Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 02:34 PM EDT

PDB ID	:	6PUM
Title	:	Structure of human MAIT A-F7 TCR in complex with human MR1-2'D-5-OP-RU
Authors	:	Awad, W.; Keller, A.N.; Rossjohn, J.
Deposited on	:	2019-07-18
Resolution	:	1.96 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:

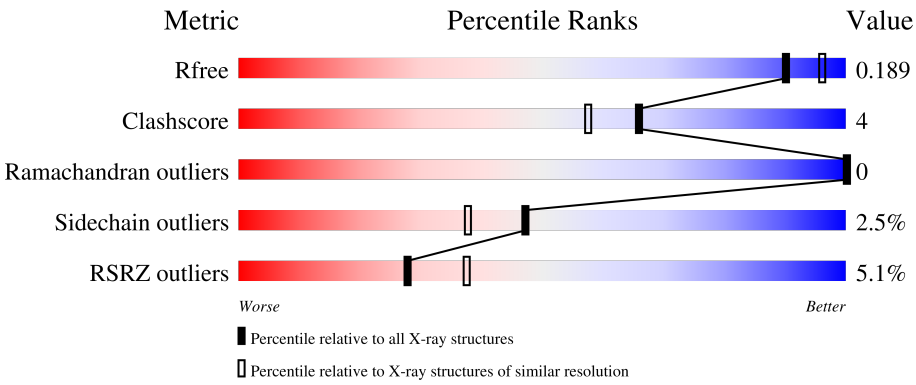
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	271	.%, 89%, 9%
1	C	271	3%, 92%, 6%
2	B	100	14%, 93%
2	F	100	.%, 95%
3	D	204	16%, 81%, 13%

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Mol	Chain	Length	Quality of chain
3	G	204	% 91% 7%
4	E	246	7% 87% 12%
4	H	246	2% 89% 9%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14699 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 Major histocompatibility complex class I-related gene protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	265	2185	1402	377	394	12	0	9	0
1	C	269	2245	1448	385	400	12	0	9	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q95460
A	261	SER	CYS	conflict	UNP Q95460
C	0	MET	-	initiating methionine	UNP Q95460
C	261	SER	CYS	conflict	UNP Q95460

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	98	777	502	133	139	3	0	1	0
2	F	99	803	516	137	147	3	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
F	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	196	1515	966	241	297	11	0	4	0

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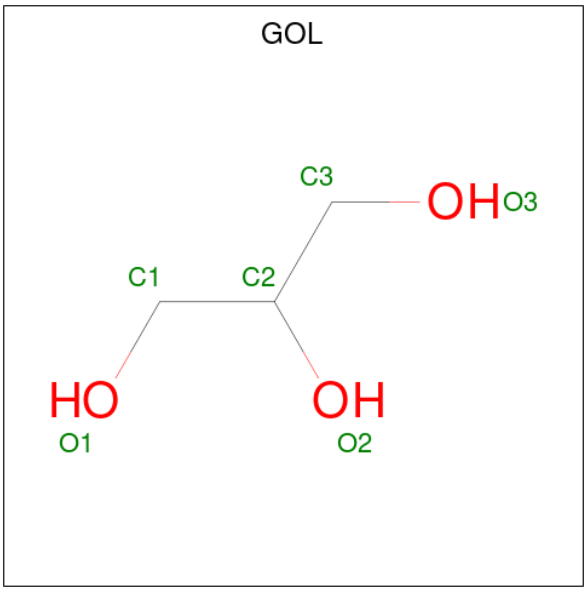
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	202	1654	1054	260	326	14	0	18	0

- Molecule 4 is a protein called TCR beta chain.

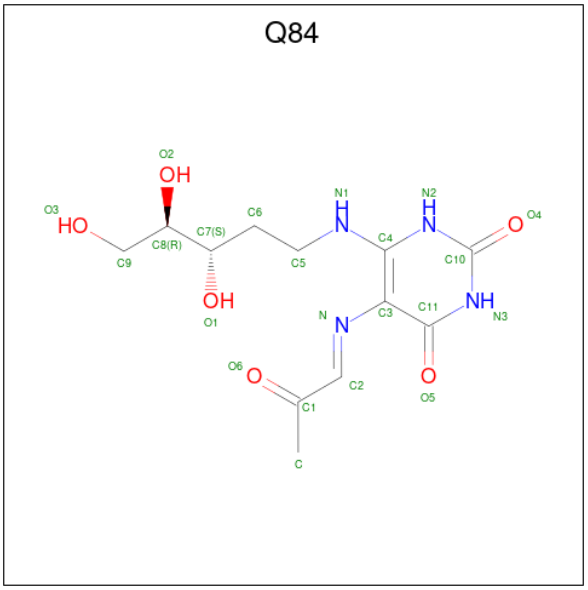
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	242	1927	1222	327	364	14	0	13	0
			Total	C	N	O	S			
4	H	244	2003	1271	341	378	13	0	20	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	3	3	0	0
			Total	C	O		
5	A	1	6	3	3	0	0
			Total	C	O		
5	C	1	6	3	3	0	0
			Total	C	O		
5	E	1	6	3	3	0	0
			Total	C	O		
5	F	1	6	3	3	0	0
			Total	C	O		
5	F	1	6	3	3	0	0

- Molecule 6 is 1,2-dideoxy-1-({2,6-dioxo-5-[(E)-(2-oxopropylidene)amino]-1,2,3,6-tetrahydro pyrimidin-4-yl}amino)-D-erythro-pentitol (three-letter code: Q84) (formula: $C_{12}H_{18}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 42 24 8 10	0	1
6	C	1	Total C N O 21 12 4 5	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0
7	B	1	Total Na 1 1	0	0
7	F	1	Total Na 1 1	0	0
7	H	1	Total Na 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	267	Total O 267 267	0	0
8	B	82	Total O 82 82	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	C	259	259	259	0	0
			Total	O		
8	D	106	106	106	0	0
			Total	O		
8	E	116	116	116	0	0
			Total	O		
8	F	102	102	102	0	0
			Total	O		
8	G	260	260	260	0	0
			Total	O		
8	H	295	295	295	0	0

3 Residue-property plots (i)

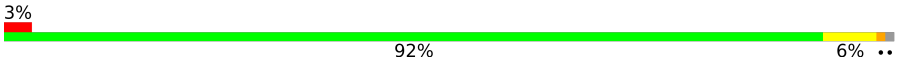
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Major histocompatibility complex class I-related gene protein

Chain A:

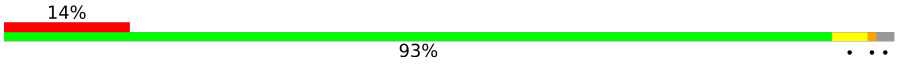
• Molecule 1: Major histocompatibility complex class I-related gene protein

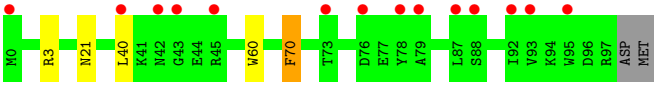
Chain C:



• Molecule 2: Beta-2-microglobulin

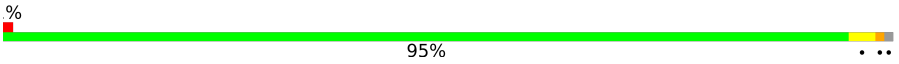
Chain B:





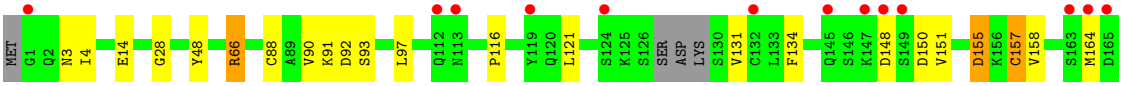
• Molecule 2: Beta-2-microglobulin

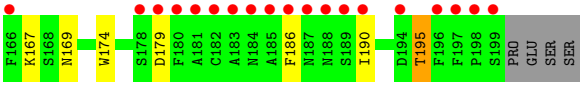
Chain F:



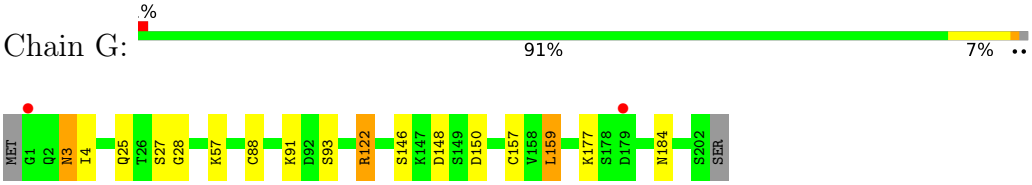
• Molecule 3: TCR alpha chain

Chain D:

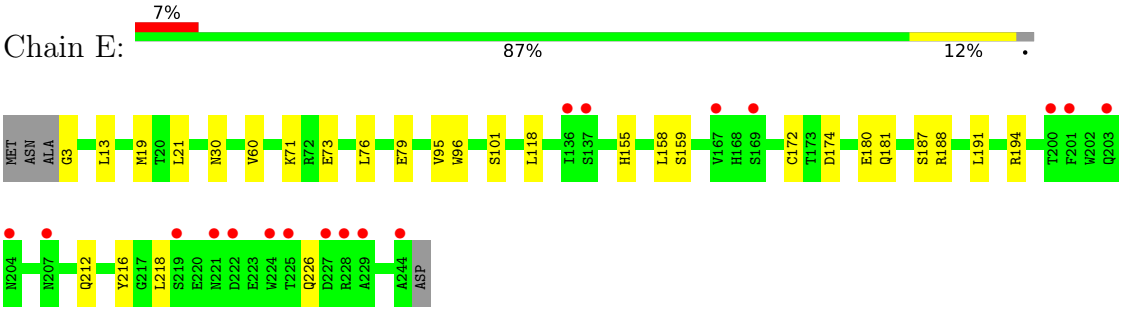




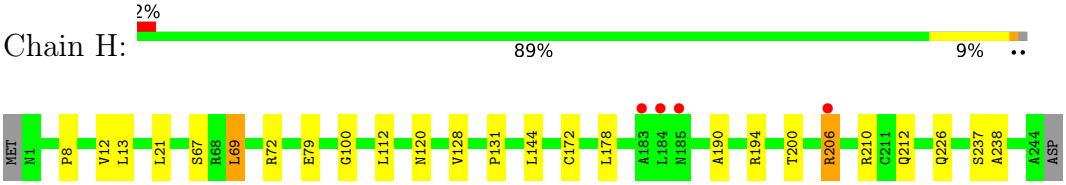
• Molecule 3: TCR alpha chain



• Molecule 4: TCR beta chain



• Molecule 4: TCR beta chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	218.06Å 70.24Å 144.02Å 90.00° 104.57° 90.00°	Depositor
Resolution (Å)	48.32 – 1.96 48.32 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.32-1.96) 99.2 (48.32-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.154 , 0.190 0.155 , 0.189	Depositor DCC
R_{free} test set	7542 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.7	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	0.97	EDS
Total number of atoms	14699	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: GOL, NA, Q84

