



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2024 – 10:17 AM EST

PDB ID : 9BU0  
Title : Structure of human MAIT A-F7 TCR in complex with human MR1-salicylaldehyde  
Authors : Awad, W.; Rossjohn, J.  
Deposited on : 2024-05-15  
Resolution : 2.89 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](mailto: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>.

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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)  
Xtrriage (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

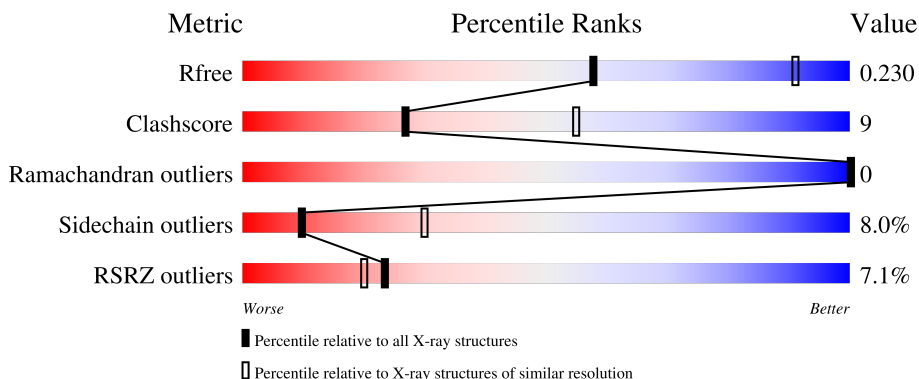
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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))
$R_{free}$	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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  $\geq 3$ , 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	 6% 76% 20% ..
1	C	271	 2% 67% 27% ..
2	B	100	 10% 61% 31% 7%
2	F	100	 3% 71% 26% ..
3	D	204	 13% 69% 22% 8%

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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
5	NK	A	301	-	-	X	-
6	GOL	A	302	-	-	X	-
6	GOL	C	302	-	-	X	-
7	ACT	F	102	-	X	-	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12615 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major histocompatibility complex class I-related gene protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	262	Total	C	N	O	S	0	8	0
			2169	1386	381	390	12			
1	C	263	Total	C	N	O	S	0	1	0
			2131	1369	368	383	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
			Total	C	N	O	S			
2	B	93	Total	C	N	O	S	0	0	0
			717	459	121	135	2			
2	F	99	Total	C	N	O	S	0	0	0
			792	505	135	149	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
			Total	C	N	O	S			
3	D	188	Total	C	N	O	S	0	1	0
			1408	905	221	273	9			

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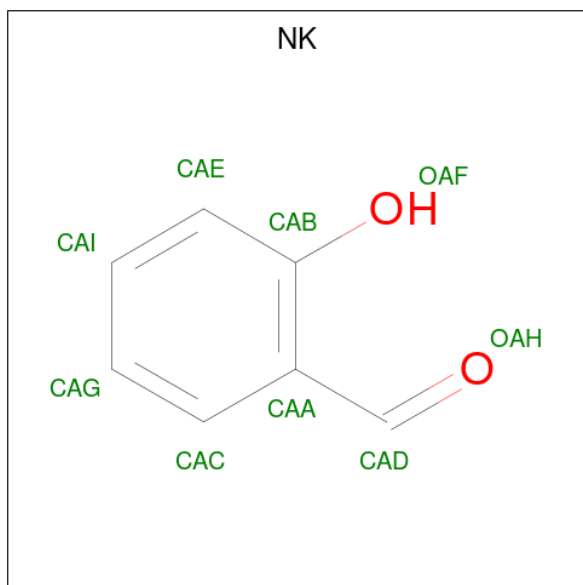
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	200	1560	990	246	313	11	0	5	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	232	1739	1101	299	330	9	0	2	0
4	H	244	1937	1224	333	367	13	0	7	0

- Molecule 5 is SALICYLALDEHYDE (three-letter code: NK) (formula: C<sub>7</sub>H<sub>6</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



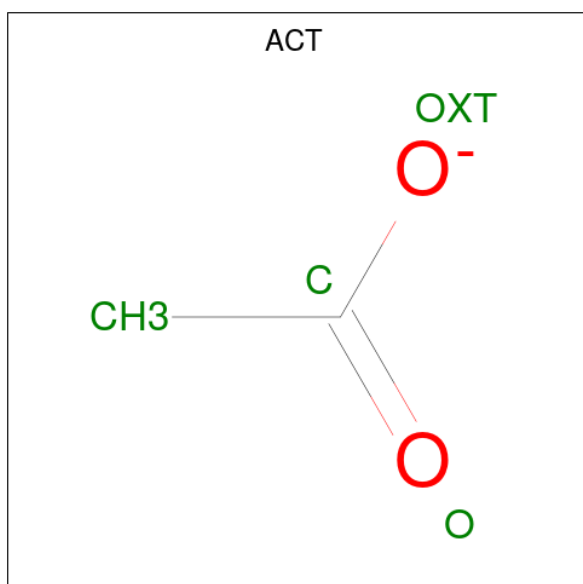
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	8	7	1	0	0
5	C	1	8	7	1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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	C	1	Total C O 6 3 3	0	0
6	F	1	Total C O 6 3 3	0	0

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



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

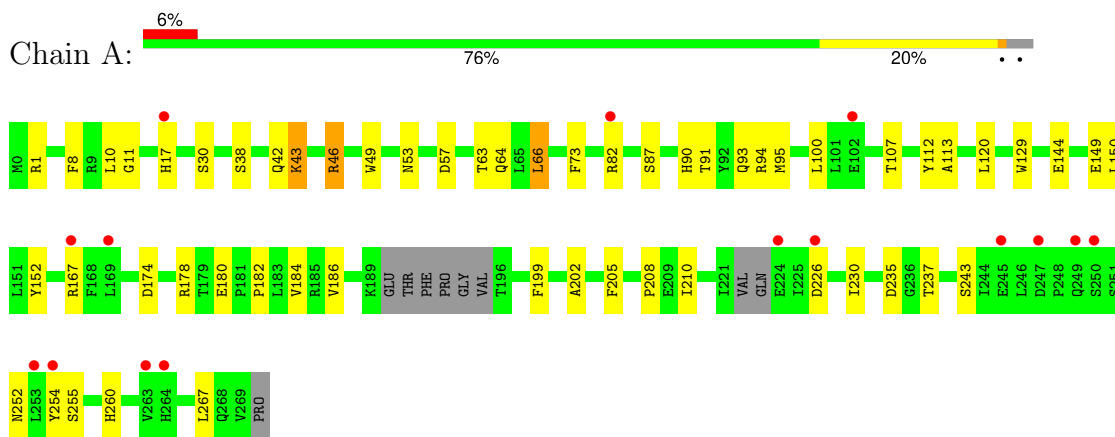
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	24	Total	O	0	0
			24	24		
8	B	7	Total	O	0	0
			7	7		
8	C	28	Total	O	0	0
			28	28		
8	D	7	Total	O	0	0
			7	7		
8	E	11	Total	O	0	0
			11	11		
8	F	8	Total	O	0	0
			8	8		
8	G	14	Total	O	0	0
			14	14		
8	H	13	Total	O	0	0
			13	13		

