Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 06:26 PM EDT

PDB ID	:	6W9U
Title	:	Structure of human MAIT A-F7 TCR in complex with patient MR1-R9H-Ac-6-FP
Authors	:	Awad, W.; Rossjohn, J.
Deposited on	:	2020-03-23
Resolution	:	1.89 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:

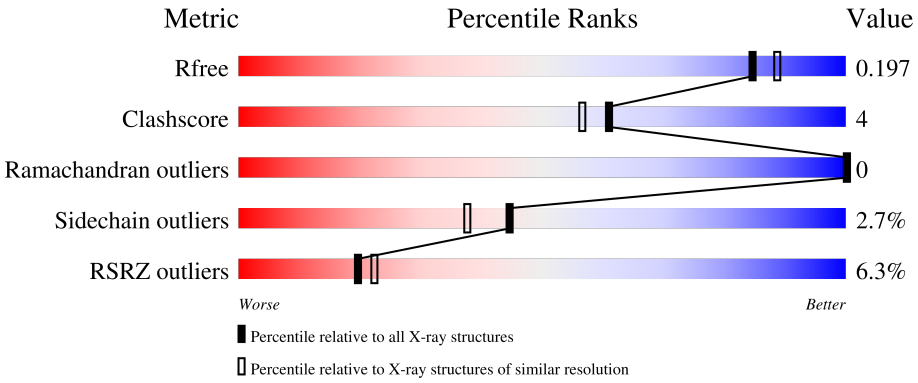
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	3% 87% 10%
1	C	271	3% 89% 10%
2	B	100	21% 92% 6%
2	F	100	93% 7%
3	D	204	20% 78% 12% 9%

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Mol	Chain	Length	Quality of chain
3	G	204	87% 10%
4	E	246	8% 84% 12%
4	H	246	2% 87% 12%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14547 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
1	A	265	Total	C	N	O	S	0	12	0
			2227	1436	383	395	13			
1	C	268	Total	C	N	O	S	0	14	0
			2270	1464	384	408	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q95460
A	9	HIS	ARG	engineered mutation	UNP Q95460
A	261	SER	CYS	conflict	UNP Q95460
C	0	MET	-	expression tag	UNP Q95460
C	9	HIS	ARG	engineered mutation	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
2	B	98	Total	C	N	O	S	0	1	0
			785	505	130	147	3			
2	F	100	Total	C	N	O	S	0	3	0
			829	532	139	154	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	expression tag	UNP P61769
F	0	MET	-	expression tag	UNP P61769

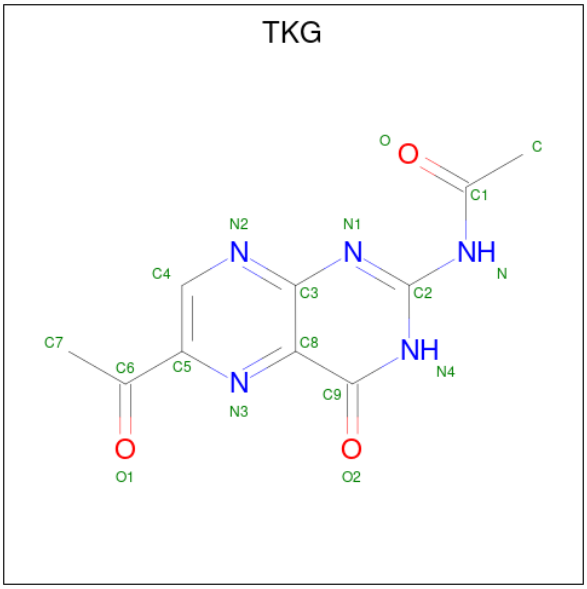
- Molecule 3 is a protein called TCR-alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	186	Total	C	N	O	S	0	4	0
			1425	918	224	274	9			
3	G	199	Total	C	N	O	S	0	20	0
			1628	1043	250	322	13			

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

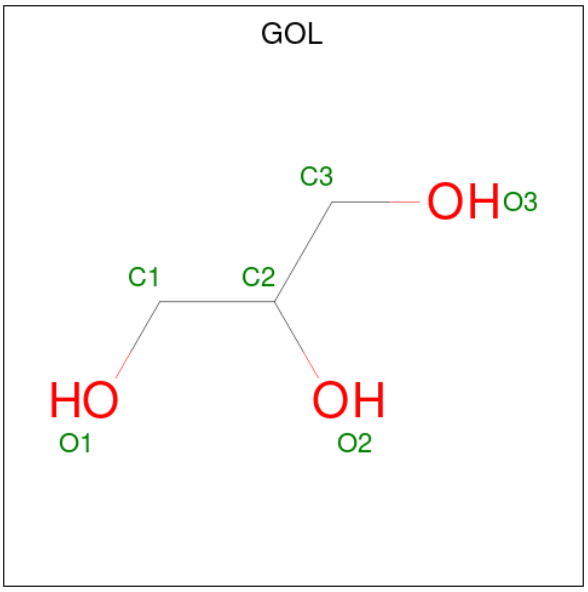
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	239	Total	C	N	O	S	0	7	0
			1869	1180	318	359	12			
4	H	244	Total	C	N	O	S	0	16	0
			1992	1265	340	374	13			

