



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 03:54 AM UTC

PDB ID : 6AD4 / pdb_00006ad4
Title : Rat Xanthine oxidoreductase, D428A variant, NADH bound form
Authors : Okamoto, K.; Kawaguchi, Y.
Deposited on : 2018-07-30
Resolution : 1.80 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

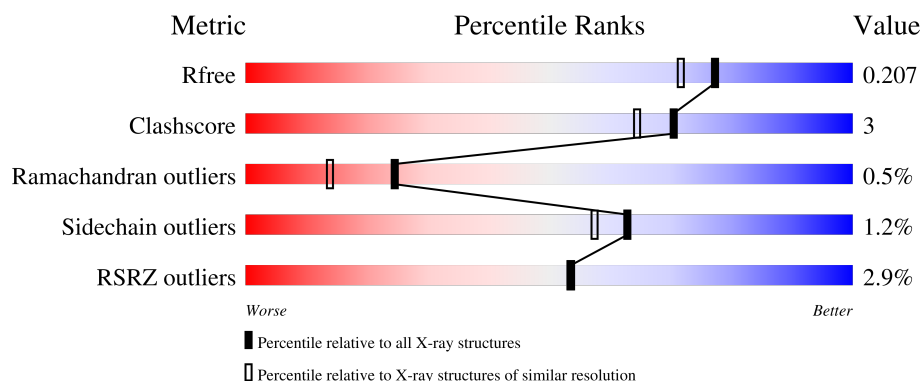
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	4% 89% 8% ..
1	B	1331	2% 89% 8% ..

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
2	URC	A	1501	-	X	-	-
2	URC	B	3003	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 21605 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.

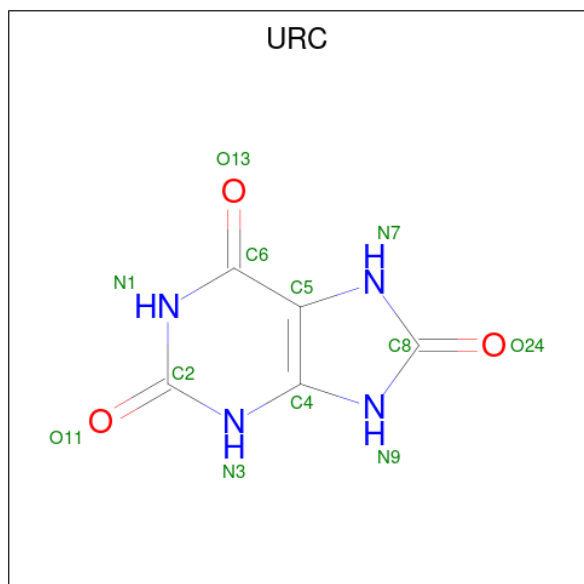
- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1300	Total	C	N	O	S	0	0	0
			10048	6366	1731	1886	65			
1	B	1291	Total	C	N	O	S	0	0	0
			9968	6319	1716	1869	64			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	428	ALA	ASP	see sequence details	UNP P22985
B	428	ALA	ASP	see sequence details	UNP P22985

- Molecule 2 is URIC ACID (CCD ID: URC) (formula: C₅H₄N₄O₃).



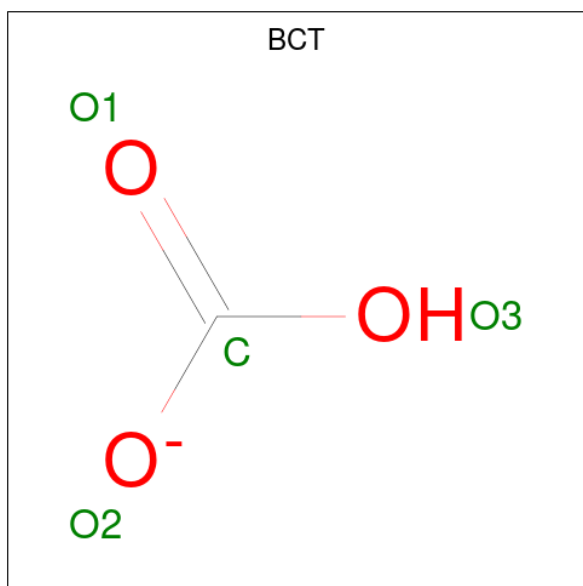
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	5	4	3		

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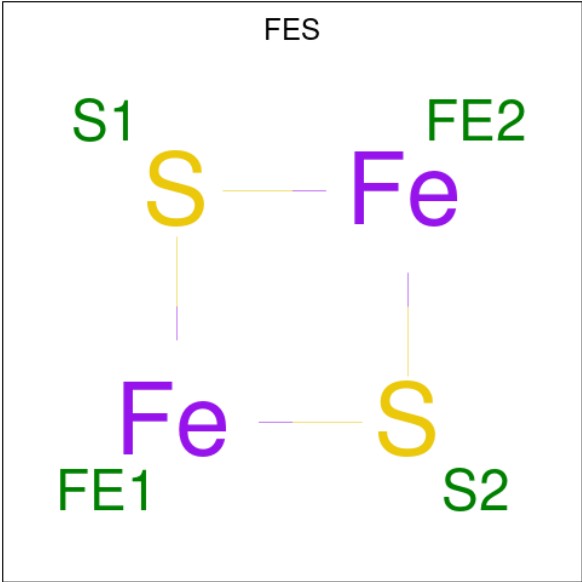
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			12	5	4	3		

- Molecule 3 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



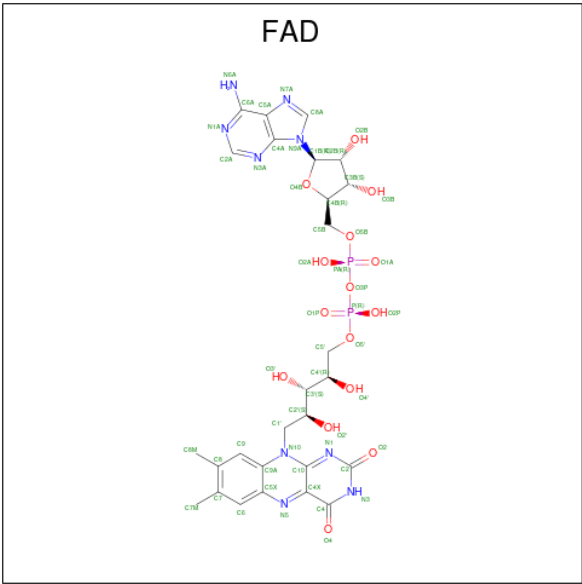
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



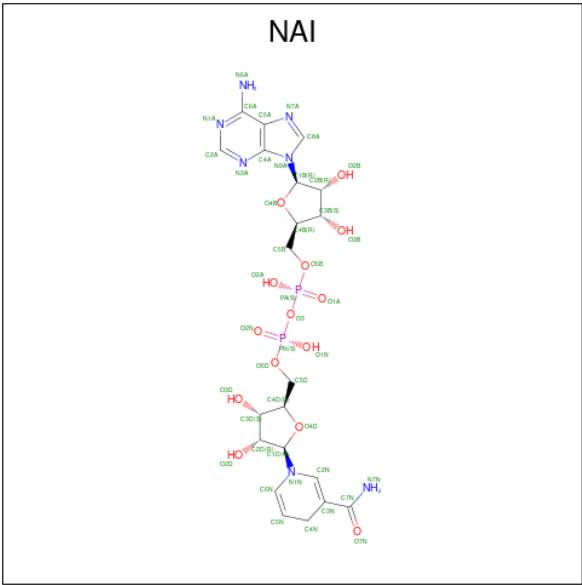
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	B	1	Total	Fe	S	0	0
			4	2	2		
4	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 6 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
6	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

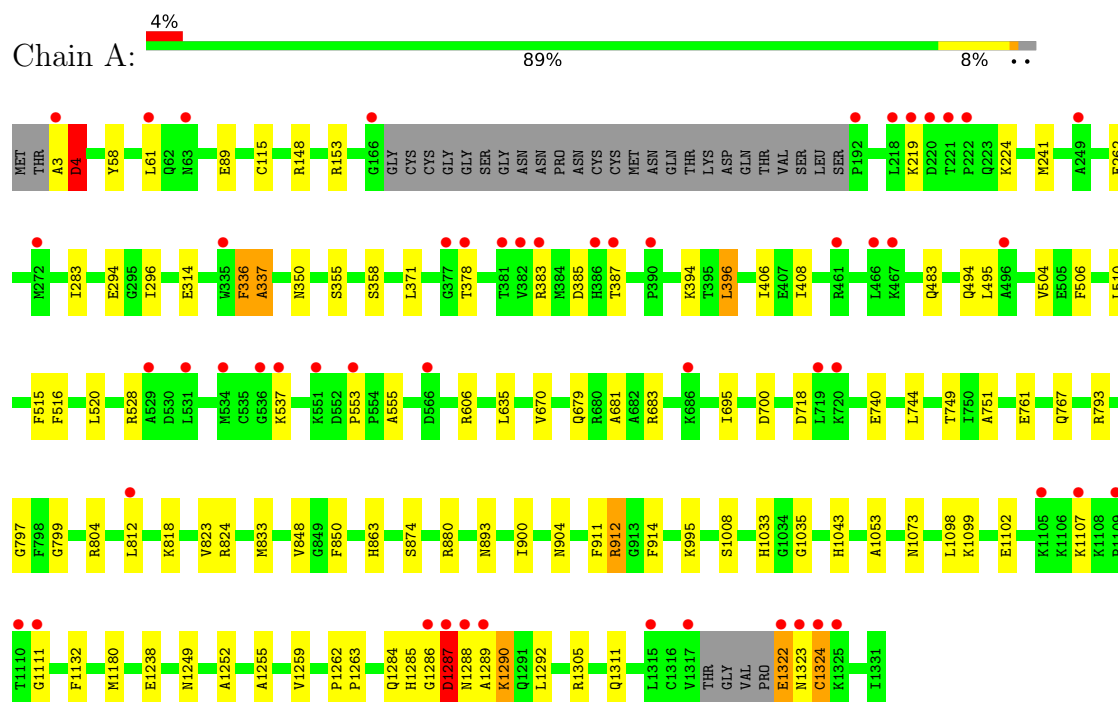
- Molecule 7 is water.

