



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:07 PM UTC

PDB ID : 9BTZ / pdb_00009btz
Title : Structure of human MAIT A-F7 TCR in complex with human MR1-nicotinaldehyde
Authors : Awad, W.; Rossjohn, J.
Deposited on : 2024-05-15
Resolution : 3.00 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

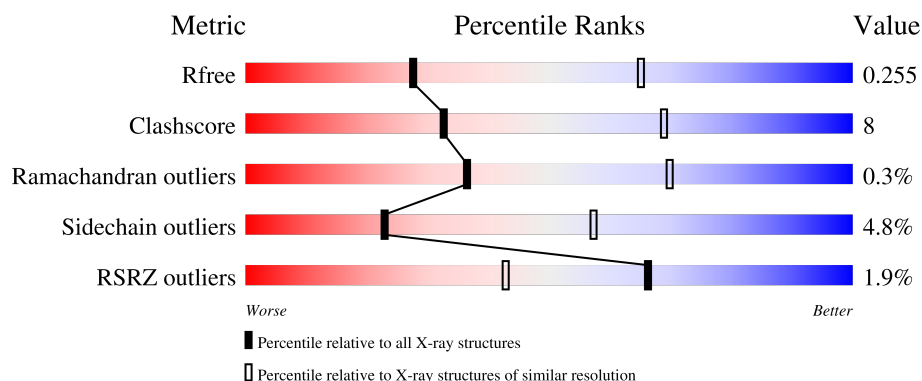
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	% 79% 18% ..
1	C	271	% 69% 27% ..
2	B	100	2% 78% 18% ..
2	F	100	81% 18% .
3	D	204	% 73% 20% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	204	% 76% 20% ..
4	E	246	4% 80% 17% ..
4	H	246	2% 81% 17% .

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
6	ACT	A	303	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12799 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	0	0
			2119	1354	365	390	10			
1	C	264	Total	C	N	O	S	0	2	0
			2182	1403	374	394	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	97	Total	C	N	O	S	0	0	0
			773	496	129	146	2			
2	F	99	Total	C	N	O	S	0	0	0
			798	509	135	151	3			

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	1	0
			1420	910	229	273	8			

Continued on next page...

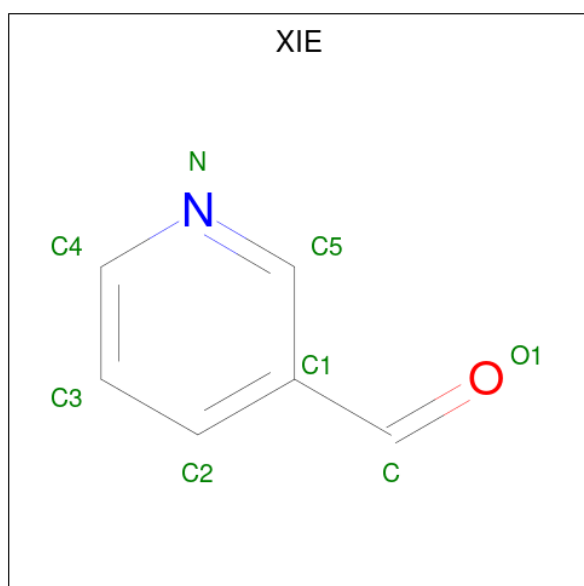
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	200	Total	C	N	O	S	0	1	0
			1531	970	245	306	10			

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

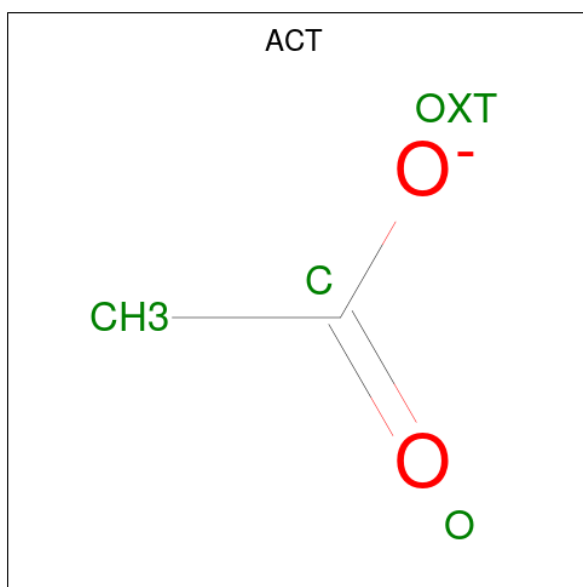
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	240	Total	C	N	O	S	0	0	0
			1834	1159	317	349	9			
4	H	245	Total	C	N	O	S	0	0	0
			1885	1190	327	359	9			

- Molecule 5 is Nicotinaldehyde (CCD ID: XIE) (formula: C_6H_5NO) (labeled as "Ligand of Interest" by depositor).



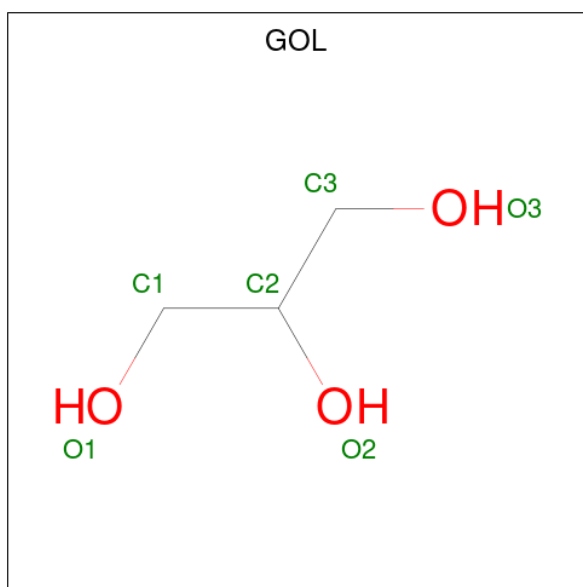
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	1
			14	12	2		
5	C	1	Total	C	N	0	1
			14	12	2		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

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

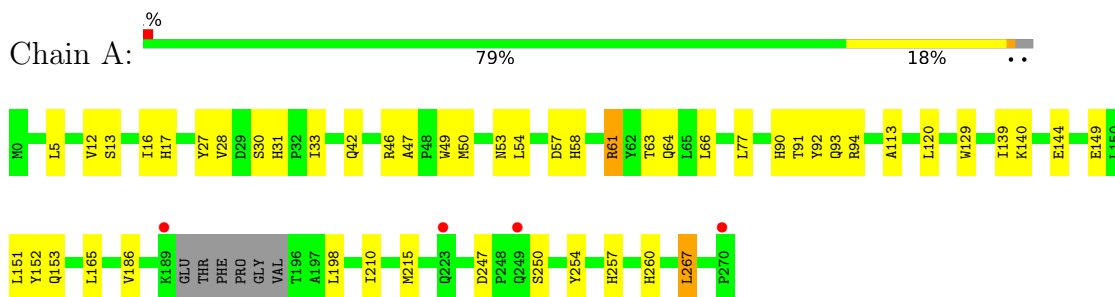
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	38	Total	O	0	0
			38	38		
9	B	5	Total	O	0	0
			5	5		
9	C	44	Total	O	0	0
			44	44		
9	D	12	Total	O	0	0
			12	12		
9	E	16	Total	O	0	0
			16	16		
9	F	18	Total	O	0	0
			18	18		
9	G	27	Total	O	0	0
			27	27		
9	H	26	Total	O	0	0
			26	26		

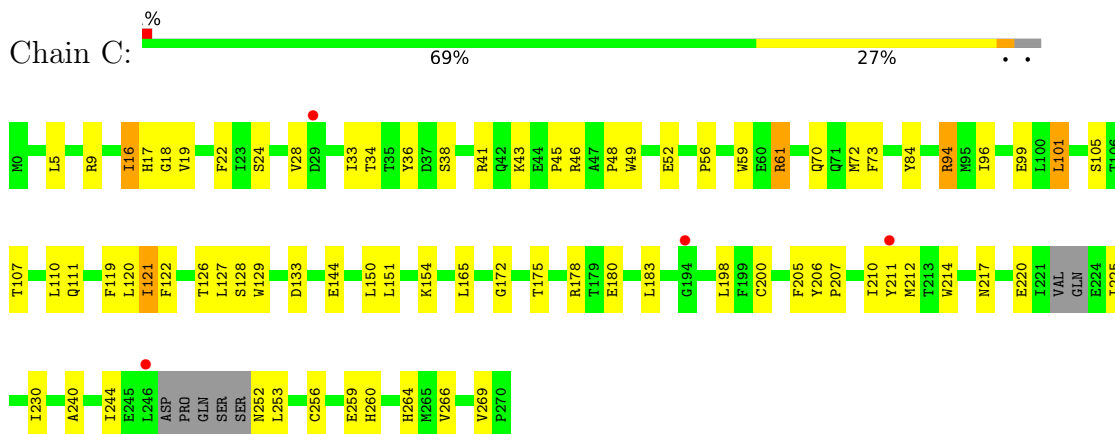
3 Residue-property plots [i](#)

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.

