Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 06:18 am BST

PDB ID	:	4RDQ
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 following versions of software and data (see references ⓘ) were used in the production of this report:

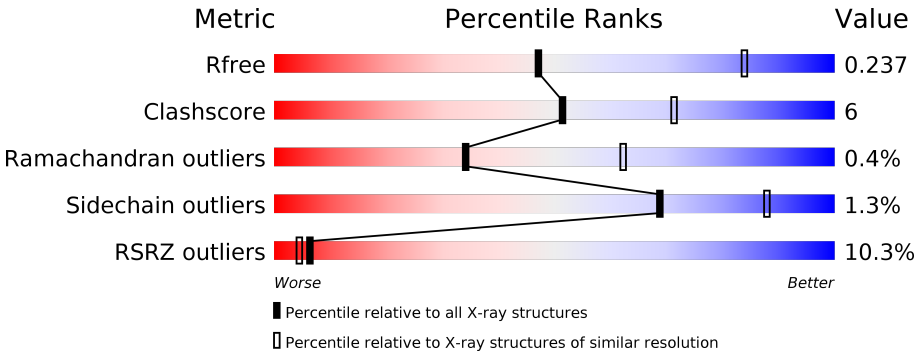
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 on 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 <=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	74% 14% • 11%
1	B	409	75% 14% • 11%
1	C	409	% 74% 15% • 11%
1	D	409	74% 15% • 11%
1	E	409	% 74% 15% • 11%
2	F	212	5% 87% 13%

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Mol	Chain	Length	Quality of chain
2	H	212	5% 83% 17%
2	J	212	49% 85% 15%
2	L	212	8% 84% 16%
2	N	212	32% 84% 16%
3	G	217	17% 86% 12%
3	I	217	3% 86% 12%
3	K	217	36% 85% 12%
3	M	217	2% 86% 12%
3	O	217	29% 87% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	B	505	-	-	-	X
5	CL	C	503	-	-	-	X
5	CL	C	505	-	-	-	X
5	CL	D	503	-	-	-	X
5	CL	D	505	-	-	-	X

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

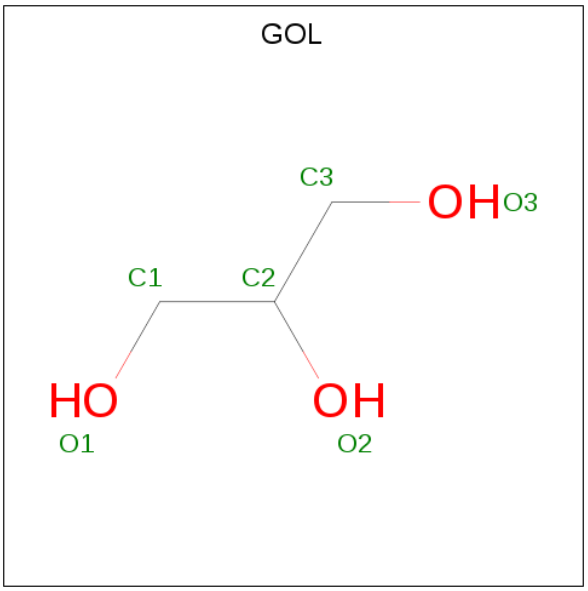
- Molecule 2 is a protein called Fab antibody fragment, light chain.

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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

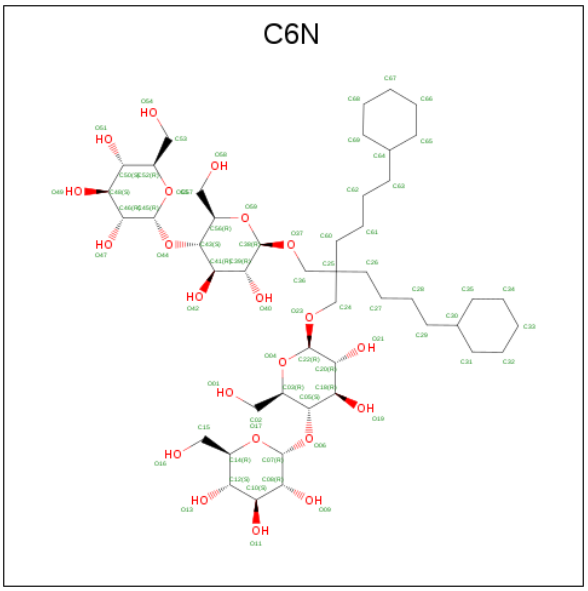
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total K 1 1	0	0
7	A	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 (three-letter code: C6N) (formula: $C_{47}H_{84}O_{22}$).



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.

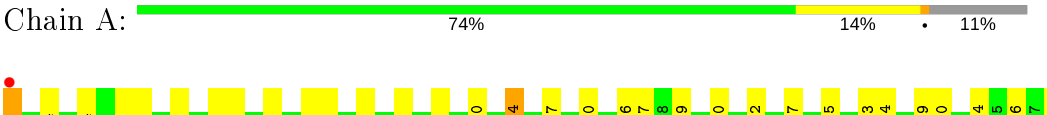
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total O 2 2	0	0
9	B	2	Total O 2 2	0	0
9	C	2	Total O 2 2	0	0
9	D	2	Total O 2 2	0	0
9	E	2	Total O 2 2	0	0

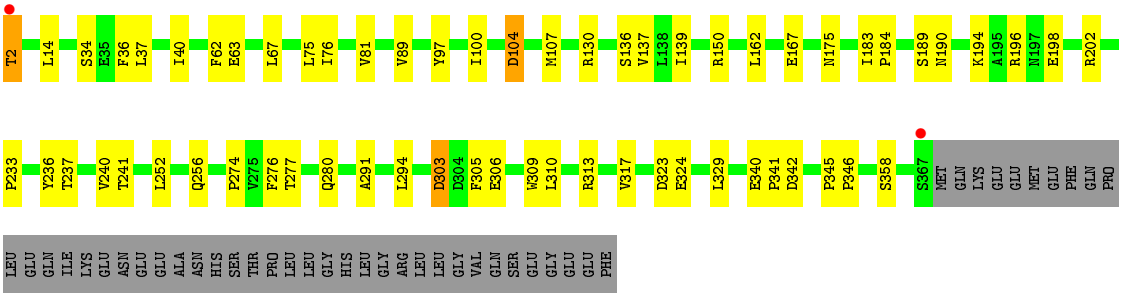
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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

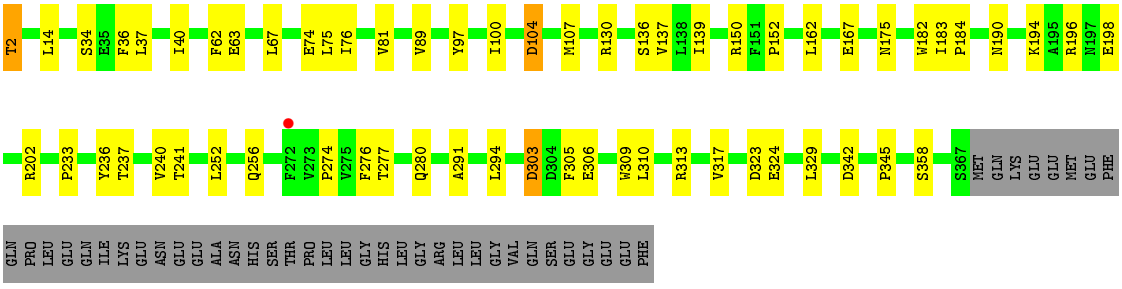
Chain A:





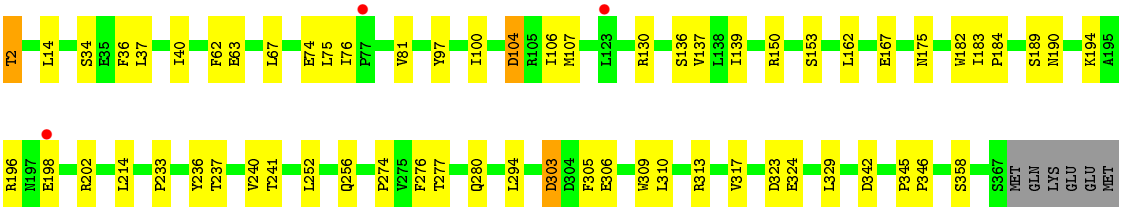
- Molecule 1: Bestrophin-1

Chain B:



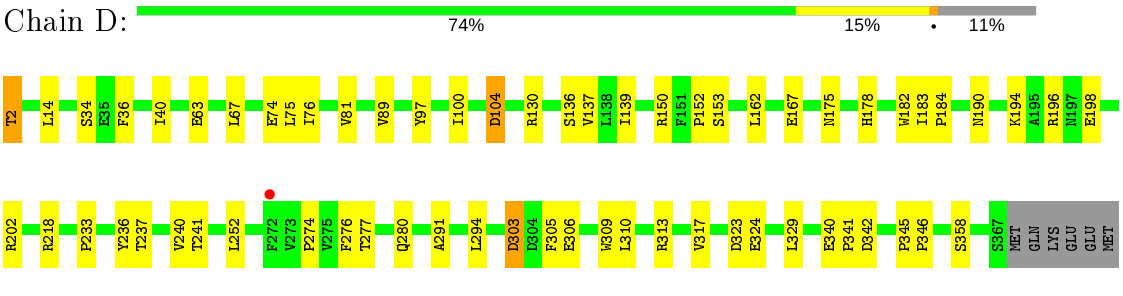
- Molecule 1: Bestrophin-1

Chain C:



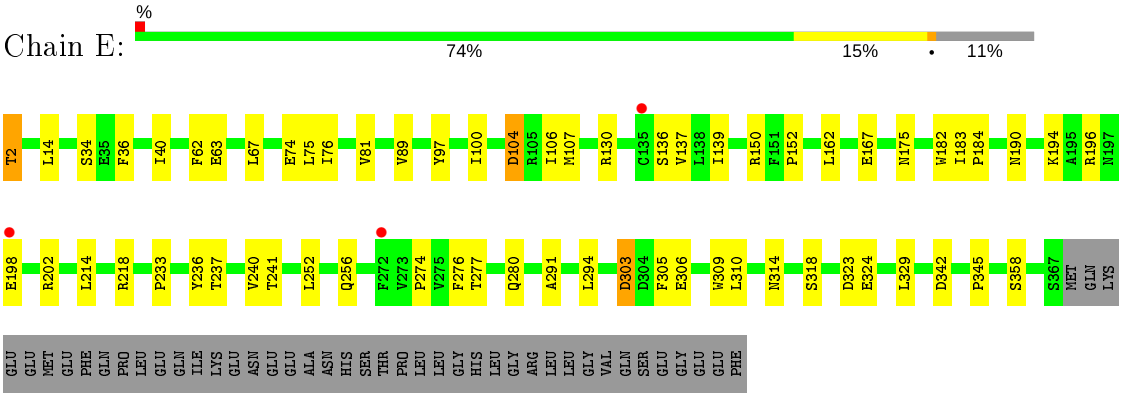
• Molecule 1: Bestrophin-1

Chain D:



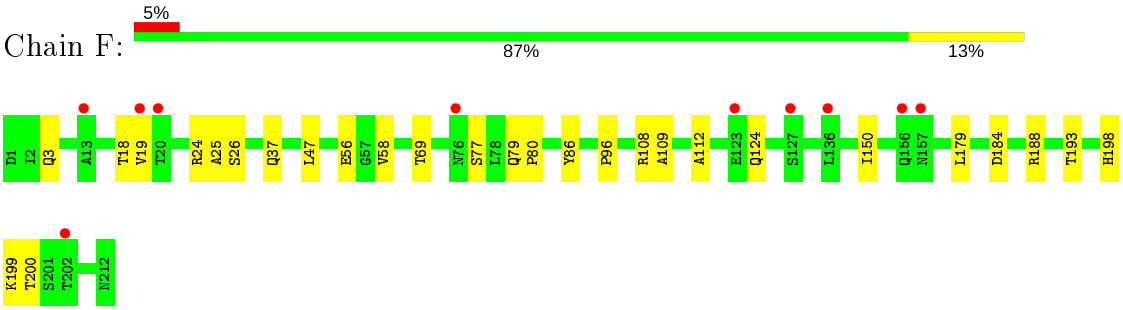
• Molecule 1: Bestrophin-1

Chain E:



