



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:22 AM UTC

PDB ID : 4RDQ / pdb_00004rdq
Title : Calcium-activated chloride channel bestrophin-1, from chicken, in complex with Fab antibody fragments, chloride and calcium
Authors : Dickson, V.K.; Pedi, L.; Long, S.B.
Deposited on : 2014-09-19
Resolution : 2.85 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

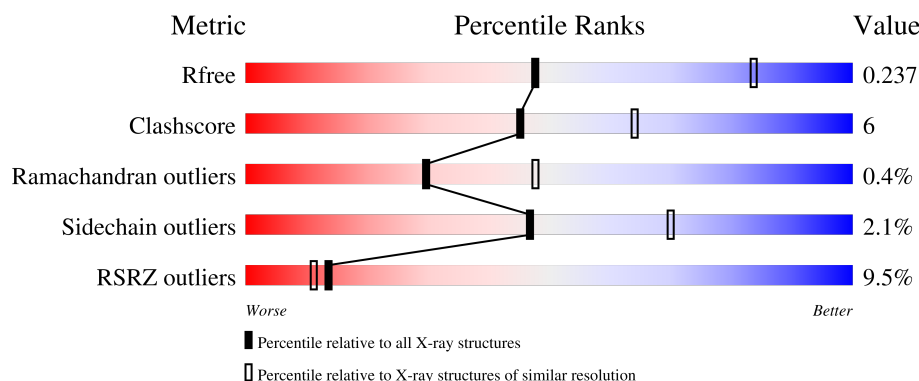
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	409	3% 73% 16% 11%
1	B	409	% 72% 16% 11%
1	C	409	2% 72% 17% 11%
1	D	409	3% 71% 17% 11%
1	E	409	4% 72% 17% 11%

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Mol	Chain	Length	Quality of chain
2	F	212	8% 86% 13%
2	H	212	11% 82% 18%
2	J	212	25% 85% 15%
2	L	212	10% 82% 18%
2	N	212	21% 83% 17%
3	G	217	13% 85% 12% •
3	I	217	8% 85% 12% •
3	K	217	22% 85% 12% •
3	M	217	9% 85% 12% •
3	O	217	22% 87% 10% •

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 31125 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 Bestrophin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2994	1962	484	535	13			
1	B	366	Total	C	N	O	S	0	0	0
			2994	1962	484	535	13			
1	C	366	Total	C	N	O	S	0	0	0
			2994	1962	484	535	13			
1	D	366	Total	C	N	O	S	0	0	0
			2994	1962	484	535	13			
1	E	366	Total	C	N	O	S	0	0	0
			2994	1962	484	535	13			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	GLU	-	expression tag	UNP E1C3A0
A	407	GLY	-	expression tag	UNP E1C3A0
A	408	GLU	-	expression tag	UNP E1C3A0
A	409	GLU	-	expression tag	UNP E1C3A0
A	410	PHE	-	expression tag	UNP E1C3A0
B	406	GLU	-	expression tag	UNP E1C3A0
B	407	GLY	-	expression tag	UNP E1C3A0
B	408	GLU	-	expression tag	UNP E1C3A0
B	409	GLU	-	expression tag	UNP E1C3A0
B	410	PHE	-	expression tag	UNP E1C3A0
C	406	GLU	-	expression tag	UNP E1C3A0
C	407	GLY	-	expression tag	UNP E1C3A0
C	408	GLU	-	expression tag	UNP E1C3A0
C	409	GLU	-	expression tag	UNP E1C3A0
C	410	PHE	-	expression tag	UNP E1C3A0
D	406	GLU	-	expression tag	UNP E1C3A0
D	407	GLY	-	expression tag	UNP E1C3A0
D	408	GLU	-	expression tag	UNP E1C3A0
D	409	GLU	-	expression tag	UNP E1C3A0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	410	PHE	-	expression tag	UNP E1C3A0
E	406	GLU	-	expression tag	UNP E1C3A0
E	407	GLY	-	expression tag	UNP E1C3A0
E	408	GLU	-	expression tag	UNP E1C3A0
E	409	GLU	-	expression tag	UNP E1C3A0
E	410	PHE	-	expression tag	UNP E1C3A0

- Molecule 2 is a protein called Fab antibody fragment, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	212	Total	C	N	O	S	0	0	0
			1591	990	266	329	6			
2	H	212	Total	C	N	O	S	0	0	0
			1591	990	266	329	6			
2	J	212	Total	C	N	O	S	0	0	0
			1591	990	266	329	6			
2	L	212	Total	C	N	O	S	0	0	0
			1591	990	266	329	6			
2	N	212	Total	C	N	O	S	0	0	0
			1591	990	266	329	6			

- Molecule 3 is a protein called Fab antibody fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	211	Total	C	N	O	S	0	0	0
			1558	991	254	305	8			
3	I	211	Total	C	N	O	S	0	0	0
			1558	991	254	305	8			
3	K	211	Total	C	N	O	S	0	0	0
			1558	991	254	305	8			
3	M	211	Total	C	N	O	S	0	0	0
			1558	991	254	305	8			
3	O	211	Total	C	N	O	S	0	0	0
			1558	991	254	305	8			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Cl	0	0
			3	3		
5	B	3	Total	Cl	0	0
			3	3		
5	C	3	Total	Cl	0	0
			3	3		
5	D	3	Total	Cl	0	0
			3	3		
5	E	3	Total	Cl	0	0
			3	3		

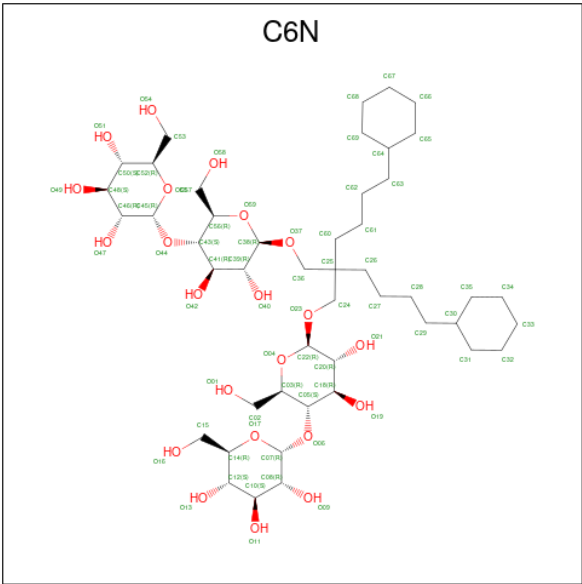
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0
6	B	1	Total Ca 1 1	0	0
6	C	1	Total Ca 1 1	0	0
6	D	1	Total Ca 1 1	0	0
6	E	1	Total Ca 1 1	0	0

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total K 1 1	0	0
7	B	1	Total K 1 1	0	0
7	C	2	Total K 2 2	0	0
7	E	1	Total K 1 1	0	0

- Molecule 8 is 6-cyclohexyl-2-(4-cyclohexylbutyl)-2-([4-O-(alpha-D-glucopyranosyl)-beta-D-glucopyranosyl]oxy)methyl)hexyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (CCD ID: C6N) (formula: C₄₇H₈₄O₂₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 69 47 22	0	0
8	B	1	Total C O 69 47 22	0	0
8	C	1	Total C O 69 47 22	0	0
8	D	1	Total C O 69 47 22	0	0
8	E	1	Total C O 69 47 22	0	0

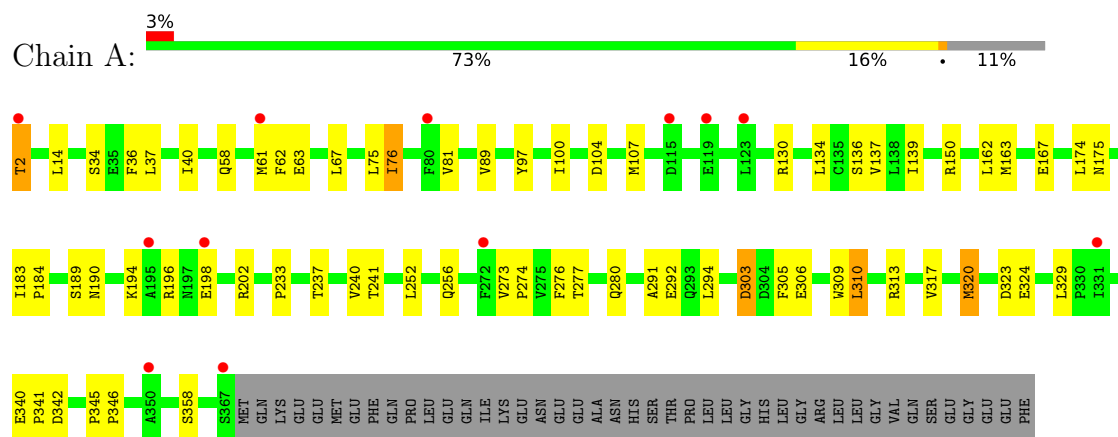
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total O 2 2	0	0
9	B	2	Total O 2 2	0	0
9	C	2	Total O 2 2	0	0
9	D	2	Total O 2 2	0	0
9	E	2	Total O 2 2	0	0

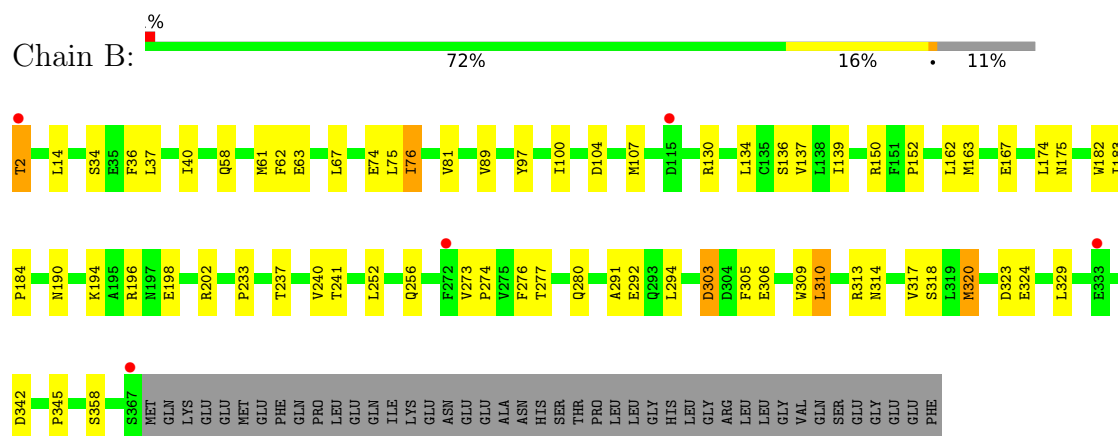
3 Residue-property plots [i](#)

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

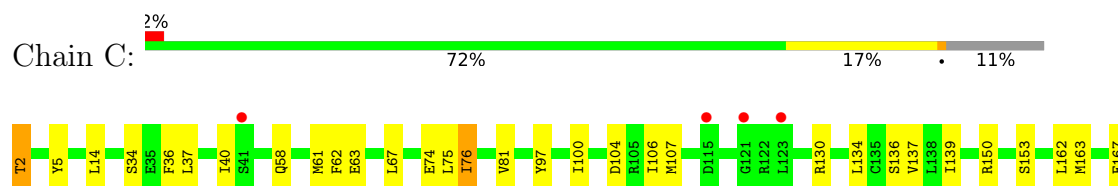
• Molecule 1: Bestrophin-1

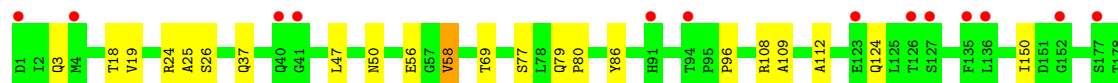


• Molecule 1: Bestrophin-1



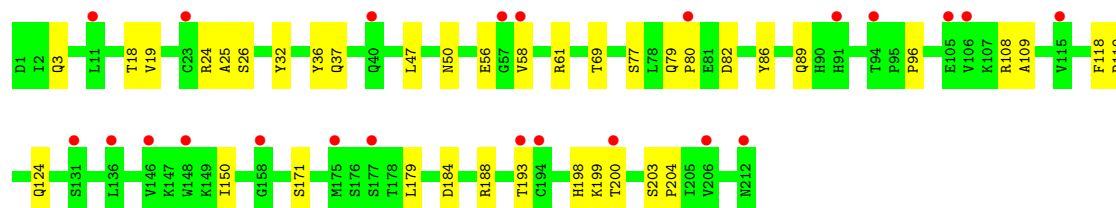
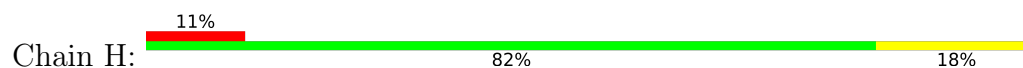
• Molecule 1: Bestrophin-1



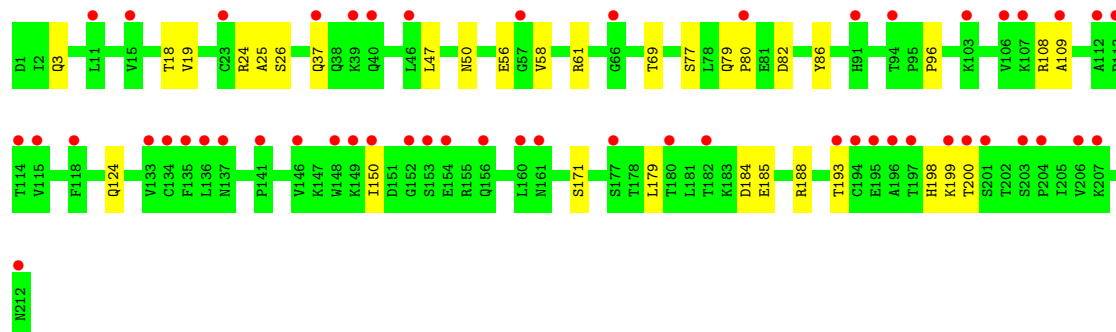
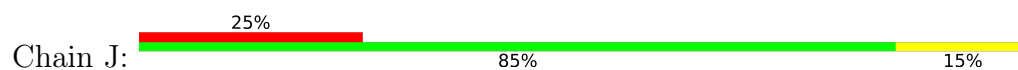




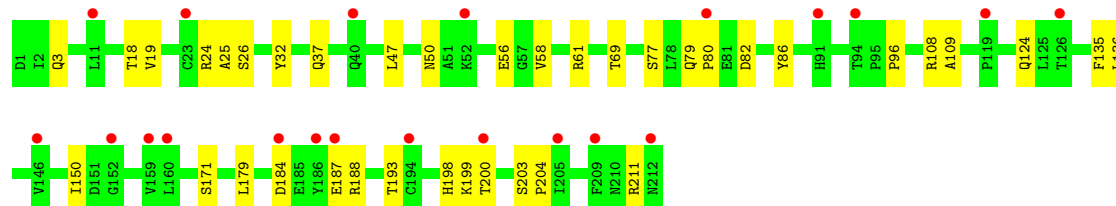
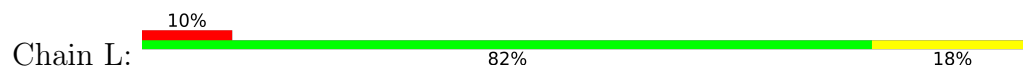
- Molecule 2: Fab antibody fragment, light chain