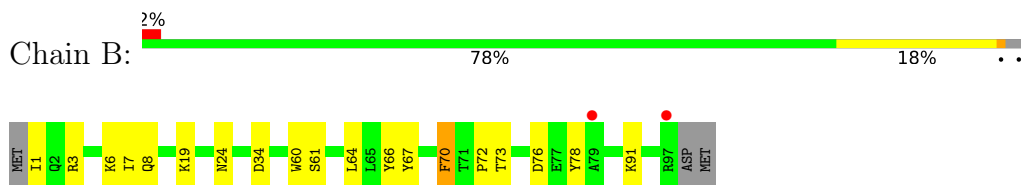
- Molecule 1: Major histocompatibility complex class I-related gene protein



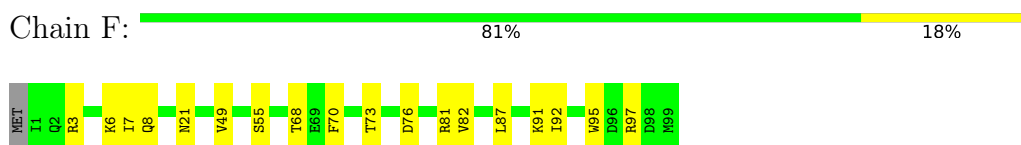
- Molecule 1: Major histocompatibility complex class I-related gene protein



- Molecule 2: Beta-2-microglobulin

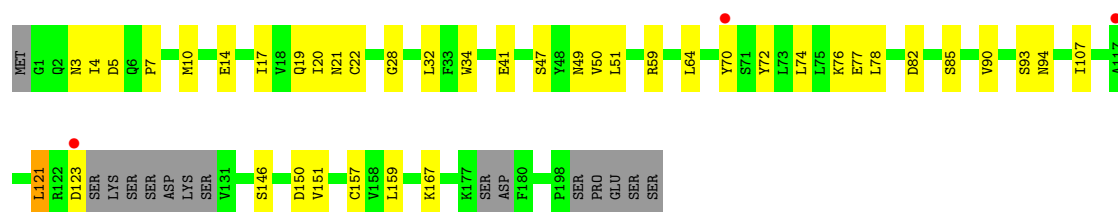


- Molecule 2: Beta-2-microglobulin



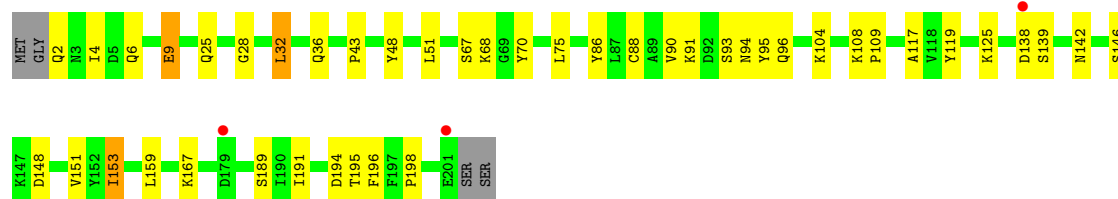
- Molecule 3: Human TCR TRAV1-2_ALPHA

Chain D: 



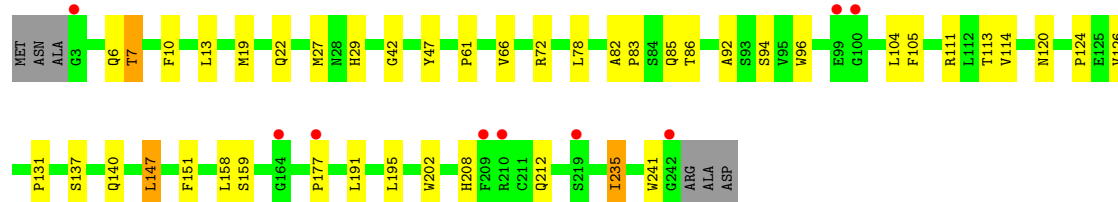
- Molecule 3: Human TCR TRAV1-2_ALPHA

Chain G: 



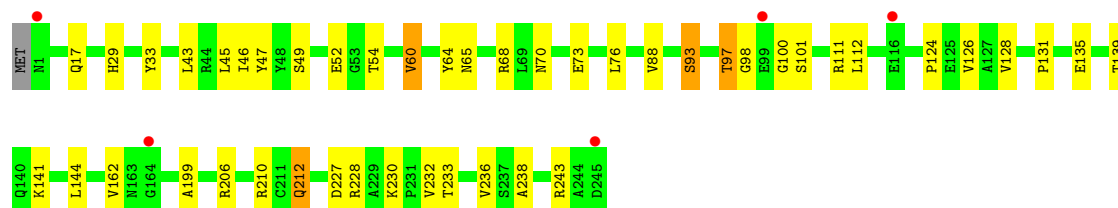
- Molecule 4: Human TCR TRBV6-1_BETA

Chain E: 



- Molecule 4: Human TCR TRBV6-1_BETA

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.57Å 69.62Å 143.34Å 90.00° 104.17° 90.00°	Depositor
Resolution (Å)	49.84 – 3.00 49.84 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.84-3.00) 98.2 (49.84-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.193 , 0.255 0.193 , 0.255	Depositor DCC
R_{free} test set	2250 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12799	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, GOL, NA, XIE

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	0.37	0/2183	0.54	0/2975
1	C	0.37	0/2255	0.54	0/3065
2	B	0.33	0/796	0.54	0/1087
2	F	0.35	0/821	0.56	0/1119
3	D	0.34	0/1454	0.55	0/1979
3	G	0.39	0/1569	0.60	0/2134
4	E	0.33	0/1885	0.52	0/2575
4	H	0.39	0/1935	0.59	0/2637
All	All	0.36	0/12898	0.55	0/17571

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	ARG	Sidechain

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	2119	0	1954	32	0
1	C	2182	0	2069	47	0
2	B	773	0	703	9	0
2	F	798	0	731	10	0
3	D	1420	0	1300	20	0
3	G	1531	0	1416	28	0
4	E	1834	0	1679	25	0
4	H	1885	0	1756	31	0
5	A	14	0	0	1	0
5	C	14	0	0	0	0
6	A	8	0	6	2	0
6	C	4	0	3	0	0
7	C	12	0	16	1	0
7	F	12	0	16	2	0
7	H	6	0	8	3	0
8	H	1	0	0	0	0
9	A	38	0	0	4	0
9	B	5	0	0	0	0
9	C	44	0	0	5	0
9	D	12	0	0	0	0
9	E	16	0	0	3	0
9	F	18	0	0	1	0
9	G	27	0	0	2	0
9	H	26	0	0	0	0
All	All	12799	0	11657	191	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 8.

