Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2023 – 10:47 PM EDT

PDB ID	:	5L2K
Title	:	Crystal structure of GEM42 TCR-CD1b-GMM complex
Authors	:	Gras, S.; Shahine, A.; Le Nours, J.; Rossjohn, J.
Deposited on	:	2016-08-02
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

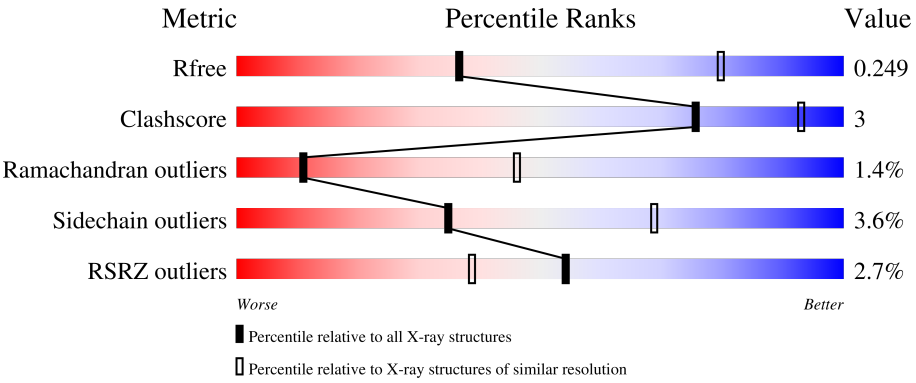
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

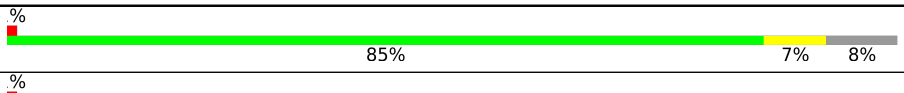
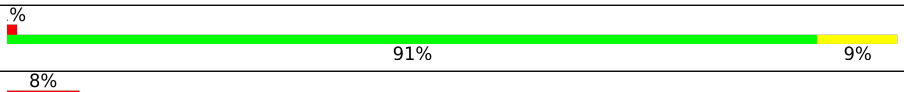
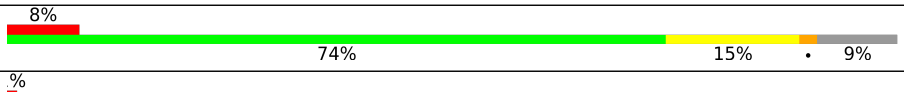
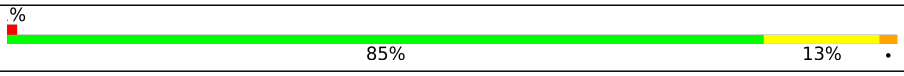
The reported resolution of this entry is 3.20 Å.

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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	300	
2	B	98	
3	D	204	
4	E	243	

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
11	70E	E	303	X	-	-	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 6497 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 T-cell surface glycoprotein CD1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	11	1	0
			2163	1386	368	399	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	ALA	ILE	engineered mutation	UNP P29016
A	279	GLY	-	expression tag	UNP P29016
A	280	SER	-	expression tag	UNP P29016
A	281	GLY	-	expression tag	UNP P29016
A	282	LEU	-	expression tag	UNP P29016
A	283	ASN	-	expression tag	UNP P29016
A	284	ASP	-	expression tag	UNP P29016
A	285	ILE	-	expression tag	UNP P29016
A	286	PHE	-	expression tag	UNP P29016
A	287	GLU	-	expression tag	UNP P29016
A	288	ALA	-	expression tag	UNP P29016
A	289	GLN	-	expression tag	UNP P29016
A	290	LYS	-	expression tag	UNP P29016
A	291	ILE	-	expression tag	UNP P29016
A	292	GLU	-	expression tag	UNP P29016
A	293	TRP	-	expression tag	UNP P29016
A	294	HIS	-	expression tag	UNP P29016
A	295	GLU	-	expression tag	UNP P29016
A	296	HIS	-	expression tag	UNP P29016
A	297	HIS	-	expression tag	UNP P29016
A	298	HIS	-	expression tag	UNP P29016
A	299	HIS	-	expression tag	UNP P29016
A	300	HIS	-	expression tag	UNP P29016
A	301	HIS	-	expression tag	UNP P29016

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			820	523	139	156	2			

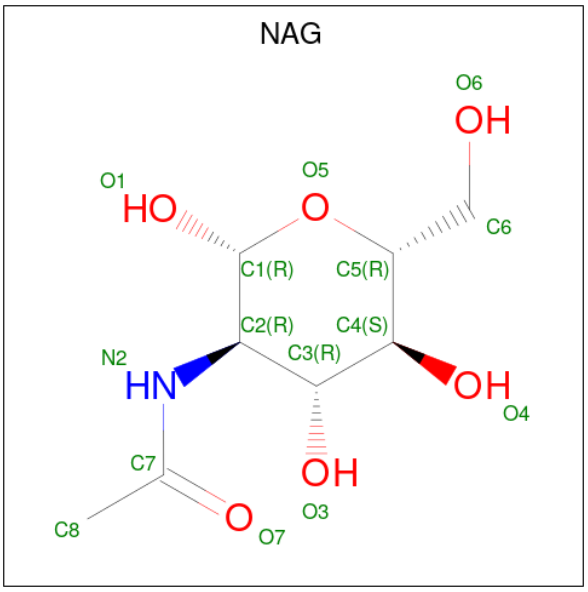
- Molecule 3 is a protein called GEM42 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	185	Total	C	N	O	S	0	0	0
			1442	903	241	289	9			

- Molecule 4 is a protein called GEM42 TCR beta chain.