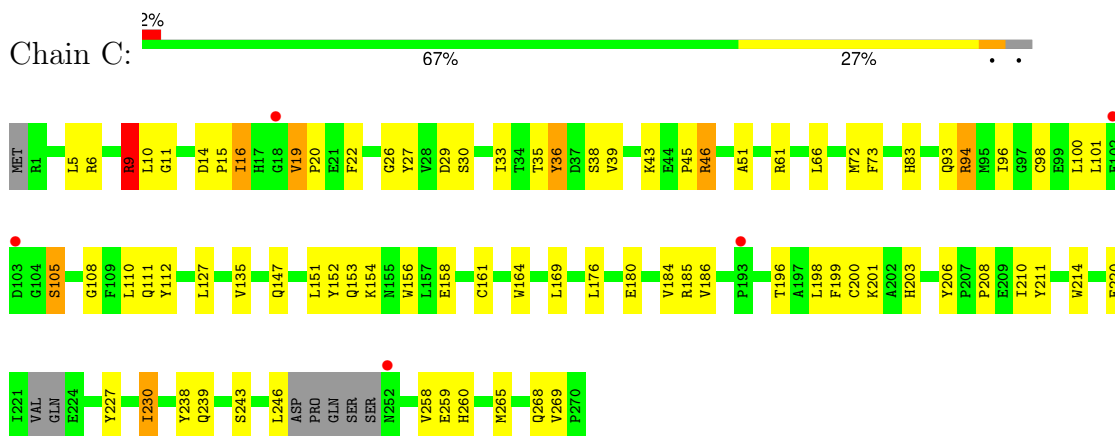
### 3 Residue-property plots [i](#)

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.

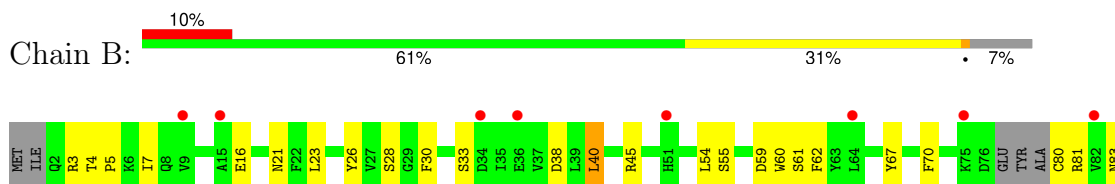
- Molecule 1: Major histocompatibility complex class I-related gene protein



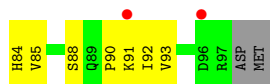
- Molecule 1: Major histocompatibility complex class I-related gene protein



- Molecule 2: Beta-2-microglobulin



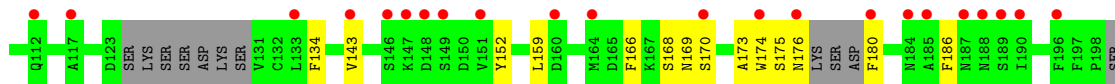




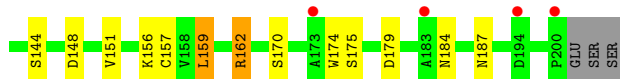
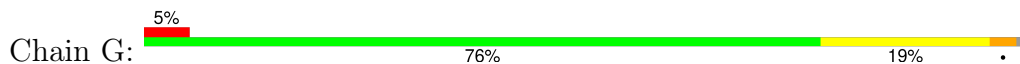
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Human TCR TRAV1-2\_ ALPHA




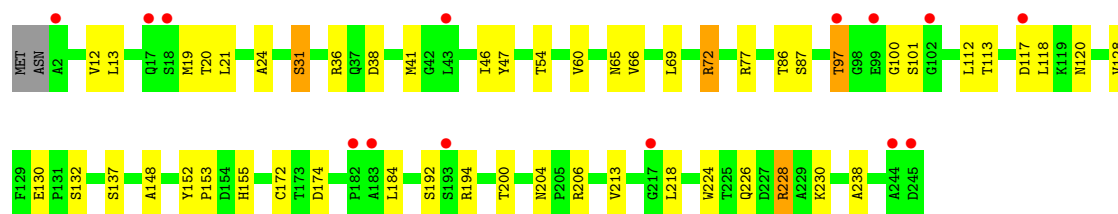
- Molecule 3: Human TCR TRAV1-2\_ ALPHA



- Molecule 4: Human TCR TRBV6-1\_ BETA



## ● Molecule 4: Human TCR TRBV6-1\_BETA

Chain H:  6% 78% 20% ..

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	217.09Å 71.19Å 144.39Å 90.00° 104.76° 90.00°	Depositor
Resolution (Å)	34.99 – 2.89 34.99 – 2.89	Depositor EDS
% Data completeness (in resolution range)	87.9 (34.99-2.89) 69.8 (34.99-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.203 , 0.238 0.204 , 0.230	Depositor DCC
$R_{free}$ test set	45688 reflections (4.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtrriage
Anisotropy	0.511	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	12615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, NK

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	0.47	0/2255	0.65	0/3064
1	C	0.48	0/2198	0.67	0/2989
2	B	0.41	0/738	0.62	0/1010
2	F	0.44	0/815	0.64	0/1112
3	D	0.48	0/1440	0.63	0/1962
3	G	0.45	0/1610	0.66	1/2185 (0.0%)
4	E	0.47	0/1789	0.65	0/2444
4	H	0.49	0/2009	0.67	0/2732
All	All	0.47	0/12854	0.65	1/17498 (0.0%)

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	C	0	1
4	E	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	92	ASP	CB-CG-OD1	5.07	122.86	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	9	ARG	Sidechain
4	E	194	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2169	0	2033	30	0
1	C	2131	0	2004	52	0
2	B	717	0	627	15	0
2	F	792	0	723	14	0
3	D	1408	0	1258	28	0
3	G	1560	0	1467	24	0
4	E	1739	0	1589	38	0
4	H	1937	0	1834	29	0
5	A	8	0	5	4	0
5	C	8	0	5	3	0
6	A	12	0	15	6	0
6	C	12	0	16	6	0
6	F	6	0	8	1	0
7	F	4	0	3	0	0
8	A	24	0	0	0	0
8	B	7	0	0	2	0
8	C	28	0	0	3	0
8	D	7	0	0	1	0
8	E	11	0	0	2	0
8	F	8	0	0	0	0
8	G	14	0	0	1	0
8	H	13	0	0	0	0
All	All	12615	0	11587	220	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 9.