All (191) 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:125:LYS:NZ	9:G:301:HOH:O	2.03	0.90
1:A:77:LEU:HD13	1:A:92:TYR:HB2	1.59	0.85
1:C:9:ARG:NH2	9:C:401:HOH:O	2.09	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:32:LEU:HD22	3:G:90:VAL:HG22	1.63	0.79
1:A:64:GLN:OE1	4:H:54:THR:OG1	2.01	0.78
4:H:29:HIS:ND1	4:H:93:SER:OG	2.16	0.77
1:A:61:ARG:NH2	3:G:94:ASN:O	2.23	0.72
7:F:301:GOL:O1	7:F:301:GOL:O3	2.06	0.71
3:D:146:SER:HB2	3:D:151:VAL:HG23	1.73	0.71
4:H:98:GLY:H	7:H:301:GOL:H32	1.56	0.70
3:G:146:SER:HB3	3:G:153:ILE:HG13	1.75	0.69
2:F:49:VAL:HG12	2:F:68:THR:HB	1.75	0.69
1:A:149:GLU:OE1	4:H:101:SER:OG	2.11	0.68
5:A:301[A]:XIE:N	9:A:401:HOH:O	2.26	0.68
1:C:24:SER:OG	9:C:402:HOH:O	2.11	0.67
4:E:42:GLY:O	9:E:301:HOH:O	2.12	0.67
3:G:148:ASP:HB3	3:G:151:VAL:HG22	1.77	0.67
3:D:32:LEU:HD12	3:D:90:VAL:HG22	1.78	0.66
4:H:49:SER:OG	4:H:68:ARG:NH2	2.25	0.66
1:C:111:GLN:HG2	1:C:121:ILE:HG23	1.76	0.66
4:E:13:LEU:HB2	4:E:114:VAL:HG12	1.78	0.65
1:A:49:TRP:O	1:A:53:ASN:ND2	2.29	0.65
2:F:7:ILE:HG12	2:F:82:VAL:HG21	1.78	0.65
4:H:128:VAL:HG23	4:H:238:ALA:HB3	1.78	0.65
4:E:131:PRO:HD2	4:E:202:TRP:CZ2	2.32	0.64
1:A:28:VAL:HG23	1:A:33:ILE:HD13	1.79	0.64
1:A:186:VAL:HG23	1:A:267:LEU:HD12	1.79	0.64
1:C:61:ARG:NH1	3:D:94:ASN:O	2.30	0.64
3:G:142:ASN:O	9:G:302:HOH:O	2.15	0.64
4:E:7:THR:HG23	4:E:22:GLN:HB2	1.79	0.63
4:H:139:THR:HG23	4:H:141:LYS:H	1.64	0.62
4:E:13:LEU:HD11	4:E:19:MET:HB2	1.80	0.62
1:A:30:SER:HB3	9:A:425:HOH:O	2.00	0.61
3:D:7:PRO:HD2	3:D:21:ASN:O	2.01	0.61
1:A:13:SER:HB3	1:A:90:HIS:H	1.66	0.60
1:A:93:GLN:HB2	1:A:113:ALA:HB3	1.82	0.60
2:F:73:THR:OG1	2:F:76:ASP:OD1	2.19	0.60
4:H:131:PRO:HD3	4:H:144:LEU:HG	1.83	0.59
4:E:83:PRO:HA	4:E:114:VAL:HG23	1.84	0.59
1:C:200:CYS:HB2	1:C:214:TRP:CZ2	2.39	0.58
4:H:210:ARG:NH1	4:H:212:GLN:OE1	2.36	0.58
1:A:198:LEU:HD12	1:A:254:TYR:HD1	1.70	0.57
3:D:14:GLU:OE1	3:D:167:LYS:HE2	2.04	0.57
4:H:135:GLU:O	4:H:139:THR:HG22	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ARG:HD3	9:A:412:HOH:O	2.04	0.56
4:E:29:HIS:HB3	4:E:94:SER:O	2.05	0.56
3:G:32:LEU:CD2	3:G:90:VAL:HG22	2.33	0.56
3:G:108:LYS:HB3	3:G:139:SER:HB3	1.88	0.56
1:C:144:GLU:HA	1:C:150:LEU:HD11	1.87	0.56
1:A:16:ILE:HG22	1:A:17:HIS:H	1.72	0.55
3:G:32:LEU:HD11	3:G:88[A]:CYS:SG	2.46	0.55
2:B:73:THR:OG1	2:B:76:ASP:OD2	2.22	0.55
1:C:211[A]:TYR:HB2	1:C:259:GLU:HB2	1.88	0.55
1:C:211[B]:TYR:HB3	1:C:259:GLU:HB2	1.88	0.54
4:E:120:ASN:HB2	9:E:307:HOH:O	2.06	0.54
3:G:36:GLN:O	3:G:43:PRO:HA	2.07	0.54
4:E:92:ALA:HA	4:E:105:PHE:O	2.07	0.54
2:B:6:LYS:HE2	2:B:8:GLN:NE2	2.22	0.54
1:C:34:THR:HB	1:C:43:LYS:HE2	1.90	0.54
4:H:97:THR:HA	7:H:301:GOL:H2	1.88	0.53
4:E:10:PHE:CE2	4:E:111:ARG:HG3	2.43	0.53
4:H:126:VAL:HG21	4:H:236:VAL:O	2.08	0.53
9:C:417:HOH:O	7:F:302:GOL:H11	2.08	0.53
1:C:96:ILE:HG13	1:C:110:LEU:HD13	1.91	0.53
2:F:87:LEU:O	9:F:401:HOH:O	2.18	0.52
1:C:151:LEU:HD22	3:D:51:LEU:HD12	1.92	0.52
1:C:175:THR:O	1:C:178:ARG:HG2	2.10	0.52
2:B:3:ARG:NH1	2:B:61:SER:HB3	2.25	0.51
1:C:210:ILE:O	4:H:206:ARG:HD2	2.10	0.51
4:E:82:ALA:O	4:E:114:VAL:HG21	2.10	0.51
1:C:41:ARG:NH1	9:C:408:HOH:O	2.43	0.51
1:C:94:ARG:HH12	7:C:302:GOL:H11	1.76	0.51
4:E:177:PRO:HG3	4:E:191:LEU:HD13	1.92	0.51
1:C:28:VAL:HG23	1:C:33:ILE:HD13	1.92	0.51
3:G:119:TYR:CE1	4:H:135:GLU:HG3	2.46	0.51
3:G:36:GLN:HG3	3:G:86:TYR:CE2	2.46	0.51
1:C:48:PRO:O	1:C:52:GLU:HG3	2.11	0.51
1:C:101:LEU:HB2	1:C:105:SER:O	2.10	0.51
3:G:196:PHE:CE2	3:G:198:PRO:HG3	2.46	0.50
4:H:46:ILE:HG22	4:H:47:TYR:HD2	1.76	0.50
4:H:70:ASN:HD21	4:H:73:GLU:HB2	1.76	0.49
1:C:61:ARG:HG2	3:D:94:ASN:HB3	1.94	0.49
1:A:27:TYR:CG	6:A:303:ACT:H3	2.47	0.49
4:E:85:GLN:HG2	9:E:313:HOH:O	2.13	0.49
1:A:152:TYR:CD2	4:H:100:GLY:HA3	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LEU:HB2	1:A:165:LEU:HD13	1.93	0.49
1:A:247:ASP:OD2	1:A:250:SER:N	2.45	0.49
4:E:86:THR:HG23	4:E:113:THR:HA	1.95	0.49
3:D:78:LEU:HD13	3:D:107:ILE:HD12	1.94	0.49
2:F:76:ASP:O	2:F:97:ARG:NH1	2.46	0.49
3:D:10:MET:HE2	3:D:20:ILE:HG12	1.94	0.48
1:A:54:LEU:HD13	1:A:58:HIS:CD2	2.48	0.48
4:E:19:MET:HB3	4:E:78:LEU:HG	1.96	0.48
1:A:91:THR:HG22	9:A:410:HOH:O	2.14	0.48
1:C:200:CYS:O	1:C:212:MET:HE1	2.14	0.48
3:D:19:GLN:HG3	3:D:72:TYR:HB2	1.95	0.48
2:B:19:LYS:O	2:B:72:PRO:HD2	2.14	0.48
3:G:4:ILE:HD13	3:G:90:VAL:HG23	1.96	0.47
3:G:191:ILE:HG22	3:G:195:THR:OG1	2.13	0.47
1:C:5:LEU:HB2	1:C:165:LEU:HD13	1.96	0.47
1:C:84:TYR:OH	1:C:133:ASP:OD2	2.15	0.47
4:E:158:LEU:HD23	4:E:159:SER:N	2.29	0.47