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	0.55	0/2277	0.64	0/3096
1	C	0.50	0/2339	0.62	0/3181
2	B	0.45	0/803	0.57	0/1096
2	F	0.49	0/829	0.63	1/1128 (0.1%)
3	D	0.46	0/1560	0.61	1/2117 (0.0%)
3	G	0.57	0/1738	0.71	1/2353 (0.0%)
4	E	0.42	0/2017	0.58	0/2748
4	H	0.58	0/2113	0.69	1/2874 (0.0%)
All	All	0.51	0/13676	0.64	4/18593 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	159	LEU	CA-CB-CG	7.04	131.48	115.30
3	D	92	ASP	CB-CG-OD1	5.84	123.56	118.30
2	F	3	ARG	NE-CZ-NH2	-5.40	117.60	120.30
4	H	69	LEU	CA-CB-CG	5.09	127.02	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2185	0	2073	16	0
1	C	2245	0	2138	15	0
2	B	777	0	720	3	0
2	F	803	0	755	3	0
3	D	1515	0	1417	18	0
3	G	1654	0	1619	10	0
4	E	1927	0	1825	18	0
4	H	2003	0	1927	28	0
5	A	12	0	16	0	0
5	C	6	0	8	1	0
5	E	6	0	8	2	0
5	F	12	0	16	0	0
6	A	42	0	0	1	0
6	C	21	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
8	A	267	0	0	9	0
8	B	82	0	0	1	0
8	C	259	0	0	6	0
8	D	106	0	0	1	0
8	E	116	0	0	4	0
8	F	102	0	0	2	0
8	G	260	0	0	2	0
8	H	295	0	0	12	0
All	All	14699	0	12522	102	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 (102) 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)
3:G:157[B]:CYS:SG	8:H:437:HOH:O	2.21	0.94
3:G:150:ASP:HB2	3:G:177:LYS:HD2	1.62	0.81
4:E:73:GLU:OE2	8:E:401:HOH:O	2.02	0.77
6:A:303[B]:Q84:O3	8:A:401:HOH:O	2.04	0.76
4:H:226:GLN:OE1	8:H:402:HOH:O	2.05	0.73
4:E:188:ARG:HD2	5:E:301:GOL:H31	1.72	0.72
4:H:178[B]:LEU:HD22	4:H:190:ALA:HB3	1.72	0.71
3:D:66[A]:ARG:NH1	8:D:301:HOH:O	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:148:ASP:HB3	3:D:151:VAL:HG12	1.73	0.69
4:H:206[A]:ARG:HH11	4:H:206[A]:ARG:HG2	1.60	0.66
1:A:72:MET:SD	8:A:632:HOH:O	2.53	0.66
1:A:249:GLN:O	8:A:402:HOH:O	2.13	0.65
3:G:148:ASP:OD2	3:G:177:LYS:NZ	2.30	0.64
1:C:264[B]:HIS:ND1	8:C:408:HOH:O	2.30	0.63
4:H:72[B]:ARG:NE	8:H:404:HOH:O	2.27	0.63
4:H:72[B]:ARG:NH1	8:H:405:HOH:O	2.33	0.61
4:H:212[A]:GLN:NE2	8:H:401:HOH:O	2.03	0.61
4:E:60[B]:VAL:HG12	8:E:424:HOH:O	2.02	0.60
2:F:31:HIS:HD2	8:F:256:HOH:O	1.85	0.59
3:G:28:GLY:HA3	3:G:93[A]:SER:OG	2.04	0.58
1:C:46[B]:ARG:NH1	8:C:409:HOH:O	2.38	0.57
4:E:95:VAL:HG12	4:E:96:TRP:CD1	2.40	0.56
2:B:3:ARG:HD2	8:B:239:HOH:O	2.04	0.56
4:H:206[B]:ARG:NH2	8:H:406:HOH:O	2.35	0.56
1:A:153:GLN:NE2	8:A:408:HOH:O	2.39	0.55
4:H:8:PRO:HD2	4:H:21:LEU:HD22	1.88	0.54
4:E:21[A]:LEU:HD12	4:E:76:LEU:HD23	1.90	0.54
4:H:210:ARG:NE	4:H:212[B]:GLN:OE1	2.37	0.54
2:F:3:ARG:HD2	8:F:265:HOH:O	2.07	0.54
3:D:28:GLY:HA3	3:D:93:SER:HB3	1.91	0.54
1:A:215:MET:HE3	1:A:218:GLY:HA2	1.90	0.53
4:H:120[A]:ASN:HB2	8:H:515:HOH:O	2.09	0.53
1:C:186:VAL:HG11	1:C:269:VAL:HG22	1.90	0.52
4:H:206[A]:ARG:NH1	8:H:408:HOH:O	2.42	0.52
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.45	0.52
1:A:246:LEU:O	8:A:403:HOH:O	2.19	0.52
3:G:3[A]:ASN:OD1	8:G:301:HOH:O	2.19	0.51
1:C:16:ILE:HD12	1:C:16:ILE:H	1.74	0.51
3:G:184:ASN:ND2	8:G:307:HOH:O	2.42	0.51
4:E:181:GLN:O	4:E:187:SER:HB2	2.11	0.51
3:D:157:CYS:SG	4:E:172[B]:CYS:HB2	2.50	0.51
4:H:12[B]:VAL:HG23	8:H:418:HOH:O	2.10	0.51
1:C:215:MET:HG3	1:C:257:HIS:CD2	2.46	0.51
4:E:174:ASP:HB2	4:E:191:LEU:HD12	1.92	0.50
4:H:206[A]:ARG:HH11	4:H:206[A]:ARG:CG	2.24	0.50
1:C:222:VAL:HA	4:H:200[A]:THR:HG21	1.93	0.50
3:D:158:VAL:HG22	3:D:169:ASN:OD1	2.13	0.48
4:H:13:LEU:CD1	4:H:112[B]:LEU:HD11	2.43	0.48
1:C:246:LEU:O	8:C:403:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:116:PRO:HB2	3:D:195:THR:HG22	1.95	0.48
1:A:0:MET:O	1:A:102:GLU:HG3	2.13	0.48
1:C:211[B]:TYR:OH	8:C:402:HOH:O	2.19	0.48
3:D:14:GLU:OE1	3:D:167:LYS:HE3	2.14	0.48
3:G:4[B]:ILE:HD11	3:G:88[B]:CYS:SG	2.53	0.48
1:A:137:HIS:O	1:A:141[A]:GLN:HG2	2.14	0.48
3:G:157[B]:CYS:HB2	4:H:172[B]:CYS:SG	2.55	0.47
4:H:128:VAL:HG23	4:H:238:ALA:HB3	1.95	0.47
4:E:30:ASN:ND2	4:E:71:LYS:HE3	2.29	0.47
4:H:120[B]:ASN:HB3	8:H:515:HOH:O	2.14	0.47
1:C:0:MET:O	1:C:102:GLU:HG3	2.15	0.47
1:A:149:GLU:HG2	8:A:551:HOH:O	2.15	0.46
4:H:212[B]:GLN:HG2	4:H:237[B]:SER:OG	2.15	0.46
1:C:221:ILE:O	4:H:200[B]:THR:HG21	2.15	0.46
1:C:1:ARG:HG2	8:C:549:HOH:O	2.15	0.45
1:C:173[A]:LYS:HE3	5:C:301:GOL:O3	2.17	0.45
3:D:121:LEU:HD23	3:D:131:VAL:HG12	1.98	0.45
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.69	0.45
4:H:67[B]:SER:OG	4:H:69:LEU:HD13	2.17	0.45
3:D:4[A]:ILE:HD11	3:D:88[A]:CYS:SG	2.58	0.44
1:A:9:ARG:NH1	8:A:415:HOH:O	2.50	0.44
3:D:48:TYR:CZ	4:E:101:SER:HA	2.52	0.44
3:D:164[B]:MET:HE1	8:E:486:HOH:O	2.17	0.44
4:E:118:LEU:HD13	4:E:218:LEU:HD22	2.00	0.44
4:E:155:HIS:HB3	4:E:216:TYR:HB2	1.99	0.44
1:C:113:ALA:HB2	2:F:60:TRP:CE2	2.53	0.44
1:C:52:GLU:OE1	8:C:404:HOH:O	2.21	0.44
1:A:160:GLU:OE2	8:A:404:HOH:O	2.21	0.43
3:D:155:ASP:OD1	3:D:155:ASP:N	2.32	0.43
2:B:21:ASN:HB3	2:B:70:PHE:CE2	2.53	0.43
3:D:91:LYS:HG2	3:D:97:LEU:HD23	1.99	0.43
1:A:200:CYS:HB2	1:A:214:TRP:CZ2	2.53	0.43
4:H:79:GLU:OE2	8:H:403:HOH:O	2.21	0.43
4:H:131:PRO:HD3	4:H:144:LEU:HG	2.00	0.43
1:C:46[A]:ARG:HD3	1:C:46[A]:ARG:HA	1.92	0.43
4:E:180:GLU:OE1	5:E:301:GOL:O3	2.25	0.43
1:A:265:MET:HE2	1:A:265:MET:HB2	1.84	0.43
4:H:210:ARG:NH1	4:H:212[B]:GLN:OE1	2.49	0.43
4:E:3:GLY:N	8:E:407:HOH:O	2.52	0.42
3:G:122:ARG:HG2	8:H:650:HOH:O	2.19	0.42
1:A:79:ARG:NE	8:A:417:HOH:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:SER:HB3	1:A:99:GLU:HG2	2.02	0.42
3:D:131:VAL:HG22	3:D:174:TRP:HB3	2.02	0.41
4:E:158:LEU:HD23	4:E:159:SER:N	2.34	0.41
4:H:13:LEU:HD12	4:H:112[B]:LEU:HD11	2.02	0.41
4:H:206[A]:ARG:HG2	4:H:206[A]:ARG:NH1	2.29	0.41
3:D:157:CYS:HB3	4:E:172[B]:CYS:SG	2.60	0.41
4:E:13:LEU:HD11	4:E:19[B]:MET:SD	2.60	0.41
3:D:4[B]:ILE:HD11	3:D:90:VAL:HB	2.03	0.41
3:D:48:TYR:CE1	4:E:101:SER:HA	2.56	0.41
3:D:134:PHE:HB2	3:D:186:PHE:CE1	2.56	0.41
3:G:91[A]:LYS:NZ	4:H:100:GLY:O	2.41	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	270/271 (100%)	266 (98%)	4 (2%)	0	100	100
1	C	274/271 (101%)	269 (98%)	5 (2%)	0	100	100
2	B	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
2	F	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	D	196/204 (96%)	191 (97%)	5 (3%)	0	100	100
3	G	218/204 (107%)	216 (99%)	2 (1%)	0	100	100
4	E	253/246 (103%)	248 (98%)	5 (2%)	0	100	100
4	H	262/246 (106%)	260 (99%)	2 (1%)	0	100	100
All	All	1668/1642 (102%)	1643 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	230/241 (95%)	226 (98%)	4 (2%)	60	55
1	C	237/241 (98%)	232 (98%)	5 (2%)	53	46
2	B	81/95 (85%)	79 (98%)	2 (2%)	47	38
2	F	86/95 (90%)	85 (99%)	1 (1%)	71	68
3	D	162/181 (90%)	153 (94%)	9 (6%)	21	9
3	G	193/181 (107%)	185 (96%)	8 (4%)	30	18
4	E	209/212 (99%)	205 (98%)	4 (2%)	57	50
4	H	220/212 (104%)	217 (99%)	3 (1%)	67	62
All	All	1418/1458 (97%)	1382 (98%)	36 (2%)	47	38