All (220) 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)
4:E:65[B]:ASN:ND2	8:E:301:HOH:O	2.08	0.85
1:C:6:ARG:NH1	1:C:29:ASP:O	2.11	0.84
2:F:73:THR:OG1	2:F:76:ASP:OD1	1.96	0.84
3:D:54:LEU:HD12	3:D:63:PHE:HB2	1.62	0.82
1:C:9:ARG:NH2	8:C:401:HOH:O	2.13	0.80
1:C:61:ARG:NH1	3:D:94:ASN:O	2.18	0.77
4:E:38:ASP:OD2	4:E:44:ARG:NH2	2.18	0.75
4:E:31:SER:HG	4:E:97:THR:HG1	1.33	0.74
1:A:64:GLN:OE1	4:H:54:THR:OG1	2.06	0.73
3:G:128:ASP:OD1	3:G:128:ASP:N	2.16	0.73
1:C:186:VAL:HG11	1:C:269:VAL:HG22	1.69	0.73
4:H:224:TRP:CD1	4:H:230:LYS:HB2	2.26	0.70
4:E:65[A]:ASN:ND2	4:E:79:GLU:OE2	2.25	0.70
3:D:36:GLN:OE1	8:D:301:HOH:O	2.10	0.69
2:B:54:LEU:HD11	2:B:62:PHE:HB3	1.75	0.69
2:F:49:VAL:HG12	2:F:68:THR:HB	1.77	0.66
3:G:43:PRO:O	8:G:301:HOH:O	2.13	0.65
4:H:86:THR:HG23	4:H:113:THR:HA	1.77	0.65
5:A:301:NK:HAG	6:A:302:GOL:O3	1.95	0.65
2:F:7:ILE:HG12	2:F:82:VAL:HG21	1.77	0.65
4:E:67:SER:OG	4:E:77:ARG:NH2	2.28	0.65
4:E:131:PRO:HD2	4:E:202:TRP:CZ2	2.32	0.64
4:E:152:TYR:HB2	4:E:188:ARG:HG2	1.80	0.64
5:C:301:NK:HAI	6:C:302:GOL:O1	1.97	0.63
3:D:7:PRO:O	3:D:103:THR:OG1	2.14	0.63
2:F:39:LEU:HD13	2:F:68:THR:HG22	1.81	0.62
1:A:94:ARG:HH22	6:A:302:GOL:H11	1.64	0.60
2:B:81:ARG:HG3	2:B:92:ILE:HG12	1.83	0.60
6:C:303:GOL:O2	2:F:96:ASP:OD1	2.15	0.60
1:A:94:ARG:HH22	6:A:302:GOL:C1	2.15	0.60
1:C:26:GLY:O	1:C:33:ILE:HG13	2.01	0.59
4:E:45:LEU:HD23	4:E:58:GLY:HA3	1.83	0.59
1:C:198:LEU:HD13	1:C:269:VAL:HG21	1.83	0.59
3:D:11:THR:HG23	3:D:106:ILE:HB	1.84	0.59
1:C:156:TRP:CZ3	1:C:161:CYS:HB2	2.38	0.58
1:A:180:GLU:O	1:A:205:PHE:HA	2.04	0.58
4:H:36:ARG:HB3	4:H:46:ILE:HD11	1.84	0.58
1:A:43:LYS:HG3	1:A:66:LEU:HD13	1.86	0.57
4:H:172[B]:CYS:SG	4:H:194:ARG:NH2	2.77	0.57
1:A:210:ILE:HG13	1:A:260:HIS:HB2	1.86	0.57
1:C:96:ILE:HG21	6:C:302:GOL:H11	1.86	0.57
1:A:235:ASP:OD1	1:A:237:THR:OG1	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ILE:HD12	2:B:91:LYS:HE3	1.87	0.56
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.40	0.56
3:G:159:LEU:HB3	4:H:172[A]:CYS:HB2	1.87	0.56
5:A:301:NK:HAI	6:A:302:GOL:C3	2.35	0.56
2:B:83:ASN:OD1	2:B:84:HIS:N	2.38	0.56
1:A:8:PHE:CE2	1:A:95[A]:MET:HG3	2.41	0.56
4:E:158:LEU:HD23	4:E:159:SER:N	2.21	0.56
1:C:96:ILE:HG13	1:C:110:LEU:HB2	1.89	0.55
3:D:17:ILE:HG12	3:D:76:LYS:HA	1.88	0.55
2:F:24:ASN:HB3	2:F:65:LEU:HD11	1.87	0.55
1:C:16:ILE:HG13	1:C:19:VAL:HG12	1.88	0.55
4:E:28:ASN:OD1	4:E:71:LYS:HE2	2.06	0.55
3:G:17:ILE:HD13	3:G:76:LYS:HG2	1.87	0.55
5:C:301:NK:HAI	6:C:302:GOL:C1	2.37	0.55
2:F:37:VAL:HG13	2:F:82:VAL:HG22	1.88	0.54
4:H:13:LEU:HD11	4:H:19[B]:MET:HG3	1.90	0.54
3:G:4[B]:ILE:HD11	3:G:90:VAL:HB	1.89	0.54
4:H:117:ASP:OD1	4:H:118:LEU:N	2.41	0.54
3:G:122:ARG:HB2	4:H:130:GLU:HB2	1.90	0.54
1:C:151:LEU:HD22	3:D:51:LEU:HD12	1.90	0.54
5:A:301:NK:HAI	6:A:302:GOL:H32	1.88	0.54
1:A:10:LEU:HD13	1:A:93:GLN:HG2	1.89	0.54
1:C:20:PRO:HB3	1:C:39:VAL:HG23	1.90	0.53
2:B:54:LEU:HD12	2:B:55:SER:H	1.73	0.53
3:D:49:ASN:OD1	3:D:62:SER:HB2	2.10	0.52
1:A:10:LEU:HD12	1:A:11:GLY:H	1.74	0.52
4:H:224:TRP:CZ2	4:H:226:GLN:HB2	2.44	0.52
1:C:22:PHE:HB3	1:C:38:SER:HB3	1.90	0.52
3:D:174:TRP:CD2	4:E:147:LEU:HD21	2.45	0.52
4:E:155:HIS:HB3	4:E:216:TYR:HB2	1.91	0.52
1:A:252:ASN:HB2	1:A:254:TYR:CE1	2.45	0.51
1:C:211:TYR:HB2	1:C:259:GLU:HB3	1.91	0.51
4:H:20:THR:OG1	4:H:77:ARG:HD3	2.09	0.51
4:E:131:PRO:HG2	4:E:142:ALA:HB1	1.92	0.51
1:C:72:MET:HG3	4:E:96:TRP:CH2	2.44	0.51
1:C:94:ARG:HG3	1:C:112:TYR:CZ	2.44	0.51
1:A:182:PRO:HB3	1:A:205:PHE:CD2	2.45	0.51
1:C:208:PRO:HG3	1:C:238:TYR:CE2	2.45	0.51
1:C:210:ILE:O	4:H:206:ARG:HD2	2.11	0.51
1:A:49:TRP:O	1:A:53:ASN:ND2	2.34	0.51
1:A:120:LEU:HB3	1:A:129:TRP:CE3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:129:LYS:HD3	3:G:174:TRP:CD1	2.45	0.51
4:E:47:TYR:HB2	4:E:66:VAL:HG11	1.93	0.50
6:F:101:GOL:O3	6:F:101:GOL:O1	2.18	0.50
4:H:174:ASP:OD2	4:H:192:SER:OG	2.20	0.50
4:E:125:GLU:O	4:E:148:ALA:HA	2.11	0.50
3:D:166:PHE:CE1	3:D:168:SER:HB3	2.47	0.49
3:D:32:LEU:HD12	3:D:90:VAL:HG22	1.94	0.49
1:C:94:ARG:HG3	1:C:112:TYR:CE2	2.47	0.49
3:D:166:PHE:HE1	3:D:168:SER:HB3	1.76	0.49
1:A:152:TYR:CE1	4:H:100:GLY:HA3	2.47	0.49
1:C:154:LYS:NZ	1:C:158:GLU:OE2	2.44	0.49
3:D:91:LYS:HA	3:D:96:GLN:O	2.12	0.49
3:G:121:LEU:N	3:G:121:LEU:HD12	2.28	0.49
1:A:144:GLU:HA	1:A:150:LEU:HD11	1.93	0.49
1:A:10:LEU:HD12	1:A:11:GLY:N	2.28	0.49
1:A:93:GLN:O	1:A:112:TYR:HA	2.13	0.49
3:G:56:GLU:HG3	3:G:61:SER:OG	2.12	0.49
3:G:120:GLN:O	4:H:132:SER:HB2	2.12	0.49
4:E:67:SER:HA	8:E:308:HOH:O	2.13	0.49
1:C:185:ARG:NH2	1:C:201:LYS:HD3	2.27	0.48
2:B:59:ASP:OD1	2:B:61:SER:OG	2.18	0.48
4:H:31:SER:OG	4:H:97:THR:OG1	2.28	0.48
1:C:96:ILE:CD1	6:C:302:GOL:H32	2.42	0.48
1:A:46:ARG:HA	1:A:46:ARG:HD3	1.49	0.48
5:A:301:NK:CAG	6:A:302:GOL:O3	2.62	0.48
2:B:80:CYS:N	2:B:93:VAL:O	2.46	0.48
3:G:87:LEU:HD23	3:G:102:GLY:HA2	1.96	0.48
4:E:11:GLN:HB3	4:E:112:LEU:CD2	2.43	0.47
1:C:46:ARG:HG2	8:C:419:HOH:O	2.14	0.47
1:C:94:ARG:HH12	6:C:302:GOL:C1	2.28	0.47
4:E:170:GLY:O	4:E:195:LEU:HA	2.15	0.47
2:F:5:PRO:HA	2:F:30:PHE:HB3	1.96	0.47
3:G:179:ASP:N	3:G:179:ASP:OD1	2.47	0.47
1:A:42:GLN:HA	1:A:63:THR:HG23	1.97	0.47
4:E:128:VAL:HG11	4:E:240:ALA:HB2	1.96	0.47
4:E:118:LEU:HD13	4:E:218:LEU:HD22	1.97	0.47
2:F:3:ARG:NH2	2:F:59:ASP:O	2.48	0.47