4:H:64:TYR:HD2	4:H:76:LEU:HD11	1.79	0.47
3:D:28:GLY:HA3	3:D:93:SER:OG	2.13	0.47
4:H:124:PRO:HG2	4:H:236:VAL:HG21	1.96	0.47
1:C:119:PHE:CD2	1:C:120:LEU:HG	2.50	0.47
1:C:210:ILE:HG13	1:C:260:HIS:HB2	1.96	0.47
2:B:64:LEU:HD13	2:B:66:TYR:HE1	1.80	0.47
1:C:126:THR:OG1	1:C:128:SER:OG	2.23	0.47
1:C:256:CYS:O	1:C:266:VAL:HA	2.15	0.47
3:D:59:ARG:HH12	3:D:82:ASP:CG	2.23	0.47
4:E:72:ARG:HE	4:E:72:ARG:HB3	1.58	0.47
4:H:232:VAL:HG23	4:H:233:THR:O	2.14	0.47
3:G:138:ASP:OD1	3:G:139:SER:N	2.48	0.46
3:G:189:SER:HB3	3:G:191:ILE:HD11	1.97	0.46
1:C:72:MET:HA	4:E:96:TRP:CH2	2.51	0.46
2:F:81:ARG:HG3	2:F:92:ILE:HG12	1.97	0.46
4:E:47:TYR:HB2	4:E:66:VAL:HG11	1.97	0.46
1:C:217:ASN:OD1	1:C:252:ASN:N	2.48	0.46
1:A:47:ALA:O	1:A:50:MET:HB2	2.16	0.46
1:A:120:LEU:HB3	1:A:129:TRP:CE3	2.50	0.46
1:A:42:GLN:HA	1:A:63:THR:HG23	1.97	0.46
1:C:264:HIS:HB2	9:C:427:HOH:O	2.15	0.46
1:C:230:ILE:HG12	1:C:240:ALA:HB2	1.96	0.45
4:H:243:ARG:HA	4:H:243:ARG:HD2	1.76	0.45
3:D:59:ARG:NH1	3:D:82:ASP:OD1	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:TYR:CE2	4:H:100:GLY:HA3	2.51	0.45
1:A:210:ILE:HG13	1:A:260:HIS:HB2	1.99	0.45
3:D:49:ASN:HB3	3:D:64:LEU:HB2	1.98	0.45
1:C:198:LEU:HD13	1:C:269:VAL:HG21	1.99	0.45
4:H:141:LYS:HA	4:H:199:ALA:N	2.32	0.45
1:A:215:MET:HE2	1:A:257:HIS:CE1	2.52	0.45
3:G:48:TYR:CE2	4:H:101:SER:HB3	2.52	0.45
3:G:28:GLY:HA3	3:G:93:SER:HB3	2.00	0.44
3:D:34:TRP:HB2	3:D:47:SER:OG	2.16	0.44
1:C:99:GLU:HB2	1:C:107:THR:OG1	2.16	0.44
4:H:33:TYR:HB3	4:H:45:LEU:HD11	1.99	0.44
4:H:98:GLY:N	7:H:301:GOL:H32	2.30	0.44
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.53	0.44
2:B:7:ILE:HD12	2:B:91:LYS:HD2	1.98	0.44
1:C:22:PHE:CG	1:C:70:GLN:HG3	2.52	0.44
1:C:225:ILE:HG12	1:C:244:ILE:HG22	1.99	0.44
3:D:3:ASN:ND2	3:D:5:ASP:OD1	2.50	0.44
1:A:27:TYR:CD1	6:A:303:ACT:H3	2.53	0.44
3:D:74:LEU:HD21	3:D:76:LYS:HE3	2.00	0.43
1:C:16:ILE:HG23	1:C:18:GLY:H	1.83	0.43
1:C:122:PHE:HB2	1:C:129:TRP:CH2	2.53	0.43
2:B:24:ASN:OD1	2:B:67:TYR:HB3	2.19	0.43
3:G:9:GLU:HB2	3:G:104:LYS:HB3	1.99	0.43
1:A:151:LEU:HD22	3:G:51:LEU:HD12	2.00	0.43
3:D:78:LEU:HD23	3:D:78:LEU:HA	1.79	0.43
4:E:212:GLN:HG3	4:E:235:ILE:HD12	2.00	0.43
1:C:56:PRO:HA	1:C:59:TRP:HD1	1.83	0.43
2:F:6:LYS:HE2	2:F:8:GLN:NE2	2.34	0.43
3:G:109:PRO:HD2	3:G:139:SER:OG	2.19	0.42
4:H:88:VAL:HG22	4:H:111:ARG:HD3	2.01	0.42
1:A:140:LYS:NZ	1:A:144:GLU:OE2	2.47	0.42
1:A:46:ARG:HD3	1:A:46:ARG:HA	1.69	0.42
1:C:49:TRP:CD2	1:C:172:GLY:HA3	2.55	0.42
4:E:6:GLN:HA	4:E:22:GLN:O	2.20	0.42
4:H:46:ILE:HD13	4:H:60:VAL:HG23	2.00	0.42
4:H:128:VAL:HG23	4:H:238:ALA:CB	2.46	0.42
3:G:117:ALA:HB2	3:G:196:PHE:HB3	2.02	0.42
1:C:122:PHE:HB2	1:C:129:TRP:CZ3	2.55	0.42
3:G:91:LYS:HG2	3:G:95:TYR:HA	2.01	0.42
1:C:206:TYR:CD1	1:C:207:PRO:HA	2.55	0.42
2:B:70:PHE:HD2	2:B:78:TYR:CZ	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ARG:HB3	1:C:46:ARG:NH1	2.35	0.41
1:C:22:PHE:HB3	1:C:38:SER:HB3	2.02	0.41
4:H:230:LYS:HE2	4:H:232:VAL:HG12	2.01	0.41
3:D:121:LEU:N	3:D:121:LEU:HD12	2.36	0.41
2:F:81:ARG:HA	2:F:91:LYS:O	2.20	0.41
1:C:22:PHE:CB	1:C:70:GLN:HG3	2.50	0.41
4:H:139:THR:HG23	4:H:141:LYS:N	2.33	0.41
1:C:180:GLU:O	1:C:205:PHE:HA	2.20	0.41
3:G:146:SER:HB2	3:G:151:VAL:HG23	2.01	0.41
4:E:126:VAL:HA	4:E:147:LEU:O	2.21	0.41
1:C:127:LEU:HD21	1:C:154:LYS:HD2	2.03	0.41
2:F:21:ASN:HB3	2:F:70:PHE:CE1	2.56	0.41
2:F:95:TRP:CE2	2:F:97:ARG:HA	2.56	0.41
3:D:5:ASP:O	3:D:22:CYS:HA	2.22	0.40
3:G:159:LEU:O	3:G:167:LYS:HA	2.21	0.40
1:A:27:TYR:HA	1:A:31:HIS:O	2.22	0.40
1:C:45:PRO:HB3	1:C:59:TRP:CH2	2.56	0.40
3:G:148:ASP:HB3	3:G:151:VAL:CG2	2.49	0.40
1:C:36:TYR:CD1	1:C:36:TYR:C	2.99	0.40
4:E:111:ARG:H	4:E:111:ARG:HG2	1.73	0.40
1:A:13:SER:CB	1:A:90:HIS:H	2.33	0.40
4:E:124:PRO:HB3	4:E:151:PHE:CD2	2.56	0.40
4:E:208:HIS:HB2	4:E:241:TRP:CZ3	2.56	0.40
3:G:68:LYS:HA	3:G:68:LYS:HD3	1.93	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	261/271 (96%)	252 (97%)	9 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	260/271 (96%)	251 (96%)	9 (4%)	0	100	100
2	B	95/100 (95%)	92 (97%)	3 (3%)	0	100	100
2	F	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
3	D	184/204 (90%)	174 (95%)	9 (5%)	1 (0%)	24	60
3	G	199/204 (98%)	191 (96%)	8 (4%)	0	100	100
4	E	238/246 (97%)	224 (94%)	13 (6%)	1 (0%)	30	65
4	H	243/246 (99%)	229 (94%)	12 (5%)	2 (1%)	16	50
All	All	1577/1642 (96%)	1508 (96%)	65 (4%)	4 (0%)	36	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	43	LEU
4	H	52	GLU
4	E	61	PRO
3	D	50	VAL

