



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:40 PM UTC

PDB ID : 2E3T / pdb_00002e3t
Title : Crystal structure of rat xanthine oxidoreductase mutant (W335A and F336L)
Authors : Asai, R.; Nishino, T.; Matsumura, T.; Okamoto, K.; Pai, E.F.; Nishino, T.
Deposited on : 2006-11-28
Resolution : 2.28 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

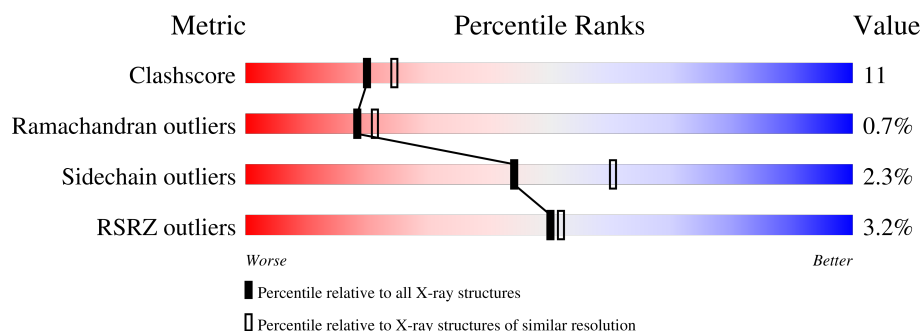
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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))
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	3% 74% 21% • •
1	B	1331	3% 74% 20% • •

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 21444 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.

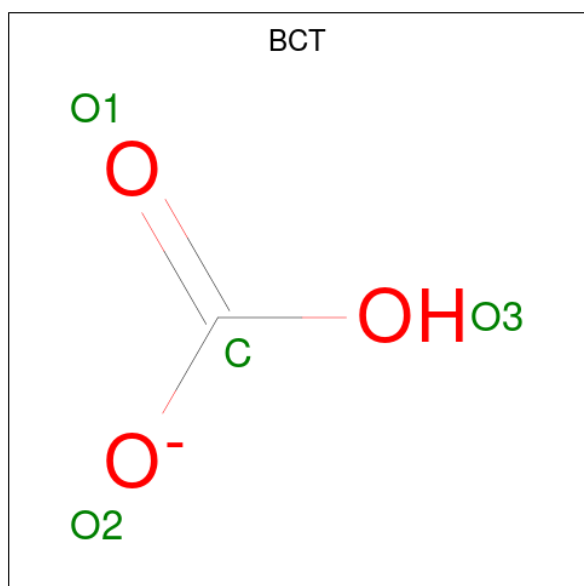
- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1291	Total	C	N	O	S	0	0	0
			9963	6309	1715	1875	64			
1	B	1281	Total	C	N	O	S	0	0	0
			9877	6255	1702	1858	62			

There are 4 discrepancies between the modelled and reference sequences:

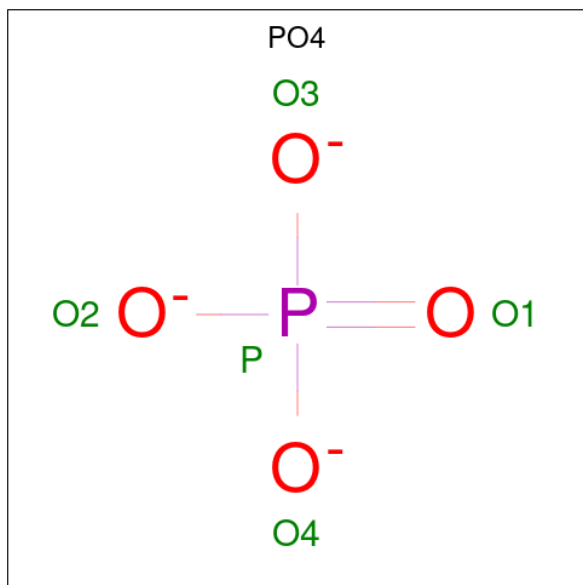
Chain	Residue	Modelled	Actual	Comment	Reference
A	335	ALA	TRP	engineered mutation	UNP P22985
A	336	LEU	PHE	engineered mutation	UNP P22985
B	335	ALA	TRP	engineered mutation	UNP P22985
B	336	LEU	PHE	engineered mutation	UNP P22985

- Molecule 2 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

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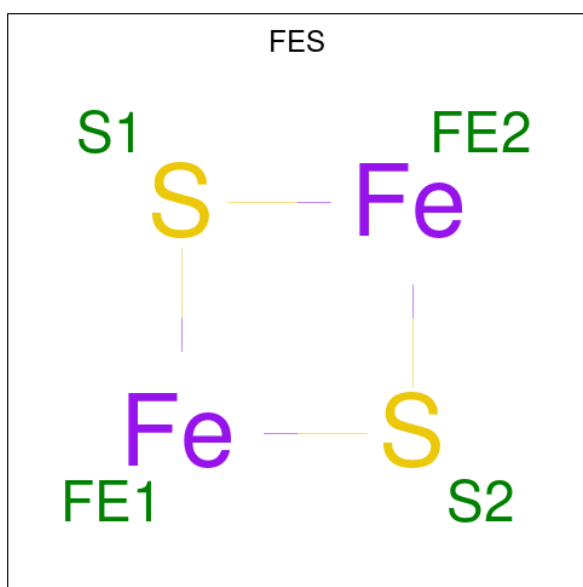
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		

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

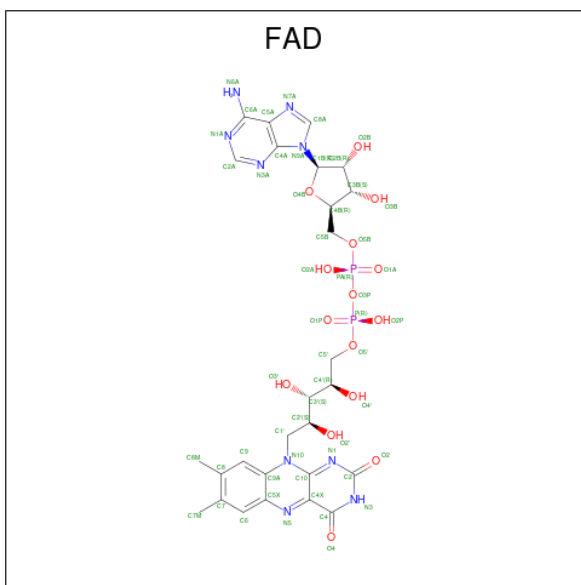
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	B	2	Total	Ca	0	0
			2	2		

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



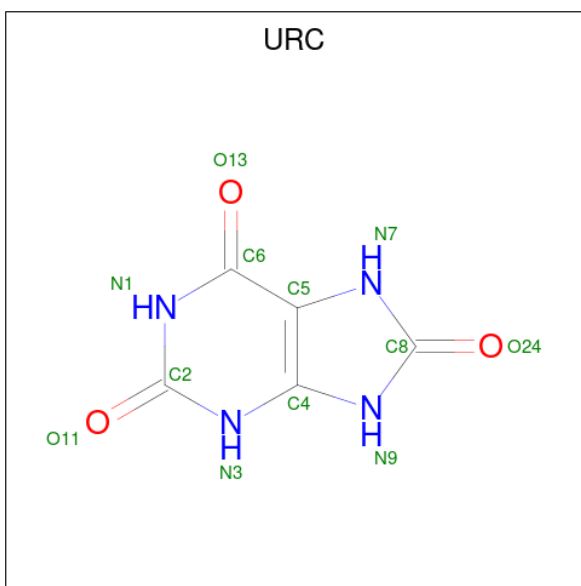
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			4	2	2		
5	A	1	Total	Fe	S	0	0
			4	2	2		
5	B	1	Total	Fe	S	0	0
			4	2	2		
5	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 7 is URIC ACID (CCD ID: URC) (formula: $C_5H_4N_4O_3$).



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

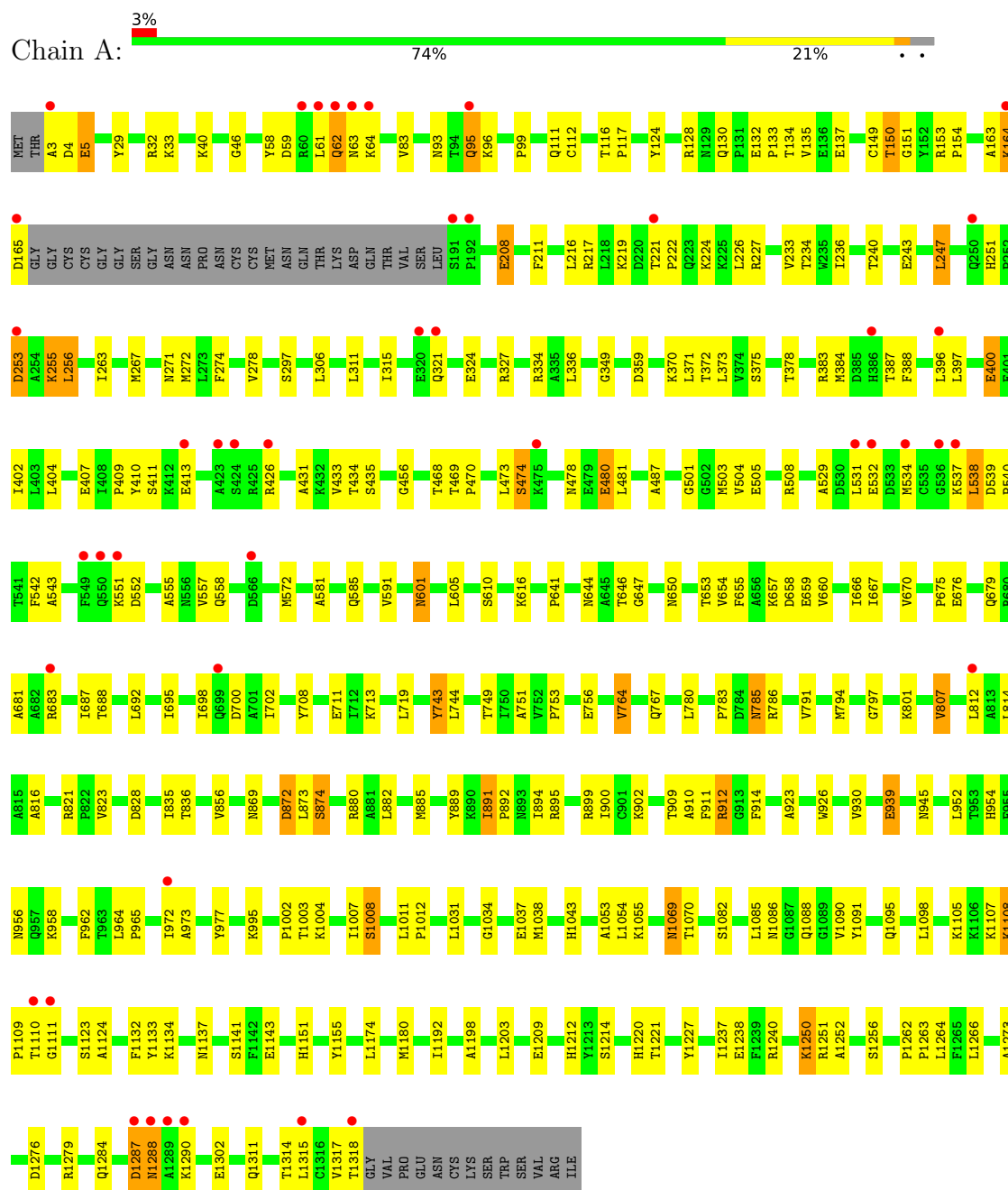
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	667	Total 667	O 667	0	0
8	B	724	Total 724	O 724	0	0