1:C:72:MET:HG3	4:E:96:TRP:CZ2	2.50	0.47
3:G:4[A]:ILE:HD11	3:G:88[A]:CYS:SG	2.55	0.47
1:C:258:VAL:HB	1:C:265[B]:MET:HG3	1.97	0.46
1:C:15:PRO:HB2	1:C:19:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:57:SER:HB3	2:F:59:ASP:OD1	2.15	0.46
3:G:2:GLN:HG2	3:G:26:THR:HA	1.97	0.46
3:D:175:SER:HB3	3:D:180:PHE:CD2	2.49	0.46
1:C:36:TYR:HB3	1:C:66:LEU:HD13	1.97	0.46
1:A:184:VAL:HG12	1:A:267:LEU:HD22	1.97	0.46
1:C:164:TRP:CZ2	3:D:93:SER:HB3	2.51	0.46
4:E:186:ASP:OD1	4:E:186:ASP:N	2.48	0.46
3:D:34:TRP:CZ3	3:D:88[B]:CYS:HB3	2.50	0.46
4:E:69:LEU:HD12	4:E:73:GLU:HB2	1.98	0.46
1:A:174:ASP:O	1:A:178:ARG:HB3	2.16	0.45
4:E:232:VAL:O	4:E:234:GLN:HG2	2.16	0.45
2:F:21:ASN:HB3	2:F:70:PHE:CE1	2.50	0.45
1:A:149:GLU:HG2	4:H:101:SER:OG	2.16	0.45
1:C:152:TYR:CD1	4:E:100:GLY:HA3	2.51	0.45
5:C:301:NK:HAE	8:C:401:HOH:O	2.16	0.45
1:C:199:PHE:CD2	1:C:243:SER:HB3	2.51	0.45
3:D:175:SER:OG	3:D:176:ASN:N	2.50	0.45
4:H:38:ASP:OD1	4:H:87:SER:OG	2.15	0.45
3:G:46:LEU:HD23	3:G:46:LEU:HA	1.66	0.44
3:G:184:ASN:HA	3:G:187:ASN:OD1	2.17	0.44
1:C:203:HIS:HB2	1:C:239:GLN:HB3	1.99	0.44
1:C:153:GLN:HE21	1:C:153:GLN:HB2	1.63	0.44
1:C:147:GLN:HE22	4:H:228:ARG:HA	1.83	0.44
2:F:81:ARG:HG3	2:F:92:ILE:HG12	1.98	0.44
4:E:124:PRO:CA	4:E:151:PHE:HB3	2.48	0.44
3:G:104:LYS:HE2	3:G:106:ILE:HD11	2.00	0.44
2:B:16:GLU:HA	8:B:105:HOH:O	2.18	0.44
2:B:23:LEU:O	2:B:67:TYR:HA	2.18	0.44
1:C:230:ILE:HD11	4:H:206:ARG:HD3	2.00	0.44
4:E:46:ILE:HG22	4:E:47:TYR:HD1	1.83	0.44
1:C:127:LEU:HD21	1:C:154:LYS:HD3	2.00	0.43
3:D:134:PHE:HB2	3:D:186:PHE:CE2	2.53	0.43
4:H:148:ALA:HB2	4:H:213:VAL:HG21	2.00	0.43
1:A:186:VAL:HG23	1:A:267:LEU:HD23	2.00	0.43
1:C:98:CYS:HA	1:C:108:GLY:HA2	2.01	0.43
1:C:169:LEU:HA	1:C:169:LEU:HD23	1.78	0.43
3:D:15:GLY:N	3:D:78:LEU:O	2.50	0.43
1:C:83:HIS:HB3	1:C:135:VAL:HG22	2.00	0.43
3:D:94:ASN:N	3:D:94:ASN:HD22	2.15	0.43
4:H:128:VAL:HG23	4:H:238:ALA:HB3	2.00	0.43
4:H:24:ALA:HA	4:H:72:ARG:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:31:GLY:HA3	3:D:48:TYR:CE1	2.54	0.43
3:G:118:VAL:HA	3:G:133:LEU:O	2.18	0.43
3:G:162:ARG:NE	3:G:162:ARG:HA	2.33	0.43
4:H:120:ASN:O	4:H:152:TYR:HD2	2.02	0.43
1:A:208:PRO:O	1:A:230:ILE:HD13	2.19	0.43
1:C:210:ILE:HG13	1:C:260:HIS:CD2	2.53	0.43
3:D:2:GLN:OE1	3:D:27:SER:N	2.48	0.43
2:F:21:ASN:HB3	2:F:70:PHE:HE1	1.84	0.43
2:F:76:ASP:O	2:F:97:ARG:NH1	2.52	0.43
1:C:200:CYS:HB2	1:C:214:TRP:CZ2	2.54	0.43
1:C:66:LEU:HA	1:C:66:LEU:HD23	1.81	0.42
1:C:10:LEU:HD12	1:C:11:GLY:H	1.83	0.42
4:H:41:MET:HE2	4:H:41:MET:HB3	1.92	0.42
4:H:47:TYR:HB2	4:H:66:VAL:HG11	2.01	0.42
1:C:220:GLU:H	1:C:220:GLU:HG2	1.54	0.42
3:D:26:THR:OG1	3:D:28:GLY:O	2.34	0.42
4:E:46:ILE:HG22	4:E:47:TYR:CD1	2.53	0.42
3:D:36:GLN:O	3:D:43:PRO:HA	2.20	0.42
4:E:181:GLN:O	4:E:187:SER:HB2	2.20	0.42
3:G:60:PHE:N	3:G:60:PHE:CD1	2.88	0.42
4:H:118:LEU:HD13	4:H:218:LEU:CD2	2.49	0.42
2:B:83:ASN:ND2	2:B:90:PRO:HG3	2.35	0.42
4:E:30:ASN:HB2	4:E:95:VAL:O	2.19	0.42
2:B:5:PRO:HB3	2:B:30:PHE:HB3	2.01	0.42
4:E:197:VAL:HG13	4:E:198:SER:O	2.20	0.42
1:A:199:PHE:CE2	1:A:243:SER:HB3	2.56	0.41
2:B:3:ARG:NH2	8:B:101:HOH:O	2.20	0.41
1:C:43:LYS:HB2	1:C:66:LEU:HD12	2.01	0.41
1:C:101:LEU:HD23	1:C:105:SER:OG	2.21	0.41
2:B:40:LEU:HD12	2:B:45:ARG:HA	2.01	0.41
1:C:5:LEU:HA	1:C:27:TYR:O	2.21	0.41
1:C:45:PRO:HG3	1:C:51:ALA:HB2	2.02	0.41
1:A:87:SER:O	1:A:90:HIS:NE2	2.51	0.41
1:C:203:HIS:CB	1:C:239:GLN:HB3	2.51	0.41
3:D:152:TYR:HB2	3:D:174:TRP:CE2	2.55	0.41
3:D:152:TYR:O	3:D:173:ALA:HA	2.20	0.41
1:C:180:GLU:HB2	1:C:206:TYR:N	2.35	0.41
4:E:11:GLN:HB3	4:E:112:LEU:HD23	2.02	0.41
3:D:34:TRP:CZ3	3:D:88[A]:CYS:HB2	2.55	0.41
4:E:197:VAL:HG22	4:E:201:PHE:HB3	2.02	0.41
3:G:151:VAL:HA	3:G:175:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:153:PRO:HG2	4:H:155:HIS:CD2	2.55	0.41
3:G:60:PHE:N	3:G:60:PHE:HD1	2.18	0.41
2:B:26:TYR:CE2	2:B:28:SER:HB3	2.55	0.41
4:E:210:ARG:HA	4:E:239:GLU:HA	2.02	0.41
3:G:30:ASN:ND2	3:G:92:ASP:O	2.54	0.41
1:C:227:TYR:OH	4:H:204:ASN:ND2	2.54	0.41
1:C:184:VAL:HG11	1:C:258:VAL:HG21	2.02	0.40
3:D:32:LEU:HD11	3:D:88[A]:CYS:SG	2.62	0.40
4:E:30:ASN:O	4:E:51[A]:SER:HA	2.21	0.40
1:A:1:ARG:H	1:A:1:ARG:HG2	1.70	0.40
4:E:10:PHE:CD2	4:E:111:ARG:HB3	2.56	0.40
4:E:69:LEU:H	4:E:69:LEU:HG	1.65	0.40
1:A:184:VAL:HG22	1:A:202:ALA:HB2	2.04	0.40
3:G:105:LEU:HA	3:G:105:LEU:HD12	1.78	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	264/271 (97%)	258 (98%)	6 (2%)	0	100	100
1	C	258/271 (95%)	249 (96%)	9 (4%)	0	100	100
2	B	89/100 (89%)	82 (92%)	7 (8%)	0	100	100
2	F	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
3	D	183/204 (90%)	167 (91%)	16 (9%)	0	100	100
3	G	203/204 (100%)	193 (95%)	10 (5%)	0	100	100
4	E	230/246 (94%)	217 (94%)	13 (6%)	0	100	100
4	H	249/246 (101%)	237 (95%)	12 (5%)	0	100	100
All	All	1573/1642 (96%)	1497 (95%)	76 (5%)	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	226/241 (94%)	211 (93%)	15 (7%)	14	39
1	C	220/241 (91%)	201 (91%)	19 (9%)	8	27
2	B	74/95 (78%)	66 (89%)	8 (11%)	5	17
2	F	85/95 (90%)	76 (89%)	9 (11%)	5	18
3	D	138/181 (76%)	128 (93%)	10 (7%)	12	35
3	G	173/181 (96%)	156 (90%)	17 (10%)	6	21
4	E	175/212 (82%)	163 (93%)	12 (7%)	13	37
4	H	208/212 (98%)	195 (94%)	13 (6%)	15	42
All	All	1299/1458 (89%)	1196 (92%)	103 (8%)	10	30

