



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 09:49 PM JST

PDB ID : 7BYD  
Title : Crystal structure of SN45 TCR in complex with lipopeptide-bound Mamu-B\*05104  
Authors : Morita, D.; Sugita, M.; Iwashita, C.  
Deposited on : 2020-04-22  
Resolution : 2.80 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

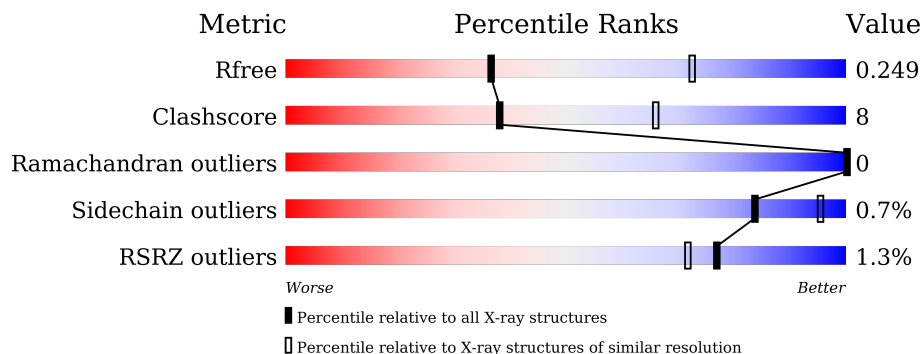
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



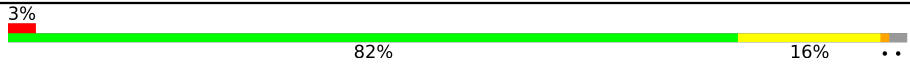
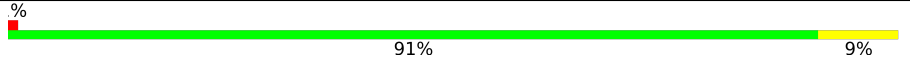
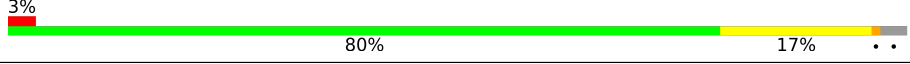
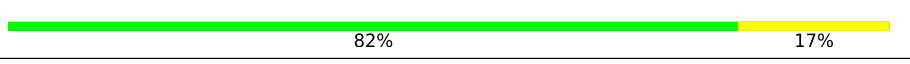
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	276	 84% 15%
1	F	276	 86% 13%
2	B	100	 81% 18%
2	G	100	 79% 21%
3	C	4	 75% 25%
3	H	4	 100%

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Mol	Chain	Length	Quality of chain
4	D	198	 3% 82% 16% ..
4	I	198	 % 91% 9%
5	E	245	 3% 80% 17% ..
5	J	245	 82% 17%

## 2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 13311 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 B protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	Total	C	N	O	S	0	2	0
			2276	1421	419	430	6			
1	F	276	Total	C	N	O	S	0	1	0
			2267	1416	418	427	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	GLU	ARG	engineered mutation	UNP B2ZHY7
A	177	GLU	LYS	engineered mutation	UNP B2ZHY7
A	223	GLU	ASP	engineered mutation	UNP B2ZHY7
F	128	GLU	ARG	engineered mutation	UNP B2ZHY7
F	177	GLU	LYS	engineered mutation	UNP B2ZHY7
F	223	GLU	ASP	engineered mutation	UNP B2ZHY7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	Total	C	N	O	S	0	1	0
			838	532	145	157	4			
2	G	100	Total	C	N	O	S	0	0	0
			827	526	141	156	4			

- Molecule 3 is a protein called GLY-GLY-ALA-ILE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	4	Total	C	N	O	0	0	0
			22	13	4	5			
3	H	4	Total	C	N	O	0	0	0
			22	13	4	5			

- Molecule 4 is a protein called SN45 T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	194	Total	C	N	O	S	0	0	0
			1501	947	248	297	9			
4	I	198	Total	C	N	O	S	0	0	0
			1530	964	253	303	10			

- Molecule 5 is a protein called SN45 T cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	238	Total	C	N	O	S	0	0	0
			1923	1227	331	357	8			
5	J	245	Total	C	N	O	S	0	0	0
			1980	1259	338	375	8			

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

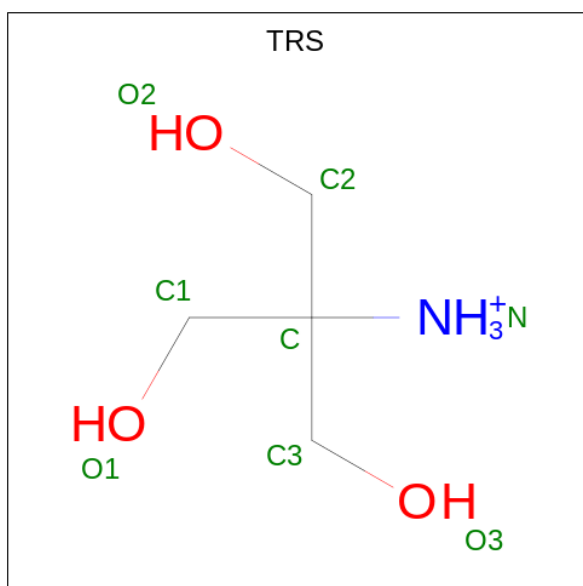
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	I	0	0
			4	4		
6	B	2	Total	I	0	0
			2	2		
6	D	1	Total	I	0	0
			1	1		
6	E	2	Total	I	0	0
			2	2		
6	F	3	Total	I	0	0
			3	3		
6	G	1	Total	I	0	0
			1	1		
6	I	4	Total	I	0	0
			4	4		
6	J	2	Total	I	0	0
			2	2		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).

