Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 01:20 AM EDT

PDB ID	:	5VXZ
Title	:	High-affinity AXL decoy receptor
Authors	:	Mathrews, I.I.; Kapur, S.; Kariolis, M.S.; Cochran, J.R.
Deposited on	:	2017-05-24
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

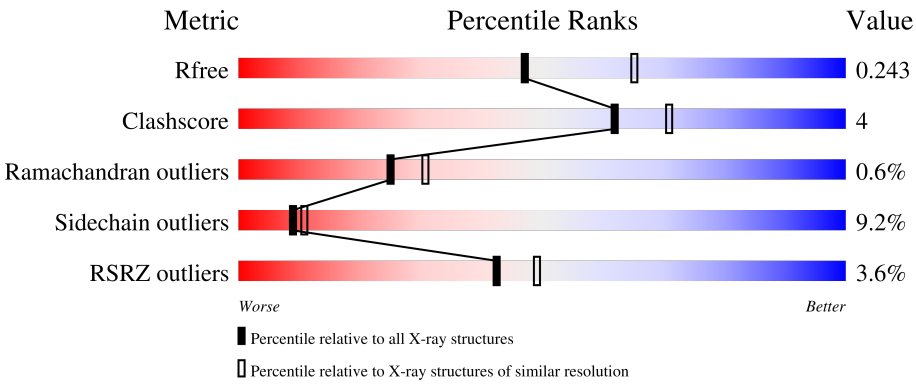
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	395	3% 80% 13% • 5%
1	B	395	2% 80% 12% • • 5%
2	C	102	10% 81% 16% •
2	D	102	6% 76% 20% •
3	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7703 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 Growth arrest-specific protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	376	2932	1868	515	535	14	0	0	0
1	B	376	2932	1868	515	535	14	0	0	0

- Molecule 2 is a protein called Tyrosine-protein kinase receptor UFO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	102	792	496	138	156	2	0	0	0
2	D	102	792	496	138	156	2	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	32	SER	GLY	engineered mutation	UNP P30530
C	72	VAL	ALA	engineered mutation	UNP P30530
C	87	GLY	ASP	engineered mutation	UNP P30530
C	92	ALA	VAL	engineered mutation	UNP P30530
C	127	ARG	GLY	engineered mutation	UNP P30530
D	32	SER	GLY	engineered mutation	UNP P30530
D	72	VAL	ALA	engineered mutation	UNP P30530
D	87	GLY	ASP	engineered mutation	UNP P30530
D	92	ALA	VAL	engineered mutation	UNP P30530
D	127	ARG	GLY	engineered mutation	UNP P30530

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	2	28	16	2	10	0	0	0
3	F	2	28	16	2	10	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	1	1	0	0
4	B	1	1	1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	1	1	1	0	0
5	B	1	2	2	0	1

- Molecule 6 is water.

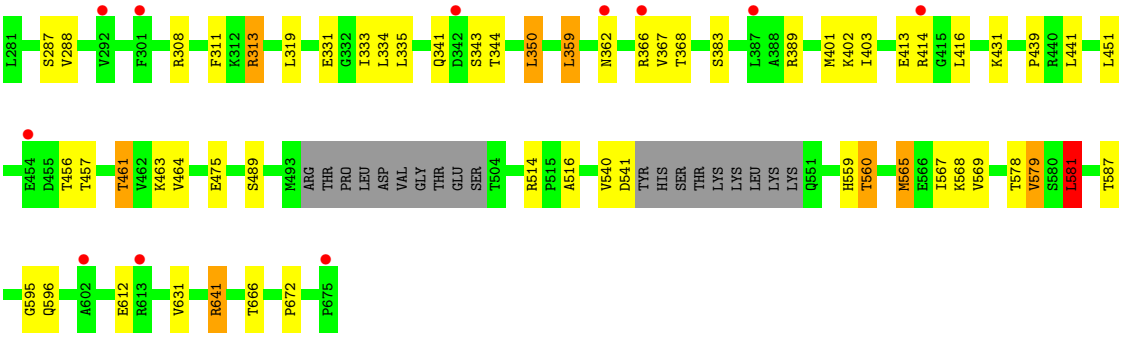
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	26	26	26	0	0
6	B	135	138	138	0	3
6	C	11	12	12	0	1
6	D	17	18	18	0	1

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.