- Molecule 5 is 1-[[6-(1-$l^{1}-oxidanylethyl)-4-$l^{3}-oxidanylidene-2,3,6,8 {a}-tetrahydropteridin-2-yl]-$l^{2}-azanyl]ethanone (three-letter code: TKG) (formula: $C_{10}H_9N_5O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			16	9	5	2		
5	C	1	Total	C	N	O	0	0
			16	9	5	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	270	Total O 270 270	0	0
8	B	70	Total O 70 70	0	0
8	C	256	Total O 256 256	0	0
8	D	104	Total O 104 104	0	0

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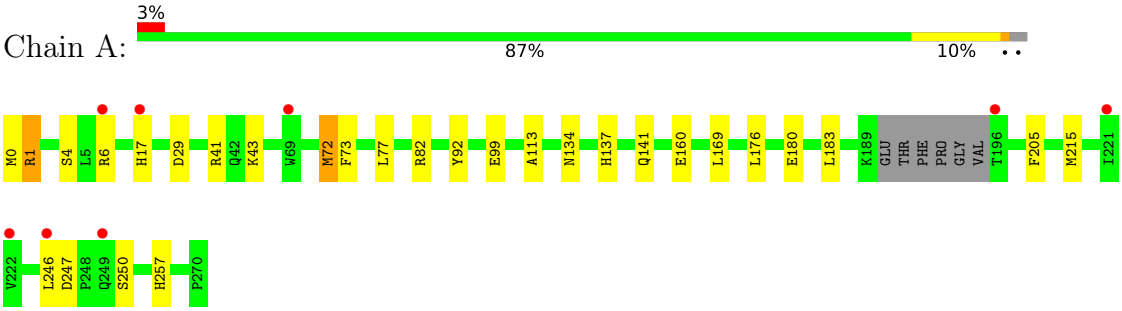
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	105	Total O 105 105	0	0
8	F	100	Total O 100 100	0	0
8	G	250	Total O 250 250	0	0
8	H	310	Total O 310 310	0	0

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.

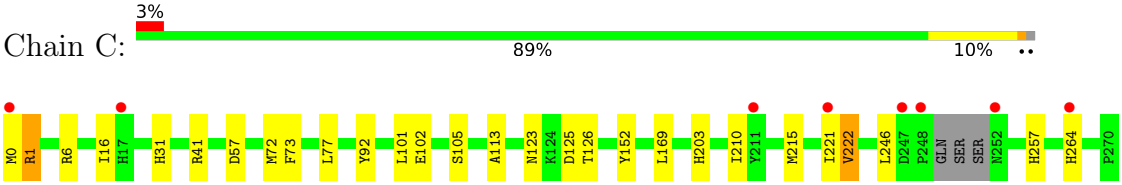
• Molecule 1: Major histocompatibility complex class I-related gene protein

Chain A:



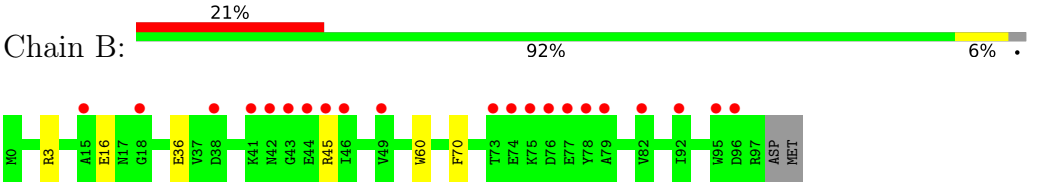
• Molecule 1: Major histocompatibility complex class I-related gene protein

Chain C:



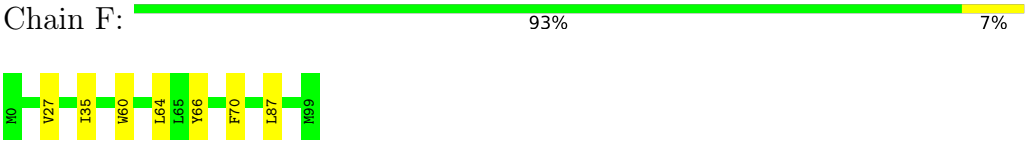
• Molecule 2: Beta-2-microglobulin

Chain B:



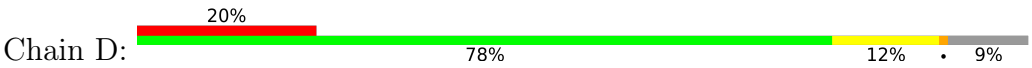
• Molecule 2: Beta-2-microglobulin

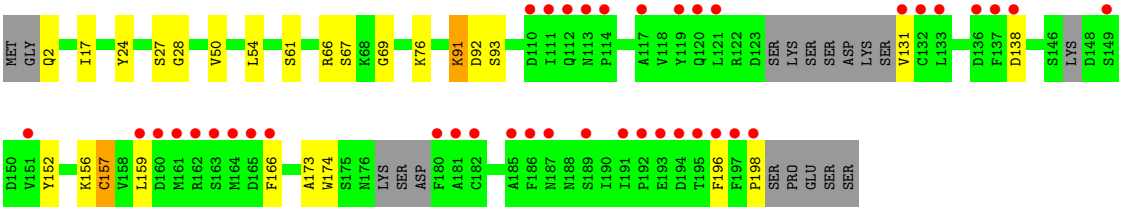
Chain F:



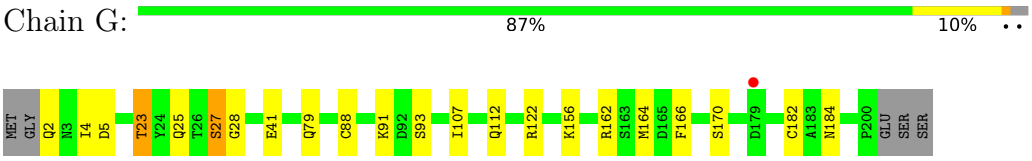
• Molecule 3: TCR-alpha chain

Chain D:

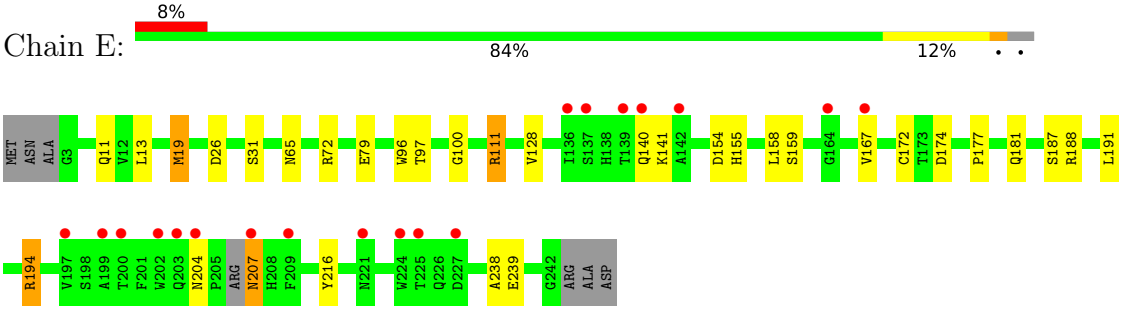




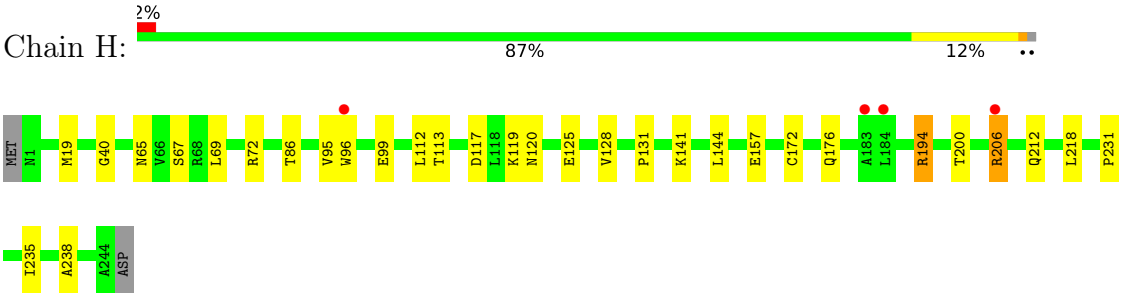
• Molecule 3: TCR-alpha chain



• 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	218.32Å 70.79Å 142.98Å 90.00° 104.59° 90.00°	Depositor
Resolution (Å)	40.11 – 1.89 46.36 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.8 (40.11-1.89) 98.8 (46.36-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.162 , 0.197 0.163 , 0.197	Depositor DCC
R_{free} test set	8492 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.9	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	14547	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 3.25% 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: CL, TKG, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.52	0/2330	0.67	2/3168 (0.1%)
1	C	0.48	0/2379	0.66	0/3233
2	B	0.39	0/811	0.57	0/1106
2	F	0.45	0/861	0.60	0/1170
3	D	0.46	0/1468	0.62	1/1995 (0.1%)
3	G	0.54	0/1723	0.69	0/2335
4	E	0.40	0/1936	0.58	0/2638
4	H	0.58	0/2091	0.67	0/2846
All	All	0.49	0/13599	0.64	3/18491 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	ARG	NE-CZ-NH2	-9.55	115.52	120.30
1	A	1	ARG	NE-CZ-NH1	5.68	123.14	120.30
3	D	92	ASP	CB-CG-OD1	5.49	123.25	118.30