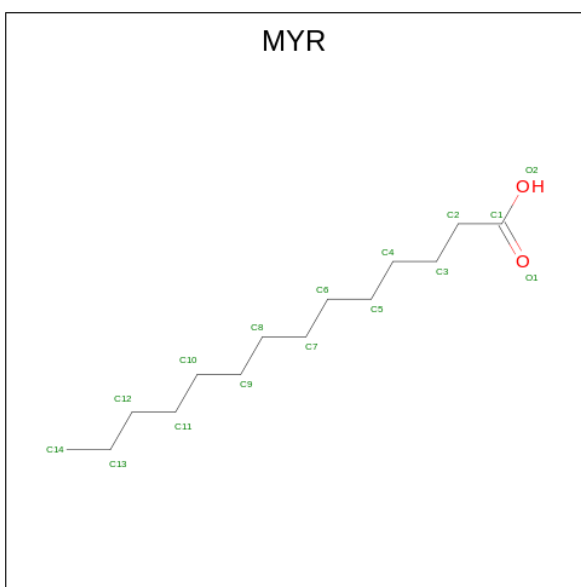


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Ca	0	0
			1	1		

- Molecule 10 is MYRISTIC ACID (three-letter code: MYR) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			15	14	1		
10	H	1	Total	C	O	0	0
			15	14	1		

- Molecule 11 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	I	1	Total	Na	0	0
			1	1		

- Molecule 12 is water.

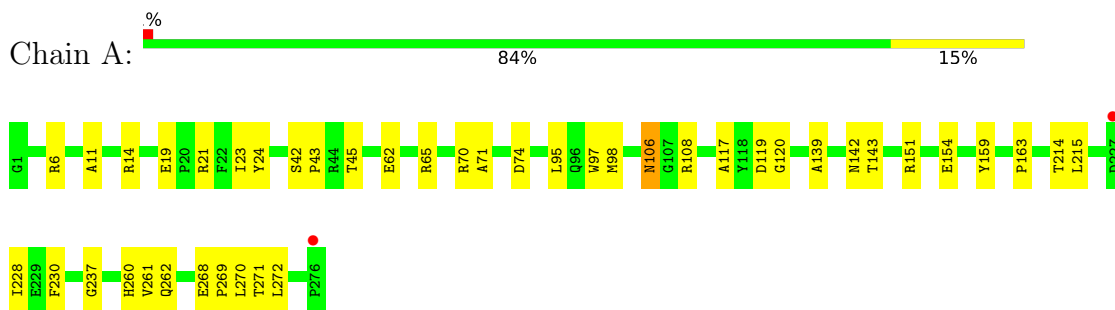
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	11	Total O 11 11	0	0
12	B	9	Total O 9 9	0	0
12	D	3	Total O 3 3	0	0
12	F	4	Total O 4 4	0	0
12	G	4	Total O 4 4	0	0
12	I	8	Total O 8 8	0	0
12	J	11	Total O 11 11	0	0



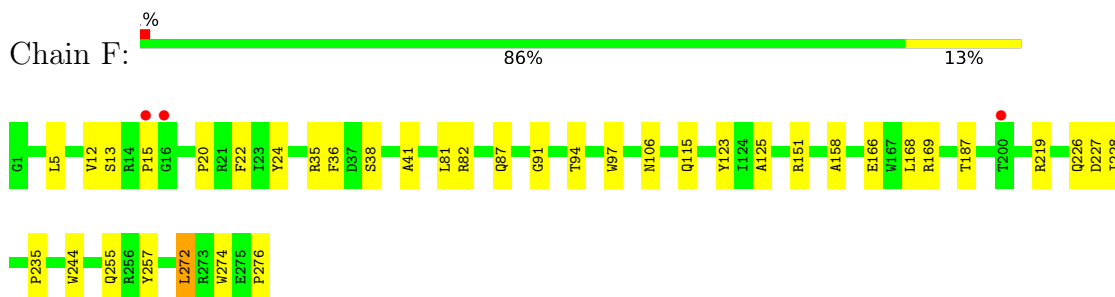
### 3 Residue-property plots [i](#)

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.

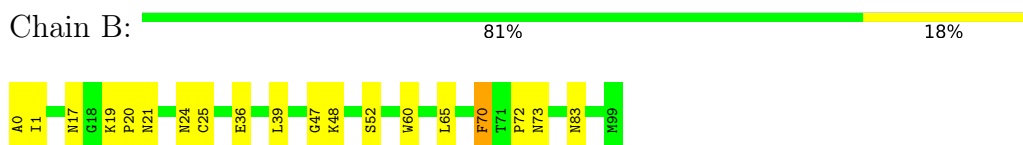
- Molecule 1: B protein



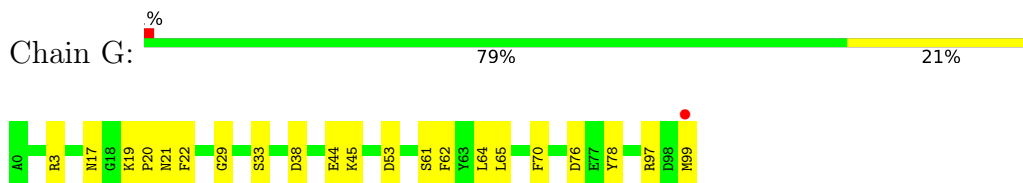
- Molecule 1: B protein



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: GLY-GLY-ALA-ILE

Chain C:  75% 25%




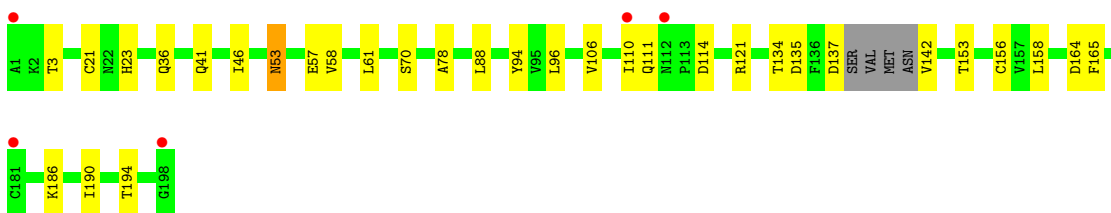
- Molecule 3: GLY-GLY-ALA-ILE

Chain H:  100%


There are no outlier residues recorded for this chain.

