



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:16 AM UTC

PDB ID : 8D7F / pdb_00008d7f
Title : FlvF from *Aspergillus flavus* in complex with Bis-Tris
Authors : Tararina, M.A.; Christianson, D.W.
Deposited on : 2022-06-07
Resolution : 2.62 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

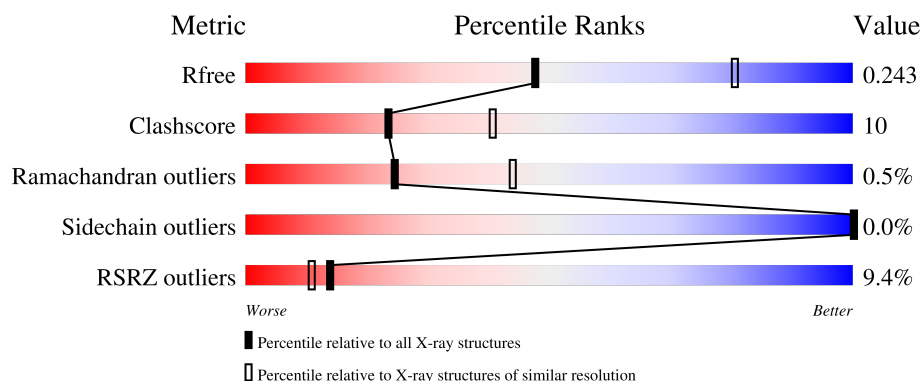
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	368	3% 81% 17% ..
1	B	368	2% 81% 16% ..
1	C	368	5% 79% 14% .. 5%
1	D	368	3% 77% 16% • 6%
1	E	368	5% 77% 15% 8%

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Mol	Chain	Length	Quality of chain
1	F	368	4% 74% 19% • 6%
1	G	368	24% 66% 23% • 9%
1	H	368	26% 62% 28% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22284 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 Terpene cyclase flvF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2939	1890	484	547	18			
1	B	361	Total	C	N	O	S	0	0	0
			2944	1895	485	547	17			
1	C	349	Total	C	N	O	S	0	1	0
			2806	1801	465	525	15			
1	D	345	Total	C	N	O	S	0	0	0
			2768	1778	456	519	15			
1	E	340	Total	C	N	O	S	0	0	0
			2756	1777	454	510	15			
1	F	345	Total	C	N	O	S	0	0	0
			2809	1809	465	520	15			
1	G	335	Total	C	N	O	S	0	0	0
			2580	1662	429	475	14			
1	H	334	Total	C	N	O	S	0	0	0
			2564	1654	428	468	14			

There are 24 discrepancies between the modelled and reference sequences:

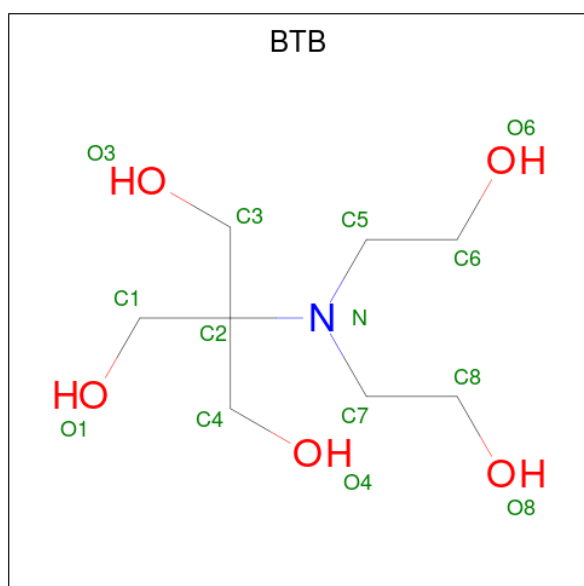
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP B8NHE1
A	0	ASN	-	expression tag	UNP B8NHE1
A	1	ALA	-	expression tag	UNP B8NHE1
B	-1	SER	-	expression tag	UNP B8NHE1
B	0	ASN	-	expression tag	UNP B8NHE1
B	1	ALA	-	expression tag	UNP B8NHE1
C	-1	SER	-	expression tag	UNP B8NHE1
C	0	ASN	-	expression tag	UNP B8NHE1
C	1	ALA	-	expression tag	UNP B8NHE1
D	-1	SER	-	expression tag	UNP B8NHE1
D	0	ASN	-	expression tag	UNP B8NHE1
D	1	ALA	-	expression tag	UNP B8NHE1
E	-1	SER	-	expression tag	UNP B8NHE1

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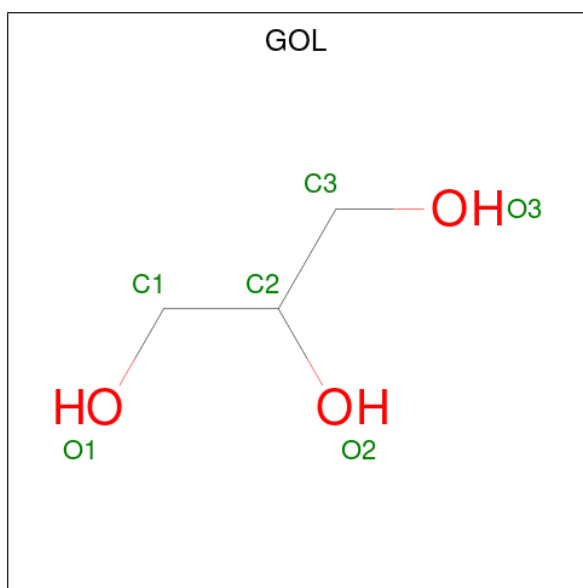
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	ASN	-	expression tag	UNP B8NHE1
E	1	ALA	-	expression tag	UNP B8NHE1
F	-1	SER	-	expression tag	UNP B8NHE1
F	0	ASN	-	expression tag	UNP B8NHE1
F	1	ALA	-	expression tag	UNP B8NHE1
G	-1	SER	-	expression tag	UNP B8NHE1
G	0	ASN	-	expression tag	UNP B8NHE1
G	1	ALA	-	expression tag	UNP B8NHE1
H	-1	SER	-	expression tag	UNP B8NHE1
H	0	ASN	-	expression tag	UNP B8NHE1
H	1	ALA	-	expression tag	UNP B8NHE1

- Molecule 2 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

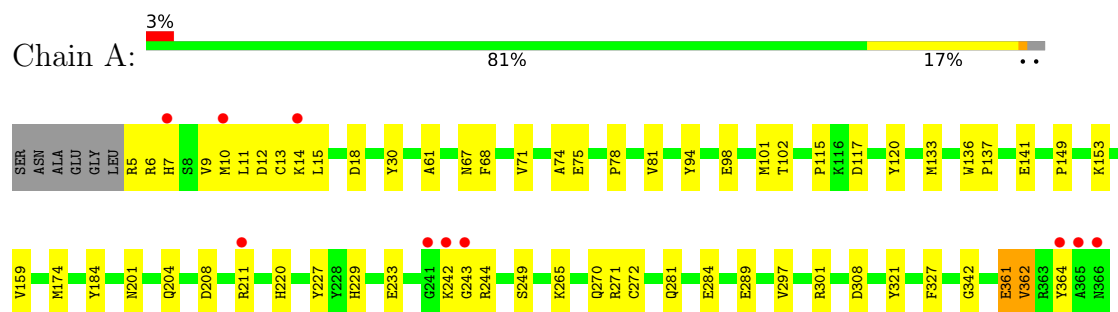


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		

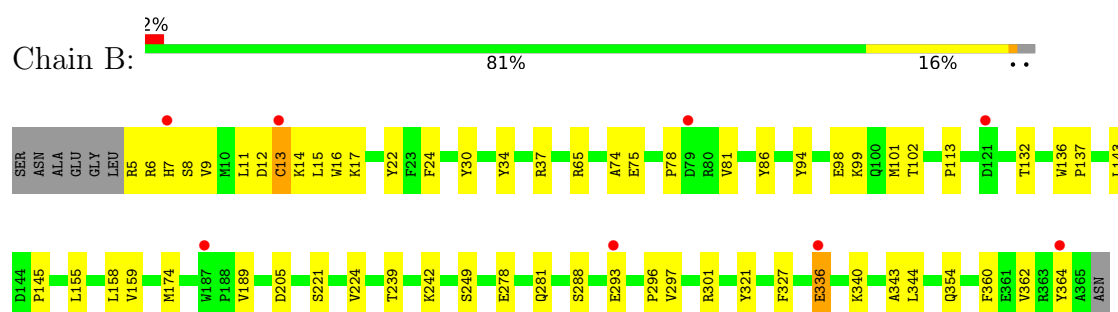
3 Residue-property plots [i](#)

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

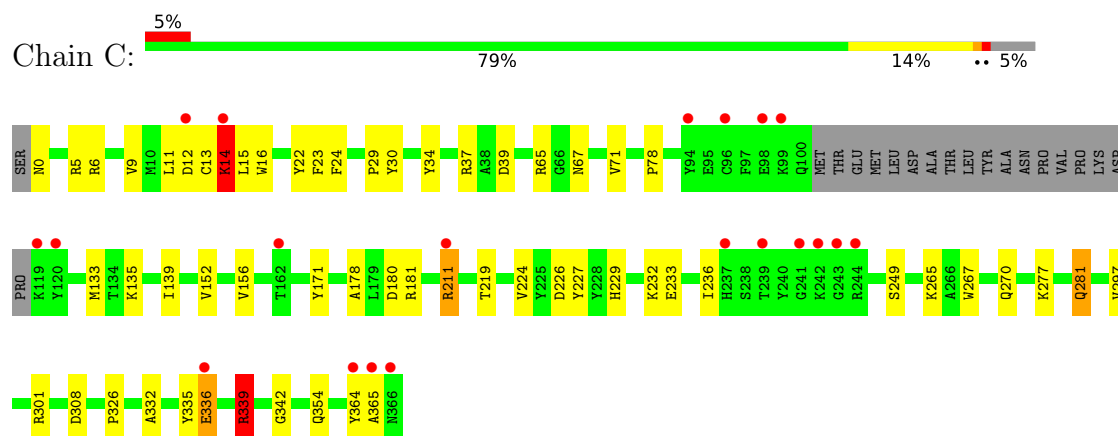
• Molecule 1: Terpene cyclase flvF



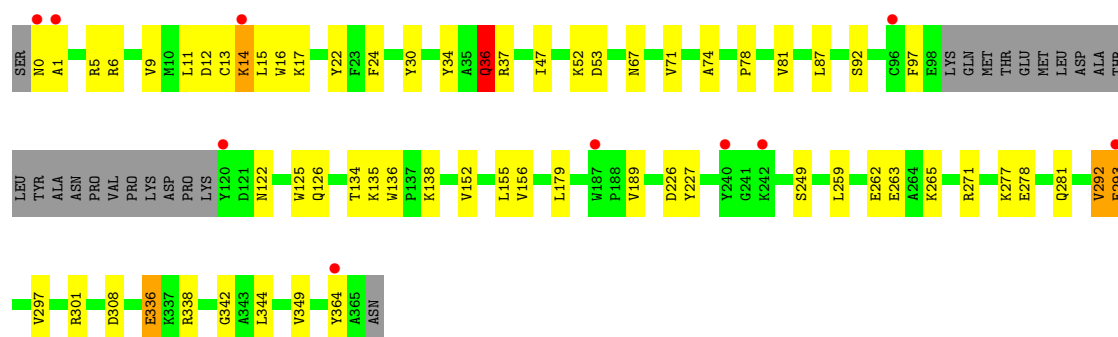
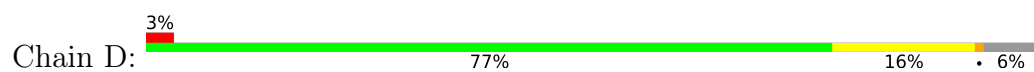
• Molecule 1: Terpene cyclase flvF



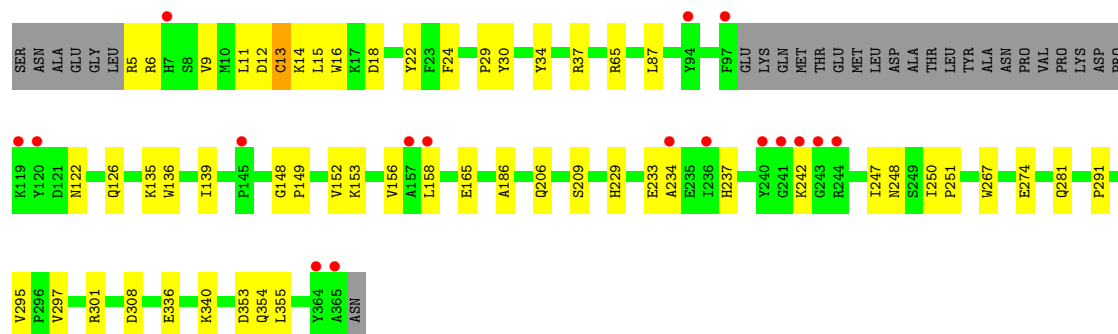
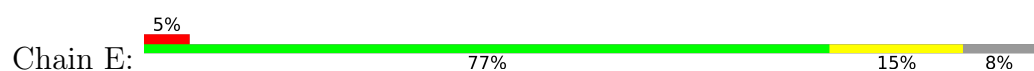
• Molecule 1: Terpene cyclase flvF



