Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2024 – 10:14 AM EST

PDB ID	:	9BTX
Title	:	Structure of human MAIT A-F7 TCR in complex with human MR1-3,4-dihydroxybenzaldehyde
Authors	:	Awad, W.; Rossjohn, J.
Deposited on	:	2024-05-15
Resolution	:	2.05 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:

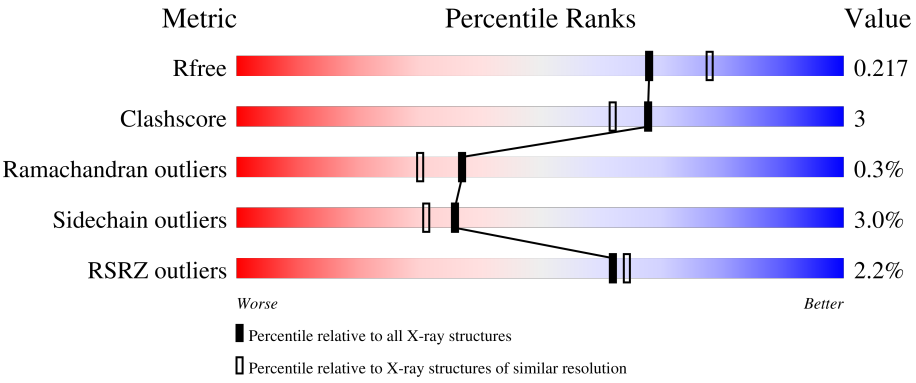
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.05 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}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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	87% 10%
1	C	271	83% 14%
2	B	100	90% 8%
2	F	100	95% 5%
3	D	204	5% 83% 9% 7%

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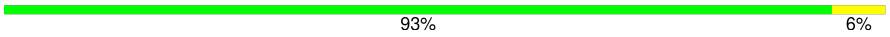
Mol	Chain	Length	Quality of chain
3	G	204	
4	E	246	
4	H	246	

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
7	ACT	C	304	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 13755 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	264	Total	C	N	O	S	0	8	0
			2183	1398	381	392	12			
1	C	265	Total	C	N	O	S	0	6	0
			2184	1408	372	393	11			

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
2	B	98	Total	C	N	O	S	0	2	0
			784	505	133	143	3			
2	F	100	Total	C	N	O	S	0	1	0
			806	516	137	149	4			

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 Human TCR TRAV1-2_ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	189	Total	C	N	O	S	0	5	0
			1448	929	231	279	9			

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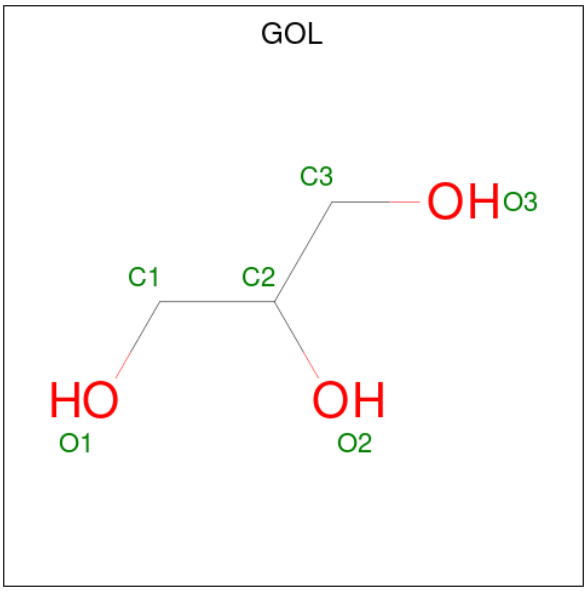
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	200	Total	C	N	O	S	0	12	0
			1605	1023	253	317	12			

- Molecule 4 is a protein called Human TCR TRBV6-1_BETA.

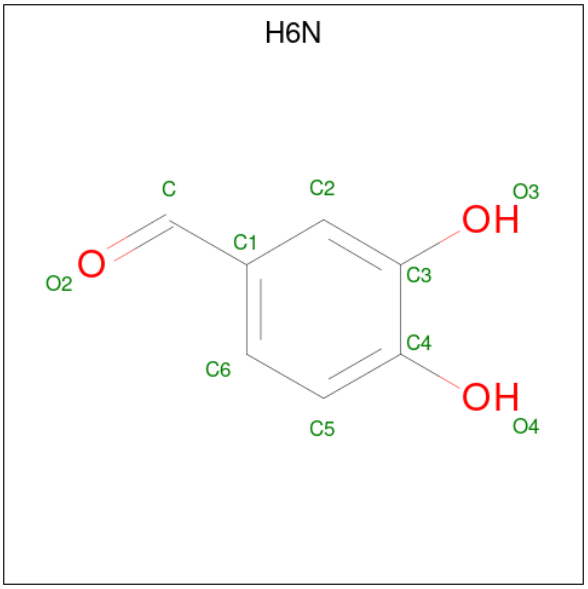
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	240	Total	C	N	O	S	0	3	0
			1839	1164	318	348	9			
4	H	245	Total	C	N	O	S	0	17	0
			1991	1261	342	373	15			

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



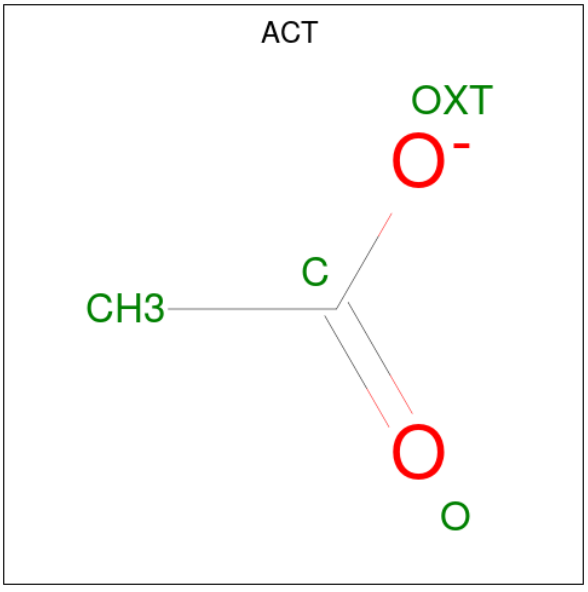
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is Protocatechuic aldehyde (three-letter code: H6N) (formula: $C_7H_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 7 2	0	0
6	C	1	Total C O 9 7 2	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	1	Total Na 1 1	0	0
8	H	1	Total Na 1 1	0	0

- Molecule 9 is water.