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	30	SER
1	A	38	SER
1	A	43	LYS
1	A	46	ARG
1	A	57	ASP
1	A	66	LEU
1	A	73	PHE
1	A	82	ARG
1	A	91	THR
1	A	100	LEU
1	A	107	THR
1	A	167	ARG
1	A	226	ASP
1	A	255	SER
2	B	4	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	21	ASN
2	B	33	SER
2	B	38	ASP
2	B	40	LEU
2	B	70	PHE
2	B	85	VAL
2	B	88	SER
1	C	9	ARG
1	C	14	ASP
1	C	16	ILE
1	C	19	VAL
1	C	30	SER
1	C	35	THR
1	C	36	TYR
1	C	46	ARG
1	C	73	PHE
1	C	93	GLN
1	C	94	ARG
1	C	100	LEU
1	C	105	SER
1	C	111	GLN
1	C	176	LEU
1	C	196	THR
1	C	230	ILE
1	C	246	LEU
1	C	268	GLN
3	D	23	THR
3	D	25	GLN
3	D	54	LEU
3	D	62	SER
3	D	67	SER
3	D	75	LEU
3	D	143	VAL
3	D	159	LEU
3	D	169	ASN
3	D	170	SER
4	E	7	THR
4	E	22	GLN
4	E	25	GLN
4	E	77	ARG
4	E	79	GLU
4	E	80	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	E	86	THR
4	E	101	SER
4	E	144	LEU
4	E	178	LEU
4	E	194	ARG
4	E	197	VAL
2	F	1	ILE
2	F	8	GLN
2	F	16	GLU
2	F	20	SER
2	F	33	SER
2	F	38	ASP
2	F	53	ASP
2	F	68	THR
2	F	70	PHE
3	G	27	SER
3	G	44	THR
3	G	54	LEU
3	G	56	GLU
3	G	60	PHE
3	G	85	SER
3	G	93	SER
3	G	128	ASP
3	G	130	SER
3	G	144	SER
3	G	148	ASP
3	G	156	LYS
3	G	157[A]	CYS
3	G	157[B]	CYS
3	G	159	LEU
3	G	162	ARG
3	G	170	SER
4	H	12	VAL
4	H	21	LEU
4	H	31	SER
4	H	60	VAL
4	H	65	ASN
4	H	69	LEU
4	H	72	ARG
4	H	97	THR
4	H	112	LEU
4	H	137	SER