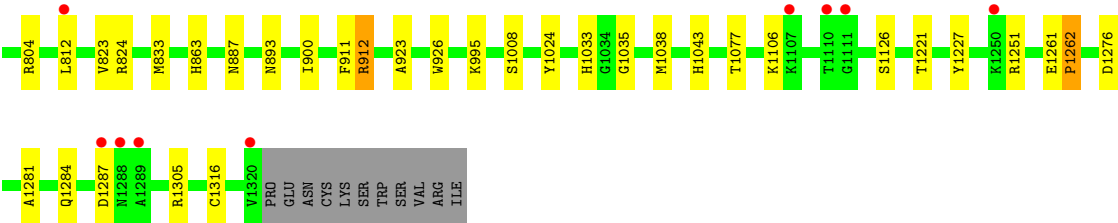
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	621	Total O 621 621	0	0
7	B	726	Total O 726 726	0	0

3 Residue-property plots

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

• Molecule 1: Xanthine dehydrogenase/oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.72Å 138.33Å 222.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 1.80 49.36 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.36-1.80) 99.7 (49.36-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.57 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.164 , 0.198 0.175 , 0.207	Depositor DCC
R_{free} test set	8609 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21605	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: FAD, NAI, BCT, URC, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.00	13/10259 (0.1%)	1.07	10/13879 (0.1%)
1	B	1.03	16/10178 (0.2%)	1.09	14/13773 (0.1%)
All	All	1.02	29/20437 (0.1%)	1.08	24/27652 (0.1%)

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	6
1	B	0	11
All	All	0	17

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1276	ASP	N-CA	7.93	1.55	1.46
1	B	1276	ASP	CG-OD2	7.34	1.39	1.25
1	A	793	ARG	CZ-NH1	7.17	1.42	1.32
1	A	337	ALA	N-CA	7.10	1.55	1.46
1	B	793	ARG	CZ-NH1	7.08	1.42	1.32
1	B	108	HIS	CE1-NE2	6.90	1.39	1.32
1	B	600	GLU	CD-OE2	6.20	1.37	1.25
1	A	408	ILE	N-CA	-6.13	1.41	1.46
1	A	1111	GLY	N-CA	6.09	1.53	1.44
1	B	793	ARG	NE-CZ	5.94	1.39	1.33
1	B	787	ILE	C-O	-5.85	1.17	1.24
1	B	124	TYR	C-O	5.80	1.30	1.24
1	B	687	ILE	N-CA	-5.64	1.39	1.46
1	A	761	GLU	CD-OE1	5.61	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1102	GLU	N-CA	5.59	1.51	1.46
1	A	848	VAL	N-CA	-5.52	1.39	1.46
1	A	89	GLU	C-O	5.46	1.31	1.24
1	B	1281	ALA	N-CA	5.36	1.52	1.46
1	A	850	PHE	N-CA	-5.32	1.39	1.45
1	B	794	MET	C-O	5.29	1.30	1.24
1	A	355	SER	N-CA	-5.22	1.39	1.45
1	A	1252	ALA	N-CA	5.21	1.52	1.45
1	B	192	PRO	N-CA	5.17	1.54	1.47
1	A	793	ARG	NE-CZ	5.13	1.38	1.33
1	A	378	THR	N-CA	5.12	1.52	1.45
1	B	863	HIS	CE1-NE2	5.07	1.37	1.32
1	B	521	THR	N-CA	5.05	1.52	1.46
1	B	303	PRO	C-O	5.05	1.29	1.23
1	B	67	HIS	CE1-NE2	5.01	1.37	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	793	ARG	NE-CZ-NH2	-21.30	100.03	119.20
1	A	793	ARG	NE-CZ-NH2	-21.23	100.09	119.20
1	B	793	ARG	NE-CZ-NH1	17.02	138.51	121.50
1	A	793	ARG	NE-CZ-NH1	16.90	138.40	121.50
1	B	793	ARG	CD-NE-CZ	11.55	140.57	124.40
1	A	793	ARG	CD-NE-CZ	11.30	140.22	124.40
1	B	1276	ASP	CA-CB-CG	10.50	123.10	112.60
1	A	4	ASP	CA-CB-CG	8.53	121.13	112.60
1	B	4	ASP	CA-CB-CG	7.43	120.03	112.60
1	A	700	ASP	CA-CB-CG	6.95	119.55	112.60
1	B	562	GLU	CB-CG-CD	6.88	124.30	112.60
1	A	553	PRO	CB-CA-C	6.65	117.42	111.17
1	B	700	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	515	PHE	CA-CB-CG	-6.01	107.79	113.80
1	B	480	GLU	CB-CG-CD	6.01	122.82	112.60
1	A	1262	PRO	N-CA-C	5.98	118.00	110.70
1	A	336	PHE	CA-CB-CG	5.53	119.33	113.80
1	B	400	GLU	CB-CG-CD	5.42	121.81	112.60
1	B	542	PHE	CA-CB-CG	5.31	119.11	113.80
1	B	192	PRO	CA-N-CD	-5.23	104.67	112.00
1	B	761	GLU	CB-CA-C	5.22	118.78	109.38
1	B	4	ASP	CA-C-O	-5.20	113.08	120.51
1	B	1262	PRO	N-CA-C	5.16	116.99	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	863	HIS	CA-CB-CG	5.01	118.81	113.80

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1287	ASP	Peptide
1	A	1305	ARG	Sidechain
1	A	148	ARG	Sidechain
1	A	3	ALA	Peptide
1	A	528	ARG	Sidechain
1	A	804	ARG	Sidechain
1	B	1251	ARG	Sidechain
1	B	128	ARG	Sidechain
1	B	1305	ARG	Sidechain
1	B	148	ARG	Sidechain
1	B	160	ARG	Sidechain
1	B	3	ALA	Peptide
1	B	32	ARG	Sidechain
1	B	334	ARG	Sidechain
1	B	383	ARG	Sidechain
1	B	535	CYS	Peptide
1	B	804	ARG	Sidechain

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	10048	0	10053	82	0
1	B	9968	0	9982	56	0
2	A	12	0	4	0	0
2	B	12	0	4	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	8	0	0	0	0
4	B	8	0	0	1	0
5	A	53	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	53	0	31	1	0
6	A	44	0	27	0	0
6	B	44	0	27	0	0
7	A	621	0	0	6	0
7	B	726	0	0	4	0
All	All	21605	0	20159	136	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 3.