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	32	PRO
1	A	73	PHE
1	A	82	ARG
2	B	40	LEU
2	B	70	PHE
1	C	73	PHE
1	C	215	MET
1	C	221	ILE
1	C	222	VAL
1	C	261	SER
3	D	3	ASN
3	D	66[A]	ARG
3	D	66[B]	ARG
3	D	150	ASP
3	D	155	ASP
3	D	157	CYS
3	D	179	ASP
3	D	190	ILE

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Mol	Chain	Res	Type
3	D	195	THR
4	E	79	GLU
4	E	194	ARG
4	E	212	GLN
4	E	226	GLN
2	F	70	PHE
3	G	3[A]	ASN
3	G	3[B]	ASN
3	G	25	GLN
3	G	27	SER
3	G	57	LYS
3	G	122	ARG
3	G	146	SER
3	G	159	LEU
4	H	194	ARG
4	H	206[A]	ARG
4	H	206[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
3	G	25	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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
5	GOL	A	301	-	5,5,5	0.98	0	5,5,5	1.15	0
5	GOL	F	102	-	5,5,5	0.61	0	5,5,5	1.26	1 (20%)
6	Q84	C	302	1	20,21,22	1.16	2 (10%)	18,27,29	0.95	1 (5%)
5	GOL	A	302	-	5,5,5	1.15	0	5,5,5	1.35	0
5	GOL	E	301	-	5,5,5	1.07	0	5,5,5	1.00	0
6	Q84	A	303[A]	1	20,21,22	1.14	2 (10%)	18,27,29	0.85	1 (5%)
5	GOL	F	101	-	5,5,5	1.03	0	5,5,5	0.94	0
5	GOL	C	301	-	5,5,5	1.00	0	5,5,5	0.87	0
6	Q84	A	303[B]	1	20,21,22	1.10	2 (10%)	18,27,29	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	301	-	-	2/4/4/4	-
5	GOL	F	102	-	-	2/4/4/4	-
6	Q84	C	302	1	-	1/15/16/17	0/1/1/1
5	GOL	A	302	-	-	3/4/4/4	-
5	GOL	E	301	-	-	2/4/4/4	-
6	Q84	A	303[A]	1	-	2/15/16/17	0/1/1/1
5	GOL	F	101	-	-	0/4/4/4	-
5	GOL	C	301	-	-	4/4/4/4	-
6	Q84	A	303[B]	1	-	5/15/16/17	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	302	Q84	C4-N1	4.20	1.38	1.32
6	A	303[B]	Q84	C4-N1	3.95	1.38	1.32
6	A	303[A]	Q84	C1-C2	-3.83	1.45	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	303[A]	Q84	C4-N1	3.03	1.36	1.32
6	A	303[B]	Q84	C1-C2	-2.74	1.46	1.49
6	C	302	Q84	C1-C2	-2.71	1.46	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	302	Q84	C-C1-C2	3.37	119.71	113.75
6	A	303[A]	Q84	C-C1-C2	2.58	118.31	113.75
5	F	102	GOL	C3-C2-C1	-2.24	103.00	111.70