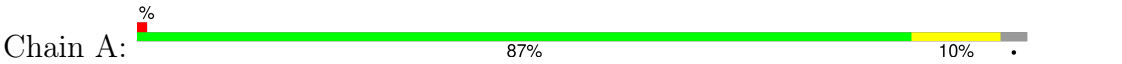
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	148	Total O 148 148	0	0
9	B	41	Total O 41 41	0	0
9	C	132	Total O 132 132	0	0
9	D	65	Total O 65 65	0	0
9	E	54	Total O 54 54	0	0
9	F	49	Total O 49 49	0	0
9	G	153	Total O 153 153	0	0
9	H	189	Total O 189 189	0	0

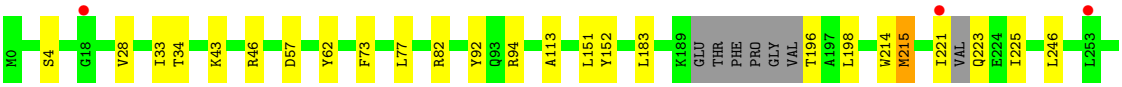
3 Residue-property plots (i)

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

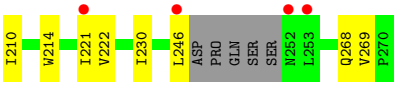
Chain A:





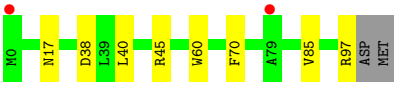
• Molecule 1: Major histocompatibility complex class I-related gene protein

Chain C:



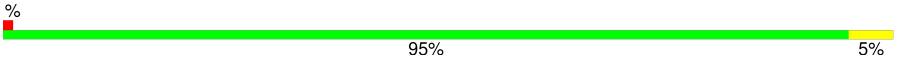
• Molecule 2: Beta-2-microglobulin

Chain B:



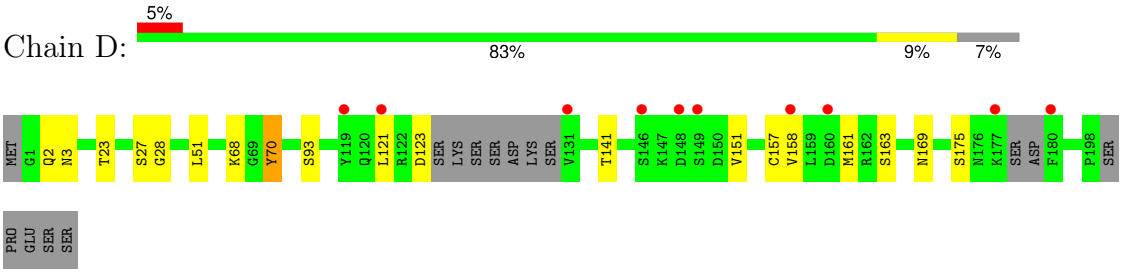
• Molecule 2: Beta-2-microglobulin

Chain F:



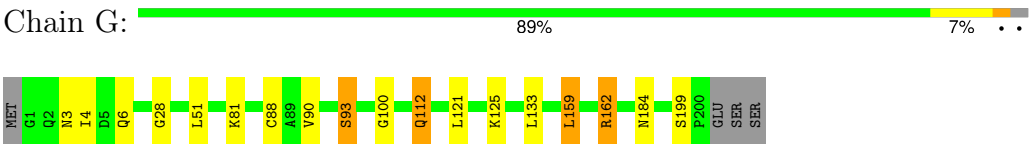
• Molecule 3: Human TCR TRAV1-2_ALPHA

Chain D:



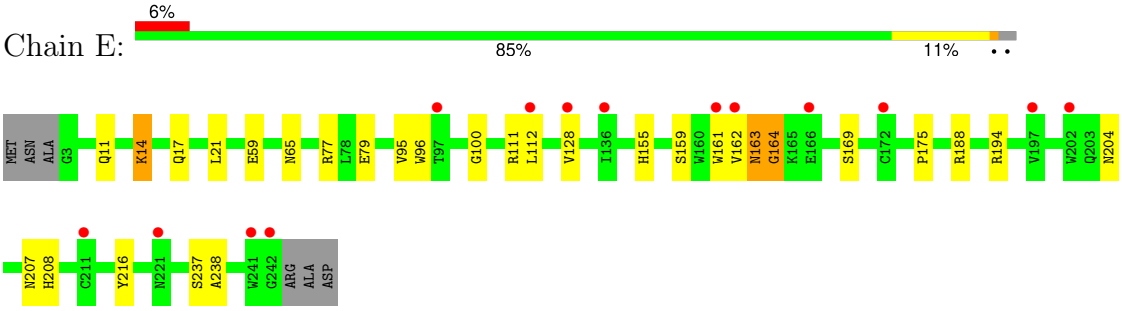
• Molecule 3: Human TCR TRAV1-2_ALPHA

Chain G:



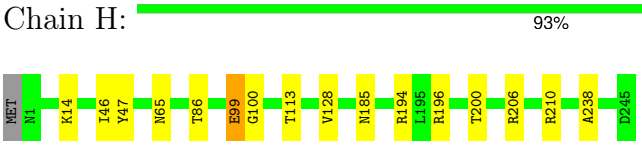
• Molecule 4: Human TCR TRBV6-1_BETA

Chain E:



• Molecule 4: Human TCR TRBV6-1_BETA

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	217.13Å 70.41Å 143.57Å 90.00° 104.61° 90.00°	Depositor
Resolution (Å)	36.19 – 2.05 36.19 – 2.05	Depositor EDS
% Data completeness (in resolution range)	94.6 (36.19-2.05) 87.0 (36.19-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.35 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.185 , 0.218 0.186 , 0.217	Depositor DCC
R_{free} test set	127722 reflections (1.32%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13755	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: ACT, NA, H6N, 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	0.25	0/2269	0.50	0/3083
1	C	0.26	0/2268	0.50	0/3086
2	B	0.24	0/813	0.49	0/1110
2	F	0.25	0/832	0.49	0/1132
3	D	0.26	0/1492	0.48	0/2029
3	G	0.27	0/1673	0.51	0/2267
4	E	0.26	0/1899	0.51	0/2594
4	H	0.28	0/2094	0.53	0/2846
All	All	0.26	0/13340	0.50	0/18147