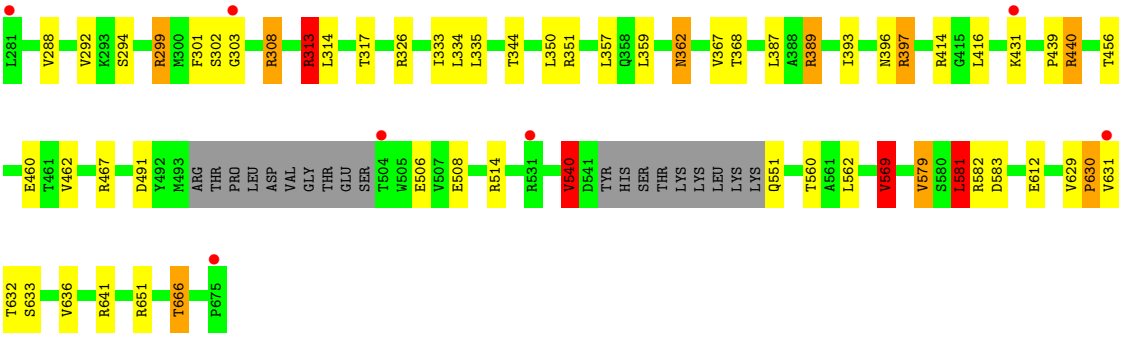
• Molecule 1: Growth arrest-specific protein 6

Chain A:



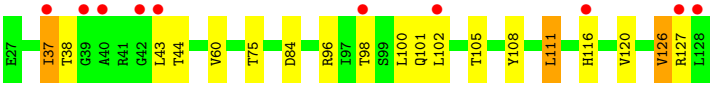
• Molecule 1: Growth arrest-specific protein 6

Chain B:



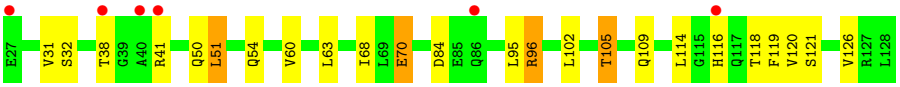
• Molecule 2: Tyrosine-protein kinase receptor UFO

Chain C:



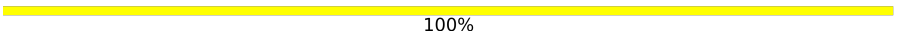
• Molecule 2: Tyrosine-protein kinase receptor UFO

Chain D:



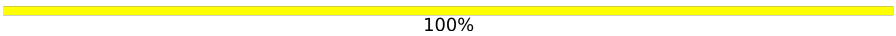
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.22Å 80.47Å 249.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.61 – 2.30 38.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.61-2.30) 99.6 (38.61-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.198 , 0.247 0.200 , 0.243	Depositor DCC
R_{free} test set	3492 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	52.8	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7703	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CA, NAG

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	0.76	0/2996	0.90	6/4077 (0.1%)
1	B	1.09	4/2996 (0.1%)	1.33	25/4077 (0.6%)
2	C	0.74	0/808	0.88	0/1102
2	D	0.96	0/808	1.03	2/1102 (0.2%)
All	All	0.92	4/7608 (0.1%)	1.10	33/10358 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	ARG	CD-NE	-6.28	1.35	1.46
1	B	301	PHE	C-O	5.70	1.34	1.23
1	B	303	GLY	N-CA	5.46	1.54	1.46
1	B	303	GLY	C-O	5.04	1.31	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	299	ARG	NE-CZ-NH2	-22.46	109.07	120.30
1	B	440	ARG	NE-CZ-NH2	-20.57	110.02	120.30
1	B	440	ARG	NE-CZ-NH1	17.14	128.87	120.30
1	B	308	ARG	NE-CZ-NH2	-14.54	113.03	120.30
1	B	308	ARG	NE-CZ-NH1	13.39	127.00	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	299	ARG	NE-CZ-NH1	12.43	126.52	120.30
1	B	581	LEU	CA-CB-CG	9.86	137.97	115.30
1	B	641	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	B	313	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	B	440	ARG	CD-NE-CZ	7.86	134.60	123.60
1	B	641	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	308	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	B	540	VAL	CB-CA-C	-7.48	97.19	111.40
1	A	308	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	299	ARG	CD-NE-CZ	6.66	132.93	123.60
1	B	389	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	491	ASP	CB-CG-OD1	6.50	124.16	118.30
1	B	440	ARG	CG-CD-NE	-6.43	98.30	111.80
1	B	313	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	514	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	514	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	B	351	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	B	326	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	299	ARG	CG-CD-NE	-5.74	99.76	111.80
1	B	569	VAL	CB-CA-C	-5.73	100.51	111.40
1	A	313	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	583	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	581	LEU	CA-CB-CG	5.51	127.98	115.30
2	D	96	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	313	ARG	CB-CG-CD	5.36	125.52	111.60
1	A	313	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	583	ASP	CB-CG-OD2	-5.11	113.70	118.30
2	D	50	GLN	CA-CB-CG	5.09	124.61	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	440	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2932	0	2933	21	0
1	B	2932	0	2933	28	0
2	C	792	0	767	8	0
2	D	792	0	767	11	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	2	0	0	1	0
6	A	26	0	0	1	0
6	B	138	0	0	5	0
6	C	12	0	0	0	0
6	D	18	0	0	2	0
All	All	7703	0	7450	66	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 4.