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	302	GOL	O1-C1-C2-C3
5	C	301	GOL	C1-C2-C3-O3
5	E	301	GOL	O1-C1-C2-C3
5	F	102	GOL	O1-C1-C2-C3
6	A	303[B]	Q84	C6-C7-C8-C9
6	A	303[B]	Q84	C6-C7-C8-O2
6	A	303[A]	Q84	C5-C6-C7-O1
6	C	302	Q84	C5-C6-C7-O1
5	F	102	GOL	O1-C1-C2-O2
5	A	301	GOL	C1-C2-C3-O3
5	C	301	GOL	O1-C1-C2-C3
5	A	302	GOL	O1-C1-C2-O2
5	E	301	GOL	O1-C1-C2-O2
6	A	303[B]	Q84	C5-C6-C7-O1
5	A	302	GOL	O2-C2-C3-O3
5	C	301	GOL	O2-C2-C3-O3
5	A	301	GOL	O2-C2-C3-O3
6	A	303[B]	Q84	O1-C7-C8-C9
5	C	301	GOL	O1-C1-C2-O2
6	A	303[A]	Q84	N1-C5-C6-C7
6	A	303[B]	Q84	N1-C5-C6-C7

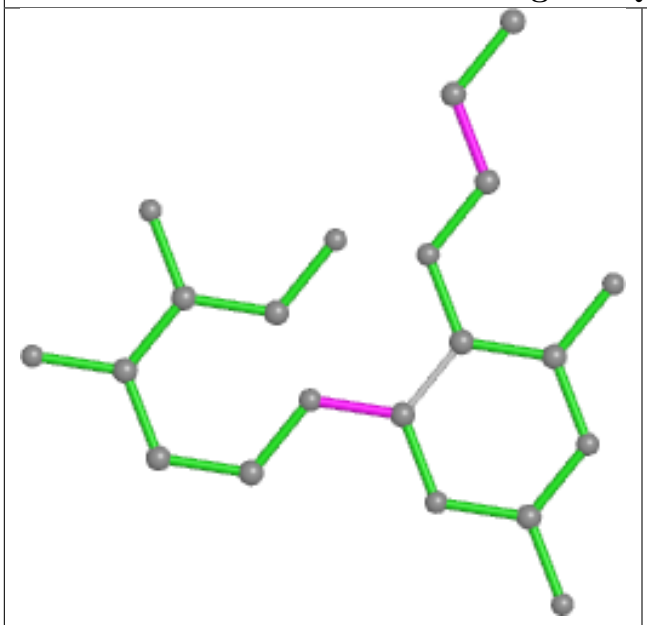
There are no ring outliers.

3 monomers are involved in 4 short contacts:

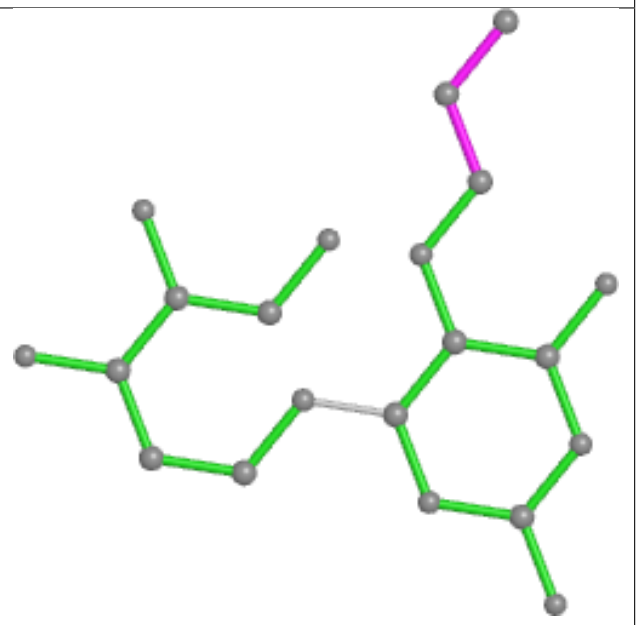
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	301	GOL	2	0
5	C	301	GOL	1	0
6	A	303[B]	Q84	1	0

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.