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	2183	0	2066	16	0
1	C	2184	0	2084	24	0
2	B	784	0	724	5	0
2	F	806	0	750	3	0
3	D	1448	0	1338	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1605	0	1545	16	0
4	E	1839	0	1697	13	0
4	H	1991	0	1908	12	0
5	A	18	0	24	1	0
5	C	6	0	8	1	0
5	F	6	0	8	0	0
5	G	6	0	8	0	0
6	A	9	0	0	0	0
6	C	9	0	0	0	0
7	A	16	0	12	3	0
7	C	8	0	6	3	0
7	D	4	0	3	0	0
8	F	1	0	0	0	0
8	H	1	0	0	0	0
9	A	148	0	0	0	0
9	B	41	0	0	2	0
9	C	132	0	0	2	0
9	D	65	0	0	1	0
9	E	54	0	0	2	0
9	F	49	0	0	0	0
9	G	153	0	0	6	0
9	H	189	0	0	3	0
All	All	13755	0	12181	87	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 (87) 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:112[B]:GLN:NE2	9:G:801:HOH:O	2.16	0.78
1:A:34:THR:HG21	7:A:304:ACT:H1	1.71	0.71
1:C:96:ILE:HD13	5:C:301:GOL:H11	1.73	0.69
3:D:151:VAL:HG23	3:D:175:SER:HB2	1.75	0.66
1:A:183:LEU:HD13	7:A:306:ACT:H1	1.76	0.66
3:D:2:GLN:HE21	3:D:27:SER:H	1.46	0.62
1:C:16:ILE:HG13	1:C:19:VAL:HG12	1.81	0.62
1:C:222:VAL:HA	4:H:200:THR:HG21	1.83	0.60
4:E:65[B]:ASN:ND2	9:E:302:HOH:O	2.34	0.59
4:H:210[B]:ARG:NH2	9:H:401:HOH:O	2.36	0.58
1:A:43:LYS:HD2	1:A:62:TYR:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HD13	1:A:92:TYR:HB2	1.85	0.56
3:G:184[A]:ASN:ND2	9:G:807:HOH:O	2.38	0.56
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.41	0.56
1:A:152:TYR:CD1	4:H:100:GLY:HA3	2.41	0.56
3:D:3[B]:ASN:ND2	9:D:802:HOH:O	2.39	0.55
4:E:204:ASN:ND2	4:E:207:ASN:OD1	2.39	0.55
1:C:28:VAL:HG23	1:C:33:ILE:HD13	1.87	0.55
1:C:77:LEU:HD13	1:C:92:TYR:HB2	1.88	0.54
1:A:28:VAL:HG23	1:A:33:ILE:HD13	1.88	0.53
3:D:158:VAL:HG22	3:D:169:ASN:HD22	1.73	0.53
3:G:125[A]:LYS:NZ	9:G:805:HOH:O	2.31	0.53
4:E:155:HIS:HB3	4:E:216:TYR:HB2	1.90	0.52
2:B:17:ASN:ND2	9:B:103:HOH:O	2.41	0.52
3:D:158:VAL:HG22	3:D:169:ASN:ND2	2.24	0.52
1:C:151:LEU:HD22	3:D:51:LEU:HD12	1.91	0.51
3:G:159[B]:LEU:HD11	4:H:196:ARG:HB2	1.92	0.51
4:H:65[A]:ASN:ND2	9:H:403:HOH:O	2.43	0.51
1:A:198:LEU:HD13	1:A:269:VAL:HG21	1.93	0.51
1:C:58:HIS:NE2	7:C:304:ACT:H2	2.26	0.50
3:G:112[A]:GLN:NE2	9:G:812:HOH:O	2.43	0.50
1:C:15:PRO:HB2	1:C:19:VAL:HG13	1.95	0.49
3:D:28:GLY:HA3	3:D:93[B]:SER:OG	2.13	0.49
1:A:215:MET:HG3	1:A:257:HIS:CD2	2.48	0.49
3:G:6:GLN:HE21	3:G:100:GLY:HA3	1.78	0.49
1:C:20:PRO:HB3	1:C:39:VAL:HG23	1.93	0.49
1:C:210:ILE:O	4:H:206[B]:ARG:HD2	2.13	0.48
3:G:3[A]:ASN:OD1	9:G:802:HOH:O	2.20	0.48
1:C:127:LEU:HD21	1:C:154:LYS:HD2	1.95	0.48
4:E:128:VAL:HG23	4:E:238:ALA:HB3	1.94	0.47
1:A:94:ARG:HH22	5:A:302:GOL:H31	1.80	0.47
1:A:4:SER:OG	7:A:305:ACT:H3	2.15	0.47
1:C:113:ALA:HB2	2:F:60:TRP:CE2	2.49	0.47
3:G:28:GLY:HA3	3:G:93[A]:SER:OG	2.14	0.47
4:H:128:VAL:HG23	4:H:238:ALA:HB3	1.96	0.47
1:A:214:TRP:H	1:A:225:ILE:HD13	1.79	0.47
1:C:198:LEU:HD13	1:C:269:VAL:HG21	1.97	0.46
3:G:81:LYS:NZ	9:G:810:HOH:O	2.42	0.46
3:G:121:LEU:HD11	3:G:133:LEU:HB2	1.97	0.46
4:H:86:THR:HG23	4:H:113:THR:HA	1.97	0.46
1:C:43:LYS:HD2	1:C:66:LEU:HD12	1.97	0.46
4:H:14[A]:LYS:NZ	9:H:407:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:6:GLN:HE22	3:G:88[A]:CYS:H	1.63	0.45
2:F:73:THR:OG1	2:F:76:ASP:OD1	2.21	0.45
3:G:6:GLN:HE22	3:G:88[B]:CYS:H	1.64	0.44
1:C:16:ILE:HD12	1:C:18:GLY:H	1.82	0.44
1:C:168:PHE:CZ	7:C:304:ACT:H3	2.52	0.44
1:A:151:LEU:HD22	3:G:51:LEU:HD12	1.98	0.44
3:D:23:THR:HG22	3:D:70:TYR:HB2	1.99	0.44
1:C:152:TYR:CD1	4:E:100:GLY:HA3	2.53	0.44
3:G:112[B]:GLN:CD	3:G:112[B]:GLN:H	2.22	0.43
4:E:21:LEU:HD11	4:E:112:LEU:HD11	1.99	0.43
3:G:162:ARG:NE	3:G:162:ARG:HA	2.34	0.43
2:B:38:ASP:OD2	2:B:45:ARG:NH1	2.52	0.43
1:C:182:PRO:HB3	1:C:205:PHE:HB3	2.01	0.43
1:C:124:LYS:NZ	9:C:402:HOH:O	2.30	0.42
4:E:159:SER:HG	4:E:161:TRP:HE1	1.67	0.42
4:E:162:VAL:O	4:E:164:GLY:N	2.51	0.42
1:A:196:THR:HG22	1:A:246:LEU:HD12	2.01	0.42
4:E:11:GLN:HB3	4:E:112:LEU:HD22	2.02	0.42
1:C:230:ILE:HD11	4:H:206[B]:ARG:HD3	2.02	0.42
4:H:46:ILE:HG22	4:H:47:TYR:HD1	1.84	0.42
4:H:99:GLU:O	4:H:99:GLU:HG3	2.18	0.42
1:C:169[A]:LEU:HD23	1:C:176:LEU:HD13	2.01	0.42
4:E:14:LYS:O	4:E:17:GLN:HB2	2.20	0.42
3:G:4[B]:ILE:HD11	3:G:90:VAL:HB	2.01	0.42
7:C:303:ACT:H3	2:F:10:TYR:HB3	2.02	0.42
4:E:188:ARG:NH2	9:E:307:HOH:O	2.49	0.42
1:A:46:ARG:HA	1:A:46:ARG:HD3	1.85	0.41
4:E:95:VAL:HG12	4:E:96:TRP:CD1	2.55	0.41
1:C:200:CYS:HB2	1:C:214:TRP:CZ2	2.55	0.41
2:B:97:ARG:H	2:B:97:ARG:HG2	1.63	0.41
1:C:186:VAL:HG11	1:C:269:VAL:HG22	2.02	0.41
4:E:163:ASN:HD21	4:E:207:ASN:HD22	1.68	0.41
1:A:221:ILE:O	1:A:223:GLN:N	2.54	0.40
2:B:85[A]:VAL:HG23	9:B:101:HOH:O	2.20	0.40
1:C:127:LEU:O	9:C:401:HOH:O	2.22	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	266/271 (98%)	262 (98%)	4 (2%)	0	100 100
1	C	267/271 (98%)	260 (97%)	6 (2%)	1 (0%)	30 23
2	B	98/100 (98%)	98 (100%)	0	0	100 100
2	F	99/100 (99%)	99 (100%)	0	0	100 100
3	D	188/204 (92%)	185 (98%)	3 (2%)	0	100 100
3	G	210/204 (103%)	206 (98%)	4 (2%)	0	100 100
4	E	241/246 (98%)	235 (98%)	3 (1%)	3 (1%)	11 4
4	H	260/246 (106%)	257 (99%)	3 (1%)	0	100 100
All	All	1629/1642 (99%)	1602 (98%)	23 (1%)	4 (0%)	37 38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	164	GLY
4	E	163	ASN
1	C	16	ILE
4	E	175	PRO

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%)	56 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	231/241 (96%)	223 (96%)	8 (4%)	31	25
2	B	83/95 (87%)	81 (98%)	2 (2%)	44	40
2	F	87/95 (92%)	86 (99%)	1 (1%)	70	71
3	D	150/181 (83%)	142 (95%)	8 (5%)	19	12
3	G	182/181 (101%)	174 (96%)	8 (4%)	24	18
4	E	191/212 (90%)	182 (95%)	9 (5%)	22	16
4	H	217/212 (102%)	214 (99%)	3 (1%)	62	63
All	All	1371/1458 (94%)	1328 (97%)	43 (3%)	36	30