All (136) 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:A:1180:MET:SD	7:A:2150:HOH:O	1.96	1.18
1:A:385:ASP:OD1	1:A:387:THR:HG22	1.44	1.15
1:B:718:ASP:H	1:B:893:ASN:HD22	1.18	0.91
1:B:749:THR:HG22	1:B:812:LEU:HD23	1.52	0.91
1:B:271:ASN:ND2	1:B:683:ARG:HH11	1.76	0.83
1:A:695:ILE:H	1:A:904:ASN:HD22	1.26	0.82
1:A:751:ALA:CB	1:A:812:LEU:CD2	2.59	0.81
1:A:751:ALA:N	1:A:812:LEU:HD21	1.97	0.80
1:A:751:ALA:CB	1:A:812:LEU:HD23	2.13	0.79
1:A:1323:ASN:HA	1:A:1324:CYS:CB	2.13	0.78
1:A:1322:GLU:HB2	1:A:1323:ASN:HB2	1.67	0.77
1:B:216:LEU:O	1:B:219:LYS:HG3	1.87	0.74
1:A:1289:ALA:O	1:A:1290:LYS:HB3	1.88	0.74
1:A:483:GLN:HE22	1:A:1311:GLN:HE22	1.37	0.73
1:A:718:ASP:H	1:A:893:ASN:HD22	1.38	0.72
1:A:1033:HIS:HE1	1:A:1043:HIS:HD2	1.35	0.72
1:B:130:GLN:HE21	1:B:132:GLU:H	1.37	0.71
1:A:751:ALA:HB2	1:A:812:LEU:CD2	2.21	0.70
1:A:751:ALA:H	1:A:812:LEU:HD21	1.54	0.70
1:A:1323:ASN:CA	1:A:1324:CYS:HB2	2.22	0.69
1:B:812:LEU:CD1	1:B:823:VAL:HG12	2.22	0.69
1:A:749:THR:HG22	1:A:812:LEU:HD22	1.75	0.68
1:A:749:THR:O	1:A:812:LEU:HD13	1.93	0.68
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	1.91	0.68
1:B:192:PRO:HD2	7:B:3620:HOH:O	1.94	0.68
1:A:262:GLU:OE1	7:A:1601:HOH:O	2.11	0.67
1:B:718:ASP:H	1:B:893:ASN:ND2	1.92	0.67
1:B:749:THR:HG22	1:B:812:LEU:CD2	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:ALA:HB3	1:A:812:LEU:HD23	1.77	0.67
1:B:812:LEU:HD11	1:B:823:VAL:C	2.21	0.66
1:A:606:ARG:HD3	1:A:679:GLN:HA	1.78	0.66
1:A:751:ALA:HB2	1:A:812:LEU:HD23	1.76	0.66
1:A:1323:ASN:CA	1:A:1324:CYS:CB	2.73	0.66
1:B:688:THR:HG23	7:B:3581:HOH:O	1.95	0.65
1:B:812:LEU:HD11	1:B:823:VAL:HG12	1.77	0.65
1:A:1323:ASN:HA	1:A:1324:CYS:HB3	1.78	0.65
1:B:606:ARG:HD3	1:B:679:GLN:HA	1.79	0.65
1:A:1323:ASN:HA	1:A:1324:CYS:HB2	1.80	0.64
1:B:749:THR:O	1:B:812:LEU:HD22	1.98	0.64
1:B:253:ASP:HB2	7:B:3312:HOH:O	1.98	0.64
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	1.96	0.63
1:B:241:MET:HE2	1:B:283:ILE:HG21	1.80	0.62
1:A:1033:HIS:CE1	1:A:1043:HIS:HD2	2.15	0.62
1:A:812:LEU:HD11	1:A:824:ARG:HA	1.79	0.62
1:A:767:GLN:HE22	1:A:799:GLY:H	1.48	0.62
1:B:812:LEU:HD21	1:B:823:VAL:O	1.99	0.62
1:B:767:GLN:HE22	1:B:799:GLY:H	1.46	0.61
1:A:1033:HIS:HD2	1:A:1035:GLY:H	1.47	0.61
1:A:751:ALA:HB3	1:A:812:LEU:CD2	2.30	0.61
1:A:1323:ASN:N	1:A:1324:CYS:HB2	2.15	0.61
1:A:695:ILE:H	1:A:904:ASN:ND2	1.99	0.60
1:B:115:CYS:HB3	1:B:744:LEU:HD22	1.82	0.60
1:B:995:LYS:HZ1	1:B:1284:GLN:HE21	1.50	0.60
1:A:1033:HIS:CE1	1:A:1043:HIS:CD2	2.92	0.58
1:A:995:LYS:HZ1	1:A:1284:GLN:HE21	1.51	0.58
1:A:1285:HIS:HD2	7:A:2177:HOH:O	1.87	0.58
1:A:1033:HIS:HE1	1:A:1043:HIS:CD2	2.19	0.57
1:A:718:ASP:H	1:A:893:ASN:ND2	2.01	0.57
1:B:271:ASN:ND2	1:B:683:ARG:NH1	2.51	0.57
1:B:115:CYS:HB3	1:B:744:LEU:CD2	2.34	0.56
1:A:1322:GLU:CB	1:A:1323:ASN:HB2	2.34	0.55
1:B:1033:HIS:HD1	1:B:1035:GLY:H	1.54	0.54
1:A:115:CYS:HB3	1:A:744:LEU:HD22	1.89	0.54
1:B:143:GLN:HE21	1:B:428:ALA:H	1.55	0.54
1:A:740:GLU:HG2	1:A:833:MET:HE3	1.90	0.53
1:A:241:MET:HE2	1:A:283:ILE:HG21	1.91	0.53
1:A:1033:HIS:CD2	1:A:1035:GLY:H	2.26	0.52
1:A:1073:ASN:HD21	1:B:1024:TYR:HA	1.75	0.52
1:B:143:GLN:HE22	1:B:335:TRP:HA	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ASP:HB2	7:A:1744:HOH:O	2.10	0.50
1:A:1289:ALA:O	1:A:1290:LYS:CB	2.59	0.50
1:A:1287:ASP:O	1:A:1287:ASP:CG	2.53	0.50
1:A:58:TYR:CE1	1:A:219:LYS:HD2	2.47	0.50
1:A:812:LEU:HD11	1:A:824:ARG:CA	2.42	0.49
1:A:812:LEU:HD11	1:A:823:VAL:O	2.12	0.49
1:A:555:ALA:O	1:A:1238:GLU:HA	2.13	0.49
1:A:874:SER:HB3	1:A:900:ILE:HG21	1.95	0.49
1:A:749:THR:O	1:A:812:LEU:CD1	2.59	0.48
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.13	0.48
1:B:740:GLU:HG2	1:B:833:MET:HE3	1.95	0.48
1:B:812:LEU:HD12	1:B:823:VAL:HG12	1.93	0.48
1:A:751:ALA:CB	1:A:812:LEU:HD21	2.40	0.48
1:A:58:TYR:CZ	1:A:219:LYS:HD2	2.49	0.47
1:A:371:LEU:HD21	1:A:406:ILE:HD12	1.97	0.47
1:B:296:ILE:CD1	1:B:314:GLU:HG3	2.45	0.47
1:A:350:ASN:ND2	1:A:358:SER:OG	2.45	0.47
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.96	0.47
1:B:1033:HIS:NE2	1:B:1043:HIS:HD2	2.13	0.46
1:A:153:ARG:HD2	1:A:153:ARG:C	2.40	0.46
1:A:337:ALA:HB2	5:A:1505:FAD:C6	2.45	0.46
1:B:508:ARG:NH1	1:B:1316:CYS:O	2.40	0.46
1:B:744:LEU:HD22	4:B:3001:FES:S1	2.56	0.46
1:B:812:LEU:HD11	1:B:824:ARG:N	2.31	0.45
1:B:1221:THR:HG22	1:B:1227:TYR:HB2	1.98	0.45
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.98	0.45
1:A:396:LEU:C	1:A:396:LEU:HD12	2.42	0.45
1:A:1292:LEU:HA	7:A:1914:HOH:O	2.17	0.45
1:B:508:ARG:HH12	1:B:1316:CYS:C	2.24	0.44
1:A:516:PHE:CZ	1:A:520:LEU:HD11	2.53	0.44
1:B:767:GLN:HE22	1:B:799:GLY:N	2.13	0.44
1:B:794:MET:HE3	1:B:1038:MET:HB3	1.99	0.44
1:B:900:ILE:HD12	1:B:900:ILE:N	2.33	0.44
1:A:115:CYS:HB3	1:A:744:LEU:CD2	2.48	0.43
1:B:469:THR:N	1:B:470:PRO:CD	2.82	0.43
1:A:495:LEU:HB2	1:A:504:VAL:HG13	1.99	0.43
1:A:1180:MET:CE	1:A:1263:PRO:HB3	2.49	0.43
1:A:880:ARG:HD2	1:A:914:PHE:HB3	2.01	0.43
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.82	0.43
1:A:635:LEU:HD21	1:A:818:LYS:HD3	2.01	0.42
1:A:1259:VAL:HG22	1:A:1259:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ALA:HB2	5:B:3005:FAD:C6	2.49	0.42
1:A:751:ALA:N	1:A:812:LEU:CD2	2.76	0.42
1:B:911:PHE:O	1:B:912:ARG:C	2.61	0.42
1:B:133:PRO:O	1:B:163:ALA:HA	2.19	0.42
1:B:271:ASN:HD22	1:B:683:ARG:NH1	2.18	0.42
1:A:1043:HIS:HE1	7:A:1870:HOH:O	2.03	0.41
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.21	0.41
1:A:296:ILE:CD1	1:A:314:GLU:HG3	2.50	0.41
1:A:911:PHE:O	1:A:912:ARG:C	2.63	0.41
1:B:1033:HIS:NE2	1:B:1043:HIS:CD2	2.88	0.41
1:A:336:PHE:O	1:A:337:ALA:C	2.63	0.41
1:B:201:LYS:HA	1:B:202:PRO:HD3	1.90	0.41
1:B:793:ARG:NH1	7:B:3116:HOH:O	2.53	0.41
1:A:296:ILE:HD11	1:A:314:GLU:HG3	2.03	0.41
1:A:506:PHE:CZ	1:A:510:LEU:HD11	2.56	0.41
1:A:718:ASP:N	1:A:893:ASN:HD22	2.13	0.41
1:A:767:GLN:HE22	1:A:799:GLY:N	2.15	0.41
1:B:650:ASN:OD1	1:B:778:LYS:NZ	2.54	0.41
1:A:1132:PHE:CG	1:B:1126:SER:HB2	2.57	0.40
1:B:130:GLN:NE2	1:B:132:GLU:H	2.13	0.40
1:A:679:GLN:HG2	1:A:683:ARG:HH11	1.86	0.40
1:B:1038:MET:CE	1:B:1077:THR:CG2	2.99	0.40
1:A:749:THR:CG2	1:A:812:LEU:HD22	2.47	0.40
1:B:923:ALA:HA	1:B:926:TRP:NE1	2.37	0.40
1:B:565:LYS:HD3	1:B:565:LYS:HA	2.01	0.40
1:B:749:THR:C	1:B:812:LEU:HD22	2.45	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	1294/1331 (97%)	1245 (96%)	41 (3%)	8 (1%)	21	11
1	B	1287/1331 (97%)	1250 (97%)	31 (2%)	6 (0%)	24	14
All	All	2581/2662 (97%)	2495 (97%)	72 (3%)	14 (0%)	24	14