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	2227	0	2120	19	0
1	C	2270	0	2176	18	0
2	B	785	0	709	3	0
2	F	829	0	787	4	0
3	D	1425	0	1316	14	0
3	G	1628	0	1595	18	0
4	E	1869	0	1737	23	0
4	H	1992	0	1910	29	0
5	A	16	0	0	0	0
5	C	16	0	0	0	0
6	A	12	0	16	0	0
6	C	6	0	8	0	0
6	F	6	0	8	0	0
7	A	1	0	0	0	0
8	A	270	0	0	4	0
8	B	70	0	0	2	0
8	C	256	0	0	7	0
8	D	104	0	0	0	0
8	E	105	0	0	6	0
8	F	100	0	0	2	0
8	G	250	0	0	7	0
8	H	310	0	0	13	0
All	All	14547	0	12382	114	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 (114) 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:28:GLY:HA3	3:G:93[B]:SER:OG	1.86	0.76
1:C:125:ASP:OD1	8:C:401:HOH:O	2.06	0.74
3:G:91:LYS:NZ	8:G:302:HOH:O	2.23	0.71
1:C:210:ILE:O	4:H:206[A]:ARG:HD2	1.90	0.70
4:H:141:LYS:NZ	8:H:305:HOH:O	2.24	0.70
1:C:6:ARG:HD3	8:C:596:HOH:O	1.92	0.69
8:C:420:HOH:O	4:H:200[B]:THR:HG22	1.93	0.68
2:F:87:LEU:O	8:F:201:HOH:O	2.12	0.67
4:H:125:GLU:OE2	8:H:301:HOH:O	2.13	0.66
1:A:41[B]:ARG:NH1	8:A:403:HOH:O	2.21	0.66
1:C:264[B]:HIS:ND1	8:C:406:HOH:O	2.30	0.65
1:C:72[A]:MET:HG3	4:E:96:TRP:CE3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:MET:HG2	4:H:96[B]:TRP:CZ2	2.34	0.62
1:A:6[B]:ARG:NH2	1:A:29:ASP:O	2.24	0.61
4:H:72:ARG:NH2	8:H:308:HOH:O	2.34	0.60
3:D:28:GLY:HA3	3:D:93[B]:SER:OG	2.03	0.58
3:G:25:GLN:NE2	8:G:313:HOH:O	2.37	0.58
1:A:77:LEU:HD13	1:A:92:TYR:HB2	1.86	0.57
4:H:172[B]:CYS:SG	4:H:194:ARG:HD3	2.44	0.57
4:E:207:ASN:N	4:E:207:ASN:HD22	2.01	0.57
3:D:157:CYS:SG	4:E:172[B]:CYS:HB2	2.44	0.56
2:B:45:ARG:NH1	8:B:103:HOH:O	2.38	0.56
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.41	0.55
4:E:13:LEU:HD11	4:E:19[B]:MET:HE2	1.89	0.55
1:A:1:ARG:HB2	8:A:524:HOH:O	2.06	0.54
1:A:215:MET:HG3	1:A:257:HIS:CD2	2.43	0.53
1:A:72:MET:HG2	4:H:96[B]:TRP:CE2	2.44	0.53
1:C:77:LEU:HD13	1:C:92:TYR:HB2	1.90	0.53
3:D:2:GLN:OE1	3:D:27:SER:N	2.39	0.53
3:G:164[A]:MET:HE3	8:H:578:HOH:O	2.09	0.52
4:H:65[B]:ASN:ND2	8:H:315:HOH:O	2.42	0.52
4:E:172[B]:CYS:SG	4:E:194:ARG:HD3	2.50	0.52
4:E:154:ASP:OD1	4:E:177:PRO:HG2	2.10	0.51
3:G:41:GLU:OE1	8:G:301:HOH:O	2.19	0.51
1:A:4:SER:HB3	1:A:99:GLU:HG2	1.91	0.51
2:F:64[B]:LEU:HD22	2:F:66:TYR:HE1	1.75	0.51
4:H:117[B]:ASP:OD1	4:H:119:LYS:HG2	2.11	0.51
1:A:72:MET:HG3	4:H:96[A]:TRP:CE3	2.46	0.51
4:H:157:GLU:OE2	8:H:303:HOH:O	2.19	0.51
4:H:200[B]:THR:HG23	8:H:503:HOH:O	2.10	0.50
3:D:196:PHE:CE2	3:D:198:PRO:HG3	2.48	0.49
3:G:28:GLY:HA3	3:G:93[A]:SER:HB3	1.94	0.49
3:G:2:GLN:OE1	3:G:27:SER:N	2.41	0.49
4:E:111:ARG:NH1	8:E:309:HOH:O	2.45	0.49
4:E:188:ARG:NH2	8:E:308:HOH:O	2.43	0.49
4:E:11:GLN:HG2	4:E:19[B]:MET:SD	2.53	0.49
4:E:65[A]:ASN:ND2	8:E:304:HOH:O	2.33	0.49
4:H:99:GLU:OE1	8:H:304:HOH:O	2.20	0.49
3:D:28:GLY:HA3	3:D:93[A]:SER:HB3	1.95	0.48
4:H:176[B]:GLN:OE1	8:H:302:HOH:O	2.19	0.48
3:G:5:ASP:HB2	3:G:23[A]:THR:HG23	1.94	0.48
3:G:184[B]:ASN:ND2	8:G:305:HOH:O	2.25	0.48
4:H:95:VAL:HG12	4:H:96[B]:TRP:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:166:PHE:CD1	4:H:141:LYS:HE2	2.49	0.48
3:D:50:VAL:O	3:D:66:ARG:HD3	2.15	0.47
3:G:122:ARG:HD2	8:H:398:HOH:O	2.13	0.47
3:D:54:LEU:HD11	3:D:61:SER:HB3	1.97	0.47
4:H:212:GLN:HG3	4:H:235:ILE:HG23	1.97	0.47
1:A:43:LYS:NZ	8:A:414:HOH:O	2.46	0.47
3:D:91:LYS:HE3	8:E:321:HOH:O	2.14	0.47
4:H:206[A]:ARG:HG3	8:H:418:HOH:O	2.15	0.47