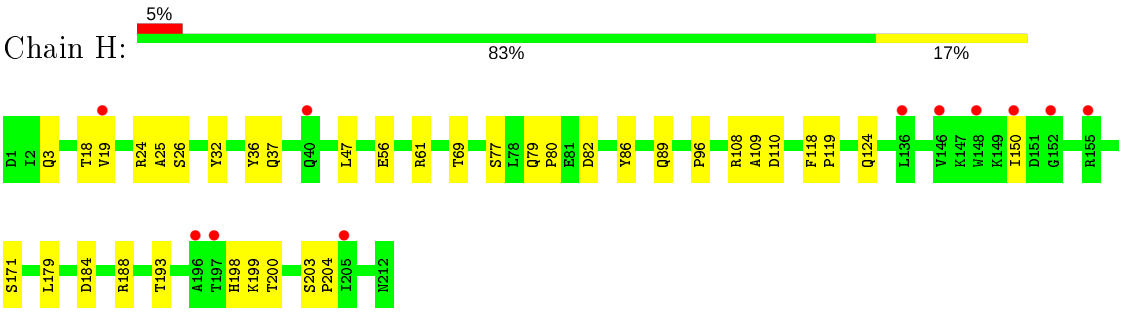
• Molecule 2: Fab antibody fragment, light chain

Chain F:



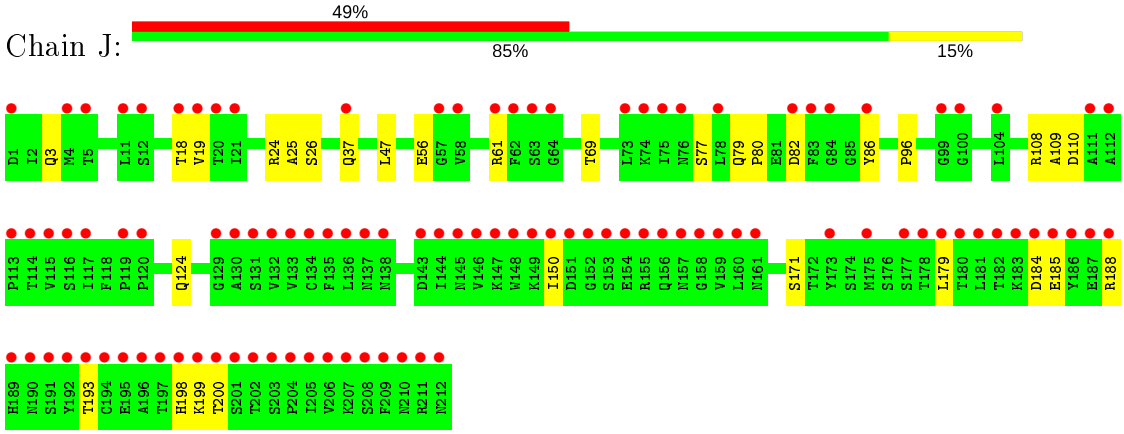
• Molecule 2: Fab antibody fragment, light chain

Chain H:



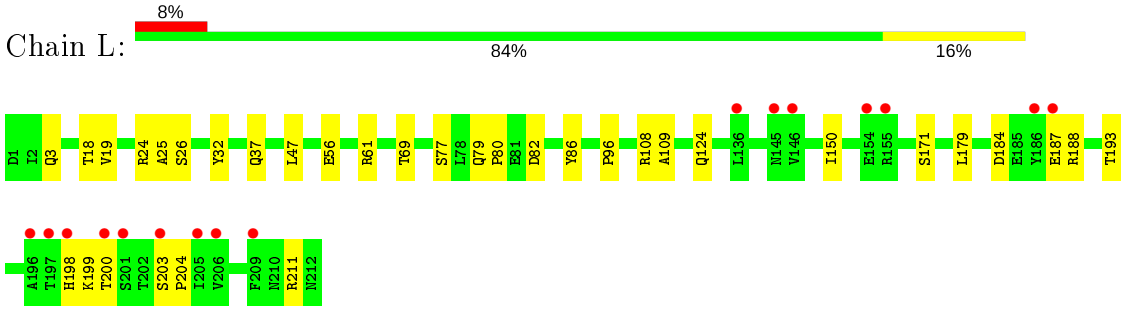
• Molecule 2: Fab antibody fragment, light chain

Chain J:



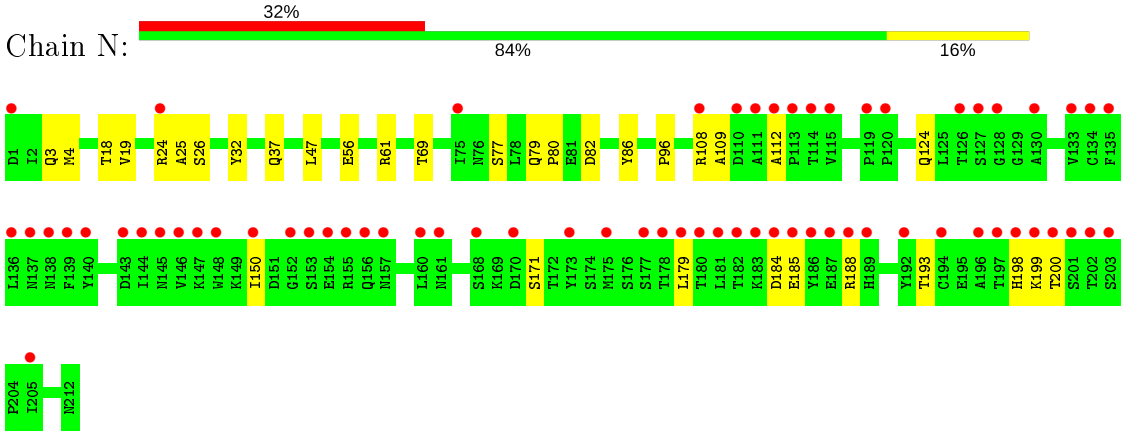
• Molecule 2: Fab antibody fragment, light chain

Chain L:



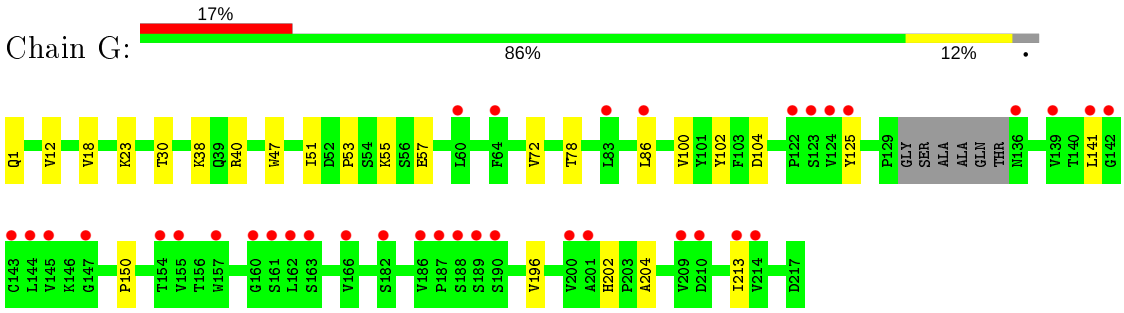
• Molecule 2: Fab antibody fragment, light chain

Chain N:



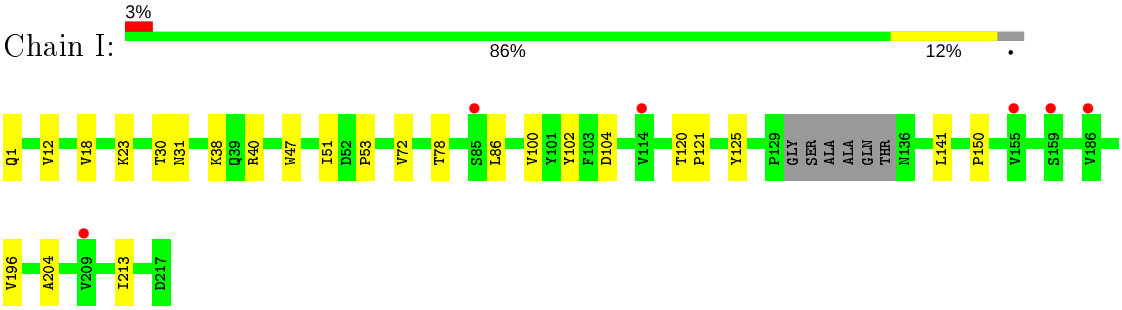
• Molecule 3: Fab antibody fragment, heavy chain

Chain G:



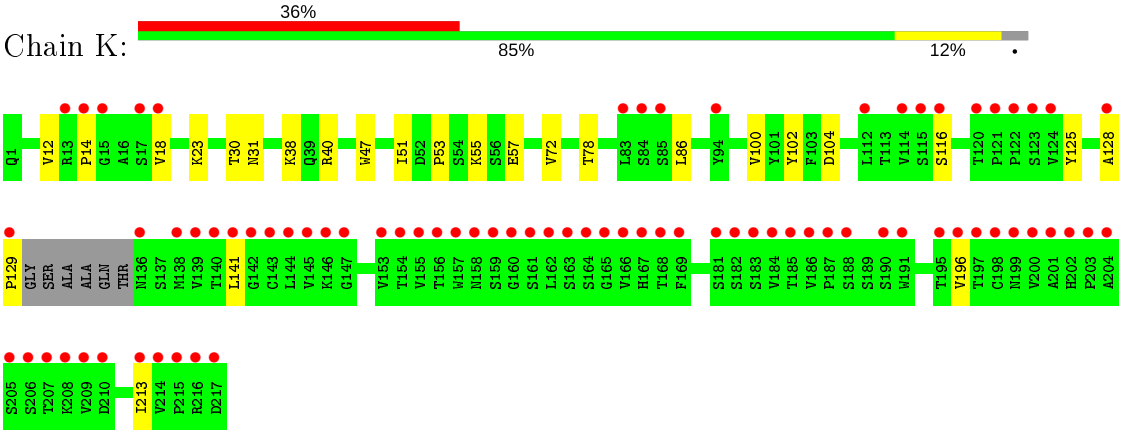
• Molecule 3: Fab antibody fragment, heavy chain

Chain I:



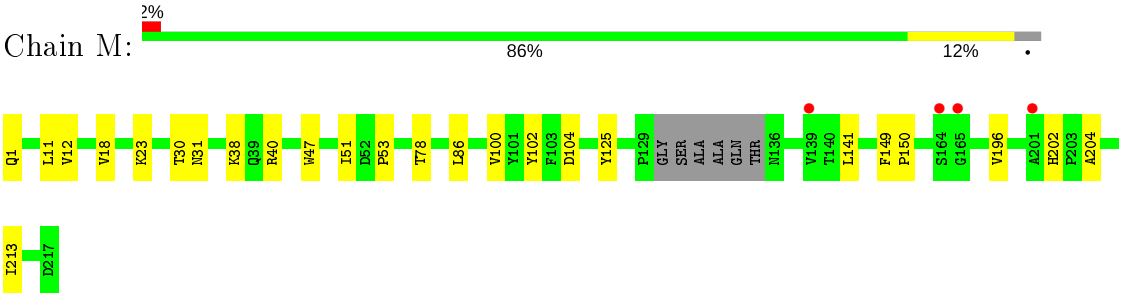
• Molecule 3: Fab antibody fragment, heavy chain

Chain K:



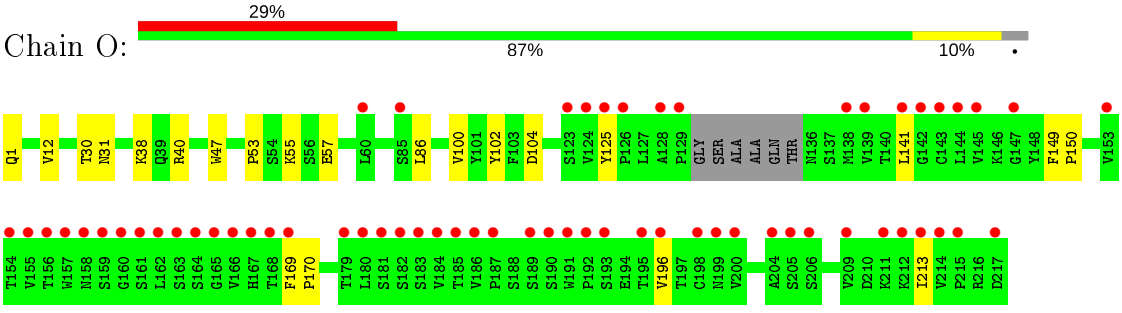
• Molecule 3: Fab antibody fragment, heavy chain

Chain M:



• Molecule 3: Fab antibody fragment, heavy chain

Chain O:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 0.222 , 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 , 56.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: C6N, GOL, K, CA, CL

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	0.23	0/3081	0.43	0/4200
1	B	0.23	0/3081	0.43	0/4200
1	C	0.23	0/3081	0.43	0/4200
1	D	0.23	0/3081	0.43	0/4200
1	E	0.23	0/3081	0.43	0/4200
2	F	0.23	0/1630	0.44	0/2225
2	H	0.23	0/1630	0.44	0/2225
2	J	0.23	0/1630	0.44	0/2225
2	L	0.23	0/1630	0.45	0/2225
2	N	0.23	0/1630	0.45	0/2225
3	G	0.22	0/1602	0.45	0/2202
3	I	0.22	0/1602	0.45	0/2202
3	K	0.22	0/1602	0.45	0/2202
3	M	0.22	0/1602	0.45	0/2202
3	O	0.22	0/1602	0.45	0/2202
All	All	0.23	0/31565	0.44	0/43135

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2994	0	2931	40	0
1	B	2994	0	2931	41	0
1	C	2994	0	2931	44	0
1	D	2994	0	2931	45	0
1	E	2994	0	2931	42	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	19	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	2	0	0	0	0
All	All	31125	0	29565	338	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 (338) 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
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
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: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
3:I:30:THR:HA	3:I:53:PRO:HB2	1.78	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O23	8:A:507:C6N:H69	2.05	0.56
8:B:507:C6N:O23	8:B:507:C6N:H69	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: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:O23	8:E:507:C6N:H69	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
2:L:79:GLN:HB3	2:L:80:PRO:HD2	1.92	0.52
1:A:175:ASN:ND2	1:D:342:ASP:OD2	2.41	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:108:ARG:NH1	2:J:109:ALA:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:198:HIS:HB3	2:F:200:THR:HG22	1.93	0.50
2:F:79:GLN:HB3	2:F:80:PRO:HD2	1.92	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:N:4:MET:HE1	2:N:25:ALA:HA	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:LEU:HD11	2:H:86:TYR:HE1	1.78	0.49
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:198:HIS:HB3	2:N:200:THR:HG22	1.94	0.48
2:N:18:THR:HG22	2:N:77:SER:H	1.78	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:108:ARG:HD2	2:L:171:SER:HB2	1.95	0.48
2:L:18:THR:HG22	2:L:77:SER:H	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:PRO:HB2	1:B:277:THR:HB	1.95	0.47
1:C:137:VAL:HG21	1:C:162:LEU:HD13	1.97	0.47
1:C:130:ARG:NH2	1:C:167:GLU:OE2	2.47	0.47
1:B:345:PRO:HB2	1:C:150:ARG:NH2	2.29	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
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: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: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
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:137:VAL:HG21	1:D:162:LEU:HD13	1.97	0.46
1:D:75:LEU:HD21	1:D:280:GLN:NE2	2.31	0.46
1:B:100:ILE:HG21	1:B:310:LEU:HD23	1.97	0.46
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:137:VAL:HG21	1:B:162:LEU:HD13	1.97	0.45
1:B:36:PHE:O	1:B:40:ILE:HG12	2.17	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:75:LEU:HD21	1:B:280:GLN:NE2	2.32	0.44
1:B:63:GLU:O	1:B:67:LEU:HG	2.18	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:N	3:M:1:GLN:OE1	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:HA	1:D:252:LEU:HD23	1.83	0.43
1:E:97:TYR:HB2	1:E:305:PHE:CZ	2.53	0.43
1:E:62:PHE:HZ	1:E:256:GLN:HG3	1.84	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
2:H:96:PRO:HD2	3:I:47:TRP:CD2	2.54	0.43
1:A:137:VAL:HG21	1:A:162:LEU:HD13	2.00	0.43
1:A:97:TYR:HB2	1:A:305:PHE:CZ	2.54	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:B:252:LEU:HD23	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
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:E:152:PRO:HB2	3:O:31:ASN:O	2.19	0.42
1:A:313:ARG:C	1:A:313:ARG:HD3	2.40	0.42
1:B:317:VAL:HG13	1:C:182:TRP:CZ2	2.55	0.42
1:E:104:ASP:HA	1:E:107:MET:HB3	2.01	0.42
1:E:2:THR:OG1	1:E:303:ASP:HA	2.19	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
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
2:L:37:GLN:HB2	2:L:47:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ARG:HD3	1:C:313:ARG:C	2.41	0.41
1:E:89:VAL:HG11	1:E:291:ALA:HA	2.02	0.41
8:E:507:C6N:H4	8:E:507:C6N:H6	1.80	0.41
3:G:1:GLN:OE1	3:G:1:GLN:N	2.45	0.41
1:D:313:ARG:C	1:D:313:ARG:HD3	2.40	0.41
1:D:340:GLU:HA	1:D:341:PRO:HD2	1.94	0.41
2:J:24:ARG:HH11	2:J:24:ARG:HG2	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:HG13	3:M:213:ILE:H	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:O	3:G:213:ILE:HD12	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:O	3:K:213:ILE:HD12	2.20	0.41
1:A:104:ASP:HA	1:A:107:MET:HB3	2.03	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:62:PHE:HZ	1:C:256:GLN:HG3	1.85	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
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
2:N:61:ARG:HD2	2:N:82:ASP:OD2	2.21	0.41
1:B:313:ARG:C	1:B:313:ARG:HD3	2.40	0.41
1:E:74:GLU:HB3	5:E:505:CL:CL	2.57	0.41
2:F:96:PRO:HD2	3:G:47:TRP:CD2	2.56	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:89:VAL:HG11	1:B:291:ALA:HA	2.02	0.40
1:B:62:PHE:HZ	1:B:256:GLN:HG3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:GLU:HB3	5:C:505:CL:CL	2.58	0.40
2:F:24:ARG:HG2	2:F:24:ARG:HH11	1.85	0.40
3:I:1:GLN:N	3:I:1:GLN:OE1	2.44	0.40
3:K:23:LYS:HG3	3:K:78:THR:HG22	2.03	0.40
1:D:153:SER:HB3	3:M:31:ASN:HB3	2.03	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
3:I:213:ILE:HG13	3:I:213:ILE:H	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%)	41	68
1	B	364/409 (89%)	349 (96%)	14 (4%)	1 (0%)	41	68
1	C	364/409 (89%)	348 (96%)	15 (4%)	1 (0%)	41	68
1	D	364/409 (89%)	349 (96%)	14 (4%)	1 (0%)	41	68
1	E	364/409 (89%)	349 (96%)	14 (4%)	1 (0%)	41	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	210/212 (99%)	192 (91%)	17 (8%)	1 (0%)	29	57
2	H	210/212 (99%)	192 (91%)	17 (8%)	1 (0%)	29	57
2	J	210/212 (99%)	191 (91%)	18 (9%)	1 (0%)	29	57
2	L	210/212 (99%)	192 (91%)	17 (8%)	1 (0%)	29	57
2	N	210/212 (99%)	192 (91%)	17 (8%)	1 (0%)	29	57
3	G	207/217 (95%)	201 (97%)	5 (2%)	1 (0%)	29	57
3	I	207/217 (95%)	200 (97%)	6 (3%)	1 (0%)	29	57
3	K	207/217 (95%)	201 (97%)	5 (2%)	1 (0%)	29	57
3	M	207/217 (95%)	201 (97%)	5 (2%)	1 (0%)	29	57
3	O	207/217 (95%)	201 (97%)	5 (2%)	1 (0%)	29	57
All	All	3905/4190 (93%)	3707 (95%)	183 (5%)	15 (0%)	34	62

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 (i)

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%)	320 (98%)	7 (2%)	53 79
1	B	327/370 (88%)	321 (98%)	6 (2%)	59 82
1	C	327/370 (88%)	320 (98%)	7 (2%)	53 79
1	D	327/370 (88%)	322 (98%)	5 (2%)	65 86
1	E	327/370 (88%)	322 (98%)	5 (2%)	65 86
2	F	173/187 (92%)	171 (99%)	2 (1%)	71 89
2	H	173/187 (92%)	170 (98%)	3 (2%)	60 83
2	J	173/187 (92%)	170 (98%)	3 (2%)	60 83
2	L	173/187 (92%)	171 (99%)	2 (1%)	71 89
2	N	173/187 (92%)	171 (99%)	2 (1%)	71 89
3	G	166/190 (87%)	166 (100%)	0	100 100
3	I	166/190 (87%)	166 (100%)	0	100 100
3	K	166/190 (87%)	166 (100%)	0	100 100
3	M	166/190 (87%)	166 (100%)	0	100 100
3	O	166/190 (87%)	166 (100%)	0	100 100
All	All	3330/3735 (89%)	3288 (99%)	42 (1%)	69 88

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	37	LEU
1	A	104	ASP
1	A	189	SER
1	A	196	ARG
1	A	236	TYR
1	A	303	ASP
1	B	2	THR
1	B	37	LEU
1	B	104	ASP
1	B	196	ARG
1	B	236	TYR
1	B	303	ASP
1	C	2	THR
1	C	37	LEU
1	C	104	ASP
1	C	189	SER
1	C	196	ARG

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Mol	Chain	Res	Type
1	C	236	TYR
1	C	303	ASP
1	D	2	THR
1	D	104	ASP
1	D	196	ARG
1	D	236	TYR
1	D	303	ASP
1	E	2	THR
1	E	104	ASP
1	E	196	ARG
1	E	236	TYR
1	E	303	ASP
2	F	19	VAL
2	F	193	THR
2	H	19	VAL
2	H	110	ASP
2	H	193	THR
2	J	19	VAL
2	J	110	ASP
2	J	193	THR
2	L	19	VAL
2	L	193	THR
2	N	19	VAL
2	N	193	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	A	326	HIS
1	B	175	ASN
1	B	326	HIS
1	C	175	ASN
1	C	326	HIS
1	D	175	ASN
1	D	326	HIS
1	E	175	ASN
1	E	326	HIS
2	F	3	GLN
2	F	38	GLN
2	F	50	ASN
2	F	89	GLN

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Mol	Chain	Res	Type
2	F	124	GLN
2	F	198	HIS
3	G	39	GLN
3	G	136	ASN
3	G	202	HIS
2	H	3	GLN
2	H	38	GLN
2	H	50	ASN
2	H	79	GLN
2	H	89	GLN
2	H	124	GLN
2	H	198	HIS
3	I	39	GLN
3	I	136	ASN
3	I	202	HIS
2	J	3	GLN
2	J	38	GLN
2	J	50	ASN
2	J	79	GLN
2	J	89	GLN
2	J	124	GLN
3	K	39	GLN
3	K	136	ASN
3	K	202	HIS
2	L	3	GLN
2	L	38	GLN
2	L	50	ASN
2	L	79	GLN
2	L	89	GLN
2	L	124	GLN
3	M	39	GLN
3	M	136	ASN
3	M	202	HIS
2	N	3	GLN
2	N	38	GLN
2	N	50	ASN
2	N	79	GLN
2	N	89	GLN
2	N	124	GLN
3	O	39	GLN
3	O	136	ASN
3	O	202	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 carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
8	C6N	E	507	-	74,74,74	0.49	0	102,104,104	1.49	16 (15%)
8	C6N	A	507	-	74,74,74	0.49	0	102,104,104	1.49	15 (14%)
8	C6N	C	508	-	74,74,74	0.49	0	102,104,104	1.49	16 (15%)
4	GOL	D	501	-	5,5,5	0.37	0	5,5,5	0.28	0
4	GOL	E	501	-	5,5,5	0.37	0	5,5,5	0.27	0
4	GOL	C	501	-	5,5,5	0.37	0	5,5,5	0.27	0
4	GOL	B	501	-	5,5,5	0.36	0	5,5,5	0.26	0
4	GOL	A	501	-	5,5,5	0.36	0	5,5,5	0.26	0
8	C6N	D	506	-	74,74,74	0.49	0	102,104,104	1.49	14 (13%)
8	C6N	B	507	-	74,74,74	0.50	0	102,104,104	1.49	14 (13%)

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
8	C6N	E	507	-	-	27/44/140/140	0/6/6/6
8	C6N	A	507	-	-	28/44/140/140	0/6/6/6
8	C6N	C	508	-	-	27/44/140/140	0/6/6/6
4	GOL	D	501	-	-	0/4/4/4	-
4	GOL	E	501	-	-	0/4/4/4	-
4	GOL	C	501	-	-	0/4/4/4	-
4	GOL	B	501	-	-	1/4/4/4	-
4	GOL	A	501	-	-	0/4/4/4	-
8	C6N	D	506	-	-	28/44/140/140	0/6/6/6
8	C6N	B	507	-	-	28/44/140/140	0/6/6/6