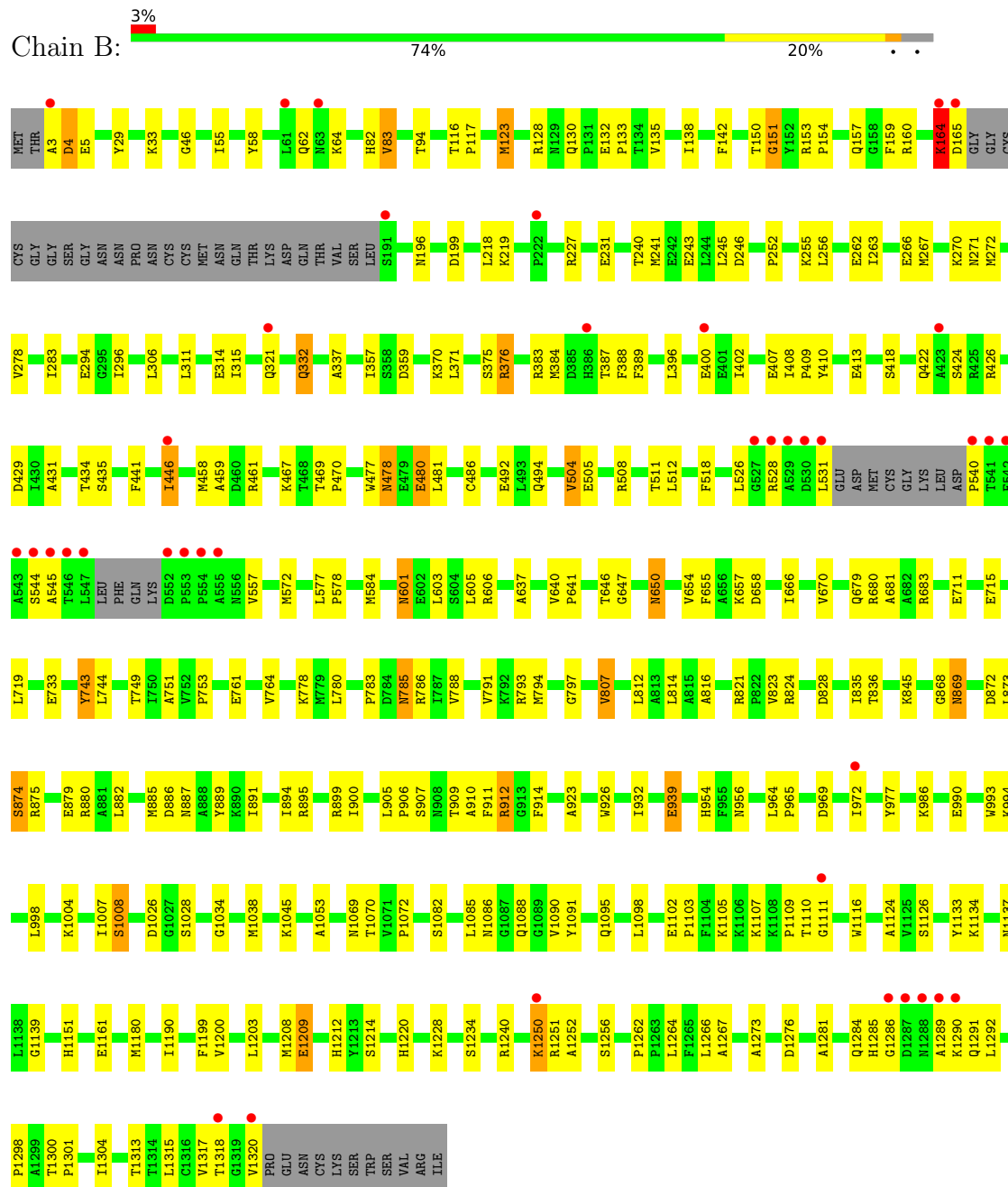
3 Residue-property plots

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



● 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	101.07Å 139.51Å 222.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.28 25.00 – 2.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.28) 95.8 (25.00-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.44 (at 2.28Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.185 , 0.229 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.4	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	21444	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: URC, CA, FES, PO4, FAD, BCT

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	0.37	0/10170	0.91	38/13763 (0.3%)
1	B	0.38	1/10081 (0.0%)	0.94	38/13642 (0.3%)
All	All	0.37	1/20251 (0.0%)	0.92	76/27405 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	123	MET	SD-CE	-5.30	1.66	1.79

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	654	VAL	N-CA-C	-9.45	101.65	110.53
1	A	835	ILE	N-CA-C	8.86	119.67	110.72
1	B	164	LYS	N-CA-C	-8.67	102.71	113.28
1	B	150	THR	N-CA-C	8.44	121.60	111.82
1	B	835	ILE	N-CA-C	8.38	120.14	111.00
1	B	1262	PRO	N-CA-C	7.97	120.42	110.70
1	A	150	THR	N-CA-C	7.80	120.87	111.82
1	B	446	ILE	N-CA-C	-7.58	105.46	112.43
1	A	654	VAL	N-CA-C	-7.50	103.48	110.53
1	A	836	THR	N-CA-C	7.25	121.98	113.20
1	A	891	ILE	CA-C-N	7.13	126.65	119.24
1	A	891	ILE	C-N-CA	7.13	126.65	119.24
1	B	956	ASN	N-CA-C	7.07	121.29	112.24
1	A	1273	ALA	N-CA-C	-7.05	103.67	111.36
1	B	836	THR	N-CA-C	7.05	121.73	113.20
1	B	389	PHE	CA-C-N	6.97	126.78	119.05
1	B	389	PHE	C-N-CA	6.97	126.78	119.05
1	B	891	ILE	CA-C-N	6.89	126.40	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	891	ILE	C-N-CA	6.89	126.40	119.24
1	B	410	TYR	N-CA-C	-6.87	101.28	110.55
1	B	874	SER	N-CA-C	6.87	119.64	111.33
1	A	956	ASN	N-CA-C	6.79	120.93	112.24
1	A	410	TYR	N-CA-C	-6.66	100.63	110.48
1	A	1262	PRO	N-CA-C	6.64	118.80	110.70
1	B	5	GLU	N-CA-C	6.53	119.95	110.28
1	B	151	GLY	N-CA-C	-6.52	106.24	115.43
1	A	869	ASN	N-CA-C	6.37	121.05	113.16
1	A	889	TYR	N-CA-C	6.29	119.71	109.59
1	B	1273	ALA	N-CA-C	-6.23	104.57	111.36
1	A	828	ASP	N-CA-C	-6.19	102.20	110.55
1	A	409	PRO	N-CA-C	6.17	121.19	111.38
1	B	1289	ALA	N-CA-C	6.15	115.56	108.49
1	B	869	ASN	N-CA-C	6.10	120.58	113.20
1	B	743	TYR	N-CA-C	-6.09	101.26	110.28
1	B	1228	LYS	N-CA-C	6.05	118.64	107.99
1	A	743	TYR	N-CA-C	-5.99	100.97	109.96
1	B	828	ASP	N-CA-C	-5.92	102.56	110.55
1	A	874	SER	N-CA-C	5.90	118.19	111.11
1	A	435	SER	N-CA-C	5.84	117.98	108.76
1	A	1137	ASN	N-CA-C	5.82	119.45	111.54
1	A	151	GLY	N-CA-C	-5.80	107.25	115.43
1	B	431	ALA	N-CA-C	5.79	119.64	112.24
1	B	504	VAL	N-CA-C	5.70	115.89	110.42
1	B	889	TYR	N-CA-C	5.67	118.72	109.59
1	A	456	GLY	N-CA-C	-5.66	102.47	111.18
1	A	1108	LYS	CA-C-N	5.65	126.90	119.84
1	A	1108	LYS	C-N-CA	5.65	126.90	119.84
1	B	1209	GLU	N-CA-C	5.63	117.86	109.25
1	B	408	ILE	CA-C-N	5.61	125.51	119.85
1	B	408	ILE	C-N-CA	5.61	125.51	119.85
1	B	1137	ASN	N-CA-C	5.58	119.14	111.54
1	B	409	PRO	N-CA-C	5.53	120.17	111.38
1	A	1174	LEU	N-CA-C	5.51	117.09	111.14
1	B	337	ALA	CB-CA-C	-5.51	110.21	116.54
1	B	1285	HIS	CB-CA-C	-5.50	108.44	116.53
1	B	435	SER	N-CA-C	5.50	117.62	108.99
1	A	5	GLU	N-CA-C	5.49	118.88	110.20
1	A	713	LYS	N-CA-C	5.43	117.34	108.76
1	B	1070	THR	N-CA-C	-5.39	106.75	113.55
1	A	112	CYS	N-CA-C	-5.28	106.09	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	ASN	CA-C-N	5.24	125.29	119.32
1	B	196	ASN	C-N-CA	5.24	125.29	119.32
1	B	387	THR	N-CA-C	5.20	118.89	112.54
1	A	1209	GLU	N-CA-C	5.19	117.19	109.25
1	A	1011	LEU	CA-C-N	5.16	126.30	119.84
1	A	1011	LEU	C-N-CA	5.16	126.30	119.84
1	A	149	CYS	N-CA-C	5.12	119.48	112.68
1	A	543	ALA	N-CA-C	5.11	117.24	111.11
1	A	40	LYS	N-CA-C	5.10	118.04	110.14
1	A	872	ASP	CB-CA-C	-5.09	110.72	116.63
1	A	591	VAL	N-CA-C	5.08	115.62	108.36
1	A	764	VAL	N-CA-C	5.07	117.12	108.86
1	A	1070	THR	N-CA-C	-5.06	107.18	113.55
1	A	1123	SER	N-CA-C	-5.06	106.80	113.17
1	A	433	VAL	N-CA-C	5.05	115.74	108.93
1	B	1026	ASP	N-CA-C	-5.02	106.93	113.16

There are no chirality outliers.

There are no planarity outliers.

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	9963	0	9972	230	0
1	B	9877	0	9888	228	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	30	0	0	1	0
3	B	25	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	8	0	0	1	0
5	B	8	0	0	1	0
6	A	53	0	28	2	0
6	B	53	0	26	3	0
7	A	12	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	12	0	4	0	0
8	A	667	0	0	7	0
8	B	724	0	0	8	0
All	All	21444	0	19922	454	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 11.