5.3.2 Protein sidechains ⓘ

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	217/241 (90%)	211 (97%)	6 (3%)	38	70
1	C	231/241 (96%)	220 (95%)	11 (5%)	23	57
2	B	82/95 (86%)	79 (96%)	3 (4%)	30	64
2	F	86/95 (90%)	84 (98%)	2 (2%)	44	74
3	D	143/181 (79%)	132 (92%)	11 (8%)	12	40
3	G	166/181 (92%)	155 (93%)	11 (7%)	15	46
4	E	189/212 (89%)	181 (96%)	8 (4%)	26	61
4	H	195/212 (92%)	185 (95%)	10 (5%)	21	55
All	All	1309/1458 (90%)	1247 (95%)	62 (5%)	23	58

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	57	ASP
1	A	66	LEU
1	A	139	ILE
1	A	153	GLN
1	A	267	LEU
2	B	1	ILE
2	B	34	ASP
2	B	70	PHE
1	C	16	ILE
1	C	17	HIS
1	C	19	VAL
1	C	61	ARG
1	C	73	PHE
1	C	94	ARG
1	C	101	LEU
1	C	121	ILE
1	C	183	LEU
1	C	220	GLU
1	C	253	LEU
3	D	4	ILE
3	D	17	ILE
3	D	41	GLU
3	D	70	TYR
3	D	77	GLU
3	D	85	SER
3	D	121	LEU
3	D	123	ASP
3	D	150	ASP
3	D	157	CYS
3	D	159	LEU
4	E	7	THR
4	E	27	MET
4	E	104	LEU
4	E	137	SER
4	E	140	GLN
4	E	147	LEU
4	E	195	LEU
4	E	235	ILE
2	F	3	ARG
2	F	55	SER
3	G	2	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	6	GLN
3	G	9	GLU
3	G	25	GLN
3	G	32	LEU
3	G	67	SER
3	G	70	TYR
3	G	75	LEU
3	G	96	GLN
3	G	153	ILE
3	G	194	ASP
4	H	17	GLN
4	H	60	VAL
4	H	65	ASN
4	H	93	SER
4	H	97	THR
4	H	112	LEU
4	H	162	VAL
4	H	212	GLN
4	H	227	ASP
4	H	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	137	HIS
1	A	187	ASN
1	C	64	GLN
1	C	117	GLN
1	C	123	ASN
1	C	148	HIS
1	C	217	ASN
1	C	260	HIS
3	D	36	GLN
3	D	49	ASN
4	E	168	HIS
4	E	214	GLN
2	F	13	HIS
3	G	94	ASN
3	G	120	GLN
3	G	184	ASN
4	H	185	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	XIE	C	301[A]	1	7,7,8	0.54	0	8,8,9	0.38	0
7	GOL	F	301	-	5,5,5	0.91	0	5,5,5	1.21	1 (20%)
5	XIE	A	301[A]	1	7,7,8	0.57	0	8,8,9	0.28	0
6	ACT	C	303	-	3,3,3	1.89	1 (33%)	3,3,3	1.10	0
6	ACT	A	303	-	3,3,3	1.11	0	3,3,3	1.07	0
7	GOL	F	302	-	5,5,5	0.90	0	5,5,5	1.18	1 (20%)
5	XIE	C	301[B]	1	7,7,8	0.53	0	8,8,9	0.38	0
6	ACT	A	302	-	3,3,3	1.74	1 (33%)	3,3,3	1.31	0
7	GOL	C	304	-	5,5,5	1.07	0	5,5,5	0.94	0
5	XIE	A	301[B]	1	7,7,8	0.61	0	8,8,9	0.59	0
7	GOL	C	302	-	5,5,5	0.69	0	5,5,5	1.32	1 (20%)
7	GOL	H	301	-	5,5,5	1.00	0	5,5,5	1.13	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	XIE	C	301[A]	1	-	-	0/1/1/1
7	GOL	F	301	-	-	0/4/4/4	-
5	XIE	A	301[A]	1	-	-	0/1/1/1
7	GOL	F	302	-	-	4/4/4/4	-
5	XIE	C	301[B]	1	-	-	0/1/1/1
7	GOL	C	304	-	-	2/4/4/4	-
5	XIE	A	301[B]	1	-	-	0/1/1/1
7	GOL	C	302	-	-	0/4/4/4	-
7	GOL	H	301	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	303	ACT	CH3-C	2.90	1.60	1.49
6	A	302	ACT	CH3-C	2.65	1.59	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	301	GOL	C3-C2-C1	-2.18	103.80	111.80
7	F	302	GOL	C3-C2-C1	-2.18	103.81	111.80
7	C	302	GOL	C3-C2-C1	-2.07	104.20	111.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

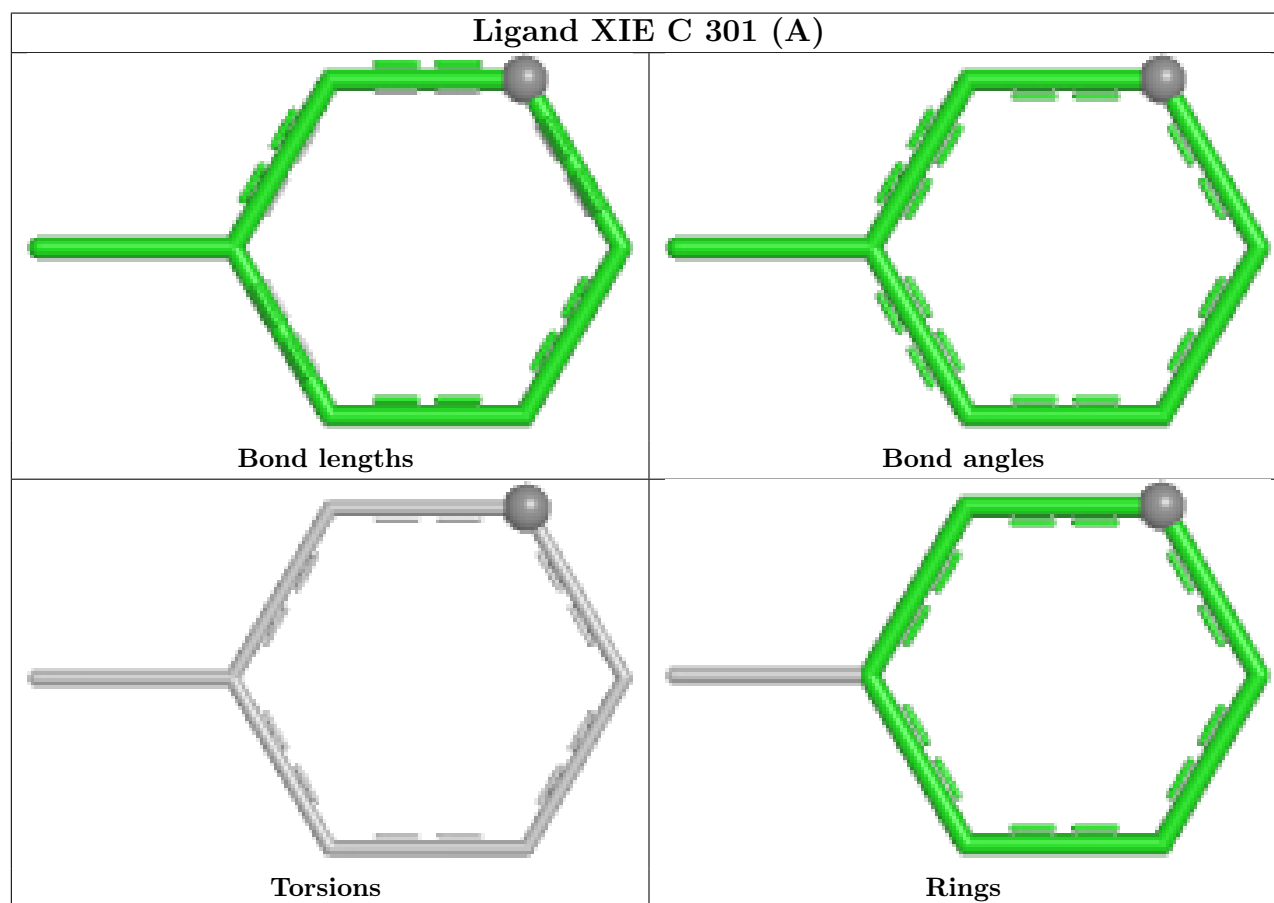
Mol	Chain	Res	Type	Atoms
7	H	301	GOL	O1-C1-C2-C3
7	C	304	GOL	O1-C1-C2-C3
7	F	302	GOL	O1-C1-C2-C3
7	F	302	GOL	C1-C2-C3-O3
7	C	304	GOL	O1-C1-C2-O2
7	H	301	GOL	O1-C1-C2-O2
7	F	302	GOL	O2-C2-C3-O3
7	F	302	GOL	O1-C1-C2-O2

There are no ring outliers.