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	1008	SER
1	A	1324	CYS
1	B	4	ASP
1	B	1008	SER
1	A	1288	ASN
1	A	1290	LYS
1	B	912	ARG
1	A	912	ARG
1	A	797	GLY
1	B	797	GLY
1	B	887	ASN
1	B	1287	ASP
1	A	1286	GLY

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	1097/1123 (98%)	1084 (99%)	13 (1%)	63	57
1	B	1088/1123 (97%)	1074 (99%)	14 (1%)	61	54
All	All	2185/2246 (97%)	2158 (99%)	27 (1%)	63	57

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	61	LEU

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Mol	Chain	Res	Type
1	A	224	LYS
1	A	294	GLU
1	A	383	ARG
1	A	394	LYS
1	A	396	LEU
1	A	494	GLN
1	A	537	LYS
1	A	1099	LYS
1	A	1107	LYS
1	A	1287	ASP
1	A	1322	GLU
1	B	4	ASP
1	B	61	LEU
1	B	99	PRO
1	B	219	LYS
1	B	224	LYS
1	B	280	PRO
1	B	308	GLU
1	B	317	LYS
1	B	467	LYS
1	B	494	GLN
1	B	535	CYS
1	B	550	GLN
1	B	659	GLU
1	B	1106	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	145	ASN
1	A	250	GLN
1	A	271	ASN
1	A	291	HIS
1	A	350	ASN
1	A	386	HIS
1	A	583	ASN
1	A	585	GLN
1	A	699	GLN
1	A	767	GLN
1	A	893	ASN
1	A	904	ASN

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Mol	Chain	Res	Type
1	A	1033	HIS
1	A	1043	HIS
1	A	1073	ASN
1	A	1137	ASN
1	A	1212	HIS
1	A	1284	GLN
1	A	1285	HIS
1	A	1311	GLN
1	B	71	ASN
1	B	130	GLN
1	B	143	GLN
1	B	145	ASN
1	B	207	GLN
1	B	250	GLN
1	B	271	ASN
1	B	350	ASN
1	B	386	HIS
1	B	550	GLN
1	B	556	ASN
1	B	583	ASN
1	B	585	GLN
1	B	705	ASN
1	B	767	GLN
1	B	893	ASN
1	B	956	ASN
1	B	1043	HIS
1	B	1137	ASN
1	B	1212	HIS
1	B	1220	HIS
1	B	1284	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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$
4	FES	B	3002	1	0,4,4	-	-	-		
5	FAD	A	1505	-	58,58,58	1.53	13 (22%)	85,89,89	1.53	15 (17%)
4	FES	B	3001	1	0,4,4	-	-	-		
3	BCT	A	1502	-	3,3,3	1.23	0	2,3,3	0.22	0
4	FES	A	1503	1	0,4,4	-	-	-		
5	FAD	B	3005	-	58,58,58	1.60	10 (17%)	85,89,89	1.45	18 (21%)
2	URC	A	1501	-	13,13,13	3.15	6 (46%)	17,19,19	2.52	8 (47%)
4	FES	A	1504	1	0,4,4	-	-	-		
3	BCT	B	3004	-	3,3,3	0.89	0	2,3,3	2.36	1 (50%)
6	NAI	A	1506	-	47,48,48	1.45	10 (21%)	64,73,73	1.79	14 (21%)
6	NAI	B	3006	-	47,48,48	1.51	7 (14%)	64,73,73	1.78	14 (21%)
2	URC	B	3003	-	13,13,13	2.90	6 (46%)	17,19,19	2.70	9 (52%)

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	A	1505	-	-	4/34/50/50	0/6/6/6
4	FES	B	3002	1	-	-	0/1/1/1
4	FES	B	3001	1	-	-	0/1/1/1
4	FES	A	1503	1	-	-	0/1/1/1
5	FAD	B	3005	-	-	2/34/50/50	0/6/6/6
2	URC	A	1501	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FES	A	1504	1	-	-	0/1/1/1
6	NAI	A	1506	-	-	2/29/72/72	0/5/5/5
6	NAI	B	3006	-	-	3/29/72/72	0/5/5/5
2	URC	B	3003	-	-	-	0/2/2/2

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	URC	C5-C4	7.20	1.51	1.37
2	B	3003	URC	C5-C4	7.12	1.51	1.37
5	B	3005	FAD	PA-O3P	5.78	1.65	1.59
6	B	3006	NAI	C5A-C4A	5.02	1.48	1.39
6	A	1506	NAI	C5A-C4A	4.86	1.47	1.39
2	A	1501	URC	O13-C6	4.60	1.32	1.23
2	A	1501	URC	O24-C8	4.20	1.32	1.23
5	B	3005	FAD	C9A-C5X	3.97	1.47	1.41
5	B	3005	FAD	C4X-N5	3.94	1.39	1.30
6	B	3006	NAI	PN-O3	3.83	1.63	1.59
5	A	1505	FAD	C4A-N9A	-3.57	1.30	1.37
2	B	3003	URC	C4-N9	3.56	1.41	1.35
2	B	3003	URC	O13-C6	3.50	1.30	1.23
2	A	1501	URC	C5-C6	3.28	1.51	1.41
2	B	3003	URC	O24-C8	3.26	1.30	1.23
2	A	1501	URC	C4-N9	3.13	1.41	1.35
5	A	1505	FAD	C9A-C5X	3.12	1.46	1.41
6	A	1506	NAI	C2N-C3N	3.00	1.43	1.35
5	B	3005	FAD	C8-C7	2.99	1.48	1.40
5	B	3005	FAD	C4A-N9A	-2.91	1.31	1.37
2	B	3003	URC	C2-N1	2.75	1.42	1.37
5	A	1505	FAD	C5X-N5	-2.74	1.34	1.39
5	A	1505	FAD	C4X-N5	2.65	1.36	1.30
5	A	1505	FAD	C8-C7	2.65	1.47	1.40
6	A	1506	NAI	C4A-N9A	-2.64	1.32	1.37
6	B	3006	NAI	C7N-C3N	2.63	1.54	1.48
5	B	3005	FAD	C10-N1	2.62	1.38	1.33
2	A	1501	URC	C2-N1	2.53	1.41	1.37
5	A	1505	FAD	C1'-C2'	2.48	1.56	1.52
5	A	1505	FAD	C7M-C7	2.47	1.55	1.51
5	A	1505	FAD	O2-C2	2.45	1.29	1.24
2	B	3003	URC	C5-C6	2.43	1.49	1.41
5	B	3005	FAD	C5A-C4A	2.42	1.43	1.39
6	A	1506	NAI	PN-O3	2.36	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1506	NAI	C8A-N7A	2.35	1.36	1.31
6	B	3006	NAI	C2N-C3N	2.30	1.41	1.35
6	B	3006	NAI	C8A-N7A	2.29	1.36	1.31
5	A	1505	FAD	C5A-C4A	2.29	1.43	1.39
6	A	1506	NAI	C5A-C6A	2.28	1.47	1.41
6	A	1506	NAI	C6N-C5N	2.23	1.39	1.33
6	A	1506	NAI	C5A-N7A	-2.22	1.35	1.39
5	B	3005	FAD	C5X-N5	-2.15	1.35	1.39
5	A	1505	FAD	C6-C7	-2.15	1.36	1.39
6	B	3006	NAI	O4D-C1D	2.11	1.46	1.42
5	A	1505	FAD	O2B-C2B	2.08	1.48	1.43
6	A	1506	NAI	PA-O3	2.05	1.61	1.59
6	B	3006	NAI	C4A-N9A	-2.03	1.33	1.37
5	B	3005	FAD	O3'-C3'	2.03	1.48	1.43
5	A	1505	FAD	C2-N3	-2.02	1.34	1.39
5	B	3005	FAD	O4B-C1B	2.02	1.46	1.42
5	A	1505	FAD	O3'-C3'	2.01	1.47	1.43
6	A	1506	NAI	O4D-C4D	-2.00	1.40	1.45