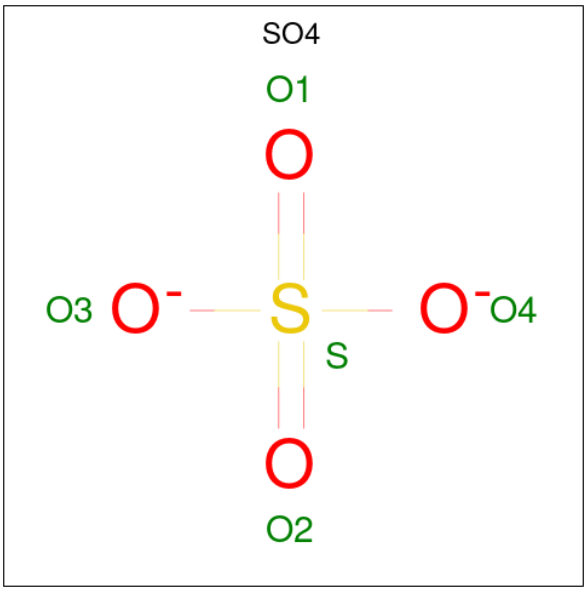
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	242	Total	C	N	O	S	0	0	0
			1916	1210	333	364	9			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0

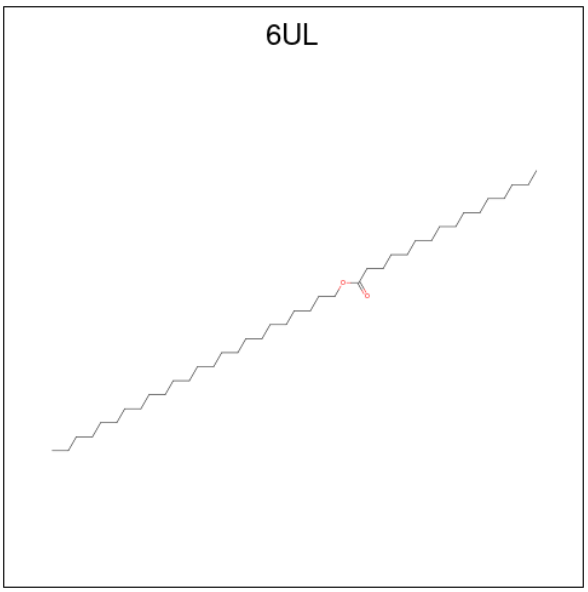
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total Cl 3 3	0	0
7	B	1	Total Cl 1 1	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Na 1 1	0	0
8	E	1	Total Na 1 1	0	0

- Molecule 9 is TETRACOSYL PALMITATE (three-letter code: 6UL) (formula: $C_{40}H_{80}O_2$).

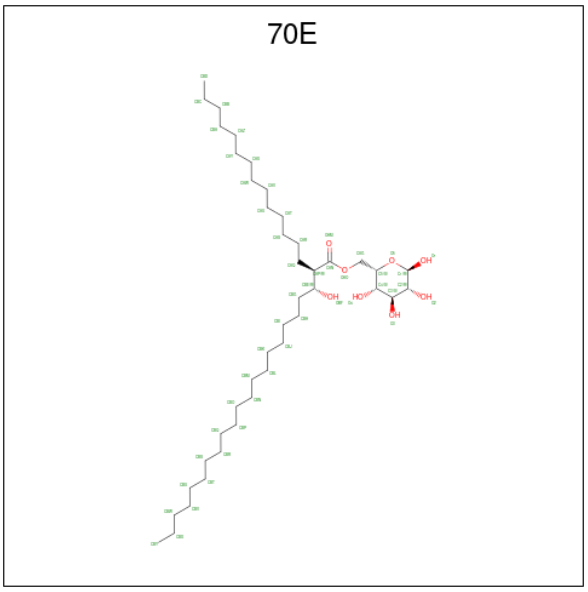


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 26 24 2	0	0

- Molecule 10 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	1	Total Cs 1 1	0	0

- Molecule 11 is 6-O-[(2R,3R)-3-hydroxy-2-tetradecyldocosanoyl]-alpha-L-idopyranose (three-letter code: 70E) (formula: $C_{42}H_{82}O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	E	1	Total C O 50 42 8	0	0

- Molecule 12 is water.