- Molecule 4: SN45 T cell receptor alpha chain

Chain D:  3% 82% 16% ..




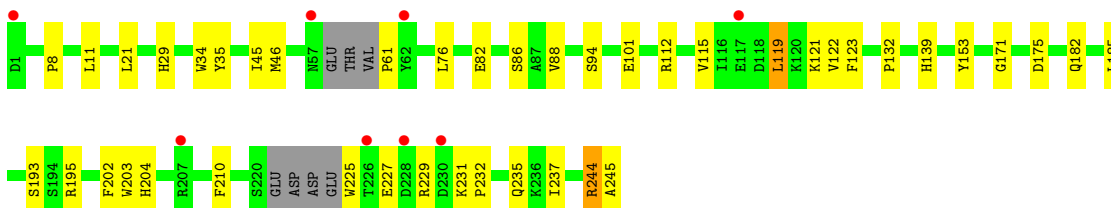
- Molecule 4: SN45 T cell receptor alpha chain

Chain I:  91% 9%




- Molecule 5: SN45 T cell receptor beta chain

Chain E:  3% 80% 17% ..



- Molecule 5: SN45 T cell receptor beta chain

Chain J:  82% 17%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.94Å 95.07Å 123.35Å 90.00° 90.89° 90.00°	Depositor
Resolution (Å)	41.96 – 2.80 41.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.96-2.80) 99.8 (41.96-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.9_1692+SVN	Depositor
R, $R_{free}$	0.185 , 0.250 0.187 , 0.249	Depositor DCC
$R_{free}$ test set	2393 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.1	Xtrriage
Anisotropy	0.174	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13311	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, TRS, CA, MYR, EDO, IOD

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	0.68	0/2344	0.74	0/3185
1	F	0.56	0/2335	0.67	0/3173
2	B	0.63	0/863	0.72	0/1167
2	G	0.56	0/852	0.66	0/1153
3	C	1.41	0/21	0.89	0/25
3	H	1.30	0/21	0.92	0/25
4	D	0.61	1/1536 (0.1%)	0.73	0/2088
4	I	0.59	0/1566	0.71	0/2130
5	E	0.61	0/1976	0.71	0/2676
5	J	0.64	0/2035	0.68	0/2761
All	All	0.62	1/13549 (0.0%)	0.70	0/18383