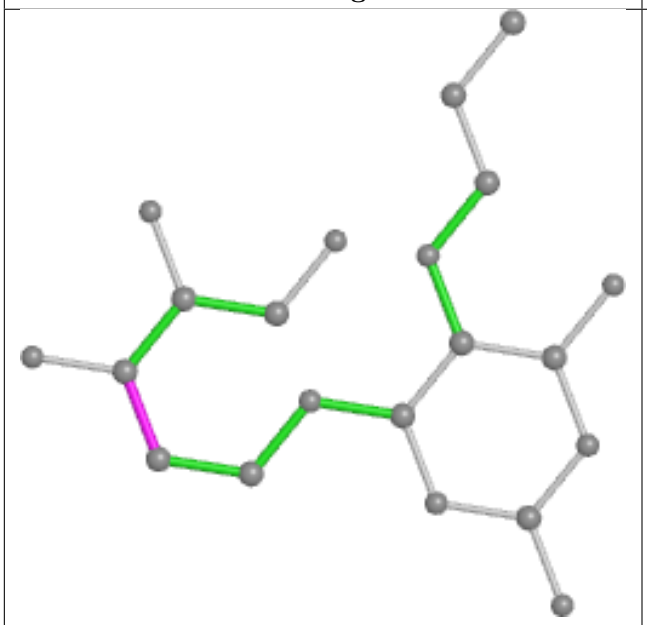
Ligand Q84 C 302



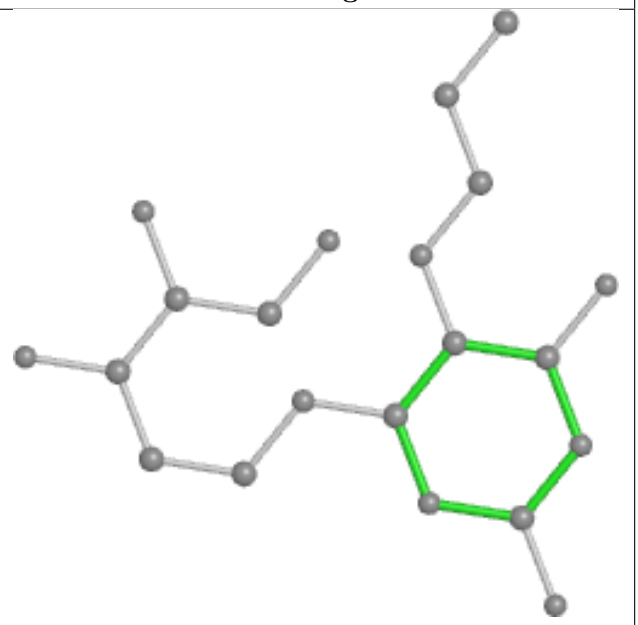
Bond lengths



Bond angles

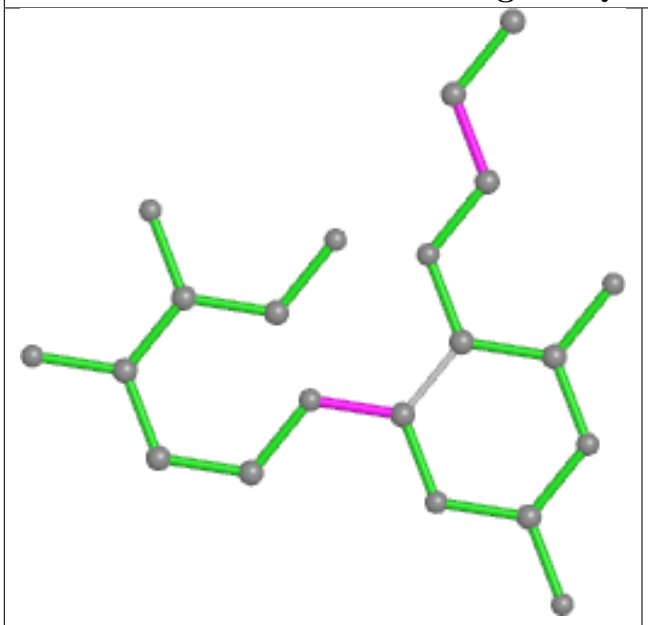


Torsions

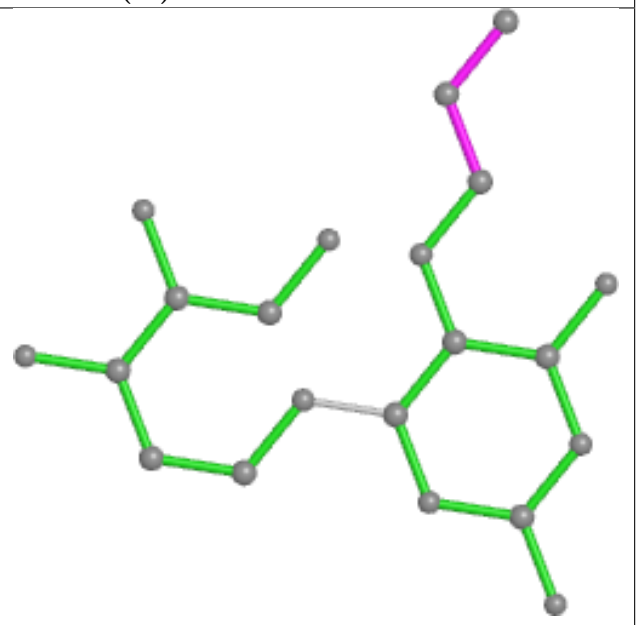


Rings

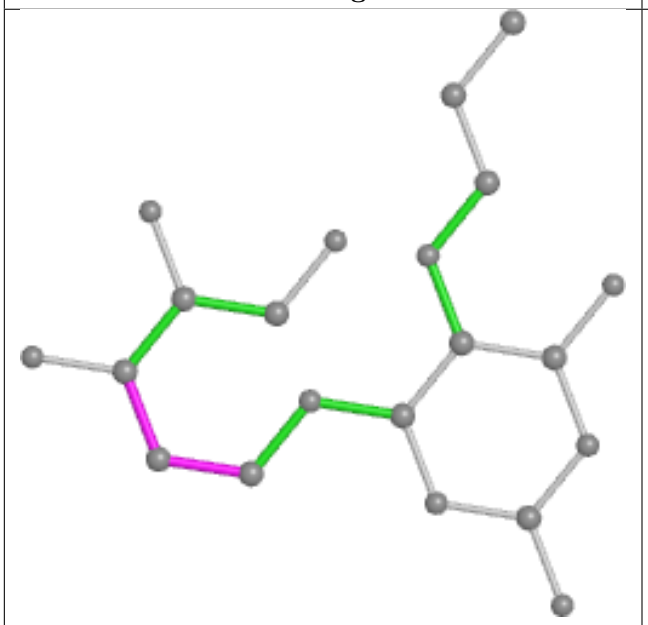
Ligand Q84 A 303 (A)