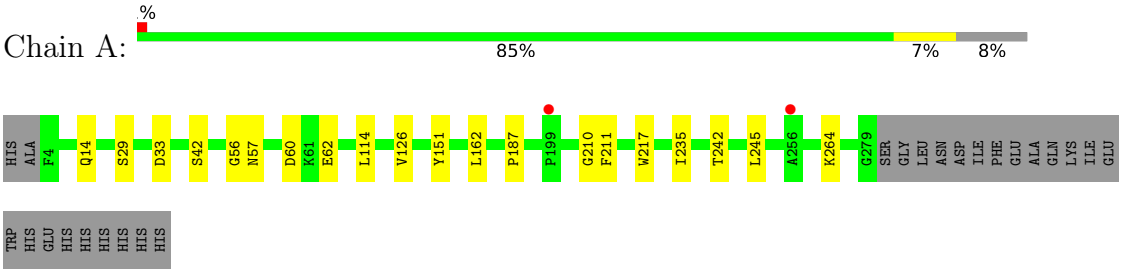
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	2	Total O 2 2	0	0
12	B	3	Total O 3 3	0	0
12	D	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

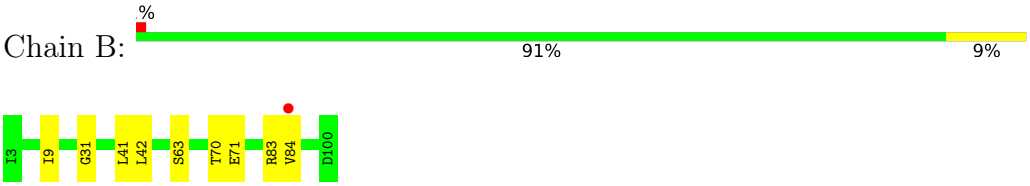
• Molecule 1: T-cell surface glycoprotein CD1b

Chain A:



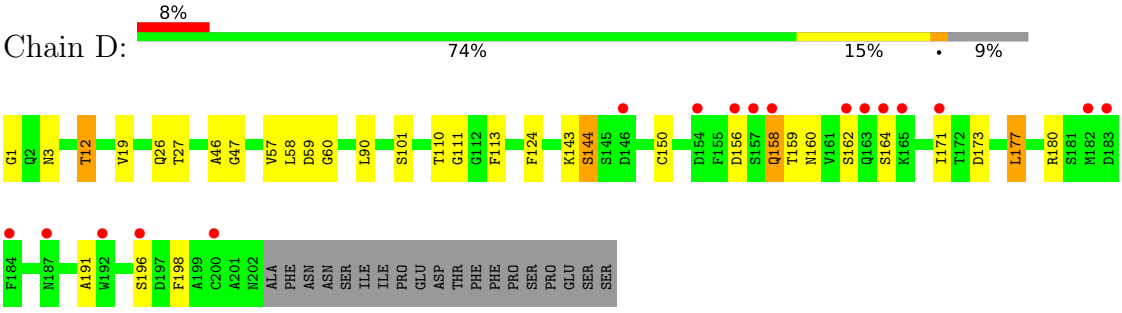
• Molecule 2: Beta-2-microglobulin

Chain B:



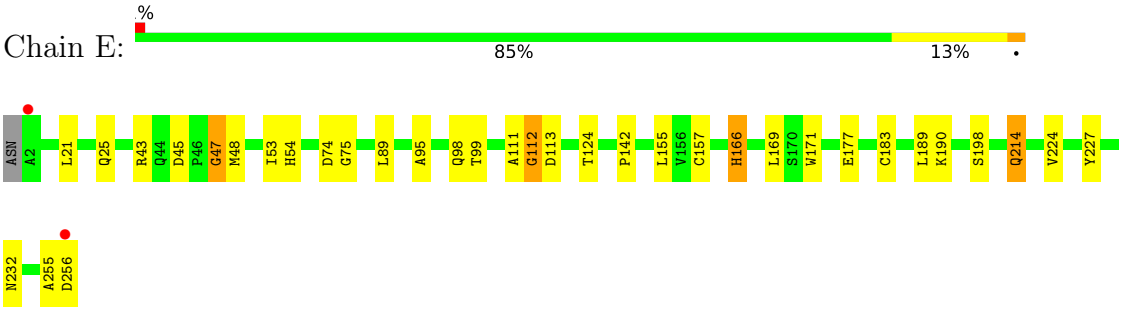
• Molecule 3: GEM42 TCR alpha chain

Chain D:



• Molecule 4: GEM42 TCR beta chain

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α, β, γ	175.00Å 175.00Å 170.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.73 – 3.20 47.73 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.73-3.20) 100.0 (47.73-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.218 , 0.239 0.227 , 0.249	Depositor DCC
R_{free} test set	1259 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	78.1	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6497	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: SO4, CS, 70E, NA, NAG, CL, 6UL

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	0.36	0/2223	0.55	0/3017
2	B	0.36	0/843	0.53	0/1142
3	D	0.37	0/1470	0.60	0/1984
4	E	0.34	0/1968	0.58	0/2676
All	All	0.36	0/6504	0.57	0/8819