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Mol	Chain	Res	Type
4	H	184	LEU
4	H	200	THR
4	H	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN
1	A	203	HIS
1	A	252	ASN
2	B	8	GLN
1	C	153	GLN
1	C	177	GLN
3	D	36	GLN
3	D	94	ASN
3	D	120	GLN
3	D	142	ASN
3	D	169	ASN
4	E	140	GLN
4	E	234	GLN
3	G	94	ASN
3	G	120	GLN
4	H	155	HIS
4	H	226	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

8 ligands are modelled in this entry.

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	NK	A	301	1	8,8,9	0.72	0	10,10,11	0.66	0
6	GOL	F	101	-	5,5,5	0.93	0	5,5,5	1.47	1 (20%)
6	GOL	A	302	-	5,5,5	1.18	1 (20%)	5,5,5	1.26	1 (20%)
5	NK	C	301	1	8,8,9	0.77	0	10,10,11	0.66	0
7	ACT	F	102	-	3,3,3	1.91	1 (33%)	3,3,3	1.80	2 (66%)
6	GOL	C	302	-	5,5,5	1.06	0	5,5,5	1.54	1 (20%)
6	GOL	A	303	-	5,5,5	0.78	0	5,5,5	1.31	1 (20%)
6	GOL	C	303	-	5,5,5	1.01	0	5,5,5	1.24	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	NK	A	301	1	-	-	0/1/1/1
6	GOL	F	101	-	-	0/4/4/4	-
6	GOL	A	302	-	-	1/4/4/4	-
5	NK	C	301	1	-	-	0/1/1/1
6	GOL	C	302	-	-	4/4/4/4	-
6	GOL	A	303	-	-	4/4/4/4	-
6	GOL	C	303	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	102	ACT	CH3-C	2.78	1.60	1.49
6	A	302	GOL	O2-C2	-2.28	1.36	1.43



All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	101	GOL	C3-C2-C1	-2.34	103.20	111.80
7	F	102	ACT	O-C-CH3	-2.31	113.05	122.53
6	A	303	GOL	C3-C2-C1	-2.19	103.77	111.80
6	C	302	GOL	C3-C2-C1	-2.17	103.85	111.80
7	F	102	ACT	OXT-C-O	2.03	129.55	122.03
6	A	302	GOL	O3-C3-C2	-2.02	101.27	110.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	302	GOL	O1-C1-C2-C3
6	C	303	GOL	O1-C1-C2-O2
6	A	303	GOL	O1-C1-C2-C3
6	A	303	GOL	C1-C2-C3-O3
6	C	302	GOL	C1-C2-C3-O3
6	C	303	GOL	O1-C1-C2-C3
6	C	302	GOL	O2-C2-C3-O3
6	A	303	GOL	O1-C1-C2-O2
6	A	303	GOL	O2-C2-C3-O3
6	C	302	GOL	O1-C1-C2-O2
6	A	302	GOL	O1-C1-C2-O2

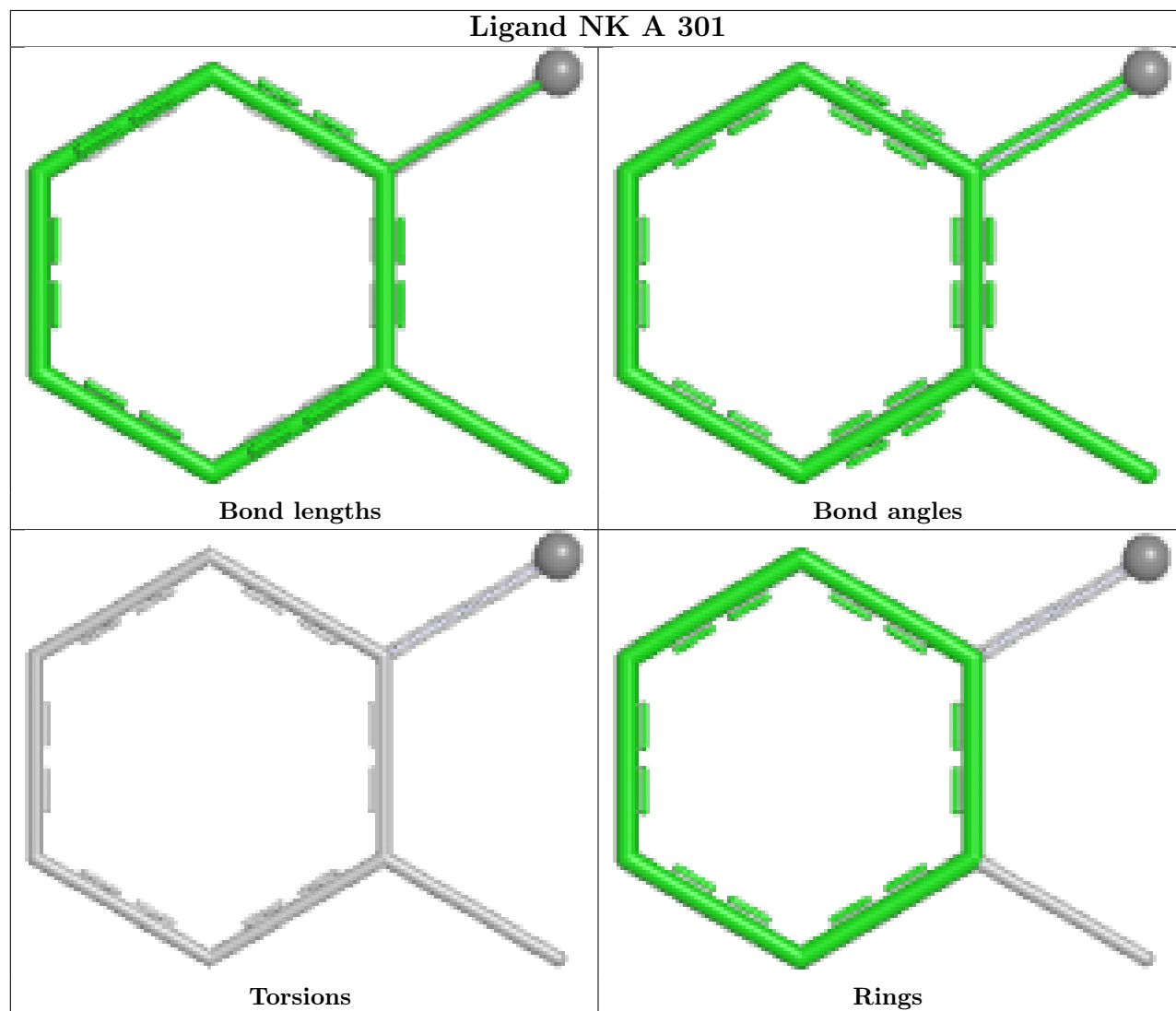
There are no ring outliers.

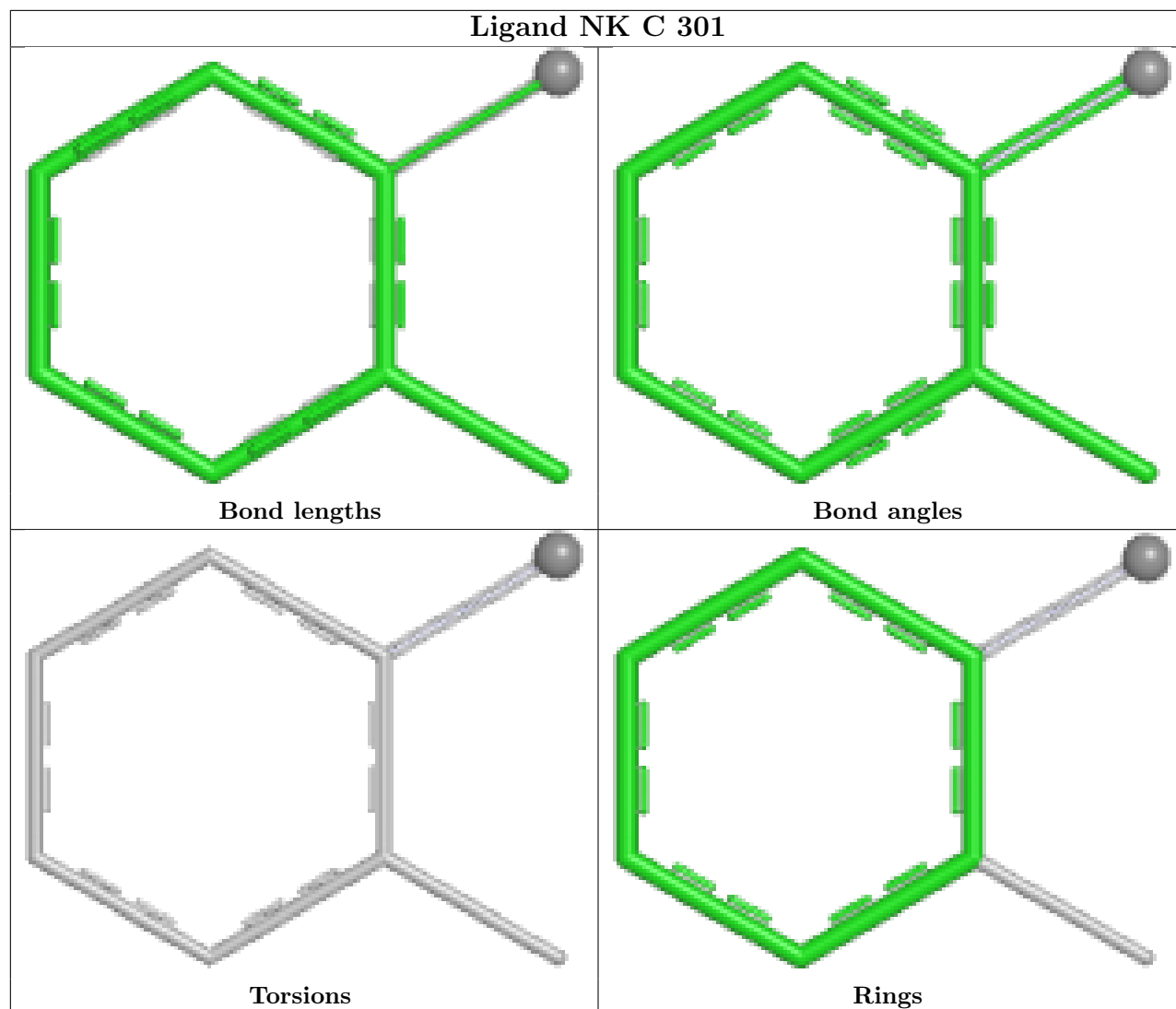
6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	301	NK	4	0
6	F	101	GOL	1	0
6	A	302	GOL	6	0
5	C	301	NK	3	0
6	C	302	GOL	5	0
6	C	303	GOL	1	0