4:H:128[B]:VAL:HG13	4:H:238:ALA:HB3	1.96	0.46
3:G:182[B]:CYS:SG	8:G:423:HOH:O	2.61	0.46
3:D:152:TYR:O	3:D:173:ALA:HA	2.15	0.46
4:H:120:ASN:HB3	8:H:442:HOH:O	2.15	0.46
4:H:218:LEU:HD22	4:H:231:PRO:HG2	1.98	0.46
3:D:159:LEU:HB3	4:E:172[B]:CYS:SG	2.56	0.46
2:B:3:ARG:HD2	8:B:143:HOH:O	2.15	0.46
3:D:131:VAL:HG12	3:D:174:TRP:HB3	1.98	0.46
1:C:101:LEU:HD12	1:C:105[A]:SER:OG	2.16	0.45
1:C:246:LEU:O	8:C:403:HOH:O	2.21	0.45
4:H:131:PRO:HD3	4:H:144:LEU:HG	1.99	0.45
3:G:4[A]:ILE:HD11	3:G:88[A]:CYS:SG	2.57	0.45
3:G:28:GLY:N	8:G:308:HOH:O	2.32	0.45
1:C:203:HIS:HD2	8:F:242:HOH:O	2.00	0.44
4:E:174:ASP:HB2	4:E:191:LEU:HD12	1.99	0.44
4:E:19[A]:MET:HE3	4:E:19[A]:MET:HB2	1.71	0.44
4:E:79:GLU:HG2	8:E:317:HOH:O	2.18	0.44
1:C:152:TYR:CE1	4:E:100:GLY:HA3	2.52	0.44
1:C:1:ARG:HA	1:C:102:GLU:HG2	2.00	0.44
1:A:160:GLU:OE2	8:A:402:HOH:O	2.21	0.44
3:D:24:TYR:CZ	3:D:69:GLY:HA2	2.54	0.43
1:C:123:ASN:OD1	1:C:126:THR:N	2.42	0.43
3:G:79:GLN:O	3:G:107[A]:ILE:HD13	2.18	0.43
1:A:72:MET:HA	4:H:96[B]:TRP:CH2	2.53	0.43
1:C:113:ALA:HB2	2:F:60:TRP:CE2	2.54	0.43
4:E:158:LEU:HD23	4:E:159:SER:N	2.34	0.43
4:H:40:GLY:HA2	8:H:565:HOH:O	2.18	0.43
1:A:247:ASP:OD1	1:A:250:SER:N	2.50	0.43
1:A:169[A]:LEU:HD23	1:A:176:LEU:HD13	2.00	0.42
1:C:222:VAL:HA	4:H:200[B]:THR:HG21	2.01	0.42
1:A:180:GLU:O	1:A:205:PHE:HA	2.19	0.42
4:E:26[A]:ASP:OD1	4:E:72:ARG:NE	2.35	0.42
1:C:41:ARG:NH1	8:C:402:HOH:O	2.10	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:23[A]:THR:HG22	8:G:415:HOH:O	2.20	0.42
4:H:19[B]:MET:SD	4:H:112:LEU:HD21	2.60	0.42
4:H:67[A]:SER:OG	4:H:69:LEU:HD23	2.20	0.42
1:A:0:MET:SD	1:A:169[B]:LEU:HD21	2.60	0.41
4:E:181:GLN:O	4:E:187:SER:HB2	2.20	0.41
4:E:128:VAL:HG23	4:E:238:ALA:HB3	2.02	0.41
3:D:166:PHE:CZ	4:E:141:LYS:HE3	2.56	0.41
1:A:246:LEU:HA	1:A:246:LEU:HD23	1.87	0.41
3:D:17[B]:ILE:HG22	3:D:76:LYS:HA	2.02	0.41
1:C:31:HIS:HE1	8:C:562:HOH:O	2.03	0.41
1:C:215[B]:MET:HG3	1:C:257:HIS:CD2	2.56	0.41
3:G:112:GLN:H	3:G:112:GLN:HG2	1.68	0.41
1:A:137:HIS:O	1:A:141[B]:GLN:HG2	2.21	0.41
2:F:27:VAL:HB	2:F:64[B]:LEU:HD12	2.02	0.41
4:E:181:GLN:NE2	8:E:302:HOH:O	2.30	0.40
3:G:156:LYS:HA	3:G:170:SER:O	2.21	0.40
4:H:86:THR:HG23	4:H:113:THR:HA	2.02	0.40
1:C:169[B]:LEU:HD12	1:C:169[B]:LEU:HA	1.93	0.40
4:E:31:SER:OG	4:E:97:THR:HG23	2.21	0.40
4:E:155:HIS:HB3	4:E:216:TYR:HB2	2.03	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	273/271 (101%)	269 (98%)	4 (2%)	0	100	100
1	C	278/271 (103%)	274 (99%)	4 (1%)	0	100	100
2	B	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
2	F	101/100 (101%)	99 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	182/204 (89%)	177 (97%)	5 (3%)	0	100	100
3	G	217/204 (106%)	213 (98%)	4 (2%)	0	100	100
4	E	242/246 (98%)	239 (99%)	3 (1%)	0	100	100
4	H	258/246 (105%)	252 (98%)	6 (2%)	0	100	100
All	All	1648/1642 (100%)	1619 (98%)	29 (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	235/241 (98%)	228 (97%)	7 (3%)	41	33
1	C	244/241 (101%)	237 (97%)	7 (3%)	42	35
2	B	81/95 (85%)	77 (95%)	4 (5%)	25	15
2	F	91/95 (96%)	89 (98%)	2 (2%)	52	47
3	D	147/181 (81%)	142 (97%)	5 (3%)	37	28
3	G	190/181 (105%)	186 (98%)	4 (2%)	53	48
4	E	199/212 (94%)	190 (96%)	9 (4%)	27	18
4	H	218/212 (103%)	215 (99%)	3 (1%)	67	65
All	All	1405/1458 (96%)	1364 (97%)	41 (3%)	44	35