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	2163	0	2079	8	0
2	B	820	0	782	4	0
3	D	1442	0	1378	11	0
4	E	1916	0	1833	18	0
5	A	42	0	39	0	0
6	A	15	0	0	0	0
6	D	5	0	0	0	0
6	E	5	0	0	0	0
7	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
8	A	1	0	0	0	0
8	E	1	0	0	0	0
9	A	26	0	42	1	0
10	D	1	0	0	0	0
11	E	50	0	0	0	0
12	A	2	0	0	0	0
12	B	3	0	0	0	0
12	D	1	0	0	0	0
All	All	6497	0	6153	39	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 3.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.77	0.66
3:D:1:GLY:CA	3:D:27:THR:HG22	2.32	0.58
1:A:217:TRP:HB3	1:A:264:LYS:HB2	1.84	0.58
3:D:3:ASN:HB2	3:D:26:GLN:HB2	1.86	0.57
2:B:31:GLY:HA2	2:B:63:SER:HB3	1.86	0.57
3:D:158:GLN:HB2	3:D:159:THR:HA	1.85	0.57
4:E:190:LYS:HE2	4:E:198:SER:HB3	1.88	0.55
3:D:1:GLY:HA2	3:D:27:THR:HG22	1.89	0.53
4:E:45:ASP:HB2	4:E:48:MET:HG2	1.92	0.51
3:D:57:VAL:HG13	3:D:58:LEU:HG	1.93	0.51
4:E:157:CYS:HB2	4:E:171:TRP:CZ2	2.46	0.50
4:E:166:HIS:HB3	4:E:227:TYR:HB2	1.95	0.49
4:E:112:GLY:HA2	4:E:113:ASP:HB2	1.95	0.49
2:B:42:LEU:HD11	2:B:83:ARG:HB2	1.95	0.49
1:A:235:ILE:HD13	1:A:245:LEU:HD13	1.94	0.48
3:D:164:SER:H	3:D:171:ILE:HD12	1.77	0.48
1:A:210:GLY:HA2	1:A:242:THR:HB	1.95	0.48
2:B:9:ILE:HG12	2:B:84:VAL:HG21	1.96	0.48
4:E:99:THR:HG23	4:E:124:THR:HA	1.95	0.48
3:D:177:LEU:HG	4:E:183:CYS:HB2	1.96	0.47
4:E:214:GLN:HG3	4:E:255:ALA:HA	1.96	0.47
4:E:47:GLY:HA2	4:E:48:MET:C	2.35	0.47
3:D:110:THR:HA	3:D:111:GLY:HA2	1.63	0.47
4:E:95:ALA:H	4:E:98:GLN:HE21	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:74:ASP:HA	4:E:75:GLY:HA2	1.75	0.45
4:E:21:LEU:HD13	4:E:89:LEU:HD23	1.99	0.45
1:A:114:LEU:HB2	1:A:162:LEU:HD11	1.99	0.45
1:A:151:TYR:HE1	4:E:111:ALA:HB2	1.82	0.45
3:D:12:THR:HG23	3:D:124:PHE:HB2	2.00	0.44
4:E:112:GLY:CA	4:E:113:ASP:HB2	2.48	0.44
4:E:142:PRO:HD3	4:E:155:LEU:HG	2.00	0.44
1:A:114:LEU:HB3	1:A:126:VAL:HB	2.00	0.43
3:D:46:ALA:HA	3:D:47:GLY:HA2	1.73	0.43
4:E:43:ARG:HB3	4:E:53:ILE:HD11	2.00	0.43
4:E:169:LEU:HG	4:E:224:VAL:HG22	2.00	0.42
1:A:14:GLN:HB2	9:A:411:6UL:HBL2	2.02	0.42
3:D:150:CYS:HB2	3:D:191:ALA:HB3	2.00	0.42
4:E:53:ILE:HG22	4:E:54:HIS:HD2	1.85	0.41
2:B:41:LEU:HD13	2:B:70:THR:HG22	2.03	0.41

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	275/300 (92%)	266 (97%)	7 (2%)	2 (1%)	22 61
2	B	96/98 (98%)	93 (97%)	3 (3%)	0	100 100
3	D	183/204 (90%)	160 (87%)	16 (9%)	7 (4%)	3 22
4	E	240/243 (99%)	224 (93%)	14 (6%)	2 (1%)	19 58
All	All	794/845 (94%)	743 (94%)	40 (5%)	11 (1%)	11 46

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	196	SER
4	E	47	GLY
1	A	56	GLY
3	D	144	SER
3	D	160	ASN
3	D	180	ARG
3	D	158	GLN
3	D	162	SER
1	A	33	ASP
3	D	60	GLY
4	E	112	GLY

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	226/246 (92%)	221 (98%)	5 (2%)	52	79
2	B	93/93 (100%)	92 (99%)	1 (1%)	73	88
3	D	160/178 (90%)	148 (92%)	12 (8%)	13	45
4	E	207/208 (100%)	200 (97%)	7 (3%)	37	70
All	All	686/725 (95%)	661 (96%)	25 (4%)	35	69

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	42	SER
1	A	57	ASN
1	A	60	ASP
1	A	62	GLU
2	B	71	GLU
3	D	12	THR
3	D	19	VAL
3	D	59	ASP
3	D	90	LEU
3	D	101	SER