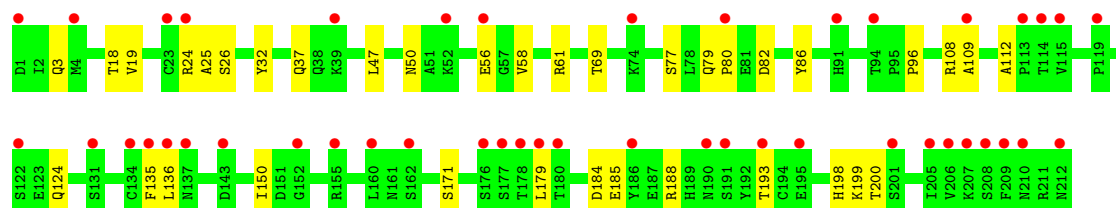
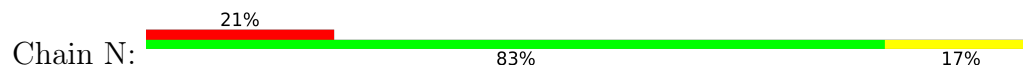
- Molecule 2: Fab antibody fragment, light chain



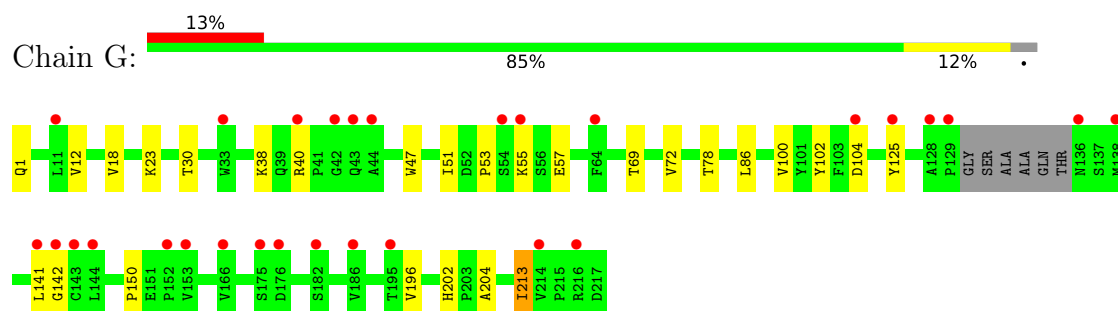
- Molecule 2: Fab antibody fragment, light chain



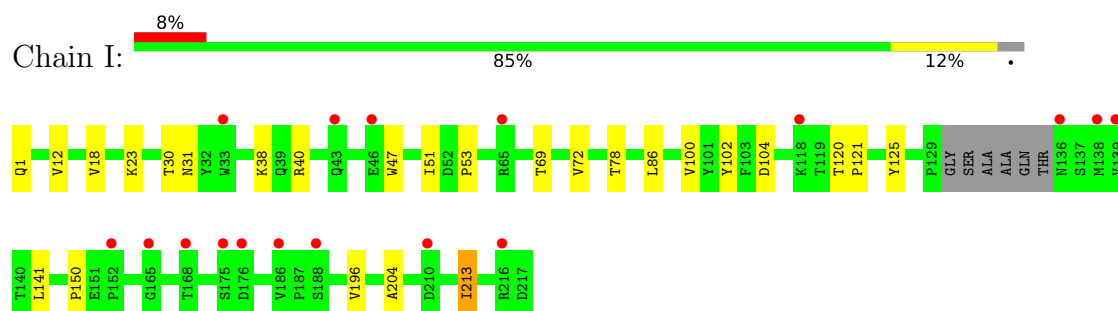
- Molecule 2: Fab antibody fragment, light chain



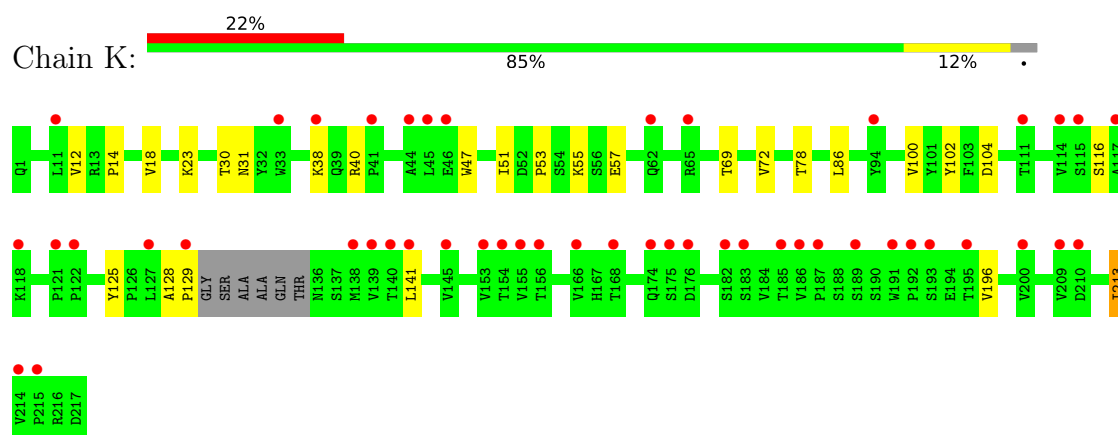
- Molecule 3: Fab antibody fragment, heavy chain



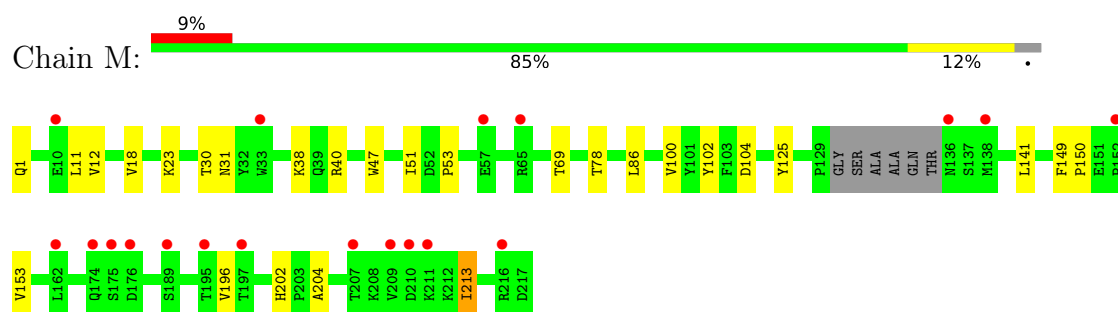
- Molecule 3: Fab antibody fragment, heavy chain



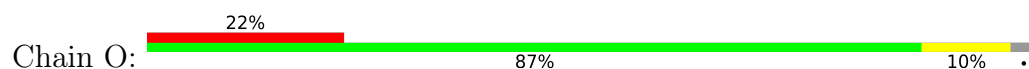
- Molecule 3: Fab antibody fragment, heavy chain

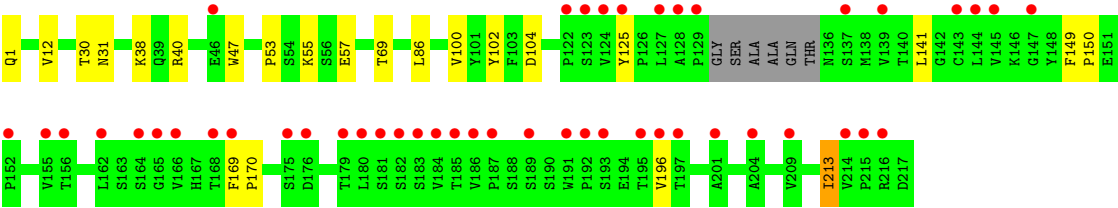


- Molecule 3: Fab antibody fragment, heavy chain



- Molecule 3: Fab antibody fragment, heavy chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.54Å 242.90Å 172.76Å 90.00° 93.68° 90.00°	Depositor
Resolution (Å)	39.89 – 2.85 39.89 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.89-2.85) 99.9 (39.89-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1678), CNS 1.3, REFMAC	Depositor
R, R_{free}	0.217 , 0.234 0.221 , 0.237	Depositor DCC
R_{free} test set	9458 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	69.8	Xtriage
Anisotropy	0.587	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31125	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: CL, CA, C6N, K, GOL

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	0.31	0/3081	0.78	1/4200 (0.0%)
1	B	0.31	0/3081	0.77	1/4200 (0.0%)
1	C	0.30	0/3081	0.77	1/4200 (0.0%)
1	D	0.31	0/3081	0.77	1/4200 (0.0%)
1	E	0.31	0/3081	0.77	1/4200 (0.0%)
2	F	0.27	0/1630	0.73	3/2225 (0.1%)
2	H	0.27	0/1630	0.73	3/2225 (0.1%)
2	J	0.27	0/1630	0.74	3/2225 (0.1%)
2	L	0.28	0/1630	0.75	3/2225 (0.1%)
2	N	0.28	0/1630	0.74	3/2225 (0.1%)
3	G	0.28	0/1602	0.74	1/2202 (0.0%)
3	I	0.28	0/1602	0.75	0/2202
3	K	0.29	0/1602	0.75	0/2202
3	M	0.29	0/1602	0.73	0/2202
3	O	0.28	0/1602	0.75	0/2202
All	All	0.29	0/31565	0.76	21/43135 (0.0%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	58	VAL	CA-C-N	5.56	125.46	119.85
2	L	58	VAL	C-N-CA	5.56	125.46	119.85
2	F	58	VAL	N-CA-C	5.48	114.93	108.96
2	N	58	VAL	N-CA-C	5.39	114.83	108.96
2	L	58	VAL	N-CA-C	5.37	114.82	108.96
2	J	58	VAL	N-CA-C	5.35	114.79	108.96
2	H	58	VAL	N-CA-C	5.34	114.78	108.96
1	E	76	ILE	CB-CA-C	-5.31	108.66	113.70
1	A	76	ILE	CB-CA-C	-5.29	108.67	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	58	VAL	CA-C-N	5.29	125.19	119.85
2	J	58	VAL	C-N-CA	5.29	125.19	119.85
2	H	58	VAL	CA-C-N	5.27	125.18	119.85
2	H	58	VAL	C-N-CA	5.27	125.18	119.85
1	C	76	ILE	CB-CA-C	-5.26	108.70	113.70
1	B	76	ILE	CB-CA-C	-5.24	108.72	113.70
1	D	76	ILE	CB-CA-C	-5.22	108.74	113.70
2	F	58	VAL	CA-C-N	5.14	125.04	119.85
2	F	58	VAL	C-N-CA	5.14	125.04	119.85
2	N	58	VAL	CA-C-N	5.11	125.01	119.85
2	N	58	VAL	C-N-CA	5.11	125.01	119.85
3	G	142	GLY	N-CA-C	5.03	118.03	110.18

There are no chirality outliers.

There are no planarity outliers.

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	2994	0	2931	44	0
1	B	2994	0	2931	46	0
1	C	2994	0	2931	50	0
1	D	2994	0	2931	51	0
1	E	2994	0	2931	48	0
2	F	1591	0	1449	16	0
2	H	1591	0	1449	20	0
2	J	1591	0	1449	17	0
2	L	1591	0	1449	20	0
2	N	1591	0	1449	20	0
3	G	1558	0	1441	18	0
3	I	1558	0	1441	18	0
3	K	1558	0	1441	17	0
3	M	1558	0	1441	20	0
3	O	1558	0	1441	14	0
4	A	6	0	8	1	0
4	B	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	6	0	8	1	0
4	D	6	0	8	1	0
4	E	6	0	8	1	0
5	A	3	0	0	0	0
5	B	3	0	0	1	0
5	C	3	0	0	1	0
5	D	3	0	0	1	0
5	E	3	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	2	0	0	0	0
7	E	1	0	0	0	0
8	A	69	0	84	1	0
8	B	69	0	84	1	0
8	C	69	0	84	2	0
8	D	69	0	84	1	0
8	E	69	0	84	2	0
9	A	2	0	0	0	0
9	B	2	0	0	0	0
9	C	2	0	0	0	0
9	D	2	0	0	0	0
9	E	2	0	0	0	0
All	All	31125	0	29565	360	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 6.