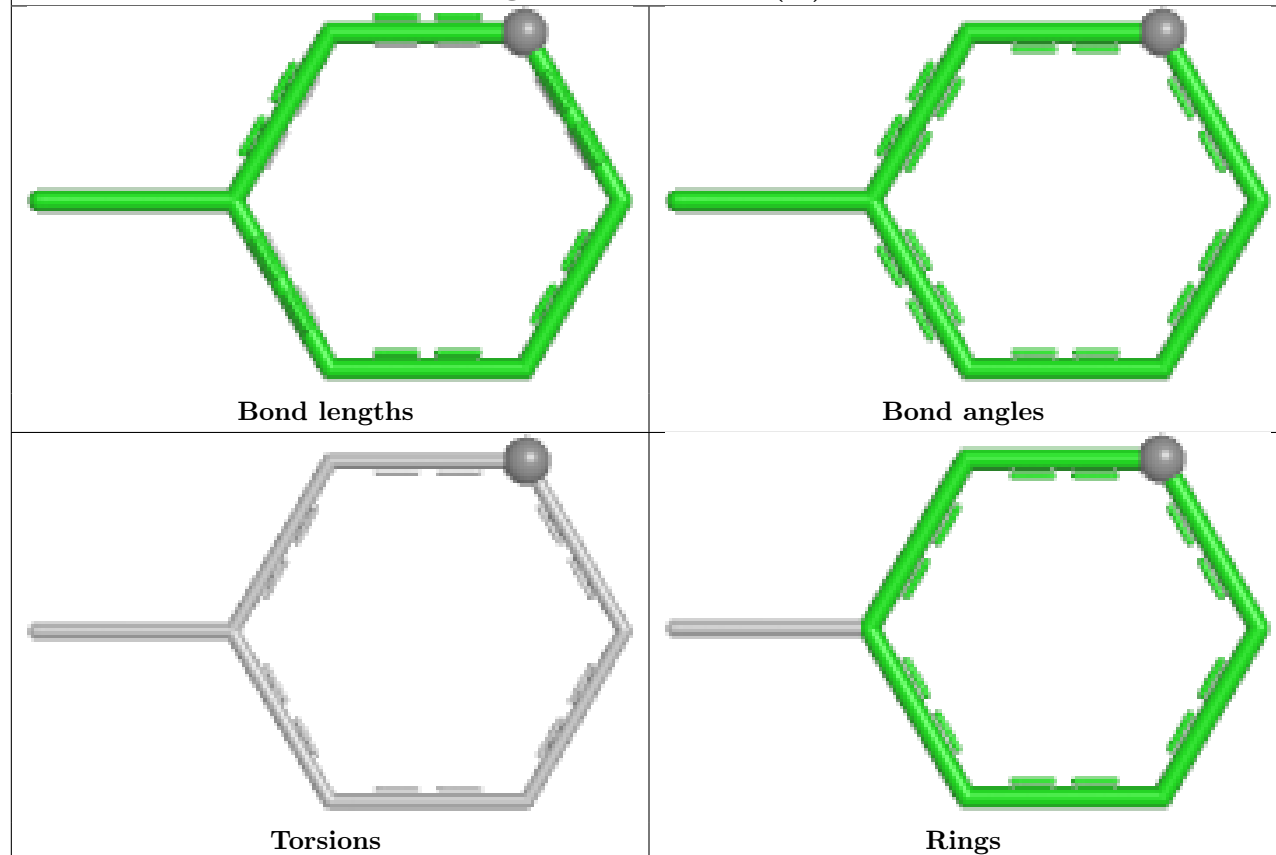
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	301	GOL	1	0
5	A	301[A]	XIE	1	0
6	A	303	ACT	2	0
7	F	302	GOL	1	0
7	C	302	GOL	1	0
7	H	301	GOL	3	0

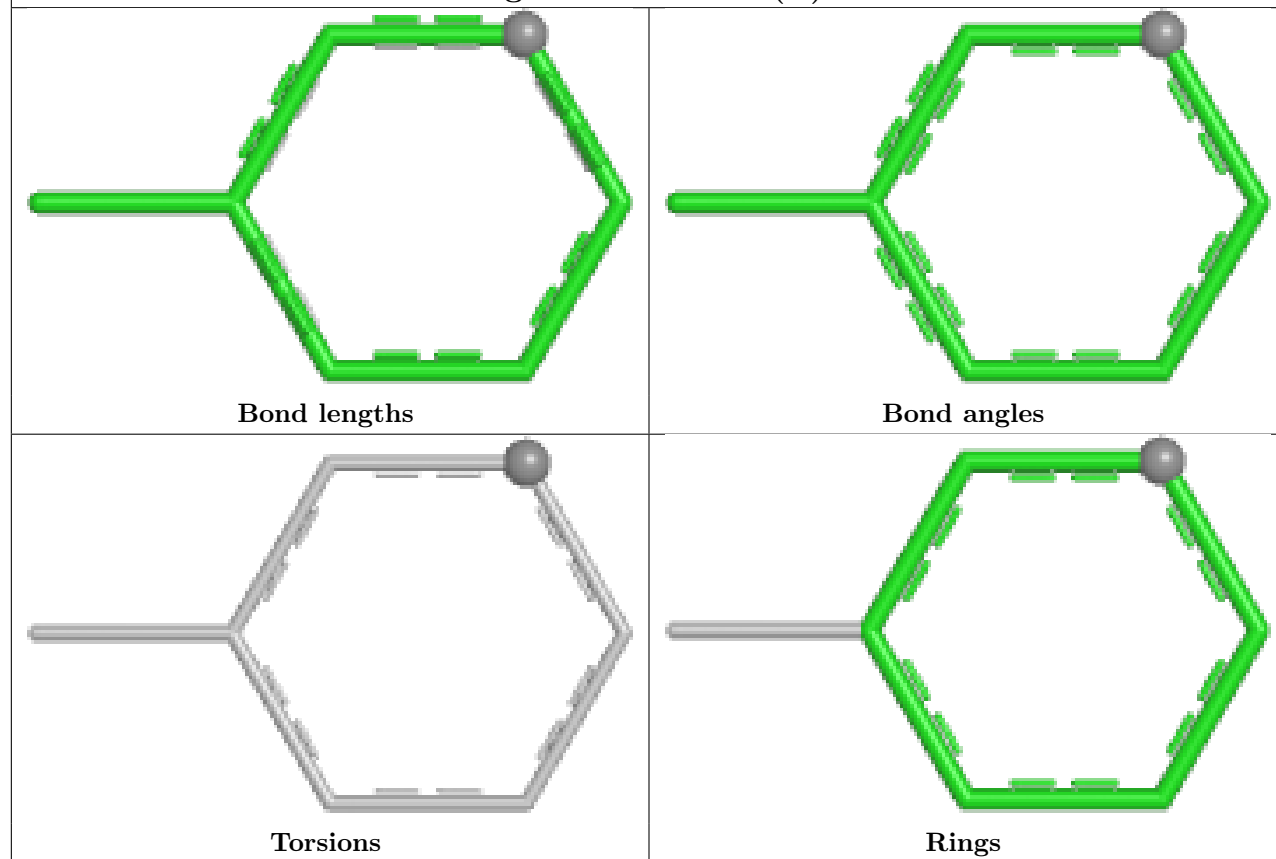
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

