



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:29 PM UTC

PDB ID : 2ZXI / pdb_00002zxi
Title : Structure of Aquifex aeolicus GidA in the form II crystal
Authors : Numata, T.; Osawa, T.
Deposited on : 2008-12-24
Resolution : 2.30 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

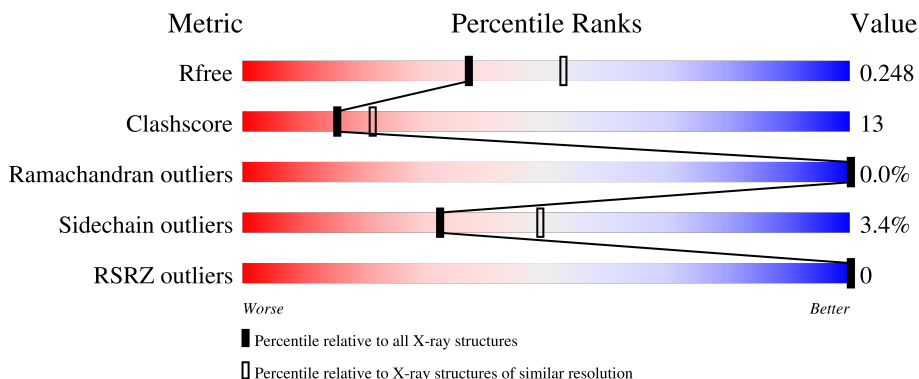
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

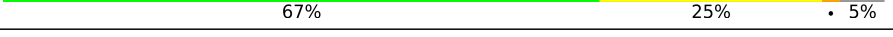
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	637	
1	B	637	
1	C	637	
1	D	637	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20580 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 tRNA uridine 5-carboxymethylaminomethyl modification enzyme mnmG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	0	0
			4801	3074	815	896	16			
1	B	606	Total	C	N	O	S	0	0	0
			4834	3093	824	901	16			
1	C	604	Total	C	N	O	S	0	0	0
			4822	3087	822	897	16			
1	D	603	Total	C	N	O	S	0	0	0
			4811	3080	818	897	16			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O66962
A	-18	GLY	-	expression tag	UNP O66962
A	-17	SER	-	expression tag	UNP O66962
A	-16	SER	-	expression tag	UNP O66962
A	-15	HIS	-	expression tag	UNP O66962
A	-14	HIS	-	expression tag	UNP O66962
A	-13	HIS	-	expression tag	UNP O66962
A	-12	HIS	-	expression tag	UNP O66962
A	-11	HIS	-	expression tag	UNP O66962
A	-10	HIS	-	expression tag	UNP O66962
A	-9	SER	-	expression tag	UNP O66962
A	-8	SER	-	expression tag	UNP O66962
A	-7	GLY	-	expression tag	UNP O66962
A	-6	LEU	-	expression tag	UNP O66962
A	-5	VAL	-	expression tag	UNP O66962
A	-4	PRO	-	expression tag	UNP O66962
A	-3	ALA	-	expression tag	UNP O66962
A	-2	GLY	-	expression tag	UNP O66962
A	-1	SER	-	expression tag	UNP O66962
A	0	HIS	-	expression tag	UNP O66962

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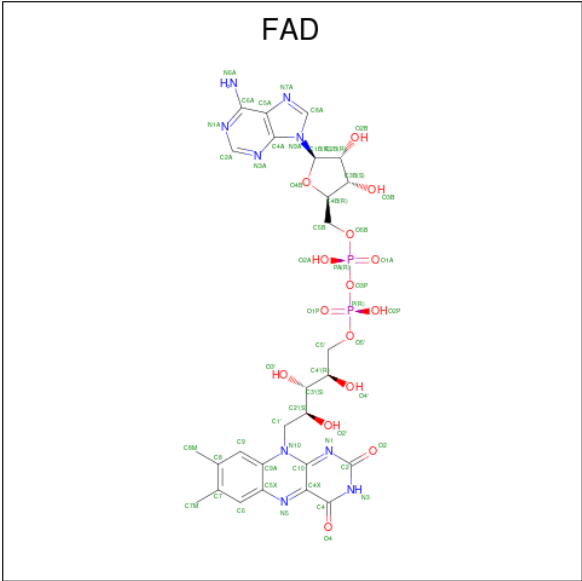
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP O66962
B	-18	GLY	-	expression tag	UNP O66962
B	-17	SER	-	expression tag	UNP O66962
B	-16	SER	-	expression tag	UNP O66962
B	-15	HIS	-	expression tag	UNP O66962
B	-14	HIS	-	expression tag	UNP O66962
B	-13	HIS	-	expression tag	UNP O66962
B	-12	HIS	-	expression tag	UNP O66962
B	-11	HIS	-	expression tag	UNP O66962
B	-10	HIS	-	expression tag	UNP O66962
B	-9	SER	-	expression tag	UNP O66962
B	-8	SER	-	expression tag	UNP O66962
B	-7	GLY	-	expression tag	UNP O66962
B	-6	LEU	-	expression tag	UNP O66962
B	-5	VAL	-	expression tag	UNP O66962
B	-4	PRO	-	expression tag	UNP O66962
B	-3	ALA	-	expression tag	UNP O66962
B	-2	GLY	-	expression tag	UNP O66962
B	-1	SER	-	expression tag	UNP O66962
B	0	HIS	-	expression tag	UNP O66962
C	-19	MET	-	expression tag	UNP O66962
C	-18	GLY	-	expression tag	UNP O66962
C	-17	SER	-	expression tag	UNP O66962
C	-16	SER	-	expression tag	UNP O66962
C	-15	HIS	-	expression tag	UNP O66962
C	-14	HIS	-	expression tag	UNP O66962
C	-13	HIS	-	expression tag	UNP O66962
C	-12	HIS	-	expression tag	UNP O66962
C	-11	HIS	-	expression tag	UNP O66962
C	-10	HIS	-	expression tag	UNP O66962
C	-9	SER	-	expression tag	UNP O66962
C	-8	SER	-	expression tag	UNP O66962
C	-7	GLY	-	expression tag	UNP O66962
C	-6	LEU	-	expression tag	UNP O66962
C	-5	VAL	-	expression tag	UNP O66962
C	-4	PRO	-	expression tag	UNP O66962
C	-3	ALA	-	expression tag	UNP O66962
C	-2	GLY	-	expression tag	UNP O66962
C	-1	SER	-	expression tag	UNP O66962
C	0	HIS	-	expression tag	UNP O66962
D	-19	MET	-	expression tag	UNP O66962
D	-18	GLY	-	expression tag	UNP O66962

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	expression tag	UNP O66962
D	-16	SER	-	expression tag	UNP O66962
D	-15	HIS	-	expression tag	UNP O66962
D	-14	HIS	-	expression tag	UNP O66962
D	-13	HIS	-	expression tag	UNP O66962
D	-12	HIS	-	expression tag	UNP O66962
D	-11	HIS	-	expression tag	UNP O66962
D	-10	HIS	-	expression tag	UNP O66962
D	-9	SER	-	expression tag	UNP O66962
D	-8	SER	-	expression tag	UNP O66962
D	-7	GLY	-	expression tag	UNP O66962
D	-6	LEU	-	expression tag	UNP O66962
D	-5	VAL	-	expression tag	UNP O66962
D	-4	PRO	-	expression tag	UNP O66962
D	-3	ALA	-	expression tag	UNP O66962
D	-2	GLY	-	expression tag	UNP O66962
D	-1	SER	-	expression tag	UNP O66962
D	0	HIS	-	expression tag	UNP O66962

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

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

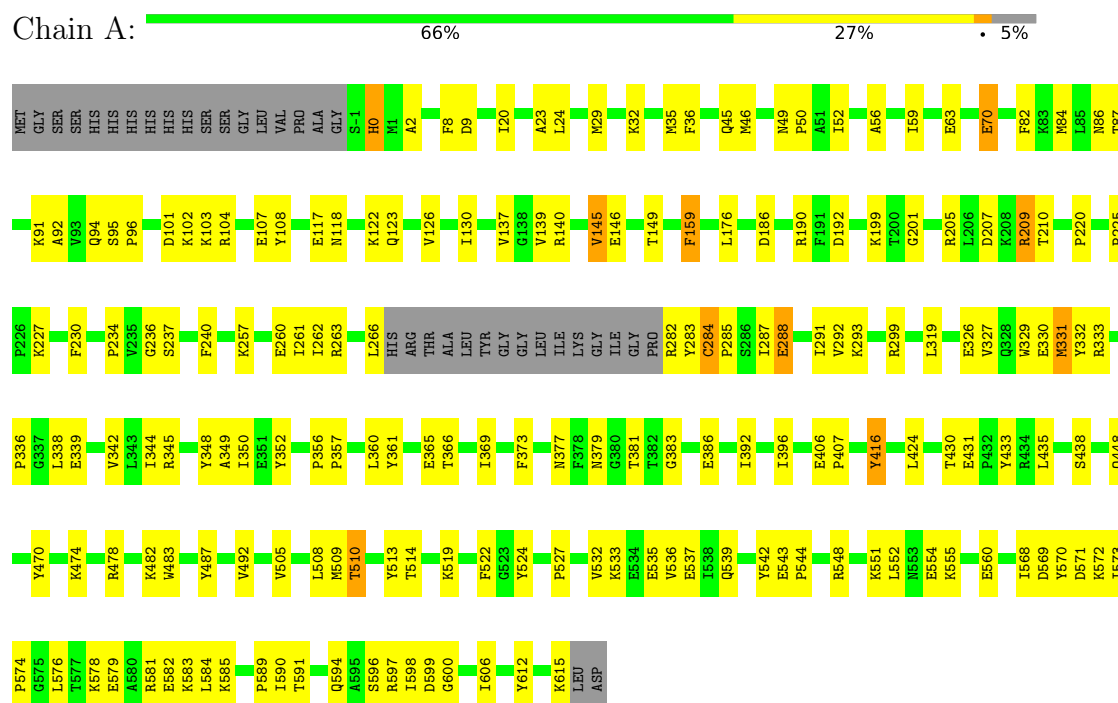
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	286	Total	O	0	0
			286	286		
3	B	275	Total	O	0	0
			275	275		
3	C	255	Total	O	0	0
			255	255		
3	D	284	Total	O	0	0
			284	284		

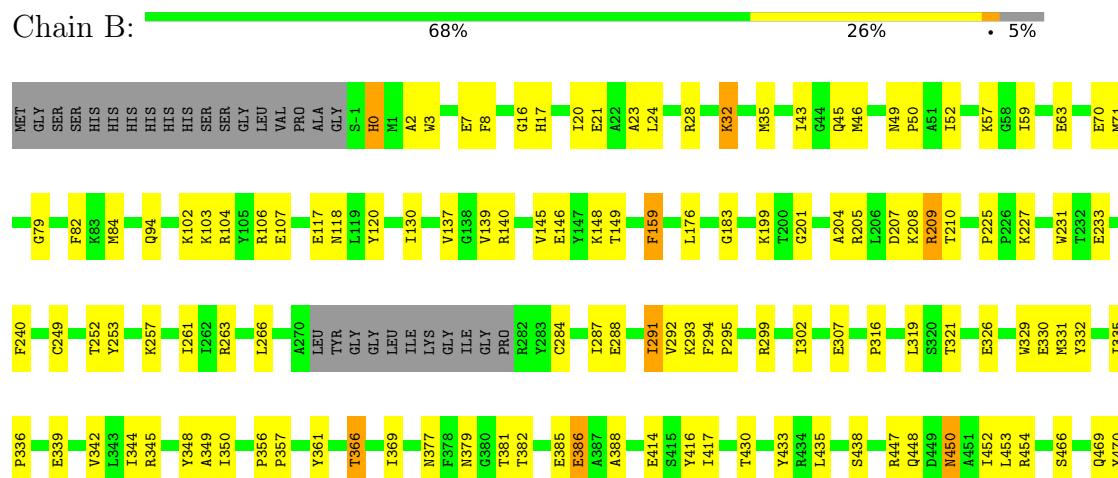
3 Residue-property plots

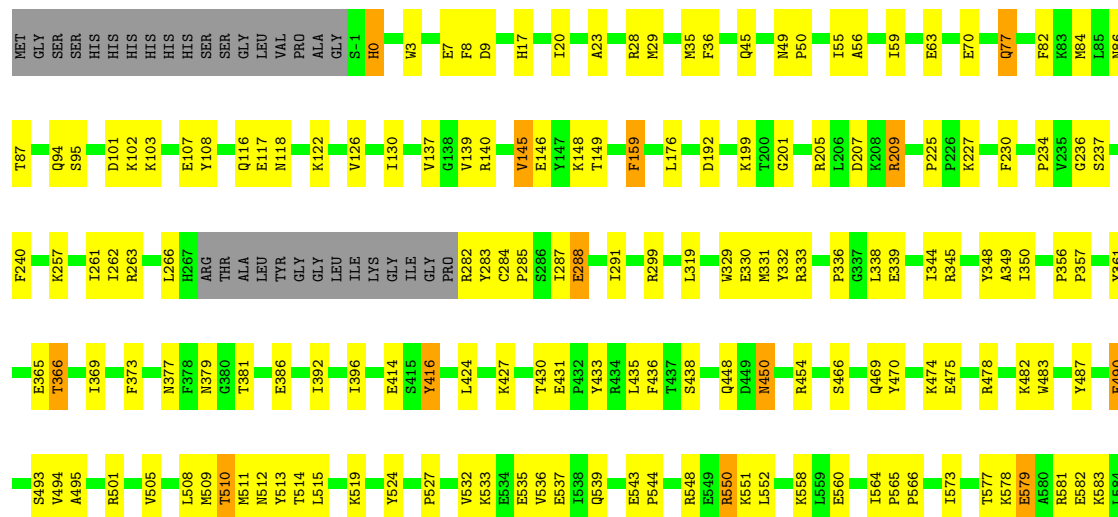
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: tRNA uridine 5-carboxymethylaminomethyl modification enzyme mmmG



- Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme mmmG





K585	
P589	
I590	
T591	
Q594	
R597	
I598	
D599	
G600	
T607	
A608	
L609	
L610	
V611	
K615	
LEU	
ASP	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.41Å 98.00Å 129.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.30 19.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.4 (19.92-2.30) 92.4 (19.92-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.29Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.209 , 0.248 0.209 , 0.248	Depositor DCC
R_{free} test set	6160 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 17.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.480 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20580	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5809e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.40	0/4901	0.90	13/6622 (0.2%)
1	B	0.40	0/4935	0.90	15/6668 (0.2%)
1	C	0.40	0/4922	0.90	18/6649 (0.3%)
1	D	0.40	0/4912	0.90	11/6637 (0.2%)
All	All	0.40	0/19670	0.90	57/26576 (0.2%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	0	HIS	N-CA-C	-8.17	103.33	113.38
1	A	344	ILE	N-CA-C	-7.92	105.49	111.90
1	C	344	ILE	N-CA-C	-7.65	105.70	111.90
1	D	344	ILE	N-CA-C	-7.63	105.72	111.90
1	A	284	CYS	CA-C-N	7.33	126.97	119.56
1	A	284	CYS	C-N-CA	7.33	126.97	119.56
1	B	344	ILE	N-CA-C	-7.31	105.98	111.90
1	B	0	HIS	N-CA-C	-7.31	104.39	113.38
1	A	361	TYR	N-CA-C	-6.94	102.15	110.13
1	D	361	TYR	N-CA-C	-6.65	102.48	110.13
1	D	0	HIS	N-CA-C	-6.55	105.33	113.38
1	D	159	PHE	N-CA-C	6.54	121.54	112.45
1	C	573	ILE	N-CA-C	6.53	113.50	107.56
1	A	573	ILE	N-CA-C	6.47	114.29	107.76
1	D	284	CYS	CA-C-N	6.46	126.09	119.56
1	D	284	CYS	C-N-CA	6.46	126.09	119.56
1	D	573	ILE	N-CA-C	6.45	114.28	107.76
1	A	0	HIS	N-CA-C	-6.38	105.54	113.38
1	B	291	ILE	N-CA-C	-6.33	106.53	113.43
1	C	291	ILE	N-CA-C	-6.33	106.53	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	PHE	N-CA-C	6.18	121.03	112.45
1	B	573	ILE	N-CA-C	6.11	113.12	107.56
1	B	284	CYS	CA-C-N	6.09	125.79	119.82
1	B	284	CYS	C-N-CA	6.09	125.79	119.82
1	C	159	PHE	N-CA-C	6.06	120.88	112.45
1	B	361	TYR	N-CA-C	-6.01	103.22	110.13
1	C	284	CYS	CA-C-N	5.99	125.69	119.82
1	C	284	CYS	C-N-CA	5.99	125.69	119.82
1	C	361	TYR	N-CA-C	-5.99	103.25	110.13
1	B	159	PHE	N-CA-C	5.97	120.75	112.45
1	B	435	LEU	N-CA-C	5.90	118.49	111.71
1	C	183	GLY	N-CA-C	5.58	119.64	112.83
1	C	430	THR	N-CA-C	-5.52	106.45	114.12
1	B	430	THR	N-CA-C	-5.45	106.63	113.72
1	C	292	VAL	N-CA-C	-5.43	105.40	113.39
1	C	356	PRO	CA-C-N	5.40	125.06	119.56
1	C	356	PRO	C-N-CA	5.40	125.06	119.56
1	B	292	VAL	N-CA-C	-5.38	105.49	113.39
1	A	514	THR	N-CA-C	-5.34	102.55	110.46
1	B	183	GLY	N-CA-C	5.31	119.31	112.83
1	A	292	VAL	N-CA-C	-5.30	107.25	111.81
1	D	514	THR	N-CA-C	-5.30	102.62	110.46
1	C	249	CYS	N-CA-C	-5.28	101.51	109.85
1	B	231	TRP	N-CA-C	5.26	119.76	113.23
1	B	249	CYS	N-CA-C	-5.25	101.55	109.85
1	C	231	TRP	N-CA-C	5.23	119.71	113.23
1	D	101	ASP	N-CA-C	-5.21	98.81	107.99
1	B	417	ILE	N-CA-C	-5.18	105.49	110.72
1	A	9	ASP	N-CA-C	-5.15	104.62	112.04
1	A	32	LYS	N-CA-C	-5.13	101.76	109.15
1	A	101	ASP	N-CA-C	-5.13	98.96	107.99
1	C	529	HIS	CA-C-N	5.12	124.56	119.24
1	C	529	HIS	C-N-CA	5.12	124.56	119.24
1	A	70	GLU	N-CA-C	5.07	119.59	113.41
1	C	417	ILE	N-CA-C	-5.06	105.61	110.72
1	D	9	ASP	N-CA-C	-5.04	104.78	112.04
1	D	70	GLU	N-CA-C	5.03	119.54	113.41

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	4801	0	4866	145	0
1	B	4834	0	4898	135	0
1	C	4822	0	4890	128	0
1	D	4811	0	4873	131	0
2	A	53	0	31	3	0
2	B	53	0	31	1	0
2	C	53	0	31	2	0
2	D	53	0	31	1	0
3	A	286	0	0	7	0
3	B	275	0	0	9	0
3	C	255	0	0	10	0
3	D	284	0	0	5	0
All	All	20580	0	19651	525	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 13.