All (454) 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)
6:B:3003:FAD:C3B	6:B:3003:FAD:C2B	1.79	1.41
1:B:3:ALA:HB1	1:B:227:ARG:H	1.16	1.05
1:A:3:ALA:HB1	1:A:227:ARG:H	1.24	1.01
1:B:123:MET:HE1	1:B:138:ILE:HG23	1.44	0.99
1:B:646:THR:HG22	1:B:647:GLY:H	1.28	0.97
1:A:646:THR:HG22	1:A:647:GLY:H	1.30	0.95
1:B:359:ASP:HA	1:B:434:THR:HG21	1.54	0.89
1:B:3:ALA:HB1	1:B:227:ARG:N	1.86	0.89
1:B:130:GLN:HE21	1:B:132:GLU:H	1.16	0.88
1:B:785:ASN:HD21	1:B:786:ARG:NH1	1.73	0.86
1:B:252:PRO:HG3	1:B:400:GLU:HG2	1.58	0.85
1:A:785:ASN:HD21	1:A:786:ARG:HH11	1.24	0.85
1:B:1088:GLN:HG2	1:B:1133:TYR:CD1	2.13	0.84
1:B:785:ASN:HD21	1:B:786:ARG:HH11	1.21	0.84
1:A:263:ILE:HG22	1:A:267:MET:HE2	1.59	0.84
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.12	0.83
1:A:359:ASP:HA	1:A:434:THR:HG21	1.58	0.83
1:A:130:GLN:HE21	1:A:132:GLU:H	1.29	0.81
1:A:555:ALA:HB3	1:A:1238:GLU:HG3	1.62	0.80
1:A:749:THR:HG22	1:A:812:LEU:HD23	1.63	0.80
1:A:939:GLU:HG2	1:A:977:TYR:CE2	2.17	0.79
1:B:1208:MET:HE1	1:B:1234:SER:HB3	1.65	0.78
1:A:557:VAL:HG12	1:A:1240:ARG:HG2	1.65	0.78
1:A:785:ASN:HD21	1:A:786:ARG:NH1	1.82	0.77
1:A:1180:MET:HE1	1:A:1266:LEU:HD12	1.66	0.77
1:B:321:GLN:HG2	1:B:413:GLU:OE2	1.85	0.77
1:B:932:ILE:O	1:B:1290:LYS:HE3	1.84	0.76
1:B:123:MET:HE2	1:B:142:PHE:CZ	2.21	0.76
1:B:785:ASN:ND2	1:B:786:ARG:HH11	1.82	0.76
1:B:650:ASN:HD21	1:B:778:LYS:NZ	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ALA:N	1:A:224:LYS:HZ1	1.85	0.75
1:A:1141:SER:OG	1:A:1143:GLU:HG2	1.87	0.75
1:B:123:MET:HE2	1:B:142:PHE:HZ	1.50	0.74
1:B:332:GLN:HA	1:B:332:GLN:HE21	1.53	0.74
1:A:785:ASN:ND2	1:A:786:ARG:HH11	1.86	0.74
1:B:650:ASN:HD21	1:B:778:LYS:HZ3	1.34	0.74
1:B:719:LEU:HD11	1:B:895:ARG:HB3	1.70	0.74
1:A:388:PHE:HA	1:A:396:LEU:HG	1.71	0.72
1:B:58:TYR:CE2	1:B:219:LYS:HG3	2.24	0.72
1:B:531:LEU:HA	1:B:540:PRO:HD2	1.73	0.71
1:B:749:THR:HG22	1:B:812:LEU:HD23	1.72	0.71
1:B:749:THR:HG22	1:B:812:LEU:CD2	2.20	0.71
1:B:939:GLU:HG2	1:B:977:TYR:CE2	2.24	0.71
1:B:1102:GLU:HB3	1:B:1103:PRO:HD3	1.72	0.71
1:A:749:THR:HG22	1:A:812:LEU:CD2	2.20	0.70
1:A:487:ALA:HA	1:A:1318:THR:HG23	1.73	0.69
1:A:3:ALA:HB1	1:A:227:ARG:N	2.05	0.69
1:B:1315:LEU:HA	1:B:1320:VAL:O	1.92	0.69
1:A:719:LEU:HD11	1:A:895:ARG:HB2	1.75	0.69
1:A:537:LYS:O	1:A:538:LEU:HB3	1.93	0.67
1:A:61:LEU:O	1:A:62:GLN:HG3	1.94	0.67
1:A:1124:ALA:HB3	1:B:1134:LYS:HD3	1.77	0.67
1:B:1180:MET:HE1	1:B:1266:LEU:HD12	1.75	0.67
1:B:271:ASN:CG	1:B:683:ARG:HD3	2.19	0.67
1:B:1203:LEU:CD2	1:B:1208:MET:HE3	2.25	0.66
1:B:1290:LYS:O	1:B:1290:LYS:HG2	1.94	0.66
1:A:375:SER:HB3	1:A:378:THR:OG1	1.95	0.66
1:B:241:MET:HE2	1:B:283:ILE:HG21	1.76	0.65
1:A:679:GLN:NE2	1:A:683:ARG:HH22	1.94	0.65
1:A:1279:ARG:HH21	1:A:1290:LYS:HD3	1.61	0.65
1:B:123:MET:HE3	1:B:159:PHE:CD2	2.31	0.65
1:A:1141:SER:HG	1:A:1143:GLU:HG2	1.60	0.65
1:A:666:ILE:CD1	1:A:807:VAL:HG13	2.27	0.64
1:B:426:ARG:HD3	1:B:1212:HIS:CG	2.32	0.64
1:B:271:ASN:HB3	1:B:683:ARG:HH11	1.62	0.64
1:B:646:THR:HG22	1:B:647:GLY:N	2.07	0.64
1:A:646:THR:HG22	1:A:647:GLY:N	2.09	0.63
1:B:272:MET:HE2	1:B:272:MET:HA	1.81	0.63
1:B:531:LEU:CA	1:B:540:PRO:HD2	2.28	0.62
1:A:646:THR:HG23	8:A:7667:HOH:O	1.99	0.62
1:B:1082:SER:HB2	3:B:6003:PO4:O2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:ASN:HD22	1:B:601:ASN:H	1.48	0.62
1:A:93:ASN:OD1	1:A:95:GLN:HG3	1.99	0.61
1:B:715:GLU:OE2	1:B:895:ARG:HD2	2.01	0.61
1:A:882:LEU:O	1:A:954:HIS:HE1	1.83	0.61
1:A:856:VAL:HG12	1:A:945:ASN:OD1	2.01	0.60
6:B:3003:FAD:C3B	6:B:3003:FAD:O2B	2.45	0.60
1:B:321:GLN:HG2	1:B:413:GLU:CD	2.27	0.60
1:B:544:SER:HB2	1:B:994:LYS:HG3	1.84	0.60
1:B:123:MET:HE3	1:B:159:PHE:CG	2.38	0.59
1:A:240:THR:OG1	1:A:243:GLU:HG3	2.02	0.59
1:B:603:LEU:HD21	1:B:821:ARG:NH2	2.18	0.59
1:A:1004:LYS:HG3	1:A:1155:TYR:CE2	2.38	0.59
1:B:271:ASN:HB3	1:B:683:ARG:NH1	2.17	0.59
1:B:650:ASN:ND2	1:B:778:LYS:NZ	2.49	0.59
1:B:1208:MET:HE1	1:B:1234:SER:CB	2.32	0.59
1:B:761:GLU:HA	1:B:788:VAL:HG13	1.85	0.59
1:A:616:LYS:HD3	1:A:659:GLU:HB3	1.85	0.58
1:B:812:LEU:HD21	1:B:823:VAL:O	2.03	0.58
1:A:785:ASN:C	1:A:785:ASN:HD22	2.12	0.58
1:A:1311:GLN:HB2	1:A:1317:VAL:HG13	1.85	0.58
1:B:885:MET:HE2	1:B:894:ILE:HD11	1.86	0.58
1:A:601:ASN:HD22	1:A:601:ASN:H	1.51	0.58
1:A:271:ASN:OD1	1:A:683:ARG:CZ	2.51	0.58
1:A:812:LEU:HD11	1:A:823:VAL:C	2.27	0.58
1:A:272:MET:HA	1:A:272:MET:HE2	1.84	0.58
1:B:650:ASN:ND2	1:B:778:LYS:HZ3	2.00	0.58
1:A:164:LYS:HB2	1:A:164:LYS:NZ	2.19	0.57
1:B:478:ASN:HD21	1:B:480:GLU:HG3	1.68	0.57
1:B:130:GLN:HE21	1:B:132:GLU:N	1.96	0.57
1:B:1088:GLN:HG2	1:B:1133:TYR:CE1	2.39	0.57
1:A:911:PHE:O	1:A:912:ARG:C	2.46	0.57
1:A:370:LYS:HE2	1:A:383:ARG:HE	1.69	0.57
1:B:486:CYS:HA	1:B:512:LEU:HD22	1.85	0.57
1:B:606:ARG:HD3	1:B:679:GLN:HA	1.86	0.57
1:B:646:THR:HG23	8:B:7280:HOH:O	2.05	0.57
1:B:886:ASP:OD1	1:B:1004:LYS:NZ	2.38	0.57
1:B:911:PHE:O	1:B:912:ARG:C	2.47	0.57
1:B:812:LEU:HD11	1:B:823:VAL:C	2.29	0.57
1:A:306:LEU:HD23	1:A:306:LEU:O	2.05	0.56
1:B:749:THR:O	1:B:812:LEU:HD22	2.05	0.56
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:O	1:A:219:LYS:HB3	2.06	0.56
1:B:446:ILE:HG12	1:B:446:ILE:O	2.04	0.56
1:B:478:ASN:C	1:B:478:ASN:HD22	2.12	0.56
1:B:954:HIS:CD2	1:B:954:HIS:H	2.23	0.56
1:B:4:ASP:HB3	8:B:7379:HOH:O	2.04	0.56
1:B:132:GLU:HB3	1:B:164:LYS:CG	2.36	0.56
1:B:446:ILE:HG12	1:B:477:TRP:H	1.69	0.56
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.87	0.56
1:A:1311:GLN:HG3	1:A:1317:VAL:CG1	2.36	0.55
1:B:882:LEU:O	1:B:954:HIS:HE1	1.89	0.55
1:B:246:ASP:OD2	1:B:376:ARG:HD2	2.06	0.55
1:A:135:VAL:HG23	1:A:165:ASP:HB3	1.88	0.55
1:B:577:LEU:HD12	1:B:578:PRO:HD2	1.88	0.55
1:A:531:LEU:HD12	1:A:534:MET:SD	2.47	0.55
1:A:1180:MET:HE3	1:A:1263:PRO:HG3	1.87	0.55
1:B:458:MET:HE2	1:B:511:THR:HG21	1.88	0.55
1:B:666:ILE:CD1	1:B:807:VAL:HG13	2.37	0.55
1:B:1250:LYS:CE	1:B:1251:ARG:HG3	2.35	0.55
1:A:59:ASP:HB3	1:A:62:GLN:HB2	1.87	0.55
1:B:640:VAL:HG23	1:B:640:VAL:O	2.07	0.55
1:B:55:ILE:HG23	1:B:83:VAL:CG1	2.36	0.55
1:B:900:ILE:N	1:B:900:ILE:HD12	2.21	0.55
1:A:58:TYR:OH	1:A:63:ASN:HA	2.07	0.54
1:B:135:VAL:HG23	1:B:165:ASP:HA	1.89	0.54
1:B:132:GLU:O	1:B:164:LYS:HE3	2.08	0.54
1:B:998:LEU:HD13	1:B:1161:GLU:HB2	1.89	0.54
1:A:58:TYR:CE2	1:A:219:LYS:HG3	2.43	0.54
1:B:370:LYS:HD2	1:B:407:GLU:OE1	2.08	0.54
1:B:55:ILE:HG23	1:B:83:VAL:HG13	1.90	0.54
1:B:164:LYS:HB2	1:B:164:LYS:NZ	2.22	0.54
1:B:332:GLN:HE21	1:B:332:GLN:CA	2.18	0.54
1:B:887:ASN:O	1:B:1004:LYS:HE2	2.08	0.54
1:B:82:HIS:CE1	1:B:218:LEU:HD13	2.43	0.53
1:B:296:ILE:CD1	1:B:314:GLU:HG3	2.39	0.53
1:B:605:LEU:C	1:B:605:LEU:HD23	2.33	0.53
1:B:332:GLN:HA	1:B:332:GLN:NE2	2.21	0.53
1:B:402:ILE:C	1:B:402:ILE:HD12	2.34	0.53
1:A:666:ILE:HD12	1:A:807:VAL:HG13	1.89	0.53
1:A:469:THR:N	1:A:470:PRO:HD2	2.23	0.53
1:B:1107:LYS:C	1:B:1109:PRO:HD3	2.33	0.53