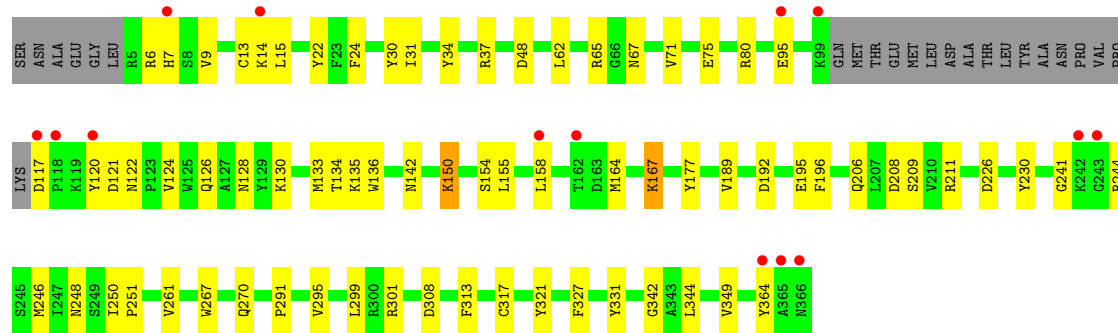
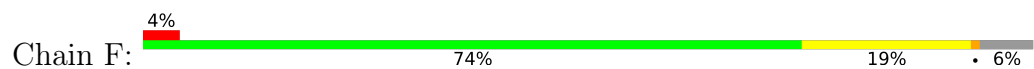
• Molecule 1: Terpene cyclase flvF



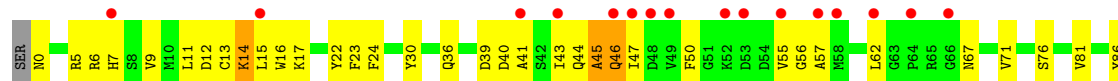
- Molecule 1: Terpene cyclase flvF

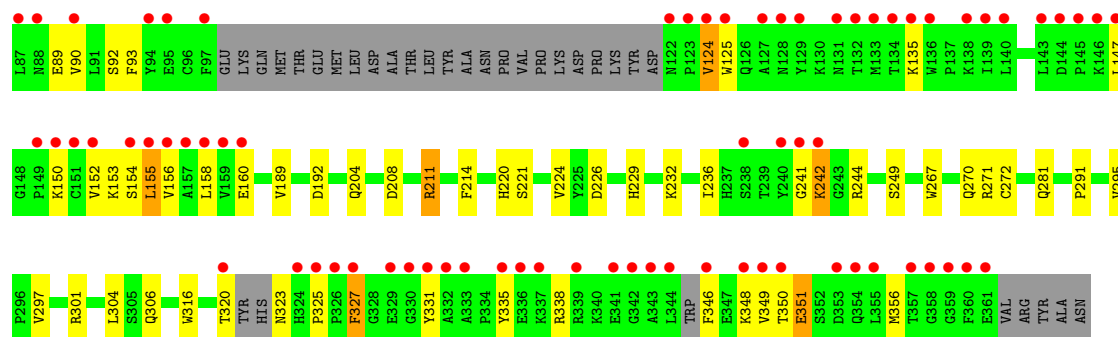


- Molecule 1: Terpene cyclase flvF

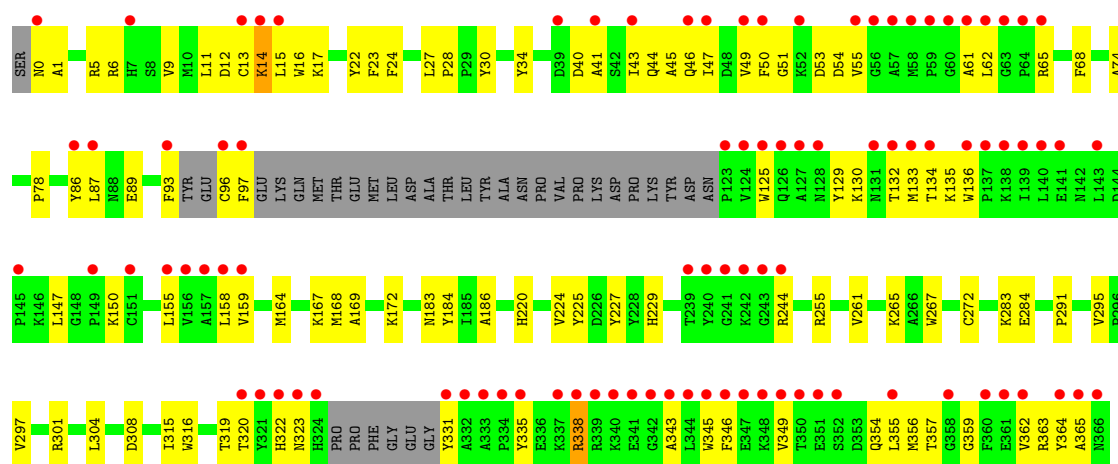


- Molecule 1: Terpene cyclase flvF





• Molecule 1: Terpene cyclase flvF



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.65Å 195.00Å 101.37Å 90.00° 106.19° 90.00°	Depositor
Resolution (Å)	97.35 – 2.62 97.35 – 2.62	Depositor EDS
% Data completeness (in resolution range)	98.8 (97.35-2.62) 98.8 (97.35-2.62)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.208 , 0.243 0.208 , 0.243	Depositor DCC
R_{free} test set	2000 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22284	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: GOL, BTB

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	0.25	0/3025	0.55	5/4110 (0.1%)
1	B	0.34	1/3030 (0.0%)	0.62	3/4113 (0.1%)
1	C	0.37	3/2889 (0.1%)	0.79	17/3927 (0.4%)
1	D	0.33	0/2847	0.72	10/3869 (0.3%)
1	E	0.29	0/2836	0.64	7/3849 (0.2%)
1	F	0.30	0/2891	0.61	2/3923 (0.1%)
1	G	0.38	0/2651	0.76	13/3612 (0.4%)
1	H	0.29	0/2633	0.63	3/3588 (0.1%)
All	All	0.32	4/22802 (0.0%)	0.67	60/30991 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	277	LYS	CD-CE	6.08	1.70	1.52
1	C	339	ARG	CD-NE	-5.75	1.38	1.46
1	C	211	ARG	CZ-NH1	5.40	1.40	1.32
1	B	340	LYS	CG-CD	-5.07	1.37	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	277	LYS	CG-CD-CE	-14.65	77.61	111.30
1	C	339	ARG	CD-NE-CZ	13.38	143.13	124.40
1	D	36	GLN	CA-CB-CG	-12.62	88.87	114.10
1	C	277	LYS	CB-CG-CD	12.44	139.91	111.30
1	B	336	GLU	CA-CB-CG	-11.88	90.34	114.10
1	D	293	GLU	CA-CB-CG	-10.96	92.18	114.10
1	E	353	ASP	CB-CA-C	-9.36	90.75	110.31
1	C	211	ARG	NE-CZ-NH2	-9.18	110.94	119.20
1	E	237	HIS	CA-C-N	-8.96	104.01	121.94
1	E	237	HIS	C-N-CA	-8.96	104.01	121.94
1	B	293	GLU	CB-CG-CD	-8.91	97.44	112.60
1	G	351	GLU	N-CA-CB	-8.57	96.60	110.14
1	G	46	GLN	CB-CG-CD	-8.40	98.31	112.60
1	C	14	LYS	CD-CE-NZ	-8.15	85.82	111.90
1	G	211	ARG	CG-CD-NE	7.93	129.44	112.00
1	F	150	LYS	CG-CD-CE	-7.80	93.37	111.30
1	C	339	ARG	NE-CZ-NH2	-7.63	112.34	119.20
1	B	340	LYS	CG-CD-CE	-7.36	94.36	111.30
1	G	211	ARG	CA-CB-CG	7.33	128.76	114.10
1	D	277	LYS	CB-CG-CD	-7.30	94.50	111.30
1	G	350	THR	CA-C-N	7.25	130.97	120.38
1	G	350	THR	C-N-CA	7.25	130.97	120.38
1	C	211	ARG	CB-CA-C	-6.93	99.24	110.74
1	C	277	LYS	CA-CB-CG	-6.91	100.27	114.10
1	D	336	GLU	CA-CB-CG	-6.91	100.28	114.10
1	G	46	GLN	CA-CB-CG	-6.79	100.51	114.10
1	C	339	ARG	CB-CG-CD	-6.74	95.81	111.30
1	A	284	GLU	CG-CD-OE2	6.64	133.67	118.40
1	C	211	ARG	CA-CB-CG	6.43	126.95	114.10
1	C	14	LYS	CA-CB-CG	6.27	126.63	114.10
1	D	262	GLU	CB-CA-C	-6.23	101.10	110.88
1	A	284	GLU	CG-CD-OE1	-6.15	104.26	118.40
1	D	53	ASP	CA-C-N	-6.01	111.60	122.54
1	D	53	ASP	C-N-CA	-6.01	111.60	122.54
1	G	160	GLU	CA-CB-CG	5.98	126.06	114.10
1	C	336	GLU	N-CA-CB	-5.94	101.38	110.12
1	C	211	ARG	CD-NE-CZ	5.93	132.70	124.40
1	H	284	GLU	CA-CB-CG	-5.89	102.32	114.10
1	A	243	GLY	N-CA-C	-5.85	108.06	115.31
1	E	5	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	C	211	ARG	NE-CZ-NH1	5.57	127.07	121.50
1	D	292	VAL	CA-C-N	-5.55	113.01	122.56
1	D	292	VAL	C-N-CA	-5.55	113.01	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	338	ARG	CG-CD-NE	-5.55	99.78	112.00
1	E	234	ALA	CA-C-N	-5.49	111.53	121.14
1	E	234	ALA	C-N-CA	-5.49	111.53	121.14
1	G	211	ARG	CB-CA-C	5.45	120.72	110.63
1	G	211	ARG	CB-CG-CD	-5.45	98.77	111.30
1	C	335	TYR	CA-C-N	5.44	127.56	120.28
1	C	335	TYR	C-N-CA	5.44	127.56	120.28
1	G	46	GLN	N-CA-C	5.39	117.23	111.36
1	G	45	ALA	CA-C-N	-5.36	112.68	120.29
1	G	45	ALA	C-N-CA	-5.36	112.68	120.29
1	F	167	LYS	N-CA-CB	-5.21	102.27	110.30
1	E	5	ARG	NE-CZ-NH1	-5.21	116.29	121.50
1	D	262	GLU	N-CA-CB	5.21	117.56	110.01
1	A	361	GLU	CA-C-N	5.20	131.34	121.97
1	A	361	GLU	C-N-CA	5.20	131.34	121.97
1	C	14	LYS	CG-CD-CE	5.15	123.14	111.30
1	H	51	GLY	N-CA-C	-5.05	106.32	112.68

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	339	ARG	Sidechain
1	D	36	GLN	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2939	0	2814	46	0
1	B	2944	0	2838	42	0
1	C	2806	0	2648	47	0
1	D	2768	0	2619	50	0
1	E	2756	0	2641	38	0
1	F	2809	0	2690	52	0
1	G	2580	0	2389	86	0
1	H	2564	0	2376	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	28	0	38	8	0
2	B	28	0	38	4	0
2	D	14	0	19	4	0
3	A	6	0	8	2	0
3	B	6	0	8	0	0
3	C	6	0	8	2	0
3	D	6	0	8	1	0
3	E	6	0	8	2	0
3	F	6	0	8	2	0
3	G	6	0	8	3	0
3	H	6	0	8	2	0
All	All	22284	0	21174	441	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 10.