All (360) 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)
2:J:185:GLU:HA	2:J:188:ARG:HD3	1.60	0.83
2:N:108:ARG:HG3	2:N:109:ALA:H	1.44	0.81
1:A:294:LEU:HD11	1:B:233:PRO:HG2	1.70	0.73
1:B:294:LEU:HD11	1:C:233:PRO:HG2	1.71	0.72
1:D:294:LEU:HD11	1:E:233:PRO:HG2	1.72	0.71
3:M:38:LYS:HE2	3:M:40:ARG:HD2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:38:LYS:HE2	3:K:40:ARG:HD2	1.73	0.71
1:C:294:LEU:HD11	1:D:233:PRO:HG2	1.73	0.70
3:O:38:LYS:HE2	3:O:40:ARG:HD2	1.74	0.70
1:A:233:PRO:HG2	1:E:294:LEU:HD11	1.72	0.70
3:G:38:LYS:HE2	3:G:40:ARG:HD2	1.74	0.69
3:I:196:VAL:HB	3:I:213:ILE:HD11	1.75	0.69
3:G:12:VAL:HG21	3:G:86:LEU:HD13	1.76	0.68
3:M:196:VAL:HB	3:M:213:ILE:HD11	1.76	0.68
1:B:76:ILE:HG12	1:C:76:ILE:HG21	1.76	0.68
3:G:196:VAL:HB	3:G:213:ILE:HD11	1.76	0.67
3:K:196:VAL:HB	3:K:213:ILE:HD11	1.77	0.67
1:E:134:LEU:HD21	1:E:163:MET:HE3	1.77	0.67
3:I:38:LYS:HE2	3:I:40:ARG:HD2	1.76	0.66
3:K:30:THR:HA	3:K:53:PRO:HB2	1.78	0.66
3:O:30:THR:HA	3:O:53:PRO:HB2	1.77	0.66
1:A:134:LEU:HD21	1:A:163:MET:HE3	1.78	0.65
1:A:76:ILE:HG12	1:B:76:ILE:HG21	1.77	0.65
3:O:196:VAL:HB	3:O:213:ILE:HD11	1.76	0.65
1:D:134:LEU:HD21	1:D:163:MET:HE3	1.78	0.65
3:I:30:THR:HA	3:I:53:PRO:HB2	1.78	0.65
1:C:58:GLN:HA	1:C:61:MET:HE3	1.79	0.65
3:M:30:THR:HA	3:M:53:PRO:HB2	1.79	0.65
1:A:76:ILE:HG21	1:E:76:ILE:HG12	1.79	0.65
1:E:58:GLN:HA	1:E:61:MET:HE3	1.80	0.64
1:D:76:ILE:HG12	1:E:76:ILE:HG21	1.78	0.64
1:C:76:ILE:HG12	1:D:76:ILE:HG21	1.79	0.64
1:A:58:GLN:HA	1:A:61:MET:HE3	1.80	0.64
1:B:58:GLN:HA	1:B:61:MET:HE3	1.80	0.63
3:G:30:THR:HA	3:G:53:PRO:HB2	1.79	0.63
3:I:12:VAL:HG21	3:I:86:LEU:HD13	1.80	0.63
1:D:58:GLN:HA	1:D:61:MET:HE3	1.81	0.63
1:B:134:LEU:HD21	1:B:163:MET:HE3	1.81	0.63
1:C:134:LEU:HD21	1:C:163:MET:HE3	1.81	0.62
3:G:102:TYR:CE1	3:G:104:ASP:HB3	2.36	0.60
3:K:12:VAL:HG21	3:K:86:LEU:HD13	1.82	0.60
2:J:108:ARG:HD2	2:J:171:SER:HB2	1.85	0.59
3:G:141:LEU:HD13	3:G:213:ILE:HD13	1.86	0.58
3:M:141:LEU:HD13	3:M:213:ILE:HD13	1.85	0.58
2:L:150:ILE:HD11	2:L:179:LEU:HD21	1.86	0.58
3:I:141:LEU:HD13	3:I:213:ILE:HD13	1.86	0.57
3:O:12:VAL:HG21	3:O:86:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ASP:OD2	1:D:175:ASN:ND2	2.37	0.57
3:K:14:PRO:HD2	3:K:116:SER:OG	2.05	0.57
1:A:183:ILE:HB	1:A:184:PRO:HD3	1.87	0.57
1:B:183:ILE:HB	1:B:184:PRO:HD3	1.87	0.57
1:C:183:ILE:HB	1:C:184:PRO:HD3	1.87	0.57
1:E:183:ILE:HB	1:E:184:PRO:HD3	1.87	0.56
3:K:141:LEU:HD13	3:K:213:ILE:HD13	1.87	0.56
8:A:507:C6N:H69	8:A:507:C6N:O23	2.05	0.56
8:B:507:C6N:H69	8:B:507:C6N:O23	2.05	0.56
3:G:102:TYR:HE1	3:G:104:ASP:HB3	1.70	0.56
3:O:141:LEU:HD13	3:O:213:ILE:HD13	1.88	0.56
1:B:175:ASN:ND2	1:E:342:ASP:OD2	2.38	0.56
8:C:508:C6N:H69	8:C:508:C6N:O23	2.05	0.55
1:C:320:MET:HE3	1:D:174:LEU:HB3	1.88	0.55
1:D:183:ILE:HB	1:D:184:PRO:HD3	1.87	0.55
8:D:506:C6N:O23	8:D:506:C6N:H69	2.05	0.55
8:E:507:C6N:H69	8:E:507:C6N:O23	2.05	0.55
3:M:12:VAL:HG21	3:M:86:LEU:HD13	1.89	0.55
2:F:150:ILE:HD11	2:F:179:LEU:HD21	1.88	0.54
2:H:198:HIS:HB3	2:H:200:THR:HG22	1.89	0.54
1:D:237:THR:O	1:D:241:THR:HG23	2.08	0.54
2:J:25:ALA:HB3	2:J:69:THR:HA	1.90	0.54
1:E:237:THR:O	1:E:241:THR:HG23	2.08	0.53
1:A:342:ASP:OD2	1:C:175:ASN:ND2	2.41	0.53
2:N:150:ILE:HD11	2:N:179:LEU:HD21	1.91	0.53
1:C:237:THR:O	1:C:241:THR:HG23	2.09	0.53
1:C:342:ASP:OD2	1:E:175:ASN:ND2	2.41	0.53
1:A:81:VAL:HG22	1:A:240:VAL:HG12	1.91	0.53
2:J:150:ILE:HD11	2:J:179:LEU:HD21	1.91	0.53
1:A:174:LEU:HB3	1:E:320:MET:HE3	1.90	0.52
2:L:79:GLN:HB3	2:L:80:PRO:HD2	1.92	0.52
1:A:320:MET:HE3	1:B:174:LEU:HB3	1.90	0.52
1:A:175:ASN:ND2	1:D:342:ASP:OD2	2.41	0.52
1:D:320:MET:HE3	1:E:174:LEU:HB3	1.92	0.52
2:H:79:GLN:HB3	2:H:80:PRO:HD2	1.92	0.52
2:N:79:GLN:HB3	2:N:80:PRO:HD2	1.92	0.52
2:H:150:ILE:HD11	2:H:179:LEU:HD21	1.91	0.52
1:B:237:THR:O	1:B:241:THR:HG23	2.10	0.51
1:C:14:LEU:HD13	1:D:34:SER:HB2	1.92	0.51
2:J:3:GLN:H	2:J:26:SER:HB3	1.75	0.51
2:J:47:LEU:HD11	2:J:86:TYR:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:108:ARG:NH1	2:J:109:ALA:O	2.44	0.51
2:L:108:ARG:NH1	2:L:109:ALA:O	2.43	0.51
1:A:237:THR:O	1:A:241:THR:HG23	2.09	0.51
1:D:274:PRO:HB2	1:D:277:THR:HB	1.92	0.51
1:A:14:LEU:HD13	1:B:34:SER:HB2	1.92	0.51
1:E:81:VAL:HG22	1:E:240:VAL:HG12	1.92	0.51
1:B:81:VAL:HG22	1:B:240:VAL:HG12	1.92	0.51
1:D:81:VAL:HG22	1:D:240:VAL:HG12	1.92	0.51
2:L:3:GLN:H	2:L:26:SER:HB3	1.75	0.51
1:B:320:MET:HE3	1:C:174:LEU:HB3	1.92	0.51
2:F:25:ALA:HB3	2:F:69:THR:HA	1.92	0.51
2:L:47:LEU:HD11	2:L:86:TYR:HE1	1.76	0.51
1:A:274:PRO:HB2	1:A:277:THR:HB	1.93	0.51
1:E:274:PRO:HB2	1:E:277:THR:HB	1.93	0.51
1:A:190:ASN:HB3	1:E:329:LEU:HD11	1.93	0.50
1:D:14:LEU:HD13	1:E:34:SER:HB2	1.93	0.50
2:F:47:LEU:HD11	2:F:86:TYR:HE1	1.77	0.50
2:J:79:GLN:HB3	2:J:80:PRO:HD2	1.92	0.50
2:L:25:ALA:HB3	2:L:69:THR:HA	1.93	0.50
2:N:3:GLN:H	2:N:26:SER:HB3	1.76	0.50
1:A:36:PHE:CZ	1:A:40:ILE:HD11	2.47	0.50
2:H:108:ARG:NH1	2:H:109:ALA:O	2.45	0.50
2:H:184:ASP:O	2:H:188:ARG:HG3	2.11	0.50
1:A:329:LEU:HD11	1:B:190:ASN:HB3	1.94	0.50
1:C:276:PHE:O	1:C:280:GLN:HG3	2.12	0.50
2:F:79:GLN:HB3	2:F:80:PRO:HD2	1.92	0.50
2:F:198:HIS:HB3	2:F:200:THR:HG22	1.93	0.50
1:C:81:VAL:HG22	1:C:240:VAL:HG12	1.93	0.50
1:C:329:LEU:HD11	1:D:190:ASN:HB3	1.93	0.50
2:N:47:LEU:HD11	2:N:86:TYR:HE1	1.76	0.50
2:F:184:ASP:O	2:F:188:ARG:HG3	2.11	0.50
2:J:198:HIS:HB3	2:J:200:THR:HG22	1.93	0.50
2:H:108:ARG:HD2	2:H:171:SER:HB2	1.94	0.49
1:A:276:PHE:O	1:A:280:GLN:HG3	2.12	0.49
1:B:14:LEU:HD13	1:C:34:SER:HB2	1.94	0.49
2:L:198:HIS:HB3	2:L:200:THR:HG22	1.93	0.49
1:B:329:LEU:HD11	1:C:190:ASN:HB3	1.94	0.49
1:D:152:PRO:HB2	3:M:31:ASN:O	2.13	0.49
1:B:276:PHE:O	1:B:280:GLN:HG3	2.13	0.49
1:B:358:SER:HA	1:C:309:TRP:NE1	2.28	0.49
2:H:47:LEU:HD11	2:H:86:TYR:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:184:ASP:O	2:N:188:ARG:HG3	2.13	0.49
1:B:36:PHE:CZ	1:B:40:ILE:HD11	2.48	0.49
1:D:130:ARG:NH2	1:D:167:GLU:OE2	2.46	0.49
1:E:130:ARG:NH2	1:E:167:GLU:OE2	2.45	0.49
1:B:130:ARG:NH2	1:B:167:GLU:OE2	2.45	0.49
1:D:276:PHE:O	1:D:280:GLN:HG3	2.12	0.49
1:E:36:PHE:CZ	1:E:40:ILE:HD11	2.48	0.49
2:J:184:ASP:O	2:J:188:ARG:HG3	2.12	0.49
2:L:124:GLN:HG3	3:M:125:TYR:CE2	2.48	0.49
2:N:25:ALA:HB3	2:N:69:THR:HA	1.94	0.49
2:J:18:THR:HG22	2:J:77:SER:H	1.78	0.49
3:M:18:VAL:HG12	3:M:86:LEU:HD11	1.94	0.49
2:N:108:ARG:HD2	2:N:171:SER:HB2	1.95	0.49
1:B:306:GLU:HA	4:B:501:GOL:H12	1.94	0.48
2:F:3:GLN:H	2:F:26:SER:HB3	1.77	0.48
2:N:18:THR:HG22	2:N:77:SER:H	1.78	0.48
2:N:198:HIS:HB3	2:N:200:THR:HG22	1.94	0.48
1:D:306:GLU:HA	4:D:501:GOL:H12	1.96	0.48
2:H:3:GLN:H	2:H:26:SER:HB3	1.76	0.48
2:N:124:GLN:HG3	3:O:125:TYR:CE2	2.49	0.48
1:D:345:PRO:HB2	1:E:150:ARG:NH2	2.29	0.48
2:H:25:ALA:HB3	2:H:69:THR:HA	1.95	0.48
2:J:124:GLN:HG3	3:K:125:TYR:CE2	2.49	0.48
2:L:184:ASP:O	2:L:188:ARG:HG3	2.14	0.48
1:C:36:PHE:CZ	1:C:40:ILE:HD11	2.48	0.48
1:E:75:LEU:HD21	1:E:280:GLN:NE2	2.29	0.48
2:L:18:THR:HG22	2:L:77:SER:H	1.78	0.48
2:L:108:ARG:HD2	2:L:171:SER:HB2	1.95	0.48
1:A:100:ILE:HG21	1:A:310:LEU:HD23	1.96	0.47
1:C:345:PRO:HB2	1:D:150:ARG:NH2	2.29	0.47
2:F:18:THR:HG22	2:F:77:SER:H	1.79	0.47
1:D:36:PHE:CZ	1:D:40:ILE:HD11	2.49	0.47
2:H:18:THR:HG22	2:H:77:SER:H	1.78	0.47
1:A:306:GLU:HA	4:A:501:GOL:H12	1.96	0.47
3:M:11:LEU:HD11	3:M:149:PHE:CE2	2.48	0.47
1:E:276:PHE:O	1:E:280:GLN:HG3	2.14	0.47
3:O:102:TYR:CE1	3:O:104:ASP:HB3	2.50	0.47
1:A:309:TRP:NE1	1:E:358:SER:HA	2.30	0.47
2:H:124:GLN:HG3	3:I:125:TYR:CE2	2.50	0.47
1:A:130:ARG:NH2	1:A:167:GLU:OE2	2.47	0.47
1:B:274:PRO:HB2	1:B:277:THR:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ARG:HD3	1:A:313:ARG:C	2.40	0.47
1:B:314:ASN:O	1:B:318:SER:OG	2.30	0.47
1:B:345:PRO:HB2	1:C:150:ARG:NH2	2.29	0.47
1:C:130:ARG:NH2	1:C:167:GLU:OE2	2.47	0.47
1:C:137:VAL:HG21	1:C:162:LEU:HD13	1.97	0.47
1:C:274:PRO:HB2	1:C:277:THR:HB	1.95	0.47
1:E:194:LYS:O	1:E:198:GLU:HG3	2.15	0.47
3:I:1:GLN:OE1	3:I:1:GLN:N	2.44	0.47
2:L:198:HIS:CD2	2:L:199:LYS:H	2.33	0.47
1:A:358:SER:HA	1:B:309:TRP:NE1	2.30	0.47
1:C:100:ILE:HG21	1:C:310:LEU:HD23	1.97	0.47
1:B:313:ARG:HD3	1:B:313:ARG:C	2.40	0.47
1:A:34:SER:HB2	1:E:14:LEU:HD13	1.96	0.46
1:C:75:LEU:HD21	1:C:280:GLN:NE2	2.30	0.46
1:D:329:LEU:HD11	1:E:190:ASN:HB3	1.95	0.46
2:F:124:GLN:HG3	3:G:125:TYR:CE2	2.50	0.46
1:C:313:ARG:HD3	1:C:313:ARG:C	2.41	0.46
1:D:100:ILE:HG21	1:D:310:LEU:HD23	1.97	0.46
1:A:150:ARG:NH2	1:E:345:PRO:HB2	2.30	0.46
1:D:313:ARG:HD3	1:D:313:ARG:C	2.40	0.46
3:M:202:HIS:CE1	3:M:204:ALA:HB3	2.51	0.46
2:N:37:GLN:HB2	2:N:47:LEU:HD11	1.97	0.46
1:C:306:GLU:HA	4:C:501:GOL:H12	1.97	0.46
3:G:18:VAL:HG12	3:G:86:LEU:HD11	1.97	0.46
1:A:346:PRO:HA	2:H:32:TYR:CE2	2.51	0.46
1:E:306:GLU:HA	4:E:501:GOL:H12	1.97	0.46
1:D:75:LEU:HD21	1:D:280:GLN:NE2	2.31	0.46
1:D:137:VAL:HG21	1:D:162:LEU:HD13	1.97	0.46
1:B:100:ILE:HG21	1:B:310:LEU:HD23	1.97	0.46
1:C:314:ASN:O	1:C:318:SER:OG	2.30	0.45
1:D:97:TYR:HB2	1:D:305:PHE:CZ	2.51	0.45
1:E:100:ILE:HG21	1:E:310:LEU:HD23	1.97	0.45
2:F:198:HIS:CD2	2:F:199:LYS:H	2.34	0.45
2:H:198:HIS:CD2	2:H:199:LYS:H	2.34	0.45
2:J:37:GLN:HB2	2:J:47:LEU:HD11	1.99	0.45
2:N:198:HIS:CD2	2:N:199:LYS:H	2.34	0.45
2:H:118:PHE:HA	2:H:119:PRO:HD3	1.83	0.45
2:J:198:HIS:CD2	2:J:199:LYS:H	2.34	0.45
2:L:203:SER:HA	2:L:204:PRO:HD3	1.88	0.45
1:B:36:PHE:O	1:B:40:ILE:HG12	2.17	0.45
1:B:137:VAL:HG21	1:B:162:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HD21	1:A:280:GLN:NE2	2.31	0.45
1:C:97:TYR:HB2	1:C:305:PHE:CZ	2.52	0.45
1:B:152:PRO:HB2	3:I:31:ASN:O	2.17	0.45
2:N:24:ARG:HG2	2:N:24:ARG:HH11	1.82	0.45
1:C:2:THR:OG1	1:C:303:ASP:HA	2.17	0.44
1:A:194:LYS:O	1:A:198:GLU:HG3	2.17	0.44
1:C:194:LYS:O	1:C:198:GLU:HG3	2.17	0.44
1:D:194:LYS:O	1:D:198:GLU:HG3	2.17	0.44
1:E:313:ARG:HD3	1:E:313:ARG:C	2.42	0.44
3:M:102:TYR:CE1	3:M:104:ASP:HB3	2.52	0.44
3:I:102:TYR:CE1	3:I:104:ASP:HB3	2.52	0.44
1:A:345:PRO:HB2	1:B:150:ARG:NH2	2.32	0.44
1:B:97:TYR:HB2	1:B:305:PHE:CZ	2.53	0.44
1:D:346:PRO:HA	2:N:32:TYR:CE2	2.53	0.44
1:B:63:GLU:O	1:B:67:LEU:HG	2.18	0.44
1:B:75:LEU:HD21	1:B:280:GLN:NE2	2.32	0.44
1:C:36:PHE:O	1:C:40:ILE:HG12	2.16	0.44
1:C:153:SER:HB3	3:K:31:ASN:HB3	2.00	0.44
2:F:108:ARG:NH1	2:F:109:ALA:O	2.50	0.44
2:H:203:SER:HA	2:H:204:PRO:HD3	1.89	0.44
1:B:104:ASP:HA	1:B:107:MET:HB3	2.00	0.44
1:E:36:PHE:O	1:E:40:ILE:HG12	2.18	0.44
3:M:1:GLN:OE1	3:M:1:GLN:N	2.44	0.44
1:C:358:SER:HA	1:D:309:TRP:NE1	2.32	0.43
1:E:136:SER:O	1:E:139:ILE:HG22	2.18	0.43
2:F:37:GLN:HB2	2:F:47:LEU:HD11	2.00	0.43
2:H:37:GLN:HB2	2:H:47:LEU:HD11	2.00	0.43
3:M:11:LEU:HD11	3:M:149:PHE:CZ	2.53	0.43
2:N:112:ALA:HA	2:N:200:THR:HG21	2.00	0.43
2:N:185:GLU:HA	2:N:188:ARG:HD3	1.98	0.43
1:A:89:VAL:HG11	1:A:291:ALA:HA	2.00	0.43
1:D:136:SER:O	1:D:139:ILE:HG22	2.18	0.43
1:D:252:LEU:HD23	1:D:252:LEU:HA	1.83	0.43
1:E:62:PHE:HZ	1:E:256:GLN:HG3	1.84	0.43
1:E:97:TYR:HB2	1:E:305:PHE:CZ	2.53	0.43
3:M:150:PRO:HD2	3:M:204:ALA:HB1	1.99	0.43
1:B:194:LYS:O	1:B:198:GLU:HG3	2.18	0.43
1:D:314:ASN:O	1:D:318:SER:OG	2.31	0.43
2:H:96:PRO:HD2	3:I:47:TRP:CD2	2.54	0.43
1:A:97:TYR:HB2	1:A:305:PHE:CZ	2.54	0.43
1:A:137:VAL:HG21	1:A:162:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:HG13	1:B:182:TRP:CZ2	2.53	0.43
1:D:2:THR:OG1	1:D:303:ASP:HA	2.19	0.43
1:D:358:SER:HA	1:E:309:TRP:NE1	2.34	0.43
2:N:96:PRO:HD2	3:O:47:TRP:CD2	2.54	0.43
1:C:323:ASP:HB3	1:C:324:GLU:OE1	2.19	0.43
2:L:96:PRO:HD2	3:M:47:TRP:CD2	2.54	0.43
1:A:2:THR:OG1	1:A:303:ASP:HA	2.19	0.43
1:A:63:GLU:O	1:A:67:LEU:HG	2.19	0.43
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.83	0.43
1:D:36:PHE:O	1:D:40:ILE:HG12	2.18	0.43
1:E:137:VAL:HG21	1:E:162:LEU:HD13	2.00	0.43
2:L:187:GLU:OE1	2:L:211:ARG:NH2	2.51	0.43
1:A:36:PHE:O	1:A:40:ILE:HG12	2.19	0.43
1:E:323:ASP:HB3	1:E:324:GLU:OE1	2.19	0.43
1:A:252:LEU:HD23	1:A:252:LEU:HA	1.83	0.43
1:E:63:GLU:O	1:E:67:LEU:HG	2.19	0.43
1:B:136:SER:O	1:B:139:ILE:HG22	2.19	0.43
1:B:323:ASP:HB3	1:B:324:GLU:OE1	2.19	0.43
1:E:252:LEU:HD23	1:E:252:LEU:HA	1.83	0.43
3:M:51:ILE:O	3:M:53:PRO:HD3	2.19	0.43
1:A:136:SER:O	1:A:139:ILE:HG22	2.18	0.42
1:B:252:LEU:HD23	1:B:252:LEU:HA	1.83	0.42
1:D:63:GLU:O	1:D:67:LEU:HG	2.19	0.42
1:A:62:PHE:HZ	1:A:256:GLN:HG3	1.85	0.42
1:C:136:SER:O	1:C:139:ILE:HG22	2.19	0.42
1:D:89:VAL:HG11	1:D:291:ALA:HA	2.01	0.42
1:E:152:PRO:HB2	3:O:31:ASN:O	2.19	0.42
3:G:150:PRO:HD2	3:G:204:ALA:HB1	2.01	0.42
3:I:23:LYS:HG3	3:I:78:THR:HG22	2.02	0.42
1:B:317:VAL:HG13	1:C:182:TRP:CZ2	2.55	0.42
1:E:2:THR:OG1	1:E:303:ASP:HA	2.19	0.42
1:E:104:ASP:HA	1:E:107:MET:HB3	2.01	0.42
3:K:102:TYR:CE1	3:K:104:ASP:HB3	2.54	0.42
1:A:340:GLU:HA	1:A:341:PRO:HD2	1.94	0.42
1:C:63:GLU:O	1:C:67:LEU:HG	2.20	0.42
3:I:18:VAL:HG12	3:I:86:LEU:HD11	2.01	0.42
2:J:96:PRO:HD2	3:K:47:TRP:CD2	2.55	0.42
2:L:61:ARG:HD2	2:L:82:ASP:OD2	2.20	0.42
3:O:1:GLN:OE1	3:O:1:GLN:N	2.44	0.42
1:B:2:THR:OG1	1:B:303:ASP:HA	2.19	0.42
1:E:106:ILE:HD11	1:E:214:LEU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:23:LYS:HG3	3:G:78:THR:HG22	2.01	0.42
2:H:24:ARG:HG2	2:H:24:ARG:HH11	1.85	0.42
3:I:120:THR:HA	3:I:121:PRO:HD3	1.89	0.42
3:O:55:LYS:HB2	3:O:57:GLU:HG3	2.02	0.42
1:D:323:ASP:HB3	1:D:324:GLU:OE1	2.20	0.42
3:I:213:ILE:HD12	3:I:213:ILE:O	2.20	0.42
1:C:5:TYR:OH	1:D:232:ILE:O	2.33	0.42
2:L:37:GLN:HB2	2:L:47:LEU:HD11	2.02	0.42
1:E:89:VAL:HG11	1:E:291:ALA:HA	2.02	0.41
8:E:507:C6N:H6	8:E:507:C6N:H4	1.80	0.41
3:G:1:GLN:OE1	3:G:1:GLN:N	2.45	0.41
1:D:340:GLU:HA	1:D:341:PRO:HD2	1.94	0.41
2:J:24:ARG:HG2	2:J:24:ARG:HH11	1.85	0.41
8:C:508:C6N:H6	8:C:508:C6N:H4	1.79	0.41
2:J:61:ARG:HD2	2:J:82:ASP:OD2	2.20	0.41
3:M:213:ILE:HD12	3:M:213:ILE:O	2.20	0.41
3:O:169:PHE:HA	3:O:170:PRO:HD3	1.92	0.41
3:K:55:LYS:HB2	3:K:57:GLU:HG3	2.02	0.41
3:M:213:ILE:H	3:M:213:ILE:HG13	1.64	0.41
3:O:213:ILE:HD12	3:O:213:ILE:O	2.21	0.41
1:C:313:ARG:HA	1:D:178:HIS:NE2	2.36	0.41
3:G:213:ILE:HD12	3:G:213:ILE:O	2.21	0.41
2:H:61:ARG:HD2	2:H:82:ASP:OD2	2.20	0.41
3:I:53:PRO:HA	3:I:72:VAL:HG21	2.03	0.41
3:K:213:ILE:HD12	3:K:213:ILE:O	2.20	0.41
1:A:104:ASP:HA	1:A:107:MET:HB3	2.03	0.41
1:C:62:PHE:HZ	1:C:256:GLN:HG3	1.85	0.41
1:C:104:ASP:HA	1:C:107:MET:HB3	2.02	0.41
1:C:106:ILE:HD11	1:C:214:LEU:HA	2.02	0.41
1:C:317:VAL:HG13	1:D:182:TRP:CZ2	2.56	0.41
3:G:150:PRO:O	3:G:202:HIS:HE1	2.04	0.41
2:L:24:ARG:HG2	2:L:24:ARG:HH11	1.85	0.41
1:C:346:PRO:HA	2:L:32:TYR:CE2	2.56	0.41
1:D:317:VAL:HG13	1:E:182:TRP:CZ2	2.56	0.41
1:E:74:GLU:HB3	5:E:505:CL:CL	2.57	0.41
1:E:130:ARG:HH22	1:E:167:GLU:CD	2.29	0.41
2:F:96:PRO:HD2	3:G:47:TRP:CD2	2.56	0.41
3:G:53:PRO:HA	3:G:72:VAL:HG21	2.03	0.41
2:H:36:TYR:HE2	2:H:89:GLN:HE21	1.69	0.41
3:I:51:ILE:O	3:I:53:PRO:HD3	2.21	0.41
3:K:18:VAL:HG12	3:K:86:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:61:ARG:HD2	2:N:82:ASP:OD2	2.21	0.41
1:A:323:ASP:HB3	1:A:324:GLU:OE1	2.20	0.41
1:D:74:GLU:HB3	5:D:505:CL:CL	2.58	0.41
3:K:53:PRO:HA	3:K:72:VAL:HG21	2.02	0.41
1:B:62:PHE:HZ	1:B:256:GLN:HG3	1.86	0.40
1:B:89:VAL:HG11	1:B:291:ALA:HA	2.02	0.40
1:C:74:GLU:HB3	5:C:505:CL:CL	2.58	0.40
1:D:153:SER:HB3	3:M:31:ASN:HB3	2.03	0.40
2:F:24:ARG:HH11	2:F:24:ARG:HG2	1.85	0.40
3:K:23:LYS:HG3	3:K:78:THR:HG22	2.03	0.40
2:L:135:PHE:C	2:L:136:LEU:HD12	2.46	0.40
1:B:74:GLU:HB3	5:B:505:CL:CL	2.58	0.40
1:C:104:ASP:OD2	1:D:218:ARG:NH2	2.51	0.40
1:D:104:ASP:OD2	1:E:218:ARG:NH2	2.48	0.40
1:E:314:ASN:O	1:E:318:SER:OG	2.30	0.40
2:F:112:ALA:HA	2:F:200:THR:HG21	2.02	0.40
3:G:55:LYS:HB2	3:G:57:GLU:HG3	2.03	0.40
3:I:150:PRO:HD2	3:I:204:ALA:HB1	2.03	0.40
3:M:23:LYS:HG3	3:M:78:THR:HG22	2.01	0.40
3:G:51:ILE:O	3:G:53:PRO:HD3	2.21	0.40
3:O:149:PHE:HA	3:O:150:PRO:HA	1.90	0.40
2:F:47:LEU:HA	2:F:58:VAL:HG21	2.04	0.40
3:K:51:ILE:O	3:K:53:PRO:HD3	2.20	0.40
2:N:135:PHE:C	2:N:136:LEU:HD12	2.47	0.40
3:I:213:ILE:H	3:I:213:ILE:HG13	1.65	0.40
3:K:128:ALA:HA	3:K:129:PRO:HD3	1.97	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	364/409 (89%)	349 (96%)	14 (4%)	1 (0%)	36	54
1	B	364/409 (89%)	349 (96%)	14 (4%)	1 (0%)	36	54
1	C	364/409 (89%)	348 (96%)	15 (4%)	1 (0%)	36	54
1	D	364/409 (89%)	349 (96%)	14 (4%)	1 (0%)	36	54
1	E	364/409 (89%)	349 (96%)	14 (4%)	1 (0%)	36	54
2	F	210/212 (99%)	192 (91%)	17 (8%)	1 (0%)	24	42
2	H	210/212 (99%)	192 (91%)	17 (8%)	1 (0%)	24	42
2	J	210/212 (99%)	191 (91%)	18 (9%)	1 (0%)	24	42
2	L	210/212 (99%)	192 (91%)	17 (8%)	1 (0%)	24	42
2	N	210/212 (99%)	192 (91%)	17 (8%)	1 (0%)	24	42
3	G	207/217 (95%)	201 (97%)	5 (2%)	1 (0%)	24	42
3	I	207/217 (95%)	200 (97%)	6 (3%)	1 (0%)	24	42
3	K	207/217 (95%)	201 (97%)	5 (2%)	1 (0%)	24	42
3	M	207/217 (95%)	201 (97%)	5 (2%)	1 (0%)	24	42
3	O	207/217 (95%)	201 (97%)	5 (2%)	1 (0%)	24	42
All	All	3905/4190 (93%)	3707 (95%)	183 (5%)	15 (0%)	30	48

