU	2.6
1	B	943	ARG	2.6
1	A	1331	ILE	2.6
1	A	413	GLU	2.6
1	A	1326	SER	2.5
1	A	428	GLU	2.5
1	A	290	VAL	2.5
1	A	982	ARG	2.5
1	A	499	ALA	2.5
1	A	812	LEU	2.5
1	A	467	LYS	2.5
1	A	426	ARG	2.5
1	B	551	LYS	2.5
1	A	335	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1328	SER	2.4
1	A	720	LYS	2.4
1	A	1329	VAL	2.4
1	A	1330	ARG	2.4
1	A	406	ILE	2.4
1	A	498	ASP	2.3
1	B	480	GLU	2.3
1	A	989	ARG	2.3
1	B	720	LYS	2.3
1	A	531	LEU	2.3
1	B	1107	LYS	2.2
1	A	321	GLN	2.2
1	A	550	GLN	2.2
1	B	1106	LYS	2.2
1	A	221	THR	2.2
1	A	377	GLY	2.2
1	A	501	GLY	2.2
1	B	812	LEU	2.2
1	A	253	ASP	2.2
1	B	192	PRO	2.1
1	A	495	LEU	2.1
1	A	553	PRO	2.1
1	B	1109	PRO	2.1
1	A	386	HIS	2.1
1	B	535	CYS	2.1
1	B	552	ASP	2.1
1	A	1250	LYS	2.1
1	B	983	GLU	2.0
1	B	566	ASP	2.0
1	B	1250	LYS	2.0
1	A	536	GLY	2.0
1	A	549	PHE	2.0
1	B	852	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

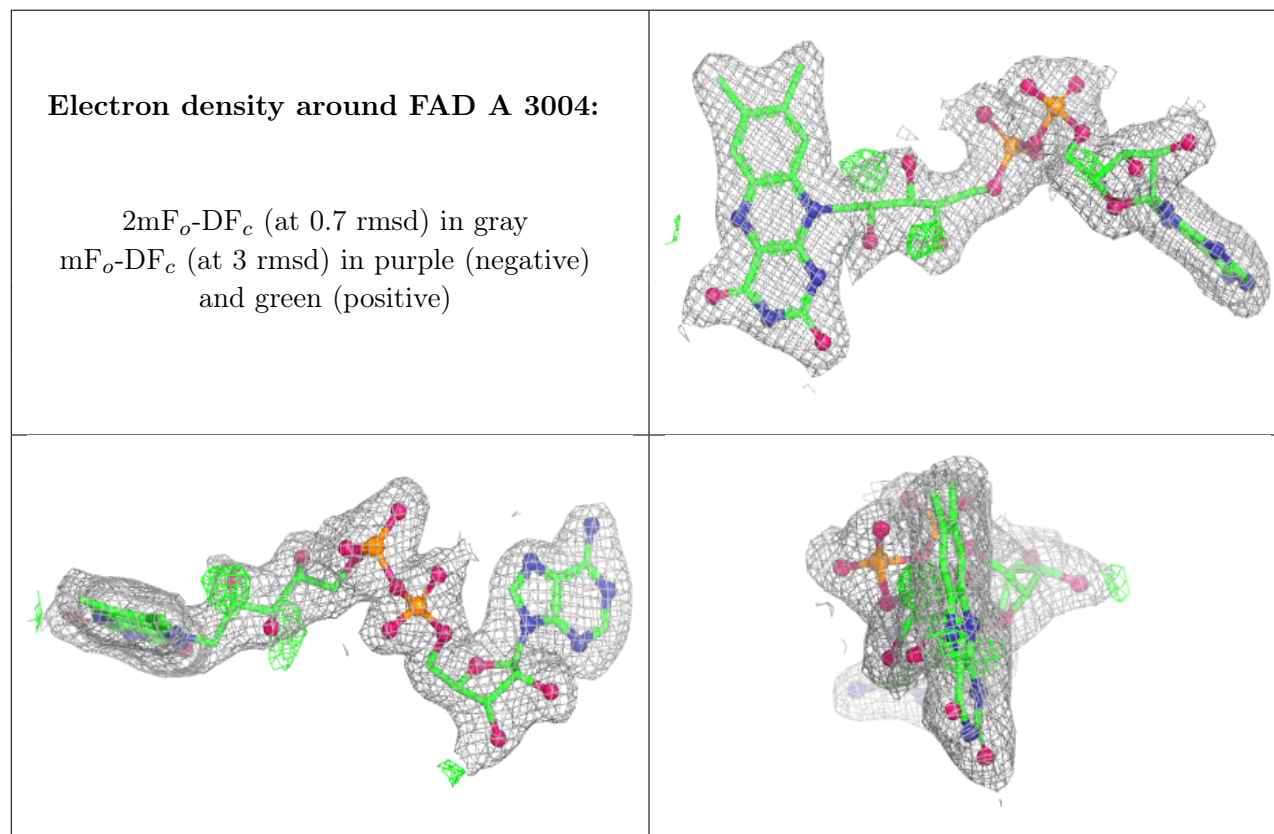
There are no oligosaccharides in this entry.