All (66) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:GLU:OE2	1:B:582:ARG:NH2	2.11	0.83
2:D:96:ARG:NH1	6:D:201:HOH:O	2.20	0.73
1:A:413:GLU:HG2	1:A:414:ARG:HG3	1.75	0.68
1:B:666:THR:CG2	6:B:833:HOH:O	2.41	0.67
1:B:396:ASN:O	1:B:397:ARG:HG3	1.99	0.62
1:B:630:PRO:HB2	1:B:632:THR:HG22	1.81	0.62
1:B:506:GLU:OE2	1:B:582:ARG:NH1	2.31	0.61
1:B:630:PRO:CB	1:B:632:THR:HG22	2.31	0.60
1:B:357:LEU:HD13	1:B:393:ILE:HD11	1.85	0.59
1:A:567:ILE:HG23	1:A:569:VAL:HG13	1.84	0.59
1:B:396:ASN:O	1:B:397:ARG:CG	2.51	0.58
1:B:299:ARG:HD3	6:B:848:HOH:O	2.04	0.57
1:B:666:THR:HG23	6:B:833:HOH:O	2.02	0.57
1:A:359:LEU:HD12	1:A:359:LEU:N	2.20	0.57
2:C:108:TYR:CE1	2:C:126:VAL:HG13	2.41	0.56
1:B:308:ARG:NH2	6:B:803:HOH:O	2.38	0.55
1:A:334:LEU:HD12	1:A:441:LEU:CD2	2.36	0.55
1:B:540:VAL:HG13	1:B:636:VAL:CG2	2.37	0.55
2:C:108:TYR:CD1	2:C:126:VAL:HG13	2.41	0.55
2:C:102:LEU:O	2:C:105:THR:HB	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ILE:HD12	1:A:439:PRO:HB3	1.91	0.53
1:B:630:PRO:C	1:B:632:THR:H	2.12	0.52
1:B:333:ILE:HD12	1:B:439:PRO:HB3	1.91	0.52
2:D:114:LEU:HD12	2:D:119:PHE:CE1	2.45	0.52
1:B:313:ARG:HG2	1:B:317:THR:OG1	2.09	0.52
1:B:456:THR:OG1	1:B:460:GLU:OE2	2.23	0.52
1:B:629:VAL:O	1:B:630:PRO:C	2.48	0.52
2:C:100:LEU:HD12	2:C:101:GLN:H	1.76	0.51
2:D:84:ASP:HA	6:D:211:HOH:O	2.11	0.51
2:D:51:LEU:N	2:D:51:LEU:HD23	2.26	0.50
2:D:63:LEU:CD2	2:D:68:ILE:HG12	2.41	0.50
1:A:559:HIS:CD2	1:A:560:THR:HG22	2.49	0.48
1:A:565:MET:HG2	1:A:595:GLY:CA	2.44	0.48
1:A:335:LEU:HD12	1:A:335:LEU:C	2.34	0.48
2:D:105:THR:HA	2:D:126:VAL:HG22	1.95	0.47
1:A:457:THR:O	1:A:461:THR:CG2	2.63	0.47
1:A:334:LEU:HD12	1:A:441:LEU:HD21	1.98	0.45
1:A:457:THR:O	1:A:461:THR:HG23	2.17	0.45
1:B:666:THR:HG22	6:B:833:HOH:O	2.11	0.45
1:A:331:GLU:HA	1:A:350:LEU:O	2.17	0.45
1:B:579:VAL:HG13	1:B:581:LEU:CD2	2.47	0.45
1:A:516:ALA:HB3	1:A:641:ARG:HB3	1.99	0.44
2:D:102:LEU:O	2:D:105:THR:HG22	2.17	0.44
1:A:540:VAL:HG22	1:A:541:ASP:N	2.33	0.44
1:B:334:LEU:HD11	1:B:350:LEU:HD13	1.99	0.44
2:C:44:THR:HB	2:C:98:THR:O	2.18	0.43
1:B:335:LEU:HD12	1:B:335:LEU:C	2.39	0.43
1:B:414:ARG:HD3	2:D:70:GLU:OE2	2.18	0.43
2:C:37:ILE:O	2:C:126:VAL:HA	2.19	0.43
1:B:359:LEU:HD12	1:B:359:LEU:C	2.40	0.42
2:D:109:GLN:HB2	2:D:121:SER:OG	2.19	0.42
1:B:292:VAL:HG22	5:B:704[B]:CL:CL	2.56	0.42
2:D:95:LEU:HD23	2:D:95:LEU:C	2.40	0.42
2:D:109:GLN:HE21	2:D:120:VAL:CG1	2.31	0.42
1:A:414:ARG:NE	6:A:801:HOH:O	2.38	0.42
1:B:630:PRO:HB3	1:B:632:THR:HG22	2.00	0.42
1:A:401:MET:HG2	1:A:403:ILE:HD11	2.02	0.42
1:A:311:PHE:CE1	2:C:75:THR:HG23	2.54	0.42
1:B:397:ARG:HH11	1:B:397:ARG:HB3	1.84	0.42
1:A:464:VAL:O	1:A:464:VAL:CG1	2.69	0.41
1:A:287:SER:HB3	1:A:672:PRO:HD2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HD12	1:A:451:LEU:HD11	2.03	0.41
1:A:579:VAL:HG13	1:A:581:LEU:CD2	2.51	0.41
1:B:294:SER:O	1:B:462:VAL:HG11	2.21	0.40
1:B:551:GLN:HB3	1:B:569:VAL:HG22	2.04	0.40
2:C:111:LEU:HD12	2:C:120:VAL:HG22	2.02	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	370/395 (94%)	356 (96%)	11 (3%)	3 (1%)	19	23
1	B	370/395 (94%)	358 (97%)	9 (2%)	3 (1%)	19	23
2	C	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
2	D	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
All	All	940/994 (95%)	908 (97%)	26 (3%)	6 (1%)	25	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	341	GLN
1	B	631	VAL
1	B	362	ASN
1	B	630	PRO
1	A	343	SER
1	A	362	ASN