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Mol	Chain	Res	Type
3	D	113	PHE
3	D	143	LYS
3	D	144	SER
3	D	156	ASP
3	D	173	ASP
3	D	177	LEU
3	D	198	PHE
4	E	25	GLN
4	E	166	HIS
4	E	177	GLU
4	E	189	LEU
4	E	214	GLN
4	E	232	ASN
4	E	256	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	105	HIS
3	D	108	ASN
4	E	25	GLN
4	E	29	HIS
4	E	54	HIS
4	E	98	GLN
4	E	237	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 7 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	$\#\|Z\| > 2$
6	SO4	E	301	-	4,4,4	0.14	0	6,6,6	0.07	0
9	6UL	A	411	-	25,25,41	0.63	0	25,25,41	0.70	0
5	NAG	A	401	1	14,14,15	1.93	3 (21%)	17,19,21	1.72	4 (23%)
5	NAG	A	402	1	14,14,15	1.87	4 (28%)	17,19,21	1.58	3 (17%)
6	SO4	D	301	-	4,4,4	0.13	0	6,6,6	0.08	0
6	SO4	A	404	-	4,4,4	0.14	0	6,6,6	0.09	0
6	SO4	A	405	-	4,4,4	0.14	0	6,6,6	0.09	0
6	SO4	A	406	-	4,4,4	0.15	0	6,6,6	0.10	0
11	70E	E	303	-	50,50,50	0.73	0	55,58,58	0.96	1 (1%)
5	NAG	A	403	1	14,14,15	1.99	4 (28%)	17,19,21	2.30	7 (41%)

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
5	NAG	A	401	1	-	3/6/23/26	0/1/1/1
5	NAG	A	402	1	-	0/6/23/26	0/1/1/1
9	6UL	A	411	-	-	15/24/24/40	-
11	70E	E	303	-	1/1/8/8	21/46/66/66	0/1/1/1
5	NAG	A	403	1	-	1/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	NAG	O5-C1	4.91	1.51	1.43
5	A	401	NAG	O5-C1	4.74	1.51	1.43
5	A	402	NAG	O5-C1	4.41	1.50	1.43
5	A	401	NAG	C7-N2	3.19	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	NAG	C7-N2	3.14	1.45	1.34
5	A	402	NAG	C7-N2	3.14	1.45	1.34
5	A	403	NAG	C3-C2	-2.28	1.47	1.52
5	A	401	NAG	C4-C3	-2.23	1.46	1.52
5	A	402	NAG	C4-C3	-2.14	1.46	1.52
5	A	403	NAG	C4-C3	-2.13	1.46	1.52
5	A	402	NAG	C3-C2	-2.12	1.48	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	403	NAG	C3-C4-C5	4.17	117.67	110.24
5	A	403	NAG	O5-C5-C6	4.10	113.63	107.20
5	A	403	NAG	C1-C2-N2	4.01	117.34	110.49
5	A	401	NAG	C1-O5-C5	3.52	116.97	112.19
5	A	403	NAG	C1-O5-C5	3.46	116.88	112.19
5	A	402	NAG	O5-C5-C6	3.43	112.58	107.20
5	A	401	NAG	O5-C5-C6	3.08	112.03	107.20
5	A	403	NAG	C2-N2-C7	2.85	126.96	122.90
5	A	402	NAG	C3-C4-C5	2.78	115.20	110.24
5	A	403	NAG	O5-C5-C4	2.71	117.41	110.83
11	E	303	70E	CAR-CAQ-CAP	-2.70	109.42	114.28
5	A	401	NAG	C3-C4-C5	2.53	114.75	110.24
5	A	401	NAG	C2-N2-C7	2.16	125.97	122.90
5	A	403	NAG	O6-C6-C5	2.15	118.68	111.29
5	A	402	NAG	C4-C3-C2	2.15	114.16	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	E	303	70E	C5

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	E	303	70E	CAN-CAP-CAQ-CAR
9	A	411	6UL	OBO-CAP-OAQ-CAR
9	A	411	6UL	CAO-CAP-OAQ-CAR
11	E	303	70E	CAP-CAQ-CAR-CAS
5	A	401	NAG	C4-C5-C6-O6
9	A	411	6UL	CAL-CAM-CAN-CAO
9	A	411	6UL	CBG-CBH-CBI-CBJ

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Mol	Chain	Res	Type	Atoms
9	A	411	6UL	CBH-CBI-CBJ-CBK
5	A	403	NAG	C1-C2-N2-C7
11	E	303	70E	CBO-CBP-CBQ-CBR
11	E	303	70E	CBQ-CBR-CBS-CBT
11	E	303	70E	CAW-CAX-CAY-CAZ
11	E	303	70E	CBS-CBT-CBU-CBV
11	E	303	70E	CAV-CAW-CAX-CAY
11	E	303	70E	CAX-CAY-CAZ-CBA
11	E	303	70E	CBJ-CBK-CBL-CBM
9	A	411	6UL	CBI-CBJ-CBK-CBL
9	A	411	6UL	CAM-CAN-CAO-CAP
9	A	411	6UL	CBD-CBE-CBF-CBG
11	E	303	70E	CBH-CBI-CBJ-CBK
9	A	411	6UL	CAT-CAU-CAV-CAW
11	E	303	70E	CBP-CBQ-CBR-CBS
9	A	411	6UL	CAS-CAT-CAU-CAV
11	E	303	70E	CAZ-CBA-CBB-CBC
11	E	303	70E	CAU-CAV-CAW-CAX
11	E	303	70E	CAY-CAZ-CBA-CBB
5	A	401	NAG	O5-C5-C6-O6
11	E	303	70E	CAQ-CAR-CAS-CAT
9	A	411	6UL	CAV-CAW-CBM-CBL
9	A	411	6UL	CAJ-CAK-CAL-CAM
11	E	303	70E	CAR-CAS-CAT-CAU
11	E	303	70E	CAS-CAT-CAU-CAV
11	E	303	70E	CBU-CBV-CBW-CBX
11	E	303	70E	CBI-CBJ-CBK-CBL
11	E	303	70E	CAN-CAP-CBE-OBF
9	A	411	6UL	CBK-CBL-CBM-CAW
5	A	401	NAG	C3-C2-N2-C7
9	A	411	6UL	CBC-CBD-CBE-CBF
11	E	303	70E	CAN-CAP-CBE-CBG
9	A	411	6UL	CBE-CBF-CBG-CBH