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	507	C6N	C45-O44-C43	-4.49	106.86	117.96
8	B	507	C6N	C45-O44-C43	-4.48	106.88	117.96
8	A	507	C6N	C45-O44-C43	-4.42	107.02	117.96
8	C	508	C6N	C45-O44-C43	-4.42	107.03	117.96
8	D	506	C6N	C45-O44-C43	-4.38	107.11	117.96
8	D	506	C6N	C38-O59-C56	3.82	121.19	113.69
8	E	507	C6N	O55-C52-C50	3.79	116.58	109.69
8	C	508	C6N	C38-O59-C56	3.79	121.12	113.69
8	A	507	C6N	C38-O59-C56	3.76	121.07	113.69
8	B	507	C6N	C38-O59-C56	3.73	121.00	113.69
8	E	507	C6N	C38-O59-C56	3.72	120.99	113.69
8	A	507	C6N	O55-C52-C50	3.69	116.40	109.69
8	C	508	C6N	O55-C52-C50	3.69	116.39	109.69
8	D	506	C6N	O55-C52-C50	3.68	116.39	109.69
8	B	507	C6N	O55-C52-C50	3.67	116.36	109.69
8	B	507	C6N	C26-C25-C36	-3.66	100.73	109.40
8	D	506	C6N	C26-C25-C36	-3.64	100.78	109.40
8	A	507	C6N	C26-C25-C36	-3.64	100.79	109.40
8	C	508	C6N	C26-C25-C36	-3.60	100.87	109.40
8	E	507	C6N	C26-C25-C36	-3.59	100.89	109.40
8	A	507	C6N	C24-O23-C22	3.33	122.02	113.36
8	B	507	C6N	C24-O23-C22	3.32	122.00	113.36
8	C	508	C6N	O37-C38-C39	3.31	113.47	108.30
8	D	506	C6N	O59-C56-C43	3.30	116.72	109.75
8	E	507	C6N	O37-C38-C39	3.28	113.42	108.30
8	D	506	C6N	C24-O23-C22	3.28	121.88	113.36
8	C	508	C6N	C24-O23-C22	3.27	121.87	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	507	C6N	O59-C56-C43	3.27	116.64	109.75
8	E	507	C6N	C24-O23-C22	3.27	121.86	113.36
8	A	507	C6N	O37-C38-C39	3.26	113.39	108.30
8	D	506	C6N	O37-C38-C39	3.26	113.39	108.30
8	B	507	C6N	O37-C38-C39	3.24	113.36	108.30
8	B	507	C6N	O59-C56-C43	3.17	116.45	109.75
8	E	507	C6N	O59-C56-C43	3.17	116.44	109.75
8	C	508	C6N	O59-C56-C43	3.16	116.41	109.75
8	E	507	C6N	O06-C05-C03	2.79	117.10	109.45
8	D	506	C6N	O06-C05-C03	2.79	117.09	109.45
8	C	508	C6N	O06-C05-C03	2.78	117.06	109.45
8	B	507	C6N	O06-C05-C03	2.74	116.95	109.45
8	A	507	C6N	O06-C05-C03	2.73	116.94	109.45
8	C	508	C6N	C67-C66-C65	-2.49	106.33	111.42
8	C	508	C6N	C60-C25-C24	2.48	115.28	109.40
8	D	506	C6N	C26-C27-C28	-2.46	105.87	113.19
8	B	507	C6N	C60-C25-C24	2.46	115.22	109.40
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	C67-C66-C65	-2.43	106.45	111.42
8	E	507	C6N	C67-C66-C65	-2.43	106.47	111.42
8	E	507	C6N	C60-C25-C24	2.42	115.14	109.40
8	D	506	C6N	C60-C25-C24	2.42	115.14	109.40
8	D	506	C6N	C67-C66-C65	-2.42	106.48	111.42
8	A	507	C6N	C67-C66-C65	-2.42	106.48	111.42
8	B	507	C6N	C26-C27-C28	-2.42	105.99	113.19
8	A	507	C6N	C26-C27-C28	-2.41	106.01	113.19
8	A	507	C6N	C60-C25-C24	2.39	115.07	109.40
8	C	508	C6N	C22-O04-C03	2.31	118.22	113.69
8	A	507	C6N	C22-O04-C03	2.30	118.20	113.69
8	E	507	C6N	C22-O04-C03	2.28	118.16	113.69
8	B	507	C6N	C22-O04-C03	2.26	118.12	113.69
8	D	506	C6N	C22-O04-C03	2.25	118.11	113.69
8	E	507	C6N	C38-C39-C41	-2.24	105.33	110.00
8	B	507	C6N	C38-C39-C41	-2.20	105.42	110.00
8	B	507	C6N	O04-C03-C05	2.18	114.35	109.75
8	A	507	C6N	O04-C03-C05	2.16	114.32	109.75
8	A	507	C6N	C38-C39-C41	-2.16	105.49	110.00
8	C	508	C6N	O04-C03-C05	2.16	114.31	109.75
8	D	506	C6N	C38-C39-C41	-2.15	105.53	110.00
8	D	506	C6N	O04-C03-C05	2.14	114.25	109.75
8	E	507	C6N	O04-C03-C05	2.13	114.24	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	508	C6N	C38-C39-C41	-2.12	105.59	110.00
8	E	507	C6N	C48-C50-C52	2.08	113.95	110.24
8	A	507	C6N	C48-C50-C52	2.03	113.86	110.24
8	C	508	C6N	C68-C69-C64	2.03	115.98	112.15
8	E	507	C6N	C68-C69-C64	2.02	115.97	112.15
8	C	508	C6N	O17-C14-C15	2.01	111.43	106.44

There are no chirality outliers.

All (139) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	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	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	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	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	C03-C05-O06-C07
8	A	507	C6N	C03-C05-O06-C07

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Mol	Chain	Res	Type	Atoms
8	C	508	C6N	C03-C05-O06-C07
8	B	507	C6N	C03-C05-O06-C07
8	D	506	C6N	C03-C05-O06-C07
8	C	508	C6N	O59-C56-C57-O58
8	B	507	C6N	O59-C56-C57-O58
8	E	507	C6N	O59-C56-C57-O58
8	C	508	C6N	O01-C02-C03-O04
8	D	506	C6N	O01-C02-C03-O04
8	A	507	C6N	O59-C56-C57-O58
8	D	506	C6N	O59-C56-C57-O58
8	E	507	C6N	O01-C02-C03-O04
8	A	507	C6N	O01-C02-C03-O04
8	B	507	C6N	O01-C02-C03-O04
8	E	507	C6N	O04-C22-O23-C24
8	A	507	C6N	O04-C22-O23-C24
8	C	508	C6N	O04-C22-O23-C24
8	B	507	C6N	O04-C22-O23-C24
8	D	506	C6N	O04-C22-O23-C24
8	B	507	C6N	O01-C02-C03-C05
8	E	507	C6N	O01-C02-C03-C05
8	A	507	C6N	O01-C02-C03-C05
8	E	507	C6N	C25-C26-C27-C28
8	A	507	C6N	C25-C26-C27-C28
8	D	506	C6N	C25-C26-C27-C28
8	A	507	C6N	C43-C56-C57-O58
8	C	508	C6N	O01-C02-C03-C05
8	D	506	C6N	O01-C02-C03-C05
8	D	506	C6N	C43-C56-C57-O58
8	E	507	C6N	C20-C22-O23-C24
8	A	507	C6N	C20-C22-O23-C24
8	C	508	C6N	C20-C22-O23-C24
8	B	507	C6N	C20-C22-O23-C24
8	D	506	C6N	C20-C22-O23-C24
8	B	507	C6N	C43-C56-C57-O58
8	C	508	C6N	C25-C26-C27-C28
8	B	507	C6N	C25-C26-C27-C28
8	E	507	C6N	C43-C56-C57-O58
8	C	508	C6N	C43-C56-C57-O58
8	E	507	C6N	C61-C62-C63-C64
8	C	508	C6N	C61-C62-C63-C64
8	B	507	C6N	C61-C62-C63-C64
8	E	507	C6N	C26-C27-C28-C29

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

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

There are no ring outliers.

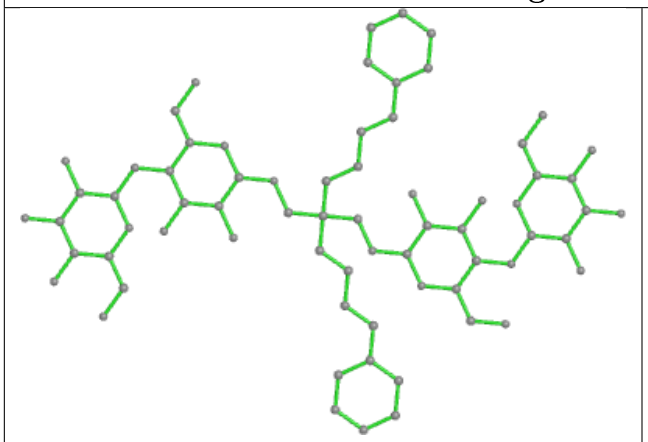
10 monomers are involved in 12 short contacts:

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

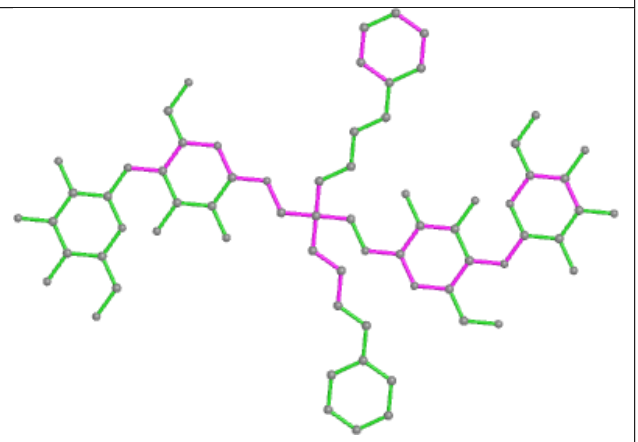
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