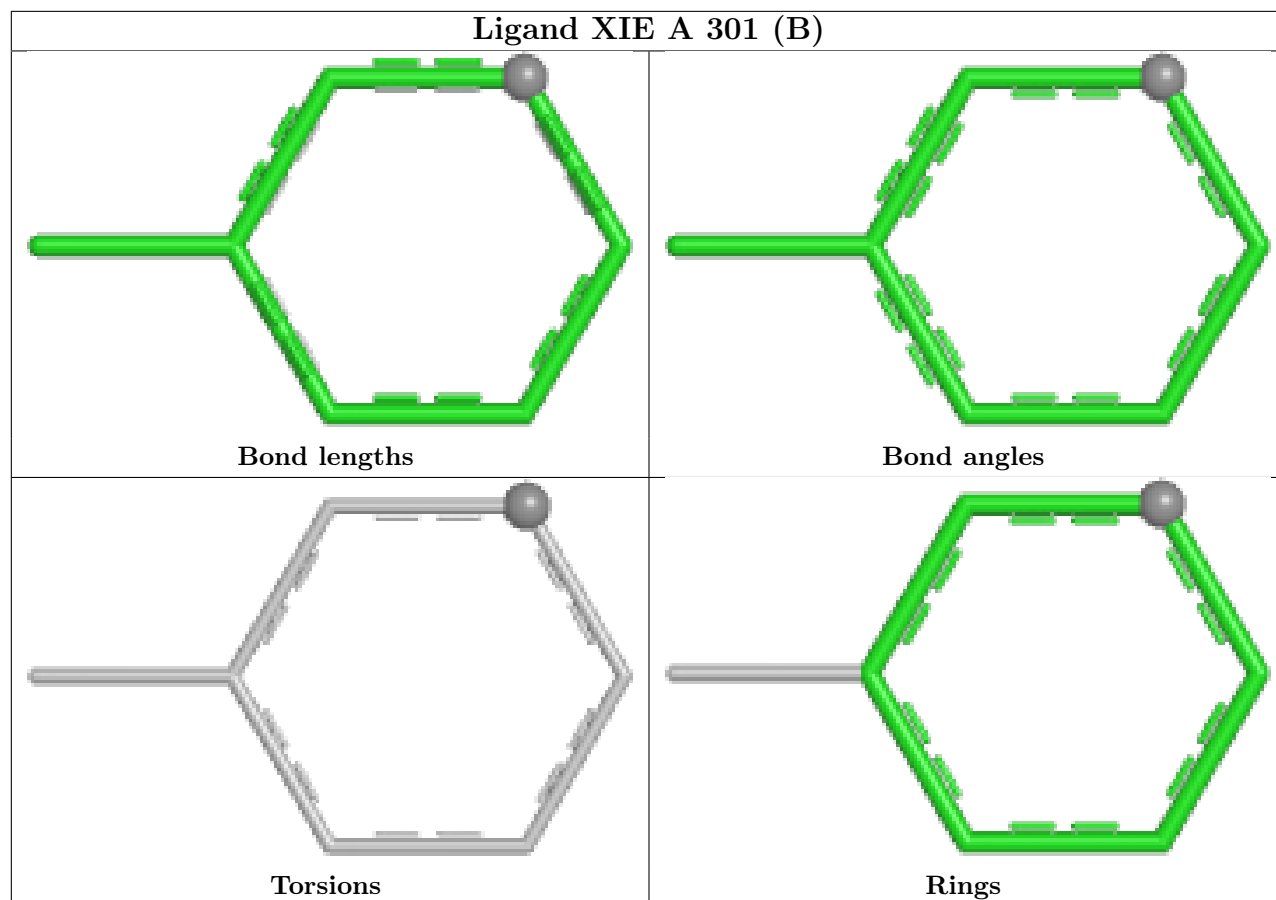


Ligand XIE A 301 (A)



Ligand XIE C 301 (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 ⓘ

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, 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%)	0.27	4 (1%) 72 49	29, 47, 82, 120	2 (0%)
1	C	264/271 (97%)	0.23	4 (1%) 72 49	26, 47, 72, 90	4 (1%)
2	B	97/100 (97%)	0.47	2 (2%) 63 40	38, 66, 91, 97	1 (1%)
2	F	99/100 (99%)	0.16	0 100 100	27, 51, 77, 83	3 (3%)
3	D	189/204 (92%)	0.41	3 (1%) 70 47	29, 54, 84, 100	1 (0%)
3	G	200/204 (98%)	0.30	3 (1%) 72 49	28, 47, 76, 95	5 (2%)
4	E	240/246 (97%)	0.38	9 (3%) 44 24	34, 56, 85, 95	3 (1%)
4	H	245/246 (99%)	0.27	5 (2%) 65 41	32, 50, 75, 97	2 (0%)
All	All	1599/1642 (97%)	0.30	30 (1%) 66 43	26, 50, 83, 120	21 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	179	ASP	3.5
4	H	245	ASP	3.2
3	G	201	GLU	3.1
1	C	211[A]	TYR	3.0
4	E	99	GLU	2.9
4	E	100	GLY	2.9
1	A	270	PRO	2.8
1	C	194	GLY	2.8
2	B	79	ALA	2.8
4	E	164	GLY	2.6
4	E	242	GLY	2.5
4	E	210	ARG	2.4
1	C	246	LEU	2.4
3	D	117	ALA	2.4
4	H	1	ASN	2.3
3	G	138	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	29	ASP	2.3
4	E	3	GLY	2.2
1	A	189	LYS	2.2
2	B	97	ARG	2.2
3	D	123	ASP	2.2
3	D	70	TYR	2.1
4	H	116	GLU	2.1
4	E	177	PRO	2.1
4	H	164	GLY	2.1
1	A	223	GLN	2.1
1	A	249	GLN	2.1
4	E	219	SER	2.1
4	E	209	PHE	2.1
4	H	99	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
6	ACT	A	302	4/4	0.68	0.22	59,62,65,67	0
5	XIE	A	301[B]	7/8	0.76	0.22	26,27,28,28	7
5	XIE	A	301[A]	7/8	0.76	0.22	27,27,28,31	7
6	ACT	C	303	4/4	0.81	0.13	38,39,51,54	0
7	GOL	H	301	6/6	0.83	0.17	52,66,67,70	0
7	GOL	C	302	6/6	0.84	0.18	41,44,45,50	6
5	XIE	C	301[A]	7/8	0.86	0.19	47,49,51,51	7
7	GOL	F	302	6/6	0.86	0.12	38,42,47,50	0
5	XIE	C	301[B]	7/8	0.86	0.19	48,49,51,51	7

Continued on next page...

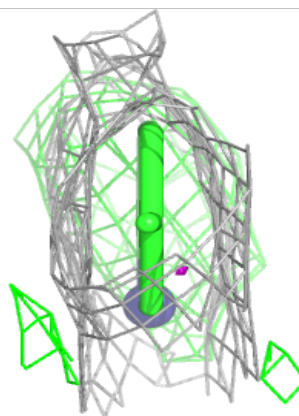
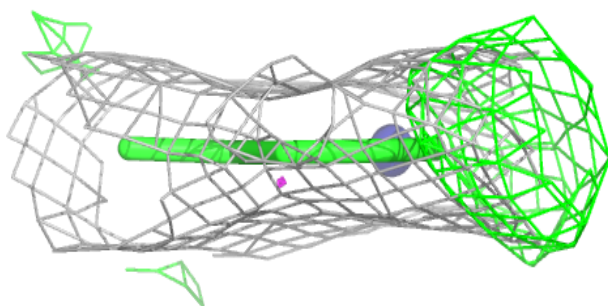
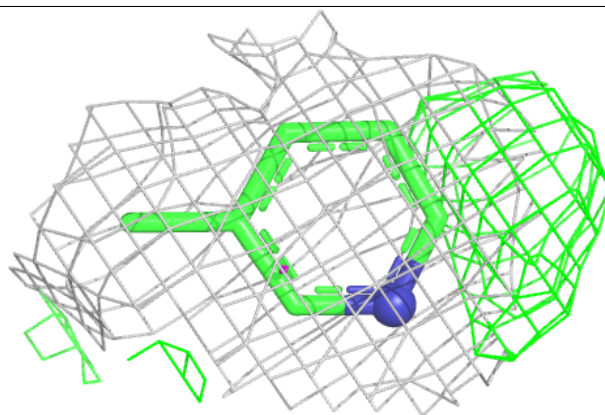
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NA	H	302	1/1	0.86	0.15	63,63,63,63	0
6	ACT	A	303	4/4	0.87	0.19	53,62,64,65	0
7	GOL	C	304	6/6	0.90	0.14	48,54,60,63	0
7	GOL	F	301	6/6	0.95	0.12	47,49,51,65	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.