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	73	PHE
1	A	82	ARG
1	A	215	MET
2	B	40	LEU
2	B	70	PHE
1	C	14	ASP
1	C	57	ASP
1	C	61	ARG
1	C	73	PHE
1	C	221	ILE
1	C	246	LEU
1	C	268[A]	GLN
1	C	268[B]	GLN
3	D	68	LYS
3	D	70	TYR
3	D	121	LEU
3	D	123	ASP
3	D	141	THR
3	D	157	CYS
3	D	161	MET
3	D	163	SER
4	E	14	LYS
4	E	59	GLU
4	E	77	ARG
4	E	79	GLU
4	E	111	ARG
4	E	169	SER

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Mol	Chain	Res	Type
4	E	194	ARG
4	E	208	HIS
4	E	237	SER
2	F	70	PHE
3	G	93[A]	SER
3	G	93[B]	SER
3	G	112[A]	GLN
3	G	112[B]	GLN
3	G	159[A]	LEU
3	G	159[B]	LEU
3	G	162	ARG
3	G	199	SER
4	H	99	GLU
4	H	185	ASN
4	H	194	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	268	GLN
1	C	85	ASN
3	D	2	GLN
3	D	96	GLN
3	D	169	ASN
3	D	187	ASN
4	E	163	ASN
4	E	204	ASN
4	E	207	ASN
3	G	2	GLN
3	G	6	GLN
4	H	22	GLN
4	H	140	GLN

5.3.3 RNA

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	302	-	5,5,5	0.78	0	5,5,5	1.29	1 (20%)
5	GOL	A	308	-	5,5,5	0.88	0	5,5,5	1.15	0
7	ACT	A	306	-	3,3,3	1.53	1 (33%)	3,3,3	1.34	0
7	ACT	C	303	-	3,3,3	1.37	0	3,3,3	1.37	0
5	GOL	A	301	-	5,5,5	0.91	0	5,5,5	1.16	0
7	ACT	A	304	-	3,3,3	1.18	0	3,3,3	1.40	0
7	ACT	D	701	-	3,3,3	1.35	0	3,3,3	1.52	0
6	H6N	C	302	1	9,9,10	0.54	0	12,12,13	0.38	0
5	GOL	G	701	-	5,5,5	0.80	0	5,5,5	1.03	0
7	ACT	A	305	-	3,3,3	1.22	0	3,3,3	1.40	0
7	ACT	A	307	-	3,3,3	1.45	1 (33%)	3,3,3	1.49	0
6	H6N	A	303	1	9,9,10	0.54	0	12,12,13	0.44	0
5	GOL	C	301	-	5,5,5	0.90	0	5,5,5	1.09	0
5	GOL	F	101	-	5,5,5	0.91	0	5,5,5	1.23	1 (20%)
7	ACT	C	304	-	3,3,3	1.31	0	3,3,3	1.46	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	302	-	-	4/4/4/4	-
5	GOL	A	308	-	-	2/4/4/4	-
5	GOL	A	301	-	-	2/4/4/4	-
6	H6N	C	302	1	-	-	0/1/1/1
5	GOL	G	701	-	-	4/4/4/4	-
6	H6N	A	303	1	-	-	0/1/1/1
5	GOL	C	301	-	-	0/4/4/4	-
5	GOL	F	101	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	306	ACT	CH3-C	2.27	1.58	1.49
7	A	307	ACT	CH3-C	2.06	1.57	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	302	GOL	C3-C2-C1	-2.23	103.63	111.80
5	F	101	GOL	C3-C2-C1	-2.04	104.31	111.80

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	GOL	O1-C1-C2-O2
5	A	301	GOL	O1-C1-C2-C3
5	A	302	GOL	C1-C2-C3-O3
5	G	701	GOL	O1-C1-C2-C3
5	G	701	GOL	C1-C2-C3-O3
5	A	302	GOL	O1-C1-C2-C3
5	A	308	GOL	O1-C1-C2-C3
5	F	101	GOL	C1-C2-C3-O3
5	G	701	GOL	O1-C1-C2-O2
5	G	701	GOL	O2-C2-C3-O3
5	A	302	GOL	O2-C2-C3-O3
5	A	302	GOL	O1-C1-C2-O2
5	F	101	GOL	O2-C2-C3-O3
5	A	308	GOL	O1-C1-C2-O2

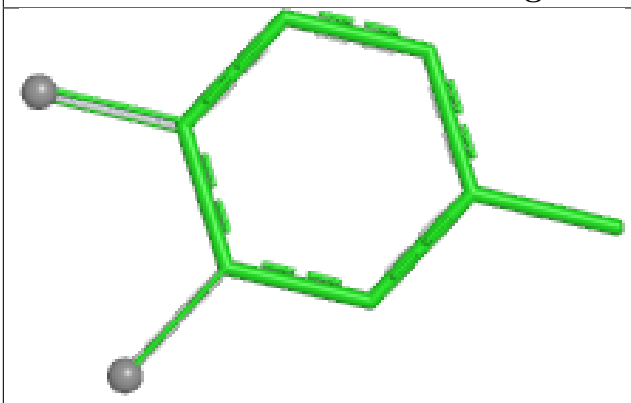
There are no ring outliers.

7 monomers are involved in 8 short contacts:

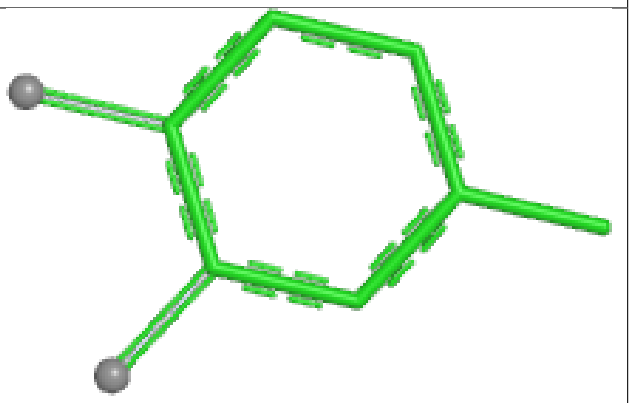
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	302	GOL	1	0
7	A	306	ACT	1	0
7	C	303	ACT	1	0
7	A	304	ACT	1	0
7	A	305	ACT	1	0
5	C	301	GOL	1	0
7	C	304	ACT	2	0

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.