All (525) 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:29:MET:HE1	1:A:396:ILE:HA	1.25	1.09
1:D:29:MET:HE1	1:D:396:ILE:HA	1.16	1.09
1:B:366:THR:HG22	1:B:369:ILE:H	1.22	1.01
1:C:366:THR:HG22	1:C:369:ILE:H	1.22	1.01
1:A:478:ARG:HH12	1:A:482:LYS:HE2	1.27	0.95
1:B:509:MET:HE3	1:B:537:GLU:HG3	1.47	0.94
1:D:594:GLN:HA	1:D:597:ARG:NH1	1.82	0.94
1:D:478:ARG:HH12	1:D:482:LYS:HE2	1.33	0.92
1:D:366:THR:HG22	1:D:369:ILE:H	1.33	0.92
1:A:49:ASN:HD22	1:A:50:PRO:CD	1.85	0.89
1:A:594:GLN:HA	1:A:597:ARG:NH1	1.87	0.89
1:A:366:THR:HG22	1:A:369:ILE:H	1.38	0.88
1:D:466:SER:H	1:D:469:GLN:HE21	1.21	0.87
1:D:49:ASN:HD22	1:D:50:PRO:CD	1.88	0.86
1:D:261:ILE:HD13	1:D:330:GLU:HG2	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ILE:HD13	1:A:330:GLU:HG2	1.61	0.82
1:D:478:ARG:NH1	1:D:482:LYS:HE2	1.94	0.82
1:B:583:LYS:NZ	1:B:600:GLY:HA3	1.95	0.82
1:A:478:ARG:NH1	1:A:482:LYS:HE2	1.95	0.80
1:B:49:ASN:HD22	1:B:50:PRO:CD	1.94	0.80
1:D:583:LYS:NZ	1:D:600:GLY:HA3	1.96	0.80
1:C:49:ASN:HD22	1:C:50:PRO:CD	1.94	0.79
1:B:357:PRO:HG3	1:B:379:ASN:O	1.81	0.79
1:B:466:SER:H	1:B:469:GLN:HE21	1.30	0.79
1:B:252:THR:HG22	1:B:253:TYR:H	1.48	0.79
1:D:594:GLN:HA	1:D:597:ARG:HH12	1.44	0.78
1:B:594:GLN:HA	1:B:597:ARG:NH1	1.99	0.78
1:C:357:PRO:HG3	1:C:379:ASN:O	1.84	0.78
1:C:583:LYS:NZ	1:C:600:GLY:HA3	1.99	0.78
1:A:583:LYS:NZ	1:A:600:GLY:HA3	1.99	0.77
1:B:49:ASN:HD22	1:B:50:PRO:N	1.82	0.77
1:C:252:THR:HG22	1:C:253:TYR:H	1.50	0.77
1:C:577:THR:HG23	1:C:580:ALA:H	1.50	0.77
1:B:509:MET:CE	1:B:537:GLU:HG3	2.15	0.76
1:D:509:MET:CE	1:D:537:GLU:HG3	2.15	0.76
1:A:509:MET:HE3	1:A:537:GLU:HG3	1.69	0.75
1:C:49:ASN:HD22	1:C:50:PRO:N	1.84	0.75
1:C:471:LYS:O	1:C:475:GLU:HG3	1.87	0.75
1:B:23:ALA:HB3	1:B:35:MET:HE3	1.69	0.73
1:A:583:LYS:HZ1	1:A:600:GLY:HA3	1.51	0.73
1:A:509:MET:CE	1:A:537:GLU:HG3	2.19	0.73
1:A:49:ASN:HD22	1:A:50:PRO:HD2	1.51	0.73
1:B:565:PRO:HB2	1:B:568:ILE:HG23	1.70	0.73
1:D:45:GLN:HG3	3:D:931:HOH:O	1.87	0.73
1:D:509:MET:HE3	1:D:537:GLU:HG3	1.72	0.71
1:A:283:TYR:CE2	1:A:285:PRO:HG3	2.25	0.71
1:A:225:PRO:HG2	1:A:240:PHE:HB2	1.72	0.70
1:D:225:PRO:HG2	1:D:240:PHE:HB2	1.72	0.70
1:A:357:PRO:HG3	1:A:379:ASN:O	1.91	0.70
1:A:87:THR:HA	1:A:94:GLN:NE2	2.06	0.70
1:C:565:PRO:HB2	1:C:568:ILE:HG23	1.73	0.70
1:D:581:ARG:O	1:D:585:LYS:HB2	1.91	0.70
1:C:23:ALA:HB3	1:C:35:MET:HE3	1.74	0.69
1:D:450:ASN:ND2	1:D:454:ARG:HE	1.89	0.69
1:D:583:LYS:HZ3	1:D:600:GLY:HA3	1.56	0.68
1:C:564:ILE:CG2	1:C:568:ILE:HD13	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:PRO:HG3	1:D:379:ASN:O	1.93	0.68
1:C:261:ILE:HD13	1:C:330:GLU:HG2	1.75	0.68
1:D:470:TYR:CE2	1:D:474:LYS:HD2	2.28	0.68
1:A:107:GLU:HG2	3:A:807:HOH:O	1.94	0.68
1:A:283:TYR:O	1:A:285:PRO:HD3	1.94	0.68
1:D:262:ILE:O	1:D:266:LEU:HG	1.93	0.67
1:D:49:ASN:HD22	1:D:50:PRO:HD2	1.57	0.67
1:C:257:LYS:HE3	3:C:878:HOH:O	1.93	0.67
1:B:583:LYS:HZ3	1:B:600:GLY:HA3	1.60	0.67
1:A:581:ARG:O	1:A:585:LYS:HB2	1.94	0.67
1:C:366:THR:CG2	1:C:369:ILE:H	2.05	0.66
1:B:564:ILE:HG23	1:B:568:ILE:HD13	1.76	0.66
1:B:590:ILE:HG13	1:B:591:THR:HG23	1.78	0.66
1:A:548:ARG:O	1:A:552:LEU:HG	1.96	0.66
1:A:29:MET:HE1	1:A:396:ILE:CA	2.14	0.66
1:B:23:ALA:CB	1:B:35:MET:HE3	2.26	0.66
1:C:590:ILE:HG13	1:C:591:THR:HG23	1.78	0.66
1:B:366:THR:CG2	1:B:369:ILE:H	2.06	0.65
1:D:466:SER:H	1:D:469:GLN:NE2	1.93	0.65
1:C:560:GLU:OE1	1:C:597:ARG:NH2	2.29	0.65
1:C:414:GLU:HG2	3:C:980:HOH:O	1.96	0.65
1:D:29:MET:HE1	1:D:396:ILE:CA	2.10	0.65
1:A:293:LYS:HD2	3:A:923:HOH:O	1.97	0.65
1:B:233:GLU:HG3	3:B:1083:HOH:O	1.97	0.65
1:C:23:ALA:CB	1:C:35:MET:HE3	2.26	0.65
1:A:20:ILE:HA	1:A:35:MET:HE1	1.77	0.64
1:C:8:PHE:O	1:C:149:THR:HA	1.98	0.64
1:D:59:ILE:O	1:D:63:GLU:HG3	1.97	0.64
1:D:478:ARG:HH12	1:D:482:LYS:CE	2.08	0.64
1:A:381:THR:HG22	1:A:433:TYR:HB3	1.80	0.64
1:B:466:SER:H	1:B:469:GLN:NE2	1.96	0.64
1:D:490:GLU:HG2	1:D:524:TYR:HE2	1.61	0.64
1:C:583:LYS:HZ2	1:C:600:GLY:HA3	1.62	0.63
1:B:8:PHE:O	1:B:149:THR:HA	1.99	0.63
1:D:49:ASN:HD22	1:D:50:PRO:N	1.96	0.63
1:B:433:TYR:OH	1:B:438:SER:HB3	1.99	0.63
1:B:564:ILE:CG2	1:B:568:ILE:HD13	2.29	0.62
1:A:29:MET:CE	1:A:396:ILE:HA	2.16	0.62
1:A:478:ARG:HH12	1:A:482:LYS:CE	2.07	0.62
1:B:583:LYS:HZ2	1:B:600:GLY:HA3	1.64	0.62
1:D:282:ARG:HB2	1:D:431:GLU:OE2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:THR:HG22	1:B:253:TYR:N	2.15	0.61
1:D:550:ARG:NH1	1:D:551:LYS:HA	2.14	0.61
1:A:560:GLU:OE1	1:A:597:ARG:NH2	2.33	0.61
1:C:50:PRO:HG3	1:C:102:LYS:HE3	1.82	0.61
1:B:49:ASN:HD22	1:B:50:PRO:HD2	1.65	0.61
1:A:49:ASN:ND2	1:A:50:PRO:HD2	2.15	0.61
1:A:207:ASP:OD1	1:A:209:ARG:HD3	2.00	0.61
1:C:564:ILE:HG23	1:C:568:ILE:HD13	1.83	0.60
1:B:0:HIS:HE1	1:B:146:GLU:OE1	1.84	0.60
1:A:583:LYS:NZ	1:A:600:GLY:CA	2.64	0.60
1:C:49:ASN:HD22	1:C:50:PRO:HD2	1.67	0.60
1:A:130:ILE:HG22	1:A:137:VAL:CG1	2.31	0.60
1:B:50:PRO:HG3	1:B:102:LYS:HE3	1.84	0.60
1:B:159:PHE:HB2	2:B:618:FAD:H8A	1.84	0.60
1:C:0:HIS:HE1	1:C:146:GLU:OE1	1.85	0.60
1:D:126:VAL:HG13	1:D:139:VAL:HG13	1.83	0.60
1:A:257:LYS:O	1:A:260:GLU:HG2	2.01	0.60
1:B:331:MET:HG3	1:B:332:TYR:N	2.16	0.60
1:C:262:ILE:O	1:C:266:LEU:HG	2.02	0.59
1:D:84:MET:HB3	1:D:87:THR:CG2	2.32	0.59
1:D:365:GLU:HB2	1:D:373:PHE:CE2	2.37	0.59
1:D:589:PRO:HG3	1:D:598:ILE:HD11	1.84	0.59
1:C:159:PHE:HB2	2:C:618:FAD:H8A	1.84	0.59
1:B:225:PRO:HG2	1:B:240:PHE:HB2	1.85	0.59
1:B:261:ILE:HD13	1:B:330:GLU:HG2	1.85	0.59
1:A:103:LYS:HD3	1:B:107:GLU:OE2	2.03	0.59
1:A:508:LEU:O	1:A:513:TYR:HB2	2.03	0.59
1:D:205:ARG:HB2	1:D:345:ARG:HB2	1.84	0.59
1:A:227:LYS:HE2	1:A:237:SER:O	2.02	0.58
1:D:84:MET:HG2	1:D:94:GLN:OE1	2.03	0.58
1:A:470:TYR:CE2	1:A:474:LYS:HD2	2.37	0.58
1:A:589:PRO:HG3	1:A:598:ILE:HD11	1.84	0.58
1:A:87:THR:HA	1:A:94:GLN:HE21	1.68	0.58
1:C:207:ASP:OD1	1:C:209:ARG:HD3	2.04	0.58
1:C:548:ARG:O	1:C:552:LEU:HG	2.03	0.58
1:D:433:TYR:OH	1:D:438:SER:HB3	2.03	0.58
1:C:252:THR:HG22	1:C:253:TYR:N	2.19	0.58
1:D:130:ILE:HG22	1:D:137:VAL:CG1	2.33	0.58
1:C:59:ILE:O	1:C:63:GLU:HG3	2.03	0.57
1:C:82:PHE:HB2	1:C:225:PRO:HB2	1.85	0.57
1:A:543:GLU:HB3	1:A:544:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ARG:HB2	1:A:345:ARG:HB2	1.86	0.57
1:A:284:CYS:HB2	3:A:923:HOH:O	2.02	0.57
1:D:416:TYR:HE1	1:D:438:SER:HG	1.52	0.57
1:C:493:SER:HA	1:C:501:ARG:O	2.05	0.57
1:C:555:LYS:HB2	3:C:772:HOH:O	2.04	0.57
1:C:254:THR:HG21	1:C:287:ILE:HD11	1.85	0.57
1:A:49:ASN:HD22	1:A:50:PRO:N	2.03	0.57
1:D:227:LYS:HE2	1:D:237:SER:O	2.04	0.57
1:D:577:THR:O	1:D:581:ARG:HG3	2.05	0.57
1:D:23:ALA:HB3	1:D:35:MET:HE3	1.87	0.56
1:A:474:LYS:HE3	3:A:728:HOH:O	2.06	0.56
1:B:20:ILE:HA	1:B:35:MET:HE1	1.86	0.56
1:C:225:PRO:HG2	1:C:240:PHE:HB2	1.87	0.56
1:D:7:GLU:OE2	1:D:148:LYS:HD2	2.04	0.56
1:D:28:ARG:HE	1:D:116:GLN:NE2	2.03	0.56
1:D:490:GLU:CG	1:D:524:TYR:HE2	2.17	0.56
1:A:126:VAL:HG13	1:A:139:VAL:HG13	1.87	0.56
1:A:535:GLU:O	1:A:539:GLN:HG3	2.05	0.56
1:D:487:TYR:CD1	1:D:505:VAL:HG11	2.41	0.56
1:D:508:LEU:O	1:D:513:TYR:HB2	2.05	0.56
1:A:433:TYR:OH	1:A:438:SER:HB3	2.05	0.56
1:A:262:ILE:O	1:A:266:LEU:HG	2.05	0.56
1:A:59:ILE:O	1:A:63:GLU:HG3	2.06	0.56
1:A:594:GLN:HA	1:A:597:ARG:HH12	1.69	0.56
1:B:82:PHE:HB2	1:B:225:PRO:HB2	1.87	0.56
1:B:49:ASN:ND2	1:B:50:PRO:HD2	2.21	0.56
1:D:50:PRO:HG3	1:D:102:LYS:HE3	1.88	0.56
1:C:433:TYR:OH	1:C:438:SER:HB3	2.05	0.55
1:C:590:ILE:H	1:C:594:GLN:NE2	2.04	0.55
1:C:326:GLU:HA	1:C:329:TRP:CE3	2.41	0.55
1:A:416:TYR:HE1	1:A:438:SER:HG	1.55	0.55
1:D:207:ASP:OD1	1:D:209:ARG:HD3	2.06	0.55
1:D:331:MET:HG3	1:D:332:TYR:N	2.20	0.55
1:B:210:THR:HG21	1:B:342:VAL:CG2	2.36	0.55
1:B:548:ARG:O	1:B:552:LEU:HG	2.06	0.55
1:C:117:GLU:O	1:C:118:ASN:HB2	2.06	0.55
1:D:509:MET:HE1	1:D:537:GLU:HG3	1.87	0.55
1:A:416:TYR:HE1	1:A:438:SER:OG	1.89	0.55
1:A:416:TYR:HE2	3:A:846:HOH:O	1.88	0.55
1:D:49:ASN:ND2	1:D:50:PRO:HD2	2.20	0.55
1:B:117:GLU:O	1:B:118:ASN:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:0:HIS:HE1	1:A:146:GLU:OE1	1.90	0.54
1:A:568:ILE:HD11	1:A:612:TYR:CE2	2.42	0.54
1:C:319:LEU:HD22	1:C:331:MET:CE	2.38	0.54
1:A:578:LYS:NZ	1:D:579:GLU:HG2	2.22	0.54
1:A:282:ARG:HB3	1:A:431:GLU:OE2	2.07	0.54
1:B:210:THR:HG21	1:B:342:VAL:HG23	1.89	0.54
1:D:583:LYS:HZ2	1:D:600:GLY:HA3	1.72	0.53
1:A:569:ASP:HB3	1:A:572:LYS:HD3	1.90	0.53
1:A:117:GLU:O	1:A:118:ASN:HB2	2.08	0.53
1:D:416:TYR:HE1	1:D:438:SER:OG	1.90	0.53
1:D:543:GLU:HB3	1:D:544:PRO:HD3	1.91	0.53
1:B:59:ILE:O	1:B:63:GLU:HG3	2.09	0.53
1:A:365:GLU:HB2	1:A:373:PHE:CE2	2.44	0.53
1:C:578:LYS:O	1:C:582:GLU:HG2	2.07	0.53
1:B:414:GLU:HG2	3:B:703:HOH:O	2.09	0.53
1:C:365:GLU:HB2	1:C:373:PHE:CE2	2.44	0.53
1:B:470:TYR:CE2	1:B:474:LYS:HD2	2.44	0.53
1:B:302:ILE:CD1	1:B:335:ILE:HD13	2.39	0.52
1:A:487:TYR:CD1	1:A:505:VAL:HG11	2.44	0.52
1:B:546:ILE:HD12	3:B:877:HOH:O	2.08	0.52
1:C:103:LYS:HE2	1:D:107:GLU:OE2	2.09	0.52
1:C:583:LYS:HZ3	1:C:600:GLY:HA3	1.69	0.52
1:C:49:ASN:ND2	1:C:50:PRO:HD2	2.23	0.52
1:D:0:HIS:HE1	1:D:146:GLU:OE1	1.93	0.52
1:B:509:MET:HE1	1:B:515:LEU:HG	1.92	0.52
1:D:82:PHE:HB2	1:D:225:PRO:HB2	1.91	0.52
1:A:583:LYS:NZ	1:A:599:ASP:O	2.36	0.52
1:D:381:THR:HG22	1:D:433:TYR:HB3	1.90	0.52
1:C:532:VAL:O	1:C:536:VAL:HG23	2.09	0.52
1:B:450:ASN:ND2	1:B:454:ARG:HE	2.08	0.52
1:B:49:ASN:HD22	1:B:49:ASN:C	2.18	0.52
1:B:532:VAL:O	1:B:536:VAL:HG23	2.10	0.52
1:C:331:MET:HG3	1:C:332:TYR:N	2.25	0.52
1:B:84:MET:HG2	1:B:94:GLN:OE1	2.09	0.51
1:D:548:ARG:O	1:D:552:LEU:HG	2.10	0.51
1:B:568:ILE:HD11	1:B:570:TYR:CZ	2.44	0.51
1:D:490:GLU:HG2	1:D:524:TYR:CE2	2.44	0.51
1:B:590:ILE:H	1:B:594:GLN:NE2	2.09	0.51
1:C:294:PHE:N	1:C:295:PRO:HD3	2.25	0.51
1:C:49:ASN:HD22	1:C:49:ASN:C	2.18	0.51
1:C:470:TYR:CE2	1:C:474:LYS:HD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ILE:O	1:A:396:ILE:HG13	2.10	0.51
1:B:287:ILE:O	1:B:291:ILE:HG23	2.11	0.51
1:C:533:LYS:HD3	1:C:533:LYS:O	2.11	0.51
1:C:377:ASN:ND2	2:C:618:FAD:H5'1	2.26	0.51
1:D:159:PHE:HB2	2:D:618:FAD:H8A	1.93	0.51
1:A:84:MET:HB3	1:A:87:THR:CG2	2.39	0.51
1:B:529:HIS:HE1	3:B:633:HOH:O	1.93	0.51
1:C:94:GLN:O	1:C:448:GLN:HG2	2.11	0.51
1:A:287:ILE:O	1:A:291:ILE:HG23	2.11	0.51
1:A:568:ILE:HD11	1:A:612:TYR:HE2	1.75	0.51
1:B:319:LEU:HD22	1:B:331:MET:CE	2.41	0.51
1:C:107:GLU:OE1	1:D:107:GLU:CD	2.54	0.51
1:A:23:ALA:HB3	1:A:35:MET:HE3	1.92	0.50
1:C:489:SER:HB3	3:C:962:HOH:O	2.12	0.50
1:B:257:LYS:HD3	3:B:681:HOH:O	2.11	0.50
1:B:509:MET:CE	1:B:515:LEU:HG	2.41	0.50
1:C:408:ILE:HD12	1:C:408:ILE:C	2.36	0.50
1:B:326:GLU:HA	1:B:329:TRP:CE3	2.47	0.50
1:A:84:MET:HE3	1:A:95:SER:C	2.37	0.50
1:A:571:ASP:HA	1:A:581:ARG:HD3	1.94	0.50
1:D:20:ILE:HA	1:D:35:MET:HE1	1.92	0.50
1:B:471:LYS:O	1:B:475:GLU:HG3	2.11	0.49
1:A:92:ALA:HB2	1:A:542:TYR:CE2	2.47	0.49
1:A:583:LYS:HZ1	1:A:600:GLY:CA	2.24	0.49
1:B:24:LEU:HD13	1:B:70:GLU:HG3	1.94	0.49
1:C:447:ARG:H	1:C:450:ASN:HD21	1.61	0.49
1:D:550:ARG:HH12	1:D:551:LYS:HA	1.75	0.49
1:D:590:ILE:HG13	1:D:591:THR:HG23	1.94	0.49
1:B:94:GLN:O	1:B:448:GLN:HG2	2.12	0.49
1:C:568:ILE:HD11	1:C:570:TYR:CZ	2.48	0.49
1:A:576:LEU:O	1:A:581:ARG:NH1	2.46	0.49
1:B:7:GLU:HG2	1:B:148:LYS:HB2	1.95	0.49
1:C:293:LYS:C	1:C:295:PRO:HD3	2.38	0.49
1:D:392:ILE:O	1:D:396:ILE:HG13	2.13	0.49
1:A:145:VAL:CG1	1:A:146:GLU:N	2.75	0.49
1:D:532:VAL:O	1:D:536:VAL:HG23	2.12	0.49
1:C:382:THR:O	1:C:386:GLU:HG3	2.11	0.49
1:B:589:PRO:HG3	1:B:598:ILE:HD11	1.95	0.49
1:D:145:VAL:CG1	1:D:146:GLU:N	2.76	0.48
1:D:287:ILE:O	1:D:291:ILE:HG23	2.13	0.48
1:B:293:LYS:C	1:B:295:PRO:HD3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:493:SER:HA	1:D:501:ARG:O	2.13	0.48
1:A:159:PHE:HB2	2:A:618:FAD:H8A	1.95	0.48
1:B:294:PHE:N	1:B:295:PRO:HD3	2.29	0.48
1:D:366:THR:CG2	1:D:369:ILE:H	2.15	0.48