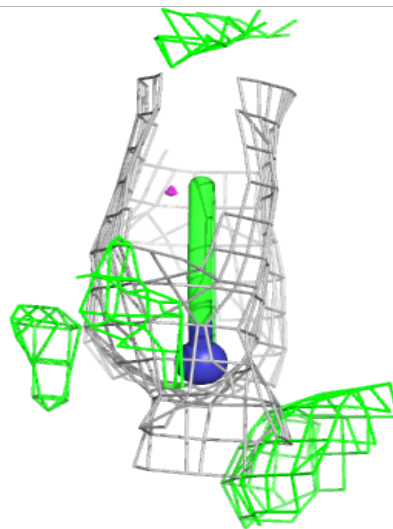
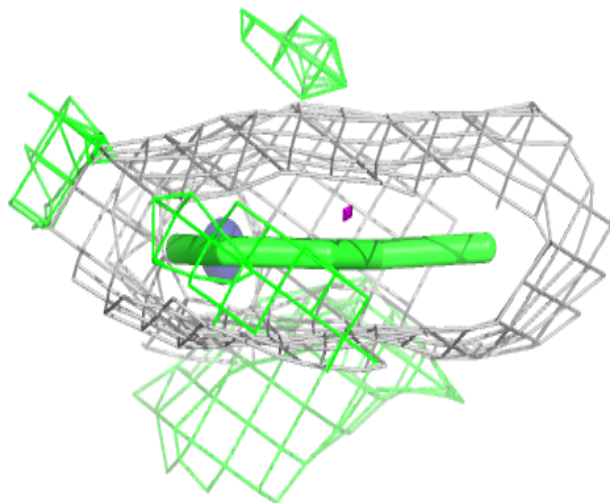
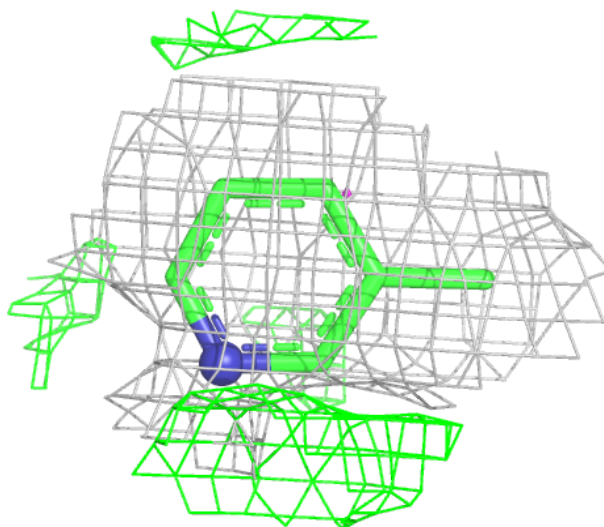
Electron density around XIE A 301 (B):

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



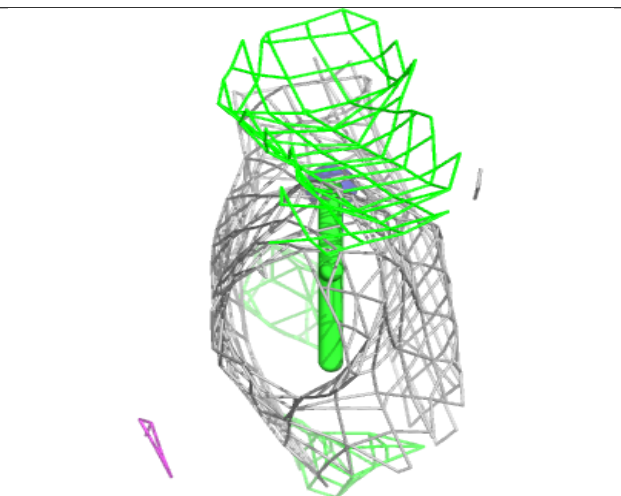
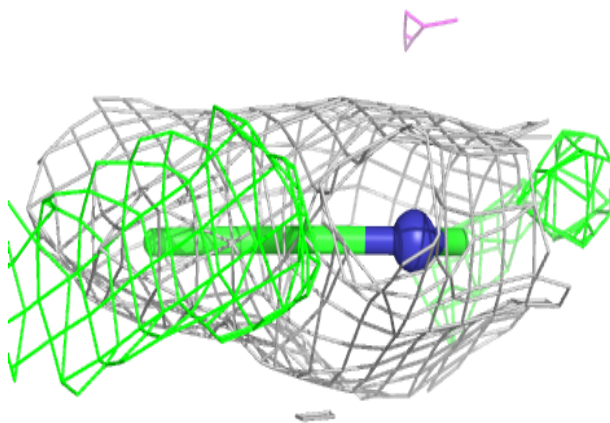
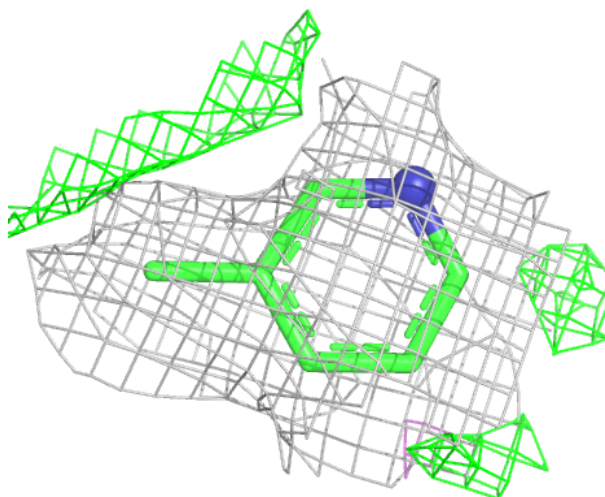
Electron density around XIE A 301 (A):

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



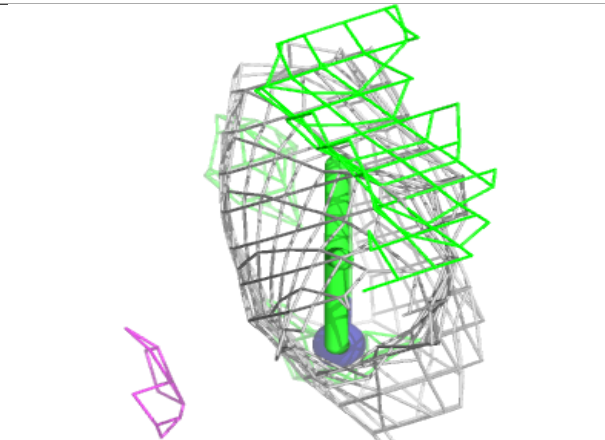
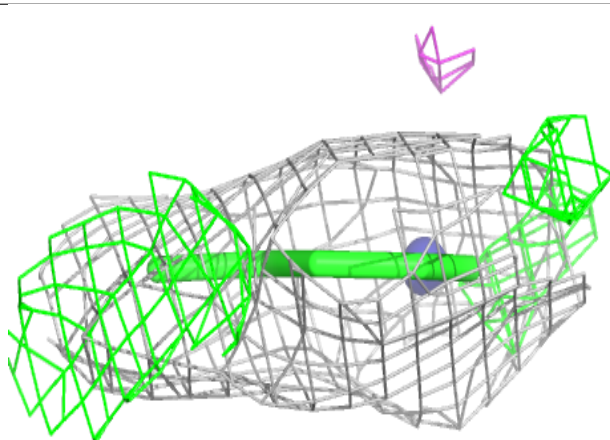
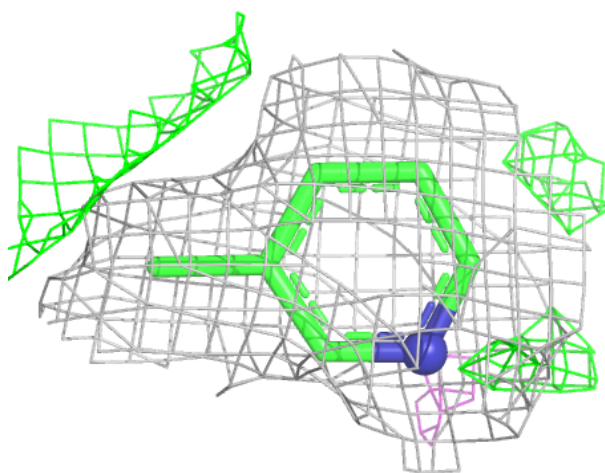
Electron density around XIE C 301 (A):

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



Electron density around XIE C 301 (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.