There are no ring outliers.

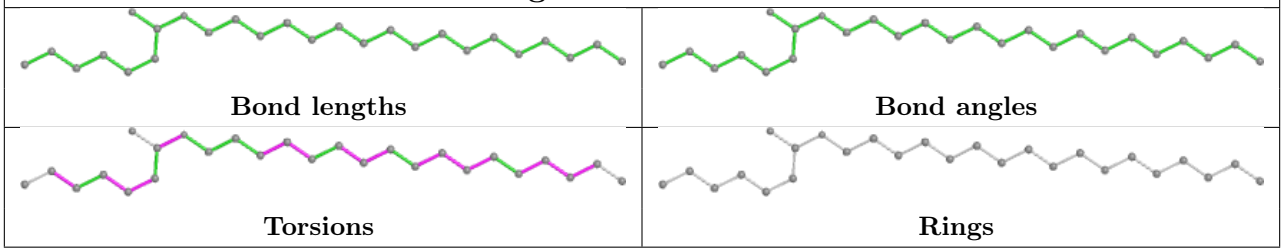
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	411	6UL	1	0

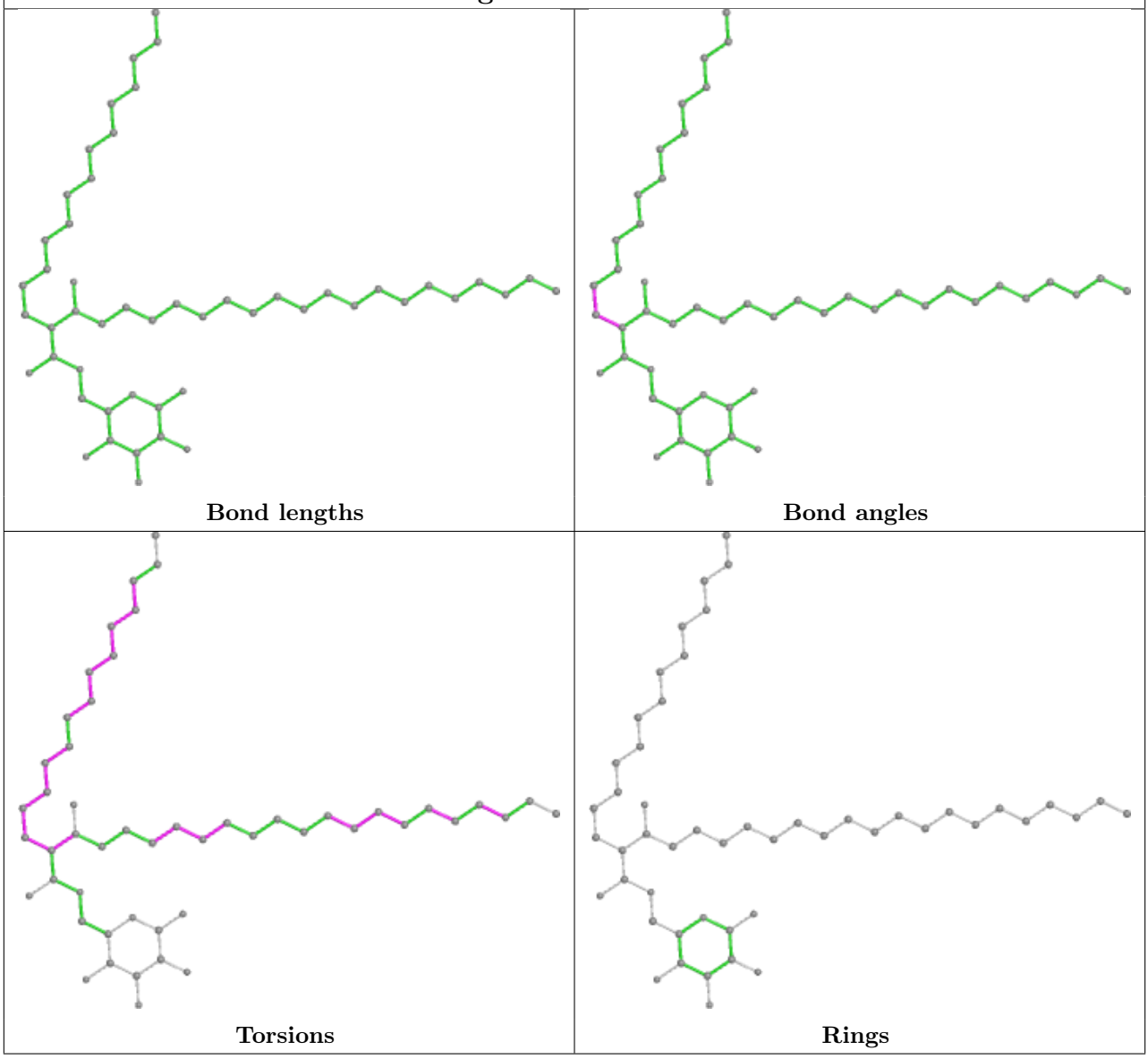
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 6UL A 411