1:A:107:GLU:CD	1:B:103:LYS:HD3	2.39	0.48
1:B:447:ARG:H	1:B:450:ASN:HD21	1.61	0.48
1:D:377:ASN:HA	1:D:381:THR:O	2.13	0.48
1:A:94:GLN:O	1:A:448:GLN:HG2	2.14	0.48
1:A:84:MET:HE1	1:A:96:PRO:HD3	1.96	0.48
1:A:532:VAL:O	1:A:536:VAL:HG23	2.13	0.48
1:C:2:ALA:HA	1:D:329:TRP:CZ3	2.48	0.48
1:C:287:ILE:O	1:C:291:ILE:HG23	2.14	0.48
1:D:117:GLU:O	1:D:118:ASN:HB2	2.13	0.48
1:D:130:ILE:HG22	1:D:137:VAL:HG13	1.95	0.48
1:A:56:ALA:HB3	1:A:435:LEU:HB3	1.96	0.48
1:A:377:ASN:HA	1:A:381:THR:O	2.13	0.48
1:C:260:GLU:HG2	1:C:264:LYS:HE3	1.95	0.48
1:C:589:PRO:HG3	1:C:598:ILE:HD11	1.96	0.48
1:A:519:LYS:HG3	1:A:524:TYR:O	2.14	0.48
1:C:581:ARG:HD2	3:C:824:HOH:O	2.14	0.48
1:A:483:TRP:CD2	1:A:527:PRO:HG3	2.49	0.48
1:D:20:ILE:HA	1:D:35:MET:CE	2.44	0.48
1:D:483:TRP:CD2	1:D:527:PRO:HG3	2.49	0.48
1:A:326:GLU:HG2	1:A:327:VAL:N	2.29	0.47
1:C:130:ILE:HD11	1:C:140:ARG:CD	2.44	0.47
1:C:491:ARG:HH11	1:C:491:ARG:HG2	1.78	0.47
1:D:94:GLN:O	1:D:448:GLN:HG2	2.14	0.47
1:D:283:TYR:O	1:D:285:PRO:HD3	2.14	0.47
1:D:519:LYS:HG3	1:D:524:TYR:O	2.14	0.47
1:A:91:LYS:HA	1:A:94:GLN:HG3	1.96	0.47
1:B:104:ARG:NH1	1:B:107:GLU:OE1	2.47	0.47
1:B:533:LYS:O	1:B:533:LYS:HD3	2.15	0.47
1:A:82:PHE:HB2	1:A:225:PRO:HB2	1.96	0.47
1:A:199:LYS:HA	1:A:350:ILE:O	2.14	0.47
1:B:130:ILE:HD11	1:B:140:ARG:CD	2.44	0.47
1:D:535:GLU:HG3	1:D:539:GLN:HE21	1.80	0.47
1:D:287:ILE:HG23	1:D:288:GLU:N	2.30	0.47
1:B:21:GLU:HG3	1:B:388:ALA:HB1	1.96	0.47
1:B:49:ASN:ND2	1:B:50:PRO:CD	2.70	0.47
1:C:491:ARG:NH1	1:C:504:SER:HB3	2.30	0.47
1:B:32:LYS:HD2	1:B:120:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:551:LYS:O	1:C:554:GLU:HG3	2.14	0.47
1:D:199:LYS:HA	1:D:350:ILE:O	2.14	0.47
1:B:490:GLU:O	1:B:505:VAL:HG23	2.15	0.47
1:D:490:GLU:CG	1:D:524:TYR:CE2	2.98	0.47
1:A:590:ILE:HG12	1:A:594:GLN:OE1	2.15	0.46
1:B:551:LYS:HD3	1:B:551:LYS:C	2.40	0.46
1:C:210:THR:HG21	1:C:342:VAL:CG2	2.45	0.46
1:C:494:VAL:O	1:C:500:THR:HA	2.16	0.46
1:A:357:PRO:HB2	1:A:424:LEU:O	2.14	0.46
1:B:28:ARG:HH12	1:B:70:GLU:HG2	1.80	0.46
1:C:319:LEU:HD13	1:C:332:TYR:CE1	2.50	0.46
1:B:319:LEU:HD11	1:B:335:ILE:CD1	2.46	0.46
1:B:555:LYS:HB2	3:B:1042:HOH:O	2.14	0.46
1:D:263:ARG:HG2	1:D:263:ARG:HH11	1.79	0.46
1:D:558:LYS:HE2	3:D:715:HOH:O	2.15	0.46
1:B:45:GLN:HA	1:B:106:ARG:HG3	1.98	0.46
1:B:207:ASP:OD1	1:B:209:ARG:HD3	2.15	0.46
1:B:416:TYR:CE1	1:B:438:SER:OG	2.69	0.46
1:B:450:ASN:HD22	1:B:450:ASN:H	1.64	0.46
1:C:568:ILE:CD1	1:C:570:TYR:CZ	2.99	0.46
1:B:201:GLY:HA2	1:B:349:ALA:HA	1.97	0.46
1:B:382:THR:O	1:B:386:GLU:HG3	2.14	0.46
1:B:543:GLU:HB3	1:B:544:PRO:HD3	1.96	0.46
1:D:23:ALA:CB	1:D:35:MET:HE3	2.45	0.46
1:A:360:LEU:HD11	1:A:379:ASN:OD1	2.16	0.46
1:C:287:ILE:HD12	1:C:319:LEU:HD23	1.96	0.46
1:D:8:PHE:O	1:D:149:THR:HA	2.16	0.46
1:D:356:PRO:HA	1:D:357:PRO:HD3	1.81	0.46
1:A:84:MET:HB3	1:A:87:THR:HG22	1.98	0.46
1:C:319:LEU:HD22	1:C:331:MET:HE1	1.97	0.46
1:C:551:LYS:HG2	3:C:880:HOH:O	2.15	0.46
1:D:201:GLY:HA2	1:D:349:ALA:HA	1.98	0.46
1:A:20:ILE:HA	1:A:35:MET:CE	2.45	0.46
1:A:123:GLN:HG2	3:A:682:HOH:O	2.16	0.46
1:A:336:PRO:HA	1:A:339:GLU:OE2	2.16	0.46
1:B:533:LYS:HD3	3:B:662:HOH:O	2.16	0.46
1:C:252:THR:HG21	1:C:336:PRO:O	2.15	0.46
1:A:108:TYR:CD2	1:A:108:TYR:C	2.94	0.46
1:C:356:PRO:HA	1:C:357:PRO:HD3	1.79	0.45
1:D:357:PRO:HB2	1:D:424:LEU:O	2.16	0.45
1:A:50:PRO:HG3	1:A:102:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:LEU:HD13	1:C:341:VAL:HG21	1.99	0.45
1:A:130:ILE:HG22	1:A:137:VAL:HG12	1.99	0.45
1:B:266:LEU:HD12	1:B:266:LEU:HA	1.81	0.45
1:C:201:GLY:HA2	1:C:349:ALA:HA	1.98	0.45
1:C:491:ARG:HG2	1:C:491:ARG:NH1	2.32	0.45
1:A:201:GLY:HA2	1:A:349:ALA:HA	1.99	0.45
1:A:319:LEU:HD13	1:A:332:TYR:CE1	2.52	0.45
1:B:205:ARG:HB2	1:B:345:ARG:HB2	1.97	0.45
1:B:287:ILE:HG23	1:B:288:GLU:N	2.30	0.45
1:C:577:THR:HG22	1:C:580:ALA:CB	2.46	0.45
1:B:208:LYS:NZ	3:B:1090:HOH:O	2.49	0.45
1:B:568:ILE:CD1	1:B:570:TYR:CZ	3.00	0.45
1:A:570:TYR:CE2	1:A:584:LEU:HB3	2.51	0.45
1:C:49:ASN:ND2	1:C:50:PRO:CD	2.71	0.45
1:C:450:ASN:ND2	1:C:454:ARG:HE	2.15	0.45
1:C:452:ILE:HG23	1:C:453:LEU:N	2.32	0.45
1:C:21:GLU:HG3	1:C:388:ALA:HB1	1.99	0.45
1:C:515:LEU:HD23	1:C:515:LEU:HA	1.83	0.45
1:D:565:PRO:HA	1:D:566:PRO:HD3	1.89	0.45
1:A:578:LYS:HZ2	1:D:579:GLU:HG2	1.81	0.45
1:A:8:PHE:O	1:A:149:THR:HA	2.17	0.44
1:A:287:ILE:HG23	1:A:288:GLU:N	2.32	0.44
1:B:3:TRP:CD1	1:B:3:TRP:N	2.84	0.44
1:A:23:ALA:CB	1:A:35:MET:HE3	2.46	0.44
1:A:24:LEU:HD13	1:A:70:GLU:HG3	1.99	0.44
1:A:283:TYR:CD2	1:A:285:PRO:HG3	2.53	0.44
1:B:50:PRO:HG2	1:B:307:GLU:HG2	1.98	0.44
1:C:101:ASP:OD1	1:C:104:ARG:HG2	2.17	0.44
1:A:366:THR:CG2	1:A:369:ILE:H	2.20	0.44
1:B:543:GLU:N	1:B:544:PRO:CD	2.81	0.44
1:B:57:LYS:HE3	1:B:385:GLU:OE1	2.18	0.44
1:B:263:ARG:HG2	1:B:263:ARG:HH11	1.82	0.44
1:B:20:ILE:HA	1:B:35:MET:CE	2.47	0.44
1:B:582:GLU:O	1:B:586:LYS:HG3	2.18	0.44
1:D:84:MET:HE3	1:D:95:SER:C	2.42	0.44
1:B:46:MET:CE	1:B:52:ILE:HD11	2.47	0.44
1:B:487:TYR:CD1	1:B:505:VAL:HG11	2.52	0.44
1:C:487:TYR:CD1	1:C:505:VAL:HG11	2.53	0.44
1:A:288:GLU:H	1:A:288:GLU:HG3	1.50	0.44
1:A:356:PRO:HA	1:A:357:PRO:HD3	1.84	0.44
1:B:377:ASN:HA	1:B:381:THR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:THR:HG21	1:C:342:VAL:HG23	1.98	0.44
1:D:230:PHE:CZ	1:D:236:GLY:HA2	2.53	0.44
1:D:483:TRP:CE2	1:D:527:PRO:HG3	2.53	0.44
1:B:227:LYS:HB2	1:B:227:LYS:HE3	1.84	0.44
1:B:356:PRO:HA	1:B:357:PRO:HD3	1.80	0.44
1:C:570:TYR:CZ	1:C:584:LEU:HB3	2.53	0.44
1:A:329:TRP:CZ3	1:B:2:ALA:HA	2.52	0.43
1:B:466:SER:OG	1:B:469:GLN:HG3	2.18	0.43
1:C:7:GLU:HG2	1:C:148:LYS:HB2	2.00	0.43
1:C:84:MET:HB3	1:C:87:THR:HG22	2.00	0.43
1:D:333:ARG:HA	1:D:338:LEU:O	2.18	0.43
1:B:577:THR:HG22	1:B:578:LYS:H	1.82	0.43
1:D:77:GLN:NE2	1:D:77:GLN:O	2.51	0.43
1:C:17:HIS:HE1	3:C:622:HOH:O	2.01	0.43
1:D:3:TRP:N	1:D:3:TRP:CD1	2.87	0.43
1:D:137:VAL:O	1:D:137:VAL:HG22	2.18	0.43
1:A:210:THR:HG21	1:A:342:VAL:HG23	2.00	0.43
1:C:416:TYR:CE1	1:C:438:SER:OG	2.72	0.43
1:C:543:GLU:HB3	1:C:544:PRO:HD3	1.99	0.43
1:C:543:GLU:N	1:C:544:PRO:CD	2.82	0.43
1:C:577:THR:HG22	1:C:580:ALA:HB2	2.01	0.43
1:A:227:LYS:HE3	1:A:227:LYS:HB2	1.74	0.43
1:B:199:LYS:HA	1:B:350:ILE:O	2.19	0.43
1:B:263:ARG:HG2	1:B:263:ARG:NH1	2.33	0.43
1:C:529:HIS:HE1	3:C:630:HOH:O	2.01	0.43
1:D:227:LYS:HD3	1:D:234:PRO:HD2	2.00	0.43
1:B:130:ILE:HD11	1:B:140:ARG:HG3	2.00	0.43
1:C:199:LYS:HA	1:C:350:ILE:O	2.19	0.43
1:C:285:PRO:HA	3:C:741:HOH:O	2.19	0.43
1:A:492:VAL:HG11	1:A:522:PHE:CE1	2.54	0.43
1:A:590:ILE:HG13	1:A:591:THR:HG23	2.01	0.43
1:B:336:PRO:HA	1:B:339:GLU:OE2	2.18	0.43
1:D:319:LEU:HD22	1:D:331:MET:HE1	2.01	0.43
1:D:450:ASN:HD21	1:D:454:ARG:HE	1.63	0.43
1:D:466:SER:N	1:D:469:GLN:HE21	2.03	0.43
1:A:49:ASN:HA	1:A:50:PRO:HD3	1.90	0.43
1:C:3:TRP:CD1	1:C:3:TRP:N	2.86	0.43
1:D:7:GLU:HB3	3:D:937:HOH:O	2.19	0.43
1:D:56:ALA:HB3	1:D:435:LEU:HB3	2.01	0.43
1:D:319:LEU:HD22	1:D:331:MET:CE	2.49	0.43
1:A:145:VAL:CG1	1:B:329:TRP:HH2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:THR:HG21	1:B:336:PRO:O	2.19	0.42
1:C:110:LYS:HE2	1:C:114:GLU:OE2	2.19	0.42
1:C:377:ASN:HA	1:C:381:THR:O	2.19	0.42
1:D:263:ARG:HG2	1:D:263:ARG:NH1	2.34	0.42
1:B:43:ILE:O	1:B:106:ARG:HG2	2.18	0.42
1:D:108:TYR:CD2	1:D:108:TYR:C	2.98	0.42
1:A:352:TYR:CD1	1:A:352:TYR:N	2.87	0.42
1:A:103:LYS:CD	1:B:107:GLU:OE2	2.67	0.42
1:B:381:THR:HG22	1:B:433:TYR:HB3	2.01	0.42
1:C:79:GLY:HA3	1:C:82:PHE:CZ	2.54	0.42
1:A:46:MET:HE3	1:A:52:ILE:HD11	2.01	0.42
1:A:331:MET:HG3	1:A:332:TYR:N	2.35	0.42
1:A:333:ARG:HA	1:A:338:LEU:O	2.19	0.42
1:B:70:GLU:O	1:B:71:MET:C	2.63	0.42
1:B:483:TRP:CD2	1:B:527:PRO:HG3	2.54	0.42
1:B:319:LEU:HD22	1:B:331:MET:HE2	2.01	0.42
1:C:254:THR:HG23	1:C:302:ILE:HD11	2.02	0.42
1:C:450:ASN:H	1:C:450:ASN:HD22	1.68	0.42
1:D:560:GLU:OE1	1:D:597:ARG:NH2	2.52	0.42
1:A:230:PHE:CZ	1:A:236:GLY:HA2	2.54	0.42
1:C:357:PRO:HB2	1:C:424:LEU:O	2.19	0.42
1:D:607:THR:O	1:D:611:VAL:HG23	2.19	0.42
1:A:227:LYS:HD3	1:A:234:PRO:HD2	2.02	0.42
1:A:263:ARG:HG2	1:A:263:ARG:HH11	1.85	0.42
1:B:16:GLY:O	1:B:20:ILE:HG13	2.20	0.42
1:B:17:HIS:HE1	3:B:620:HOH:O	2.03	0.42
1:C:70:GLU:O	1:C:71:MET:C	2.63	0.42
1:D:257:LYS:O	1:D:261:ILE:HG13	2.19	0.42
1:B:473:VAL:O	1:B:477:GLU:HB2	2.19	0.41
1:D:130:ILE:HD11	1:D:140:ARG:CD	2.50	0.41
1:A:572:LYS:O	1:A:574:PRO:HD3	2.20	0.41
1:D:427:LYS:NZ	3:D:966:HOH:O	2.52	0.41
1:A:126:VAL:HG13	1:A:139:VAL:CG1	2.49	0.41
1:A:176:LEU:HB2	1:A:348:TYR:CE1	2.55	0.41
1:A:377:ASN:ND2	2:A:618:FAD:H5'1	2.35	0.41
1:A:583:LYS:HZ2	1:A:600:GLY:HA3	1.83	0.41
1:A:585:LYS:HD2	1:A:585:LYS:HA	1.86	0.41
1:B:471:LYS:HE3	1:B:471:LYS:HB2	1.87	0.41
1:B:594:GLN:HA	1:B:597:ARG:HH12	1.78	0.41
1:C:411:ARG:HB3	1:C:413:ASP:OD1	2.20	0.41
1:D:176:LEU:HB2	1:D:348:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:LYS:HB2	1:D:227:LYS:HE3	1.78	0.41
1:A:579:GLU:OE2	1:D:578:LYS:HD3	2.20	0.41
1:B:319:LEU:HD22	1:B:331:MET:HE1	2.02	0.41
1:C:373:PHE:O	1:C:374:HIS:HD2	2.04	0.41
1:D:436:PHE:CD2	1:D:436:PHE:C	2.98	0.41
1:A:186:ASP:O	1:A:190:ARG:HB2	2.20	0.41
1:A:510:THR:O	1:A:510:THR:CG2	2.65	0.41
1:B:508:LEU:O	1:B:513:TYR:HB2	2.21	0.41
1:C:16:GLY:O	1:C:20:ILE:HG13	2.20	0.41
1:C:96:PRO:HB2	1:C:228:PHE:CE2	2.56	0.41
1:B:594:GLN:HA	1:B:597:ARG:CZ	2.50	0.41
1:C:145:VAL:CG1	1:C:146:GLU:N	2.83	0.41
1:C:262:ILE:CG2	1:C:291:ILE:HD11	2.50	0.41
1:D:49:ASN:HA	1:D:50:PRO:HD3	1.90	0.41
1:D:509:MET:HE1	1:D:515:LEU:HG	2.03	0.41
1:A:36:PHE:HA	1:A:122:LYS:O	2.20	0.41
1:A:210:THR:HG21	1:A:342:VAL:CG2	2.50	0.41
1:A:583:LYS:HB3	1:A:583:LYS:HE2	1.90	0.41
1:B:176:LEU:HB2	1:B:348:TYR:CE1	2.56	0.41
1:C:298:GLU:HG3	1:C:299:ARG:HG2	2.01	0.41
1:C:588:LYS:HD2	3:C:1010:HOH:O	2.19	0.41
1:A:383:GLY:HA2	2:A:618:FAD:O2	2.21	0.41
1:B:79:GLY:HA3	1:B:82:PHE:CZ	2.56	0.41
1:B:507:THR:HG22	1:B:511:MET:HE3	2.02	0.41
1:D:336:PRO:HA	1:D:339:GLU:OE2	2.21	0.41
1:D:511:MET:O	1:D:512:ASN:HB2	2.21	0.41
1:A:45:GLN:HG3	3:A:866:HOH:O	2.20	0.41
1:C:130:ILE:HD11	1:C:140:ARG:HD2	2.03	0.41
1:C:329:TRP:HH2	1:D:145:VAL:CG1	2.34	0.41
1:C:381:THR:HG22	1:C:433:TYR:HB3	2.02	0.41
1:D:28:ARG:HE	1:D:116:GLN:HE22	1.69	0.41
1:D:36:PHE:HA	1:D:122:LYS:O	2.20	0.41
1:D:564:ILE:HD11	1:D:609:LEU:HD21	2.03	0.41
1:A:107:GLU:OE1	1:B:107:GLU:CD	2.64	0.41
1:A:406:GLU:HA	1:A:407:PRO:HD3	1.92	0.41
1:B:570:TYR:CZ	1:B:584:LEU:HB3	2.56	0.41
1:C:20:ILE:HA	1:C:35:MET:HE1	2.03	0.41
1:C:84:MET:HG2	1:C:94:GLN:OE1	2.21	0.41
1:C:204:ALA:O	1:C:316:PRO:HD2	2.21	0.40
1:C:565:PRO:HA	1:C:566:PRO:HD3	1.87	0.40
1:D:17:HIS:HD2	3:D:632:HOH:O	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:LEU:HB2	1:D:348:TYR:CZ	2.56	0.40
1:A:130:ILE:HD11	1:A:140:ARG:CD	2.51	0.40
1:A:551:LYS:O	1:A:554:GLU:HG3	2.21	0.40
1:B:319:LEU:HD13	1:B:332:TYR:CE1	2.57	0.40
1:C:23:ALA:HB3	1:C:35:MET:CE	2.49	0.40
1:C:473:VAL:O	1:C:477:GLU:HB2	2.21	0.40
1:A:130:ILE:HG22	1:A:137:VAL:HG13	2.01	0.40
1:B:452:ILE:HG23	1:B:453:LEU:N	2.37	0.40
1:B:492:VAL:HG12	1:B:493:SER:N	2.37	0.40
1:C:286:SER:O	1:C:287:ILE:C	2.65	0.40
1:C:298:GLU:HG3	1:C:299:ARG:CG	2.51	0.40
1:D:494:VAL:HG12	1:D:495:ALA:N	2.36	0.40
1:A:2:ALA:HA	1:B:329:TRP:CZ3	2.56	0.40
1:A:555:LYS:HA	1:A:555:LYS:HD3	1.89	0.40
1:D:510:THR:O	1:D:510:THR:CG2	2.66	0.40
1:A:492:VAL:HG11	1:A:522:PHE:CD1	2.56	0.40
1:A:596:SER:HA	1:A:606:ILE:HD11	2.03	0.40
1:B:204:ALA:O	1:B:316:PRO:HD2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	598/637 (94%)	577 (96%)	21 (4%)	0	100	100
1	B	602/637 (94%)	586 (97%)	16 (3%)	0	100	100
1	C	598/637 (94%)	582 (97%)	16 (3%)	0	100	100
1	D	599/637 (94%)	580 (97%)	18 (3%)	1 (0%)	43	55
All	All	2397/2548 (94%)	2325 (97%)	71 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	55	ILE