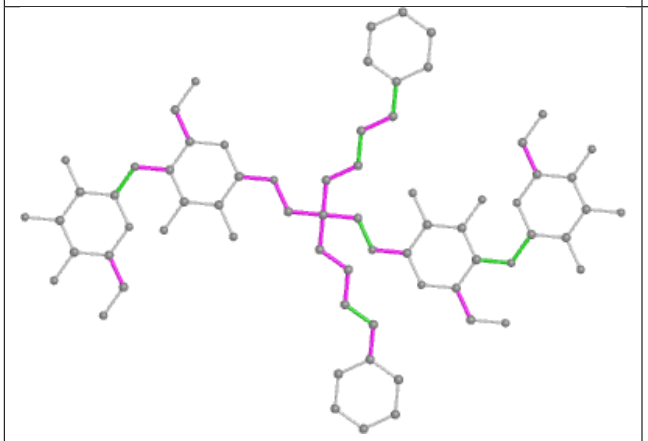
Ligand C6N E 507



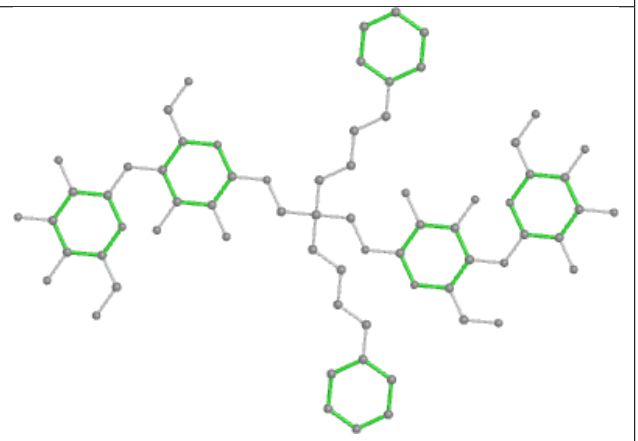
Bond lengths



Bond angles

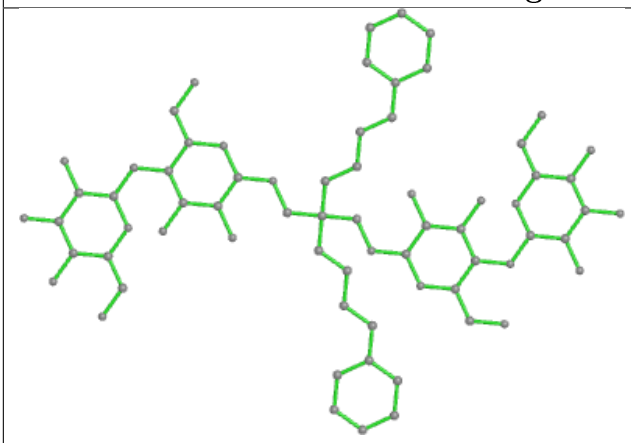


Torsions

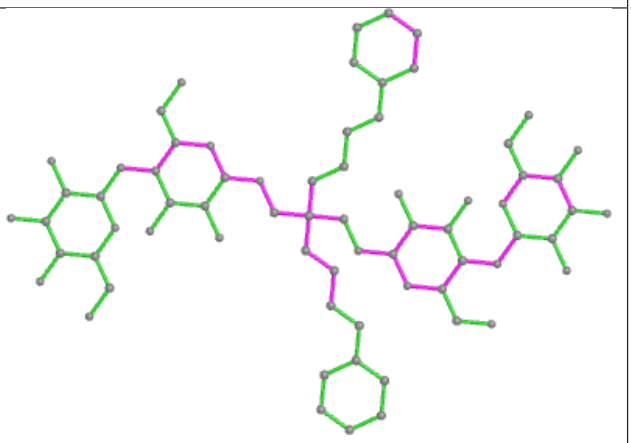


Rings

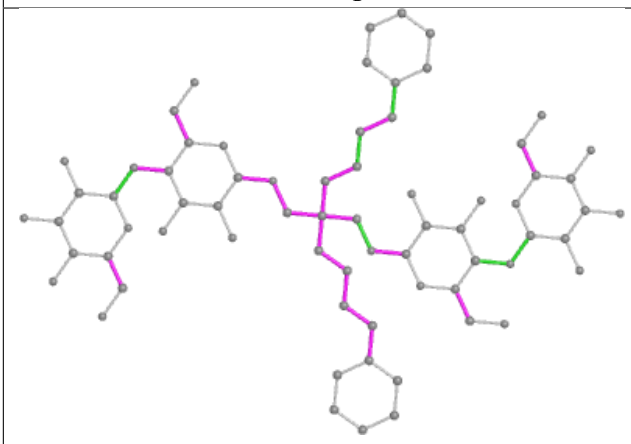
Ligand C6N A 507



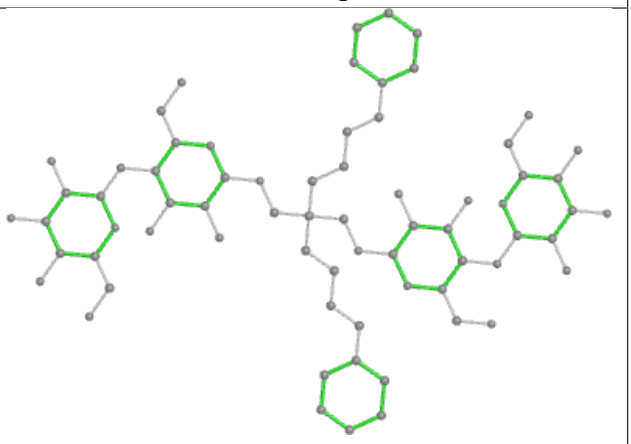
Bond lengths



Bond angles

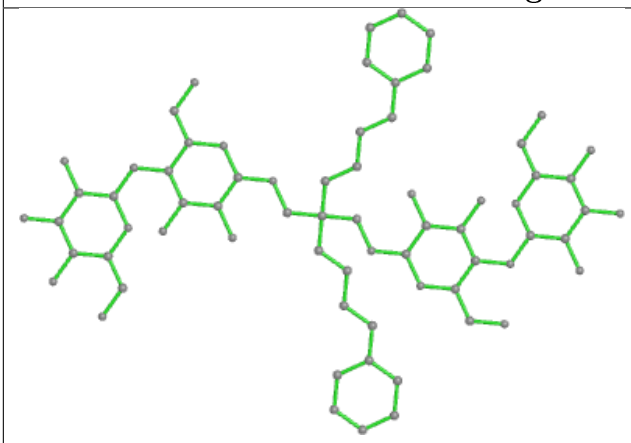


Torsions

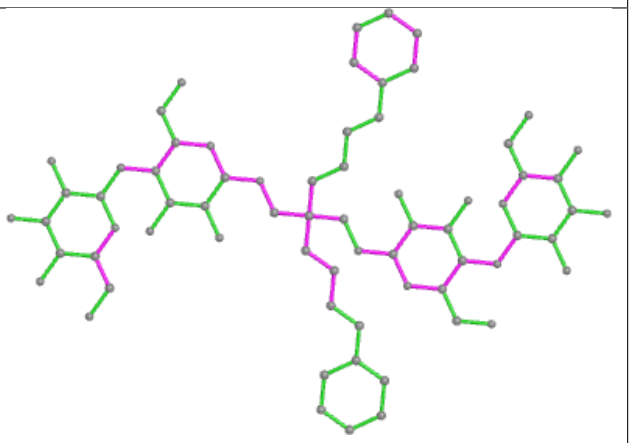


Rings

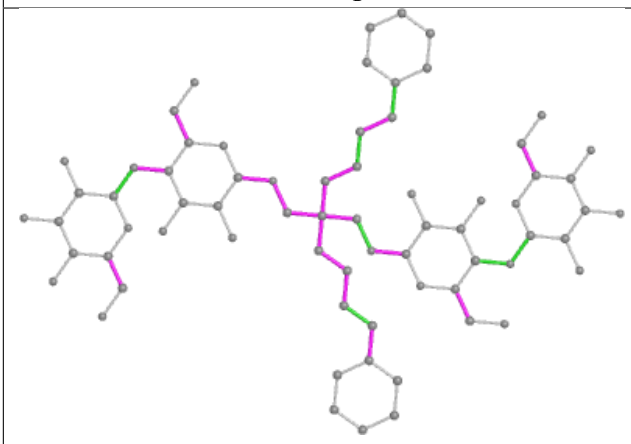
Ligand C6N C 508



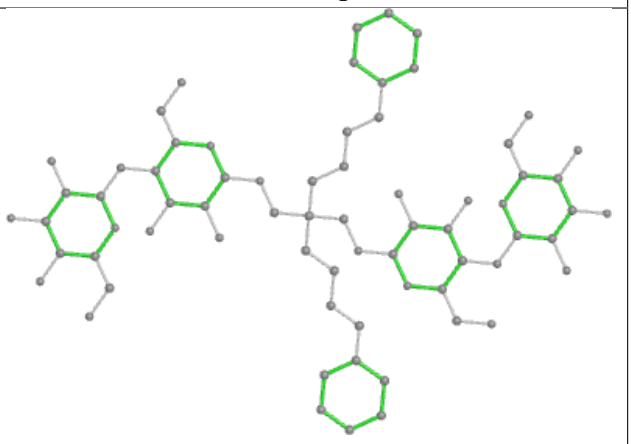
Bond lengths



Bond angles

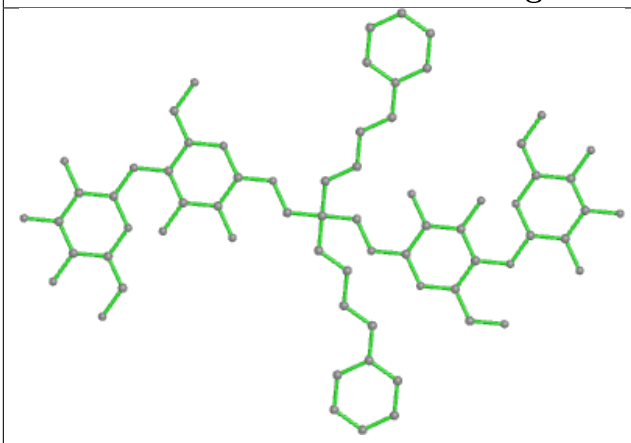


Torsions

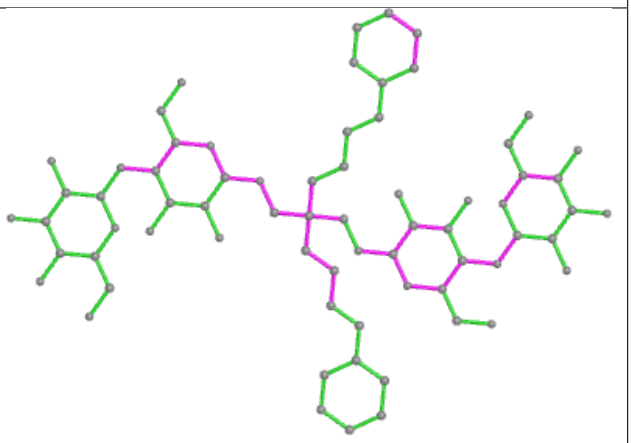


Rings

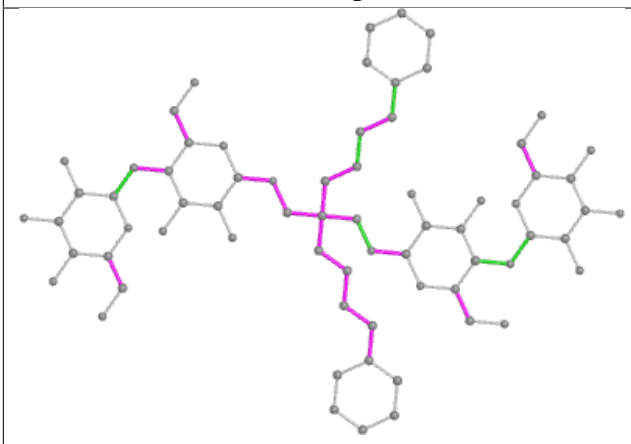
Ligand C6N D 506



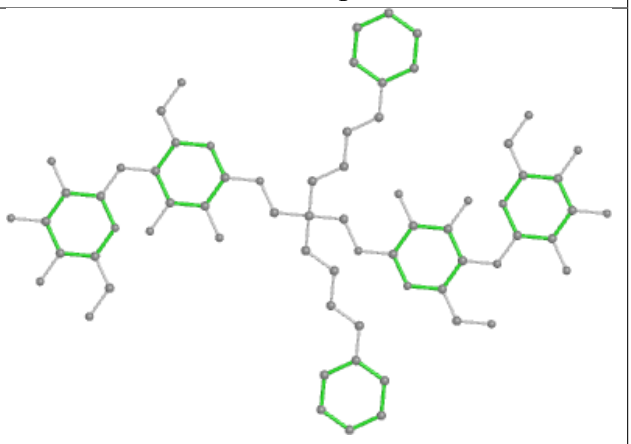
Bond lengths



Bond angles

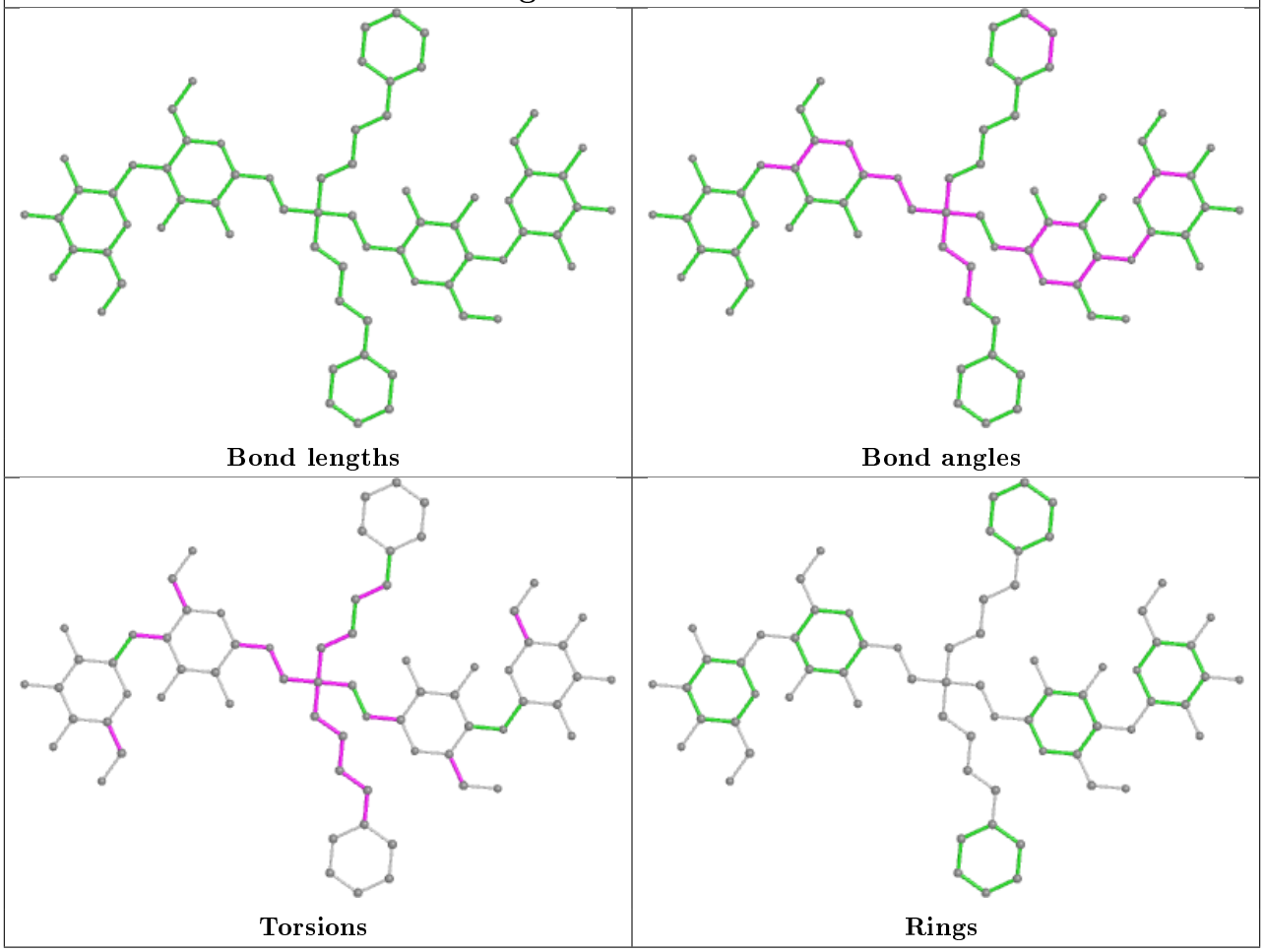


Torsions



Rings

Ligand C6N B 507



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.04	2 (0%) 91 90	45, 69, 98, 187	0
1	B	366/409 (89%)	0.11	1 (0%) 94 94	47, 71, 100, 171	0
1	C	366/409 (89%)	0.14	3 (0%) 86 85	44, 69, 94, 174	0
1	D	366/409 (89%)	0.02	1 (0%) 94 94	44, 64, 94, 193	0
1	E	366/409 (89%)	0.09	3 (0%) 86 85	42, 66, 99, 170	0
2	F	212/212 (100%)	0.27	10 (4%) 31 27	73, 115, 148, 168	0
2	H	212/212 (100%)	0.33	11 (5%) 27 22	72, 106, 141, 164	0
2	J	212/212 (100%)	3.19	104 (49%) 0 0	75, 190, 288, 332	0
2	L	212/212 (100%)	0.36	16 (7%) 14 10	59, 98, 132, 142	0
2	N	212/212 (100%)	1.59	67 (31%) 0 0	67, 148, 256, 333	0
3	G	211/217 (97%)	0.70	36 (17%) 1 1	62, 119, 165, 200	0
3	I	211/217 (97%)	0.15	6 (2%) 53 48	70, 106, 151, 172	0
3	K	211/217 (97%)	2.10	79 (37%) 0 0	74, 160, 283, 318	0
3	M	211/217 (97%)	0.13	4 (1%) 66 64	55, 96, 157, 181	0
3	O	211/217 (97%)	1.70	62 (29%) 0 0	58, 120, 269, 333	0
All	All	3945/4190 (94%)	0.60	405 (10%) 6 4	42, 88, 228, 333	0

All (405) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	166	VAL	20.7
3	O	143	CYS	19.1
2	J	146	VAL	16.1
2	J	153	SER	15.4
2	J	148	TRP	15.1
2	J	194	CYS	14.3
2	J	181	LEU	14.2

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Mol	Chain	Res	Type	RSRZ
2	J	200	THR	13.4
3	O	182	SER	13.4
3	O	144	LEU	13.1