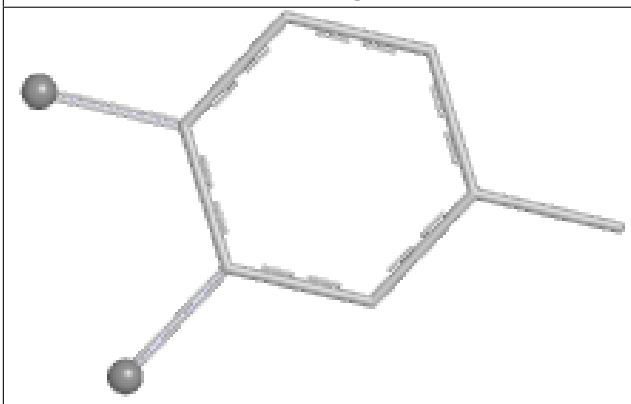
Ligand H6N C 302



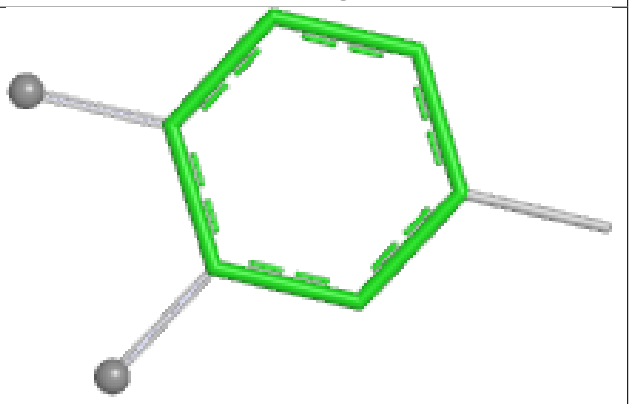
Bond lengths



Bond angles

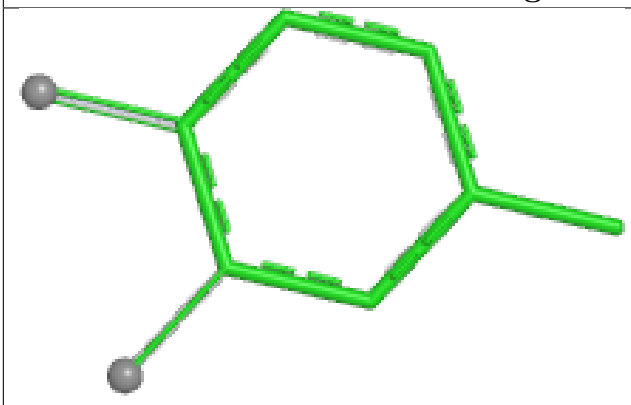


Torsions

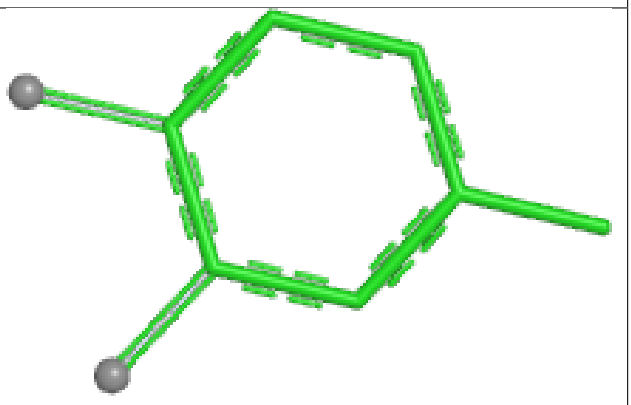


Rings

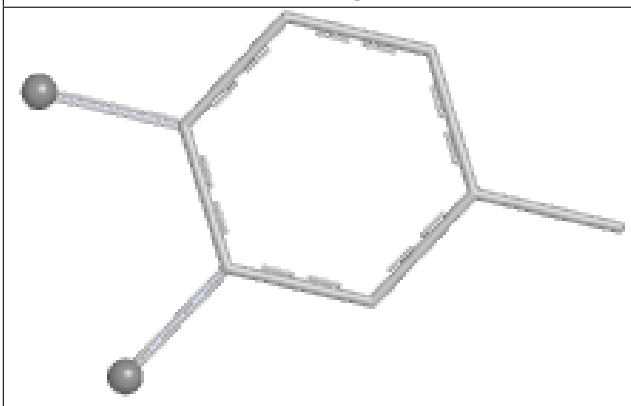
Ligand H6N A 303



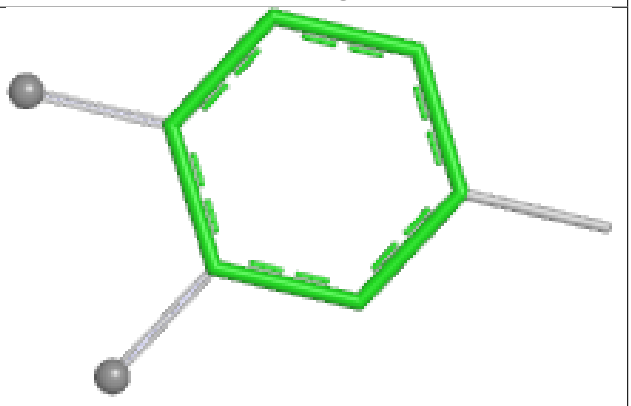
Bond lengths



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	264/271 (97%)	0.02	4 (1%) 71 74	24, 46, 85, 95	10 (3%)
1	C	265/271 (97%)	0.05	4 (1%) 71 74	24, 46, 65, 89	26 (9%)
2	B	98/100 (98%)	0.47	2 (2%) 64 68	41, 68, 94, 97	2 (2%)
2	F	100/100 (100%)	-0.02	1 (1%) 79 81	31, 51, 76, 81	3 (3%)
3	D	189/204 (92%)	0.48	10 (5%) 33 35	21, 60, 100, 113	9 (4%)
3	G	200/204 (98%)	-0.18	0 100 100	23, 40, 63, 78	20 (10%)
4	E	240/246 (97%)	0.57	14 (5%) 30 32	31, 65, 105, 120	10 (4%)
4	H	245/246 (99%)	-0.15	0 100 100	24, 42, 62, 85	24 (9%)
All	All	1601/1642 (97%)	0.14	35 (2%) 62 64	21, 49, 90, 120	104 (6%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	119	TYR	4.7
1	A	221	ILE	4.1
1	C	221	ILE	3.9
4	E	242	GLY	3.9
3	D	148	ASP	3.4
4	E	128	VAL	3.3
4	E	202	TRP	2.8
4	E	162	VAL	2.8
3	D	177	LYS	2.7
4	E	172	CYS	2.7
3	D	160	ASP	2.6
1	C	253	LEU	2.6
4	E	166	GLU	2.5
4	E	97	THR	2.4
4	E	241	TRP	2.4
3	D	146	SER	2.3