1:A:508:ARG:CZ	1:A:1315:LEU:HD11	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1107:LYS:C	1:A:1108:LYS:HD2	2.34	0.53
1:A:972:ILE:HG13	1:A:973:ALA:N	2.24	0.53
1:A:885:MET:HE2	1:A:894:ILE:HD11	1.91	0.53
1:A:874:SER:HB3	1:A:900:ILE:HG21	1.90	0.52
1:B:1317:VAL:HG23	1:B:1318:THR:N	2.24	0.52
1:A:306:LEU:HD23	1:A:306:LEU:C	2.34	0.52
1:A:785:ASN:HD22	1:A:786:ARG:N	2.07	0.52
1:A:1082:SER:HB2	3:A:6002:PO4:O4	2.09	0.52
1:B:923:ALA:HA	1:B:926:TRP:NE1	2.25	0.52
1:A:749:THR:O	1:A:812:LEU:HD22	2.08	0.52
1:B:388:PHE:HA	1:B:396:LEU:HG	1.92	0.52
1:B:785:ASN:C	1:B:785:ASN:HD22	2.15	0.52
1:B:1091:TYR:O	1:B:1095:GLN:HG2	2.09	0.52
1:B:1053:ALA:O	1:B:1098:LEU:HD11	2.10	0.52
1:A:900:ILE:N	1:A:900:ILE:HD12	2.25	0.52
1:A:124:TYR:OH	1:A:208:GLU:HG3	2.09	0.52
1:B:240:THR:OG1	1:B:243:GLU:HG3	2.10	0.51
1:A:111:GLN:NE2	1:A:150:THR:HA	2.25	0.51
1:A:555:ALA:O	1:A:1238:GLU:HA	2.10	0.51
1:A:581:ALA:O	1:A:585:GLN:HG3	2.09	0.51
1:A:667:ILE:HD13	1:A:687:ILE:HD13	1.92	0.51
1:B:153:ARG:C	1:B:153:ARG:HD2	2.35	0.51
1:B:62:GLN:OE1	1:B:64:LYS:HE3	2.10	0.51
1:B:157:GLN:HA	1:B:160:ARG:NH1	2.26	0.51
1:A:812:LEU:HD11	1:A:823:VAL:HG12	1.93	0.51
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.11	0.51
1:A:1221:THR:CG2	1:A:1227:TYR:HB2	2.41	0.51
1:B:666:ILE:HD11	1:B:807:VAL:HG13	1.91	0.51
1:A:163:ALA:C	1:A:165:ASP:H	2.19	0.51
1:A:217:ARG:C	1:A:219:LYS:H	2.18	0.51
1:B:601:ASN:HD22	1:B:601:ASN:N	2.07	0.51
1:A:487:ALA:CA	1:A:1318:THR:HG23	2.41	0.51
1:A:400:GLU:H	1:A:400:GLU:CD	2.20	0.50
1:A:601:ASN:HD22	1:A:601:ASN:N	2.09	0.50
1:A:812:LEU:CD1	1:A:823:VAL:HG12	2.40	0.50
1:A:267:MET:HE1	8:A:7168:HOH:O	2.10	0.50
1:A:695:ILE:HG23	1:A:700:ASP:HB3	1.92	0.50
1:B:467:LYS:HB2	1:B:492:GLU:CD	2.36	0.50
1:B:469:THR:N	1:B:470:PRO:HD2	2.26	0.50
1:B:764:VAL:O	1:B:791:VAL:HG22	2.10	0.50
1:B:132:GLU:HB3	1:B:164:LYS:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:NH1	1:A:675:PRO:HD2	2.27	0.50
1:A:253:ASP:OD2	1:A:253:ASP:N	2.45	0.50
1:B:969:ASP:O	1:B:972:ILE:HG12	2.12	0.50
1:A:321:GLN:HG2	1:A:413:GLU:OE1	2.12	0.50
1:A:995:LYS:NZ	1:A:1284:GLN:NE2	2.60	0.50
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.92	0.50
1:A:426:ARG:HD3	1:A:1212:HIS:CG	2.46	0.50
1:A:1054:LEU:O	1:A:1055:LYS:HB2	2.11	0.50
1:A:3:ALA:CB	1:A:227:ARG:H	2.11	0.50
1:A:478:ASN:ND2	1:A:480:GLU:H	2.10	0.50
1:B:481:LEU:C	1:B:481:LEU:HD23	2.37	0.50
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.93	0.49
1:A:1134:LYS:HD3	1:B:1124:ALA:HB3	1.92	0.49
1:B:426:ARG:O	1:B:426:ARG:HG2	2.11	0.49
1:B:1203:LEU:C	1:B:1203:LEU:HD23	2.37	0.49
1:A:1037:GLU:HB2	1:A:1043:HIS:CD2	2.47	0.49
1:B:761:GLU:HG3	1:B:788:VAL:HG13	1.93	0.49
1:B:1086:ASN:O	1:B:1090:VAL:HG23	2.11	0.49
1:B:785:ASN:HD22	1:B:786:ARG:N	2.10	0.49
1:A:1004:LYS:HG3	1:A:1155:TYR:HE2	1.77	0.49
1:A:537:LYS:O	1:A:538:LEU:CB	2.60	0.49
1:A:387:THR:O	1:A:396:LEU:HD21	2.12	0.49
1:A:1311:GLN:HG3	1:A:1317:VAL:HG13	1.93	0.49
1:B:733:GLU:OE1	1:B:845:LYS:HE2	2.12	0.49
1:A:1003:THR:HG22	1:A:1266:LEU:HD21	1.94	0.49
1:B:655:PHE:HE2	1:B:814:LEU:HD23	1.77	0.49
1:B:909:THR:OG1	1:B:910:ALA:N	2.43	0.49
1:A:164:LYS:HB2	1:A:164:LYS:HZ2	1.77	0.49
1:A:311:LEU:O	1:A:315:ILE:HG13	2.13	0.49
1:B:733:GLU:HG2	1:B:845:LYS:HG2	1.95	0.49
1:B:749:THR:HG22	1:B:812:LEU:HD22	1.93	0.49
1:B:812:LEU:HD11	1:B:824:ARG:N	2.27	0.49
1:A:1107:LYS:O	1:A:1108:LYS:HD2	2.13	0.49
1:B:1208:MET:CE	1:B:1234:SER:HB3	2.37	0.49
1:A:756:GLU:OE2	1:B:793:ARG:NH2	2.46	0.48
1:A:1180:MET:HE1	1:A:1266:LEU:CD1	2.39	0.48
1:B:266:GLU:O	1:B:270:LYS:HB2	2.13	0.48
1:A:605:LEU:HD23	1:A:605:LEU:C	2.38	0.48
1:A:954:HIS:H	1:A:954:HIS:CD2	2.30	0.48
1:B:422:GLN:HG2	1:B:424:SER:H	1.78	0.48
1:A:558:GLN:HB3	1:A:1192:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:GLU:CD	1:B:793:ARG:HH22	2.21	0.48
1:A:1287:ASP:O	1:A:1288:ASN:HB2	2.11	0.48
1:A:431:ALA:HB2	1:A:501:GLY:HA3	1.93	0.48
1:B:601:ASN:H	1:B:601:ASN:ND2	2.11	0.48
1:B:880:ARG:HD2	1:B:914:PHE:O	2.14	0.48
1:A:785:ASN:ND2	1:A:786:ARG:HG2	2.29	0.48
1:A:794:MET:HE3	1:A:1038:MET:HB3	1.96	0.48
1:A:1132:PHE:CG	1:B:1126:SER:HB2	2.48	0.48
1:A:62:GLN:O	1:A:64:LYS:HG3	2.13	0.48
1:A:711:GLU:HA	1:A:899:ARG:CD	2.44	0.48
1:B:1214:SER:HB3	1:B:1220:HIS:NE2	2.29	0.48
1:B:1313:THR:O	1:B:1317:VAL:HG22	2.14	0.48
1:A:481:LEU:C	1:A:481:LEU:HD23	2.38	0.48
1:B:164:LYS:O	1:B:165:ASP:HB2	2.14	0.48
1:B:531:LEU:CB	1:B:540:PRO:HD2	2.43	0.47
1:A:667:ILE:CD1	1:A:687:ILE:HD13	2.43	0.47
1:B:245:LEU:HD22	1:B:375:SER:HA	1.95	0.47
1:B:1045:LYS:HE3	1:B:1190:ILE:HG21	1.97	0.47
1:B:646:THR:HG21	8:B:7201:HOH:O	2.14	0.47
1:A:251:HIS:C	1:A:253:ASP:H	2.23	0.47
1:A:552:ASP:HB2	1:A:1237:ILE:HD13	1.95	0.47
1:A:711:GLU:HA	1:A:899:ARG:HD3	1.97	0.47
1:A:1203:LEU:HD23	1:A:1203:LEU:C	2.40	0.47
1:B:528:ARG:HH11	1:B:528:ARG:HG2	1.80	0.47
1:A:217:ARG:C	1:A:219:LYS:N	2.72	0.47
1:B:874:SER:HB3	1:B:900:ILE:HG21	1.96	0.47
1:B:794:MET:HE3	1:B:1038:MET:HB3	1.97	0.47
1:B:1007:ILE:O	1:B:1008:SER:CB	2.63	0.47
1:A:557:VAL:HG12	1:A:1240:ARG:CG	2.41	0.47
1:A:236:ILE:HD12	1:A:247:LEU:HD11	1.97	0.46
1:B:572:MET:HE2	8:B:7077:HOH:O	2.14	0.46
1:A:372:THR:HG21	1:A:404:LEU:HD23	1.96	0.46
1:B:657:LYS:O	1:B:658:ASP:HB2	2.14	0.46
1:A:370:LYS:CE	1:A:383:ARG:HH21	2.29	0.46
1:B:441:PHE:CZ	1:B:526:LEU:HD11	2.50	0.46
1:A:5:GLU:HG2	8:A:7612:HOH:O	2.16	0.46
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.30	0.46
1:B:531:LEU:HD23	1:B:531:LEU:C	2.41	0.46
1:B:641:PRO:HG2	1:B:780:LEU:HA	1.96	0.46
1:A:487:ALA:CB	1:A:1318:THR:HG23	2.45	0.46
1:B:637:ALA:O	1:B:640:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:964:LEU:HB3	1:A:965:PRO:HD3	1.97	0.46
1:A:1007:ILE:O	1:A:1008:SER:CB	2.64	0.46
1:B:1209:GLU:O	1:B:1298:PRO:HG3	2.16	0.45
1:A:251:HIS:C	1:A:253:ASP:N	2.72	0.45
1:A:812:LEU:HD21	1:A:823:VAL:O	2.16	0.45
1:B:231:GLU:OE2	1:B:680:ARG:NH1	2.49	0.45
1:B:545:ALA:HB2	1:B:993:TRP:HB2	1.97	0.45
1:A:646:THR:HG21	8:A:7078:HOH:O	2.15	0.45
1:A:1069:ASN:C	1:A:1069:ASN:HD22	2.24	0.45
1:A:1221:THR:HG22	1:A:1227:TYR:HB2	1.97	0.45
1:B:646:THR:CG2	1:B:647:GLY:H	2.09	0.45
1:B:1281:ALA:O	1:B:1284:GLN:HB3	2.16	0.45
1:B:1318:THR:HG22	1:B:1320:VAL:H	1.80	0.45
1:B:371:LEU:HD11	1:B:384:MET:HE3	1.99	0.45
1:B:1250:LYS:HE3	1:B:1251:ARG:HG3	1.97	0.45
1:A:909:THR:OG1	1:A:910:ALA:N	2.42	0.45
1:B:296:ILE:HD11	1:B:314:GLU:HG3	1.98	0.45
1:B:875:ARG:O	1:B:879:GLU:HG3	2.16	0.45
1:B:711:GLU:HA	1:B:899:ARG:HD2	1.97	0.45
1:B:812:LEU:HD11	1:B:823:VAL:HG12	1.98	0.45
1:B:1252:ALA:HB3	1:B:1256:SER:O	2.17	0.45
1:A:255:LYS:HG3	1:A:274:PHE:CD1	2.52	0.45
1:B:263:ILE:HG22	1:B:267:MET:HE2	1.98	0.45
1:B:478:ASN:C	1:B:478:ASN:ND2	2.75	0.45
1:A:256:LEU:HD22	1:A:278:VAL:CG1	2.47	0.45
1:A:373:LEU:HD22	1:A:397:LEU:HD11	1.98	0.45
1:A:749:THR:C	1:A:812:LEU:HD22	2.42	0.45
1:A:529:ALA:HB3	1:A:531:LEU:HD23	1.99	0.45