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	ARG
1	B	202	ARG
1	C	202	ARG
1	D	202	ARG
1	E	202	ARG
2	F	56	GLU
2	H	56	GLU
2	J	56	GLU
2	L	56	GLU
2	N	56	GLU
3	G	100	VAL
3	I	100	VAL
3	K	100	VAL
3	M	100	VAL
3	O	100	VAL

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	327/370 (88%)	318 (97%)	9 (3%)	38	62
1	B	327/370 (88%)	319 (98%)	8 (2%)	43	67
1	C	327/370 (88%)	318 (97%)	9 (3%)	38	62
1	D	327/370 (88%)	318 (97%)	9 (3%)	38	62
1	E	327/370 (88%)	318 (97%)	9 (3%)	38	62
2	F	173/187 (92%)	170 (98%)	3 (2%)	53	75
2	H	173/187 (92%)	170 (98%)	3 (2%)	53	75
2	J	173/187 (92%)	170 (98%)	3 (2%)	53	75
2	L	173/187 (92%)	170 (98%)	3 (2%)	53	75
2	N	173/187 (92%)	170 (98%)	3 (2%)	53	75
3	G	166/190 (87%)	164 (99%)	2 (1%)	63	80
3	I	166/190 (87%)	164 (99%)	2 (1%)	63	80
3	K	166/190 (87%)	164 (99%)	2 (1%)	63	80
3	M	166/190 (87%)	163 (98%)	3 (2%)	51	73
3	O	166/190 (87%)	164 (99%)	2 (1%)	63	80
All	All	3330/3735 (89%)	3260 (98%)	70 (2%)	47	70

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	37	LEU
1	A	189	SER
1	A	196	ARG
1	A	273	VAL
1	A	292	GLU
1	A	303	ASP
1	A	310	LEU
1	A	320	MET
1	B	2	THR

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Mol	Chain	Res	Type
1	B	37	LEU
1	B	196	ARG
1	B	273	VAL
1	B	292	GLU
1	B	303	ASP
1	B	310	LEU
1	B	320	MET
1	C	2	THR
1	C	37	LEU
1	C	189	SER
1	C	196	ARG
1	C	273	VAL
1	C	292	GLU
1	C	303	ASP
1	C	310	LEU
1	C	320	MET
1	D	2	THR
1	D	37	LEU
1	D	189	SER
1	D	196	ARG
1	D	273	VAL
1	D	292	GLU
1	D	303	ASP
1	D	310	LEU
1	D	320	MET
1	E	2	THR
1	E	37	LEU
1	E	189	SER
1	E	196	ARG
1	E	273	VAL
1	E	292	GLU
1	E	303	ASP
1	E	310	LEU
1	E	320	MET
2	F	19	VAL
2	F	50	ASN
2	F	193	THR
3	G	69	THR
3	G	213	ILE
2	H	19	VAL
2	H	50	ASN
2	H	193	THR