All (441) 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:E:242:LYS:HD2	1:E:242:LYS:O	1.27	1.25
1:F:208:ASP:OD1	1:F:211:ARG:CZ	1.91	1.17
1:G:46:GLN:NE2	1:G:93:PHE:CZ	2.16	1.13
1:F:150:LYS:NZ	1:F:195:GLU:OE1	1.84	1.11
1:G:46:GLN:NE2	1:G:93:PHE:HZ	1.48	1.10
1:G:44:GLN:HG3	1:G:356:MET:HG2	1.35	1.04
1:B:15:LEU:HB3	1:B:65:ARG:HD3	1.50	0.93
1:G:325:PRO:HA	1:G:327:PHE:H	1.32	0.93
1:D:87:LEU:HD13	1:D:136:TRP:CZ3	2.07	0.90
1:E:242:LYS:O	1:E:242:LYS:CD	2.18	0.89
1:D:87:LEU:CD1	1:D:136:TRP:CZ3	2.56	0.88
1:G:204:GLN:OE1	1:G:211:ARG:NH2	2.08	0.87
1:A:13:CYS:O	1:A:15:LEU:N	2.07	0.87
1:D:13:CYS:O	1:D:15:LEU:N	2.08	0.86
1:B:158:LEU:HB3	2:B:401:BTB:H12	1.59	0.85
1:C:13:CYS:O	1:C:15:LEU:N	2.10	0.85
1:A:204:GLN:OE1	1:A:211:ARG:NH2	2.12	0.83
1:G:36:GLN:NE2	1:G:338:ARG:HD3	1.93	0.83
1:G:45:ALA:HB1	1:G:90:VAL:HG13	1.61	0.83
1:F:208:ASP:OD1	1:F:211:ARG:NH1	2.13	0.82
1:D:292:VAL:HG23	1:D:293:GLU:HG3	1.62	0.81
1:G:46:GLN:CD	1:G:93:PHE:HZ	1.88	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:LEU:HB3	1:F:65:ARG:HD3	1.61	0.81
1:D:87:LEU:HD11	1:D:136:TRP:CH2	2.17	0.80
1:H:0:ASN:O	1:H:6:ARG:NH1	2.16	0.79
1:A:208:ASP:HA	1:A:211:ARG:HG3	1.65	0.78
1:D:0:ASN:O	1:D:6:ARG:NH1	2.17	0.78
1:H:343:ALA:HB1	1:H:362:VAL:HG21	1.65	0.78
1:E:15:LEU:HB3	1:E:65:ARG:HD3	1.65	0.77
1:C:11:LEU:HD23	1:C:12:ASP:O	1.83	0.77
1:C:34:TYR:HB3	1:C:37:ARG:HD3	1.67	0.77
1:D:87:LEU:HD13	1:D:136:TRP:CE3	2.20	0.77
1:B:336:GLU:O	1:B:336:GLU:HG3	1.81	0.77
1:H:13:CYS:O	1:H:15:LEU:N	2.19	0.75
1:D:336:GLU:O	1:D:336:GLU:HG3	1.86	0.74
1:H:169:ALA:HA	1:H:255:ARG:HH12	1.53	0.73
1:D:87:LEU:CD1	1:D:136:TRP:CH2	2.71	0.73
1:H:135:LYS:NZ	1:H:354:GLN:O	2.20	0.73
1:G:62:LEU:HD22	1:G:331:TYR:CD1	2.24	0.73
1:F:208:ASP:OD1	1:F:211:ARG:NH2	2.23	0.72
1:D:36:GLN:HG3	1:D:36:GLN:O	1.89	0.71
2:A:402:BTB:HO4	2:A:402:BTB:HO1	1.36	0.71
1:C:332:ALA:O	1:C:336:GLU:HG3	1.91	0.71
1:F:208:ASP:HA	1:F:211:ARG:HG3	1.72	0.71
1:H:357:THR:HB	1:H:363:ARG:HB3	1.72	0.71
1:D:226:ASP:OD2	1:D:249:SER:OG	2.07	0.70
1:E:149:PRO:O	1:E:153:LYS:HG2	1.92	0.70
1:G:13:CYS:O	1:G:15:LEU:N	2.20	0.70
1:H:343:ALA:HB3	1:H:345:TRP:CZ2	2.26	0.70
1:G:124:VAL:HG13	1:G:125:TRP:H	1.57	0.70
1:G:5:ARG:O	1:G:301:ARG:NH2	2.25	0.69
1:D:36:GLN:NE2	1:D:338:ARG:HD2	2.07	0.69
1:A:281:GLN:NE2	1:G:281:GLN:OE1	2.26	0.68
1:E:229:HIS:ND1	1:E:233:GLU:HG3	2.08	0.68
1:B:6:ARG:HH11	1:B:9:VAL:HG11	1.59	0.68
1:E:122:ASN:O	1:E:126:GLN:HG3	1.94	0.68
1:G:46:GLN:O	1:G:50:PHE:N	2.23	0.67
1:D:87:LEU:CD1	1:D:136:TRP:CE3	2.78	0.67
1:F:267:TRP:CD1	3:F:401:GOL:H32	2.31	0.66
1:C:9:VAL:HG21	1:C:30:TYR:HB3	1.75	0.66
1:F:164:MET:O	1:F:167:LYS:HB2	1.96	0.66
1:G:36:GLN:HE21	1:G:338:ARG:HD3	1.60	0.66
1:C:5:ARG:O	1:C:301:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:46:GLN:HA	1:G:46:GLN:OE1	1.96	0.66
1:F:13:CYS:SG	1:F:14:LYS:N	2.66	0.65
1:G:11:LEU:HD23	1:G:12:ASP:O	1.95	0.65
2:A:402:BTB:O1	2:A:402:BTB:O4	2.10	0.65
1:C:135:LYS:HE3	1:C:139:ILE:HD11	1.78	0.65
1:H:65:ARG:HD3	1:H:319:THR:HG21	1.79	0.65
1:C:281[B]:GLN:OE1	1:E:281:GLN:NE2	2.29	0.64
1:H:6:ARG:NH2	1:H:308:ASP:OD1	2.30	0.64
1:F:117:ASP:HB3	1:F:120:TYR:HD2	1.63	0.64
1:E:11:LEU:HD23	1:E:12:ASP:O	1.99	0.63
1:D:34:TYR:HB3	1:D:37:ARG:HD3	1.81	0.63
1:D:5:ARG:O	1:D:301:ARG:NH2	2.31	0.63
1:G:241:GLY:O	1:G:242:LYS:HB2	1.99	0.62
1:A:159:VAL:HA	2:A:401:BTB:H42	1.80	0.62
1:C:9:VAL:CG2	1:C:30:TYR:HB3	2.29	0.62
1:F:158:LEU:HD11	1:F:189:VAL:HG21	1.81	0.62
1:F:130:LYS:O	1:F:134:THR:HG23	2.00	0.61
1:F:133:MET:HE3	1:F:136:TRP:HE1	1.65	0.61
1:A:78:PRO:O	1:A:81:VAL:HG12	2.00	0.61
1:G:242:LYS:NZ	1:G:242:LYS:HB3	2.16	0.61
1:H:158:LEU:HD21	1:H:183:ASN:HB3	1.82	0.61
1:G:43:ILE:O	1:G:47:ILE:HG13	2.01	0.60
1:E:34:TYR:HB3	1:E:37:ARG:HD3	1.82	0.60
1:A:242:LYS:HD2	1:A:242:LYS:O	2.01	0.60
1:F:154:SER:OG	1:F:192:ASP:OD2	2.12	0.60
1:C:267:TRP:CD1	3:C:401:GOL:H32	2.36	0.60
1:F:9:VAL:HG21	1:F:30:TYR:HB3	1.84	0.60
1:B:159:VAL:HA	2:B:401:BTB:H31	1.84	0.60
1:E:6:ARG:HE	1:E:9:VAL:HG11	1.68	0.59
1:B:11:LEU:HD23	1:B:12:ASP:O	2.02	0.59
1:H:316:TRP:CZ2	1:H:320:THR:HG21	2.38	0.59
1:G:46:GLN:CD	1:G:93:PHE:CZ	2.73	0.59
1:B:343:ALA:HB1	1:B:362:VAL:HG21	1.84	0.58
1:E:9:VAL:HG21	1:E:30:TYR:HB3	1.85	0.58
1:E:135:LYS:NZ	1:E:354:GLN:O	2.35	0.58
1:G:348:LYS:O	1:G:351:GLU:HB2	2.03	0.58
1:D:92:SER:HA	2:D:401:BTB:H82	1.86	0.58
1:A:115:PRO:HG3	1:A:244:ARG:HG3	1.85	0.58
1:E:9:VAL:CG2	1:E:30:TYR:HB3	2.34	0.58
1:H:89:GLU:OE2	1:H:331:TYR:OH	2.20	0.58
1:D:9:VAL:HG21	1:D:30:TYR:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:VAL:CG2	1:F:30:TYR:HB3	2.34	0.58
1:C:342:GLY:O	1:C:364:TYR:HB3	2.04	0.57
1:H:267:TRP:CD1	3:H:401:GOL:H31	2.39	0.57
1:H:11:LEU:HD12	1:H:12:ASP:N	2.19	0.57
1:A:18:ASP:CG	1:C:0:ASN:HA	2.29	0.57
1:F:135:LYS:HE3	1:F:349:VAL:HG22	1.87	0.57
1:D:11:LEU:HD23	1:D:12:ASP:O	2.04	0.57
1:B:98:GLU:O	1:B:102:THR:HG23	2.05	0.57
1:A:174:MET:HE1	1:A:249:SER:HB2	1.87	0.56
1:C:6:ARG:NH2	1:C:308:ASP:OD1	2.37	0.56
1:G:267:TRP:CD1	3:G:401:GOL:H31	2.40	0.56
1:A:5:ARG:O	1:A:301:ARG:NH2	2.38	0.56
1:A:6:ARG:NH2	1:A:308:ASP:OD1	2.38	0.56
1:F:34:TYR:HB3	1:F:37:ARG:HD3	1.86	0.56
1:G:62:LEU:HD22	1:G:331:TYR:CE1	2.40	0.56
1:H:43:ILE:HD11	1:H:345:TRP:NE1	2.21	0.56
1:H:346:PHE:CZ	1:H:357:THR:HA	2.41	0.56
1:E:13:CYS:O	1:E:16:TRP:NE1	2.38	0.56
1:E:153:LYS:HA	1:E:156:VAL:HG22	1.85	0.56
1:H:62:LEU:O	1:H:320:THR:OG1	2.24	0.56
1:A:208:ASP:OD1	1:A:211:ARG:NE	2.36	0.56
1:D:9:VAL:CG2	1:D:30:TYR:HB3	2.36	0.56
1:B:174:MET:HE1	1:B:249:SER:HB2	1.89	0.55
1:G:62:LEU:HD22	1:G:331:TYR:HD1	1.72	0.55
1:B:9:VAL:CG2	1:B:30:TYR:HB3	2.37	0.55
1:E:135:LYS:HD3	1:E:139:ILE:HD11	1.88	0.55
1:G:55:VAL:HG11	1:G:335:TYR:HD2	1.71	0.55
1:F:155:LEU:HA	1:F:158:LEU:HD12	1.88	0.55
1:A:201:ASN:ND2	1:B:354:GLN:OE1	2.39	0.55
1:C:332:ALA:O	1:C:336:GLU:HB2	2.05	0.55
1:C:13:CYS:C	1:C:15:LEU:H	2.14	0.55
1:D:36:GLN:HE21	1:D:338:ARG:CD	2.18	0.55
1:G:9:VAL:CG2	1:G:30:TYR:HB3	2.36	0.55
1:H:9:VAL:CG2	1:H:30:TYR:HB3	2.37	0.55
1:G:325:PRO:HA	1:G:327:PHE:N	2.13	0.54
1:C:365:ALA:C	1:F:130:LYS:HD3	2.32	0.54
1:E:148:GLY:O	1:E:152:VAL:HG23	2.06	0.54
1:G:9:VAL:HG21	1:G:30:TYR:HB3	1.90	0.54
1:G:50:PHE:CE2	1:G:57:ALA:HB3	2.42	0.54
1:D:271:ARG:HD3	3:D:402:GOL:H31	1.89	0.54
1:G:23:PHE:CD2	1:G:224:VAL:HG12	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:LYS:HE3	1:C:236:ILE:HD11	1.89	0.54
1:H:40:ASP:OD1	1:H:338:ARG:NH2	2.41	0.54
1:B:9:VAL:HG21	1:B:30:TYR:HB3	1.90	0.54
1:C:67:ASN:O	1:C:71:VAL:HG22	2.08	0.54
1:D:14:LYS:HG3	1:D:17:LYS:HB2	1.90	0.53
1:H:9:VAL:HG21	1:H:30:TYR:HB3	1.90	0.53
1:G:6:ARG:HH11	1:G:9:VAL:HG11	1.72	0.53
1:H:320:THR:HG23	1:H:322:HIS:H	1.74	0.53
1:D:16:TRP:CE3	1:D:17:LYS:HA	2.43	0.53
1:D:78:PRO:O	1:D:81:VAL:HG12	2.09	0.53
1:B:13:CYS:SG	1:B:14:LYS:N	2.79	0.53
1:B:296:PRO:HG3	1:H:172:LYS:HD2	1.91	0.53
1:A:94:TYR:CE2	2:A:401:BTB:H82	2.43	0.53
1:D:134:THR:O	1:D:138:LYS:HD3	2.08	0.53
1:H:61:ALA:HB1	1:H:68:PHE:HB3	1.90	0.53
1:H:261:VAL:O	1:H:265:LYS:HG3	2.09	0.53
1:D:36:GLN:NE2	1:D:338:ARG:CD	2.70	0.53
1:F:177:TYR:OH	1:F:226:ASP:OD2	2.23	0.52
1:B:239:THR:O	1:B:242:LYS:HE2	2.09	0.52
1:G:220:HIS:CD2	1:G:272:CYS:HB3	2.45	0.52
1:G:6:ARG:HG2	1:G:304:LEU:HD13	1.90	0.52
1:H:16:TRP:CH2	1:H:28:PRO:HB3	2.45	0.52
1:H:93:PHE:HB2	1:H:129:TYR:OH	2.09	0.52
1:B:155:LEU:HD13	1:B:189:VAL:HG21	1.92	0.52
1:H:16:TRP:CE3	1:H:17:LYS:HA	2.45	0.52
1:H:158:LEU:HD13	1:H:186:ALA:HA	1.91	0.52
1:H:55:VAL:HB	1:H:335:TYR:CE2	2.45	0.52
1:G:39:ASP:OD1	1:G:67:ASN:HB2	2.10	0.52
1:G:56:GLY:N	1:G:331:TYR:CD2	2.78	0.52
1:H:41:ALA:HB1	1:H:86:TYR:HB2	1.91	0.52
1:G:152:VAL:O	1:G:156:VAL:HG13	2.10	0.52
1:H:5:ARG:O	1:H:301:ARG:NH2	2.42	0.52
1:C:6:ARG:HE	1:C:9:VAL:HG11	1.75	0.51
1:F:48:ASP:O	1:F:128:ASN:HB3	2.10	0.51
1:D:36:GLN:O	1:D:36:GLN:CG	2.54	0.51
1:B:34:TYR:HB3	1:B:37:ARG:HD3	1.91	0.51
1:D:278:GLU:O	1:D:281:GLN:HG3	2.10	0.51
1:E:291:PRO:O	1:E:295:VAL:HG23	2.11	0.51
1:A:289:GLU:HB2	1:G:271:ARG:CZ	2.40	0.51
1:C:171:TYR:OH	1:C:180:ASP:OD2	2.25	0.51
1:D:1:ALA:HB2	1:D:6:ARG:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:208:ASP:HA	1:F:211:ARG:CG	2.39	0.51
1:G:16:TRP:CE3	1:G:17:LYS:HA	2.46	0.51
1:F:342:GLY:O	1:F:364:TYR:HB3	2.10	0.51
1:G:208:ASP:HA	1:G:211:ARG:HD2	1.93	0.51
1:B:278:GLU:O	1:B:281:GLN:HG3	2.10	0.51
1:B:8:SER:HB3	1:B:34:TYR:HE2	1.76	0.51
1:F:230:TYR:CG	1:F:250:ILE:HD12	2.45	0.51
1:A:117:ASP:HB3	1:A:120:TYR:HD2	1.77	0.50
1:G:55:VAL:HG12	1:G:331:TYR:CD2	2.47	0.50
1:B:297:VAL:O	1:B:301:ARG:HG3	2.11	0.50
1:C:15:LEU:HB3	1:C:65:ARG:HD3	1.92	0.50
1:F:95:GLU:CD	1:F:95:GLU:H	2.20	0.50
1:A:297:VAL:O	1:A:301:ARG:HG3	2.11	0.50
1:H:46:GLN:O	1:H:50:PHE:N	2.20	0.50
1:H:6:ARG:HG2	1:H:304:LEU:HD13	1.93	0.50
1:E:242:LYS:HD2	1:E:242:LYS:C	2.25	0.50
1:G:56:GLY:N	1:G:331:TYR:HD2	2.09	0.50
1:H:11:LEU:CD1	1:H:28:PRO:HB2	2.42	0.50
1:A:361:GLU:O	1:A:362:VAL:HG22	2.12	0.49
1:C:23:PHE:CD2	1:C:224:VAL:HG23	2.47	0.49
1:D:97:PHE:CD1	1:D:126:GLN:HG2	2.47	0.49
1:H:357:THR:HB	1:H:363:ARG:CB	2.39	0.49
1:A:11:LEU:HD23	1:A:12:ASP:O	2.12	0.49
1:H:343:ALA:CB	1:H:362:VAL:HG21	2.39	0.49
1:E:6:ARG:NH2	1:E:308:ASP:OD1	2.45	0.49
1:F:158:LEU:HD11	1:F:189:VAL:CG2	2.41	0.49
1:B:5:ARG:O	1:B:301:ARG:NH2	2.46	0.49
1:G:153:LYS:HA	1:G:156:VAL:HG22	1.94	0.49
1:A:270:GLN:HB3	3:A:403:GOL:O1	2.13	0.49
1:F:6:ARG:NH2	1:F:308:ASP:OD1	2.45	0.49
1:H:13:CYS:O	1:H:14:LYS:C	2.55	0.49
1:D:152:VAL:O	1:D:156:VAL:HG23	2.13	0.49
1:G:226:ASP:OD2	1:G:249:SER:OG	2.20	0.49
1:A:7:HIS:HB2	1:B:145:PRO:HG2	1.95	0.49
1:G:36:GLN:HE22	1:G:338:ARG:HD3	1.75	0.48
1:A:9:VAL:HG11	1:A:75:GLU:HG2	1.93	0.48
1:D:6:ARG:NH2	1:D:308:ASP:OD1	2.46	0.48
1:F:62:LEU:HB2	1:F:331:TYR:CZ	2.48	0.48
1:C:181:ARG:NH2	1:C:226:ASP:OD1	2.42	0.48
1:E:267:TRP:CE2	3:E:401:GOL:H12	2.47	0.48