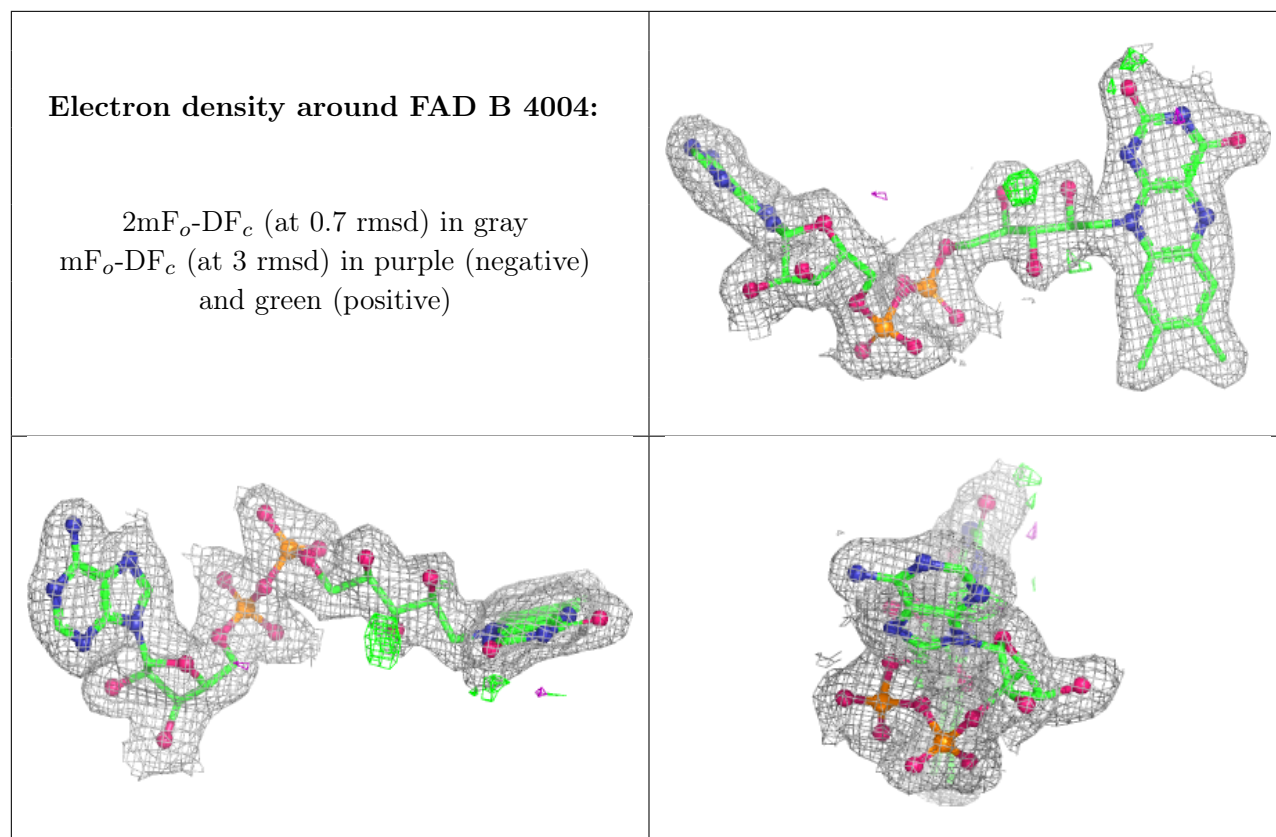
6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FAD	A	3004	53/53	0.96	0.07	19,26,34,41	0
4	FAD	B	4004	53/53	0.98	0.05	13,16,20,27	0
2	FES	A	3001	4/4	0.99	0.04	19,20,21,22	0
3	CA	A	3003	1/1	0.99	0.05	22,22,22,22	0
2	FES	A	3002	4/4	1.00	0.01	15,17,18,18	0
3	CA	B	4003	1/1	1.00	0.04	19,19,19,19	0
2	FES	B	4001	4/4	1.00	0.03	17,18,19,21	0
2	FES	B	4002	4/4	1.00	0.02	14,14,14,15	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.