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	319/337 (95%)	289 (91%)	30 (9%)	8 10
1	B	319/337 (95%)	295 (92%)	24 (8%)	13 17
2	C	89/89 (100%)	79 (89%)	10 (11%)	6 6
2	D	89/89 (100%)	78 (88%)	11 (12%)	4 5
All	All	816/852 (96%)	741 (91%)	75 (9%)	9 11

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	VAL
1	A	313	ARG
1	A	344	THR
1	A	350	LEU
1	A	359	LEU
1	A	366	ARG
1	A	367	VAL
1	A	368	THR
1	A	383	SER
1	A	389	ARG
1	A	402	LYS
1	A	416	LEU
1	A	431	LYS
1	A	456	THR
1	A	461	THR
1	A	463	LYS
1	A	475	GLU
1	A	489	SER
1	A	560	THR
1	A	565	MET
1	A	568	LYS
1	A	578	THR
1	A	579	VAL
1	A	581	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	587	THR
1	A	596	GLN
1	A	612	GLU
1	A	631	VAL
1	A	641	ARG
1	A	666	THR
1	B	288	VAL
1	B	302	SER
1	B	313	ARG
1	B	314	LEU
1	B	344	THR
1	B	362	ASN
1	B	367	VAL
1	B	368	THR
1	B	387	LEU
1	B	389	ARG
1	B	397	ARG
1	B	416	LEU
1	B	431	LYS
1	B	467	ARG
1	B	540	VAL
1	B	560	THR
1	B	562	LEU
1	B	569	VAL
1	B	579	VAL
1	B	581	LEU
1	B	612	GLU
1	B	633	SER
1	B	651	ARG
1	B	666	THR
2	C	37	ILE
2	C	38	THR
2	C	43	LEU
2	C	60	VAL
2	C	84	ASP
2	C	96	ARG
2	C	111	LEU
2	C	116	HIS
2	C	126	VAL
2	C	127	ARG
2	D	31	VAL
2	D	32	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	38	THR
2	D	41	ARG
2	D	51	LEU
2	D	54	GLN
2	D	60	VAL
2	D	70	GLU
2	D	105	THR
2	D	116	HIS
2	D	118	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	459	GLN
1	A	605	GLN
1	B	435	GLN