1:G:41:ALA:HB1	1:G:86:TYR:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:TYR:CE2	1:B:24:PHE:HB2	2.48	0.48
1:B:94:TYR:HD1	1:B:101:MET:SD	2.36	0.48
1:H:0:ASN:OD1	1:H:283:LYS:NZ	2.46	0.48
1:D:6:ARG:HE	1:D:9:VAL:HG11	1.79	0.48
1:F:241:GLY:O	1:F:244:ARG:HB2	2.14	0.48
1:F:321:TYR:O	1:F:327:PHE:HA	2.14	0.48
1:H:355:LEU:HB3	1:H:356:MET:HG3	1.96	0.48
1:G:135:LYS:HD2	1:G:349:VAL:HG22	1.96	0.48
1:G:242:LYS:HB3	1:G:242:LYS:HZ2	1.79	0.48
1:A:98:GLU:O	1:A:102:THR:HG23	2.14	0.48
1:D:47:ILE:HG12	1:D:52:LYS:HA	1.95	0.48
1:D:344:LEU:HD22	1:D:364:TYR:HB2	1.95	0.48
1:E:18:ASP:CG	1:G:0:ASN:H2	2.17	0.48
1:G:23:PHE:HD2	1:G:224:VAL:HG12	1.79	0.48
1:E:18:ASP:OD2	1:G:0:ASN:N	2.35	0.48
1:A:136:TRP:CG	1:A:137:PRO:HD3	2.50	0.47
1:H:22:TYR:OH	1:H:27:LEU:O	2.30	0.47
1:F:9:VAL:HG23	1:F:31:ILE:O	2.13	0.47
1:G:7:HIS:CD2	1:G:301:ARG:NH2	2.83	0.47
1:H:1:ALA:HB2	1:H:6:ARG:HD2	1.96	0.47
1:B:7:HIS:CD2	1:B:301:ARG:NH2	2.83	0.47
1:F:126:GLN:O	1:F:130:LYS:HG3	2.14	0.47
1:C:135:LYS:NZ	1:C:354:GLN:O	2.38	0.47
1:G:46:GLN:OE1	1:G:93:PHE:CZ	2.67	0.47
1:G:338:ARG:HA	1:G:338:ARG:HD2	1.69	0.47
1:B:16:TRP:CE3	1:B:17:LYS:HA	2.50	0.47
1:D:155:LEU:HD13	1:D:189:VAL:HG21	1.96	0.47
1:E:336:GLU:HG3	1:E:340:LYS:HE2	1.97	0.47
1:H:297:VAL:O	1:H:301:ARG:HG3	2.15	0.47
1:B:99:LYS:HE2	1:B:113:PRO:HB3	1.96	0.47
1:F:9:VAL:HG11	1:F:75:GLU:HG2	1.96	0.47
1:E:87:LEU:HD13	1:E:136:TRP:CZ3	2.50	0.47
1:G:291:PRO:O	1:G:295:VAL:HG23	2.15	0.47
1:H:43:ILE:HD11	1:H:345:TRP:CE2	2.49	0.47
1:F:313:PHE:CZ	1:F:317:CYS:SG	3.08	0.46
1:G:270:GLN:HB3	3:G:401:GOL:O3	2.15	0.46
1:H:227:TYR:CE2	1:H:265:LYS:HB3	2.50	0.46
1:A:242:LYS:C	1:A:244:ARG:H	2.22	0.46
1:G:232:LYS:O	1:G:236:ILE:HG13	2.14	0.46
1:C:229:HIS:CD2	1:C:233:GLU:HG3	2.50	0.46
1:G:346:PHE:HB3	1:G:351:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:CYS:SG	1:C:14:LYS:HB3	2.55	0.46
1:B:221:SER:HA	1:B:224:VAL:HG12	1.97	0.46
1:F:291:PRO:O	1:F:295:VAL:HG23	2.15	0.46
1:C:226:ASP:OD2	1:C:249:SER:OG	2.23	0.46
1:G:9:VAL:HG22	1:G:30:TYR:HD2	1.80	0.46
1:G:154:SER:O	1:G:189:VAL:HG22	2.14	0.46
1:H:45:ALA:HB2	1:H:86:TYR:CG	2.51	0.46
1:H:343:ALA:HA	1:H:365:ALA:HB3	1.96	0.46
1:B:78:PRO:O	1:B:81:VAL:HG12	2.15	0.46
1:B:344:LEU:HG	1:B:364:TYR:HB2	1.96	0.46
1:F:121:ASP:OD1	1:F:126:GLN:NE2	2.49	0.46
1:H:133:MET:CE	1:H:136:TRP:HE1	2.28	0.46
1:A:242:LYS:C	1:A:244:ARG:N	2.72	0.46
2:D:401:BTB:H71	2:D:401:BTB:H42	1.66	0.46
1:H:23:PHE:CD2	1:H:224:VAL:HG23	2.51	0.46
2:B:401:BTB:H52	2:B:401:BTB:H42	1.66	0.46
1:F:250:ILE:HD13	1:F:261:VAL:HG23	1.98	0.45
1:H:17:LYS:HD3	1:H:17:LYS:C	2.41	0.45
1:C:15:LEU:O	1:C:65:ARG:NH1	2.47	0.45
1:D:342:GLY:O	1:D:364:TYR:HB3	2.16	0.45
1:G:297:VAL:O	1:G:301:ARG:HG3	2.16	0.45
1:D:122:ASN:HB3	1:D:125:TRP:HB2	1.98	0.45
1:E:274:GLU:OE2	3:E:401:GOL:O2	2.35	0.45
1:G:220:HIS:O	1:G:224:VAL:HG22	2.16	0.45
1:H:9:VAL:HG23	1:H:74:ALA:HB1	1.97	0.45
1:A:9:VAL:HG23	1:A:74:ALA:HB1	1.98	0.45
2:A:402:BTB:H31	2:A:402:BTB:H51	1.52	0.45
1:D:9:VAL:HG23	1:D:74:ALA:HB1	1.98	0.45
1:G:22:TYR:CE2	1:G:24:PHE:HB2	2.50	0.45
1:G:229:HIS:NE2	1:G:323:ASN:OD1	2.50	0.45
1:H:316:TRP:CE2	1:H:320:THR:HG21	2.51	0.45
1:C:133:MET:HE2	1:C:133:MET:HB3	1.76	0.45
1:G:43:ILE:HA	1:G:331:TYR:OH	2.16	0.45
1:B:99:LYS:O	1:B:102:THR:OG1	2.31	0.45
1:G:40:ASP:O	1:G:43:ILE:HG12	2.17	0.45
1:H:132:THR:HA	1:H:349:VAL:HG21	1.98	0.45
1:H:225:TYR:O	1:H:229:HIS:HB2	2.16	0.45
1:B:336:GLU:O	1:B:336:GLU:CG	2.49	0.45
1:G:76:SER:HB2	1:G:81:VAL:HB	1.98	0.45
1:H:362:VAL:O	1:H:362:VAL:HG13	2.16	0.45
1:A:9:VAL:CG2	1:A:30:TYR:HB3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ALA:HB1	1:A:68:PHE:HB3	1.99	0.44
1:E:250:ILE:HB	1:E:251:PRO:HD3	1.97	0.44
1:H:17:LYS:HD3	1:H:17:LYS:O	2.18	0.44
2:A:402:BTB:H72	2:A:402:BTB:H62	1.71	0.44
1:F:158:LEU:CD1	1:F:189:VAL:HG21	2.47	0.44
1:A:321:TYR:O	1:A:327:PHE:HA	2.17	0.44
2:D:401:BTB:H52	2:D:401:BTB:H32	1.61	0.44
1:H:34:TYR:CE2	1:H:78:PRO:HG3	2.53	0.44
1:H:87:LEU:HD11	1:H:136:TRP:CE3	2.51	0.44
1:C:178:ALA:HB1	1:C:219:THR:HG23	2.00	0.44
1:G:241:GLY:O	1:G:244:ARG:HG3	2.17	0.44
1:G:316:TRP:CZ2	1:G:320:THR:HG21	2.53	0.44
1:D:135:LYS:HD3	1:D:349:VAL:HG22	1.99	0.44
1:E:297:VAL:O	1:E:301:ARG:HG3	2.18	0.44
1:G:67:ASN:O	1:G:71:VAL:HG22	2.16	0.44
1:H:22:TYR:CZ	1:H:24:PHE:HB2	2.52	0.44
1:H:43:ILE:CD1	1:H:345:TRP:CE2	3.00	0.44
1:A:101:MET:HG3	1:A:133:MET:HE2	1.99	0.44
1:G:13:CYS:O	1:G:15:LEU:HG	2.18	0.44
1:A:227:TYR:CE2	1:A:265:LYS:HB3	2.52	0.44
1:G:150:LYS:HD3	1:G:192:ASP:OD1	2.18	0.44
1:G:208:ASP:OD1	1:G:211:ARG:CZ	2.66	0.44
1:H:316:TRP:CH2	1:H:320:THR:HG21	2.53	0.44
1:A:141:GLU:HG2	1:A:149:PRO:HG3	2.00	0.43
2:A:401:BTB:H32	2:A:401:BTB:H71	1.46	0.43
1:F:80:ARG:NH1	1:F:196:PHE:O	2.47	0.43
1:H:155:LEU:O	1:H:159:VAL:HG13	2.18	0.43
1:C:39:ASP:OD1	1:C:67:ASN:HB2	2.17	0.43
1:H:46:GLN:HA	1:H:49:VAL:CG2	2.48	0.43
1:C:227:TYR:CE2	1:C:265:LYS:HB3	2.54	0.43
1:G:316:TRP:CH2	1:G:320:THR:HG21	2.54	0.43
1:H:11:LEU:HD11	1:H:28:PRO:HB2	2.00	0.43
1:D:297:VAL:O	1:D:301:ARG:HG3	2.19	0.43
1:A:6:ARG:HE	1:A:9:VAL:HG11	1.84	0.43
1:A:208:ASP:HA	1:A:211:ARG:HE	1.83	0.43
1:C:22:TYR:CZ	1:C:24:PHE:HB2	2.53	0.43
1:C:211:ARG:HE	1:C:211:ARG:HB2	1.33	0.43
1:C:232:LYS:O	1:C:236:ILE:HG13	2.19	0.43
1:C:297:VAL:O	1:C:301:ARG:HG3	2.18	0.43
1:C:332:ALA:O	1:C:336:GLU:CG	2.65	0.43
1:F:122:ASN:OD1	1:F:124:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:LEU:HD23	1:G:147:LEU:HA	1.89	0.43
1:A:13:CYS:C	1:A:15:LEU:N	2.74	0.43
1:A:67:ASN:O	1:A:71:VAL:HG22	2.18	0.43
1:A:220:HIS:CD2	1:A:272:CYS:HB3	2.53	0.43
1:B:86:TYR:OH	1:B:132:THR:HG23	2.19	0.43
1:H:6:ARG:HE	1:H:9:VAL:HG11	1.84	0.43
1:E:248:ASN:O	1:E:251:PRO:HD2	2.19	0.43
1:F:299:LEU:HD12	1:F:299:LEU:HA	1.87	0.42
1:H:53:ASP:OD1	1:H:53:ASP:N	2.52	0.42
1:C:229:HIS:CE1	1:C:232:LYS:HD3	2.54	0.42
1:D:13:CYS:C	1:D:15:LEU:N	2.75	0.42
1:G:211:ARG:HH11	1:G:211:ARG:HD3	1.64	0.42
1:G:221:SER:HA	1:G:224:VAL:HG22	2.01	0.42
1:H:50:PHE:HD2	1:H:54:ASP:O	2.02	0.42
1:C:152:VAL:O	1:C:156:VAL:HG23	2.19	0.42
1:C:339:ARG:HH11	1:C:339:ARG:HB3	1.84	0.42
1:H:164:MET:O	1:H:168:MET:N	2.52	0.42
1:A:184:TYR:CE2	2:A:401:BTB:H51	2.55	0.42
2:B:401:BTB:H42	2:B:401:BTB:O6	2.19	0.42
1:C:22:TYR:CE2	1:C:24:PHE:HB2	2.54	0.42
1:H:164:MET:SD	1:H:184:TYR:HB2	2.58	0.42
1:D:9:VAL:CG2	1:D:74:ALA:HB1	2.50	0.42
1:D:22:TYR:CE2	1:D:24:PHE:HB2	2.54	0.42
2:D:401:BTB:O4	2:D:401:BTB:O1	2.35	0.42
1:H:220:HIS:CD2	1:H:272:CYS:HB3	2.55	0.42
1:A:153:LYS:HA	1:A:153:LYS:HD2	1.89	0.42
1:F:344:LEU:HG	1:F:364:TYR:HB2	2.01	0.42
1:G:267:TRP:NE1	3:G:401:GOL:H31	2.35	0.42
1:H:47:ILE:HD11	1:H:335:TYR:HE1	1.83	0.42
1:F:206:GLN:O	1:F:209:SER:OG	2.29	0.42
1:G:214:PHE:CD2	1:G:306:GLN:HG3	2.54	0.42
1:B:9:VAL:HG12	1:B:75:GLU:OE2	2.20	0.42
1:B:143:LEU:HD12	1:B:360:PHE:CZ	2.55	0.42
1:C:229:HIS:HD2	1:C:233:GLU:OE2	2.03	0.42
1:D:259:LEU:HD22	1:D:263:GLU:HB3	2.01	0.42
1:E:13:CYS:SG	1:E:14:LYS:N	2.92	0.42
1:H:164:MET:O	1:H:168:MET:HG2	2.20	0.42
1:G:36:GLN:O	1:G:36:GLN:HG3	2.19	0.42
1:H:291:PRO:O	1:H:295:VAL:HG23	2.20	0.42
1:E:165:GLU:HB2	1:E:247:ILE:HD11	2.02	0.42
1:F:7:HIS:CD2	1:F:301:ARG:NH2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:125:TRP:O	1:H:129:TYR:HB2	2.20	0.42
1:A:342:GLY:O	1:A:364:TYR:HB3	2.20	0.41
1:B:136:TRP:CG	1:B:137:PRO:HD3	2.55	0.41
1:B:205:ASP:OD2	1:H:167:LYS:NZ	2.52	0.41
1:D:67:ASN:O	1:D:71:VAL:HG22	2.20	0.41
1:F:270:GLN:HB3	3:F:401:GOL:O3	2.20	0.41
1:A:271:ARG:HD3	3:A:403:GOL:H31	2.01	0.41
1:E:16:TRP:CE2	1:E:29:PRO:HD2	2.56	0.41
1:H:147:LEU:O	1:H:150:LYS:HB2	2.20	0.41
1:E:22:TYR:CE2	1:E:24:PHE:HB2	2.56	0.41
1:G:44:GLN:HB3	1:G:86:TYR:CE2	2.54	0.41
1:H:22:TYR:CE2	1:H:24:PHE:HB2	2.56	0.41
1:E:14:LYS:HE2	1:G:14:LYS:CB	2.50	0.41
1:F:142:ASN:N	1:F:142:ASN:HD22	2.19	0.41
1:C:270:GLN:HB3	3:C:401:GOL:O3	2.21	0.41
1:G:89:GLU:O	1:G:92:SER:OG	2.36	0.41
1:F:67:ASN:O	1:F:71:VAL:HG22	2.20	0.41
1:H:96:CYS:HB3	1:H:97:PHE:HD1	1.84	0.41
1:C:37:ARG:CZ	1:C:78:PRO:HB2	2.50	0.41
1:H:130:LYS:O	1:H:134:THR:OG1	2.26	0.41
1:A:10:MET:HE3	1:A:11:LEU:H	1.86	0.41
1:E:206:GLN:O	1:E:209:SER:HB3	2.21	0.41
1:H:315:ILE:HD12	1:H:315:ILE:HA	1.89	0.41
1:B:6:ARG:HD3	1:B:9:VAL:HG13	2.03	0.41
1:B:9:VAL:HG23	1:B:74:ALA:HB1	2.03	0.41
1:B:17:LYS:HA	1:B:17:LYS:HD2	1.91	0.41
1:C:16:TRP:CE2	1:C:29:PRO:HD2	2.55	0.41
1:C:281[A]:GLN:NE2	1:E:281:GLN:HB3	2.36	0.41
1:D:87:LEU:HD12	1:D:136:TRP:CD2	2.56	0.41
1:D:138:LYS:HB2	1:D:138:LYS:HE2	1.83	0.41
1:D:179:LEU:HD23	1:D:179:LEU:HA	1.82	0.41
1:E:158:LEU:HD11	1:E:186:ALA:HA	2.03	0.41
1:F:22:TYR:CE2	1:F:24:PHE:HB2	2.56	0.41
1:F:208:ASP:HA	1:F:211:ARG:NE	2.36	0.41
1:F:246:MET:HE3	1:F:251:PRO:HG3	2.02	0.41
1:G:155:LEU:HA	1:G:158:LEU:HB2	2.02	0.41
1:H:6:ARG:HB3	1:H:9:VAL:HG12	2.02	0.41
1:H:46:GLN:HE22	1:H:93:PHE:HE2	1.67	0.41
1:H:97:PHE:CD1	1:H:97:PHE:N	2.89	0.41
1:B:288:SER:HG	3:H:401:GOL:HO1	1.69	0.40
1:C:326:PRO:HG3	1:H:244:ARG:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:ASN:O	1:F:251:PRO:HD2	2.21	0.40
1:B:321:TYR:O	1:B:327:PHE:HA	2.21	0.40
1:A:229:HIS:CD2	1:A:233:GLU:HG3	2.56	0.40
1:E:355:LEU:HD23	1:E:355:LEU:HA	1.95	0.40
1:G:55:VAL:HG11	1:G:335:TYR:CD2	2.55	0.40
1:G:220:HIS:NE2	1:G:272:CYS:HB3	2.36	0.40
1:A:6:ARG:HB3	1:A:9:VAL:CG1	2.51	0.40
1:D:227:TYR:CE2	1:D:265:LYS:HB3	2.56	0.40
1:H:44:GLN:NE2	1:H:346:PHE:H	2.20	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	360/368 (98%)	345 (96%)	13 (4%)	2 (1%)	21	39
1	B	359/368 (98%)	344 (96%)	14 (4%)	1 (0%)	36	56
1	C	346/368 (94%)	332 (96%)	13 (4%)	1 (0%)	36	56
1	D	341/368 (93%)	332 (97%)	8 (2%)	1 (0%)	36	56
1	E	336/368 (91%)	322 (96%)	13 (4%)	1 (0%)	36	56
1	F	341/368 (93%)	325 (95%)	16 (5%)	0	100	100
1	G	327/368 (89%)	307 (94%)	15 (5%)	5 (2%)	8	16
1	H	326/368 (89%)	310 (95%)	12 (4%)	4 (1%)	10	21
All	All	2736/2944 (93%)	2617 (96%)	104 (4%)	15 (0%)	24	44