1:B:606:ARG:CD	1:B:679:GLN:HA	2.46	0.45
1:B:964:LEU:HB3	1:B:965:PRO:HD3	1.97	0.45
1:B:1110:THR:O	1:B:1111:GLY:C	2.60	0.45
1:B:751:ALA:H	1:B:812:LEU:HD21	1.82	0.45
1:A:64:LYS:NZ	1:A:64:LYS:HB3	2.32	0.44
1:A:751:ALA:H	1:A:812:LEU:HD21	1.82	0.44
1:B:263:ILE:HD11	6:B:3003:FAD:H3B	1.99	0.44
1:A:130:GLN:O	1:A:133:PRO:HD3	2.17	0.44
1:A:504:VAL:HG23	1:A:505:GLU:N	2.33	0.44
1:B:123:MET:HE3	1:B:159:PHE:HB3	1.99	0.44
1:B:557:VAL:HG22	1:B:1240:ARG:HG2	1.99	0.44
1:B:749:THR:C	1:B:812:LEU:HD22	2.43	0.44
1:B:711:GLU:HA	1:B:899:ARG:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:986:LYS:O	1:B:990:GLU:HG3	2.17	0.44
1:A:1088:GLN:NE2	8:A:7582:HOH:O	2.49	0.44
1:A:1314:THR:O	1:A:1315:LEU:HB2	2.17	0.44
1:B:130:GLN:NE2	1:B:132:GLU:H	1.99	0.44
1:B:400:GLU:HB2	8:B:7626:HOH:O	2.18	0.44
1:B:939:GLU:CG	1:B:977:TYR:CE2	2.97	0.44
1:A:3:ALA:N	1:A:224:LYS:NZ	2.60	0.44
1:A:58:TYR:CZ	1:A:63:ASN:HA	2.52	0.44
1:A:349:GLY:C	6:A:2003:FAD:H5'1	2.42	0.44
1:A:952:LEU:HD23	1:A:958:LYS:HA	2.00	0.44
1:A:1086:ASN:O	1:A:1090:VAL:HG23	2.18	0.44
1:B:872:ASP:CG	1:B:873:LEU:H	2.25	0.44
1:B:1264:LEU:C	1:B:1264:LEU:HD23	2.43	0.44
1:A:1034:GLY:HA3	8:A:7049:HOH:O	2.17	0.44
1:A:1088:GLN:HG2	1:A:1133:TYR:CE1	2.50	0.44
1:B:753:PRO:HD3	1:B:816:ALA:HB1	1.99	0.44
1:A:880:ARG:HD2	1:A:914:PHE:O	2.18	0.44
1:A:939:GLU:HG2	1:A:977:TYR:CZ	2.52	0.44
1:A:962:PHE:CE2	1:A:965:PRO:HD3	2.52	0.44
1:B:812:LEU:CD1	1:B:823:VAL:HG12	2.48	0.44
1:A:95:GLN:OE1	1:A:96:LYS:HB2	2.17	0.43
1:A:211:PHE:CD2	1:A:216:LEU:HD13	2.53	0.43
1:A:641:PRO:HG2	1:A:780:LEU:HA	1.99	0.43
1:A:767:GLN:HG3	1:A:801:LYS:HB2	1.99	0.43
1:B:793:ARG:HG2	8:B:7042:HOH:O	2.18	0.43
1:A:324:GLU:HB2	1:A:411:SER:CB	2.48	0.43
1:B:128:ARG:HB3	1:B:128:ARG:NH1	2.33	0.43
1:A:503:MET:HG2	1:A:1302:GLU:OE2	2.18	0.43
1:A:315:ILE:HD13	1:A:327:ARG:HG2	1.99	0.43
1:A:751:ALA:N	1:A:812:LEU:HD21	2.33	0.43
1:B:459:ALA:C	1:B:461:ARG:H	2.26	0.43
1:B:1034:GLY:HA3	8:B:7040:HOH:O	2.19	0.43
1:A:402:ILE:C	1:A:402:ILE:HD12	2.44	0.43
1:A:601:ASN:H	1:A:601:ASN:ND2	2.16	0.43
1:A:601:ASN:O	1:A:821:ARG:HD2	2.19	0.43
1:B:151:GLY:HA2	1:B:1200:VAL:HG21	1.99	0.43
1:B:153:ARG:N	1:B:154:PRO:HD2	2.34	0.43
1:B:751:ALA:N	1:B:812:LEU:HD21	2.34	0.43
1:B:1088:GLN:CG	1:B:1133:TYR:CD1	2.94	0.43
1:B:504:VAL:HG23	1:B:505:GLU:N	2.34	0.43
1:B:357:ILE:CD1	1:B:429:ASP:HA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:PHE:HA	1:A:396:LEU:CG	2.44	0.43
1:A:753:PRO:HD3	1:A:816:ALA:HB1	1.99	0.43
1:B:29:TYR:CE1	1:B:33:LYS:HG2	2.54	0.43
1:B:1300:THR:O	1:B:1304:ILE:HG13	2.18	0.43
1:A:3:ALA:HA	1:A:226:LEU:HD22	2.00	0.43
1:A:153:ARG:HD2	1:A:153:ARG:C	2.44	0.42
1:A:616:LYS:HG2	1:A:692:LEU:HD11	2.02	0.42
1:A:688:THR:HG23	8:A:7329:HOH:O	2.19	0.42
1:A:872:ASP:CG	1:A:873:LEU:H	2.26	0.42
1:B:252:PRO:CG	1:B:400:GLU:HG2	2.39	0.42
1:B:785:ASN:ND2	1:B:786:ARG:HG2	2.34	0.42
1:B:1151:HIS:NE2	1:B:1251:ARG:HB3	2.33	0.42
1:A:644:ASN:O	1:A:653:THR:HA	2.20	0.42
1:A:1088:GLN:HG2	1:A:1133:TYR:CG	2.51	0.42
1:A:1264:LEU:C	1:A:1264:LEU:HD23	2.44	0.42
1:B:82:HIS:NE2	1:B:218:LEU:HD13	2.33	0.42
1:B:256:LEU:HD22	1:B:278:VAL:HG13	2.00	0.42
1:A:666:ILE:HD11	1:A:807:VAL:CG1	2.49	0.42
1:A:926:TRP:O	1:A:930:VAL:HG23	2.19	0.42
1:B:1300:THR:HB	1:B:1301:PRO:HD2	2.02	0.42
1:A:698:ILE:O	1:A:702:ILE:HG13	2.20	0.42
1:A:1143:GLU:OE1	1:A:1143:GLU:N	2.48	0.42
1:A:1250:LYS:CE	1:A:1251:ARG:HG3	2.49	0.42
1:B:164:LYS:HB2	1:B:164:LYS:HZ2	1.85	0.42
1:A:749:THR:HG23	1:A:764:VAL:HG22	2.02	0.42
1:B:785:ASN:ND2	1:B:785:ASN:C	2.78	0.42
1:B:640:VAL:O	1:B:640:VAL:CG2	2.68	0.42
1:A:29:TYR:CZ	1:A:33:LYS:HG2	2.55	0.42
1:B:783:PRO:HB2	1:B:785:ASN:ND2	2.35	0.42
1:A:657:LYS:O	1:A:658:ASP:HB2	2.20	0.42
1:A:785:ASN:ND2	1:A:785:ASN:C	2.77	0.42
1:A:128:ARG:NE	1:A:208:GLU:HG2	2.35	0.41
1:A:336:LEU:HG	6:A:2003:FAD:C4	2.49	0.41
1:A:532:GLU:OE1	1:A:537:LYS:HA	2.20	0.41
1:B:94:THR:HG21	1:B:584:MET:HG2	2.02	0.41
1:B:508:ARG:HG2	1:B:508:ARG:HH11	1.84	0.41
1:B:3:ALA:O	1:B:4:ASP:C	2.63	0.41
1:A:321:GLN:HG2	1:A:413:GLU:CD	2.45	0.41
1:A:711:GLU:CA	1:A:899:ARG:HD3	2.50	0.41
1:B:785:ASN:ND2	1:B:786:ARG:NH1	2.49	0.41
1:A:1110:THR:O	1:A:1111:GLY:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1199:PHE:CE1	1:B:1267:ALA:HA	2.55	0.41
1:A:153:ARG:N	1:A:154:PRO:HD2	2.35	0.41
1:A:297:SER:HA	1:A:407:GLU:HA	2.03	0.41
1:B:1004:LYS:HE2	1:B:1004:LYS:HB3	1.86	0.41
1:A:32:ARG:HH22	1:A:676:GLU:CD	2.27	0.41
1:A:1198:ALA:HB3	1:A:1263:PRO:HB2	2.02	0.41
1:A:1279:ARG:NH2	1:A:1290:LYS:HD3	2.33	0.41
1:B:262:GLU:O	1:B:266:GLU:HG3	2.20	0.41
1:B:1291:GLN:HG2	1:B:1292:LEU:N	2.36	0.41
1:A:655:PHE:HE2	1:A:814:LEU:HD23	1.85	0.41
1:A:891:ILE:HA	1:A:892:PRO:HD3	1.91	0.41
1:A:1180:MET:HE3	1:A:1263:PRO:HB3	2.02	0.41
1:A:233:VAL:HG12	1:A:234:THR:N	2.35	0.41
1:A:539:ASP:HB3	1:A:542:PHE:CD1	2.56	0.41
1:A:708:TYR:CE1	1:A:902:LYS:HA	2.56	0.41
1:A:719:LEU:HD11	1:A:895:ARG:CB	2.46	0.41
1:A:911:PHE:C	1:A:911:PHE:CD2	2.99	0.41
1:A:1107:LYS:C	1:A:1109:PRO:HD3	2.46	0.41
1:A:46:GLY:CA	5:A:2002:FES:S1	3.09	0.41
1:A:116:THR:HB	1:A:117:PRO:HD3	2.03	0.41
1:A:610:SER:HB2	1:A:660:VAL:HG11	2.02	0.41
1:A:1105:LYS:HE3	1:A:1105:LYS:HB2	1.91	0.41
1:A:1214:SER:HB3	1:A:1220:HIS:NE2	2.36	0.41
1:B:116:THR:HB	1:B:117:PRO:HD3	2.03	0.41
1:B:130:GLN:O	1:B:133:PRO:HD3	2.21	0.41
1:B:311:LEU:O	1:B:315:ILE:HG13	2.21	0.41
1:B:418:SER:HB2	1:B:518:PHE:CD1	2.56	0.41
1:B:1102:GLU:HB3	1:B:1103:PRO:CD	2.48	0.41
1:B:1105:LYS:HA	1:B:1116:TRP:NE1	2.36	0.41
1:B:1200:VAL:O	1:B:1203:LEU:HB3	2.21	0.41
1:A:3:ALA:HA	1:A:226:LEU:CD2	2.51	0.41
1:A:764:VAL:O	1:A:791:VAL:HG22	2.21	0.41
1:A:1252:ALA:HB3	1:A:1256:SER:O	2.20	0.41
1:B:504:VAL:HG22	8:B:7235:HOH:O	2.21	0.41
1:B:531:LEU:HB2	1:B:540:PRO:HD2	2.03	0.41
1:B:868:GLY:HA3	1:B:907:SER:HA	2.04	0.41
1:A:132:GLU:O	1:A:164:LYS:HE3	2.21	0.40
1:B:123:MET:CE	1:B:138:ILE:HG23	2.33	0.40
1:A:221:THR:HA	1:A:222:PRO:HD3	1.93	0.40
1:A:783:PRO:HB3	1:B:1028:SER:HB3	2.03	0.40
1:A:1151:HIS:NE2	1:A:1251:ARG:HB3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:GLU:HG3	1:B:370:LYS:NZ	2.36	0.40
1:B:531:LEU:HG	1:B:540:PRO:HB2	2.03	0.40
1:A:371:LEU:HD11	1:A:384:MET:HE3	2.02	0.40
1:A:1311:GLN:CG	1:A:1317:VAL:HG13	2.52	0.40
1:B:905:LEU:O	1:B:906:PRO:C	2.64	0.40
1:A:134:THR:OG1	1:A:137:GLU:HG3	2.22	0.40
1:A:473:LEU:O	1:A:474:SER:CB	2.69	0.40
1:A:1091:TYR:O	1:A:1095:GLN:HG2	2.22	0.40
1:B:132:GLU:HB3	1:B:164:LYS:HD3	2.02	0.40
1:A:132:GLU:HB3	1:A:164:LYS:HD3	2.04	0.40
1:A:334:ARG:NH1	1:A:334:ARG:HB3	2.36	0.40
1:A:468:THR:C	1:A:470:PRO:HD2	2.47	0.40
1:A:539:ASP:HA	1:A:540:PRO:HD3	1.97	0.40
1:B:46:GLY:HA2	5:B:2002:FES:S1	2.62	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	1287/1331 (97%)	1220 (95%)	57 (4%)	10 (1%)	16	18
1	B	1273/1331 (96%)	1220 (96%)	46 (4%)	7 (0%)	24	29
All	All	2560/2662 (96%)	2440 (95%)	103 (4%)	17 (1%)	18	21