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	514/540 (95%)	498 (97%)	16 (3%)	35	52
1	B	517/540 (96%)	502 (97%)	15 (3%)	37	55
1	C	516/540 (96%)	497 (96%)	19 (4%)	30	45
1	D	515/540 (95%)	494 (96%)	21 (4%)	27	41
All	All	2062/2160 (96%)	1991 (97%)	71 (3%)	32	49

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	104	ARG
1	A	145	VAL
1	A	192	ASP
1	A	209	ARG
1	A	220	PRO
1	A	288	GLU
1	A	299	ARG
1	A	331	MET
1	A	386	GLU
1	A	416	TYR
1	A	430	THR
1	A	510	THR
1	A	533	LYS
1	A	582	GLU
1	A	615	LYS
1	B	32	LYS
1	B	137	VAL
1	B	139	VAL
1	B	145	VAL
1	B	209	ARG

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Mol	Chain	Res	Type
1	B	299	ARG
1	B	321	THR
1	B	366	THR
1	B	386	GLU
1	B	450	ASN
1	B	550	ARG
1	B	577	THR
1	B	579	GLU
1	B	582	GLU
1	B	606	ILE
1	C	52	ILE
1	C	88	ARG
1	C	103	LYS
1	C	104	ARG
1	C	137	VAL
1	C	139	VAL
1	C	145	VAL
1	C	209	ARG
1	C	288	GLU
1	C	298	GLU
1	C	299	ARG
1	C	321	THR
1	C	366	THR
1	C	386	GLU
1	C	441	GLU
1	C	450	ASN
1	C	533	LYS
1	C	558	LYS
1	C	567	ASP
1	D	77	GLN
1	D	86	ASN
1	D	103	LYS
1	D	145	VAL
1	D	192	ASP
1	D	209	ARG
1	D	288	GLU
1	D	299	ARG
1	D	366	THR
1	D	386	GLU
1	D	414	GLU
1	D	416	TYR
1	D	430	THR

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Mol	Chain	Res	Type
1	D	450	ASN
1	D	475	GLU
1	D	490	GLU
1	D	510	THR
1	D	533	LYS
1	D	550	ARG
1	D	579	GLU
1	D	582	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	17	HIS
1	A	45	GLN
1	A	49	ASN
1	A	94	GLN
1	A	377	ASN
1	A	529	HIS
1	B	0	HIS
1	B	17	HIS
1	B	49	ASN
1	B	77	GLN
1	B	115	ASN
1	B	161	ASN
1	B	248	ASN
1	B	300	HIS
1	B	450	ASN
1	B	469	GLN
1	B	512	ASN
1	B	529	HIS
1	B	594	GLN
1	C	0	HIS
1	C	17	HIS
1	C	49	ASN
1	C	77	GLN
1	C	115	ASN
1	C	134	ASN
1	C	161	ASN
1	C	248	ASN
1	C	300	HIS
1	C	340	ASN