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	LYS

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Mol	Chain	Res	Type
1	A	362	VAL
1	C	14	LYS
1	D	14	LYS
1	G	14	LYS
1	G	155	LEU
1	H	14	LYS
1	B	13	CYS
1	E	13	CYS
1	G	124	VAL
1	H	359	GLY
1	H	364	TYR
1	G	242	LYS
1	G	327	PHE
1	H	323	ASN

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	310/318 (98%)	310 (100%)	0	100	100
1	B	312/318 (98%)	312 (100%)	0	100	100
1	C	290/318 (91%)	288 (99%)	2 (1%)	76	89
1	D	287/318 (90%)	287 (100%)	0	100	100
1	E	289/318 (91%)	289 (100%)	0	100	100
1	F	295/318 (93%)	295 (100%)	0	100	100
1	G	253/318 (80%)	253 (100%)	0	100	100
1	H	249/318 (78%)	249 (100%)	0	100	100
All	All	2285/2544 (90%)	2283 (100%)	2 (0%)	100	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	281[A]	GLN

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Mol	Chain	Res	Type
1	C	281[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	112	ASN
1	A	201	ASN
1	A	281	GLN
1	B	100	GLN
1	B	193	ASN
1	B	270	GLN
1	C	7	HIS
1	C	229	HIS
1	D	36	GLN
1	E	36	GLN
1	E	88	ASN
1	E	170	HIS
1	E	270	GLN
1	E	281	GLN
1	F	7	HIS
1	F	88	ASN
1	F	142	ASN
1	G	281	GLN
1	H	7	HIS

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

13 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	$\# Z > 2$
3	GOL	E	401	-	5,5,5	0.58	0	5,5,5	0.31	0
3	GOL	G	401	-	5,5,5	0.57	0	5,5,5	0.34	0
2	BTB	A	401	-	13,13,13	0.51	0	7,16,16	1.07	0
3	GOL	H	401	-	5,5,5	0.57	0	5,5,5	0.33	0
2	BTB	B	401	-	13,13,13	0.46	0	7,16,16	0.67	0
3	GOL	F	401	-	5,5,5	0.57	0	5,5,5	0.47	0
3	GOL	C	401	-	5,5,5	0.56	0	5,5,5	0.43	0
3	GOL	D	402	-	5,5,5	0.57	0	5,5,5	0.44	0
2	BTB	B	402	-	13,13,13	0.52	0	7,16,16	1.11	1 (14%)
2	BTB	D	401	-	13,13,13	0.55	0	7,16,16	0.82	0
3	GOL	A	403	-	5,5,5	0.55	0	5,5,5	0.28	0
3	GOL	B	403	-	5,5,5	0.55	0	5,5,5	0.63	0
2	BTB	A	402	-	13,13,13	0.57	0	7,16,16	0.74	0

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
3	GOL	E	401	-	-	2/4/4/4	-
3	GOL	G	401	-	-	0/4/4/4	-
2	BTB	A	401	-	-	11/21/21/21	-
3	GOL	H	401	-	-	2/4/4/4	-
2	BTB	B	401	-	-	15/21/21/21	-
3	GOL	F	401	-	-	2/4/4/4	-
3	GOL	C	401	-	-	2/4/4/4	-
3	GOL	D	402	-	-	2/4/4/4	-
2	BTB	B	402	-	-	10/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BTB	D	401	-	-	7/21/21/21	-
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	B	403	-	-	0/4/4/4	-
2	BTB	A	402	-	-	12/21/21/21	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	BTB	O3-C3-C2	-2.25	106.11	111.40

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	BTB	O1-C1-C2-C3
2	A	401	BTB	O1-C1-C2-C4
2	A	401	BTB	O1-C1-C2-N
2	A	401	BTB	C1-C2-N-C5
2	A	401	BTB	C1-C2-N-C7
2	A	401	BTB	C3-C2-N-C5
2	A	401	BTB	C3-C2-N-C7
2	A	401	BTB	C4-C2-N-C5
2	A	401	BTB	C4-C2-N-C7
2	A	402	BTB	O1-C1-C2-C3
2	A	402	BTB	O1-C1-C2-C4
2	A	402	BTB	O1-C1-C2-N
2	A	402	BTB	C1-C2-C3-O3
2	A	402	BTB	C4-C2-C3-O3
2	A	402	BTB	N-C2-C3-O3
2	A	402	BTB	C1-C2-C4-O4
2	A	402	BTB	C3-C2-C4-O4
2	A	402	BTB	N-C2-C4-O4
2	B	401	BTB	O1-C1-C2-C3
2	B	401	BTB	O1-C1-C2-C4
2	B	401	BTB	O1-C1-C2-N
2	B	401	BTB	C1-C2-C4-O4
2	B	401	BTB	C3-C2-C4-O4
2	B	401	BTB	N-C2-C4-O4
2	B	401	BTB	C1-C2-N-C5