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	72	MET
1	A	73	PHE
1	A	82	ARG
1	A	134[A]	ASN
1	A	134[B]	ASN

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Mol	Chain	Res	Type
1	A	183	LEU
2	B	16[A]	GLU
2	B	16[B]	GLU
2	B	36	GLU
2	B	70	PHE
1	C	0	MET
1	C	1	ARG
1	C	16	ILE
1	C	57	ASP
1	C	73	PHE
1	C	221	ILE
1	C	222	VAL
3	D	67	SER
3	D	91	LYS
3	D	138	ASP
3	D	156	LYS
3	D	157	CYS
4	E	19[A]	MET
4	E	19[B]	MET
4	E	111	ARG
4	E	140	GLN
4	E	167	VAL
4	E	194	ARG
4	E	204	ASN
4	E	207	ASN
4	E	239	GLU
2	F	35	ILE
2	F	70	PHE
3	G	23[A]	THR
3	G	23[B]	THR
3	G	27	SER
3	G	162	ARG
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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	TKG	A	301	1	16,17,19	0.41	0	18,24,27	0.60	0
6	GOL	C	302	-	5,5,5	0.81	0	5,5,5	0.92	0
6	GOL	F	101	-	5,5,5	0.41	0	5,5,5	1.43	1 (20%)
6	GOL	A	302	-	5,5,5	1.27	1 (20%)	5,5,5	0.99	0
6	GOL	A	303	-	5,5,5	1.07	0	5,5,5	0.88	0
5	TKG	C	301	1	16,17,19	0.36	0	18,24,27	0.94	2 (11%)

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	TKG	A	301	1	-	0/4/4/8	0/2/2/2
6	GOL	C	302	-	-	2/4/4/4	-
6	GOL	F	101	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	302	-	-	0/4/4/4	-
6	GOL	A	303	-	-	0/4/4/4	-
5	TKG	C	301	1	-	0/4/4/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	302	GOL	C3-C2	2.31	1.61	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	101	GOL	C3-C2-C1	-2.46	102.14	111.70
5	C	301	TKG	C4-C5-N3	2.39	122.51	120.24
5	C	301	TKG	C9-C8-N3	2.22	122.81	118.18

There are no chirality outliers.

All (6) torsion outliers are listed below:

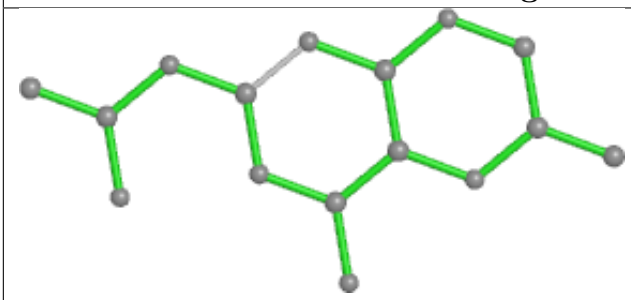
Mol	Chain	Res	Type	Atoms
6	F	101	GOL	O1-C1-C2-C3
6	C	302	GOL	C1-C2-C3-O3
6	F	101	GOL	C1-C2-C3-O3
6	F	101	GOL	O1-C1-C2-O2
6	C	302	GOL	O2-C2-C3-O3
6	F	101	GOL	O2-C2-C3-O3

There are no ring outliers.

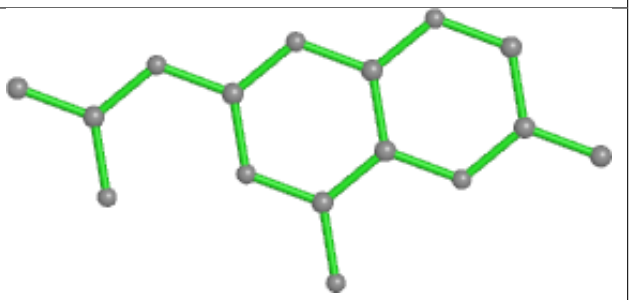
No monomer is involved in short contacts.