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1505	FAD	C4A-N9A-C8A	5.37	111.38	105.74
6	B	3006	NAI	C5A-C4A-N3A	-5.33	119.37	126.72
2	B	3003	URC	N7-C8-N9	5.33	114.77	107.22
2	B	3003	URC	N3-C2-N1	4.89	123.42	115.74
2	A	1501	URC	N7-C8-N9	4.83	114.06	107.22
6	A	1506	NAI	C5A-C4A-N3A	-4.71	120.23	126.72
2	A	1501	URC	N3-C2-N1	4.70	123.13	115.74
6	A	1506	NAI	N3A-C2A-N1A	-4.60	121.63	128.58
6	A	1506	NAI	N3A-C4A-N9A	4.56	134.92	127.17
6	B	3006	NAI	N3A-C4A-N9A	4.39	134.64	127.17
6	A	1506	NAI	C2A-N3A-C4A	4.26	122.24	111.83
6	B	3006	NAI	C4A-N9A-C8A	4.23	110.17	105.74
5	A	1505	FAD	O2A-PA-O3P	3.84	117.66	107.27
6	A	1506	NAI	C4A-N9A-C8A	3.75	109.67	105.74
6	B	3006	NAI	C2A-N3A-C4A	3.74	120.97	111.83
5	A	1505	FAD	O4'-C4'-C3'	-3.64	100.72	109.25
2	A	1501	URC	N9-C4-N3	3.63	136.93	128.19
2	B	3003	URC	O24-C8-N7	-3.55	119.11	125.56
5	B	3005	FAD	C4A-N9A-C8A	3.52	109.44	105.74
6	A	1506	NAI	O3-PN-O2N	-3.45	100.33	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3005	FAD	C5A-C4A-N3A	-3.40	122.03	126.72
6	B	3006	NAI	C4A-C5A-N7A	-3.31	106.80	110.58
6	B	3006	NAI	N3A-C2A-N1A	-3.31	123.58	128.58
5	A	1505	FAD	N3A-C4A-N9A	3.28	132.75	127.17
5	A	1505	FAD	N9A-C8A-N7A	-3.27	109.30	113.94
2	B	3003	URC	N9-C4-N3	3.24	135.99	128.19
3	B	3004	BCT	O2-C-O1	3.19	127.83	119.68
2	B	3003	URC	O11-C2-N3	-3.10	116.36	121.86
6	B	3006	NAI	N9A-C8A-N7A	-3.08	109.57	113.94
6	B	3006	NAI	C6A-C5A-N7A	3.03	137.93	132.09
5	B	3005	FAD	N3A-C4A-N9A	3.03	132.31	127.17
2	B	3003	URC	O13-C6-C5	-3.01	120.00	127.26
5	B	3005	FAD	C4-N3-C2	-2.93	120.43	125.64
2	B	3003	URC	C6-N1-C2	-2.89	122.39	126.37
5	B	3005	FAD	O4-C4-C4X	-2.84	119.02	126.53
6	B	3006	NAI	C3D-C2D-C1D	2.83	106.82	101.46
2	A	1501	URC	C6-N1-C2	-2.82	122.49	126.37
6	A	1506	NAI	O1N-PN-O3	2.81	114.87	107.27
6	A	1506	NAI	C3N-C2N-N1N	-2.79	119.10	123.20
6	B	3006	NAI	O2A-PA-O3	2.78	114.78	107.27
5	A	1505	FAD	C5A-C4A-N3A	-2.76	122.92	126.72
5	B	3005	FAD	O4'-C4'-C3'	-2.73	102.86	109.25
6	A	1506	NAI	C5A-C6A-N6A	-2.70	116.59	123.29
5	A	1505	FAD	C2B-C1B-N9A	2.63	119.84	113.30
5	A	1505	FAD	C2B-C3B-C4B	2.62	107.67	102.61
5	A	1505	FAD	C4A-N9A-C1B	-2.58	120.60	126.63
6	B	3006	NAI	C5A-N7A-C8A	2.56	107.48	103.45
5	B	3005	FAD	O4B-C1B-N9A	-2.56	103.17	108.09
5	B	3005	FAD	N6A-C6A-N1A	2.55	124.05	118.38
5	B	3005	FAD	C2B-C1B-N9A	2.53	119.60	113.30
2	A	1501	URC	O13-C6-C5	-2.53	121.16	127.26
2	B	3003	URC	O13-C6-N1	2.52	124.86	120.11
2	A	1501	URC	C5-C4-N3	-2.47	117.13	122.94
5	B	3005	FAD	C5'-C4'-C3'	2.47	116.88	112.22
6	A	1506	NAI	C6A-C5A-N7A	2.41	136.73	132.09
6	A	1506	NAI	N6A-C6A-N1A	2.37	123.66	118.38
2	A	1501	URC	O24-C8-N7	-2.37	121.25	125.56
5	B	3005	FAD	C4-C4X-N5	2.33	121.42	118.21
6	B	3006	NAI	C2B-C1B-N9A	2.29	119.00	113.30
5	A	1505	FAD	C7M-C7-C8	2.29	125.44	120.76
5	A	1505	FAD	N6A-C6A-N1A	2.29	123.47	118.38
5	A	1505	FAD	O4B-C1B-N9A	-2.28	103.71	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	3006	NAI	O7N-C7N-C3N	-2.27	116.62	120.90
5	B	3005	FAD	C4X-C10-N1	-2.26	119.05	124.59
5	B	3005	FAD	N3-C2-N1	2.25	124.28	119.50
2	B	3003	URC	C5-C4-N9	-2.24	105.14	108.31
5	B	3005	FAD	C5A-C6A-N6A	-2.24	117.74	123.29
6	B	3006	NAI	O1N-PN-O3	2.20	113.22	107.27
5	B	3005	FAD	C4X-C4-N3	2.17	118.78	113.25
6	A	1506	NAI	N9A-C8A-N7A	-2.17	110.85	113.94
5	B	3005	FAD	C10-C4X-N5	-2.14	120.44	124.81
5	B	3005	FAD	C4A-N9A-C1B	-2.13	121.64	126.63
6	A	1506	NAI	O2B-C2B-C1B	-2.13	102.78	110.10
5	A	1505	FAD	C9A-N10-C10	-2.10	117.56	120.75
5	A	1505	FAD	C5A-N7A-C8A	2.08	106.72	103.45
5	A	1505	FAD	C8M-C8-C9	-2.06	115.94	119.57
5	B	3005	FAD	C4X-C10-N10	2.06	119.44	116.48
6	A	1506	NAI	O5D-C5D-C4D	-2.03	102.09	108.99
2	A	1501	URC	O11-C2-N3	-2.01	118.29	121.86

There are no chirality outliers.

All (11) torsion outliers are listed below:

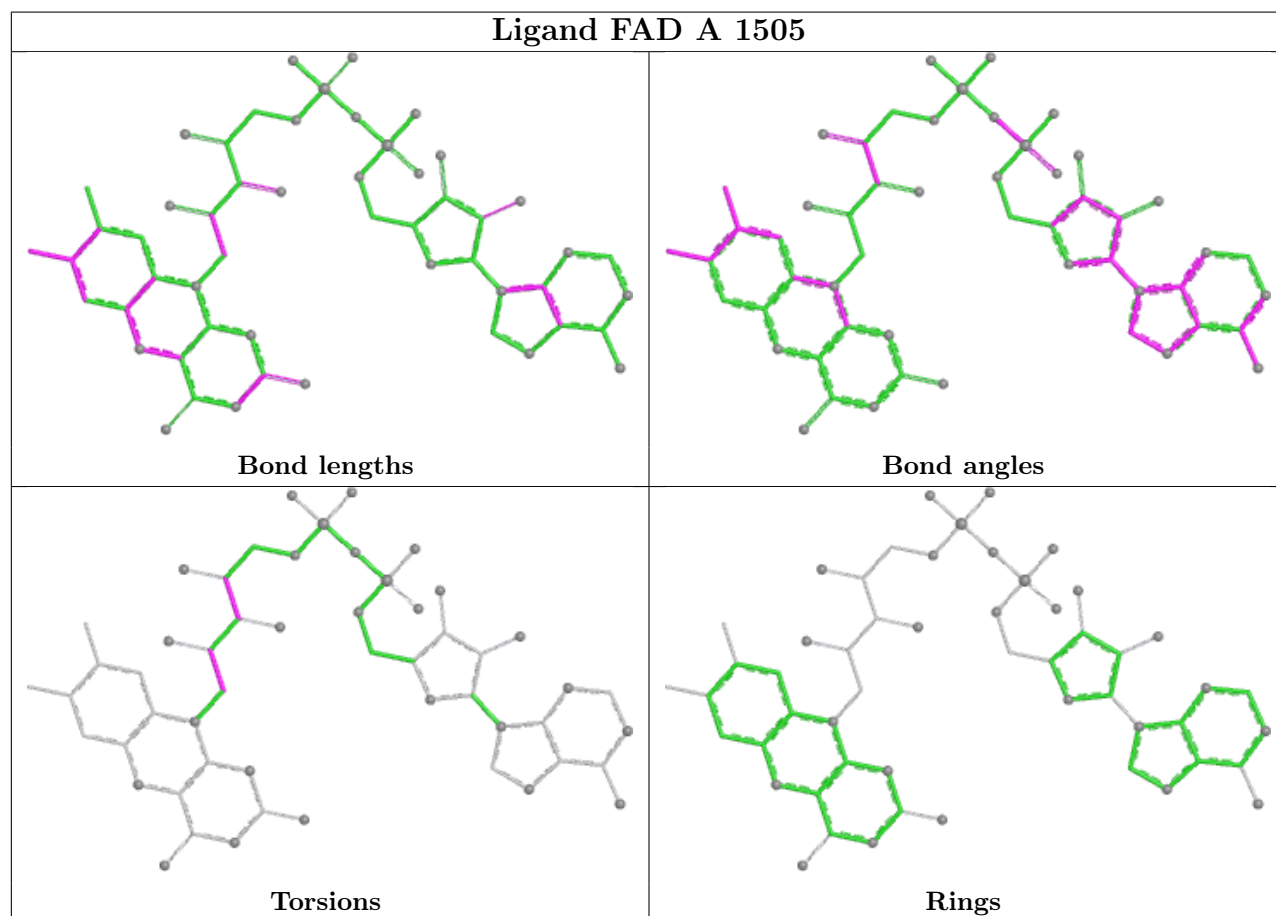
Mol	Chain	Res	Type	Atoms
5	A	1505	FAD	N10-C1'-C2'-O2'
5	A	1505	FAD	N10-C1'-C2'-C3'
5	B	3005	FAD	N10-C1'-C2'-O2'
5	B	3005	FAD	N10-C1'-C2'-C3'
5	A	1505	FAD	C2'-C3'-C4'-C5'
5	A	1505	FAD	C2'-C3'-C4'-O4'
6	A	1506	NAI	C2D-C1D-N1N-C6N
6	A	1506	NAI	O4D-C1D-N1N-C6N
6	B	3006	NAI	C2D-C1D-N1N-C6N
6	B	3006	NAI	O4D-C1D-N1N-C6N
6	B	3006	NAI	PA-O3-PN-O1N