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	41	GLN	C-N	-6.90	1.20	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2276	0	2121	31	0
1	F	2267	0	2116	32	0
2	B	838	0	800	14	0
2	G	827	0	788	19	0
3	C	22	0	21	1	0
3	H	22	0	21	0	0
4	D	1501	0	1433	31	0
4	I	1530	0	1463	11	0
5	E	1923	0	1871	38	0
5	J	1980	0	1914	34	0
6	A	4	0	0	0	0
6	B	2	0	0	1	0
6	D	1	0	0	0	0
6	E	2	0	0	1	0
6	F	3	0	0	1	0
6	G	1	0	0	1	0
6	I	4	0	0	2	0
6	J	2	0	0	0	0
7	A	4	0	6	0	0
7	F	4	0	6	0	0
7	G	4	0	6	1	0
7	I	4	0	6	0	0
8	B	8	0	12	4	0
9	B	1	0	0	0	0
10	C	15	0	27	2	0
10	H	15	0	27	2	0
11	I	1	0	0	0	0
12	A	11	0	0	0	0
12	B	9	0	0	0	0
12	D	3	0	0	0	0
12	F	4	0	0	0	0
12	G	4	0	0	1	0
12	I	8	0	0	0	0
12	J	11	0	0	0	0
All	All	13311	0	12638	196	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 (196) 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)
5:E:244:ARG:HG2	5:E:244:ARG:HH11	1.23	1.02
5:E:225:TRP:CD1	5:E:231:LYS:HB3	2.02	0.94
1:F:187:THR:HG22	1:F:272:LEU:HD11	1.49	0.92
5:J:67:LYS:HD2	5:J:77:HIS:CD2	2.06	0.90
1:A:214:THR:OG1	1:A:262:GLN:HB3	1.72	0.90
5:E:101:GLU:N	5:E:101:GLU:OE1	2.09	0.84
1:F:187:THR:CG2	1:F:272:LEU:HD11	2.08	0.82
1:F:187:THR:HG22	1:F:272:LEU:CD1	2.12	0.80
2:B:72:PRO:HB2	6:B:101:IOD:I	2.52	0.79
2:B:52:SER:HB3	8:B:103:TRS:H22	1.65	0.79
1:A:228:ILE:HD12	1:A:228:ILE:O	1.83	0.79
4:I:36:GLN:HB2	4:I:46:ILE:HD11	1.66	0.77
4:D:164:ASP:O	4:D:165:PHE:CD1	2.38	0.76
2:G:65:LEU:HD23	7:G:102:EDO:H22	1.70	0.73
1:F:272:LEU:HD23	1:F:272:LEU:N	2.07	0.69
1:F:15:PRO:HG3	1:F:91:GLY:O	1.94	0.68
4:D:36:GLN:HB2	4:D:46:ILE:HD11	1.76	0.68
5:J:67:LYS:CD	5:J:77:HIS:HD2	2.08	0.66
1:F:187:THR:CG2	1:F:272:LEU:CD1	2.70	0.66
5:J:116:ILE:HD11	5:J:119:LEU:HD23	1.77	0.66
5:J:67:LYS:CD	5:J:77:HIS:CD2	2.78	0.66
5:E:244:ARG:HG2	5:E:244:ARG:NH1	1.98	0.65
1:A:106:ASN:HD22	1:A:108:ARG:HB2	1.60	0.65
5:J:64:PHE:CE2	5:J:78:ILE:HD12	2.32	0.65
4:I:15:GLN:O	4:I:77:VAL:HG22	1.98	0.64
2:B:48:LYS:O	2:B:48:LYS:HG2	1.97	0.63
8:B:103:TRS:O3	8:B:103:TRS:O2	2.13	0.62
1:A:214:THR:OG1	1:A:262:GLN:CB	2.46	0.62
1:A:151:ARG:HE	1:A:154:GLU:HG3	1.67	0.60
4:D:142:VAL:O	4:D:142:VAL:HG13	2.01	0.60
5:J:52:LYS:HE2	5:J:70:ASP:HA	1.84	0.59
1:A:11:ALA:HB3	1:A:95:LEU:HB3	1.85	0.59
5:J:56:LEU:HD21	5:J:58:GLU:CG	2.33	0.59
5:E:225:TRP:NE1	5:E:231:LYS:HB3	2.17	0.59
4:D:61:LEU:HD11	4:D:70:SER:HB2	1.84	0.58
4:D:186:LYS:HZ3	4:D:190:ILE:HG22	1.69	0.58
1:F:115:GLN:HG2	1:F:125:ALA:HB1	1.85	0.56
5:E:61:PRO:HG3	1:F:41:ALA:HB1	1.87	0.56
5:J:56:LEU:C	5:J:56:LEU:HD23	2.25	0.56
2:G:38:ASP:HB3	2:G:45:LYS:HG2	1.86	0.56
5:E:82:GLU:O	5:E:115:VAL:HG21	2.06	0.56
5:E:225:TRP:CG	5:E:231:LYS:HB3	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:LEU:HD22	4:D:96:LEU:HD22	1.88	0.56
5:E:29:HIS:HB3	5:E:94:SER:O	2.06	0.56
2:G:17:ASN:OD1	2:G:97:ARG:NH1	2.39	0.56
5:J:13:ARG:HH21	5:J:17:LYS:HB3	1.71	0.56
4:I:137:ASP:HB2	6:I:203:IOD:I	2.76	0.55
4:D:156:CYS:HB3	5:E:195:ARG:HH22	1.70	0.55
5:E:175:ASP:OD2	5:E:193:SER:OG	2.21	0.55
1:F:219:ARG:HD2	1:F:257:TYR:CZ	2.42	0.55
5:J:29:HIS:HB3	5:J:94:SER:O	2.06	0.54
4:D:57:GLU:HG2	4:D:58:VAL:HG13	1.89	0.54
5:J:155:ASP:OD1	5:J:155:ASP:N	2.39	0.54
4:D:121:ARG:HB2	4:D:121:ARG:NH1	2.23	0.54
4:D:3:THR:HB	4:D:21:CYS:SG	2.47	0.53
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.43	0.53
1:A:270:LEU:HD22	1:A:272:LEU:HD22	1.89	0.53
6:G:101:IOD:I	12:G:204:HOH:O	2.89	0.53
5:E:182:GLN:HB3	6:E:302:IOD:I	2.79	0.53
5:J:56:LEU:HD21	5:J:58:GLU:HG3	1.91	0.52
1:F:82:ARG:HG2	1:F:87:GLN:HB2	1.92	0.52
1:A:45:THR:HG23	10:C:101:MYR:H132	1.93	0.51
1:A:139:ALA:O	1:A:142:ASN:HB2	2.11	0.51
5:J:132:PRO:HD2	5:J:203:TRP:CZ2	2.46	0.51
5:J:25:GLN:HG2	5:J:27:LEU:H	1.76	0.51
4:I:12:TYR:O	4:I:15:GLN:HG2	2.11	0.51
5:J:56:LEU:HD21	5:J:58:GLU:HG2	1.93	0.50
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.93	0.50
5:J:34:TRP:O	5:J:45:ILE:HD12	2.11	0.50
5:E:244:ARG:NH1	5:E:244:ARG:CG	2.72	0.50
4:D:186:LYS:NZ	4:D:190:ILE:HG22	2.25	0.50
1:A:119:ASP:HB3	2:B:0:ALA:HA	1.94	0.49
1:A:237:GLY:HA2	8:B:103:TRS:H11	1.93	0.49
4:I:160:MET:HE1	5:J:142:LYS:HD3	1.93	0.49
4:D:78:ALA:O	4:D:106:VAL:HG11	2.12	0.49
1:A:65:ARG:HD2	4:D:94:TYR:OH	2.12	0.49
2:G:70:PHE:CE1	2:G:78:TYR:CZ	3.01	0.48
1:F:166:GLU:OE1	1:F:169:ARG:NH1	2.46	0.48
2:G:33:SER:HB3	2:G:62:PHE:CZ	2.48	0.48
5:J:67:LYS:HD2	5:J:77:HIS:NE2	2.27	0.48
4:D:53:ASN:ND2	4:D:53:ASN:H	2.11	0.48
1:F:81:LEU:HD21	1:F:123:TYR:CZ	2.47	0.48
4:I:3:THR:HB	4:I:21:CYS:SG	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:PHE:HB2	1:F:38:SER:HB3	1.96	0.48
1:F:35:ARG:HD3	2:G:53:ASP:OD2	2.14	0.48
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.49	0.48
1:A:70:ARG:NH2	1:A:74:ASP:OD1	2.45	0.47
4:D:53:ASN:ND2	4:D:53:ASN:N	2.61	0.47
5:E:121:LYS:HE3	5:E:153:TYR:CE2	2.49	0.47
1:F:228:ILE:HD12	1:F:228:ILE:O	2.14	0.47
5:J:63:ARG:NH2	5:J:85:ASP:OD2	2.47	0.47
1:A:268:GLU:HB2	1:A:269:PRO:HD2	1.97	0.47
5:J:20:SER:HB2	5:J:77:HIS:CE1	2.50	0.47
1:F:187:THR:HG21	1:F:272:LEU:HD11	1.95	0.47
5:E:88:VAL:HG22	5:E:112:ARG:HG2	1.97	0.47
1:A:151:ARG:HA	1:A:151:ARG:HD2	1.54	0.47
1:A:159:TYR:CD1	1:A:163:PRO:HG2	2.50	0.47
4:D:186:LYS:O	4:D:186:LYS:HG3	2.14	0.47
1:A:6:ARG:HD3	1:A:98:MET:HE3	1.96	0.46
1:F:272:LEU:N	1:F:272:LEU:CD2	2.78	0.46
1:A:120:GLY:HA3	2:B:1:ILE:HG13	1.97	0.46
8:B:103:TRS:HO2	8:B:103:TRS:HO3	1.54	0.46
4:D:158:LEU:HD11	5:E:171:GLY:C	2.35	0.46
5:E:112:ARG:HB3	5:E:112:ARG:NH2	2.30	0.46
4:I:152:ILE:HG22	4:I:153:THR:O	2.15	0.46
2:G:70:PHE:HE1	2:G:78:TYR:CZ	2.33	0.46
1:A:106:ASN:ND2	1:A:108:ARG:HB2	2.29	0.46
1:F:151:ARG:HA	1:F:151:ARG:HD2	1.28	0.46
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.98	0.45
4:D:134:THR:HG22	4:D:135:ASP:CG	2.36	0.45
2:G:19:LYS:HD3	2:G:19:LYS:C	2.37	0.45
4:D:190:ILE:HD11	4:D:194:THR:HG21	1.97	0.45
2:G:3:ARG:HB3	2:G:29:GLY:O	2.17	0.45
2:G:29:GLY:HA2	2:G:61:SER:HB2	1.99	0.45
4:D:153:THR:HG21	5:E:193:SER:OG	2.17	0.45
5:E:121:LYS:O	5:E:123:PHE:HD1	1.99	0.45
5:E:202:PHE:HE2	5:E:210:PHE:HE1	1.65	0.45
4:D:53:ASN:H	4:D:53:ASN:HD22	1.65	0.44
1:F:274:TRP:O	1:F:276:PRO:HD3	2.18	0.44
5:J:6:GLN:HB2	5:J:109:PRO:HD2	1.99	0.44
1:F:272:LEU:HD23	1:F:272:LEU:H	1.81	0.44
5:J:13:ARG:NH2	5:J:17:LYS:HB3	2.32	0.44
1:F:5:LEU:HB2	1:F:168:LEU:HD13	1.99	0.44
4:D:121:ARG:HB2	4:D:121:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:21:LEU:HB2	5:E:76:LEU:HB3	2.00	0.44
2:G:70:PHE:CE1	2:G:78:TYR:CE1	3.06	0.44
1:F:12:VAL:HG13	1:F:94:THR:HG22	1.99	0.44
5:E:35:TYR:CZ	5:E:45:ILE:HD13	2.53	0.44
5:J:20:SER:HB2	5:J:77:HIS:ND1	2.33	0.44
5:J:175:ASP:HB2	5:J:192:LEU:HD12	1.99	0.44
5:E:8:PRO:HG2	5:E:11:LEU:HD13	2.00	0.43
5:E:122:VAL:O	5:E:232:PRO:HG2	2.18	0.43
1:F:158:ALA:HB1	6:I:202:IOD:I	2.88	0.43
5:E:132:PRO:HD2	5:E:203:TRP:CZ2	2.53	0.43
5:J:156:HIS:HB3	5:J:217:TYR:HB2	2.00	0.43
4:D:110:ILE:HG13	4:D:137:ASP:HA	2.01	0.43
4:D:158:LEU:HD11	5:E:171:GLY:O	2.19	0.43
5:E:86:SER:OG	5:E:115:VAL:HG22	2.19	0.43
1:F:97:TRP:CZ3	10:H:101:MYR:H71	2.54	0.43
5:E:202:PHE:HE2	5:E:210:PHE:CE1	2.37	0.43
5:E:34:TRP:HB3	5:E:46:MET:HE3	2.00	0.43
2:B:36:GLU:HB3	2:B:83:ASN:HB2	2.00	0.43
5:E:204:HIS:CD2	5:E:245:ALA:HB3	2.54	0.43
1:F:255:GLN:NE2	1:F:274:TRP:O	2.52	0.43
2:G:19:LYS:HD3	2:G:20:PRO:N	2.33	0.43
4:D:53:ASN:N	4:D:53:ASN:HD22	2.17	0.42
2:G:21:ASN:OD1	2:G:22:PHE:N	2.45	0.42
2:G:64:LEU:HD23	2:G:64:LEU:HA	1.83	0.42
1:A:143:THR:OG1	3:C:5:ILE:HG23	2.20	0.42
2:B:19:LYS:HA	2:B:20:PRO:HD3	1.90	0.42
1:F:20:PRO:HG3	6:F:303:IOD:I	2.89	0.42
1:F:235:PRO:HG2	2:G:65:LEU:HD22	2.01	0.42
4:I:145:SER:HA	4:I:187:ASP:OD2	2.20	0.42
4:D:186:LYS:HZ2	4:D:190:ILE:H	1.66	0.42
5:E:11:LEU:HD12	5:E:11:LEU:HA	1.92	0.42
1:F:106:ASN:OD1	1:F:106:ASN:N	2.47	0.42
5:E:21:LEU:HD12	5:E:76:LEU:HD23	2.02	0.42
5:J:205:ASN:HA	5:J:206:PRO:HD3	1.86	0.42
1:A:19:GLU:OE2	1:A:19:GLU:HA	2.19	0.42
4:D:134:THR:HG22	4:D:135:ASP:N	2.35	0.42
5:E:119:LEU:HD13	5:E:119:LEU:N	2.35	0.42
5:J:21:LEU:HD12	5:J:76:LEU:HD23	2.02	0.42
5:J:6:GLN:CB	5:J:109:PRO:HD2	2.50	0.42
5:J:157:VAL:HA	5:J:215:GLN:O	2.20	0.42
1:A:228:ILE:HD13	1:A:230:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:HIS:CE1	1:A:271:THR:HG23	2.54	0.42
2:B:17:ASN:OD1	2:B:73:ASN:HA	2.20	0.41
2:G:33:SER:HB3	2:G:62:PHE:CE2	2.55	0.41
4:D:190:ILE:HG13	4:D:194:THR:OG1	2.20	0.41
5:E:185:LEU:HD22	2:G:44:GLU:HB2	2.02	0.41
1:A:62:GLU:HG3	1:A:65:ARG:NH1	2.35	0.41
2:B:47:GLY:HA2	5:J:186:GLU:HG2	2.02	0.41
4:I:17:VAL:CG2	4:I:77:VAL:HG11	2.50	0.41
1:A:42:SER:HA	1:A:43:PRO:HD2	1.73	0.41
4:D:111:GLN:H	4:D:111:GLN:HG2	1.62	0.41
5:E:235:GLN:OE1	5:E:237:ILE:HD11	2.20	0.41
2:G:76:ASP:HB3	2:G:78:TYR:CE1	2.54	0.41
4:D:114:ASP:OD1	5:E:139:HIS:NE2	2.54	0.41
1:A:97:TRP:CH2	10:C:101:MYR:H71	2.55	0.41
5:E:112:ARG:HB3	5:E:112:ARG:HH21	1.86	0.41
5:E:227:GLU:HG2	5:E:229:ARG:CZ	2.51	0.41
1:F:226:GLN:O	1:F:227:ASP:HB2	2.20	0.41
5:J:76:LEU:HD12	5:J:76:LEU:HA	1.86	0.41
1:A:120:GLY:HA3	2:B:1:ILE:CG1	2.51	0.41
1:F:13:SER:OG	1:F:15:PRO:HD3	2.21	0.41
4:D:121:ARG:HH11	4:D:121:ARG:CB	2.34	0.41
1:A:24:TYR:OH	1:A:71:ALA:HA	2.20	0.40
10:H:101:MYR:H32	10:H:101:MYR:H61	1.63	0.40
4:I:48:GLN:NE2	5:J:102:VAL:HG13	2.36	0.40
1:A:215:LEU:HD12	1:A:261:VAL:HG22	2.02	0.40
1:F:24:TYR:HB2	1:F:36:PHE:HB3	2.02	0.40
1:F:244:TRP:HE1	2:G:99:MET:CG	2.34	0.40
5:J:83:LEU:HD21	5:J:117:GLU:HG3	2.04	0.40
1:A:21:ARG:HE	1:A:23:ILE:HD11	1.86	0.40
4:I:193:ASP:OD1	4:I:193:ASP:N	2.45	0.40
5:J:182:GLN:HB2	5:J:188:SER:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	276/276 (100%)	270 (98%)	6 (2%)	0	100	100
1	F	275/276 (100%)	269 (98%)	6 (2%)	0	100	100
2	B	99/100 (99%)	98 (99%)	1 (1%)	0	100	100
2	G	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	2/4 (50%)	2 (100%)	0	0	100	100
3	H	2/4 (50%)	2 (100%)	0	0	100	100
4	D	190/198 (96%)	184 (97%)	6 (3%)	0	100	100
4	I	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
5	E	232/245 (95%)	225 (97%)	7 (3%)	0	100	100
5	J	243/245 (99%)	239 (98%)	4 (2%)	0	100	100
All	All	1613/1646 (98%)	1575 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/229 (101%)	229 (99%)	2 (1%)	78	94
1	F	230/229 (100%)	229 (100%)	1 (0%)	91	97
2	B	94/93 (101%)	93 (99%)	1 (1%)	73	92
2	G	93/93 (100%)	93 (100%)	0	100	100
3	C	1/1 (100%)	1 (100%)	0	100	100
3	H	1/1 (100%)	1 (100%)	0	100	100
4	D	169/173 (98%)	167 (99%)	2 (1%)	71	92
4	I	173/173 (100%)	172 (99%)	1 (1%)	86	96
5	E	211/218 (97%)	209 (99%)	2 (1%)	78	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	J	218/218 (100%)	217 (100%)	1 (0%)	88	96
All	All	1421/1428 (100%)	1411 (99%)	10 (1%)	84	95