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)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	3,1	14,14,15	0.75	0	17,19,21	1.74	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	2	3	14,14,15	0.83	1 (7%)	17,19,21	1.91	2 (11%)
3	NAG	F	1	3,1	14,14,15	0.93	0	17,19,21	1.55	2 (11%)
3	NAG	F	2	3	14,14,15	1.06	2 (14%)	17,19,21	2.28	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	C1-C2	2.46	1.56	1.52
3	F	2	NAG	O3-C3	-2.18	1.37	1.43
3	F	2	NAG	C1-C2	-2.18	1.49	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2	NAG	C1-O5-C5	7.17	121.91	112.19
3	E	2	NAG	O5-C5-C6	5.43	115.71	107.20
3	E	2	NAG	C1-C2-N2	3.47	116.41	110.49
3	F	2	NAG	O3-C3-C4	-3.45	102.36	110.35
3	F	1	NAG	O5-C1-C2	-3.21	106.21	111.29
3	E	1	NAG	O6-C6-C5	-3.02	100.94	111.29
3	E	1	NAG	O5-C1-C2	-3.00	106.55	111.29
3	F	2	NAG	O4-C4-C5	2.85	116.38	109.30
3	E	1	NAG	C3-C4-C5	-2.84	105.18	110.24
3	F	1	NAG	C1-O5-C5	2.69	115.84	112.19
3	F	2	NAG	O7-C7-C8	-2.33	117.74	122.06
3	E	1	NAG	O7-C7-N2	2.20	126.00	121.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

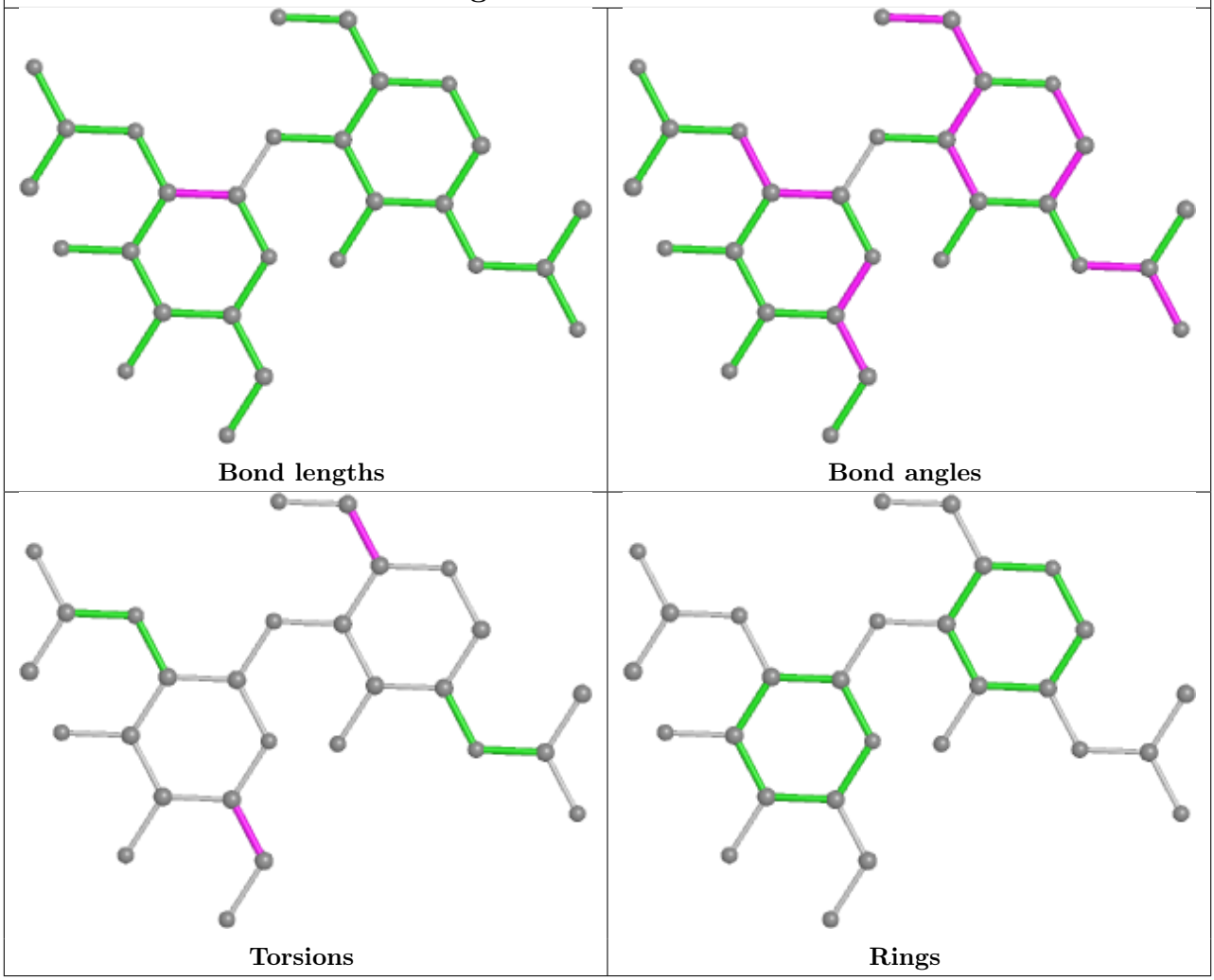
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6