Ligand 70E E 303



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	276/300 (92%)	-0.10	2 (0%)	87	81	43, 73, 112, 122	3 (1%)
2	B	98/98 (100%)	0.37	1 (1%)	82	72	58, 94, 116, 128	0
3	D	185/204 (90%)	0.38	17 (9%)	9	5	45, 71, 137, 149	9 (4%)
4	E	242/243 (99%)	-0.06	2 (0%)	86	78	51, 73, 105, 123	0
All	All	801/845 (94%)	0.08	22 (2%)	54	39	43, 75, 120, 149	12 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	164	SER	6.2
3	D	156	ASP	4.9
3	D	163	GLN	4.4
1	A	256	ALA	4.0
4	E	2	ALA	3.5
3	D	200	CYS	3.3
3	D	184	PHE	3.3
4	E	256	ASP	3.1
3	D	182	MET	3.0
3	D	158	GLN	2.8
3	D	192	TRP	2.7
3	D	187	ASN	2.6
3	D	162	SER	2.5
3	D	157	SER	2.4
3	D	165	LYS	2.4
3	D	146	ASP	2.3
1	A	199	PRO	2.2
3	D	196	SER	2.2
3	D	171	ILE	2.2
3	D	154	ASP	2.1
2	B	84	VAL	2.1
3	D	183	ASP	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

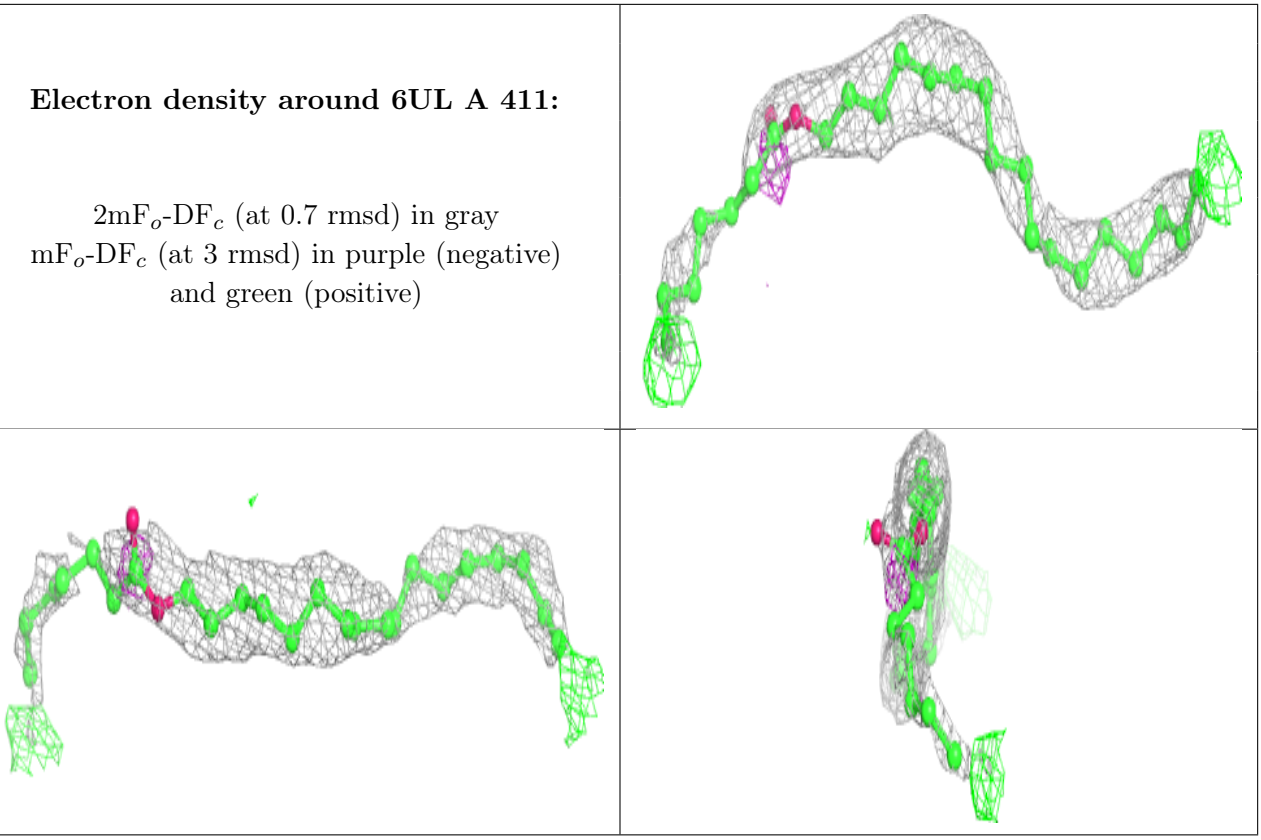
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	SO4	D	301	5/5	0.74	0.24	148,148,148,148	0
7	CL	B	201	1/1	0.76	0.27	98,98,98,98	0
6	SO4	E	301	5/5	0.78	0.31	169,169,170,170	0
7	CL	A	408	1/1	0.80	0.14	87,87,87,87	0
7	CL	A	409	1/1	0.81	0.27	93,93,93,93	0
7	CL	A	407	1/1	0.81	0.14	96,96,96,96	0
5	NAG	A	403	14/15	0.83	0.28	97,98,100,101	0
6	SO4	A	404	5/5	0.85	0.23	129,129,129,129	0
9	6UL	A	411	26/42	0.85	0.47	54,57,67,68	0
5	NAG	A	402	14/15	0.88	0.33	108,109,110,110	0
8	NA	A	410	1/1	0.91	0.22	64,64,64,64	0
11	70E	E	303	50/50	0.92	0.39	54,58,67,69	0
5	NAG	A	401	14/15	0.94	0.17	61,62,64,64	0
8	NA	E	302	1/1	0.94	0.53	43,43,43,43	0
6	SO4	A	405	5/5	0.94	0.17	97,98,98,98	0
6	SO4	A	406	5/5	0.94	0.18	116,116,116,116	0
10	CS	D	302	1/1	0.97	0.11	145,145,145,145	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.