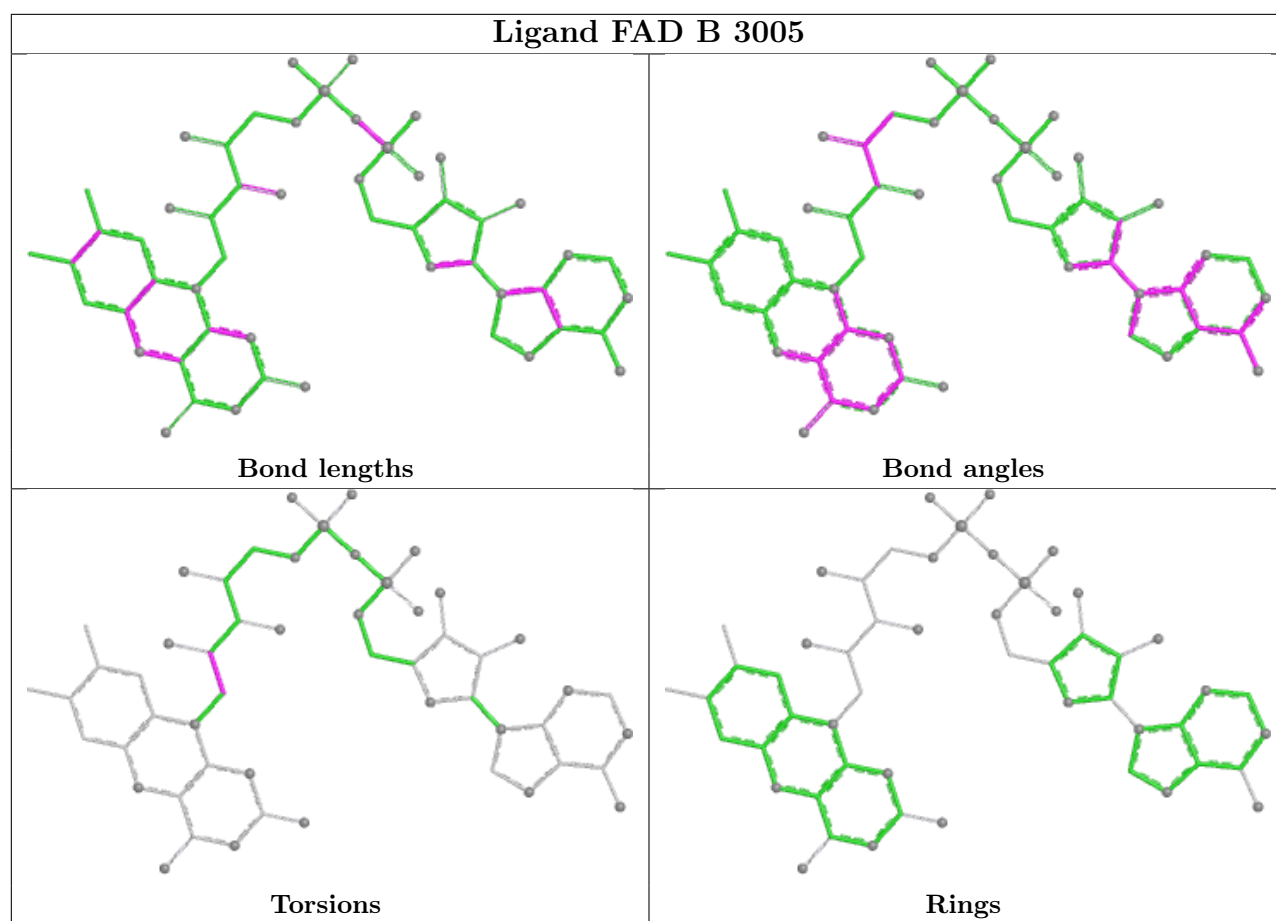
There are no ring outliers.

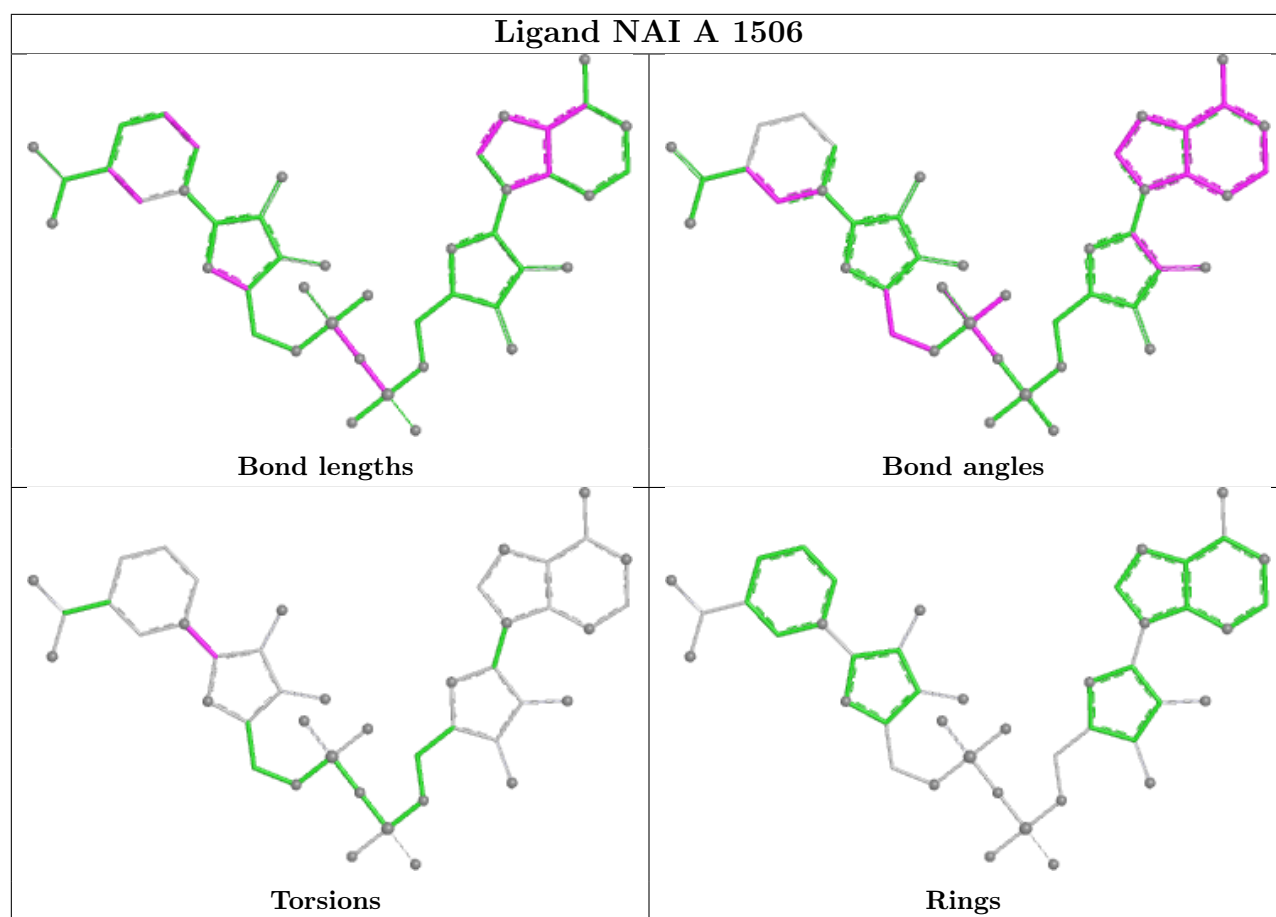
3 monomers are involved in 3 short contacts:

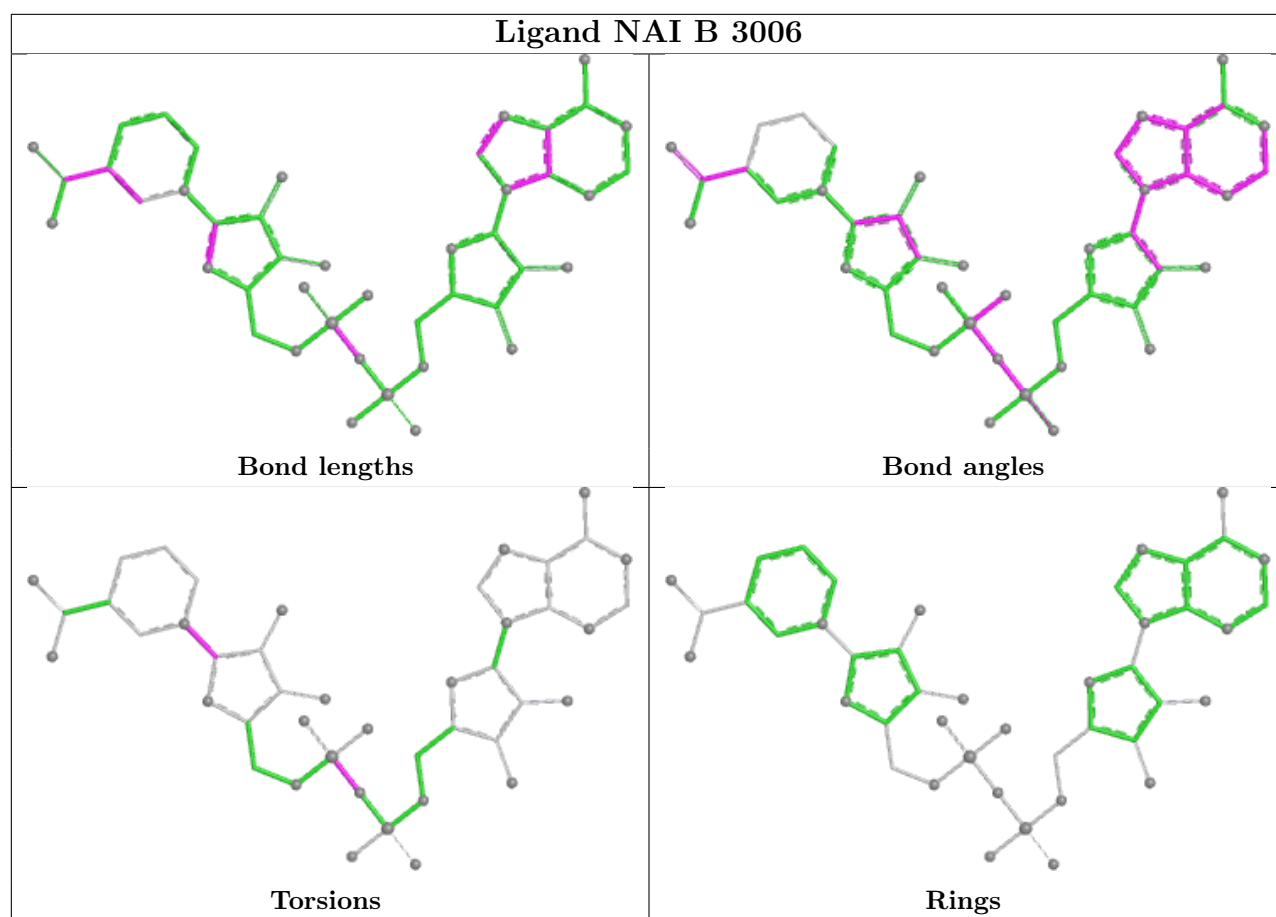
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1505	FAD	1	0
4	B	3001	FES	1	0
5	B	3005	FAD	1	0

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	1300/1331 (97%)	-0.01	52 (4%)	42 41	11, 21, 43, 81	0
1	B	1291/1331 (96%)	-0.26	24 (1%)	66 66	11, 17, 35, 65	0
All	All	2591/2662 (97%)	-0.14	76 (2%)	53 53	11, 19, 40, 81	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1289	ALA	7.4
1	A	1317	VAL	6.3
1	B	61	LEU	6.0
1	A	192	PRO	6.0
1	A	61	LEU	4.8
1	B	1287	ASP	4.7
1	A	1287	ASP	4.7
1	B	1111	GLY	4.5
1	B	1289	ALA	4.5
1	A	3	ALA	4.5
1	A	1111	GLY	4.3
1	A	1110	THR	4.1
1	B	3	ALA	4.0
1	A	1286	GLY	3.9
1	B	1320	VAL	3.8
1	A	1323	ASN	3.8
1	B	1288	ASN	3.7
1	A	1325	LYS	3.6
1	A	1322	GLU	3.6
1	B	1110	THR	3.5
1	A	466	LEU	3.2
1	A	1324	CYS	3.2
1	B	222	PRO	3.1
1	A	534	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	218	LEU	3.0
1	A	387	THR	2.9
1	A	222	PRO	2.9
1	A	1288	ASN	2.8
1	A	386	HIS	2.8
1	B	192	PRO	2.8
1	A	272	MET	2.8
1	A	529	ALA	2.8
1	A	335	TRP	2.8
1	A	537	LYS	2.7
1	B	812	LEU	2.7
1	A	536	GLY	2.7
1	A	1105	LYS	2.7
1	B	535	CYS	2.7
1	B	221	THR	2.6
1	A	553	PRO	2.6
1	A	218	LEU	2.6
1	A	531	LEU	2.6
1	A	1315	LEU	2.6
1	A	390	PRO	2.6
1	B	1250	LYS	2.5
1	B	220	ASP	2.5
1	B	164	LYS	2.5
1	B	473	LEU	2.5
1	A	166	GLY	2.5
1	A	381	THR	2.5
1	A	383	ARG	2.4
1	A	812	LEU	2.4
1	A	1107	LYS	2.4
1	A	220	ASP	2.4
1	B	1107	LYS	2.3
1	A	221	THR	2.3
1	B	565	LYS	2.3
1	B	530	ASP	2.3
1	B	566	ASP	2.3
1	A	720	LYS	2.3
1	A	378	THR	2.2
1	A	63	ASN	2.2
1	A	461	ARG	2.2
1	B	62	GLN	2.1
1	A	467	LYS	2.1
1	A	1109	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	249	ALA	2.1
1	A	382	VAL	2.1
1	A	719	LEU	2.1
1	A	566	ASP	2.1
1	A	496	ALA	2.1
1	A	551	LYS	2.0
1	A	686	LYS	2.0
1	B	536	GLY	2.0
1	A	219	LYS	2.0
1	A	377	GLY	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](#)

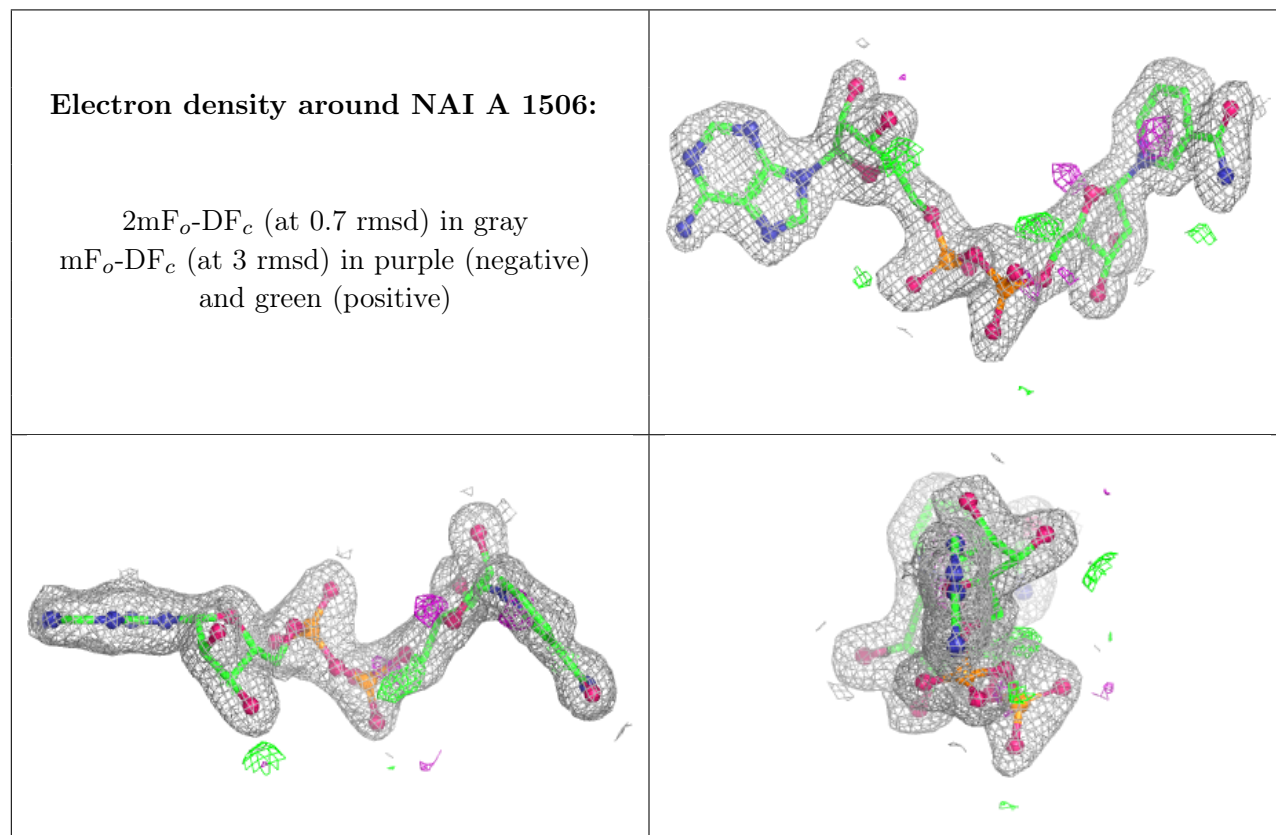
There are no oligosaccharides in this entry.