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Mol	Chain	Res	Type
3	I	69	THR
3	I	213	ILE
2	J	19	VAL
2	J	50	ASN
2	J	193	THR
3	K	69	THR
3	K	213	ILE
2	L	19	VAL
2	L	50	ASN
2	L	193	THR
3	M	69	THR
3	M	153	VAL
3	M	213	ILE
2	N	19	VAL
2	N	50	ASN
2	N	193	THR
3	O	69	THR
3	O	213	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	A	326	HIS
1	A	327	GLN
1	B	175	ASN
1	B	208	GLN
1	B	326	HIS
1	C	175	ASN
1	C	208	GLN
1	C	326	HIS
1	D	175	ASN
1	D	208	GLN
1	D	326	HIS
1	D	327	GLN
1	E	175	ASN
1	E	208	GLN
1	E	326	HIS
1	E	344	GLN
2	F	3	GLN
2	F	37	GLN
2	F	38	GLN

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Mol	Chain	Res	Type
2	F	50	ASN
2	F	89	GLN
2	F	138	ASN
2	F	161	ASN
2	F	198	HIS
3	G	39	GLN
3	G	77	ASN
3	G	202	HIS
2	H	3	GLN
2	H	38	GLN
2	H	50	ASN
2	H	89	GLN
2	H	138	ASN
2	H	161	ASN
2	H	198	HIS
3	I	39	GLN
3	I	77	ASN
3	I	202	HIS
2	J	3	GLN
2	J	37	GLN
2	J	38	GLN
2	J	50	ASN
2	J	89	GLN
2	J	138	ASN
2	J	161	ASN
2	J	210	ASN
3	K	39	GLN
3	K	77	ASN
3	K	202	HIS
2	L	3	GLN
2	L	38	GLN
2	L	50	ASN
2	L	89	GLN
2	L	138	ASN
2	L	161	ASN
3	M	39	GLN
3	M	77	ASN
3	M	202	HIS
2	N	3	GLN
2	N	37	GLN
2	N	38	GLN
2	N	50	ASN

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Mol	Chain	Res	Type
2	N	89	GLN
2	N	138	ASN
2	N	161	ASN
2	N	198	HIS
3	O	39	GLN
3	O	77	ASN
3	O	202	HIS

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](#)

Of 35 ligands modelled in this entry, 25 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	C	501	-	5,5,5	0.38	0	5,5,5	0.31	0
8	C6N	C	508	-	74,74,74	0.49	0	98,104,104	1.45	13 (13%)
4	GOL	A	501	-	5,5,5	0.37	0	5,5,5	0.30	0
4	GOL	E	501	-	5,5,5	0.38	0	5,5,5	0.30	0
8	C6N	A	507	-	74,74,74	0.49	0	98,104,104	1.45	13 (13%)
8	C6N	D	506	-	74,74,74	0.49	0	98,104,104	1.45	12 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	C6N	E	507	-	74,74,74	0.48	0	98,104,104	1.45	13 (13%)
8	C6N	B	507	-	74,74,74	0.49	0	98,104,104	1.45	12 (12%)
4	GOL	B	501	-	5,5,5	0.37	0	5,5,5	0.29	0
4	GOL	D	501	-	5,5,5	0.37	0	5,5,5	0.31	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
4	GOL	C	501	-	-	0/4/4/4	-
8	C6N	C	508	-	-	27/44/140/140	0/6/6/6
4	GOL	A	501	-	-	0/4/4/4	-
4	GOL	E	501	-	-	0/4/4/4	-
8	C6N	A	507	-	-	28/44/140/140	0/6/6/6
8	C6N	D	506	-	-	28/44/140/140	0/6/6/6
8	C6N	E	507	-	-	27/44/140/140	0/6/6/6
8	C6N	B	507	-	-	28/44/140/140	0/6/6/6
4	GOL	B	501	-	-	1/4/4/4	-
4	GOL	D	501	-	-	0/4/4/4	-

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	507	C6N	C45-O44-C43	-4.69	106.86	117.98
8	B	507	C6N	C45-O44-C43	-4.68	106.88	117.98
8	A	507	C6N	C45-O44-C43	-4.62	107.02	117.98
8	C	508	C6N	C45-O44-C43	-4.62	107.03	117.98
8	D	506	C6N	C45-O44-C43	-4.58	107.11	117.98
8	D	506	C6N	C38-O59-C56	3.82	121.19	113.72
8	E	507	C6N	O55-C52-C50	3.82	116.58	109.70
8	C	508	C6N	C38-O59-C56	3.79	121.12	113.72
8	A	507	C6N	C38-O59-C56	3.76	121.07	113.72
8	B	507	C6N	C38-O59-C56	3.73	121.00	113.72
8	E	507	C6N	C38-O59-C56	3.72	120.99	113.72
8	A	507	C6N	O55-C52-C50	3.72	116.40	109.70
8	C	508	C6N	O55-C52-C50	3.72	116.39	109.70
8	D	506	C6N	O55-C52-C50	3.71	116.39	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	507	C6N	O55-C52-C50	3.69	116.36	109.70
8	A	507	C6N	C24-O23-C22	3.43	122.02	113.31
8	B	507	C6N	C24-O23-C22	3.42	122.00	113.31
8	C	508	C6N	O37-C38-C39	3.42	113.47	108.27
8	E	507	C6N	O37-C38-C39	3.39	113.42	108.27
8	D	506	C6N	O59-C56-C43	3.38	116.72	109.72
8	D	506	C6N	C24-O23-C22	3.38	121.88	113.31
8	A	507	C6N	O37-C38-C39	3.37	113.39	108.27
8	C	508	C6N	C24-O23-C22	3.37	121.87	113.31
8	D	506	C6N	O37-C38-C39	3.37	113.39	108.27
8	E	507	C6N	C24-O23-C22	3.37	121.86	113.31
8	A	507	C6N	O59-C56-C43	3.35	116.64	109.72
8	B	507	C6N	O37-C38-C39	3.35	113.36	108.27
8	B	507	C6N	O59-C56-C43	3.25	116.45	109.72
8	E	507	C6N	O59-C56-C43	3.25	116.44	109.72
8	C	508	C6N	O59-C56-C43	3.24	116.41	109.72
8	E	507	C6N	O06-C05-C03	2.91	117.10	109.48
8	D	506	C6N	O06-C05-C03	2.90	117.09	109.48
8	C	508	C6N	O06-C05-C03	2.89	117.06	109.48
8	B	507	C6N	O06-C05-C03	2.85	116.95	109.48
8	A	507	C6N	O06-C05-C03	2.84	116.94	109.48
8	C	508	C6N	C67-C66-C65	-2.47	106.33	111.42
8	D	506	C6N	C26-C27-C28	-2.46	105.87	113.19
8	C	508	C6N	C26-C27-C28	-2.44	105.92	113.19
8	E	507	C6N	C26-C27-C28	-2.44	105.93	113.19
8	B	507	C6N	C26-C27-C28	-2.42	105.99	113.19
8	B	507	C6N	C67-C66-C65	-2.42	106.45	111.42
8	A	507	C6N	C26-C27-C28	-2.41	106.01	113.19
8	E	507	C6N	C67-C66-C65	-2.41	106.47	111.42
8	D	506	C6N	C67-C66-C65	-2.40	106.48	111.42
8	A	507	C6N	C67-C66-C65	-2.40	106.48	111.42
8	C	508	C6N	C22-O04-C03	2.31	118.22	113.72
8	A	507	C6N	C22-O04-C03	2.30	118.20	113.72
8	E	507	C6N	C22-O04-C03	2.27	118.16	113.72
8	B	507	C6N	C22-O04-C03	2.25	118.12	113.72
8	D	506	C6N	C22-O04-C03	2.25	118.11	113.72
8	B	507	C6N	O04-C03-C05	2.24	114.35	109.72
8	E	507	C6N	C38-C39-C41	-2.22	105.33	110.01
8	A	507	C6N	O04-C03-C05	2.22	114.32	109.72
8	C	508	C6N	O04-C03-C05	2.22	114.31	109.72
8	D	506	C6N	O04-C03-C05	2.19	114.25	109.72
8	E	507	C6N	O04-C03-C05	2.19	114.24	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	507	C6N	C38-C39-C41	-2.18	105.42	110.01
8	A	507	C6N	C38-C39-C41	-2.15	105.49	110.01
8	D	506	C6N	C38-C39-C41	-2.13	105.53	110.01
8	C	508	C6N	C38-C39-C41	-2.10	105.59	110.01
8	E	507	C6N	C48-C50-C52	2.05	113.95	110.23
8	C	508	C6N	O17-C14-C15	2.02	111.43	106.44
8	A	507	C6N	C48-C50-C52	2.00	113.86	110.23

There are no chirality outliers.

All (139) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	507	C6N	C25-C24-O23-C22
8	A	507	C6N	C24-C25-C60-C61
8	A	507	C6N	C26-C25-C60-C61
8	A	507	C6N	C36-C25-C60-C61
8	A	507	C6N	O59-C38-O37-C36
8	B	507	C6N	C25-C24-O23-C22
8	B	507	C6N	C60-C25-C26-C27
8	B	507	C6N	C24-C25-C60-C61
8	B	507	C6N	C26-C25-C60-C61
8	B	507	C6N	C36-C25-C60-C61
8	B	507	C6N	O59-C38-O37-C36
8	C	508	C6N	C25-C24-O23-C22
8	C	508	C6N	C60-C25-C26-C27
8	C	508	C6N	C24-C25-C60-C61
8	C	508	C6N	C26-C25-C60-C61
8	C	508	C6N	C36-C25-C60-C61
8	C	508	C6N	O59-C38-O37-C36
8	D	506	C6N	C25-C24-O23-C22
8	D	506	C6N	C60-C25-C26-C27
8	D	506	C6N	C24-C25-C60-C61
8	D	506	C6N	C26-C25-C60-C61
8	D	506	C6N	C36-C25-C60-C61
8	D	506	C6N	O59-C38-O37-C36
8	E	507	C6N	C25-C24-O23-C22
8	E	507	C6N	C60-C25-C26-C27
8	E	507	C6N	C24-C25-C60-C61
8	E	507	C6N	C26-C25-C60-C61
8	E	507	C6N	C36-C25-C60-C61
8	E	507	C6N	O59-C38-O37-C36
8	A	507	C6N	C03-C05-O06-C07

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Mol	Chain	Res	Type	Atoms
8	B	507	C6N	C03-C05-O06-C07
8	C	508	C6N	C03-C05-O06-C07
8	D	506	C6N	C03-C05-O06-C07
8	E	507	C6N	C03-C05-O06-C07
8	C	508	C6N	O01-C02-C03-O04
8	D	506	C6N	O01-C02-C03-O04
8	A	507	C6N	O01-C02-C03-O04
8	B	507	C6N	O01-C02-C03-O04
8	B	507	C6N	O59-C56-C57-O58
8	C	508	C6N	O59-C56-C57-O58
8	E	507	C6N	O01-C02-C03-O04
8	E	507	C6N	O59-C56-C57-O58
8	A	507	C6N	O59-C56-C57-O58
8	D	506	C6N	O59-C56-C57-O58
8	A	507	C6N	O04-C22-O23-C24
8	B	507	C6N	O04-C22-O23-C24
8	C	508	C6N	O04-C22-O23-C24
8	D	506	C6N	O04-C22-O23-C24
8	E	507	C6N	O04-C22-O23-C24
8	B	507	C6N	O01-C02-C03-C05
8	A	507	C6N	O01-C02-C03-C05
8	C	508	C6N	O01-C02-C03-C05
8	E	507	C6N	O01-C02-C03-C05
8	A	507	C6N	C43-C56-C57-O58
8	D	506	C6N	O01-C02-C03-C05
8	D	506	C6N	C43-C56-C57-O58
8	A	507	C6N	C20-C22-O23-C24
8	B	507	C6N	C20-C22-O23-C24
8	C	508	C6N	C20-C22-O23-C24
8	D	506	C6N	C20-C22-O23-C24
8	E	507	C6N	C20-C22-O23-C24
8	A	507	C6N	C25-C26-C27-C28
8	D	506	C6N	C25-C26-C27-C28
8	E	507	C6N	C25-C26-C27-C28
8	B	507	C6N	C43-C56-C57-O58
8	C	508	C6N	C43-C56-C57-O58
8	E	507	C6N	C43-C56-C57-O58
8	B	507	C6N	C25-C26-C27-C28
8	C	508	C6N	C25-C26-C27-C28
8	E	507	C6N	C61-C62-C63-C64
8	C	508	C6N	C61-C62-C63-C64
8	B	507	C6N	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
8	A	507	C6N	C61-C62-C63-C64
8	D	506	C6N	C61-C62-C63-C64
8	C	508	C6N	C26-C27-C28-C29
8	D	506	C6N	C26-C27-C28-C29
8	A	507	C6N	C26-C27-C28-C29
8	E	507	C6N	C26-C27-C28-C29
8	B	507	C6N	C26-C27-C28-C29
8	B	507	C6N	C28-C29-C30-C35
8	C	508	C6N	C28-C29-C30-C35
8	D	506	C6N	C28-C29-C30-C35
8	E	507	C6N	C28-C29-C30-C35
8	A	507	C6N	C28-C29-C30-C35
8	E	507	C6N	O55-C52-C53-O54
8	C	508	C6N	O55-C52-C53-O54
8	B	507	C6N	O55-C52-C53-O54
8	A	507	C6N	O55-C52-C53-O54
8	D	506	C6N	O55-C52-C53-O54
8	A	507	C6N	C25-C60-C61-C62
8	C	508	C6N	C28-C29-C30-C31
8	D	506	C6N	C25-C60-C61-C62
8	A	507	C6N	C39-C38-O37-C36
8	E	507	C6N	C39-C38-O37-C36
8	D	506	C6N	O17-C14-C15-O16
8	B	507	C6N	C28-C29-C30-C31
8	D	506	C6N	C28-C29-C30-C31
8	E	507	C6N	C28-C29-C30-C31
8	B	507	C6N	O17-C14-C15-O16
8	C	508	C6N	O17-C14-C15-O16
8	B	507	C6N	C25-C60-C61-C62
8	C	508	C6N	C25-C60-C61-C62
8	E	507	C6N	C25-C60-C61-C62
8	A	507	C6N	O17-C14-C15-O16
8	E	507	C6N	O17-C14-C15-O16
8	A	507	C6N	C60-C25-C26-C27
8	A	507	C6N	C28-C29-C30-C31
8	B	507	C6N	C39-C38-O37-C36
8	D	506	C6N	C39-C38-O37-C36
8	C	508	C6N	C39-C38-O37-C36
8	B	507	C6N	C60-C25-C36-O37
8	C	508	C6N	C26-C25-C36-O37
8	C	508	C6N	C60-C25-C36-O37
8	E	507	C6N	C60-C25-C36-O37

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Mol	Chain	Res	Type	Atoms
8	C	508	C6N	C36-C25-C26-C27
8	E	507	C6N	C36-C25-C26-C27
8	B	507	C6N	O23-C24-C25-C36
8	C	508	C6N	O23-C24-C25-C36
8	D	506	C6N	O23-C24-C25-C36
4	B	501	GOL	O1-C1-C2-O2
8	E	507	C6N	O23-C24-C25-C36
8	A	507	C6N	O23-C24-C25-C36
8	A	507	C6N	C36-C25-C26-C27
8	B	507	C6N	C36-C25-C26-C27
8	D	506	C6N	C36-C25-C26-C27
8	D	506	C6N	C27-C28-C29-C30
8	A	507	C6N	C27-C28-C29-C30
8	A	507	C6N	O23-C24-C25-C60
8	A	507	C6N	C26-C25-C36-O37
8	A	507	C6N	C60-C25-C36-O37
8	B	507	C6N	O23-C24-C25-C60
8	B	507	C6N	C26-C25-C36-O37
8	C	508	C6N	O23-C24-C25-C60
8	D	506	C6N	O23-C24-C25-C60
8	D	506	C6N	C26-C25-C36-O37
8	D	506	C6N	C60-C25-C36-O37
8	E	507	C6N	O23-C24-C25-C60
8	E	507	C6N	C26-C25-C36-O37
8	B	507	C6N	C27-C28-C29-C30