There are no ring outliers.

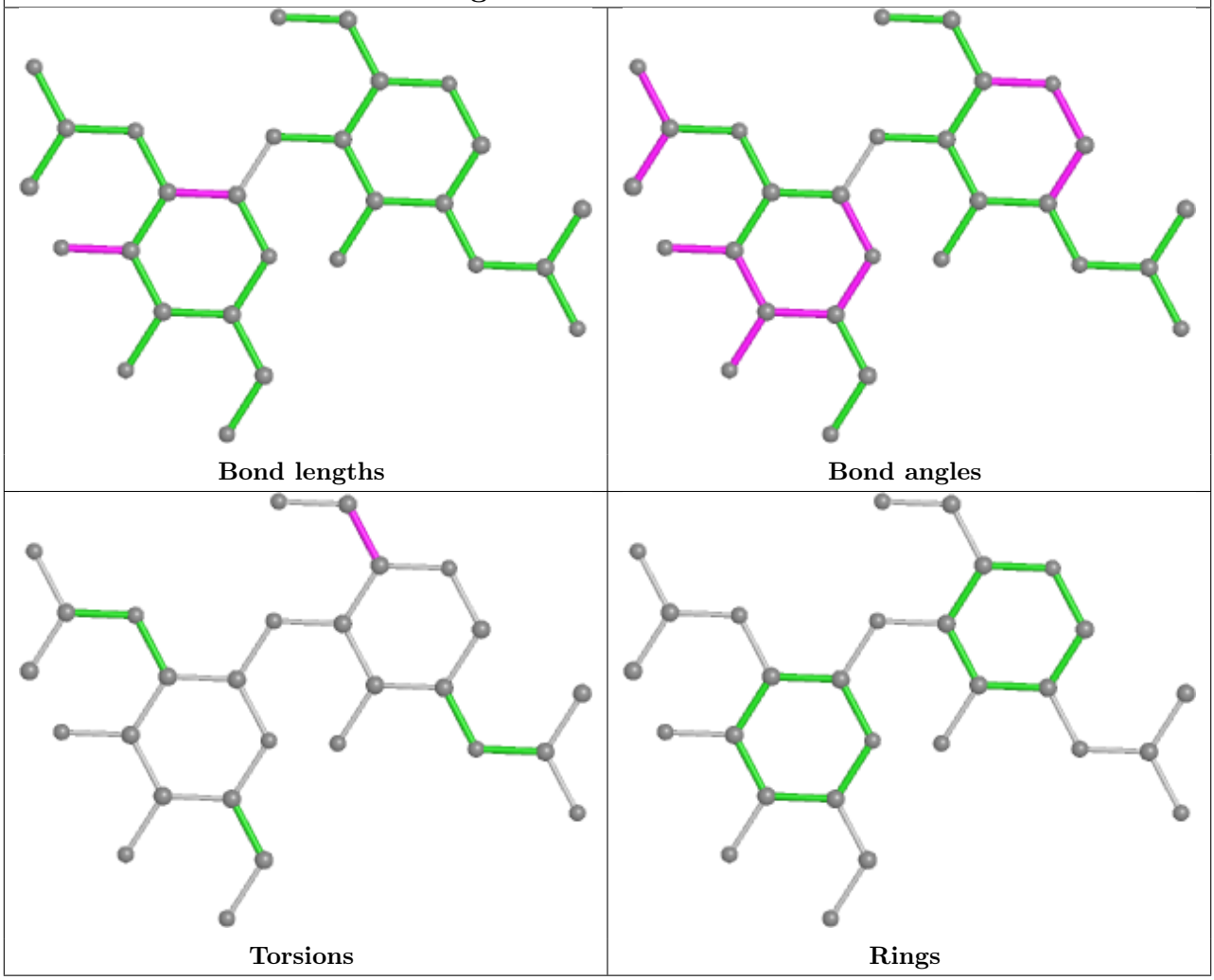
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain E



Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	376/395 (95%)	0.01	11 (2%) 51 58	43, 70, 98, 126	0
1	B	376/395 (95%)	-0.16	7 (1%) 66 73	30, 43, 72, 103	0
2	C	102/102 (100%)	-0.00	10 (9%) 7 10	50, 67, 101, 140	0
2	D	102/102 (100%)	0.09	6 (5%) 22 28	38, 66, 97, 147	0
All	All	956/994 (96%)	-0.05	34 (3%) 42 49	30, 59, 97, 147	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	LEU	4.9
2	C	128	LEU	4.5
1	B	631	VAL	4.5
2	D	116	HIS	4.3
1	A	675	PRO	4.0
2	C	116	HIS	3.4
1	A	301	PHE	3.2
1	A	454	GLU	3.0
1	A	387	LEU	3.0
2	C	127	ARG	2.7
1	A	362	ASN	2.7
1	B	504	THR	2.6
2	D	38	THR	2.6
1	B	675	PRO	2.5
2	D	41	ARG	2.5
2	C	102	LEU	2.4
1	B	531	ARG	2.3
2	D	86	GLN	2.3
1	A	292	VAL	2.3
2	C	98	THR	2.2
2	C	37	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	27	GLU	2.2
1	B	303	GLY	2.2
2	C	42	GLY	2.1
2	C	39	GLY	2.1
2	C	43	LEU	2.1
1	A	366	ARG	2.1
1	A	342	ASP	2.0
2	C	40	ALA	2.0
1	A	602	ALA	2.0
1	B	431	LYS	2.0
1	A	414	ARG	2.0
1	A	613	ARG	2.0
2	D	40	ALA	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)

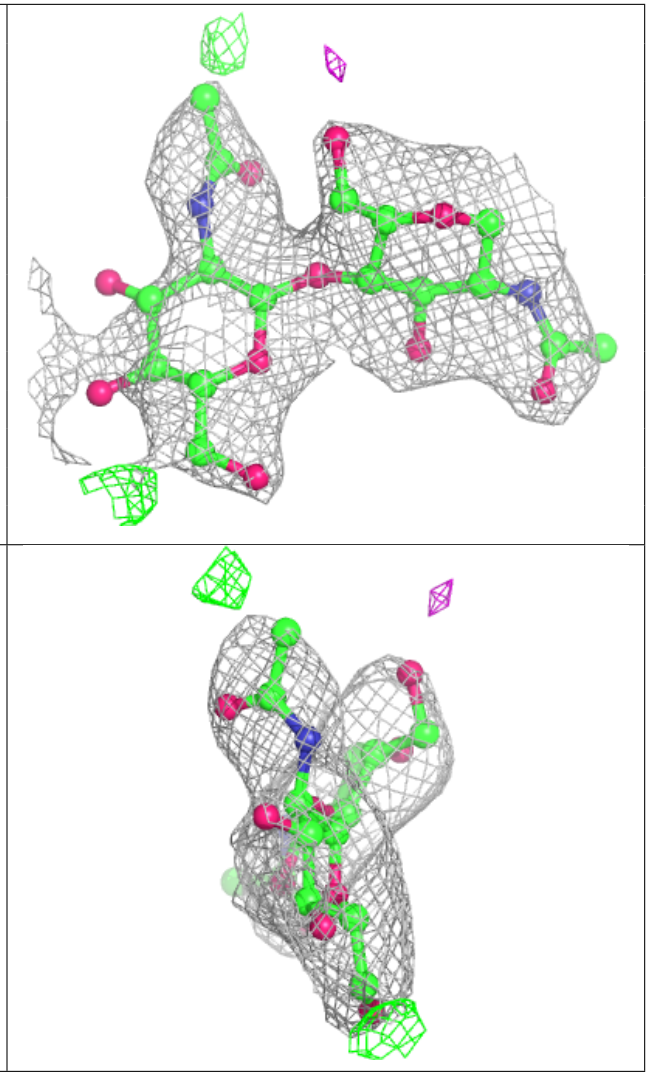
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	E	2	14/15	0.82	0.20	94,110,130,137	0
3	NAG	F	2	14/15	0.92	0.14	46,63,83,83	0
3	NAG	E	1	14/15	0.94	0.12	60,73,87,96	0
3	NAG	F	1	14/15	0.96	0.08	37,47,59,60	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