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	106	ASN
2	B	70	PHE
4	D	23	HIS
4	D	53	ASN
5	E	119	LEU
5	E	244	ARG
1	F	272	LEU
4	I	178	ASP
5	J	25	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
4	D	53	ASN
1	F	255	GLN
5	J	25	GLN
5	J	77	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 28 ligands modelled in this entry, 21 are monoatomic - leaving 7 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
7	EDO	G	102	-	3,3,3	0.41	0	2,2,2	0.47	0
10	MYR	H	101	3	14,14,15	0.39	0	13,13,15	0.96	0
8	TRS	B	103	-	7,7,7	0.51	0	9,9,9	1.09	0
10	MYR	C	101	3	14,14,15	0.36	0	13,13,15	0.75	0
7	EDO	A	305	-	3,3,3	0.62	0	2,2,2	0.28	0
7	EDO	I	205	-	3,3,3	0.53	0	2,2,2	0.45	0
7	EDO	F	304	-	3,3,3	0.51	0	2,2,2	0.34	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
7	EDO	G	102	-	-	1/1/1/1	-
10	MYR	H	101	3	-	6/11/12/13	-
8	TRS	B	103	-	-	2/9/9/9	-
10	MYR	C	101	3	-	6/11/12/13	-
7	EDO	A	305	-	-	0/1/1/1	-
7	EDO	I	205	-	-	1/1/1/1	-
7	EDO	F	304	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	102	EDO	O1-C1-C2-O2