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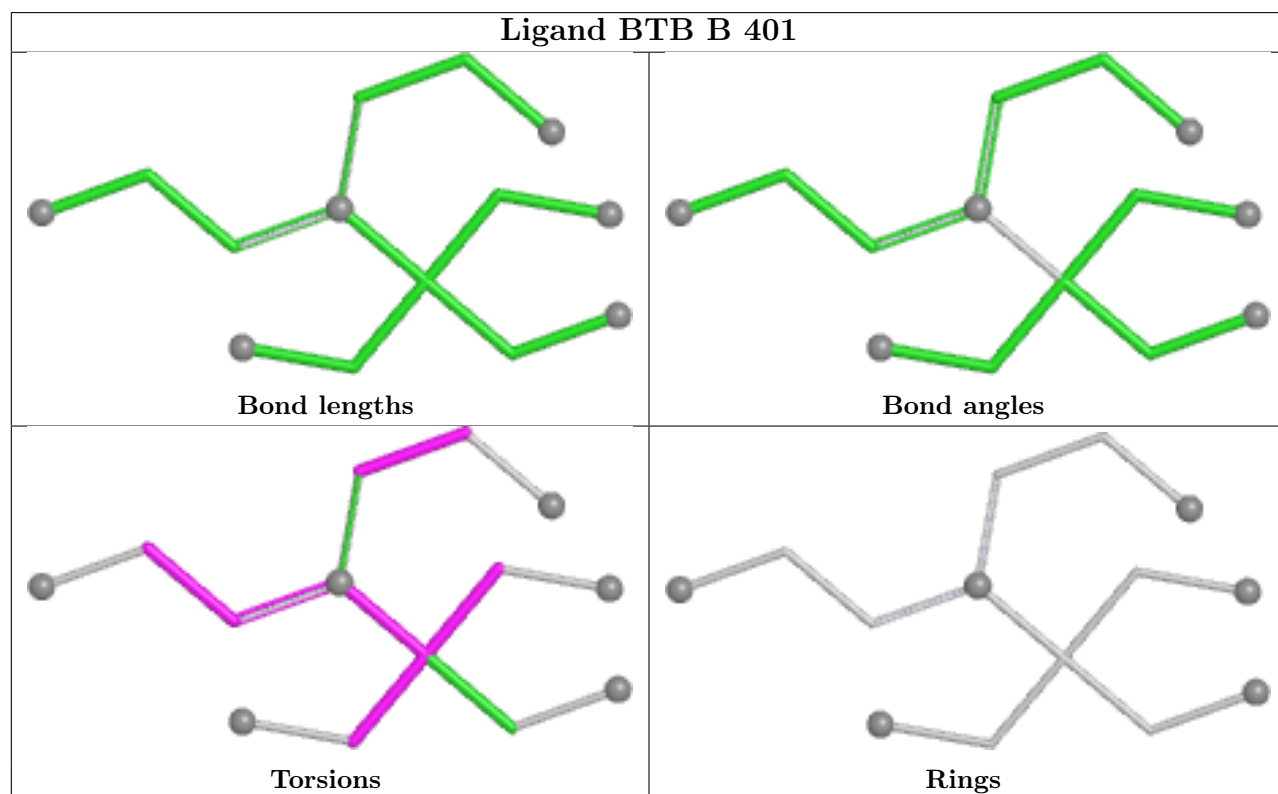
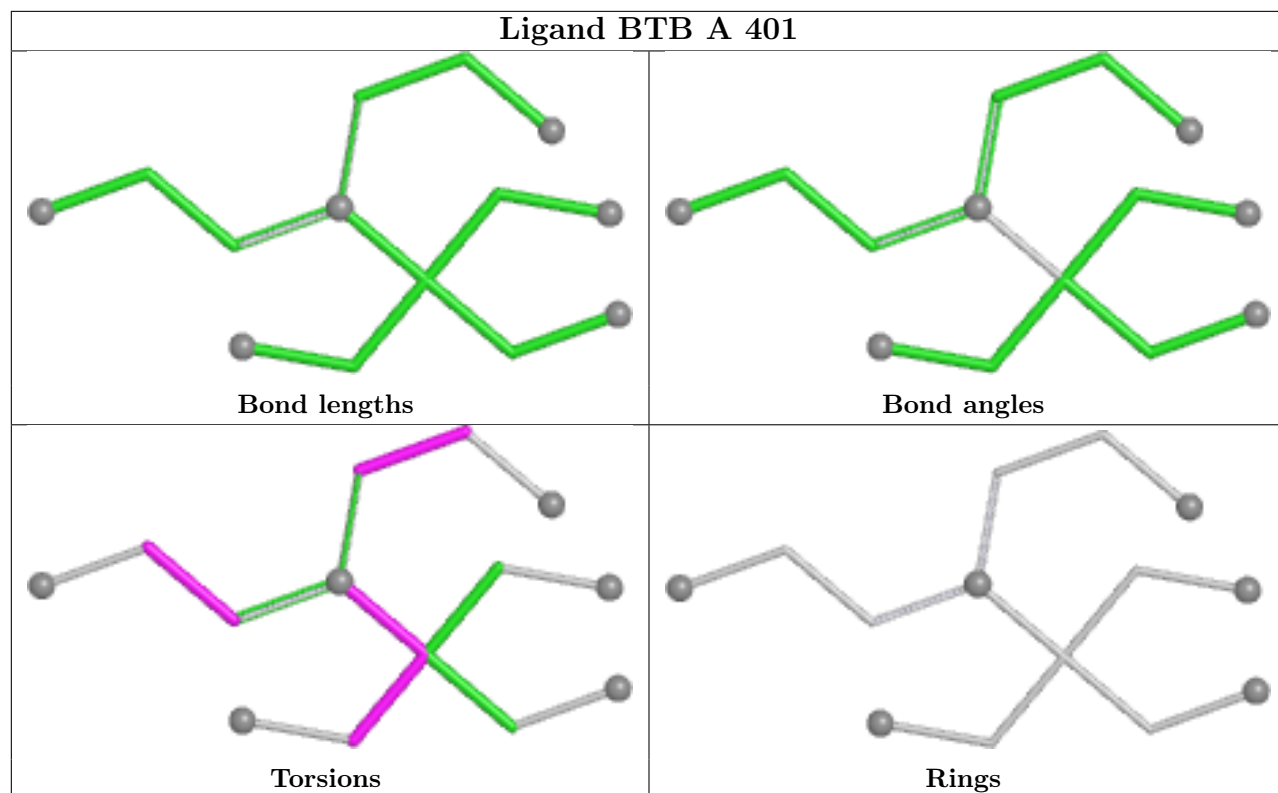
Mol	Chain	Res	Type	Atoms
2	B	401	BTB	C1-C2-N-C7
2	B	401	BTB	C3-C2-N-C5
2	B	401	BTB	C3-C2-N-C7
2	B	401	BTB	C4-C2-N-C5
2	B	401	BTB	C4-C2-N-C7
2	B	402	BTB	O1-C1-C2-C3
2	B	402	BTB	O1-C1-C2-C4
2	B	402	BTB	O1-C1-C2-N
2	B	402	BTB	C1-C2-C4-O4
2	B	402	BTB	C3-C2-C4-O4
2	B	402	BTB	N-C2-C4-O4
2	D	401	BTB	O1-C1-C2-C3
2	D	401	BTB	O1-C1-C2-C4
2	D	401	BTB	O1-C1-C2-N
2	D	401	BTB	C1-C2-C3-O3
2	D	401	BTB	C4-C2-C3-O3
2	D	401	BTB	N-C2-C3-O3
3	A	403	GOL	C1-C2-C3-O3
3	C	401	GOL	C1-C2-C3-O3
3	D	402	GOL	C1-C2-C3-O3
3	E	401	GOL	C1-C2-C3-O3
3	F	401	GOL	C1-C2-C3-O3
3	H	401	GOL	C1-C2-C3-O3
2	A	401	BTB	N-C5-C6-O6
2	A	402	BTB	N-C7-C8-O8
2	B	401	BTB	N-C5-C6-O6
2	B	401	BTB	N-C7-C8-O8
3	A	403	GOL	O2-C2-C3-O3
3	E	401	GOL	O2-C2-C3-O3
2	B	402	BTB	N-C7-C8-O8
3	C	401	GOL	O2-C2-C3-O3
3	F	401	GOL	O2-C2-C3-O3
2	A	402	BTB	N-C5-C6-O6
2	A	402	BTB	C6-C5-N-C7
3	D	402	GOL	O2-C2-C3-O3
3	H	401	GOL	O2-C2-C3-O3
2	D	401	BTB	N-C7-C8-O8
2	A	401	BTB	N-C7-C8-O8
2	B	401	BTB	C8-C7-N-C2
2	B	402	BTB	C1-C2-N-C5
2	B	402	BTB	C3-C2-N-C5
2	B	402	BTB	C4-C2-N-C5

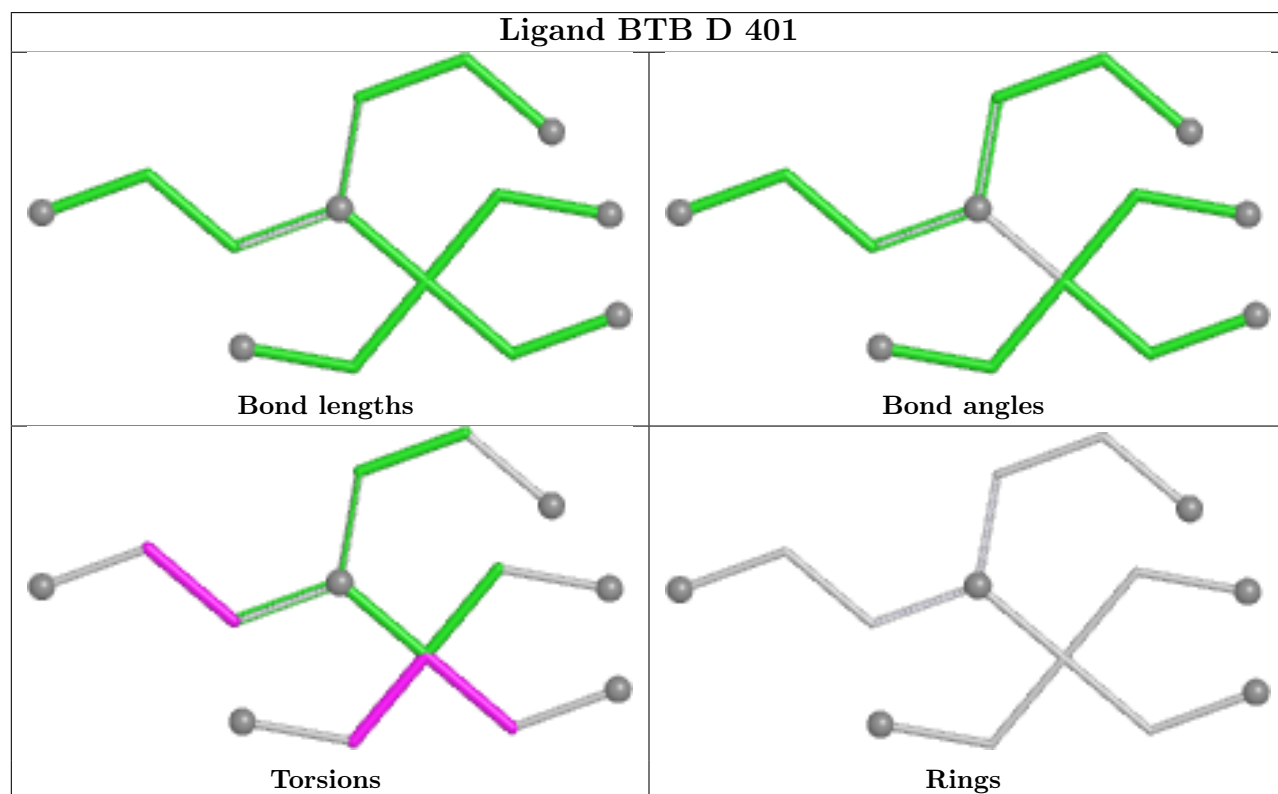
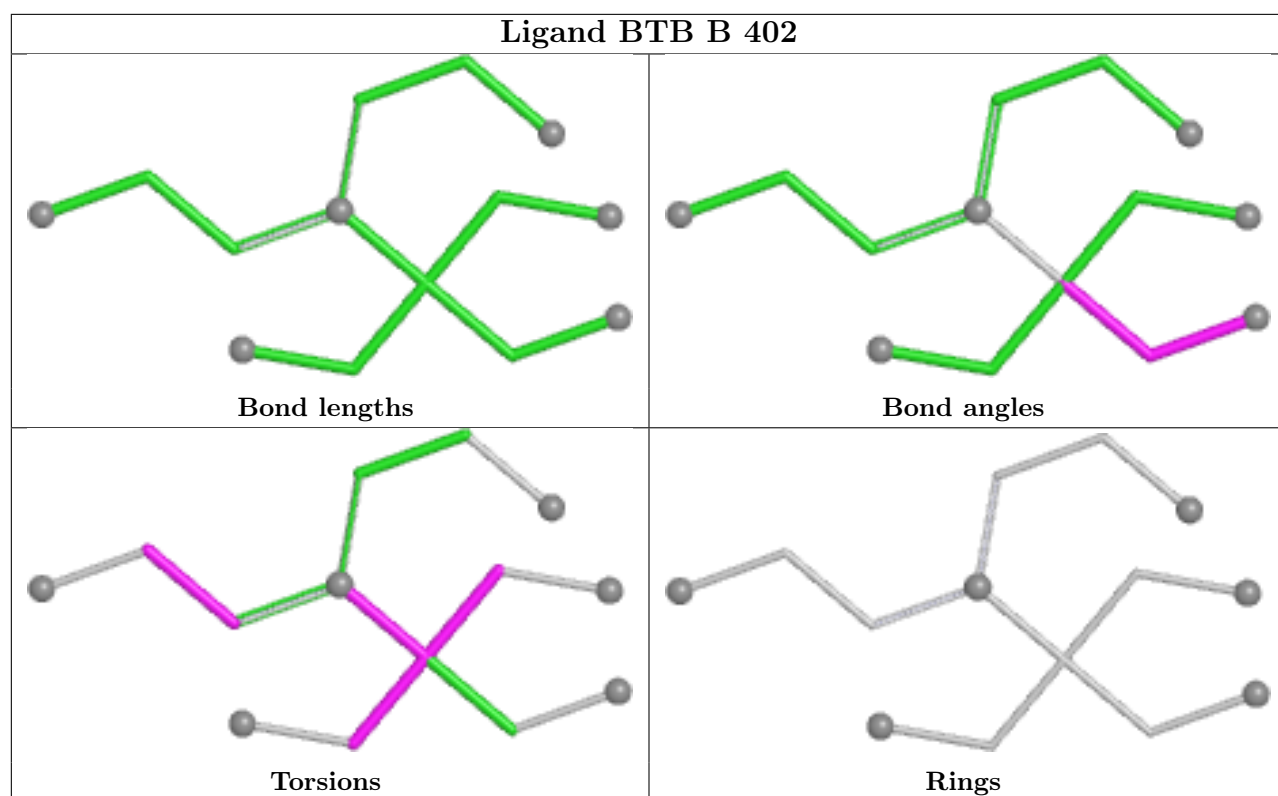
There are no ring outliers.