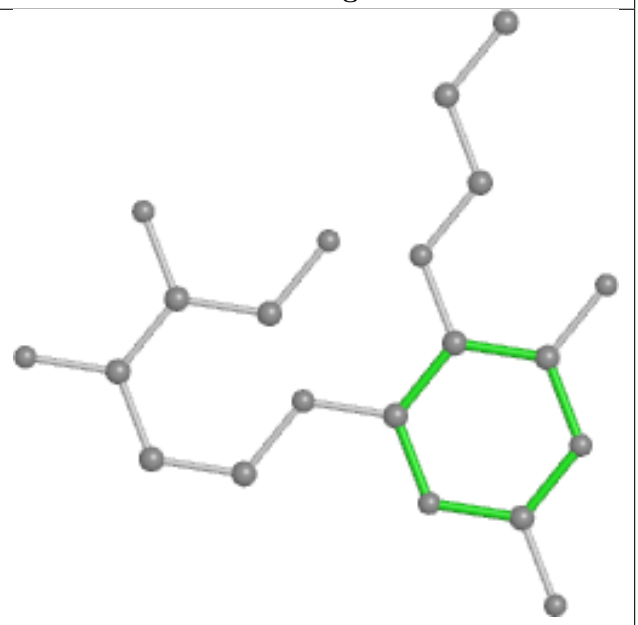
Bond lengths



Bond angles

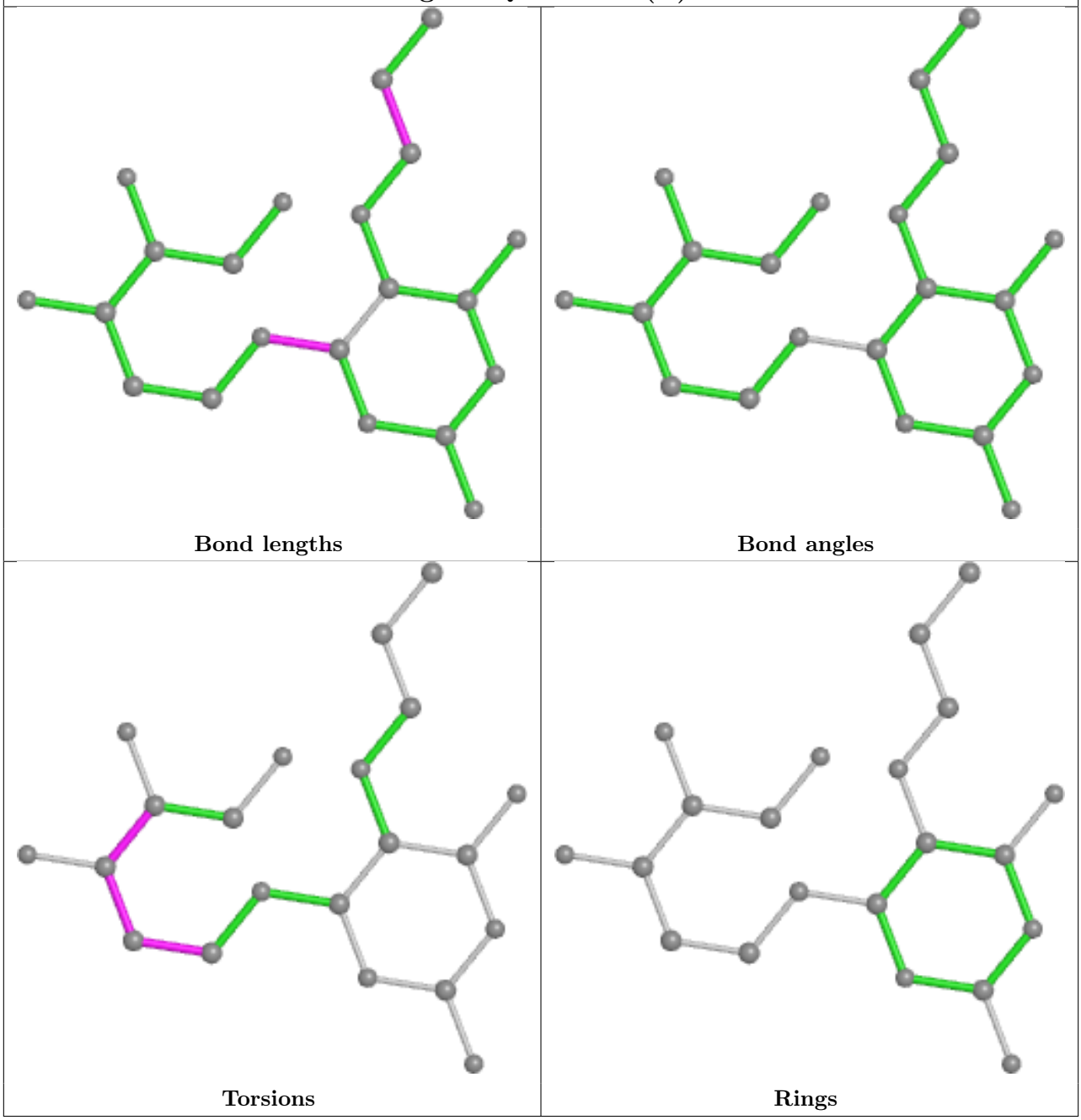


Torsions



Rings

Ligand Q84 A 303 (B)



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	265/271 (97%)	-0.17	3 (1%)	80	85	26, 41, 80, 97	4 (1%)
1	C	269/271 (99%)	-0.14	9 (3%)	46	56	28, 40, 68, 94	9 (3%)
2	B	98/100 (98%)	0.62	14 (14%)	2	4	33, 58, 86, 93	1 (1%)
2	F	99/100 (99%)	-0.26	1 (1%)	82	87	30, 43, 65, 78	2 (2%)
3	D	196/204 (96%)	0.53	32 (16%)	1	2	33, 56, 97, 122	4 (2%)
3	G	202/204 (99%)	-0.37	2 (0%)	82	87	24, 35, 61, 92	7 (3%)
4	E	242/246 (98%)	0.11	18 (7%)	14	22	36, 58, 96, 118	7 (2%)
4	H	244/246 (99%)	-0.13	4 (1%)	72	79	25, 36, 53, 81	6 (2%)
All	All	1615/1642 (98%)	-0.02	83 (5%)	28	37	24, 43, 85, 122	40 (2%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	227	ASP	5.1
4	E	224	TRP	4.4
3	D	179	ASP	4.4
3	D	163	SER	4.1
3	D	164[A]	MET	4.0
2	B	78	TYR	3.7
3	D	166	PHE	3.6
3	G	1	GLY	3.6
2	B	43	GLY	3.5
1	C	17	HIS	3.5
3	D	190	ILE	3.5
2	B	76	ASP	3.5
3	D	180	PHE	3.4
2	B	92	ILE	3.3
1	A	196	THR	3.3
4	E	204	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
4	E	225	THR	3.2
3	D	149	SER	3.2
4	E	200	THR	3.2
3	D	182	CYS	3.2
2	B	45	ARG	3.2
3	D	181	ALA	3.2
3	D	186	PHE	3.1
3	D	1	GLY	3.1
4	E	201	PHE	3.1
4	E	221	ASN	3.1
1	C	211[A]	TYR	3.1
1	A	221	ILE	3.0
3	D	148	ASP	3.0
1	C	247	ASP	3.0
2	B	73	THR	3.0
3	D	185	ALA	2.9
3	D	197	PHE	2.9
1	C	251	SER	2.9
3	D	147	LYS	2.9
3	D	113	ASN	2.9
1	C	16	ILE	2.8
3	D	119	TYR	2.8
1	C	252	ASN	2.8
3	D	184	ASN	2.8
3	D	178	SER	2.8
1	A	222	VAL	2.8
3	D	196	PHE	2.7
1	C	248	PRO	2.7
3	D	112	GLN	2.7
3	D	188	ASN	2.6
4	H	185	ASN	2.6
1	C	0	MET	2.6
4	E	219	SER	2.6
2	B	93	VAL	2.6
4	E	137	SER	2.5
3	D	165	ASP	2.4
3	D	199	SER	2.4
2	B	42	ASN	2.4
3	D	198	PRO	2.4
2	B	88	SER	2.3
2	B	40	LEU	2.3
4	E	167	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	183	ALA	2.3
4	H	183	ALA	2.3
2	B	87	LEU	2.3
4	E	203	GLN	2.3
3	D	189	SER	2.3
4	E	222	ASP	2.3
4	E	207	ASN	2.2
4	E	229	ALA	2.2
4	E	136	ILE	2.2
2	B	0	MET	2.2
2	B	95	TRP	2.2
4	E	244	ALA	2.2
3	D	132	CYS	2.2
3	D	124	SER	2.1
3	D	187	ASN	2.1
3	G	179	ASP	2.1
2	F	0	MET	2.1
4	E	228	ARG	2.1
2	B	79	ALA	2.1
4	E	169	SER	2.1
4	H	184	LEU	2.1
3	D	145	GLN	2.1
3	D	194	ASP	2.0
1	C	222	VAL	2.0
4	H	206[A]	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