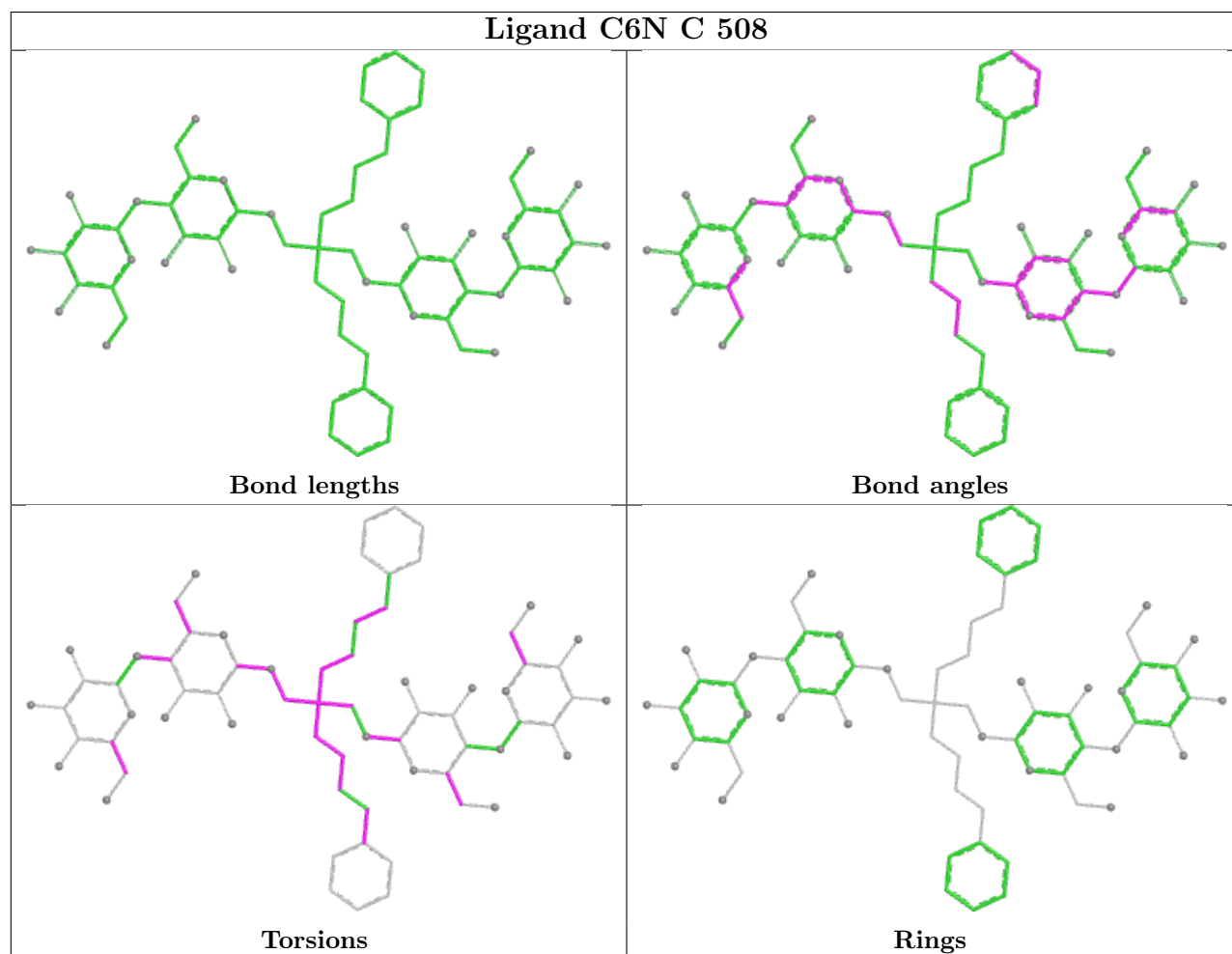
There are no ring outliers.

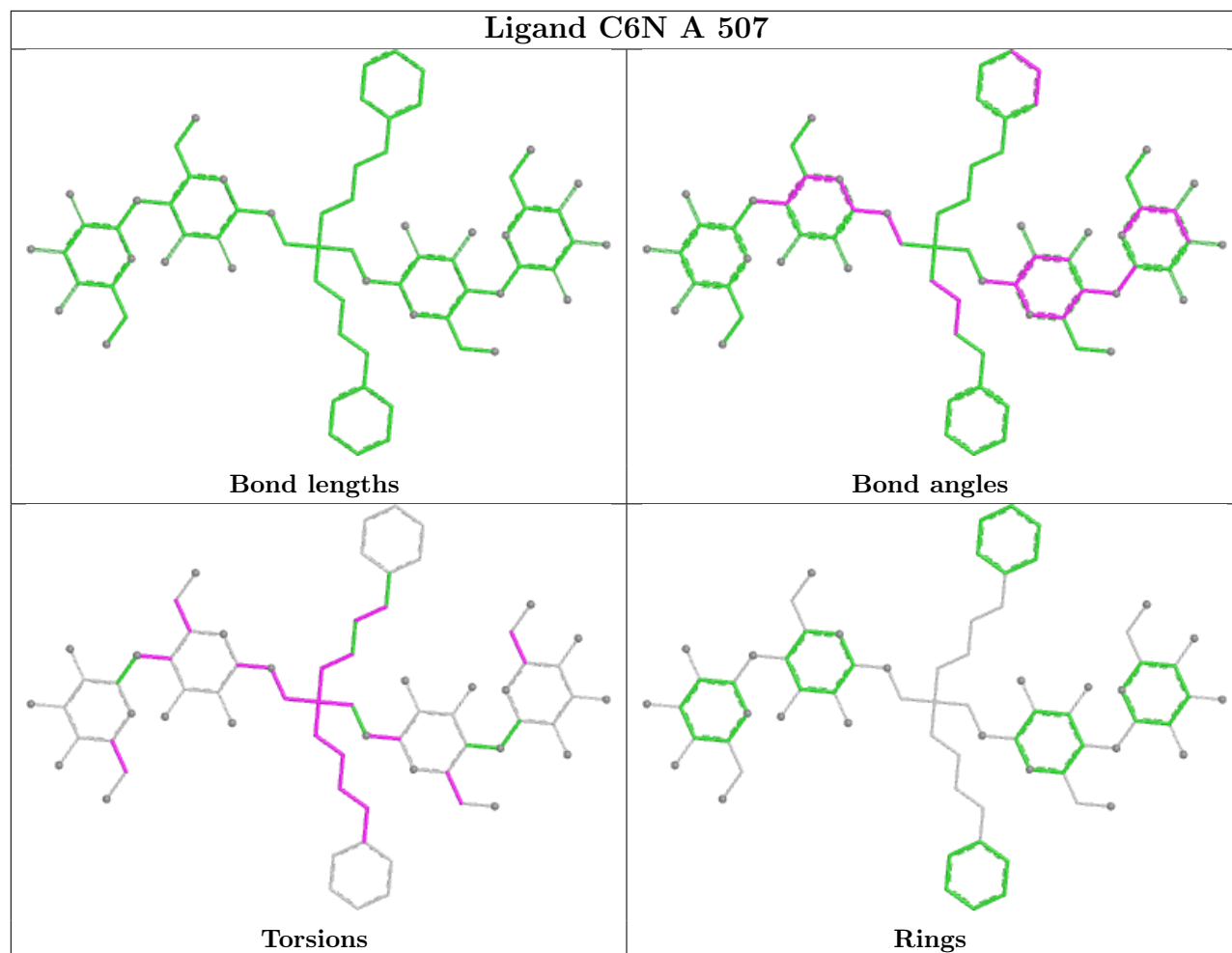
10 monomers are involved in 12 short contacts:

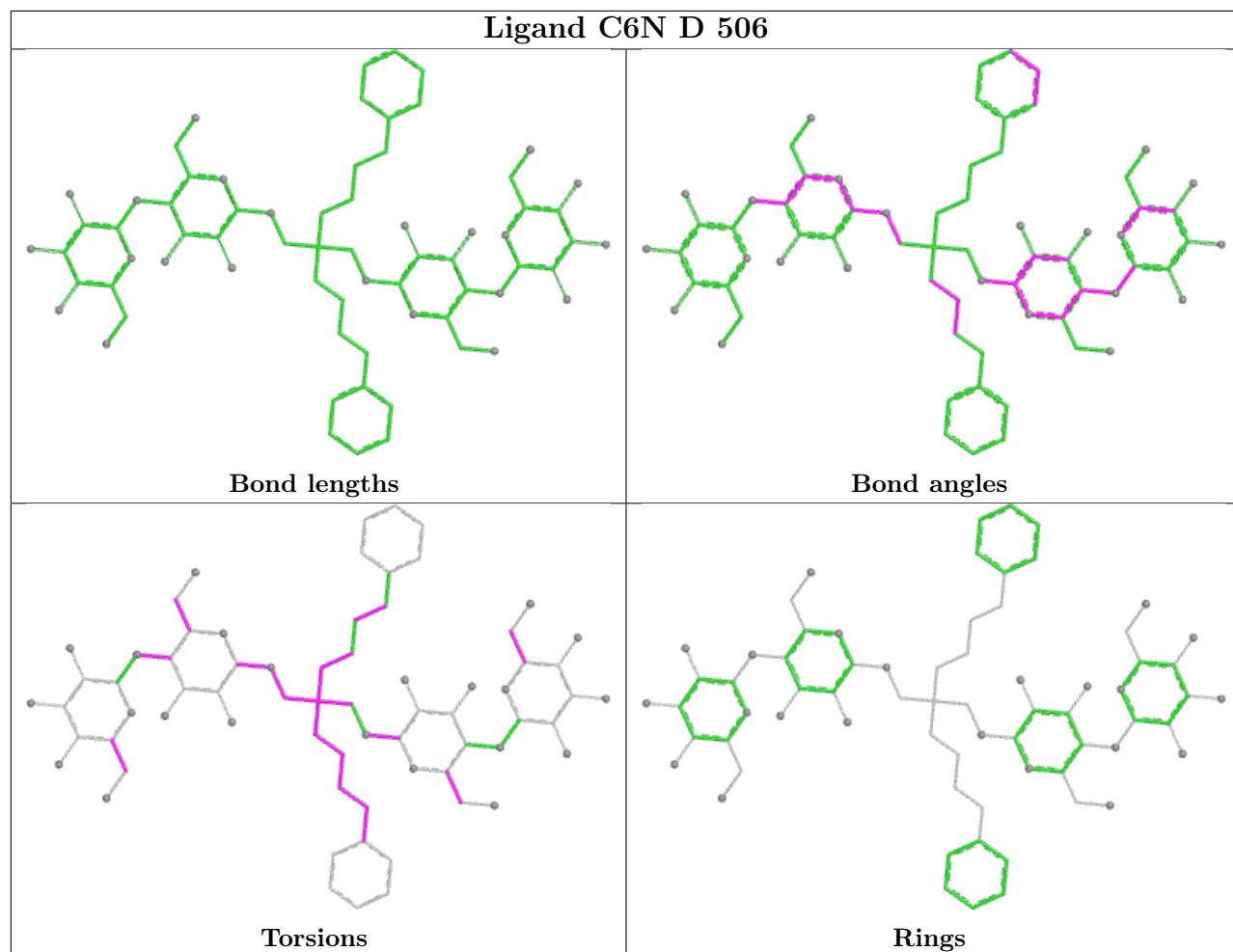
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	501	GOL	1	0
8	C	508	C6N	2	0
4	A	501	GOL	1	0
4	E	501	GOL	1	0
8	A	507	C6N	1	0
8	D	506	C6N	1	0
8	E	507	C6N	2	0
8	B	507	C6N	1	0
4	B	501	GOL	1	0
4	D	501	GOL	1	0

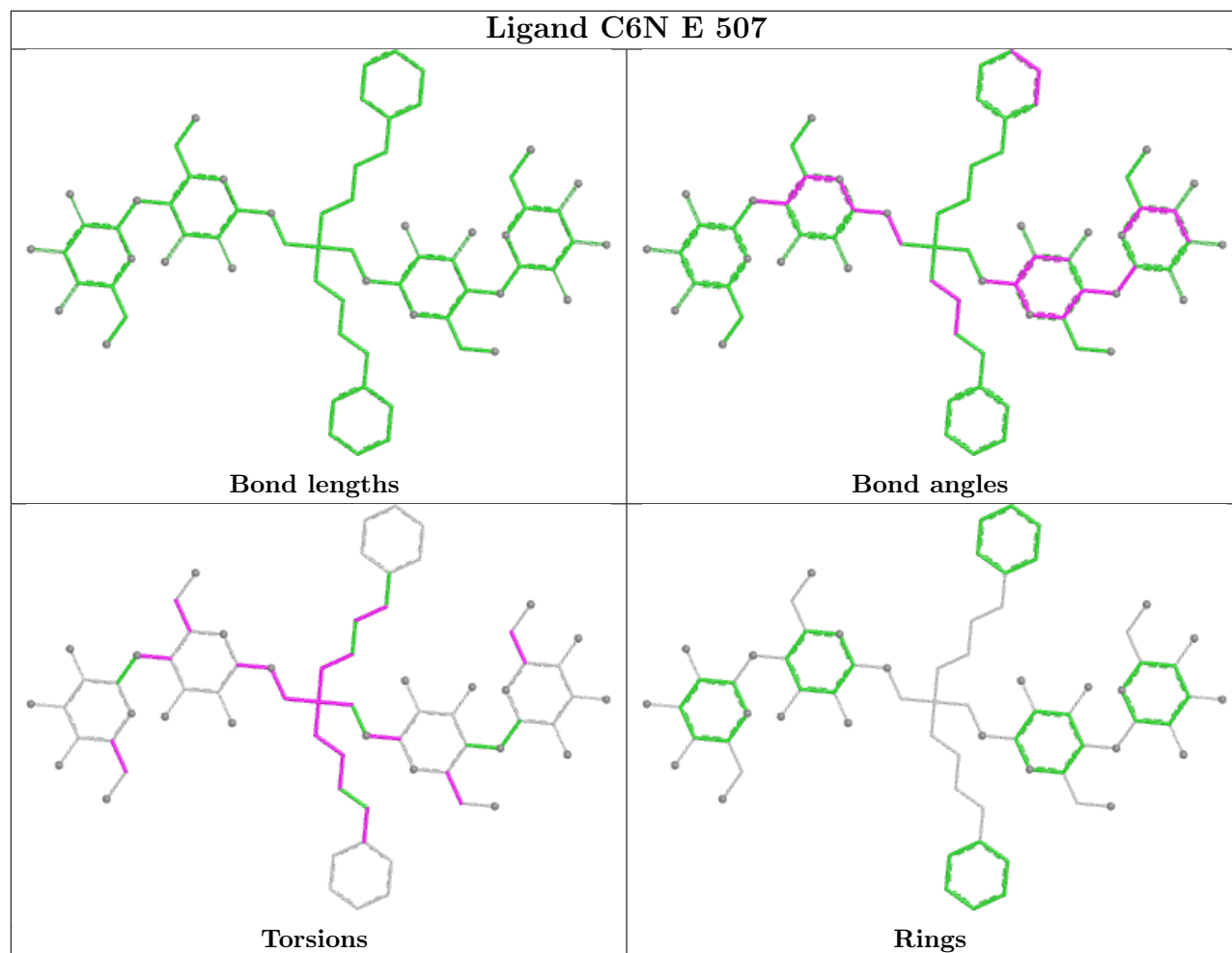
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