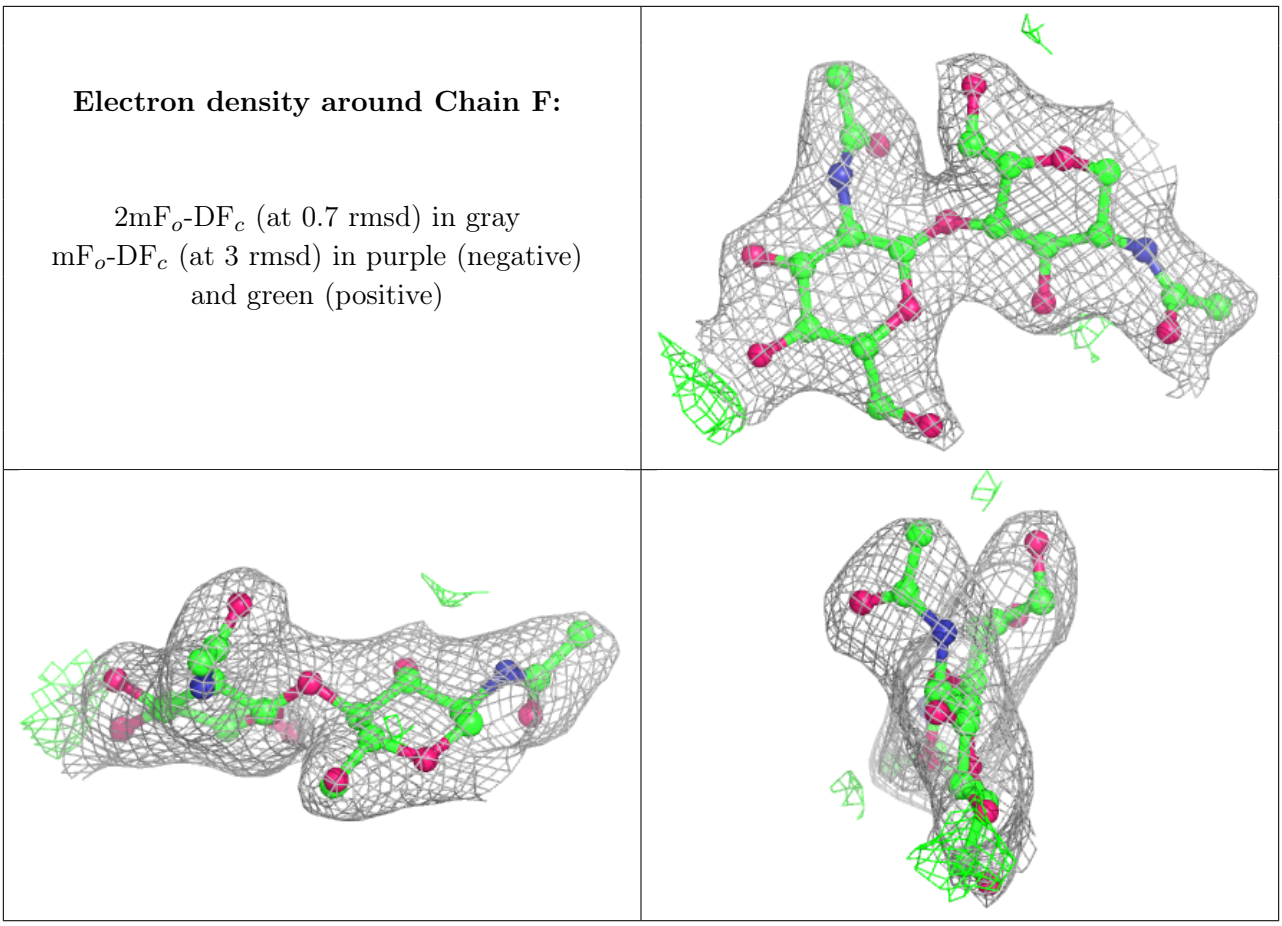
Electron density around Chain E:

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



Electron density around Chain F:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	B	704[A]	1/1	0.82	0.22	57,57,57,57	1
5	CL	B	704[B]	1/1	0.82	0.22	65,65,65,65	1
5	CL	A	704	1/1	0.83	0.10	104,104,104,104	0
4	CA	A	703	1/1	0.99	0.12	58,58,58,58	0
4	CA	B	703	1/1	1.00	0.17	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.