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	1008	SER
1	A	1287	ASP
1	A	1288	ASN

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Mol	Chain	Res	Type
1	B	4	ASP
1	B	1008	SER
1	A	62	GLN
1	A	912	ARG
1	B	912	ARG
1	B	1286	GLY
1	A	797	GLY
1	B	376	ARG
1	B	797	GLY
1	A	538	LEU
1	A	474	SER
1	B	1139	GLY
1	A	1012	PRO

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	1089/1123 (97%)	1063 (98%)	26 (2%)	43	59
1	B	1079/1123 (96%)	1056 (98%)	23 (2%)	47	63
All	All	2168/2246 (96%)	2119 (98%)	49 (2%)	44	60

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	VAL
1	A	95	GLN
1	A	99	PRO
1	A	164	LYS
1	A	208	GLU
1	A	247	LEU
1	A	253	ASP
1	A	255	LYS
1	A	256	LEU
1	A	400	GLU

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Mol	Chain	Res	Type
1	A	480	GLU
1	A	551	LYS
1	A	572	MET
1	A	601	ASN
1	A	650	ASN
1	A	743	TYR
1	A	744	LEU
1	A	785	ASN
1	A	807	VAL
1	A	939	GLU
1	A	1002	PRO
1	A	1031	LEU
1	A	1069	ASN
1	A	1085	LEU
1	A	1250	LYS
1	A	1276	ASP
1	B	83	VAL
1	B	164	LYS
1	B	199	ASP
1	B	255	LYS
1	B	306	LEU
1	B	332	GLN
1	B	383	ARG
1	B	478	ASN
1	B	480	GLU
1	B	494	GLN
1	B	601	ASN
1	B	650	ASN
1	B	743	TYR
1	B	744	LEU
1	B	785	ASN
1	B	807	VAL
1	B	869	ASN
1	B	939	GLU
1	B	1069	ASN
1	B	1072	PRO
1	B	1085	LEU
1	B	1250	LYS
1	B	1276	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	130	GLN
1	A	145	ASN
1	A	207	GLN
1	A	332	GLN
1	A	350	ASN
1	A	422	GLN
1	A	449	GLN
1	A	472	GLN
1	A	478	ASN
1	A	583	ASN
1	A	585	GLN
1	A	601	ASN
1	A	642	ASN
1	A	650	ASN
1	A	679	GLN
1	A	747	ASN
1	A	785	ASN
1	A	954	HIS
1	A	956	ASN
1	A	1069	ASN
1	A	1088	GLN
1	A	1284	GLN
1	B	63	ASN
1	B	130	GLN
1	B	145	ASN
1	B	223	GLN
1	B	251	HIS
1	B	260	ASN
1	B	332	GLN
1	B	350	ASN
1	B	386	HIS
1	B	478	ASN
1	B	601	ASN
1	B	642	ASN
1	B	650	ASN
1	B	705	ASN
1	B	747	ASN
1	B	785	ASN
1	B	869	ASN
1	B	954	HIS
1	B	1069	ASN
1	B	1086	ASN

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Mol	Chain	Res	Type
1	B	1148	ASN
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 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	$\# Z > 2$
7	URC	A	4001	-	13,13,13	2.08	5 (38%)	17,19,19	1.68	5 (29%)
5	FES	A	2001	1	0,4,4	-	-	-		
2	BCT	A	5001	-	3,3,3	0.55	0	2,3,3	1.56	0
3	PO4	A	6002	-	4,4,4	1.78	1 (25%)	6,6,6	0.47	0
3	PO4	A	6008	-	4,4,4	1.67	0	6,6,6	0.46	0
7	URC	B	4002	-	13,13,13	2.09	5 (38%)	17,19,19	1.67	4 (23%)
3	PO4	B	6005	-	4,4,4	1.71	0	6,6,6	0.47	0
5	FES	B	2001	1	0,4,4	-	-	-		
3	PO4	B	6003	-	4,4,4	1.83	2 (50%)	6,6,6	0.47	0
3	PO4	B	6010	-	4,4,4	1.71	0	6,6,6	0.46	0
3	PO4	B	6007	-	4,4,4	1.73	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FES	A	2002	1	0,4,4	-	-	-		
3	PO4	A	6001	-	4,4,4	1.71	0	6,6,6	0.47	0
6	FAD	B	3003	-	58,58,58	4.49	28 (48%)	85,89,89	2.13	29 (34%)
3	PO4	A	6004	-	4,4,4	1.66	0	6,6,6	0.46	0
3	PO4	A	6006	-	4,4,4	1.70	0	6,6,6	0.46	0
3	PO4	A	6009	-	4,4,4	1.65	0	6,6,6	0.46	0
6	FAD	A	2003	-	58,58,58	3.69	23 (39%)	85,89,89	2.11	31 (36%)
3	PO4	B	6011	-	4,4,4	1.71	1 (25%)	6,6,6	0.46	0
2	BCT	B	5002	-	3,3,3	0.59	0	2,3,3	1.54	0
5	FES	B	2002	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
7	URC	B	4002	-	-	-	0/2/2/2
6	FAD	B	3003	-	-	4/34/50/50	0/6/6/6
5	FES	B	2001	1	-	-	0/1/1/1
7	URC	A	4001	-	-	-	0/2/2/2
6	FAD	A	2003	-	-	1/34/50/50	0/6/6/6
5	FES	A	2001	1	-	-	0/1/1/1
5	FES	A	2002	1	-	-	0/1/1/1
5	FES	B	2002	1	-	-	0/1/1/1

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	3003	FAD	C5'-C4'	-22.77	1.20	1.51
6	A	2003	FAD	C5'-C4'	-16.53	1.29	1.51
6	B	3003	FAD	P-O3P	-14.09	1.44	1.59
6	A	2003	FAD	P-O3P	-12.66	1.45	1.59
6	B	3003	FAD	C2B-C3B	9.66	1.79	1.53
6	A	2003	FAD	O2B-C2B	-8.76	1.21	1.43
6	B	3003	FAD	O2B-C2B	-7.23	1.25	1.43
6	B	3003	FAD	C5B-C4B	-5.82	1.34	1.51
6	A	2003	FAD	C2B-C1B	-5.46	1.36	1.53
6	A	2003	FAD	C4X-N5	5.35	1.42	1.30
6	A	2003	FAD	C10-N1	5.28	1.43	1.33
6	B	3003	FAD	C4X-N5	5.12	1.41	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	3003	FAD	C10-N1	4.96	1.43	1.33
6	B	3003	FAD	O4B-C1B	4.77	1.53	1.42
6	A	2003	FAD	PA-O3P	4.77	1.64	1.59
7	A	4001	URC	C5-N7	-4.55	1.30	1.37
7	B	4002	URC	C5-N7	-4.40	1.30	1.37
6	B	3003	FAD	C2B-C1B	-4.29	1.40	1.53
6	A	2003	FAD	O5'-C5'	-4.01	1.29	1.44
6	A	2003	FAD	C1B-N9A	3.80	1.56	1.46
6	A	2003	FAD	O4B-C1B	3.71	1.50	1.42
6	B	3003	FAD	C6-C7	3.57	1.44	1.39
6	B	3003	FAD	P-O5'	-3.30	1.46	1.59
6	A	2003	FAD	C9A-N10	3.25	1.46	1.41
6	A	2003	FAD	C6-C7	3.25	1.44	1.39
6	B	3003	FAD	C9A-N10	3.24	1.46	1.41
6	B	3003	FAD	C9-C9A	3.20	1.44	1.39
7	B	4002	URC	C5-C6	3.17	1.51	1.41
6	A	2003	FAD	C9-C9A	3.11	1.44	1.39
7	A	4001	URC	C5-C6	3.09	1.51	1.41
6	B	3003	FAD	P-O1P	2.98	1.61	1.50
6	B	3003	FAD	C3B-C4B	2.96	1.60	1.53
7	A	4001	URC	C4-N9	-2.95	1.30	1.35
7	B	4002	URC	C4-N9	-2.88	1.30	1.35
6	B	3003	FAD	C5A-N7A	-2.84	1.33	1.39
7	B	4002	URC	C8-N7	-2.81	1.32	1.38
7	B	4002	URC	C8-N9	-2.81	1.32	1.38
7	A	4001	URC	C8-N9	-2.77	1.32	1.38
6	A	2003	FAD	C10-N10	2.75	1.43	1.37
6	B	3003	FAD	C10-N10	2.75	1.43	1.37
6	A	2003	FAD	C5A-N7A	-2.74	1.34	1.39
7	A	4001	URC	C8-N7	-2.64	1.32	1.38
6	A	2003	FAD	C9A-C5X	2.58	1.45	1.41
6	B	3003	FAD	C4A-N3A	2.56	1.39	1.34
6	A	2003	FAD	C4-N3	2.54	1.43	1.38
6	B	3003	FAD	PA-O5B	-2.51	1.49	1.59
6	B	3003	FAD	O5B-C5B	2.51	1.54	1.44
6	B	3003	FAD	C6-C5X	2.50	1.43	1.40
6	B	3003	FAD	O5'-C5'	-2.44	1.35	1.44
6	B	3003	FAD	PA-O2A	-2.38	1.44	1.55
6	A	2003	FAD	PA-O2A	-2.36	1.44	1.55
6	B	3003	FAD	C9A-C5X	2.33	1.45	1.41
6	B	3003	FAD	O3B-C3B	-2.29	1.37	1.43
6	A	2003	FAD	C4A-N9A	-2.24	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2003	FAD	C4A-N3A	2.22	1.38	1.34
6	B	3003	FAD	C4A-N9A	-2.18	1.33	1.37
3	B	6003	PO4	P-O4	-2.12	1.48	1.54
6	A	2003	FAD	C8-C7	2.11	1.46	1.40
3	B	6003	PO4	P-O2	-2.07	1.48	1.54
6	A	2003	FAD	C6-C5X	2.06	1.43	1.40
6	B	3003	FAD	C9-C8	2.05	1.42	1.39
3	A	6002	PO4	P-O4	-2.04	1.48	1.54
6	A	2003	FAD	O3B-C3B	-2.04	1.37	1.43
6	B	3003	FAD	C8-C7	2.03	1.45	1.40
3	B	6011	PO4	P-O3	-2.02	1.48	1.54