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Mol	Chain	Res	Type	RSRZ
4	E	136	ILE	2.3
1	A	253	LEU	2.3
3	D	149	SER	2.3
2	F	99	MET	2.3
3	D	131	VAL	2.3
3	D	121	LEU	2.2
4	E	211	CYS	2.2
1	A	18	GLY	2.2
3	D	180	PHE	2.2
2	B	79	ALA	2.2
1	A	270	PRO	2.2
2	B	0	MET	2.2
1	C	246	LEU	2.1
4	E	112	LEU	2.1
4	E	197	VAL	2.1
1	C	252	ASN	2.1
3	D	158	VAL	2.1
4	E	221	ASN	2.0
4	E	161	TRP	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
7	ACT	A	306	4/4	0.69	0.20	54,61,65,70	0
7	ACT	D	701	4/4	0.79	0.17	49,59,62,65	0
7	ACT	C	303	4/4	0.84	0.17	55,60,61,65	0
7	ACT	A	304	4/4	0.86	0.20	44,45,48,48	4

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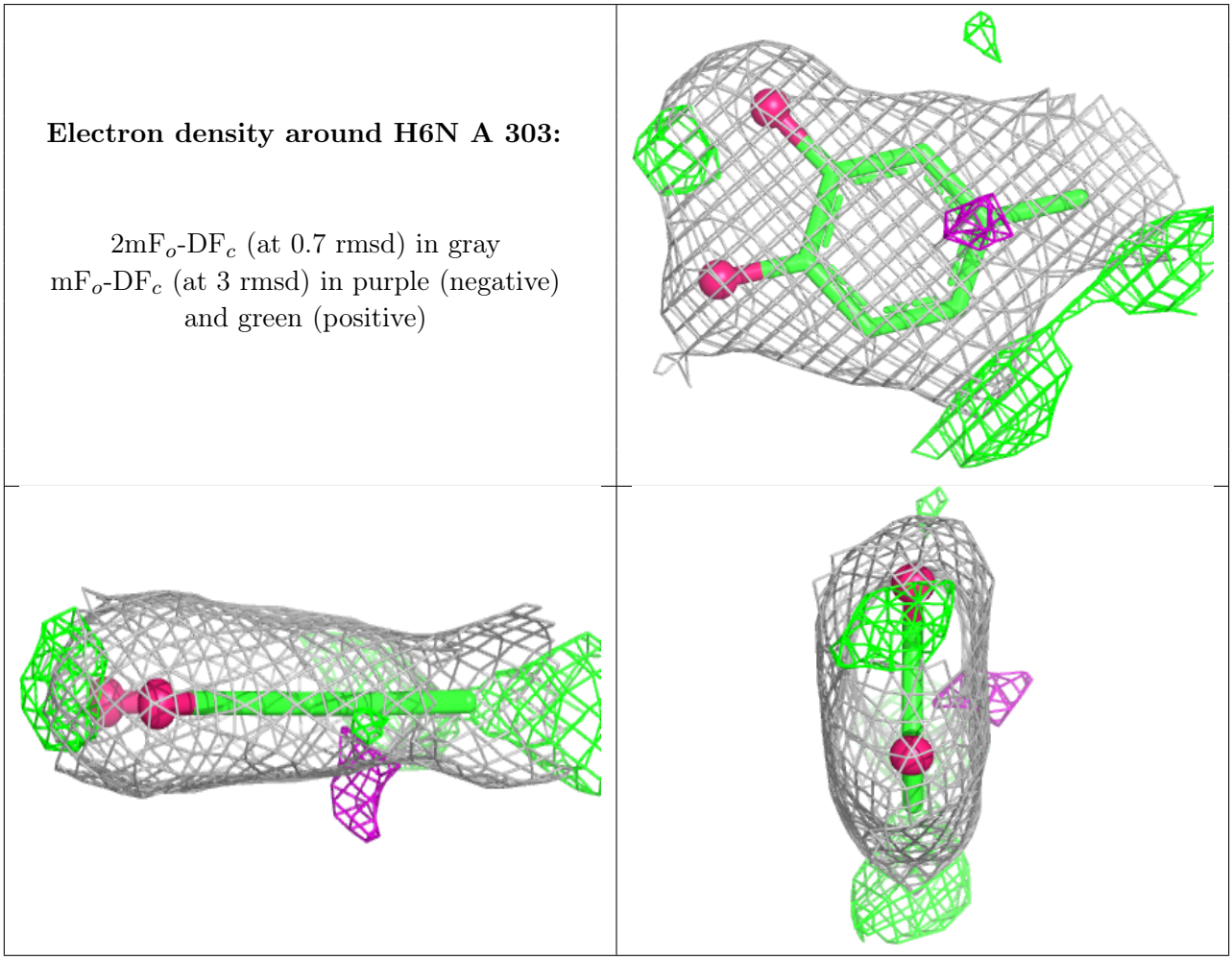
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	G	701	6/6	0.86	0.15	46,54,59,61	0
6	H6N	A	303	9/10	0.87	0.12	41,43,48,49	0
5	GOL	C	301	6/6	0.88	0.15	44,53,56,56	6
7	ACT	A	307	4/4	0.88	0.17	59,63,65,68	0
6	H6N	C	302	9/10	0.89	0.12	47,51,54,59	0
7	ACT	A	305	4/4	0.89	0.15	47,58,61,67	0
5	GOL	A	302	6/6	0.91	0.14	43,48,48,49	6
7	ACT	C	304	4/4	0.91	0.17	52,53,54,58	4
5	GOL	A	308	6/6	0.91	0.11	52,59,62,64	0
5	GOL	A	301	6/6	0.93	0.10	46,47,52,55	0
5	GOL	F	101	6/6	0.93	0.13	38,45,50,51	6
8	NA	F	102	1/1	0.97	0.06	56,56,56,56	0
8	NA	H	301	1/1	0.99	0.03	44,44,44,44	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.