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Mol	Chain	Res	Type
1	C	377	ASN
1	C	450	ASN
1	C	512	ASN
1	C	529	HIS
1	C	594	GLN
1	D	0	HIS
1	D	17	HIS
1	D	49	ASN
1	D	77	GLN
1	D	116	GLN
1	D	118	ASN
1	D	134	ASN
1	D	161	ASN
1	D	450	ASN
1	D	469	GLN
1	D	512	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
2	FAD	C	618	-	58,58,58	1.81	15 (25%)	85,89,89	1.95	23 (27%)
2	FAD	B	618	-	58,58,58	1.84	16 (27%)	85,89,89	1.95	22 (25%)
2	FAD	D	618	-	58,58,58	1.84	18 (31%)	85,89,89	1.95	23 (27%)
2	FAD	A	618	-	58,58,58	1.81	16 (27%)	85,89,89	1.95	24 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	618	-	-	5/34/50/50	0/6/6/6
2	FAD	B	618	-	-	5/34/50/50	0/6/6/6
2	FAD	D	618	-	-	5/34/50/50	0/6/6/6
2	FAD	A	618	-	-	5/34/50/50	0/6/6/6

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	618	FAD	C4X-N5	4.96	1.41	1.30
2	B	618	FAD	C4X-N5	4.86	1.41	1.30
2	D	618	FAD	C4X-N5	4.64	1.40	1.30
2	A	618	FAD	C4X-N5	4.58	1.40	1.30
2	C	618	FAD	C6-C7	4.45	1.45	1.39
2	B	618	FAD	C6-C7	4.36	1.45	1.39
2	A	618	FAD	O4-C4	-4.34	1.15	1.23
2	D	618	FAD	O4-C4	-4.26	1.15	1.23
2	A	618	FAD	C6-C7	4.20	1.45	1.39
2	D	618	FAD	C6-C7	4.18	1.45	1.39
2	B	618	FAD	C1'-C2'	3.62	1.57	1.52
2	B	618	FAD	C10-N10	3.56	1.45	1.37
2	C	618	FAD	O4-C4	-3.50	1.16	1.23
2	B	618	FAD	O4-C4	-3.49	1.16	1.23
2	A	618	FAD	C9-C9A	3.29	1.44	1.39
2	D	618	FAD	C1'-C2'	3.25	1.57	1.52
2	D	618	FAD	C9-C9A	3.23	1.44	1.39
2	C	618	FAD	C10-N10	3.18	1.44	1.37
2	D	618	FAD	C10-N10	3.13	1.44	1.37
2	B	618	FAD	P-O2P	-3.11	1.40	1.55
2	C	618	FAD	P-O2P	-3.11	1.41	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	618	FAD	P-O2P	-3.08	1.41	1.55
2	C	618	FAD	C1'-C2'	3.08	1.56	1.52
2	A	618	FAD	P-O2P	-3.03	1.41	1.55
2	D	618	FAD	O4B-C4B	-3.00	1.38	1.45
2	A	618	FAD	C10-N10	2.97	1.43	1.37
2	C	618	FAD	O4B-C4B	-2.95	1.38	1.45
2	A	618	FAD	PA-O2A	-2.92	1.41	1.55
2	A	618	FAD	O4B-C4B	-2.86	1.38	1.45
2	C	618	FAD	C9-C9A	2.84	1.44	1.39
2	C	618	FAD	C6-C5X	2.84	1.44	1.40
2	B	618	FAD	C9-C9A	2.79	1.44	1.39
2	D	618	FAD	PA-O2A	-2.77	1.42	1.55
2	B	618	FAD	O4B-C4B	-2.74	1.38	1.45
2	B	618	FAD	C6-C5X	2.74	1.44	1.40
2	C	618	FAD	PA-O2A	-2.72	1.42	1.55
2	B	618	FAD	PA-O2A	-2.63	1.43	1.55
2	A	618	FAD	C1'-C2'	2.59	1.56	1.52
2	A	618	FAD	PA-O1A	-2.45	1.42	1.50
2	A	618	FAD	C6-C5X	2.43	1.43	1.40
2	D	618	FAD	C6-C5X	2.42	1.43	1.40
2	B	618	FAD	C10-N1	2.41	1.38	1.33
2	D	618	FAD	C5A-N7A	-2.37	1.34	1.39
2	C	618	FAD	C10-N1	2.37	1.38	1.33
2	D	618	FAD	O3'-C3'	-2.32	1.37	1.43
2	C	618	FAD	PA-O1A	-2.23	1.43	1.50
2	D	618	FAD	PA-O1A	-2.23	1.43	1.50
2	B	618	FAD	C5A-C4A	2.21	1.43	1.39
2	A	618	FAD	C5A-N7A	-2.18	1.35	1.39
2	B	618	FAD	PA-O1A	-2.18	1.43	1.50
2	D	618	FAD	P-O1P	-2.17	1.43	1.50
2	B	618	FAD	C5A-N7A	-2.14	1.35	1.39
2	A	618	FAD	C10-N1	2.11	1.37	1.33
2	C	618	FAD	C2-N1	2.11	1.41	1.36
2	B	618	FAD	C2'-C3'	2.10	1.57	1.53
2	C	618	FAD	C5A-N7A	-2.09	1.35	1.39
2	A	618	FAD	O3'-C3'	-2.09	1.37	1.43
2	D	618	FAD	C10-N1	2.08	1.37	1.33
2	D	618	FAD	C9A-C5X	2.07	1.44	1.41
2	C	618	FAD	C5A-C4A	2.06	1.42	1.39
2	D	618	FAD	C5A-C4A	2.04	1.42	1.39
2	A	618	FAD	P-O1P	-2.03	1.43	1.50
2	A	618	FAD	C2-N1	2.02	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	618	FAD	C2'-C3'	2.02	1.56	1.53
2	B	618	FAD	P-O1P	-2.01	1.43	1.50

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	618	FAD	C5A-C4A-N3A	-5.23	119.52	126.72
2	D	618	FAD	C5A-C4A-N3A	-5.09	119.71	126.72
2	C	618	FAD	C5A-C4A-N3A	-5.09	119.71	126.72
2	A	618	FAD	C5A-C4A-N3A	-5.04	119.78	126.72
2	D	618	FAD	N3A-C2A-N1A	-4.65	121.54	128.58
2	A	618	FAD	N3A-C2A-N1A	-4.63	121.57	128.58
2	B	618	FAD	N3A-C4A-N9A	4.58	134.96	127.17
2	D	618	FAD	N3A-C4A-N9A	4.51	134.84	127.17
2	B	618	FAD	N3A-C2A-N1A	-4.50	121.78	128.58
2	C	618	FAD	N3A-C2A-N1A	-4.49	121.78	128.58
2	A	618	FAD	N3A-C4A-N9A	4.49	134.80	127.17
2	D	618	FAD	C4-N3-C2	-4.45	117.73	125.64
2	C	618	FAD	N3A-C4A-N9A	4.45	134.73	127.17
2	C	618	FAD	C4-N3-C2	-4.45	117.74	125.64
2	A	618	FAD	C4-N3-C2	-4.43	117.77	125.64
2	B	618	FAD	C4-N3-C2	-4.43	117.77	125.64
2	C	618	FAD	C4-C4X-N5	3.97	123.69	118.21
2	B	618	FAD	C4-C4X-N5	3.94	123.66	118.21
2	A	618	FAD	C4-C4X-N5	3.92	123.63	118.21
2	C	618	FAD	C10-C4X-N5	-3.87	116.91	124.81
2	B	618	FAD	C10-C4X-N5	-3.87	116.91	124.81
2	D	618	FAD	C4-C4X-N5	3.81	123.47	118.21
2	D	618	FAD	C4'-C3'-C2'	3.78	119.86	113.57
2	B	618	FAD	C2A-N3A-C4A	3.78	121.05	111.83
2	A	618	FAD	C4'-C3'-C2'	3.77	119.85	113.57
2	A	618	FAD	C10-C4X-N5	-3.77	117.10	124.81
2	D	618	FAD	C10-C4X-N5	-3.75	117.14	124.81
2	D	618	FAD	C2A-N3A-C4A	3.73	120.93	111.83
2	C	618	FAD	C5A-N7A-C8A	3.71	109.28	103.45
2	A	618	FAD	C2A-N3A-C4A	3.70	120.87	111.83
2	C	618	FAD	C2A-N3A-C4A	3.70	120.86	111.83
2	B	618	FAD	C5A-N7A-C8A	3.69	109.26	103.45
2	A	618	FAD	C4X-C4-N3	3.65	122.54	113.25
2	D	618	FAD	C5A-N7A-C8A	3.63	109.15	103.45
2	A	618	FAD	C5A-N7A-C8A	3.59	109.09	103.45
2	D	618	FAD	C4X-C4-N3	3.58	122.37	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	618	FAD	C4X-C4-N3	3.52	122.22	113.25
2	C	618	FAD	C5X-N5-C4X	3.45	123.67	118.09
2	B	618	FAD	C5X-N5-C4X	3.45	123.67	118.09
2	B	618	FAD	C4X-C4-N3	3.43	121.99	113.25
2	B	618	FAD	C4'-C3'-C2'	3.41	119.25	113.57
2	A	618	FAD	C4X-C10-N10	3.37	121.31	116.48
2	D	618	FAD	C4X-C10-N10	3.34	121.27	116.48
2	D	618	FAD	C4X-C10-N1	-3.31	116.47	124.59
2	A	618	FAD	O4-C4-N3	-3.29	113.94	120.11
2	D	618	FAD	C5X-N5-C4X	3.28	123.40	118.09
2	A	618	FAD	C5X-N5-C4X	3.26	123.36	118.09
2	A	618	FAD	C4X-C10-N1	-3.26	116.60	124.59
2	B	618	FAD	C4X-C10-N10	3.26	121.15	116.48
2	B	618	FAD	C4X-C10-N1	-3.25	116.61	124.59
2	C	618	FAD	O4-C4-N3	-3.25	114.00	120.11
2	C	618	FAD	C4X-C10-N1	-3.25	116.62	124.59
2	C	618	FAD	C4X-C10-N10	3.22	121.09	116.48
2	D	618	FAD	O4-C4-N3	-3.20	114.10	120.11
2	C	618	FAD	C4'-C3'-C2'	3.14	118.80	113.57
2	B	618	FAD	O4-C4-N3	-3.11	114.26	120.11
2	B	618	FAD	C4A-C5A-N7A	-2.92	107.25	110.58
2	C	618	FAD	C4A-C5A-N7A	-2.91	107.26	110.58
2	C	618	FAD	C4A-N9A-C1B	-2.86	119.94	126.63
2	A	618	FAD	C4A-C5A-N7A	-2.82	107.36	110.58
2	B	618	FAD	C10-N1-C2	2.82	122.95	116.85
2	C	618	FAD	C10-N1-C2	2.81	122.93	116.85
2	D	618	FAD	C4A-C5A-N7A	-2.80	107.38	110.58
2	B	618	FAD	C9A-C9-C8	2.79	124.83	119.22
2	C	618	FAD	C9A-C9-C8	2.76	124.78	119.22
2	D	618	FAD	C10-N1-C2	2.74	122.78	116.85
2	A	618	FAD	C4A-N9A-C1B	-2.73	120.25	126.63
2	A	618	FAD	C10-N1-C2	2.72	122.74	116.85
2	C	618	FAD	N9A-C8A-N7A	-2.69	110.12	113.94
2	B	618	FAD	C4A-N9A-C1B	-2.64	120.46	126.63
2	D	618	FAD	C4A-N9A-C1B	-2.63	120.49	126.63
2	A	618	FAD	C9A-C9-C8	2.62	124.48	119.22
2	D	618	FAD	C9A-C9-C8	2.61	124.46	119.22
2	A	618	FAD	N9A-C8A-N7A	-2.55	110.32	113.94
2	B	618	FAD	N9A-C8A-N7A	-2.54	110.33	113.94
2	D	618	FAD	N9A-C8A-N7A	-2.53	110.34	113.94
2	C	618	FAD	C9A-C5X-N5	-2.44	119.86	122.45
2	B	618	FAD	C9A-C5X-N5	-2.30	120.01	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	618	FAD	O5'-C5'-C4'	2.29	115.48	109.36
2	A	618	FAD	C9A-C5X-N5	-2.26	120.05	122.45
2	A	618	FAD	O5'-C5'-C4'	2.23	115.30	109.36
2	C	618	FAD	C1B-N9A-C8A	2.22	132.03	127.09
2	C	618	FAD	O5'-C5'-C4'	2.22	115.29	109.36
2	A	618	FAD	O2'-C2'-C3'	2.22	114.44	109.25
2	D	618	FAD	C9A-C5X-N5	-2.17	120.15	122.45
2	D	618	FAD	O2'-C2'-C3'	2.15	114.27	109.25
2	C	618	FAD	O2'-C2'-C3'	2.10	114.16	109.25
2	A	618	FAD	C1B-N9A-C8A	2.09	131.73	127.09
2	B	618	FAD	C1B-N9A-C8A	2.07	131.68	127.09
2	B	618	FAD	O2'-C2'-C3'	2.06	114.08	109.25
2	A	618	FAD	O3'-C3'-C2'	-2.04	104.29	108.93
2	D	618	FAD	C1B-N9A-C8A	2.03	131.59	127.09

There are no chirality outliers.