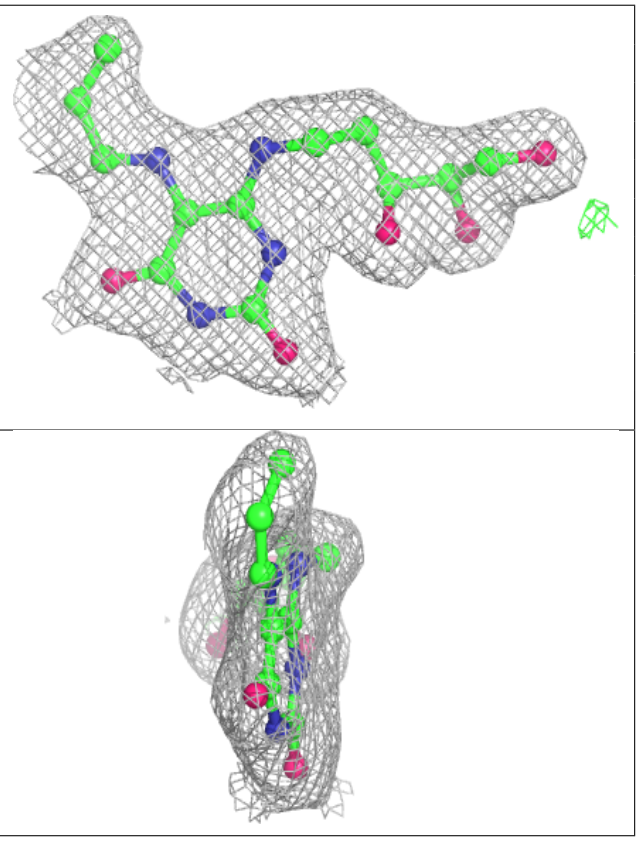
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	A	301	6/6	0.85	0.11	58,61,63,67	0
5	GOL	E	301	6/6	0.89	0.29	57,66,68,69	0
7	NA	B	101	1/1	0.89	0.27	65,65,65,65	0
5	GOL	C	301	6/6	0.90	0.32	59,64,66,70	6
5	GOL	A	302	6/6	0.92	0.19	46,54,55,58	0
7	NA	A	304	1/1	0.93	0.08	46,46,46,46	0
5	GOL	F	101	6/6	0.94	0.11	32,37,38,39	6
5	GOL	F	102	6/6	0.96	0.13	35,45,48,51	0
7	NA	F	103	1/1	0.96	0.20	44,44,44,44	0
6	Q84	C	302	21/22	0.97	0.12	28,33,37,40	0
6	Q84	A	303[A]	21/22	0.98	0.12	25,28,30,31	21
6	Q84	A	303[B]	21/22	0.98	0.12	23,28,30,41	21
7	NA	H	301	1/1	0.99	0.05	39,39,39,39	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.

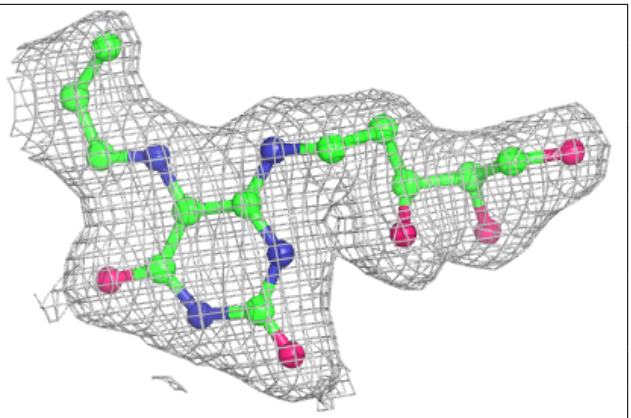
Electron density around Q84 C 302:

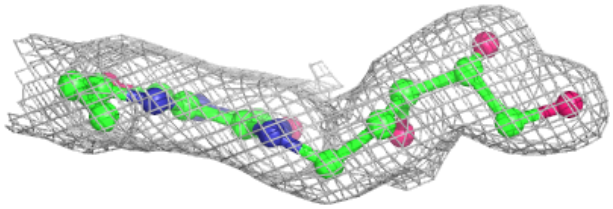
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

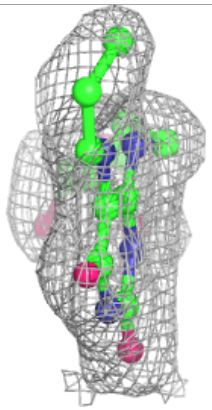


Electron density around Q84 A 303 (A):

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

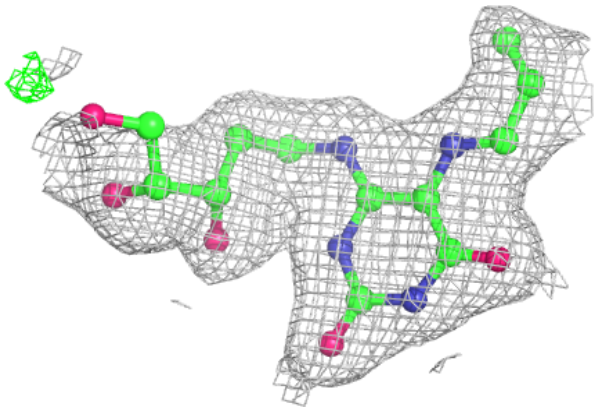


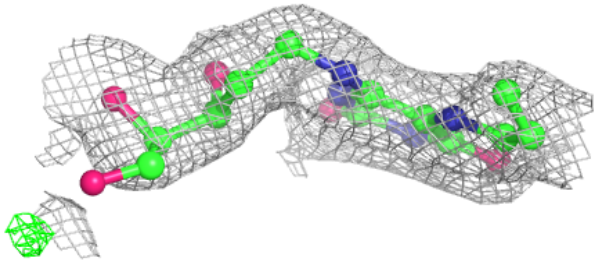


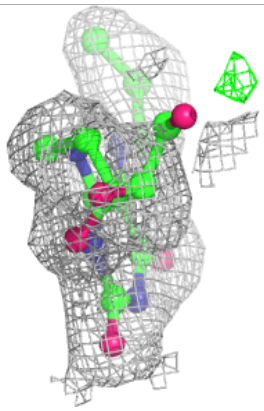


Electron density around Q84 A 303 (B):

$2mF_o$-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.