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

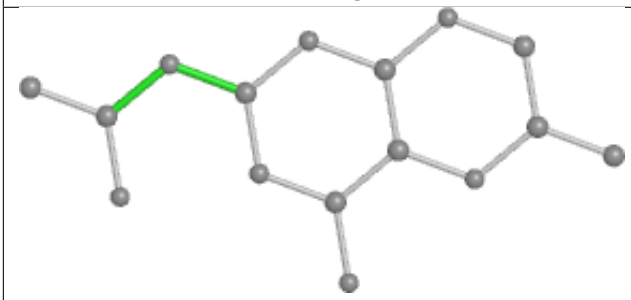
Ligand TKG A 301



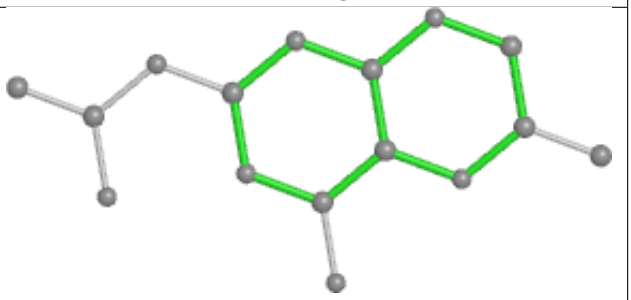
Bond lengths



Bond angles

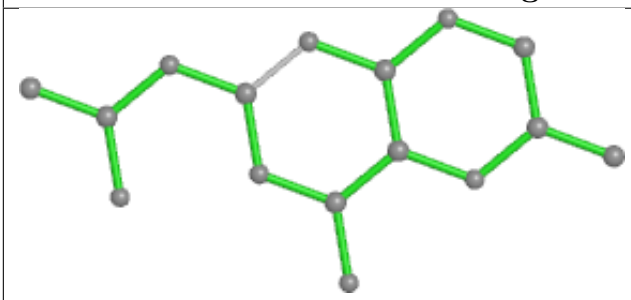


Torsions

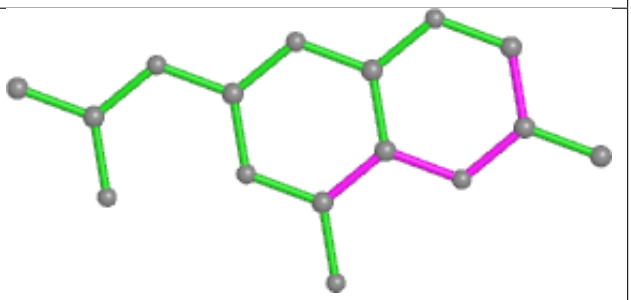


Rings

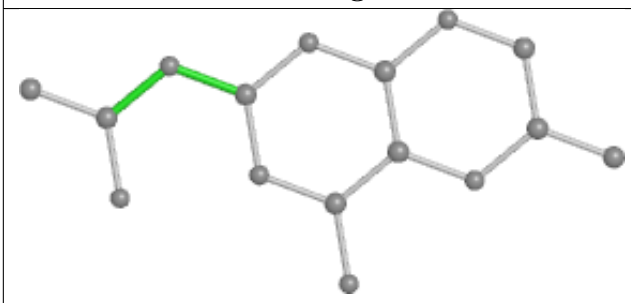
Ligand TKG C 301



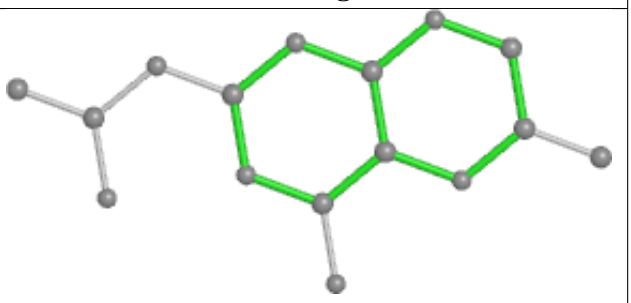
Bond lengths



Bond angles



Torsions



Rings

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	265/271 (97%)	-0.12	8 (3%) 50 53	27, 41, 75, 83	10 (3%)
1	C	268/271 (98%)	-0.19	8 (2%) 50 53	29, 41, 61, 91	20 (7%)
2	B	98/100 (98%)	0.85	21 (21%) 0 0	34, 61, 86, 92	4 (4%)
2	F	100/100 (100%)	-0.33	0 100 100	31, 43, 62, 66	8 (8%)
3	D	186/204 (91%)	0.74	40 (21%) 0 0	34, 54, 90, 98	7 (3%)
3	G	199/204 (97%)	-0.33	1 (0%) 91 92	26, 35, 58, 65	11 (5%)
4	E	239/246 (97%)	0.12	19 (7%) 12 14	38, 58, 98, 109	9 (3%)
4	H	244/246 (99%)	-0.21	4 (1%) 72 74	27, 36, 52, 68	11 (4%)
All	All	1599/1642 (97%)	0.01	101 (6%) 20 22	26, 43, 83, 109	80 (5%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	197	PHE	5.8
3	D	163	SER	5.6
2	B	78	TYR	5.3
3	D	119	TYR	4.9
3	D	196	PHE	4.9
4	E	136	ILE	4.6
3	D	180	PHE	4.5
4	E	197	VAL	4.4
2	B	79	ALA	4.3
3	D	117	ALA	4.3
4	E	142	ALA	4.1
3	D	166	PHE	4.1
3	D	164	MET	4.0
4	E	224	TRP	4.0
3	D	181	ALA	3.9
3	D	149	SER	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	43	GLY	3.9
3	D	159	LEU	3.8
4	E	204	ASN	3.7
3	D	112	GLN	3.7
3	D	198	PRO	3.7
3	D	132	CYS	3.7
1	A	222	VAL	3.7
4	H	184	LEU	3.7
4	E	200	THR	3.6
3	D	162	ARG	3.6
2	B	76	ASP	3.6
4	E	199	ALA	3.4
3	D	182	CYS	3.4
2	B	46	ILE	3.4
2	B	42	ASN	3.3
4	H	96[A]	TRP	3.2
3	D	194	ASP	3.2
4	E	167	VAL	3.2
3	D	192	PRO	3.1
4	E	202	TRP	3.1
3	D	121	LEU	3.1
4	E	225	THR	3.1
3	D	165	ASP	3.1
2	B	77	GLU	3.0
2	B	73	THR	3.0
1	C	252	ASN	3.0
3	D	137	PHE	3.0
2	B	82	VAL	3.0
2	B	92	ILE	2.9
4	E	137	SER	2.8
1	A	69[A]	TRP	2.8
3	D	131	VAL	2.8
3	D	138	ASP	2.8
4	E	164	GLY	2.8
3	D	186	PHE	2.8
4	E	140	GLN	2.7
2	B	44	GLU	2.7
1	A	196	THR	2.7
4	E	227	ASP	2.7
2	B	75	LYS	2.7
1	A	249	GLN	2.6
3	D	195	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	45	ARG	2.6
3	D	191	ILE	2.6
4	E	221	ASN	2.5
1	C	211[A]	TYR	2.5
3	D	160	ASP	2.5
2	B	95	TRP	2.5
3	D	161	MET	2.5
3	D	133	LEU	2.5
3	D	120	GLN	2.4
1	C	247	ASP	2.4
3	D	111	ILE	2.4
3	D	136	ASP	2.4
3	D	187	ASN	2.4
2	B	18	GLY	2.4
3	D	113	ASN	2.4
2	B	96	ASP	2.3
4	E	203	GLN	2.3
3	D	114	PRO	2.3
3	D	110	ASP	2.3
3	D	189	SER	2.3
1	C	221	ILE	2.3
4	H	183	ALA	2.3
2	B	41	LYS	2.3
1	C	17	HIS	2.3
1	C	248	PRO	2.2
4	E	207	ASN	2.2
1	A	17	HIS	2.2
3	G	179	ASP	2.2
1	A	6[A]	ARG	2.2
1	A	246	LEU	2.2
2	B	15	ALA	2.1
1	C	0	MET	2.1
3	D	185	ALA	2.1
4	H	206[A]	ARG	2.1
2	B	49	VAL	2.1
3	D	151	VAL	2.1
1	A	221	ILE	2.1
2	B	38	ASP	2.1
3	D	193	GLU	2.1
4	E	139	THR	2.0
4	E	209	PHE	2.0
1	C	264[A]	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	74	GLU	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)