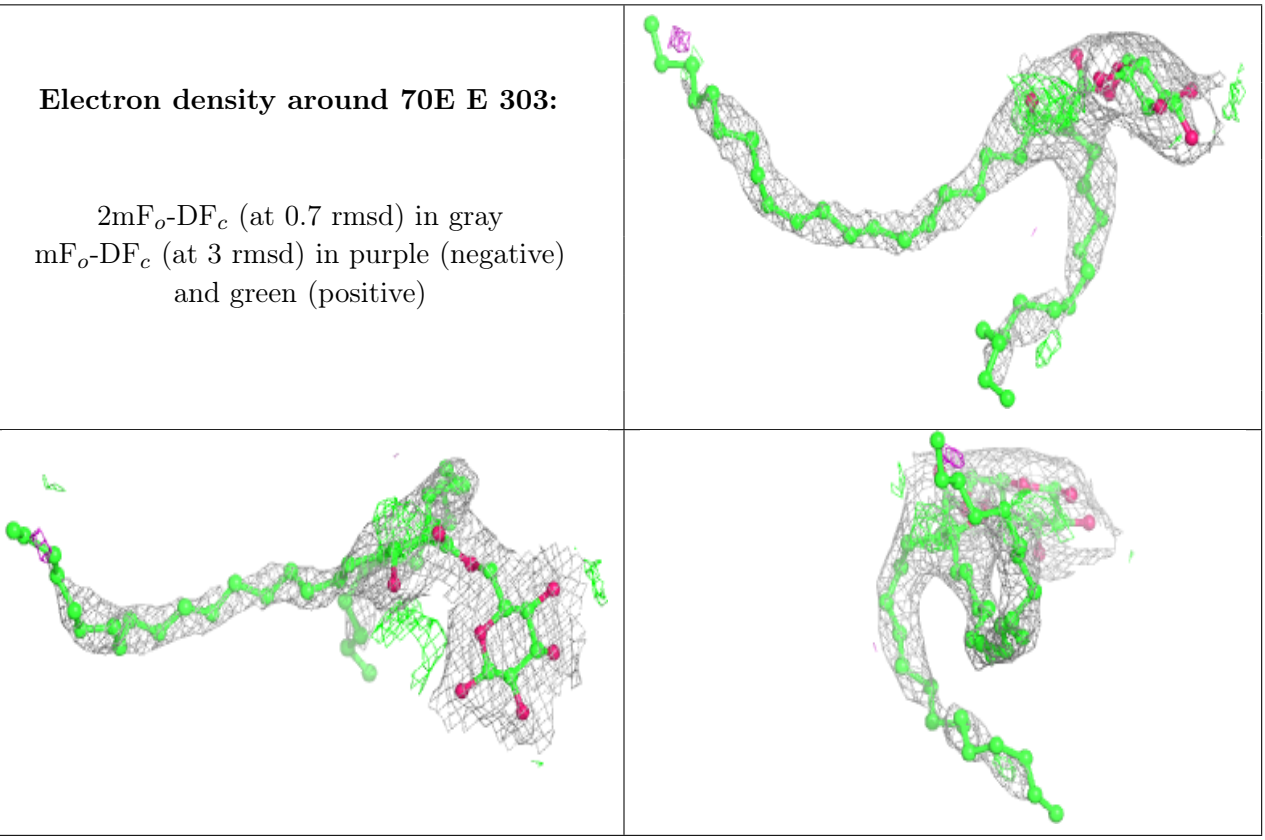
Electron density around 6UL A 411:

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



Electron density around 70E E 303:

$2mF_o$-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.