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.

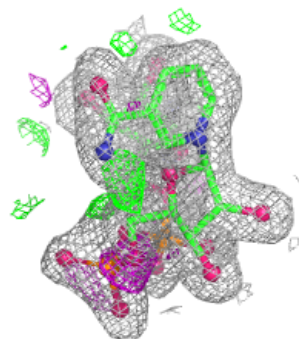
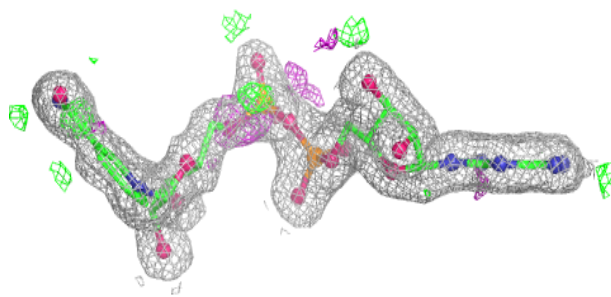
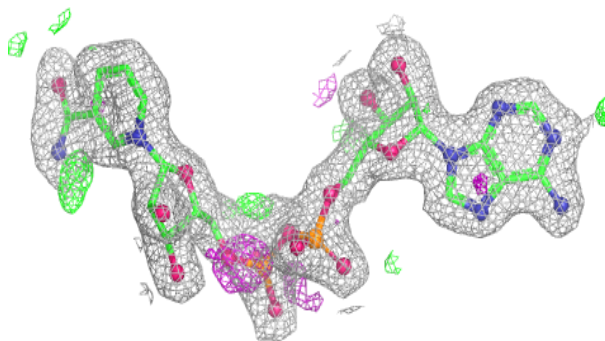
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	URC	A	1501	12/12	0.91	0.09	20,25,29,29	0
2	URC	B	3003	12/12	0.93	0.07	18,22,26,26	0
6	NAI	A	1506	44/44	0.93	0.09	23,32,39,43	0
6	NAI	B	3006	44/44	0.93	0.08	20,23,30,35	0
3	BCT	A	1502	4/4	0.97	0.07	18,21,23,25	0
5	FAD	A	1505	53/53	0.97	0.06	17,20,24,25	0
3	BCT	B	3004	4/4	0.98	0.05	14,15,17,19	0
5	FAD	B	3005	53/53	0.98	0.04	13,14,16,17	0
4	FES	A	1504	4/4	0.99	0.05	16,17,17,18	0
4	FES	B	3001	4/4	0.99	0.06	15,15,17,18	0
4	FES	A	1503	4/4	1.00	0.01	13,14,14,14	0
4	FES	B	3002	4/4	1.00	0.01	11,11,11,12	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.

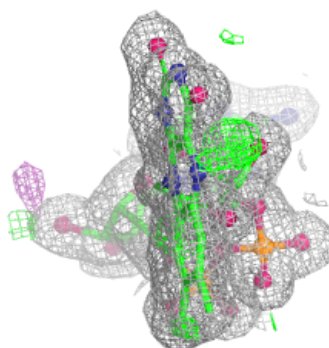
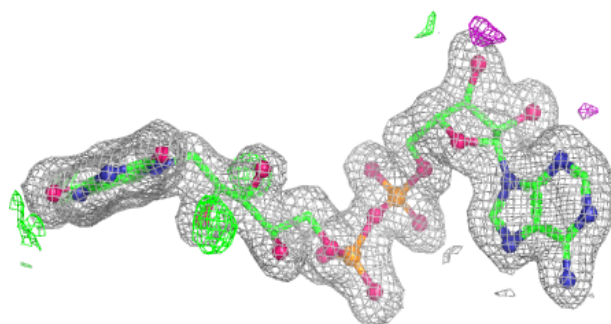
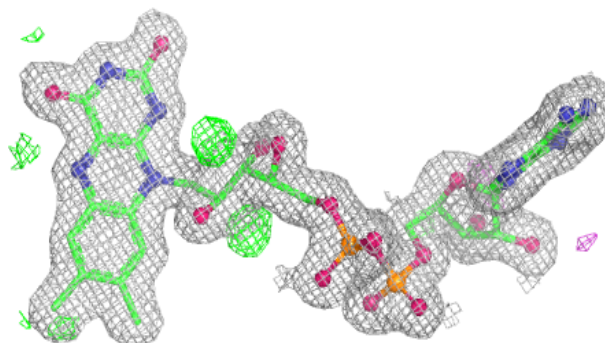


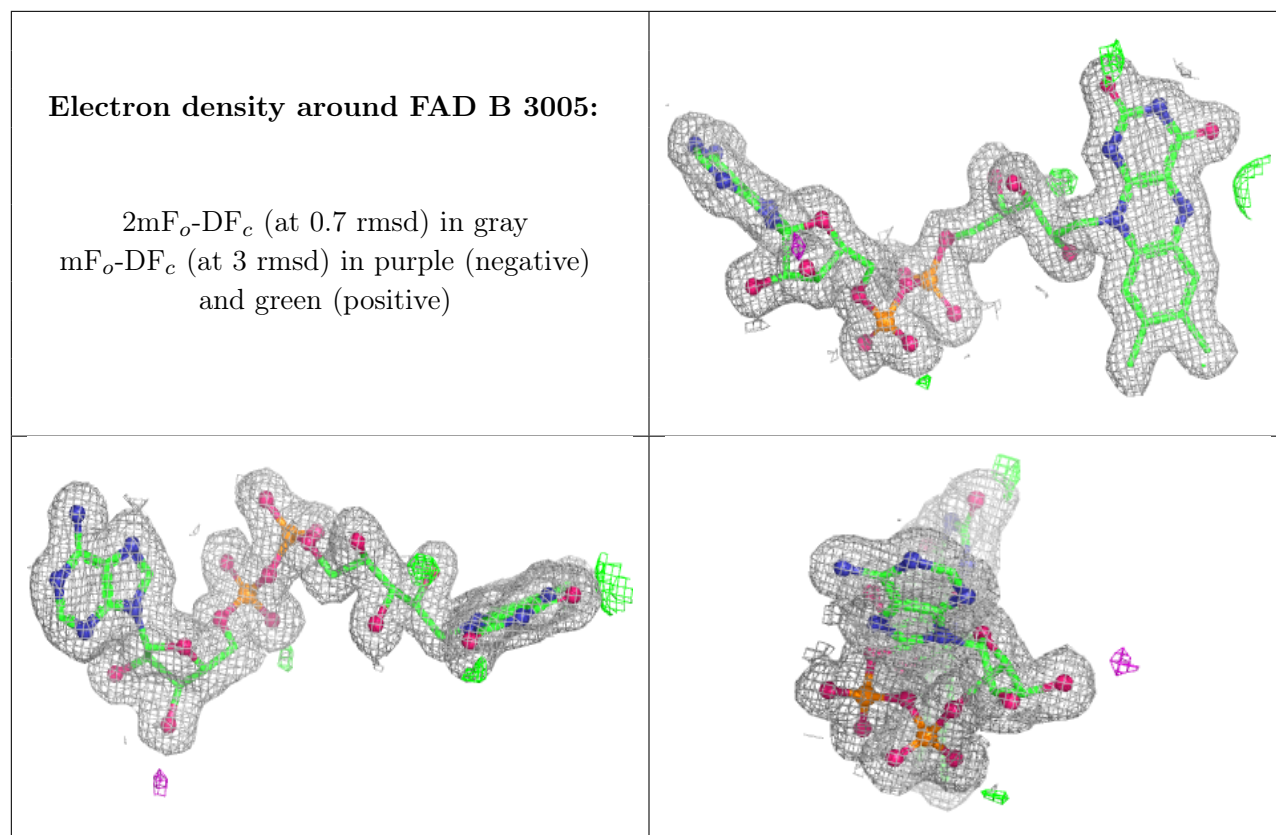
Electron density around NAI B 3006:

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

**Electron density around FAD A 1505:**

$2mF_o-DF_c$ (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.