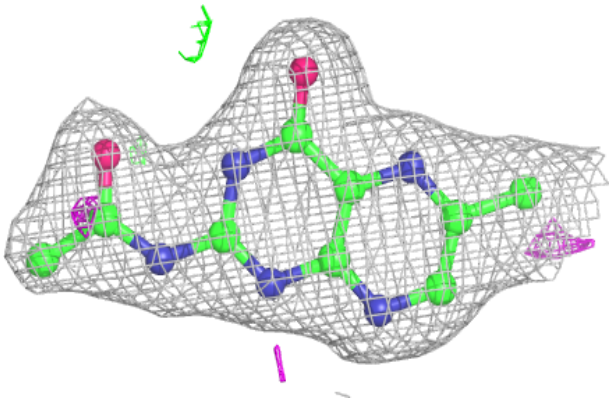
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

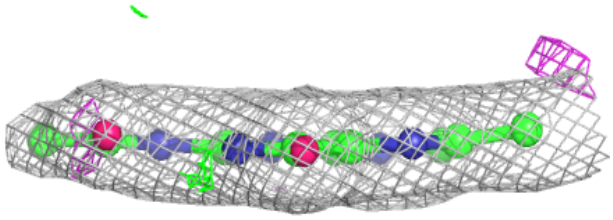
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	C	302	6/6	0.86	0.24	36,47,53,53	6
6	GOL	A	303	6/6	0.89	0.17	41,50,56,57	0
6	GOL	A	302	6/6	0.89	0.13	37,38,40,42	0
6	GOL	F	101	6/6	0.94	0.12	35,44,57,61	0
5	TKG	A	301	16/18	0.97	0.09	25,35,40,41	0
5	TKG	C	301	16/18	0.97	0.11	33,42,50,50	0
7	CL	A	304	1/1	0.97	0.07	43,43,43,43	0

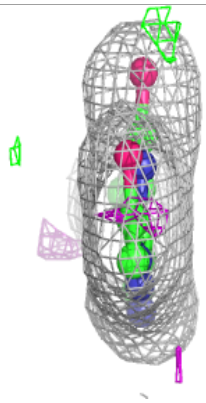
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TKG A 301:

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

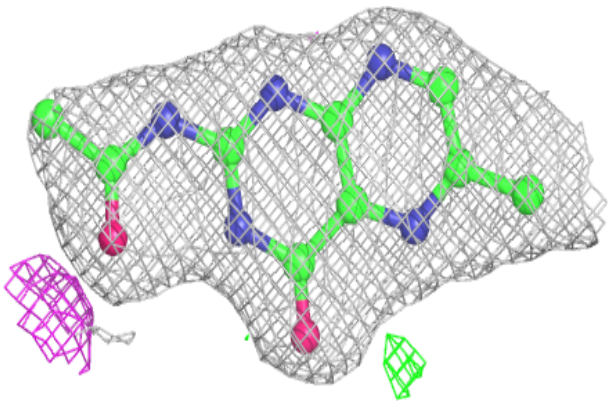


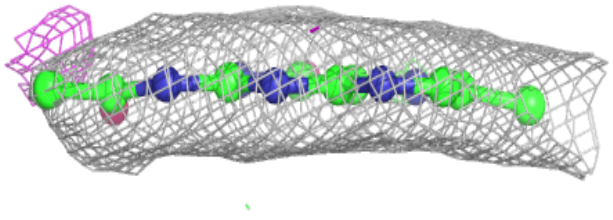


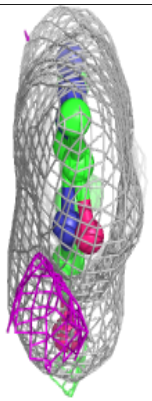


Electron density around TKG C 301:

$2mF_o$-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.