2	J	193	THR	13.0
2	J	150	ILE	12.7
2	J	115	VAL	12.6
3	K	200	VAL	12.4
2	J	145	ASN	12.0
3	K	141	LEU	11.6
3	O	129	PRO	11.6
2	N	155	ARG	11.5
3	O	155	VAL	11.2
2	J	152	GLY	11.2
2	J	155	ARG	11.0
3	K	155	VAL	10.6
2	J	197	THR	10.5
3	O	165	GLY	10.5
3	O	156	THR	10.4
3	O	124	VAL	10.4
2	J	136	LEU	10.3
3	O	184	VAL	10.1
3	K	201	ALA	10.1
2	J	196	ALA	9.9
3	K	184	VAL	9.5
2	J	156	GLN	9.5
2	J	154	GLU	9.4
3	K	182	SER	9.3
2	N	113	PRO	9.2
3	K	183	SER	9.1
3	K	143	CYS	9.0
2	J	135	PHE	8.6
2	J	132	VAL	8.6
2	N	146	VAL	8.6
2	J	192	TYR	8.6
3	O	166	VAL	8.5
2	J	114	THR	8.5
2	J	177	SER	8.4
3	O	185	THR	8.4
2	J	175	MET	8.4
2	J	113	PRO	8.3
2	J	149	LYS	8.2
3	O	141	LEU	8.2

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Mol	Chain	Res	Type	RSRZ
2	J	201	SER	8.2
3	K	204	ALA	8.0
3	K	168	THR	7.9
2	J	206	VAL	7.8
2	J	186	TYR	7.7
2	J	205	ILE	7.7
3	O	147	GLY	7.7
2	J	151	ASP	7.6
2	J	134	CYS	7.5
2	J	133	VAL	7.5
3	K	139	VAL	7.5
3	O	168	THR	7.4
3	K	144	LEU	7.3
2	N	181	LEU	7.3
3	O	125	TYR	7.2
3	K	186	VAL	7.2
3	K	209	VAL	7.2
2	J	180	THR	7.0
2	J	204	PRO	7.0
3	O	186	VAL	6.9
3	K	156	THR	6.9
2	N	197	THR	6.9
2	N	186	TYR	6.8
2	N	114	THR	6.8
2	J	144	ILE	6.6
2	J	199	LYS	6.6
3	K	165	GLY	6.6
3	O	169	PHE	6.5
3	O	167	HIS	6.5
2	J	112	ALA	6.4
2	J	182	THR	6.4
3	O	187	PRO	6.3
3	K	140	THR	6.3
3	O	198	CYS	6.3
2	J	187	GLU	6.2
2	N	156	GLN	6.2
3	O	145	VAL	6.2
2	J	179	LEU	6.2
2	N	154	GLU	6.1
3	K	214	VAL	6.0
3	G	143	CYS	6.0
2	N	135	PHE	6.0

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Mol	Chain	Res	Type	RSRZ
3	K	164	SER	6.0
3	K	124	VAL	6.0
3	O	200	VAL	5.9
3	O	123	SER	5.9
2	N	137	ASN	5.9
3	K	154	THR	5.8
2	J	147	LYS	5.8
2	N	198	HIS	5.8
2	N	161	ASN	5.8
3	O	183	SER	5.8
3	K	159	SER	5.7
3	K	213	ILE	5.7
2	J	207	LYS	5.7
3	O	163	SER	5.7
2	J	159	VAL	5.6
2	J	19	VAL	5.6
3	O	181	SER	5.5
2	N	136	LEU	5.5
2	J	117	ILE	5.5
2	N	145	ASN	5.5
2	J	137	ASN	5.5
3	O	214	VAL	5.5
2	N	153	SER	5.4
2	L	205	ILE	5.4
3	K	163	SER	5.4
3	O	157	TRP	5.4
3	K	123	SER	5.3
2	J	75	ILE	5.3
2	N	112	ALA	5.3
2	N	202	THR	5.2
3	K	153	VAL	5.2
3	O	159	SER	5.2
3	O	213	ILE	5.2
2	N	179	LEU	5.2
2	N	177	SER	5.1
2	J	157	ASN	5.1
2	J	208	SER	5.1
2	J	120	PRO	5.1
3	K	158	ASN	5.1
2	N	185	GLU	5.1
2	N	150	ILE	5.0
2	J	131	SER	5.0