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	3003	FAD	N3A-C2A-N1A	-7.01	117.97	128.58
6	A	2003	FAD	N3A-C2A-N1A	-6.85	118.22	128.58
6	B	3003	FAD	O2P-P-O3P	5.18	121.27	107.27
6	A	2003	FAD	C5A-C4A-N3A	-5.08	119.72	126.72
6	B	3003	FAD	C5A-C4A-N3A	-4.96	119.89	126.72
6	B	3003	FAD	P-O5'-C5'	4.59	147.66	121.35
6	A	2003	FAD	C2A-N3A-C4A	4.47	122.75	111.83
6	B	3003	FAD	C2A-N3A-C4A	4.36	122.49	111.83
6	A	2003	FAD	O3B-C3B-C2B	4.22	125.35	111.82
6	A	2003	FAD	O2B-C2B-C1B	3.97	123.79	110.10
6	B	3003	FAD	C5B-C4B-C3B	3.70	128.52	115.21
6	B	3003	FAD	O4B-C1B-C2B	3.69	114.52	106.62
6	B	3003	FAD	N3A-C4A-N9A	3.60	133.29	127.17
6	A	2003	FAD	N3A-C4A-N9A	3.57	133.23	127.17
6	A	2003	FAD	C3B-C2B-C1B	-3.44	94.96	101.46
6	A	2003	FAD	C2'-C1'-N10	3.43	126.42	110.20
6	B	3003	FAD	C2'-C1'-N10	3.38	126.18	110.20
7	A	4001	URC	O13-C6-C5	-3.17	119.61	127.26
6	A	2003	FAD	C2B-C3B-C4B	3.16	108.72	102.61
6	A	2003	FAD	C4-N3-C2	-3.13	120.09	125.64
6	B	3003	FAD	C4'-C3'-C2'	3.11	118.74	113.57
6	B	3003	FAD	C4-N3-C2	-3.11	120.12	125.64
7	B	4002	URC	O13-C6-C5	-3.05	119.89	127.26
6	A	2003	FAD	C1'-C2'-C3'	3.02	117.85	109.66
6	B	3003	FAD	C1'-C2'-C3'	2.99	117.77	109.66
6	B	3003	FAD	C4X-C4-N3	2.97	120.81	113.25
6	A	2003	FAD	C4X-C4-N3	2.92	120.68	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	4002	URC	N3-C2-N1	2.89	120.29	115.74
6	A	2003	FAD	O4B-C1B-C2B	2.88	112.78	106.62
7	A	4001	URC	N3-C2-N1	2.88	120.27	115.74
6	A	2003	FAD	C4A-C5A-N7A	-2.87	107.30	110.58
6	A	2003	FAD	C4'-C3'-C2'	2.81	118.25	113.57
6	B	3003	FAD	C4A-C5A-N7A	-2.79	107.40	110.58
6	A	2003	FAD	O4B-C4B-C3B	-2.72	99.76	105.15
6	B	3003	FAD	C2A-N1A-C6A	2.70	123.17	118.73
6	B	3003	FAD	C5A-N7A-C8A	2.55	107.45	103.45
6	B	3003	FAD	C9A-C5X-N5	-2.54	119.76	122.45
6	A	2003	FAD	C5A-N7A-C8A	2.52	107.41	103.45
6	B	3003	FAD	O2B-C2B-C1B	2.51	118.76	110.10
6	A	2003	FAD	C2A-N1A-C6A	2.51	122.85	118.73
6	A	2003	FAD	C5B-C4B-C3B	2.51	124.24	115.21
6	A	2003	FAD	C9A-C5X-N5	-2.49	119.81	122.45
7	A	4001	URC	C6-N1-C2	-2.49	122.94	126.37
6	B	3003	FAD	C3B-C2B-C1B	-2.44	96.84	101.46
6	A	2003	FAD	N9A-C8A-N7A	-2.43	110.48	113.94
6	A	2003	FAD	O5'-C5'-C4'	2.41	115.78	109.36
6	B	3003	FAD	C8M-C8-C9	-2.39	115.35	119.57
7	B	4002	URC	C6-N1-C2	-2.39	123.07	126.37
6	B	3003	FAD	N9A-C8A-N7A	-2.38	110.56	113.94
6	B	3003	FAD	C5X-N5-C4X	2.37	121.92	118.09
6	B	3003	FAD	C10-C4X-N5	-2.29	120.13	124.81
6	B	3003	FAD	O4-C4-C4X	-2.29	120.49	126.53
6	A	2003	FAD	C10-C4X-N5	-2.28	120.16	124.81
6	A	2003	FAD	C8M-C8-C9	-2.26	115.58	119.57
6	B	3003	FAD	O3'-C3'-C2'	-2.25	103.81	108.93
6	A	2003	FAD	O4-C4-C4X	-2.24	120.61	126.53
6	A	2003	FAD	O2B-C2B-C3B	-2.24	104.63	111.82
6	A	2003	FAD	C5X-N5-C4X	2.24	121.71	118.09
6	B	3003	FAD	C10-N1-C2	2.21	121.64	116.85
6	A	2003	FAD	C10-N1-C2	2.21	121.63	116.85
6	B	3003	FAD	C4X-C10-N1	-2.19	119.23	124.59
7	B	4002	URC	C5-C4-N9	-2.17	105.24	108.31
7	A	4001	URC	O13-C6-N1	2.17	124.19	120.11
6	B	3003	FAD	C6-C5X-C9A	2.17	122.02	119.05
7	A	4001	URC	C5-C4-N9	-2.11	105.33	108.31
6	A	2003	FAD	C4X-C10-N1	-2.10	119.44	124.59
6	A	2003	FAD	C6-C5X-C9A	2.05	121.86	119.05
6	A	2003	FAD	O3'-C3'-C2'	-2.01	104.36	108.93
6	B	3003	FAD	C5'-C4'-C3'	2.01	116.01	112.22

There are no chirality outliers.

All (5) torsion outliers are listed below:

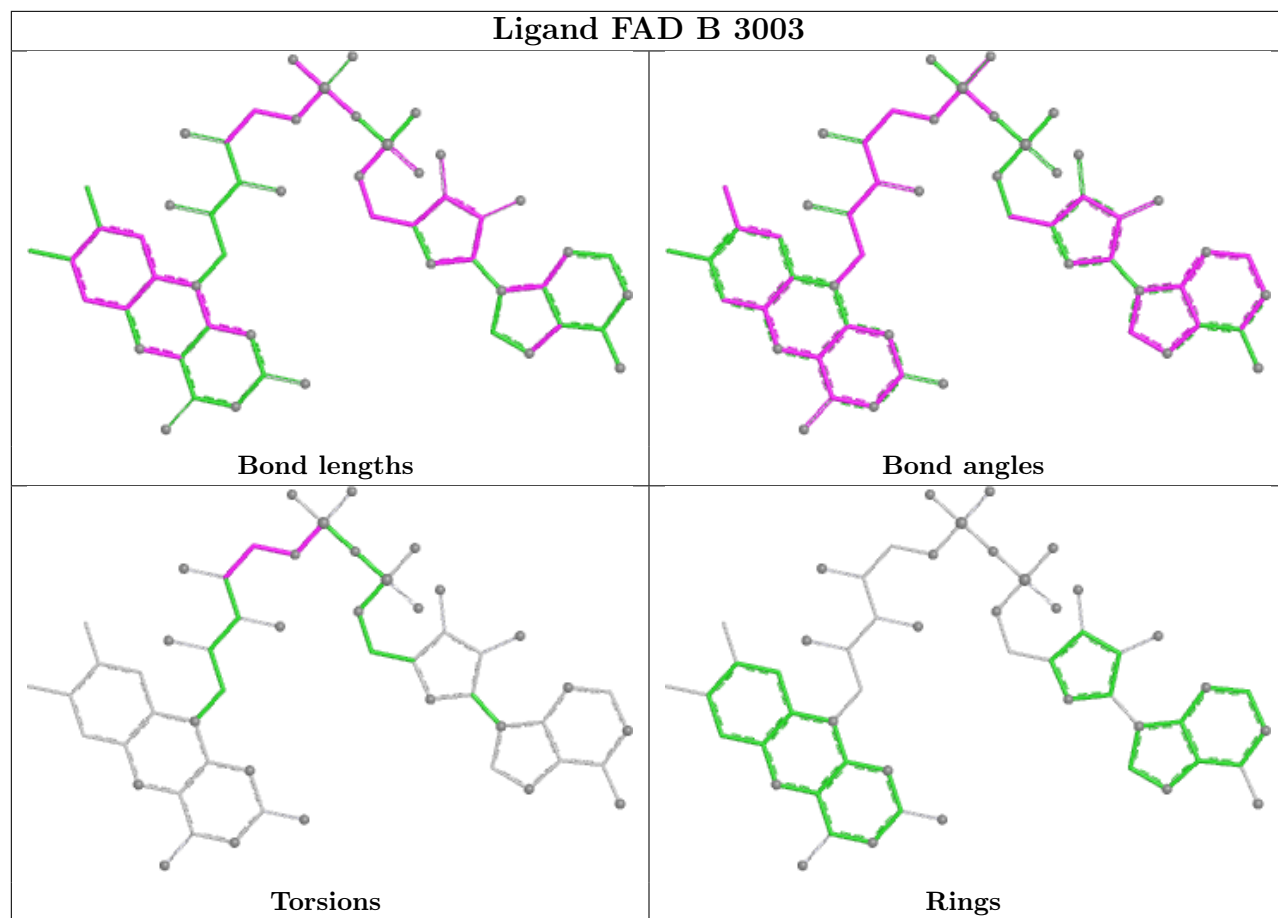
Mol	Chain	Res	Type	Atoms
6	B	3003	FAD	O4'-C4'-C5'-O5'
6	B	3003	FAD	C3'-C4'-C5'-O5'
6	B	3003	FAD	C5'-O5'-P-O1P
6	A	2003	FAD	C4'-C5'-O5'-P
6	B	3003	FAD	C4'-C5'-O5'-P