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





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	262/271 (96%)	0.60	15 (5%) 30 26	14, 34, 62, 85	14 (5%)
1	C	263/271 (97%)	0.54	5 (1%) 66 60	17, 31, 48, 65	20 (7%)
2	B	93/100 (93%)	1.08	10 (10%) 12 11	23, 51, 71, 77	3 (3%)
2	F	99/100 (99%)	0.66	3 (3%) 52 47	25, 37, 53, 64	2 (2%)
3	D	188/204 (92%)	0.97	26 (13%) 8 7	13, 40, 71, 83	9 (4%)
3	G	200/204 (98%)	0.80	10 (5%) 35 30	19, 36, 55, 72	15 (7%)
4	E	232/246 (94%)	0.89	30 (12%) 9 7	18, 40, 70, 80	7 (3%)
4	H	244/246 (99%)	0.66	14 (5%) 30 26	18, 34, 51, 71	14 (5%)
All	All	1581/1642 (96%)	0.74	113 (7%) 23 20	13, 36, 64, 85	84 (5%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	148	ASP	5.1
1	C	103	ASP	5.1
4	H	99	GLU	4.7
3	D	189	SER	4.3
4	E	128	VAL	4.0
4	H	245	ASP	4.0
4	H	102	GLY	3.8
3	D	149	SER	3.8
1	A	250	SER	3.7
1	A	224	GLU	3.6
4	E	220	GLU	3.5
1	A	249	GLN	3.4
3	D	160	ASP	3.3
3	G	138	ASP	3.3
3	D	190	ILE	3.2
3	D	1	GLY	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	D	196	PHE	3.2
2	B	36	GLU	3.2
4	E	164	GLY	3.2
4	E	200	THR	3.1
4	E	210	ARG	3.1
3	D	176	ASN	3.0
1	C	18	GLY	2.9
3	G	173	ALA	2.9
4	H	117	ASP	2.9
3	D	164	MET	2.9
4	E	227	ASP	2.9
4	E	137	SER	2.9
4	E	98	GLY	2.8
4	H	217	GLY	2.8
2	B	82	VAL	2.8
1	A	102	GLU	2.8
1	A	253	LEU	2.8
3	D	188	ASN	2.7
2	B	9	VAL	2.7
2	F	99	MET	2.7
3	D	146	SER	2.7
4	H	244	ALA	2.7
1	C	102	GLU	2.7
4	E	162	VAL	2.7
3	D	187	ASN	2.7
2	B	15	ALA	2.6
2	F	87	LEU	2.6
3	D	180	PHE	2.6
3	D	184	ASN	2.6
4	E	163	ASN	2.6
4	E	201	PHE	2.6
1	A	245	GLU	2.6
2	B	96	ASP	2.6
4	E	117	ASP	2.6
2	B	64	LEU	2.6
3	D	174	TRP	2.6
3	G	194	ASP	2.6
4	E	221	ASN	2.6
4	E	143	THR	2.6
3	D	185	ALA	2.5
3	D	133	LEU	2.5
4	H	2	ALA	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	E	224	TRP	2.5
1	A	169	LEU	2.5
4	E	238	ALA	2.5
2	F	88	SER	2.4
1	A	264[A]	HIS	2.4
3	D	170	SER	2.4
4	H	17	GLN	2.4
4	H	97	THR	2.4
1	C	193	PRO	2.4
3	G	200	PRO	2.4
4	E	110	SER	2.4
4	E	185	ASN	2.4
1	A	226	ASP	2.4
3	G	130	SER	2.3
4	E	129	PHE	2.3
3	G	113	ASN	2.3
3	D	42	ALA	2.3
3	D	117	ALA	2.3
1	A	82	ARG	2.3
4	E	126	VAL	2.3
4	H	43	LEU	2.3
1	A	17	HIS	2.2
1	C	252	ASN	2.2
4	E	22	GLN	2.2
4	E	130	GLU	2.2
4	E	241	TRP	2.2
3	D	147	LYS	2.2
3	D	52	ASP	2.2
4	E	26	ASP	2.2
2	B	51	HIS	2.2
4	E	82	ALA	2.2
4	H	183	ALA	2.2
4	E	239	GLU	2.2
3	G	3	ASN	2.1
2	B	75	LYS	2.1
1	A	247	ASP	2.1
3	D	112	GLN	2.1
4	E	240	ALA	2.1
4	H	182	PRO	2.1
4	E	97	THR	2.1
4	E	218	LEU	2.1
1	A	263	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	143	VAL	2.1
3	G	12	ALA	2.1
3	G	183	ALA	2.1
1	A	254	TYR	2.1
3	D	151	VAL	2.1
1	A	167	ARG	2.1
2	B	34	ASP	2.0
4	E	52	GLU	2.0
3	G	4[A]	ILE	2.0
2	B	91	LYS	2.0
4	H	18	SER	2.0
4	H	193	SER	2.0
3	D	90	VAL	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.