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Mol	Chain	Res	Type	RSRZ
3	K	157	TRP	5.0
3	K	208	LYS	4.9
2	J	203	SER	4.9
3	O	139	VAL	4.9
2	L	197	THR	4.9
2	N	182	THR	4.8
2	N	148	TRP	4.8
3	O	128	ALA	4.7
3	K	167	HIS	4.7
3	K	207	THR	4.7
2	N	205	ILE	4.6
2	J	161	ASN	4.6
3	K	129	PRO	4.6
2	N	196	ALA	4.6
3	K	205	SER	4.6
2	N	134	CYS	4.6
1	A	367	SER	4.6
3	K	198	CYS	4.6
2	N	130	ALA	4.6
2	J	191	SER	4.5
2	J	209	PHE	4.5
2	N	184	ASP	4.5
3	G	210	ASP	4.5
3	K	15	GLY	4.5
2	J	130	ALA	4.4
2	J	184	ASP	4.4
3	O	158	ASN	4.4
2	N	144	ILE	4.4
3	O	164	SER	4.4
3	O	142	GLY	4.4
2	N	200	THR	4.4
3	O	161	SER	4.4
3	O	217	ASP	4.3
2	J	178	THR	4.3
2	N	120	PRO	4.3
2	N	138	ASN	4.2
3	O	160	GLY	4.2
2	J	189	HIS	4.2
2	J	195	GLU	4.2
2	J	73	LEU	4.2
2	N	175	MET	4.2
3	K	160	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
2	L	196	ALA	4.2
3	G	200	VAL	4.1
3	K	206	SER	4.1
2	N	111	ALA	4.1
3	G	144	LEU	4.1
2	N	173	TYR	4.1
3	K	83	LEU	4.1
2	J	138	ASN	4.0
2	J	190	ASN	4.0
2	J	198	HIS	4.0
2	N	199	LYS	4.0
3	K	18	VAL	4.0
2	N	140	TYR	4.0
3	O	162	LEU	3.9
3	O	195	THR	3.9
3	G	213	ILE	3.9
3	O	180	LEU	3.9
2	N	188	ARG	3.8
3	G	209	VAL	3.8
2	N	201	SER	3.8
3	K	199	ASN	3.8
3	K	114	VAL	3.8
2	J	185	GLU	3.8
3	O	189	SER	3.8
3	K	185	THR	3.8
2	H	150	ILE	3.8
3	O	191	TRP	3.8
2	J	158	GLY	3.8
2	J	62	PHE	3.8
2	N	115	VAL	3.8
3	O	209	VAL	3.8
2	J	63	SER	3.7
3	K	181	SER	3.7
2	J	58	VAL	3.7
3	K	195	THR	3.7
3	K	136	ASN	3.7
3	G	141	LEU	3.7
3	K	162	LEU	3.7
3	I	186	VAL	3.7
2	H	148	TRP	3.7
2	N	203	SER	3.7
3	K	142	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
3	K	210	ASP	3.6
2	N	139	PHE	3.5
3	O	138	MET	3.5
2	J	12	SER	3.5
3	K	169	PHE	3.5
3	K	17	SER	3.4
2	J	202	THR	3.4
2	J	20	THR	3.4
2	L	200	THR	3.4
2	N	194	CYS	3.4
2	H	197	THR	3.3
3	G	160	GLY	3.3
2	N	147	LYS	3.3
3	G	186	VAL	3.3
2	L	203	SER	3.3
3	K	202	HIS	3.3
3	K	128	ALA	3.3
2	H	155	ARG	3.2
2	J	18	THR	3.2
2	N	178	THR	3.2
2	N	24	ARG	3.2
3	K	116	SER	3.2
3	K	196	VAL	3.2
3	K	122	PRO	3.2
3	O	215	PRO	3.2
3	G	155	VAL	3.1
2	J	119	PRO	3.1
2	J	37	GLN	3.1
3	I	159	SER	3.1
3	O	199	ASN	3.1
2	J	21	ILE	3.1
2	J	116	SER	3.1
3	G	163	SER	3.1
3	K	145	VAL	3.1
3	K	187	PRO	3.1
2	J	86	TYR	3.1
3	G	161	SER	3.0
3	K	85	SER	3.0
2	F	13	ALA	3.0
2	N	187	GLU	3.0
2	J	143	ASP	3.0
3	K	14	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
2	N	189	HIS	3.0
2	L	146	VAL	3.0
3	G	157	TRP	3.0
3	O	126	PRO	3.0
3	K	188	SER	3.0
3	K	203	PRO	2.9
2	J	173	TYR	2.9
2	J	212	ASN	2.9
2	L	155	ARG	2.9
2	J	11	LEU	2.9
3	G	182	SER	2.9
2	J	76	ASN	2.9
3	I	209	VAL	2.9
1	E	135	CYS	2.9
3	K	84	SER	2.9
3	G	166	VAL	2.9
3	G	83	LEU	2.9
2	L	187	GLU	2.9
3	K	161	SER	2.8
2	J	5	THR	2.8
2	L	198	HIS	2.8
3	G	124	VAL	2.8
3	G	145	VAL	2.8
3	G	189	SER	2.8
2	H	196	ALA	2.8
2	N	119	PRO	2.8
2	L	145	ASN	2.8
2	N	143	ASP	2.8
2	J	104	LEU	2.8
3	O	211	LYS	2.8
2	N	152	GLY	2.8
2	J	188	ARG	2.7
3	O	193	SER	2.7
2	J	111	ALA	2.7
2	J	1	ASP	2.7
2	N	160	LEU	2.7
3	O	192	PRO	2.7
3	G	139	VAL	2.7
3	G	125	TYR	2.7
3	G	162	LEU	2.7
2	J	57	GLY	2.7
2	N	170	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
3	O	153	VAL	2.7
2	N	192	TYR	2.7
3	G	122	PRO	2.7
2	J	100	GLY	2.7
2	J	129	GLY	2.7
2	N	157	ASN	2.7
2	N	180	THR	2.7
2	N	128	GLY	2.7
2	N	133	VAL	2.6
3	G	190	SER	2.6
2	N	75	ILE	2.6
3	O	196	VAL	2.6
1	E	272	PHE	2.6
3	M	139	VAL	2.6
1	D	272	PHE	2.6
3	G	201	ALA	2.6
3	K	215	PRO	2.6
3	K	190	SER	2.6
2	L	136	LEU	2.5
3	G	188	SER	2.5
2	J	74	LYS	2.5
3	G	142	GLY	2.5
2	L	206	VAL	2.5
2	F	123	GLU	2.5
3	K	138	MET	2.5
3	O	179	THR	2.5
3	G	123	SER	2.5
2	J	210	ASN	2.5
3	G	154	THR	2.5
2	J	61	ARG	2.5
2	J	99	GLY	2.5
1	B	272	PHE	2.4
3	G	187	PRO	2.4
2	F	127	SER	2.4
2	N	108	ARG	2.4
2	H	19	VAL	2.4
3	K	112	LEU	2.4
3	K	115	SER	2.4
2	N	168	SER	2.4
2	J	83	PHE	2.4
3	K	121	PRO	2.4
3	M	165	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	40	GLN	2.4
3	O	206	SER	2.4
2	H	146	VAL	2.4
3	K	94	TYR	2.4
3	K	120	THR	2.4
3	O	204	ALA	2.4
3	K	216	ARG	2.4
2	N	1	ASP	2.3
2	N	110	ASP	2.3
3	K	217	ASP	2.3
3	G	60	LEU	2.3
2	F	19	VAL	2.3
3	O	205	SER	2.3
3	G	147	GLY	2.3
3	O	60	LEU	2.3
2	J	211	ARG	2.3
3	I	114	VAL	2.3
3	G	86	LEU	2.3
3	O	212	LYS	2.3
2	H	136	LEU	2.3
2	F	157	ASN	2.3
2	N	127	SER	2.2
3	I	85	SER	2.2
3	K	197	THR	2.2
2	F	76	ASN	2.2
2	F	202	THR	2.2
3	O	154	THR	2.2
2	F	156	GLN	2.2
3	K	13	ARG	2.2
3	G	64	PHE	2.2
2	F	136	LEU	2.2
1	A	2	THR	2.2
2	J	64	GLY	2.2
3	K	146	LYS	2.2
2	L	154	GLU	2.2
2	N	183	LYS	2.2
3	G	214	VAL	2.2
2	L	209	PHE	2.1
2	H	205	ILE	2.1
3	G	136	ASN	2.1
1	E	198	GLU	2.1
3	O	190	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	82	ASP	2.1
3	M	164	SER	2.1
2	F	20	THR	2.1
2	J	160	LEU	2.1
2	H	152	GLY	2.1
3	O	85	SER	2.1
2	J	78	LEU	2.1
2	J	84	GLY	2.1
3	M	201	ALA	2.1
2	J	4	MET	2.1
3	K	147	GLY	2.1
2	L	201	SER	2.1
1	C	77	PRO	2.1
1	C	198	GLU	2.1
3	K	191	TRP	2.1
2	L	186	TYR	2.0
2	N	126	THR	2.0
3	I	155	VAL	2.0
1	C	123	LEU	2.0
2	J	183	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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, 95^{th} 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	C	505	1/1	0.51	0.51	111,111,111,111	0
5	CL	B	505	1/1	0.54	0.63	128,128,128,128	0
5	CL	D	503	1/1	0.59	0.46	124,124,124,124	0

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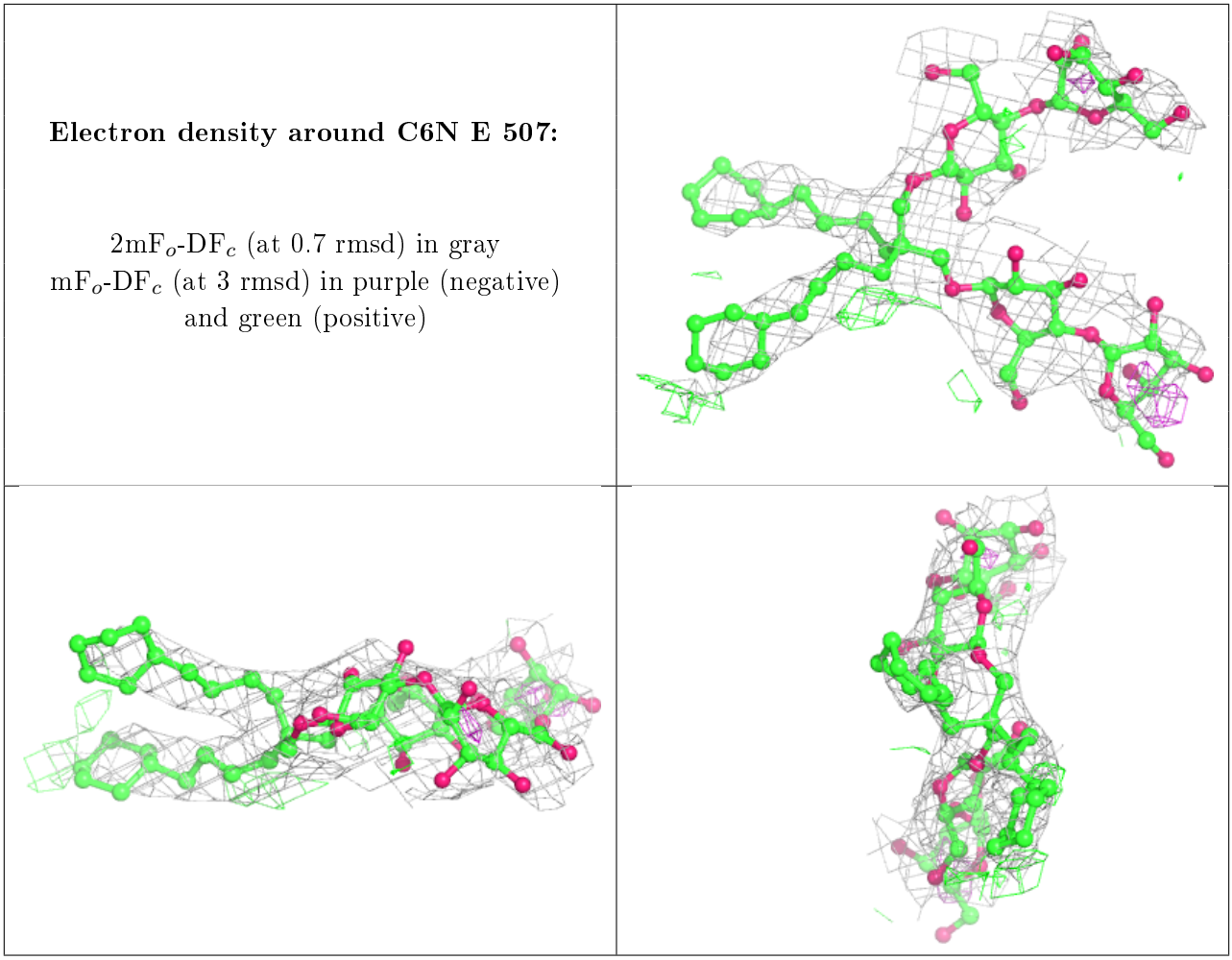
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	D	505	1/1	0.60	0.58	110,110,110,110	0
5	CL	E	505	1/1	0.65	0.36	101,101,101,101	0
5	CL	C	503	1/1	0.69	0.42	109,109,109,109	0
5	CL	A	505	1/1	0.72	0.40	112,112,112,112	0
8	C6N	E	507	69/69	0.76	0.34	113,142,162,166	0
5	CL	B	503	1/1	0.81	0.80	110,110,110,110	0
8	C6N	D	506	69/69	0.81	0.26	97,125,145,148	0
4	GOL	D	501	6/6	0.82	0.41	81,87,97,102	0
8	C6N	A	507	69/69	0.82	0.31	107,137,158,162	0
5	CL	E	503	1/1	0.83	0.31	128,128,128,128	0
8	C6N	B	507	69/69	0.83	0.38	116,145,167,171	0
4	GOL	C	501	6/6	0.84	0.40	95,99,110,116	0
4	GOL	E	501	6/6	0.84	0.36	78,82,93,98	0
8	C6N	C	508	69/69	0.84	0.33	105,132,154,158	0
4	GOL	B	501	6/6	0.85	0.35	100,107,116,122	0
5	CL	A	503	1/1	0.88	0.36	105,105,105,105	0
4	GOL	A	501	6/6	0.88	0.37	104,108,118,123	0
7	K	A	506	1/1	0.90	0.19	87,87,87,87	0
7	K	C	507	1/1	0.92	0.18	86,86,86,86	0
7	K	C	506	1/1	0.94	0.17	88,88,88,88	0
7	K	E	506	1/1	0.94	0.14	79,79,79,79	0
7	K	B	506	1/1	0.95	0.14	88,88,88,88	0
5	CL	E	504	1/1	0.96	0.07	65,65,65,65	0
5	CL	B	504	1/1	0.96	0.21	69,69,69,69	0
6	CA	E	502	1/1	0.98	0.17	54,54,54,54	0
5	CL	D	504	1/1	0.98	0.12	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	0.98	0.16	64,64,64,64	0
5	CL	A	502	1/1	0.99	0.14	67,67,67,67	0
6	CA	B	502	1/1	0.99	0.21	62,62,62,62	0
6	CA	A	504	1/1	0.99	0.19	59,59,59,59	0
6	CA	D	502	1/1	0.99	0.17	52,52,52,52	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.