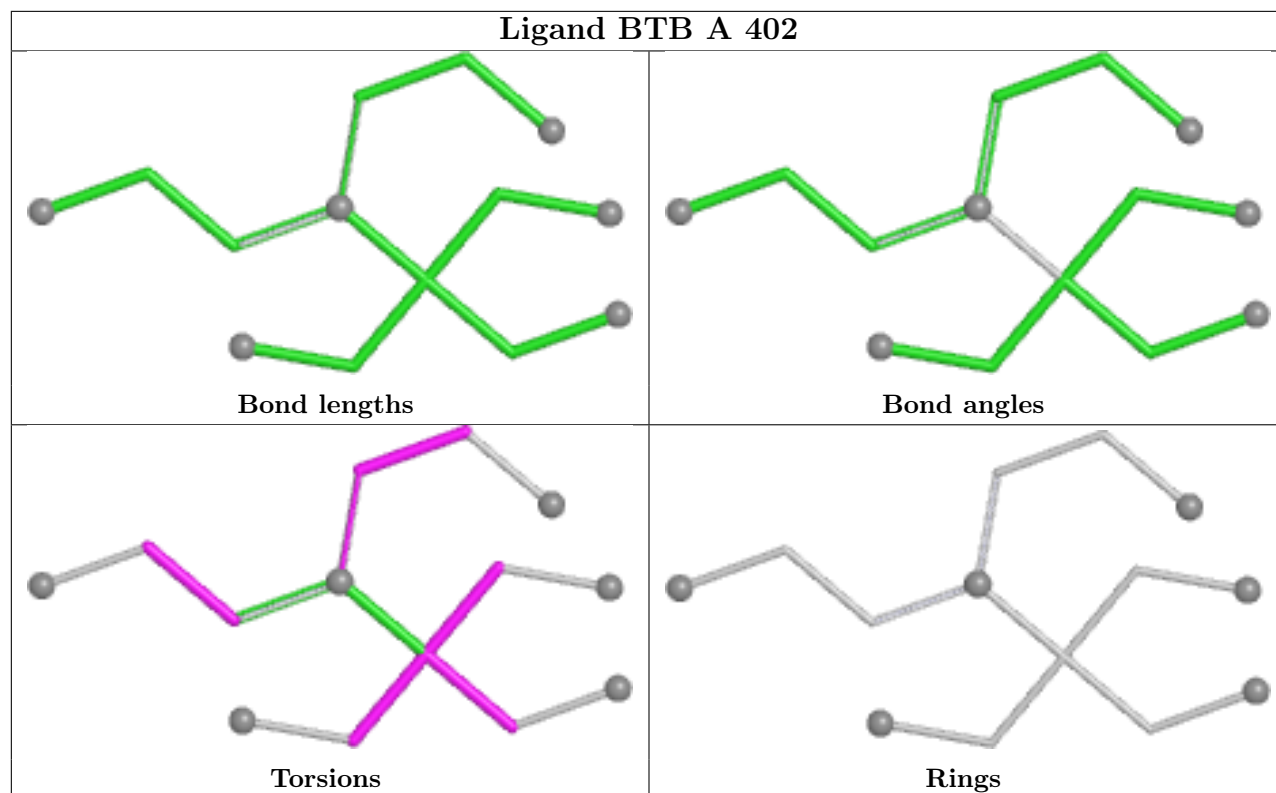
11 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	401	GOL	2	0
3	G	401	GOL	3	0
2	A	401	BTB	4	0
3	H	401	GOL	2	0
2	B	401	BTB	4	0
3	F	401	GOL	2	0
3	C	401	GOL	2	0
3	D	402	GOL	1	0
2	D	401	BTB	4	0
3	A	403	GOL	2	0
2	A	402	BTB	4	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	362/368 (98%)	-0.07	10 (2%) 55 50	20, 36, 61, 106	0
1	B	361/368 (98%)	-0.05	8 (2%) 62 57	21, 34, 63, 80	0
1	C	349/368 (94%)	0.07	20 (5%) 29 24	22, 40, 76, 104	1 (0%)
1	D	345/368 (93%)	0.09	10 (2%) 53 48	21, 40, 71, 102	0
1	E	340/368 (92%)	0.22	17 (5%) 34 29	26, 41, 81, 111	0
1	F	345/368 (93%)	0.18	14 (4%) 41 36	23, 40, 87, 131	0
1	G	335/368 (91%)	1.05	88 (26%) 1 1	25, 57, 139, 162	0
1	H	334/368 (90%)	1.15	94 (28%) 1 1	26, 60, 142, 185	0
All	All	2771/2944 (94%)	0.32	261 (9%) 14 11	20, 42, 118, 185	1 (0%)

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	364	TYR	5.8
1	F	366	ASN	5.8
1	H	323	ASN	5.4
1	H	364	TYR	5.3
1	G	343	ALA	5.2
1	H	366	ASN	5.1
1	H	360	PHE	4.7
1	G	353	ASP	4.6
1	E	244	ARG	4.6
1	H	321	TYR	4.5
1	H	324	HIS	4.4
1	C	364	TYR	4.4
1	G	358	GLY	4.4
1	F	364	TYR	4.2
1	G	151	CYS	4.2
1	G	326	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	335	TYR	4.1
1	H	352	SER	4.1
1	H	334	PRO	4.0
1	H	347	GLU	4.0
1	H	7	HIS	4.0
1	D	364	TYR	4.0
1	H	243	GLY	3.9
1	H	345	TRP	3.7
1	H	365	ALA	3.7
1	H	123	PRO	3.7
1	C	120	TYR	3.7
1	H	244	ARG	3.7
1	G	155	LEU	3.6
1	G	122	ASN	3.6
1	H	136	TRP	3.6
1	G	341	GLU	3.6
1	F	158	LEU	3.6
1	G	344	LEU	3.6
1	H	355	LEU	3.6
1	C	14	LYS	3.6
1	H	0	ASN	3.6
1	G	66	GLY	3.6
1	G	145	PRO	3.6
1	D	293	GLU	3.6
1	H	143	LEU	3.6
1	H	350	THR	3.5
1	G	136	TRP	3.5
1	H	344	LEU	3.5
1	G	128	ASN	3.5
1	H	341	GLU	3.4
1	H	125	TRP	3.4
1	H	139	ILE	3.4
1	G	361	GLU	3.4
1	H	137	PRO	3.4
1	H	322	HIS	3.4
1	H	349	VAL	3.4
1	G	125	TRP	3.4
1	F	118	PRO	3.4
1	G	127	ALA	3.4
1	G	94	TYR	3.4
1	E	7	HIS	3.4
1	D	187	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	211	ARG	3.3
1	H	93	PHE	3.3
1	D	120	TYR	3.3
1	E	158	LEU	3.3
1	G	339	ARG	3.3
1	G	332	ALA	3.3
1	G	131	ASN	3.3
1	H	362	VAL	3.3
1	H	14	LYS	3.3
1	G	97	PHE	3.3
1	G	62	LEU	3.3
1	A	241	GLY	3.3
1	H	358	GLY	3.3
1	H	343	ALA	3.3
1	H	320	THR	3.2
1	H	241	GLY	3.2
1	G	349	VAL	3.2
1	H	242	LYS	3.2
1	H	340	LYS	3.2
1	H	339	ARG	3.2
1	H	351	GLU	3.2
1	G	154	SER	3.2
1	H	333	ALA	3.2
1	G	146	LYS	3.1
1	H	158	LEU	3.1
1	G	149	PRO	3.1
1	G	41	ALA	3.1
1	H	335	TYR	3.1
1	G	140	LEU	3.1
1	H	97	PHE	3.1
1	A	10	MET	3.1
1	A	364	TYR	3.1
1	G	359	GLY	3.1
1	H	332	ALA	3.1
1	H	331	TYR	3.1
1	C	12	ASP	3.1
1	H	64	PRO	3.1
1	H	149	PRO	3.1
1	C	241	GLY	3.1
1	F	162	THR	3.1
1	H	239	THR	3.1
1	G	46	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	132	THR	3.0
1	G	333	ALA	3.0
1	G	49	VAL	3.0
1	E	364	TYR	3.0
1	G	159	VAL	3.0
1	G	43	ILE	3.0
1	G	346	PHE	3.0
1	G	360	PHE	3.0
1	G	147	LEU	2.9
1	G	329	GLU	2.9
1	H	141	GLU	2.9
1	A	243	GLY	2.9
1	E	240	TYR	2.9
1	H	56	GLY	2.9
1	C	365	ALA	2.9
1	H	126	GLN	2.9
1	D	240	TYR	2.9
1	H	57	ALA	2.9
1	H	138	LYS	2.9
1	H	155	LEU	2.9
1	G	133	MET	2.8
1	G	123	PRO	2.8
1	E	234	ALA	2.8
1	G	7	HIS	2.8
1	H	134	THR	2.8
1	H	55	VAL	2.8
1	H	124	VAL	2.8
1	C	96	CYS	2.8
1	G	87	LEU	2.8
1	E	365	ALA	2.8
1	H	49	VAL	2.8
1	H	159	VAL	2.8
1	H	63	GLY	2.7
1	H	13	CYS	2.7
1	G	47	ILE	2.7
1	G	330	GLY	2.7
1	D	0	ASN	2.7
1	G	124	VAL	2.7
1	G	48	ASP	2.7
1	G	129	TYR	2.7
1	D	96	CYS	2.7
1	H	151	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	327	PHE	2.7
1	H	157	ALA	2.7
1	H	15	LEU	2.6
1	H	60	GLY	2.6
1	F	365	ALA	2.6
1	G	55	VAL	2.6
1	G	152	VAL	2.6
1	F	7	HIS	2.6
1	E	243	GLY	2.6
1	H	131	ASN	2.6
1	G	320	THR	2.6
1	H	346	PHE	2.6
1	G	324	HIS	2.6
1	H	342	GLY	2.6
1	H	50	PHE	2.6
1	G	139	ILE	2.6
1	H	87	LEU	2.6
1	C	242	LYS	2.6
1	A	366	ASN	2.6
1	G	143	LEU	2.5
1	A	14	LYS	2.5
1	E	242	LYS	2.5
1	G	138	LYS	2.5
1	G	337	LYS	2.5
1	H	361	GLU	2.5
1	F	243	GLY	2.5
1	G	357	THR	2.5
1	H	338	ARG	2.5
1	C	243	GLY	2.5
1	C	119	LYS	2.5
1	H	96	CYS	2.5
1	G	64	PRO	2.5
1	F	14	LYS	2.4
1	G	15	LEU	2.4
1	G	158	LEU	2.4
1	H	133	MET	2.4
1	F	120	TYR	2.4
1	E	119	LYS	2.4
1	G	354	GLN	2.4
1	H	128	ASN	2.4
1	H	39	ASP	2.4
1	C	336	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	59	PRO	2.4
1	G	52	LYS	2.4
1	G	331	TYR	2.4
1	C	366	ASN	2.4
1	C	94	TYR	2.4
1	G	157	ALA	2.4
1	H	41	ALA	2.4
1	H	43	ILE	2.4
1	E	94	TYR	2.3
1	E	120	TYR	2.3
1	H	140	LEU	2.3
1	F	242	LYS	2.3
1	G	238	SER	2.3
1	G	325	PRO	2.3
1	H	65	ARG	2.3
1	H	58	MET	2.3
1	F	99	LYS	2.3
1	G	242	LYS	2.3
1	G	240	TYR	2.3
1	H	337	LYS	2.3
1	B	121	ASP	2.3
1	G	156	VAL	2.3
1	D	1	ALA	2.3
1	C	239	THR	2.3
1	H	47	ILE	2.2
1	G	134	THR	2.2
1	B	293	GLU	2.2
1	B	187	TRP	2.2
1	E	97	PHE	2.2
1	G	135	LYS	2.2
1	B	13	CYS	2.2
1	G	95	GLU	2.2
1	H	46	GLN	2.2
1	B	79	ASP	2.2
1	G	53	ASP	2.2
1	G	241	GLY	2.2
1	H	52	LYS	2.2
1	H	61	ALA	2.2
1	A	242	LYS	2.2
1	B	7	HIS	2.2
1	A	365	ALA	2.2
1	B	336	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	244	ARG	2.2
1	G	348	LYS	2.2
1	F	117	ASP	2.2
1	G	90	VAL	2.2
1	G	160	GLU	2.1
1	H	86	TYR	2.1
1	G	342	GLY	2.1
1	A	7	HIS	2.1
1	G	132	THR	2.1
1	G	355	LEU	2.1
1	C	98	GLU	2.1
1	G	336	GLU	2.1
1	D	14	LYS	2.1
1	G	58	MET	2.1
1	C	237	HIS	2.1
1	E	236	ILE	2.1
1	G	144	ASP	2.1
1	G	57	ALA	2.1
1	C	99	LYS	2.1
1	G	88	ASN	2.1
1	E	241	GLY	2.1
1	C	211	ARG	2.0
1	E	157	ALA	2.0
1	H	348	LYS	2.0
1	C	162	THR	2.0
1	E	145	PRO	2.0
1	H	145	PRO	2.0
1	H	62	LEU	2.0
1	H	240	TYR	2.0
1	F	95	GLU	2.0
1	D	242	LYS	2.0
1	G	150	LYS	2.0
1	H	127	ALA	2.0
1	G	350	THR	2.0
1	H	156	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