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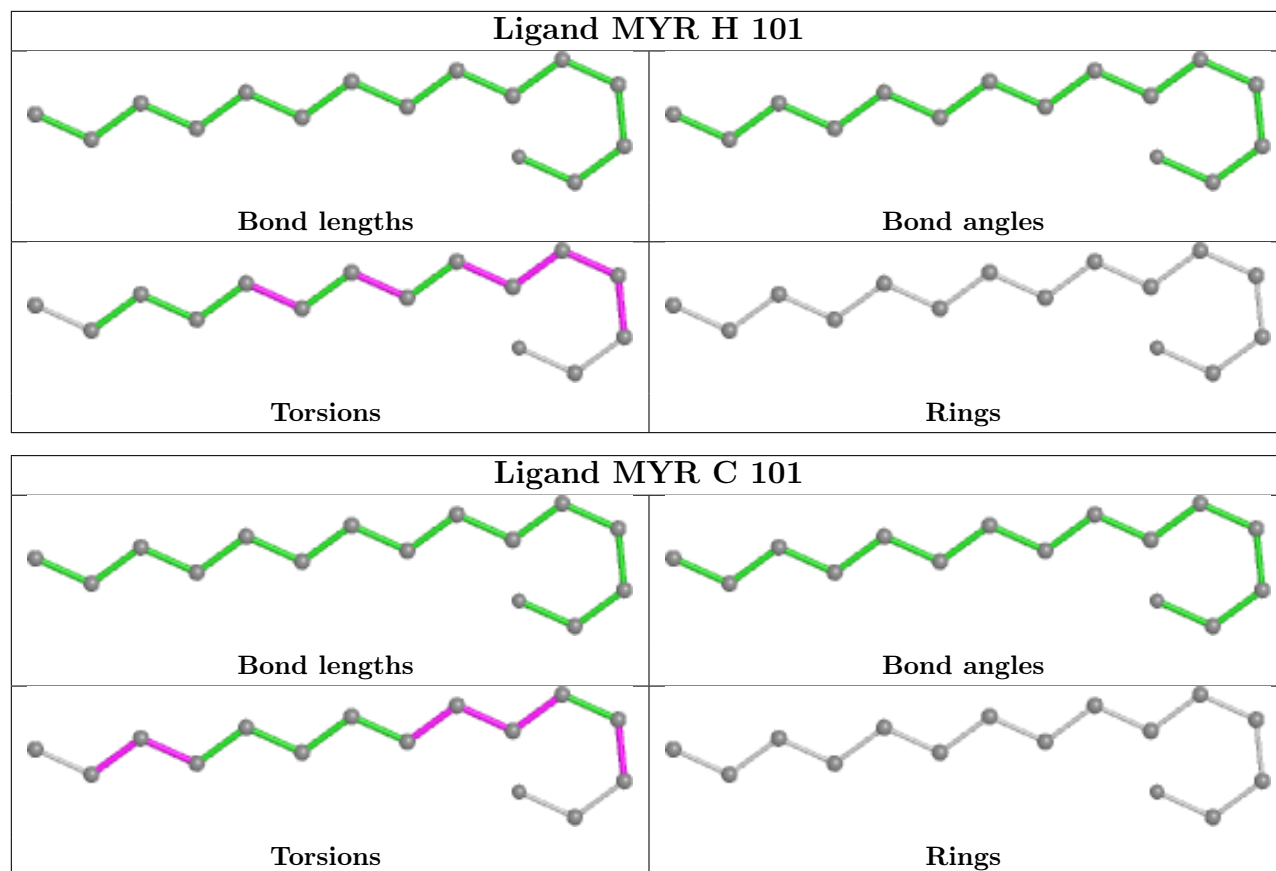
Mol	Chain	Res	Type	Atoms
10	H	101	MYR	C1-C2-C3-C4
10	H	101	MYR	C3-C4-C5-C6
10	C	101	MYR	C4-C5-C6-C7
10	C	101	MYR	C3-C4-C5-C6
10	C	101	MYR	C5-C6-C7-C8
10	H	101	MYR	C11-C10-C9-C8
7	I	205	EDO	O1-C1-C2-O2
10	H	101	MYR	C2-C3-C4-C5
10	H	101	MYR	C4-C5-C6-C7
10	C	101	MYR	C10-C11-C12-C13
10	C	101	MYR	C11-C12-C13-C14
10	H	101	MYR	C6-C7-C8-C9
8	B	103	TRS	N-C-C1-O1
10	C	101	MYR	C1-C2-C3-C4
8	B	103	TRS	C2-C-C1-O1