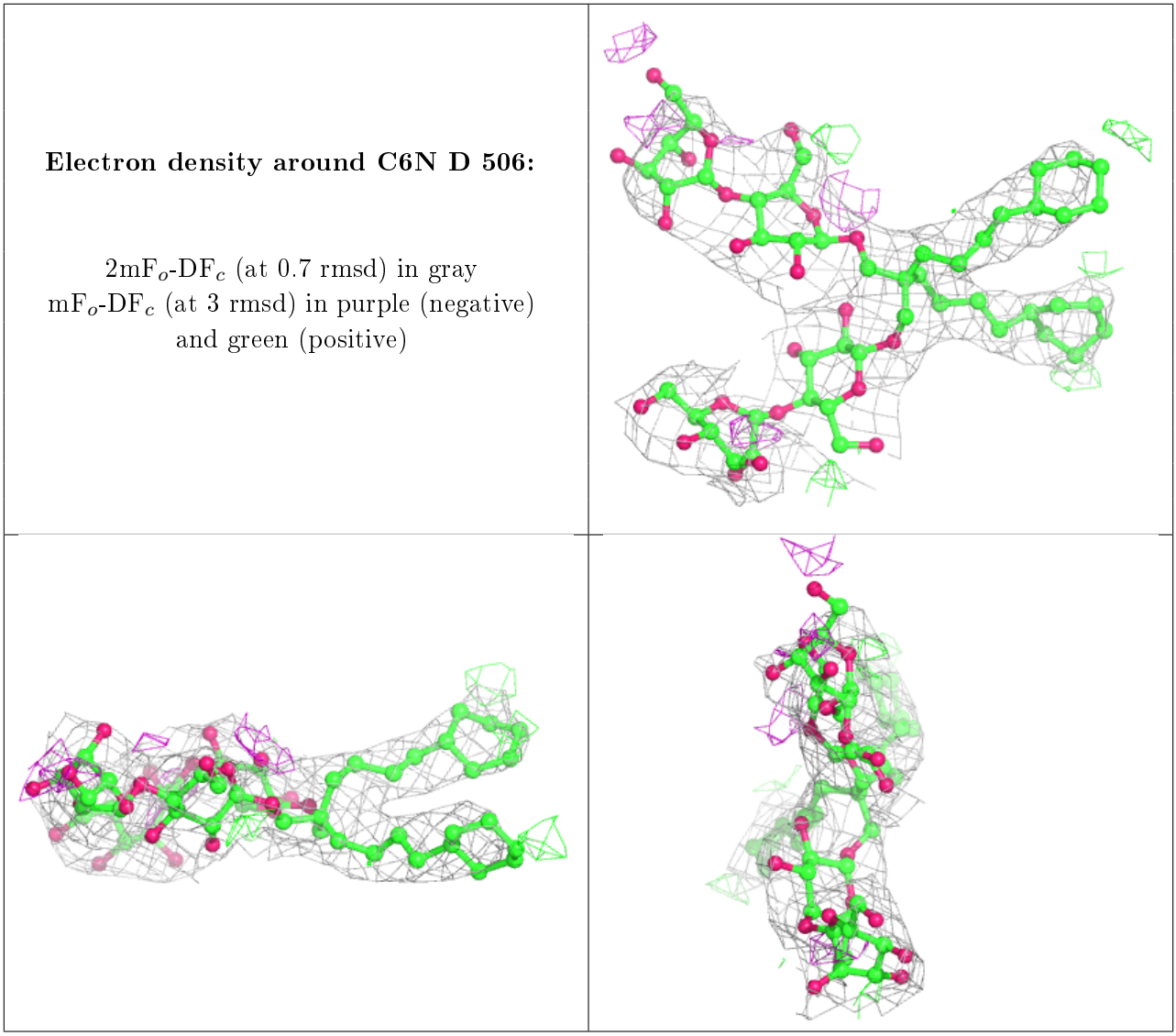
Electron density around C6N E 507:

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



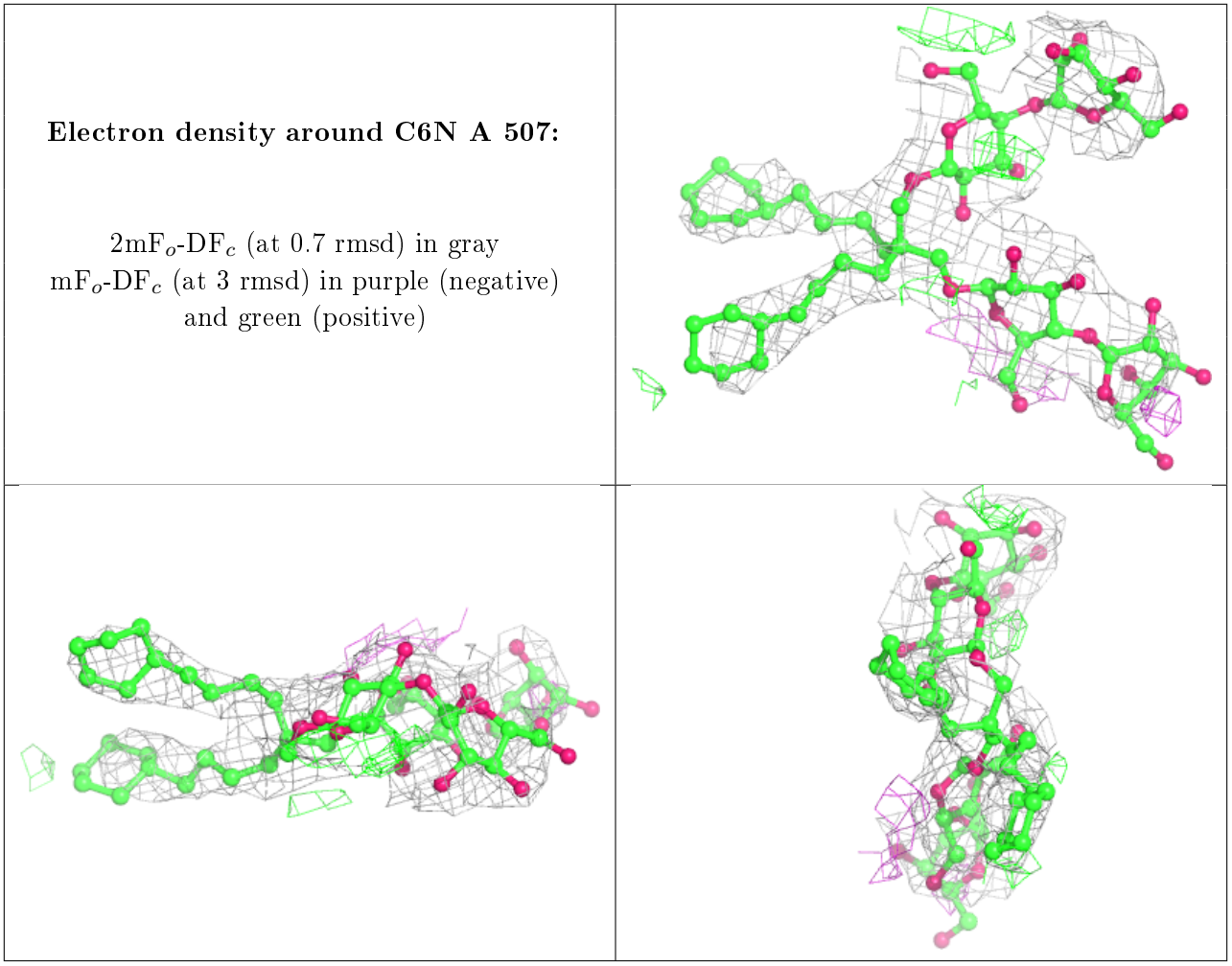
Electron density around C6N D 506:

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



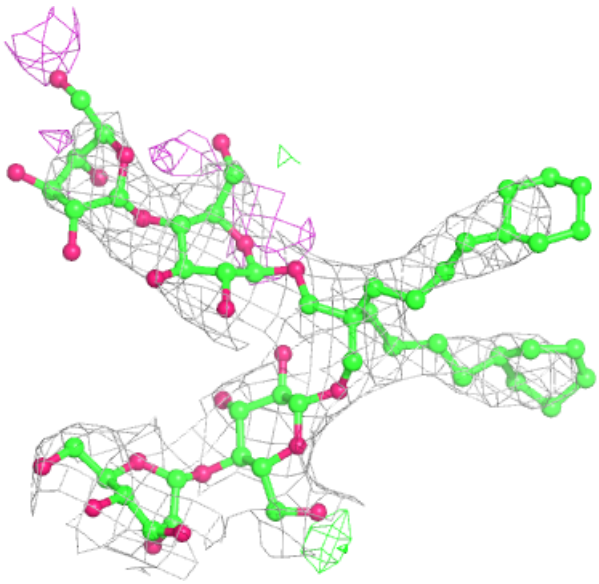
Electron density around C6N A 507:

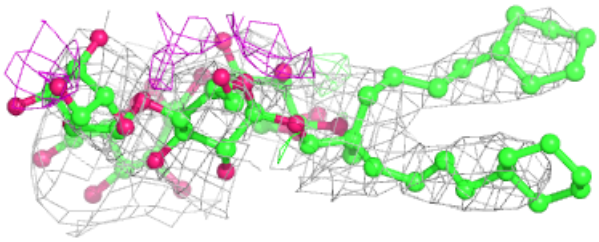
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

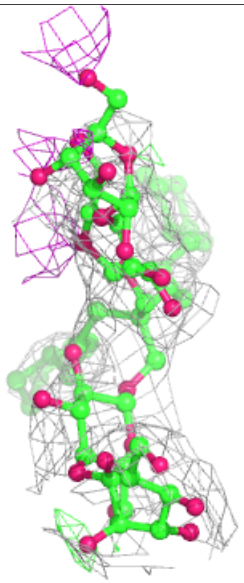


Electron density around C6N B 507:

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

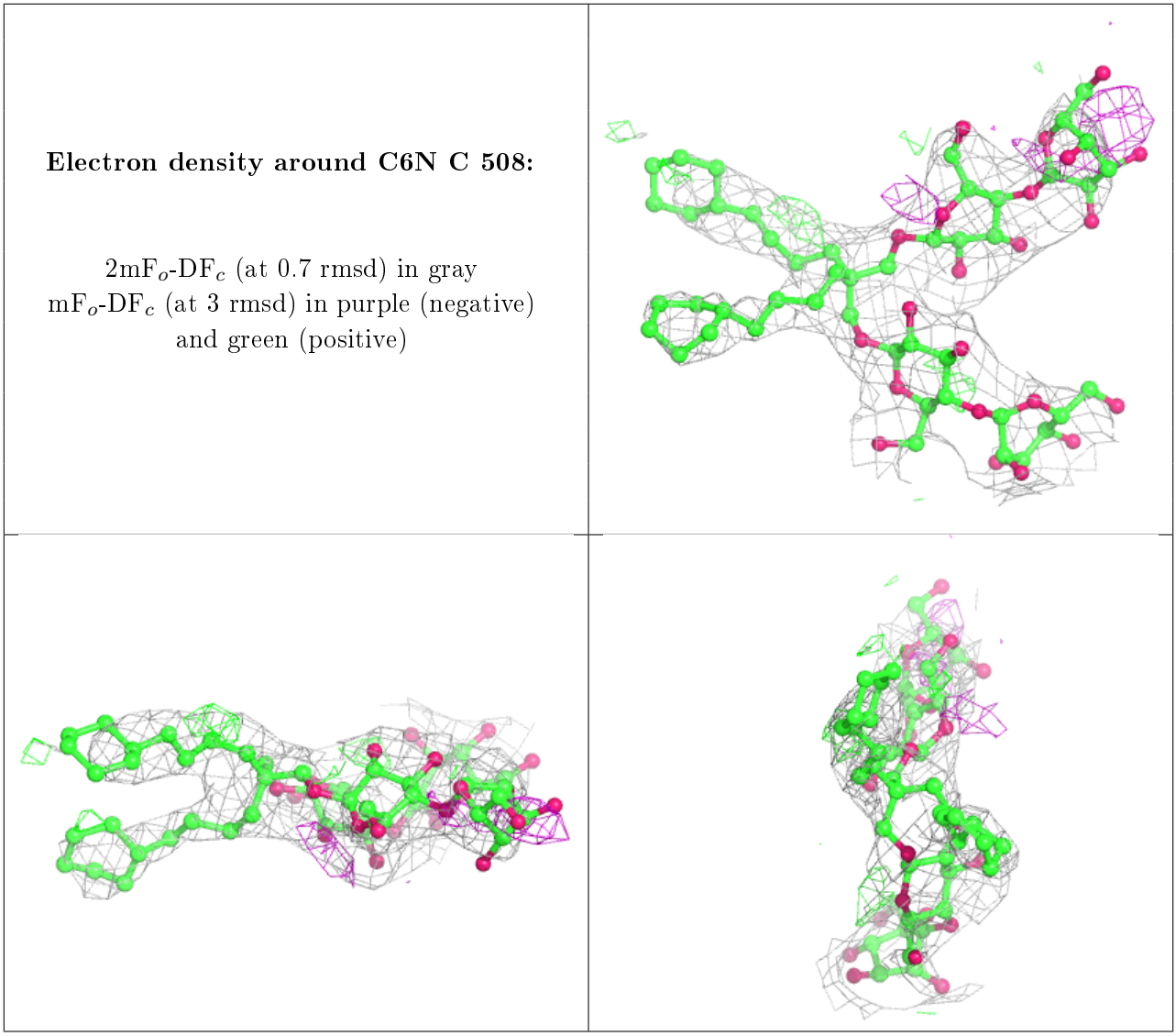






Electron density around C6N C 508:

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



6.5 Other polymers (i)

There are no such residues in this entry.