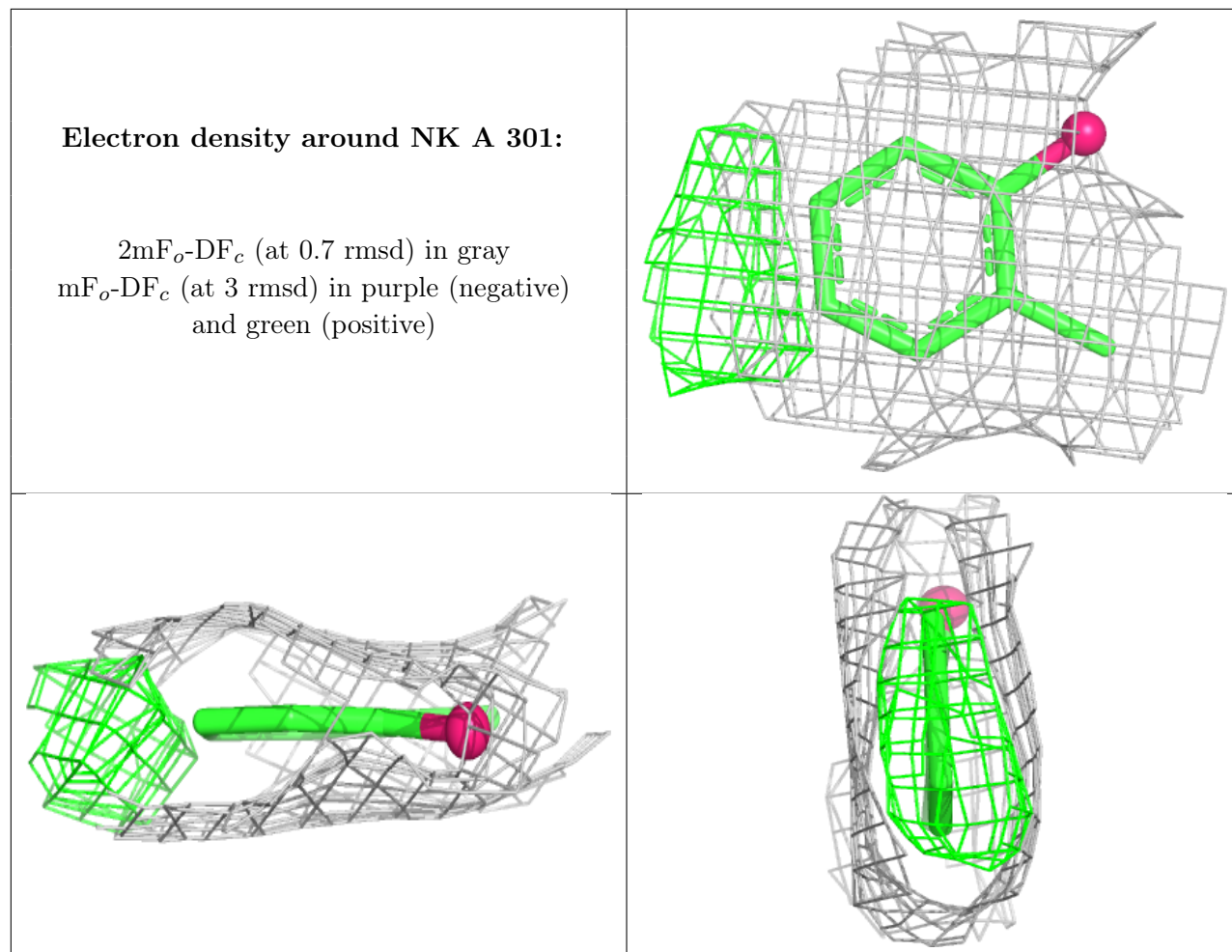
## 6.4 Ligands [i](#)

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<sup>th</sup> 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.

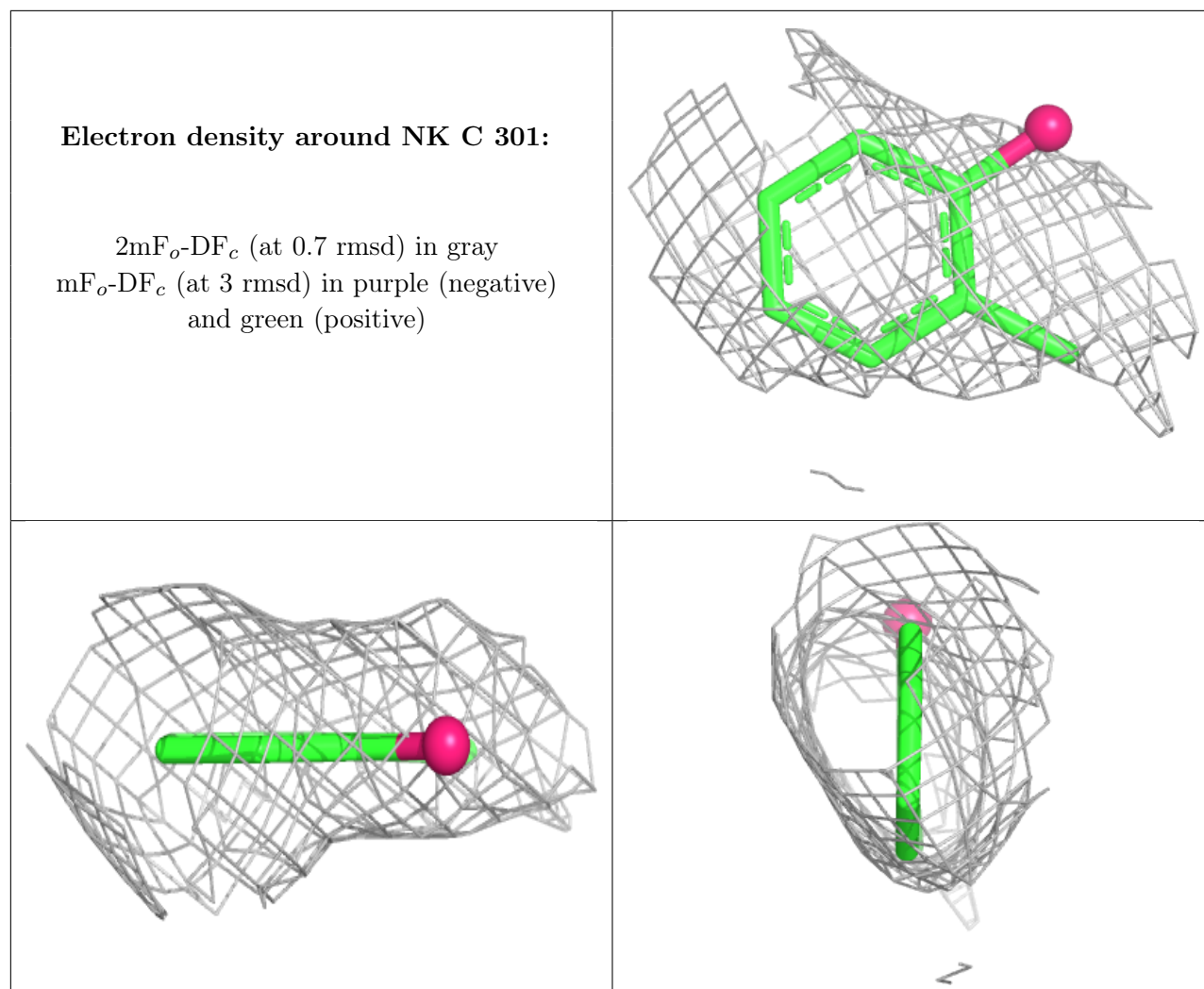
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	A	302	6/6	0.77	0.20	17,23,26,28	6
5	NK	A	301	8/9	0.83	0.18	19,21,27,27	0
6	GOL	A	303	6/6	0.85	0.10	42,45,47,53	0
7	ACT	F	102	4/4	0.87	0.14	16,20,29,30	0
6	GOL	C	302	6/6	0.88	0.19	31,34,47,48	0
5	NK	C	301	8/9	0.88	0.15	30,34,40,41	0
6	GOL	F	101	6/6	0.90	0.14	23,27,28,28	6
6	GOL	C	303	6/6	0.90	0.17	32,40,41,43	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.







## 6.5 Other polymers [i](#)

There are no such residues in this entry.