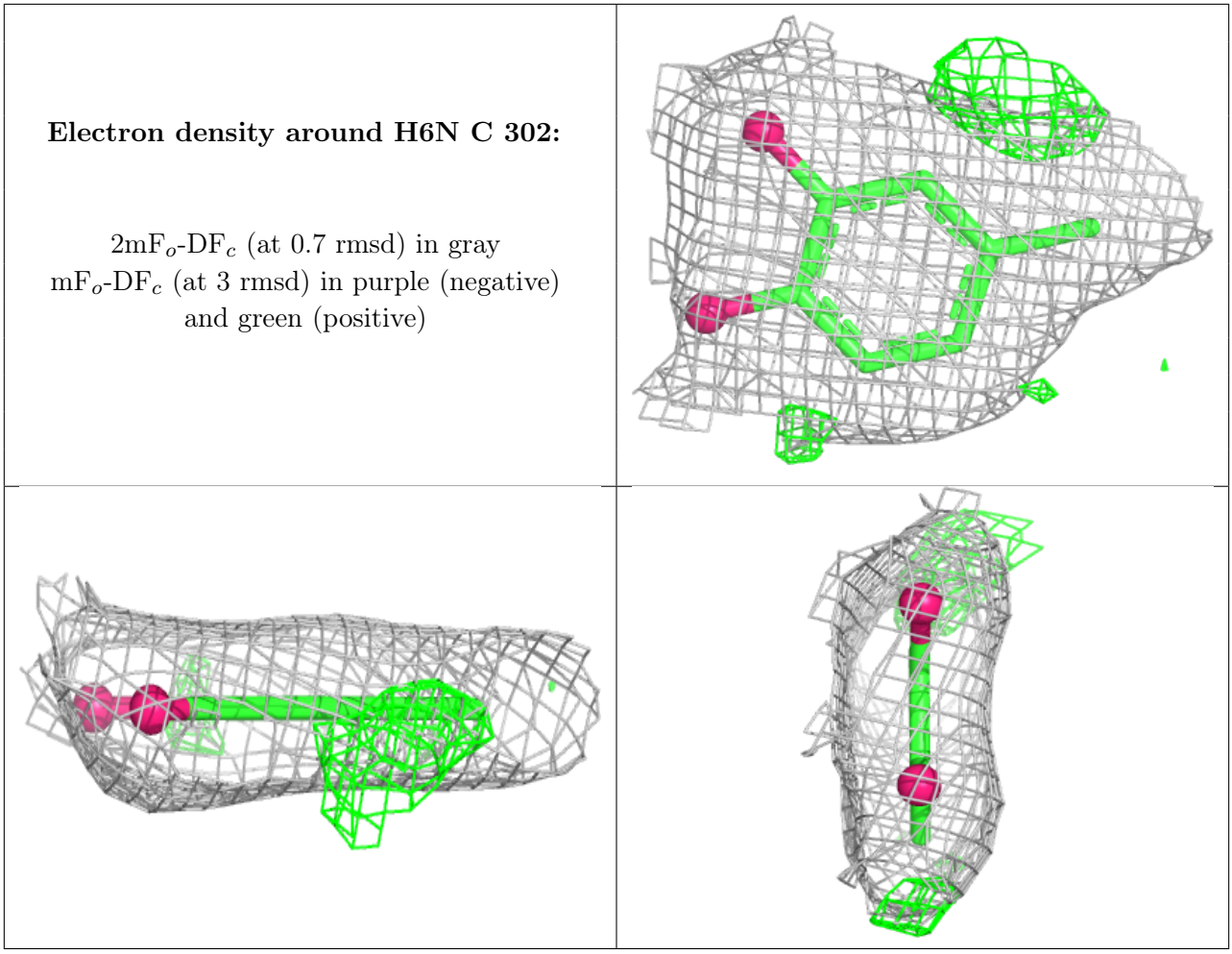
Electron density around H6N A 303:

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



Electron density around H6N 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)



6.5 Other polymers

There are no such residues in this entry.