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	102	EDO	1	0
10	H	101	MYR	2	0
8	B	103	TRS	4	0
10	C	101	MYR	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 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	276/276 (100%)	-0.37	2 (0%) 87 84	13, 33, 67, 88	0
1	F	276/276 (100%)	-0.17	3 (1%) 80 75	22, 46, 85, 101	0
2	B	100/100 (100%)	-0.52	0 100 100	13, 27, 60, 83	0
2	G	100/100 (100%)	-0.36	1 (1%) 82 77	25, 42, 71, 87	0
3	C	4/4 (100%)	-0.35	0 100 100	37, 39, 39, 41	0
3	H	4/4 (100%)	-0.17	0 100 100	50, 52, 56, 57	0
4	D	194/198 (97%)	0.12	5 (2%) 56 46	23, 61, 99, 120	0
4	I	198/198 (100%)	-0.43	1 (0%) 91 88	15, 31, 62, 87	0
5	E	238/245 (97%)	-0.02	8 (3%) 45 35	28, 57, 98, 123	0
5	J	245/245 (100%)	-0.41	1 (0%) 92 91	16, 34, 60, 101	0
All	All	1635/1646 (99%)	-0.25	21 (1%) 77 72	13, 41, 88, 123	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	207	ARG	3.9
4	D	198	GLY	3.9
4	D	1	ALA	3.4
5	E	228	ASP	3.4
5	E	1	ASP	3.3
5	E	226	THR	3.1
1	F	16	GLY	2.7
5	E	62	TYR	2.7
4	I	198	GLY	2.6
5	E	230	ASP	2.6
4	D	110	ILE	2.4
1	F	15	PRO	2.4
4	D	181	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	57	ASN	2.3
4	D	112	ASN	2.2
1	A	227	ASP	2.2
1	A	276	PRO	2.1
5	E	117	GLU	2.1
1	F	200	THR	2.0
5	J	62	TYR	2.0
2	G	99	MET	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.