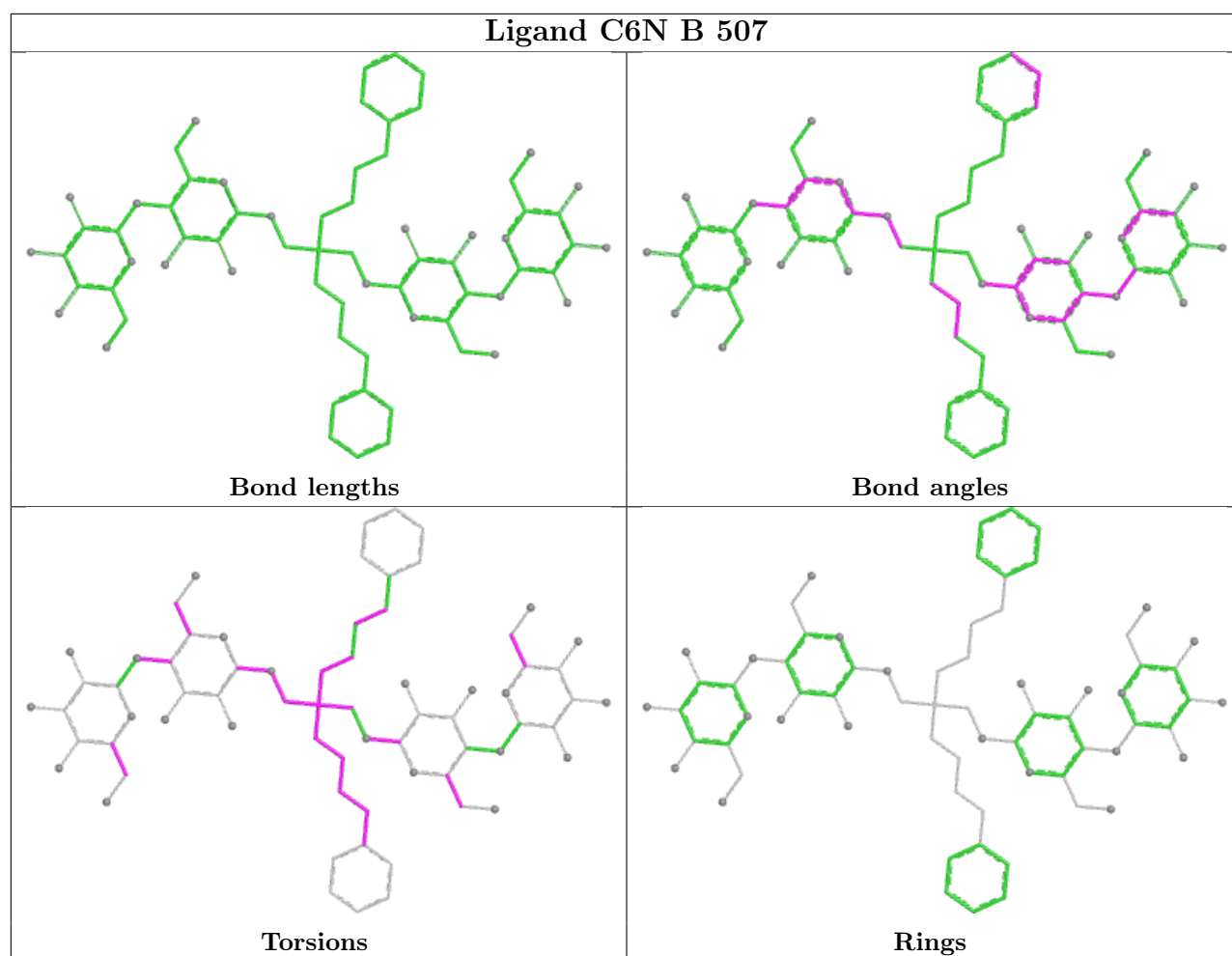
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	366/409 (89%)	0.25	12 (3%) 49 40	45, 69, 98, 187	0
1	B	366/409 (89%)	0.25	5 (1%) 73 67	47, 71, 100, 171	0
1	C	366/409 (89%)	0.22	10 (2%) 56 47	44, 69, 94, 174	0
1	D	366/409 (89%)	0.22	12 (3%) 49 40	44, 64, 94, 193	0
1	E	366/409 (89%)	0.24	16 (4%) 39 30	42, 66, 99, 170	0
2	F	212/212 (100%)	0.85	18 (8%) 16 12	73, 115, 148, 168	0
2	H	212/212 (100%)	0.78	23 (10%) 11 8	72, 106, 141, 164	0
2	J	212/212 (100%)	1.36	53 (25%) 2 1	75, 190, 288, 332	0
2	L	212/212 (100%)	0.75	21 (9%) 13 10	59, 98, 132, 142	0
2	N	212/212 (100%)	1.24	45 (21%) 2 2	67, 148, 256, 333	0
3	G	211/217 (97%)	1.00	29 (13%) 6 5	62, 119, 165, 200	0
3	I	211/217 (97%)	0.72	17 (8%) 18 13	70, 106, 151, 172	0
3	K	211/217 (97%)	1.31	48 (22%) 2 2	74, 160, 282, 318	0
3	M	211/217 (97%)	0.79	19 (9%) 15 12	55, 96, 157, 181	0
3	O	211/217 (97%)	1.18	47 (22%) 2 2	58, 120, 269, 333	0
All	All	3945/4190 (94%)	0.64	375 (9%) 14 11	42, 88, 228, 333	0

All (375) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	144	LEU	7.4
3	O	182	SER	6.3
3	K	166	VAL	5.7
3	M	176	ASP	5.6
3	O	129	PRO	5.3
3	K	168	THR	5.3
2	N	178	THR	5.2

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Mol	Chain	Res	Type	RSRZ
3	K	129	PRO	5.0
2	J	106	VAL	5.0
3	O	176	ASP	4.9
3	O	181	SER	4.8
2	H	40	GLN	4.8
3	O	143	CYS	4.7
2	N	177	SER	4.6
2	N	206	VAL	4.6
3	O	209	VAL	4.6
3	K	176	ASP	4.5
3	K	155	VAL	4.4
2	J	91	HIS	4.4
3	G	152	PRO	4.4
1	C	367	SER	4.4
2	N	135	PHE	4.4
3	G	176	ASP	4.3
2	J	146	VAL	4.3
3	O	155	VAL	4.2
2	N	195	GLU	4.2
1	E	367	SER	4.1
3	G	143	CYS	4.1
2	J	135	PHE	4.1
2	L	205	ILE	4.0
1	B	367	SER	4.0
2	N	207	LYS	4.0
3	O	214	VAL	4.0
3	K	182	SER	3.9
3	I	138	MET	3.8
3	K	175	SER	3.8
3	K	183	SER	3.8
2	F	40	GLN	3.8
2	F	212	ASN	3.8
2	J	193	THR	3.8
2	J	136	LEU	3.8
1	D	367	SER	3.7
2	F	127	SER	3.7
1	E	350	ALA	3.7
3	K	139	VAL	3.7
3	O	124	VAL	3.7
2	J	11	LEU	3.7
2	L	187	GLU	3.7
2	N	180	THR	3.6

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Mol	Chain	Res	Type	RSRZ
3	M	174	GLN	3.6
2	N	1	ASP	3.6
3	I	176	ASP	3.6
3	O	195	THR	3.6
2	N	24	ARG	3.6
3	M	175	SER	3.6
3	O	186	VAL	3.6
3	O	187	PRO	3.6
2	J	114	THR	3.5
2	F	94	THR	3.5
2	J	197	THR	3.5
2	J	153	SER	3.5
3	O	204	ALA	3.5
2	J	195	GLU	3.5
3	G	64	PHE	3.4
3	M	138	MET	3.4
3	K	193	SER	3.4
3	I	168	THR	3.4
2	N	131	SER	3.4
2	N	143	ASP	3.4
3	G	128	ALA	3.4
2	J	200	THR	3.4
3	G	43	GLN	3.4
3	K	156	THR	3.4
3	G	141	LEU	3.3
3	K	200	VAL	3.3
3	K	209	VAL	3.3
3	G	40	ARG	3.3
3	G	138	MET	3.3
2	F	126	THR	3.3
2	H	148	TRP	3.3
2	N	160	LEU	3.3
2	J	109	ALA	3.3
3	O	127	LEU	3.3
2	J	40	GLN	3.3
2	N	191	SER	3.3
3	G	129	PRO	3.2
3	K	215	PRO	3.2
3	K	189	SER	3.2
3	K	186	VAL	3.2
1	D	220	GLN	3.2
2	J	94	THR	3.2

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Mol	Chain	Res	Type	RSRZ
3	G	33	TRP	3.2
2	J	160	LEU	3.2
3	K	111	THR	3.2
3	K	185	THR	3.2
3	K	192	PRO	3.2
3	O	189	SER	3.1
3	K	65	ARG	3.1
1	A	115	ASP	3.1
2	L	91	HIS	3.1
3	K	195	THR	3.1
3	K	117	ALA	3.1
2	N	176	SER	3.0
2	L	152	GLY	3.0
3	M	10	GLU	3.0
2	J	148	TRP	3.0
3	M	216	ARG	3.0
3	O	215	PRO	3.0
2	N	91	HIS	3.0
2	N	52	LYS	3.0
2	N	186	TYR	3.0
2	H	177	SER	3.0
2	N	122	SER	3.0
2	F	123	GLU	3.0
2	H	106	VAL	3.0
3	O	191	TRP	2.9
2	J	150	ILE	2.9
3	K	187	PRO	2.9
2	H	94	THR	2.9
3	O	162	LEU	2.9
3	I	136	ASN	2.9
2	F	41	GLY	2.9
3	O	165	GLY	2.9
3	I	43	GLN	2.9
2	L	212	ASN	2.9
2	H	58	VAL	2.9
2	L	94	THR	2.9
2	N	114	THR	2.9
3	G	195	THR	2.9
2	J	206	VAL	2.8
3	I	216	ARG	2.8
3	M	210	ASP	2.8
3	O	183	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	N	23	CYS	2.8
3	K	41	PRO	2.8
2	J	107	LYS	2.8
2	F	177	SER	2.8
2	J	66	GLY	2.8
2	N	152	GLY	2.8
3	K	153	VAL	2.8
2	N	208	SER	2.8
2	J	103	LYS	2.8
1	B	272	PHE	2.8
2	N	137	ASN	2.8
1	B	2	THR	2.8
2	N	193	THR	2.8
3	O	197	THR	2.8
2	H	105	GLU	2.7
3	G	125	TYR	2.7
1	D	2	THR	2.7
2	F	1	ASP	2.7
3	O	168	THR	2.7
3	O	125	TYR	2.7
2	J	180	THR	2.7
3	M	195	THR	2.7
3	O	156	THR	2.7
3	M	57	GLU	2.7
2	N	94	THR	2.7
1	E	203	ASP	2.7
2	J	141	PRO	2.7
3	O	123	SER	2.7
3	O	139	VAL	2.7
2	H	23	CYS	2.7
2	J	194	CYS	2.7
2	N	134	CYS	2.7
2	N	212	ASN	2.7
2	H	146	VAL	2.7
3	K	145	VAL	2.7
3	K	214	VAL	2.7
3	I	175	SER	2.7
3	K	138	MET	2.6
2	H	194	CYS	2.6
2	L	200	THR	2.6
3	K	154	THR	2.6
1	E	123	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	198	GLU	2.6
1	E	353	GLU	2.6
2	J	15	VAL	2.6
3	I	210	ASP	2.6
3	K	118	LYS	2.6
3	K	141	LEU	2.6
3	K	44	ALA	2.6
2	F	91	HIS	2.6
2	J	23	CYS	2.6
3	K	140	THR	2.6
2	J	161	ASN	2.6
3	M	136	ASN	2.6
2	J	112	ALA	2.6
1	D	99	SER	2.6
2	H	91	HIS	2.6
2	F	136	LEU	2.6
3	K	127	LEU	2.6
3	O	184	VAL	2.6
1	A	272	PHE	2.6
1	A	367	SER	2.5
2	N	162	SER	2.5
2	J	39	LYS	2.5
2	J	57	GLY	2.5
3	G	144	LEU	2.5
3	I	139	VAL	2.5
3	O	145	VAL	2.5
1	D	268	GLU	2.5
3	O	179	THR	2.5
2	J	149	LYS	2.5
1	C	121	GLY	2.5
2	H	11	LEU	2.5
3	K	11	LEU	2.5
3	M	197	THR	2.5
2	H	212	ASN	2.5
2	J	199	LYS	2.5
3	M	209	VAL	2.5
1	E	33	TYR	2.5
2	N	209	PHE	2.5
2	L	23	CYS	2.5
3	M	211	LYS	2.5
2	J	152	GLY	2.5
2	J	201	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	N	119	PRO	2.5
1	D	366	ILE	2.5
3	O	185	THR	2.5
1	C	115	ASP	2.4
1	C	342	ASP	2.4
2	J	204	PRO	2.4
1	D	121	GLY	2.4
3	O	147	GLY	2.4
3	K	115	SER	2.4
3	O	169	PHE	2.4
3	K	94	TYR	2.4
1	A	2	THR	2.4
2	J	113	PRO	2.4
2	L	80	PRO	2.4
3	K	210	ASP	2.4
2	F	206	VAL	2.4
3	O	166	VAL	2.4
3	O	216	ARG	2.4
2	L	52	LYS	2.4
2	L	209	PHE	2.4
3	I	46	GLU	2.4
3	K	38	LYS	2.4
1	E	2	THR	2.4
2	H	175	MET	2.4
2	N	4	MET	2.4
1	A	331	ILE	2.4
3	O	122	PRO	2.4
2	N	74	LYS	2.4
3	O	128	ALA	2.4
2	N	136	LEU	2.4
1	D	261	GLU	2.4
2	L	40	GLN	2.4
3	M	189	SER	2.4
1	A	195	ALA	2.3
1	A	350	ALA	2.3
2	N	56	GLU	2.3
2	F	208	SER	2.3
3	K	191	TRP	2.3
1	C	331	ILE	2.3
2	N	205	ILE	2.3
2	L	119	PRO	2.3
3	O	196	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	80	PHE	2.3
2	F	4	MET	2.3
2	J	203	SER	2.3
3	M	33	TRP	2.3
3	O	152	PRO	2.3
3	I	186	VAL	2.3
2	H	57	GLY	2.3
2	H	158	GLY	2.3
1	E	272	PHE	2.3
2	F	135	PHE	2.3
1	A	198	GLU	2.3
1	B	333	GLU	2.3
1	C	123	LEU	2.3
3	O	137	SER	2.3
2	N	113	PRO	2.3
3	G	42	GLY	2.3
1	A	80	PHE	2.3
2	J	46	LEU	2.3
2	L	11	LEU	2.3
3	M	162	LEU	2.3
1	C	366	ILE	2.3
2	L	194	CYS	2.3
3	G	55	LYS	2.3
2	H	193	THR	2.3
2	H	200	THR	2.3
3	G	216	ARG	2.3
2	L	186	TYR	2.3
3	M	152	PRO	2.3
1	A	123	LEU	2.2
3	K	174	GLN	2.2
3	I	65	ARG	2.2
2	J	80	PRO	2.2
2	N	201	SER	2.2
3	K	121	PRO	2.2
3	G	11	LEU	2.2
1	E	331	ILE	2.2
2	J	115	VAL	2.2
3	G	166	VAL	2.2
3	M	207	THR	2.2
3	O	175	SER	2.2
1	E	268	GLU	2.2
1	E	360	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	M	65	ARG	2.2
1	B	115	ASP	2.2
2	J	133	VAL	2.2
2	L	146	VAL	2.2
2	J	182	THR	2.2
1	E	202	ARG	2.2
2	N	210	ASN	2.2
1	A	61	MET	2.2
2	L	126	THR	2.2
2	F	152	GLY	2.2
1	E	135	CYS	2.2
2	L	160	LEU	2.2
3	K	45	LEU	2.2
2	N	155	ARG	2.1
2	J	212	ASN	2.1
3	G	214	VAL	2.1
1	D	203	ASP	2.1
3	I	165	GLY	2.1
1	C	41	SER	2.1
1	E	349	ALA	2.1
2	J	154	GLU	2.1
2	J	156	GLN	2.1
3	G	136	ASN	2.1
3	I	152	PRO	2.1
3	G	104	ASP	2.1
2	H	136	LEU	2.1
3	G	44	ALA	2.1
3	I	188	SER	2.1
3	G	153	VAL	2.1
2	H	80	PRO	2.1
1	D	115	ASP	2.1
3	K	33	TRP	2.1
1	A	119	GLU	2.1
1	C	261	GLU	2.1
2	F	205	ILE	2.1
2	H	131	SER	2.1
2	J	177	SER	2.1
2	N	39	LYS	2.1
3	K	114	VAL	2.1
2	N	80	PRO	2.1
3	K	122	PRO	2.1
3	O	192	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	190	ASN	2.1
2	J	118	PHE	2.1
3	G	142	GLY	2.1
3	O	201	ALA	2.1
3	O	46	GLU	2.1
1	D	23	GLN	2.0
2	J	134	CYS	2.0
2	J	207	LYS	2.0
3	G	175	SER	2.0
3	O	164	SER	2.0
1	D	332	LEU	2.0
2	F	210	ASN	2.0
2	N	179	LEU	2.0
3	O	180	LEU	2.0
3	K	46	GLU	2.0
3	I	118	LYS	2.0
2	H	115	VAL	2.0
2	J	37	GLN	2.0
3	G	54	SER	2.0
3	G	182	SER	2.0
3	G	186	VAL	2.0
3	K	62	GLN	2.0
3	O	193	SER	2.0
2	J	137	ASN	2.0
2	J	196	ALA	2.0
2	N	109	ALA	2.0
1	C	303	ASP	2.0
2	L	184	ASP	2.0
3	I	33	TRP	2.0
2	H	206	VAL	2.0
2	L	159	VAL	2.0
2	N	115	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