All (20) torsion outliers are listed below:

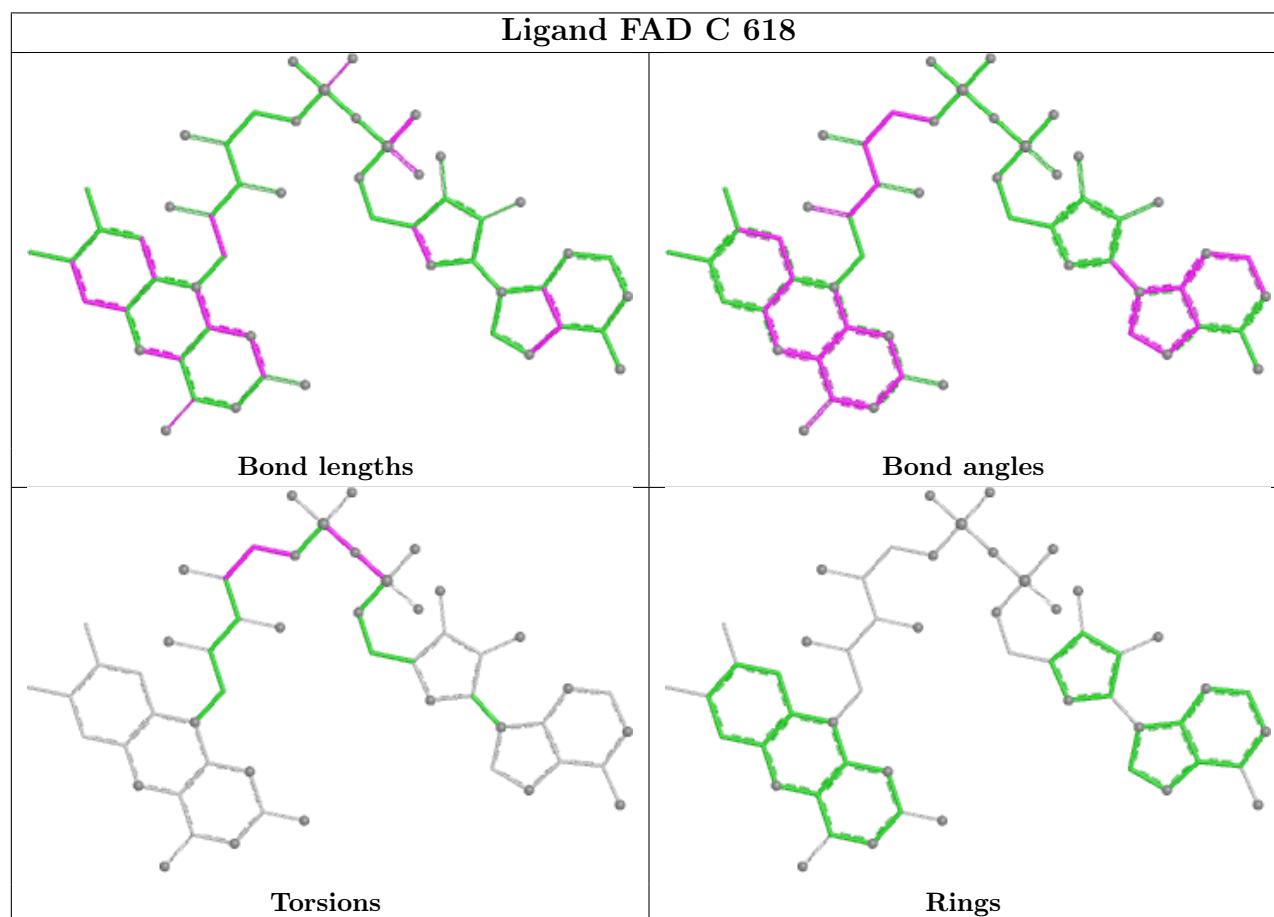
Mol	Chain	Res	Type	Atoms
2	A	618	FAD	C3'-C4'-C5'-O5'
2	A	618	FAD	O4'-C4'-C5'-O5'
2	A	618	FAD	C4'-C5'-O5'-P
2	B	618	FAD	C3'-C4'-C5'-O5'
2	B	618	FAD	O4'-C4'-C5'-O5'
2	B	618	FAD	C4'-C5'-O5'-P
2	C	618	FAD	C3'-C4'-C5'-O5'
2	C	618	FAD	O4'-C4'-C5'-O5'
2	C	618	FAD	C4'-C5'-O5'-P
2	D	618	FAD	C3'-C4'-C5'-O5'
2	D	618	FAD	O4'-C4'-C5'-O5'
2	D	618	FAD	C4'-C5'-O5'-P
2	A	618	FAD	PA-O3P-P-O5'
2	B	618	FAD	PA-O3P-P-O5'
2	C	618	FAD	PA-O3P-P-O5'
2	D	618	FAD	PA-O3P-P-O5'
2	A	618	FAD	P-O3P-PA-O2A
2	C	618	FAD	P-O3P-PA-O2A
2	B	618	FAD	P-O3P-PA-O2A
2	D	618	FAD	P-O3P-PA-O2A

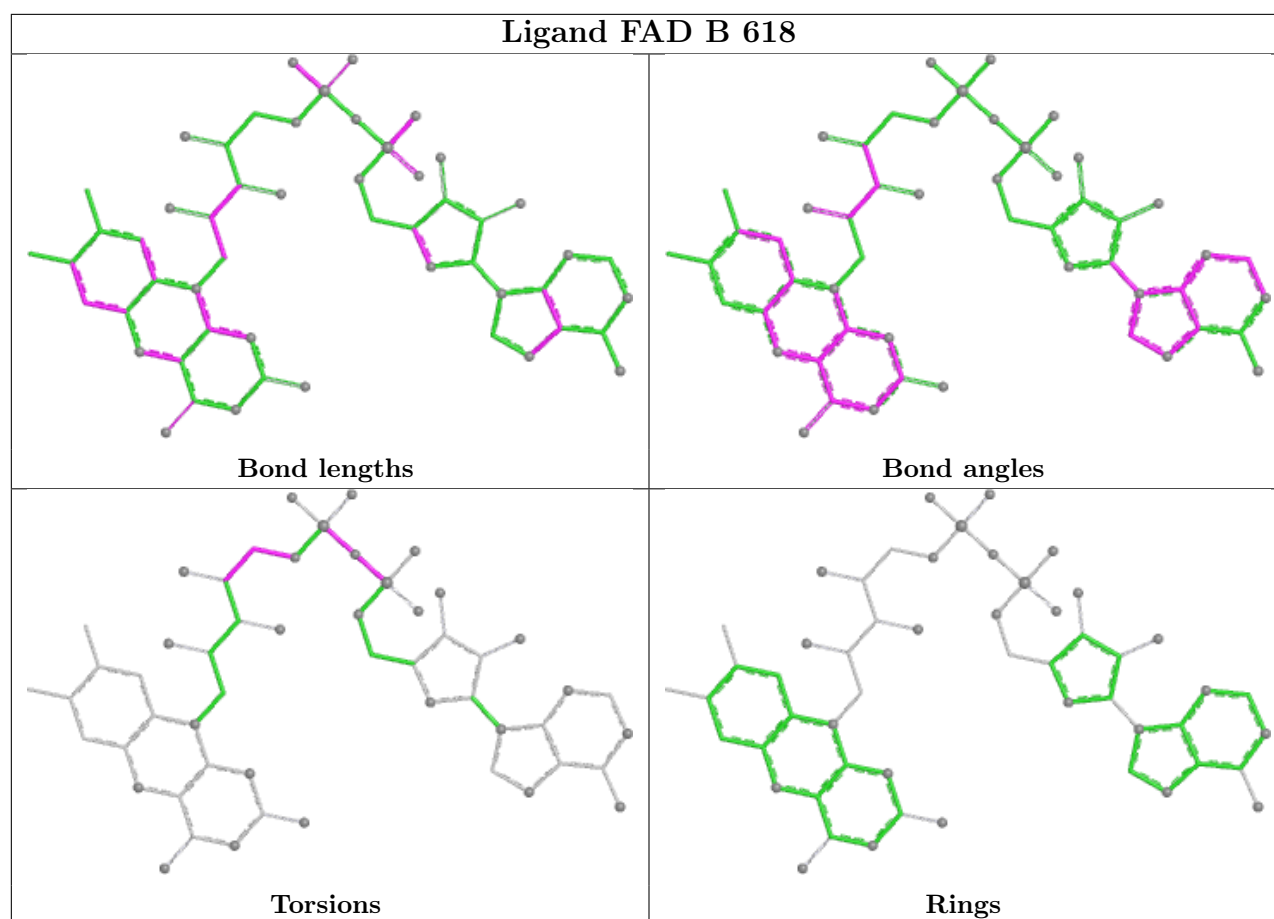
There are no ring outliers.

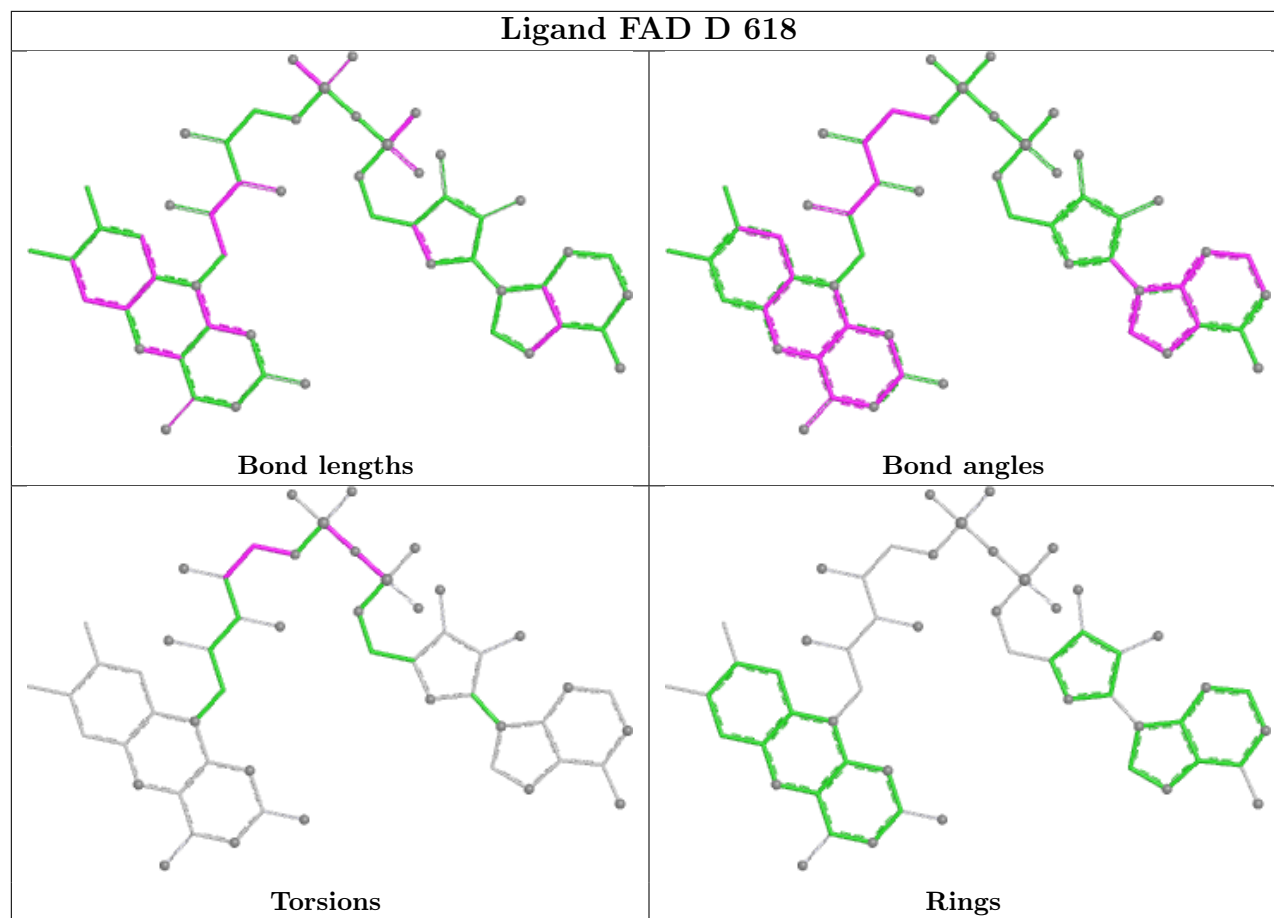
4 monomers are involved in 7 short contacts:

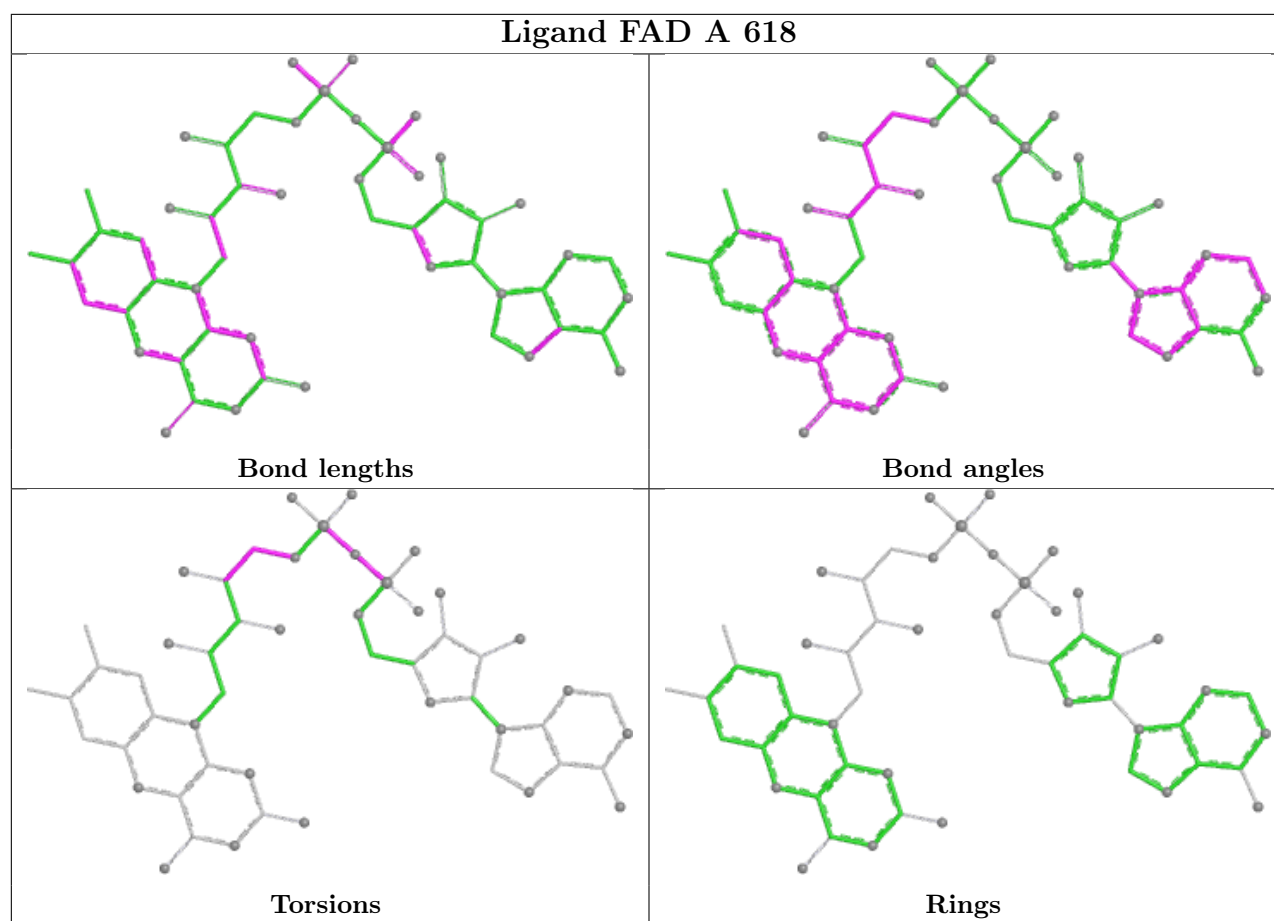
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	618	FAD	2	0
2	B	618	FAD	1	0
2	D	618	FAD	1	0
2	A	618	FAD	3	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	602/637 (94%)	-1.58	0 100 100	12, 25, 57, 79	0
1	B	606/637 (95%)	-1.60	0 100 100	11, 24, 54, 77	0
1	C	604/637 (94%)	-1.60	0 100 100	11, 24, 54, 77	0
1	D	603/637 (94%)	-1.58	0 100 100	10, 25, 58, 78	0
All	All	2415/2548 (94%)	-1.59	0 100 100	10, 25, 56, 79	0

There are no RSRZ outliers to report.

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](#)

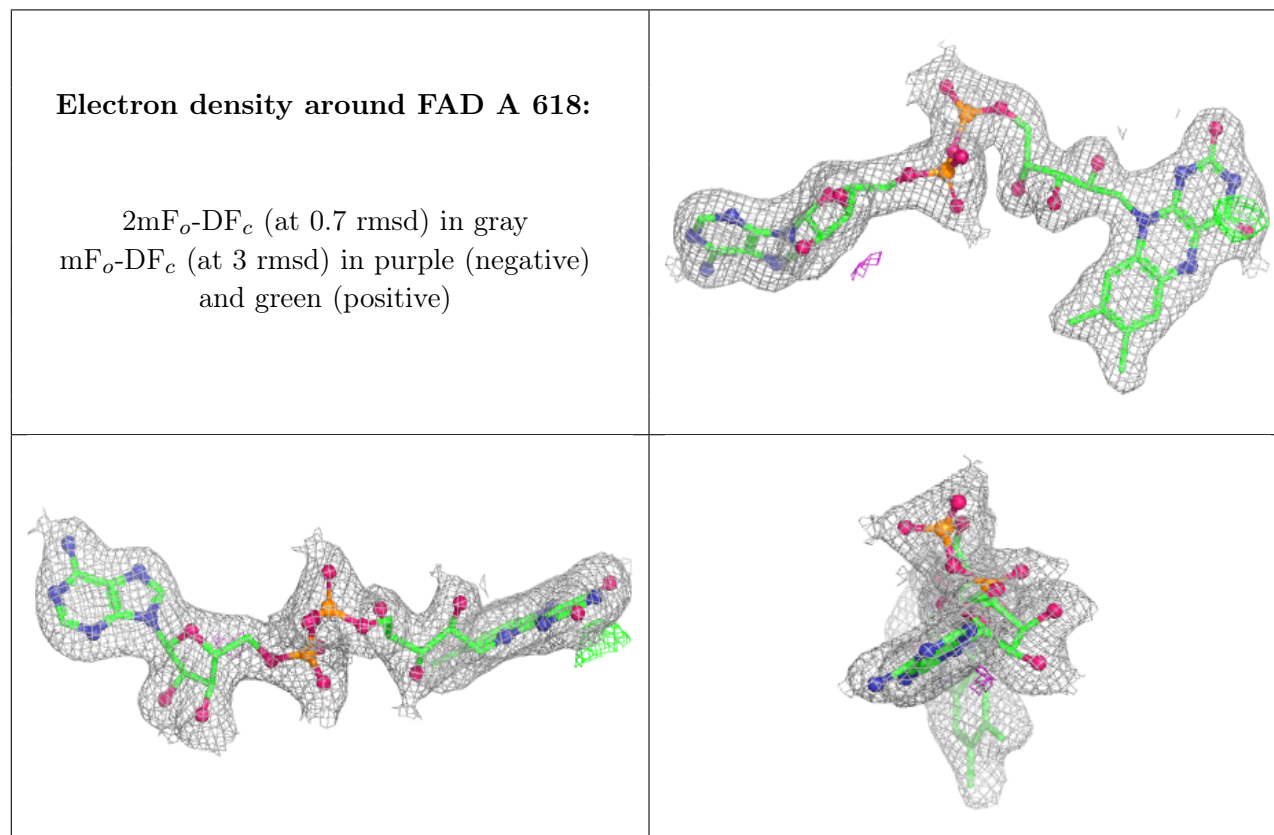
There are no oligosaccharides in this entry.

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.

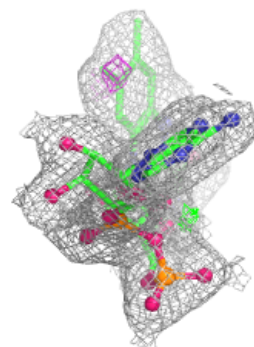
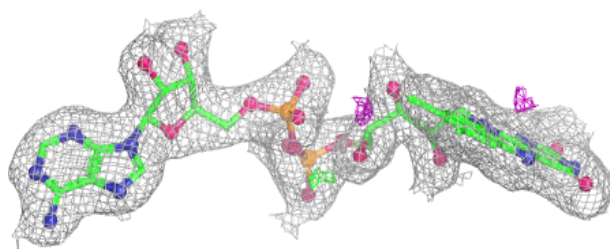
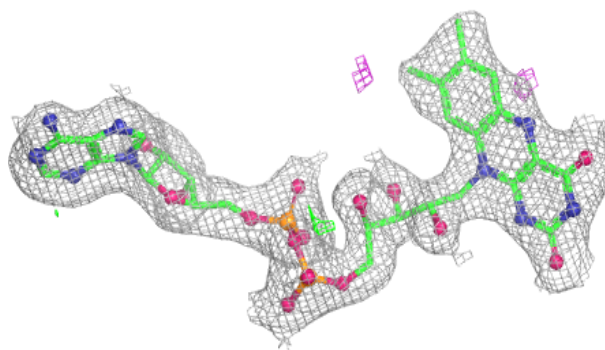
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	A	618	53/53	1.00	0.02	11,16,20,25	0
2	FAD	B	618	53/53	1.00	0.02	9,16,25,27	0
2	FAD	C	618	53/53	1.00	0.02	10,17,25,28	0
2	FAD	D	618	53/53	1.00	0.02	10,16,22,26	0

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.

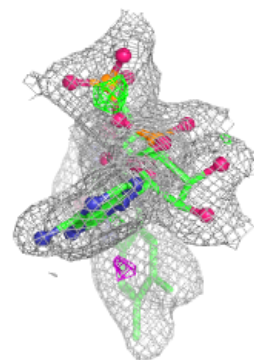
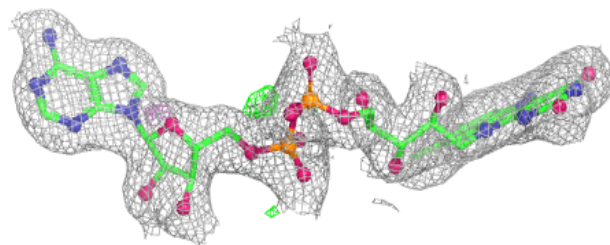
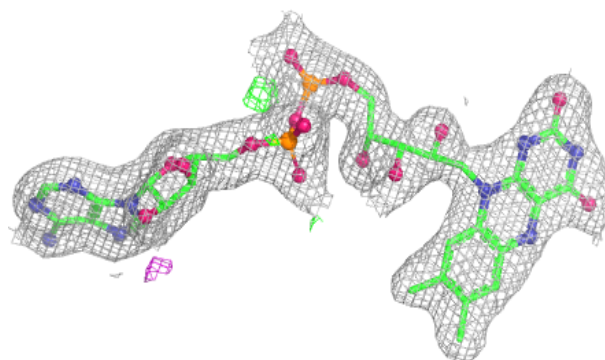


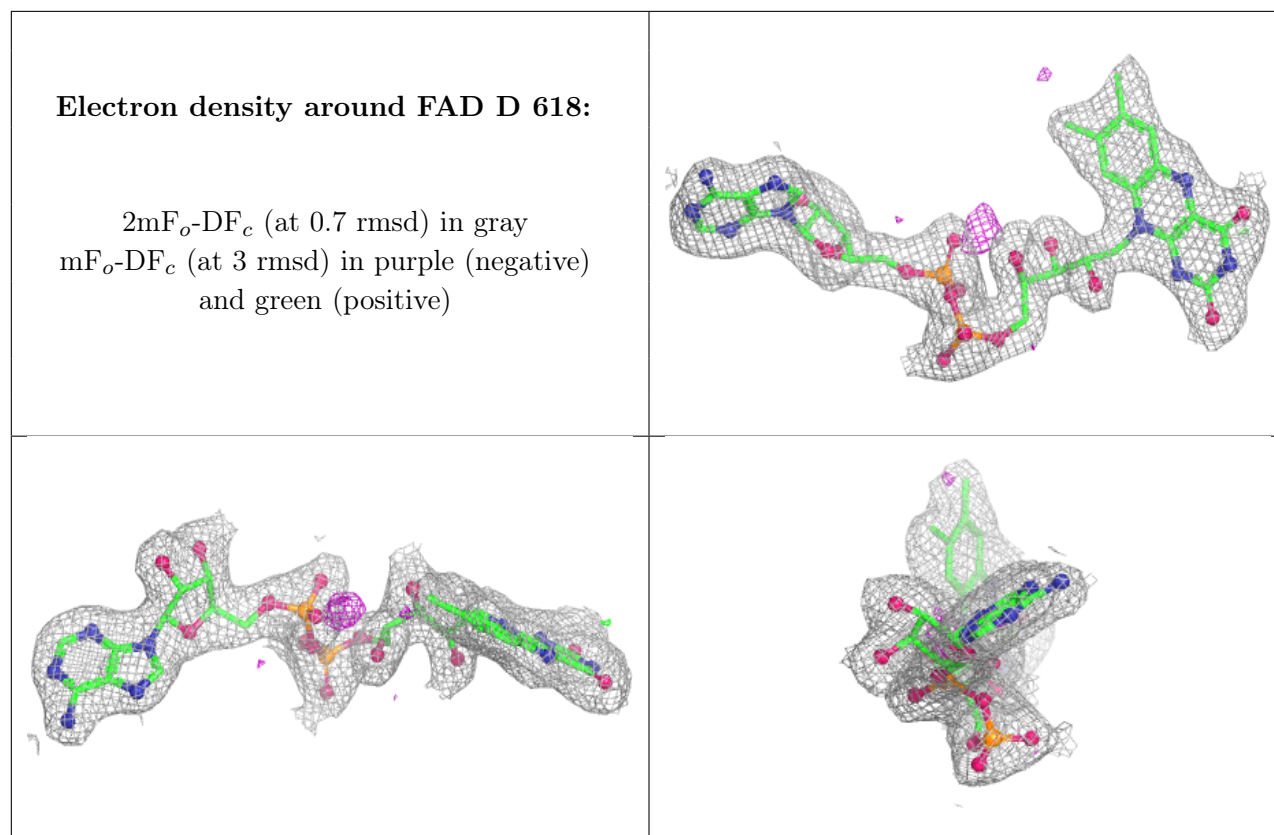
Electron density around FAD B 618:

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

**Electron density around FAD C 618:**

$2mF_o-DF_c$ (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.