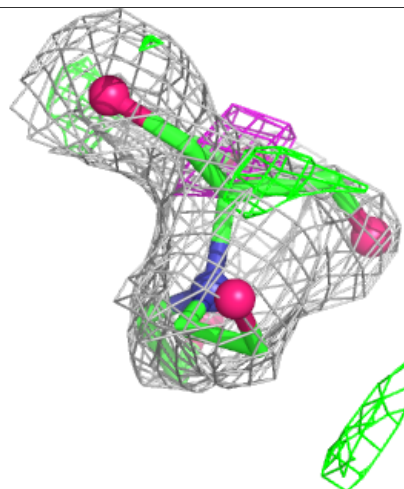
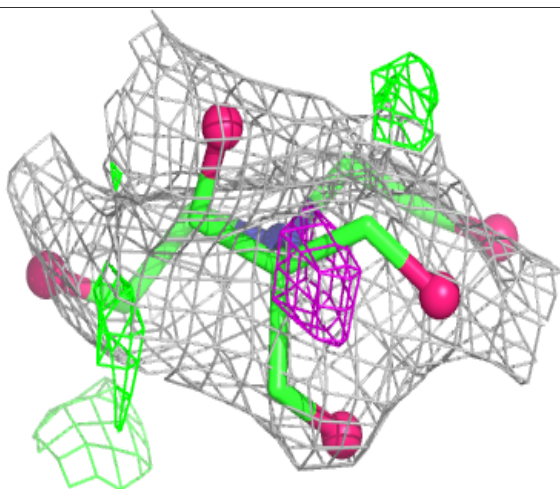
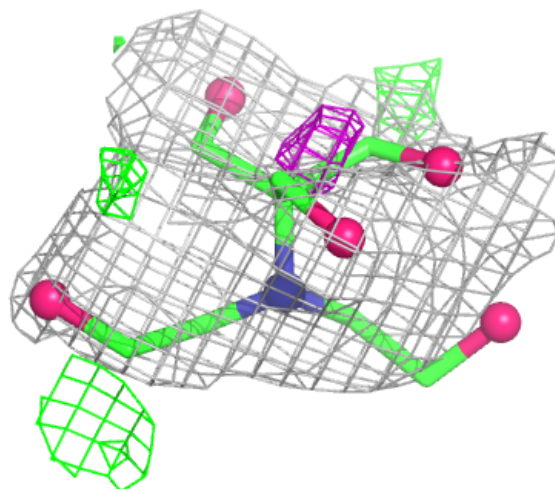
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BTB	A	401	14/14	0.69	0.22	67,72,78,86	0
2	BTB	B	401	14/14	0.77	0.20	56,63,70,72	0
2	BTB	B	402	14/14	0.83	0.20	53,62,69,73	0
2	BTB	D	401	14/14	0.83	0.15	54,62,81,81	0
3	GOL	F	401	6/6	0.84	0.16	42,45,48,59	0
3	GOL	B	403	6/6	0.87	0.18	35,37,43,47	0
2	BTB	A	402	14/14	0.88	0.15	52,57,64,66	0
3	GOL	H	401	6/6	0.89	0.11	48,51,52,64	0
3	GOL	A	403	6/6	0.91	0.12	34,36,42,45	0
3	GOL	D	402	6/6	0.94	0.08	28,34,37,43	0
3	GOL	G	401	6/6	0.94	0.12	40,45,50,50	0
3	GOL	E	401	6/6	0.94	0.09	31,33,39,41	0
3	GOL	C	401	6/6	0.95	0.06	32,39,41,45	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.

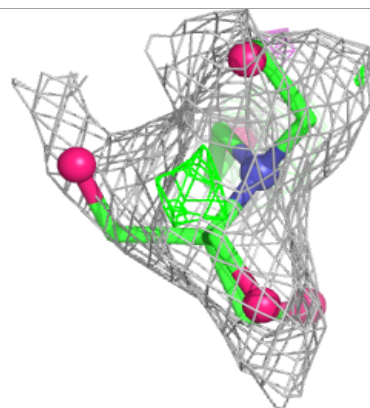
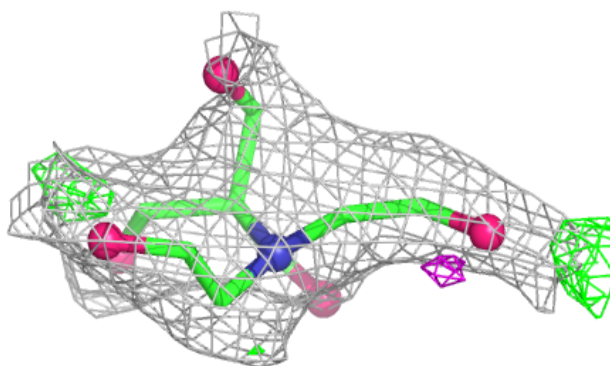
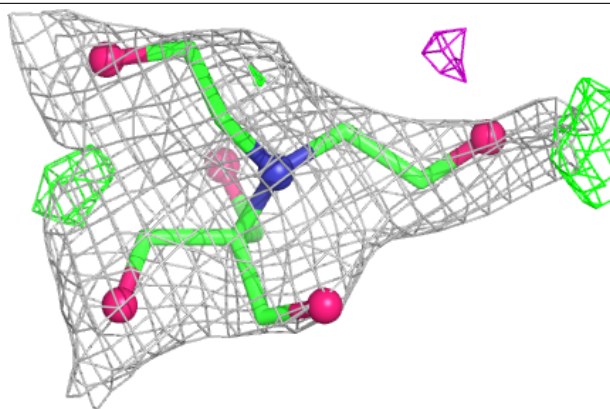
Electron density around BTB A 401:

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



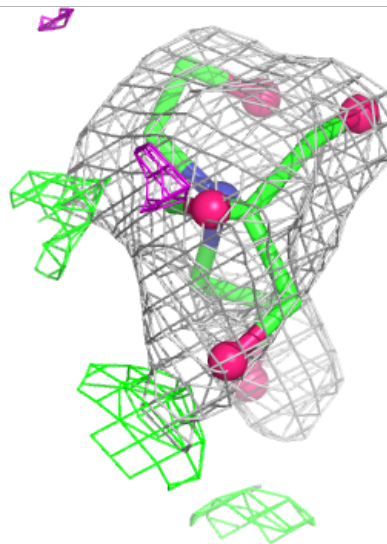
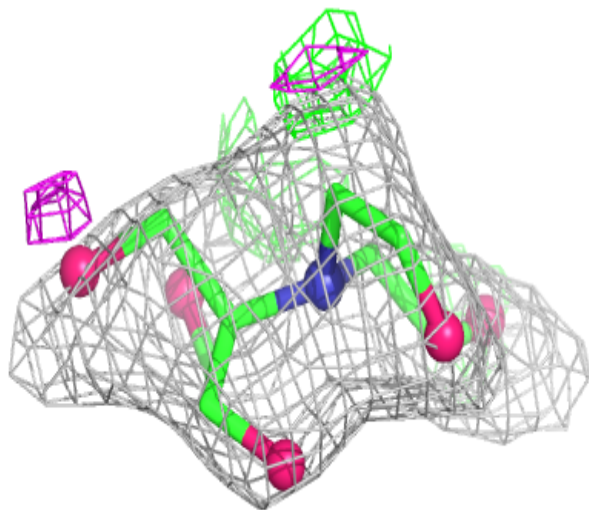
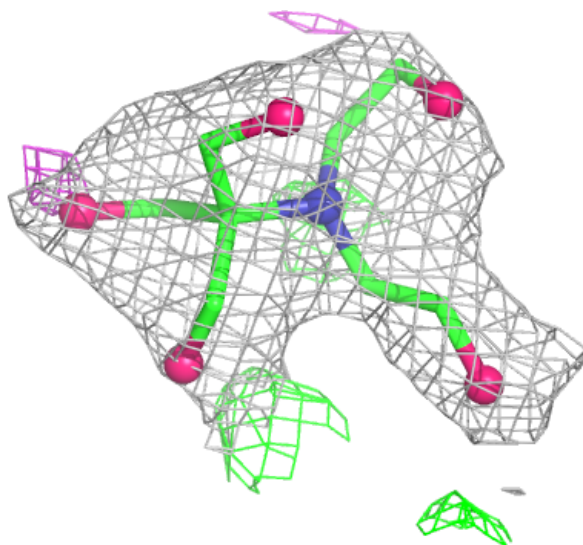
Electron density around BTB B 401:

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



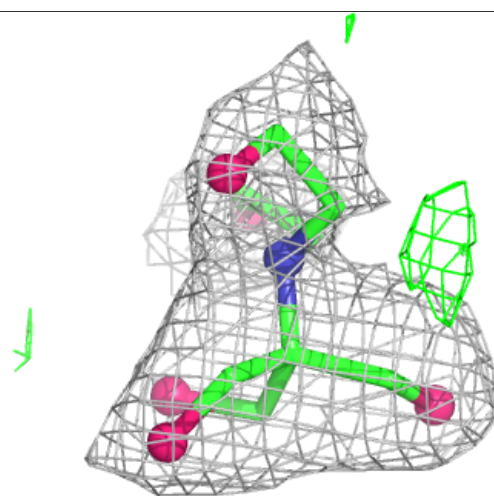
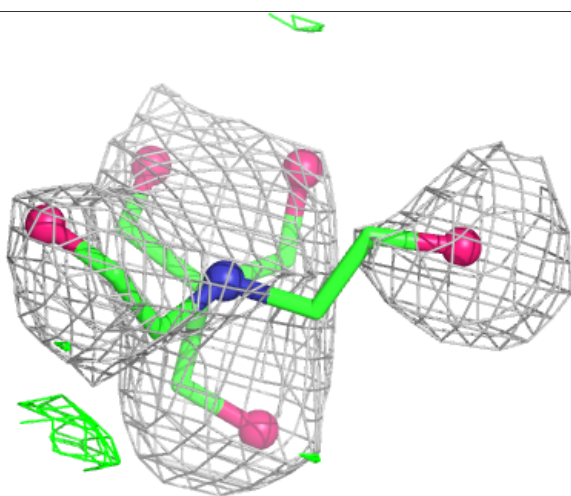
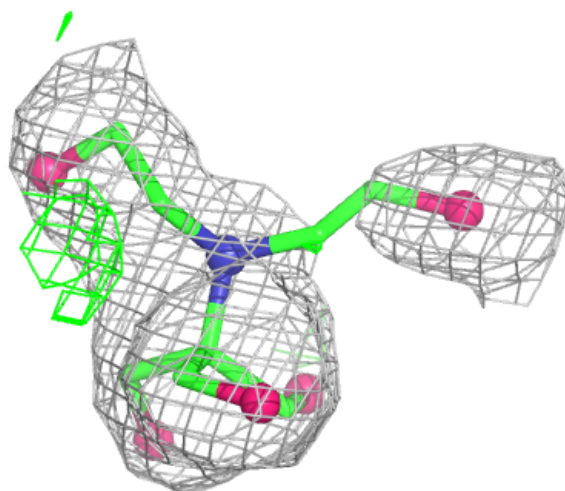
Electron density around BTB B 402:

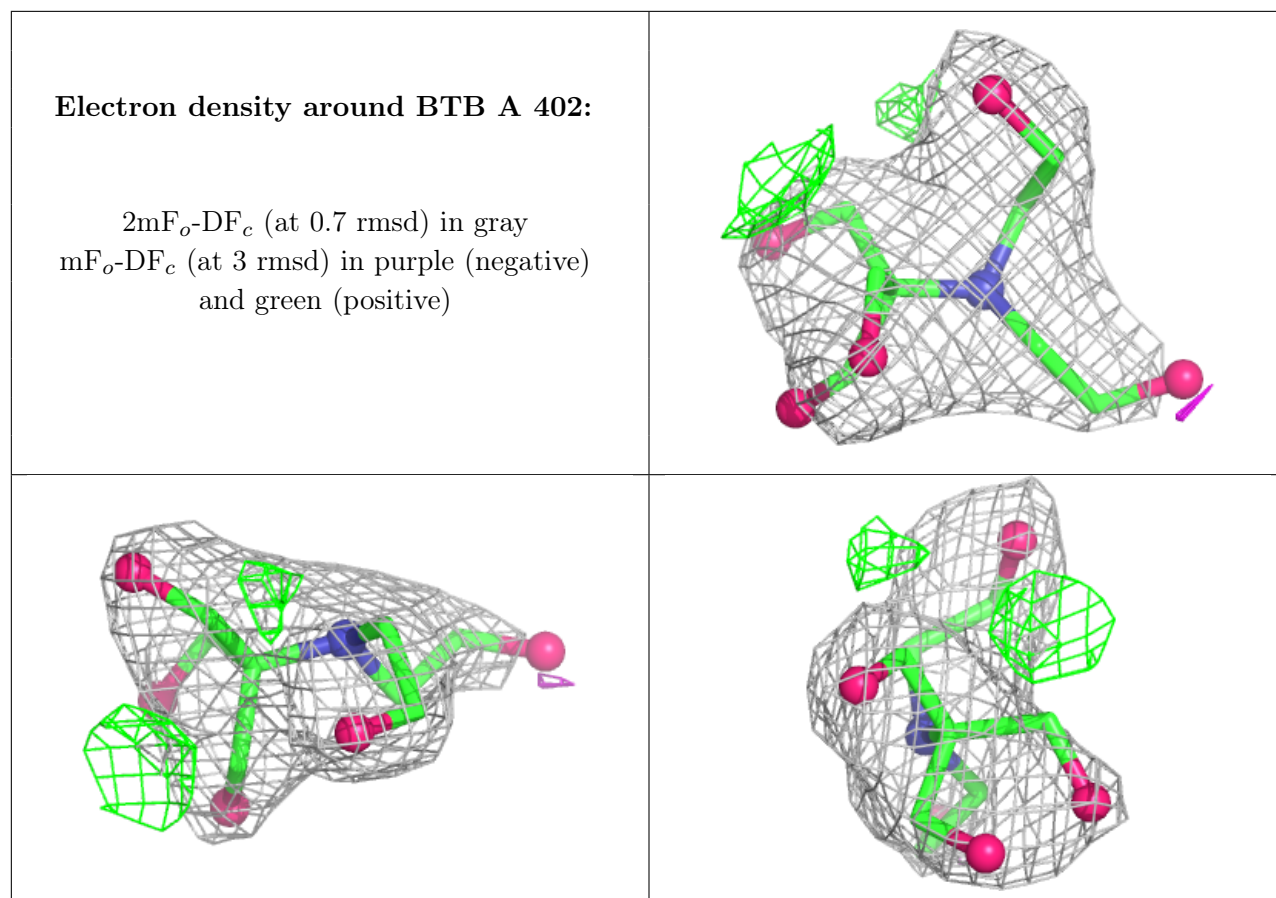
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BTB D 401:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.