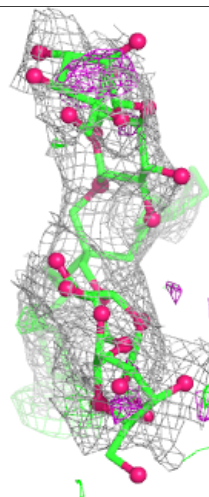
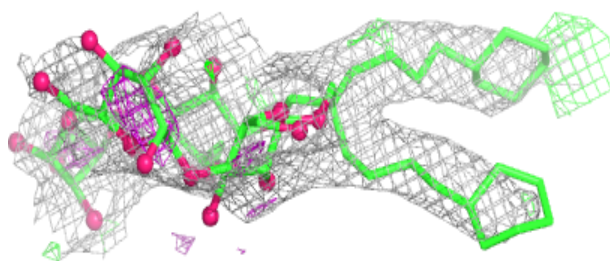
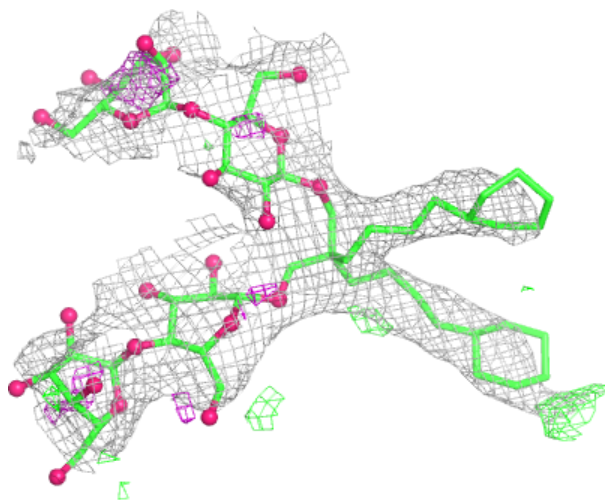
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CL	B	505	1/1	0.47	0.22	128,128,128,128	0
4	GOL	C	501	6/6	0.76	0.33	95,99,110,116	0
5	CL	C	505	1/1	0.76	0.14	111,111,111,111	0
8	C6N	E	507	69/69	0.76	0.19	113,142,162,166	0
8	C6N	D	506	69/69	0.78	0.17	97,125,145,148	0
8	C6N	B	507	69/69	0.79	0.18	116,145,167,171	0
8	C6N	C	508	69/69	0.79	0.17	105,132,154,158	0
4	GOL	A	501	6/6	0.80	0.29	104,108,118,123	0
8	C6N	A	507	69/69	0.80	0.17	107,137,158,162	0
5	CL	D	505	1/1	0.81	0.12	110,110,110,110	0
4	GOL	D	501	6/6	0.81	0.30	81,87,97,102	0
4	GOL	E	501	6/6	0.82	0.27	78,82,93,98	0
4	GOL	B	501	6/6	0.83	0.30	100,107,116,122	0
5	CL	C	503	1/1	0.86	0.23	109,109,109,109	0
5	CL	B	503	1/1	0.86	0.28	110,110,110,110	0
5	CL	E	503	1/1	0.88	0.23	128,128,128,128	0
5	CL	D	503	1/1	0.88	0.23	124,124,124,124	0
5	CL	A	503	1/1	0.88	0.10	105,105,105,105	0
5	CL	A	505	1/1	0.89	0.20	112,112,112,112	0
7	K	B	506	1/1	0.91	0.10	88,88,88,88	0
5	CL	E	505	1/1	0.91	0.10	101,101,101,101	0
7	K	C	507	1/1	0.94	0.14	86,86,86,86	0
7	K	A	506	1/1	0.94	0.12	87,87,87,87	0
5	CL	B	504	1/1	0.95	0.20	69,69,69,69	0
7	K	C	506	1/1	0.95	0.08	88,88,88,88	0
7	K	E	506	1/1	0.96	0.11	79,79,79,79	0
5	CL	E	504	1/1	0.96	0.12	65,65,65,65	0
5	CL	A	502	1/1	0.97	0.09	67,67,67,67	0
5	CL	D	504	1/1	0.97	0.09	58,58,58,58	0
5	CL	C	504	1/1	0.98	0.07	66,66,66,66	0
6	CA	C	502	1/1	0.99	0.03	64,64,64,64	0
6	CA	D	502	1/1	1.00	0.02	52,52,52,52	0
6	CA	E	502	1/1	1.00	0.03	54,54,54,54	0
6	CA	B	502	1/1	1.00	0.04	62,62,62,62	0
6	CA	A	504	1/1	1.00	0.03	59,59,59,59	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.

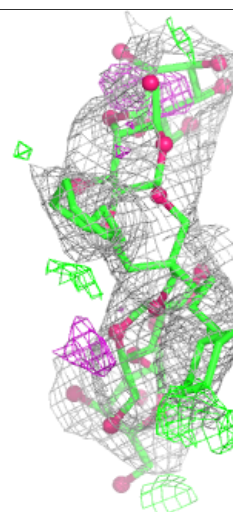
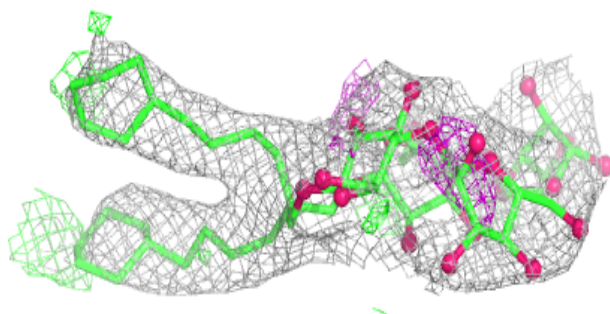
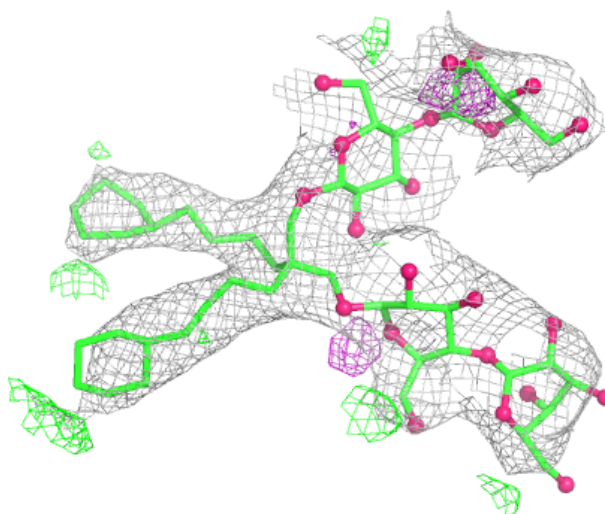
Electron density around C6N E 507:

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



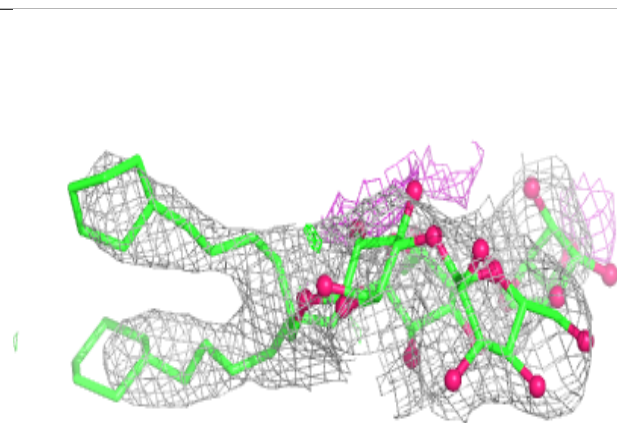
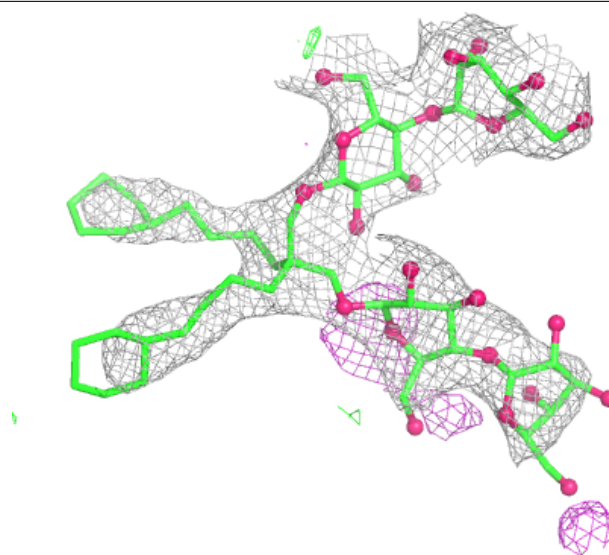
Electron density around C6N D 506:

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



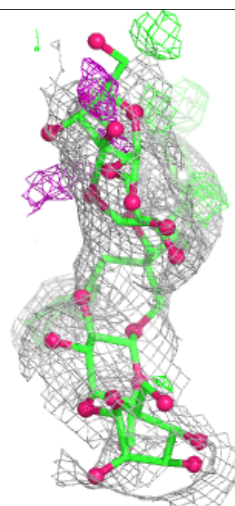
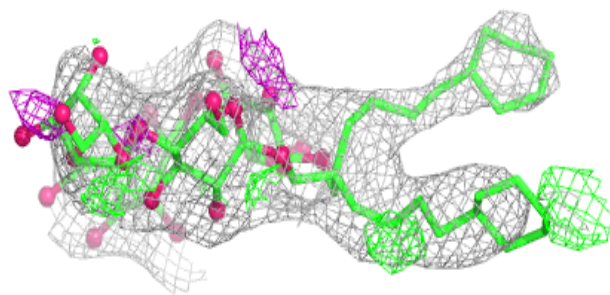
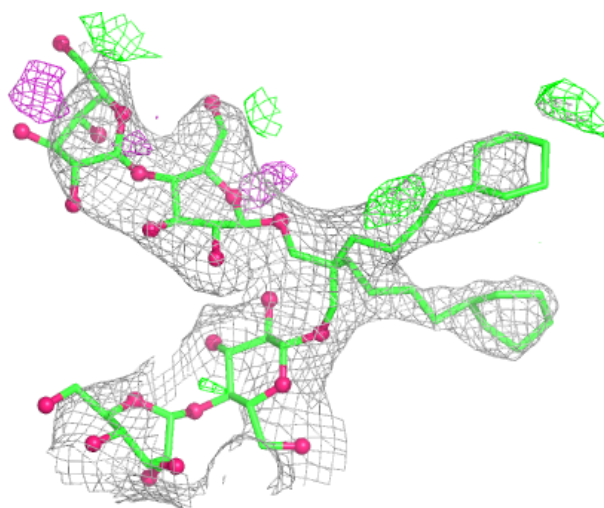
Electron density around C6N B 507:

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



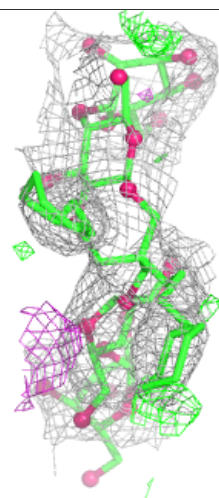
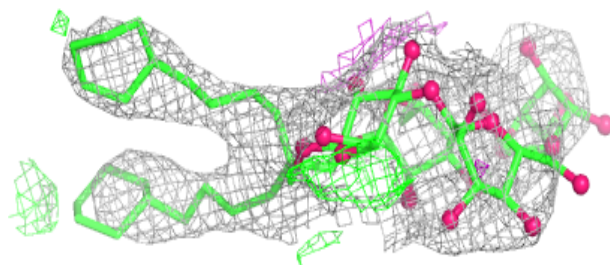
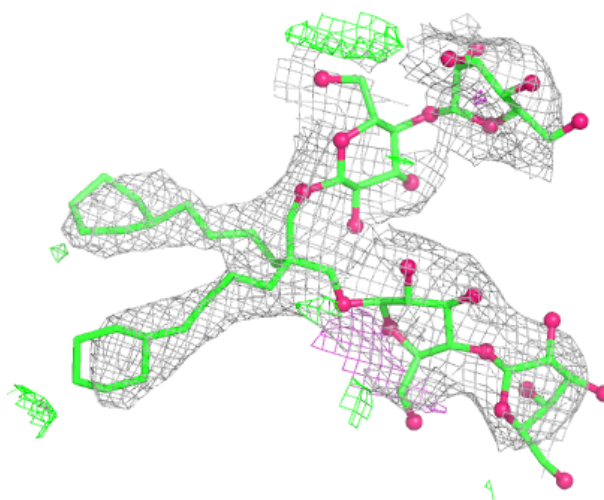
Electron density around C6N C 508:

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



Electron density around C6N A 507:

$2mF_o-DF_c$ (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.