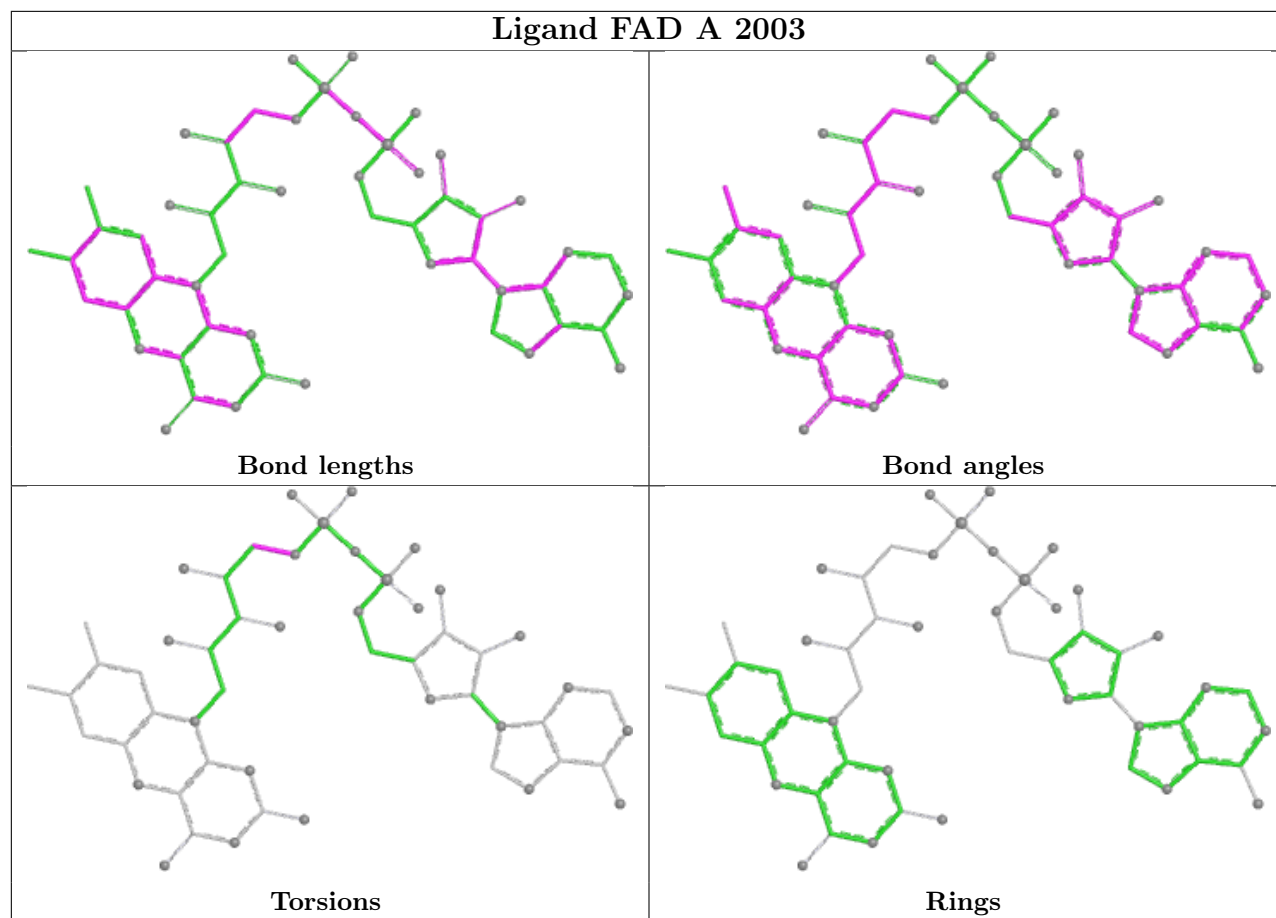
There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	6002	PO4	1	0
3	B	6003	PO4	1	0
5	A	2002	FES	1	0
6	B	3003	FAD	3	0
6	A	2003	FAD	2	0
5	B	2002	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	1291/1331 (96%)	-0.12	44 (3%)	48 50	14, 29, 57, 96	0
1	B	1281/1331 (96%)	-0.21	39 (3%)	52 54	13, 26, 53, 116	0
All	All	2572/2662 (96%)	-0.17	83 (3%)	50 52	13, 28, 55, 116	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	529	ALA	7.0
1	B	540	PRO	6.0
1	A	1289	ALA	5.9
1	A	61	LEU	5.7
1	B	531	LEU	5.6
1	B	553	PRO	5.6
1	B	541	THR	5.4
1	B	554	PRO	5.4
1	B	547	LEU	5.1
1	B	542	PHE	5.1
1	B	543	ALA	4.6
1	B	555	ALA	4.6
1	A	165	ASP	4.3
1	B	530	ASP	4.3
1	B	1320	VAL	4.2
1	B	1318	THR	4.1
1	B	544	SER	4.1
1	B	61	LEU	4.0
1	B	165	ASP	4.0
1	B	1288	ASN	3.9
1	A	1111	GLY	3.9
1	A	423	ALA	3.7
1	A	221	THR	3.6
1	B	546	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	424	SER	3.4
1	B	528	ARG	3.4
1	A	1288	ASN	3.3
1	B	191	SER	3.2
1	A	95	GLN	3.2
1	A	1290	LYS	3.1
1	B	1289	ALA	3.1
1	A	1318	THR	3.1
1	B	446	ILE	3.1
1	B	63	ASN	3.0
1	A	551	LYS	3.0
1	A	1287	ASP	3.0
1	A	192	PRO	3.0
1	B	3	ALA	3.0
1	B	1287	ASP	3.0
1	B	972	ILE	2.9
1	A	549	PHE	2.8
1	B	1286	GLY	2.8
1	B	164	LYS	2.8
1	B	545	ALA	2.8
1	A	550	GLN	2.7
1	A	426	ARG	2.7
1	B	1290	LYS	2.6
1	A	532	GLU	2.6
1	A	191	SER	2.6
1	A	3	ALA	2.6
1	B	552	ASP	2.5
1	A	1315	LEU	2.5
1	B	222	PRO	2.5
1	B	527	GLY	2.4
1	A	321	GLN	2.4
1	A	413	GLU	2.3
1	A	699	GLN	2.3
1	B	321	GLN	2.3
1	A	396	LEU	2.3
1	A	164	LYS	2.3
1	B	423	ALA	2.3
1	A	536	GLY	2.3
1	B	1111	GLY	2.3
1	A	60	ARG	2.2
1	A	812	LEU	2.2
1	A	566	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	250	GLN	2.2
1	A	972	ILE	2.2
1	A	253	ASP	2.2
1	B	400	GLU	2.2
1	B	1250	LYS	2.2
1	A	63	ASN	2.1
1	A	683	ARG	2.1
1	A	537	LYS	2.1
1	A	320	GLU	2.1
1	A	62	GLN	2.1
1	B	386	HIS	2.1
1	A	1110	THR	2.1
1	A	534	MET	2.0
1	A	386	HIS	2.0
1	A	531	LEU	2.0
1	A	64	LYS	2.0
1	A	475	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 [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
3	PO4	A	6009	5/5	0.71	0.12	85,86,86,87	0
3	PO4	A	6004	5/5	0.73	0.18	97,97,98,99	0
3	PO4	A	6006	5/5	0.82	0.14	80,80,81,81	0
3	PO4	B	6005	5/5	0.85	0.16	82,83,84,84	0
3	PO4	B	6010	5/5	0.86	0.16	69,70,71,71	0
3	PO4	A	6008	5/5	0.89	0.12	73,74,74,75	0

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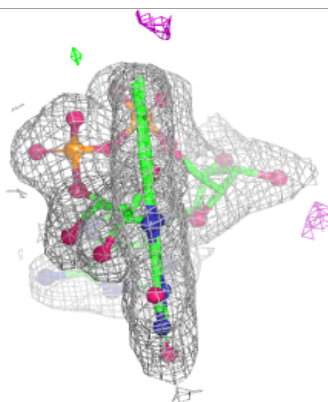
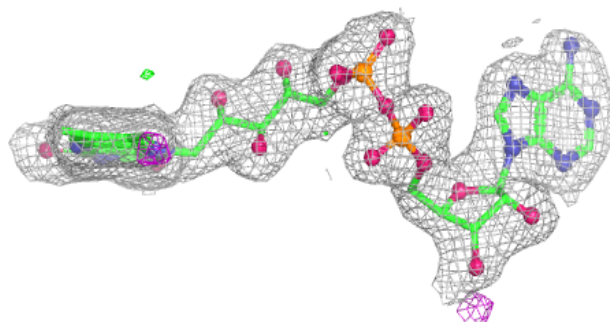
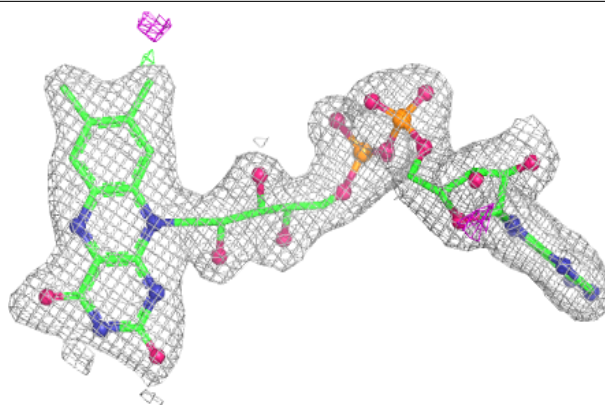
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	A	6001	5/5	0.89	0.11	46,48,51,51	0
3	PO4	B	6007	5/5	0.92	0.10	72,72,73,73	0
7	URC	A	4001	12/12	0.92	0.08	31,34,35,38	0
7	URC	B	4002	12/12	0.92	0.08	32,34,39,39	0
3	PO4	B	6011	5/5	0.95	0.12	49,50,51,53	0
6	FAD	A	2003	53/53	0.96	0.06	20,28,31,37	0
3	PO4	A	6002	5/5	0.96	0.09	34,37,39,42	0
5	FES	A	2001	4/4	0.96	0.06	31,32,32,34	0
3	PO4	B	6003	5/5	0.97	0.07	32,33,39,40	0
6	FAD	B	3003	53/53	0.97	0.06	14,22,26,28	0
2	BCT	B	5002	4/4	0.97	0.05	22,22,23,24	0
5	FES	B	2001	4/4	0.97	0.05	26,30,30,33	0
2	BCT	A	5001	4/4	0.98	0.05	23,25,25,26	0
4	CA	A	7003	1/1	0.98	0.06	22,22,22,22	0
5	FES	B	2002	4/4	0.99	0.02	19,20,20,21	0
4	CA	B	7004	1/1	0.99	0.03	22,22,22,22	0
4	CA	A	7002	1/1	0.99	0.03	23,23,23,23	0
5	FES	A	2002	4/4	0.99	0.02	20,20,21,21	0
4	CA	B	7001	1/1	0.99	0.03	21,21,21,21	0

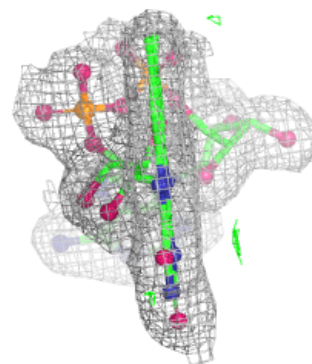
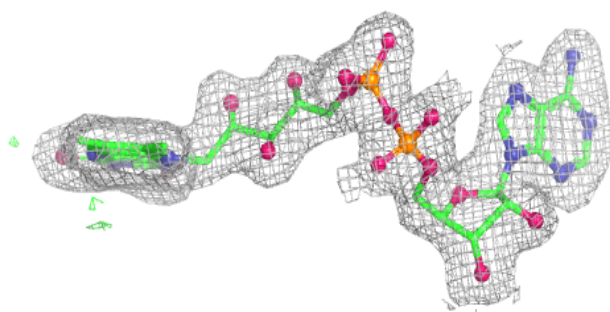
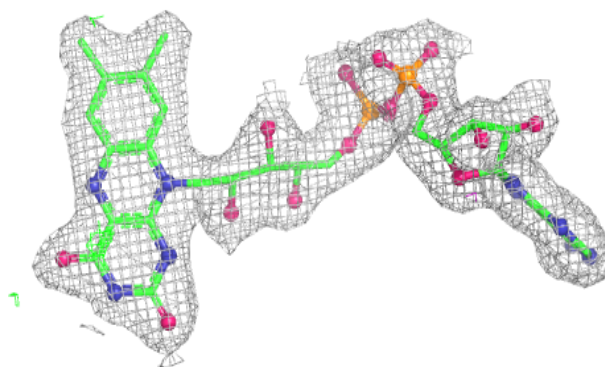
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD A 2003:

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

**Electron density around FAD B 3003:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.