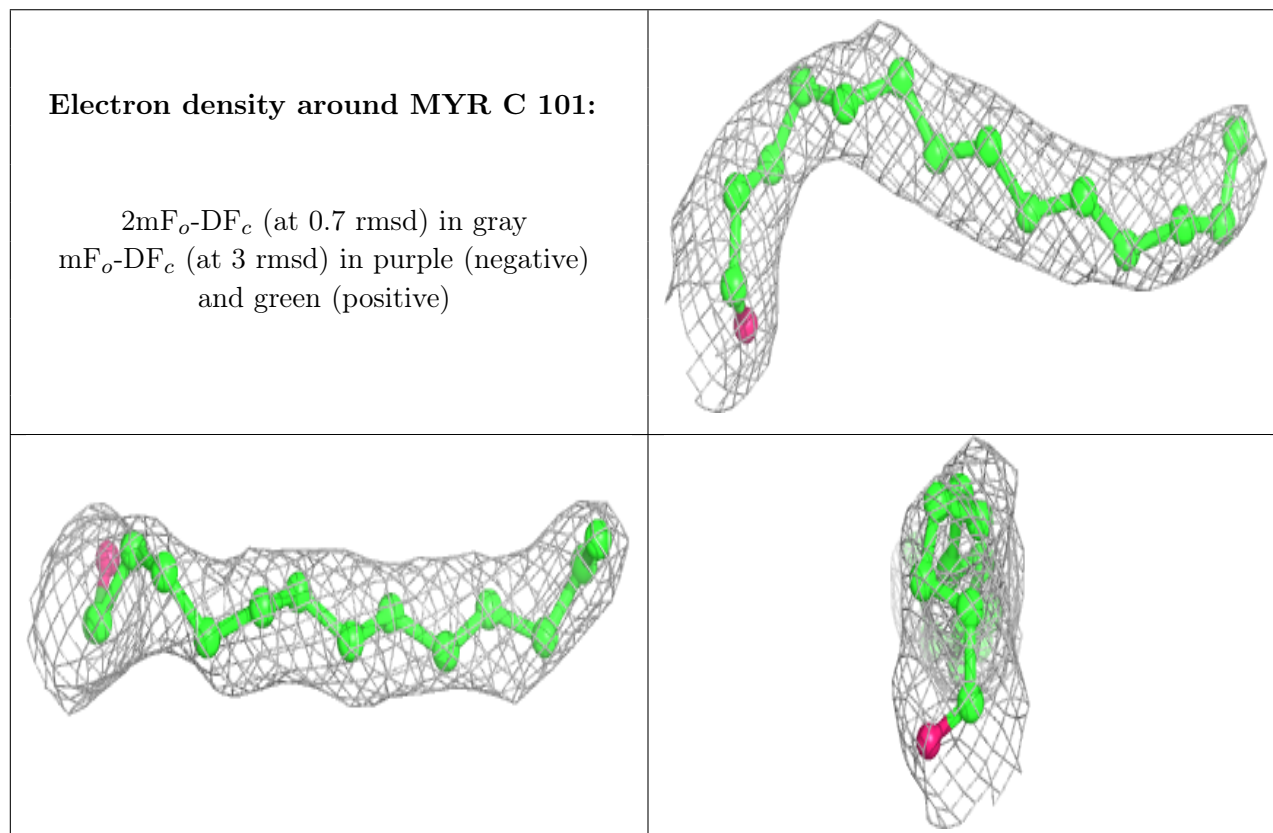
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	IOD	F	303	1/1	0.82	0.12	147,147,147,147	0
7	EDO	F	304	4/4	0.87	0.27	43,46,54,60	0
7	EDO	A	305	4/4	0.88	0.20	33,39,39,40	0
7	EDO	I	205	4/4	0.91	0.26	26,29,34,42	0
9	CA	B	104	1/1	0.91	0.07	58,58,58,58	0
8	TRS	B	103	8/8	0.95	0.19	23,36,49,60	0
6	IOD	A	303	1/1	0.95	0.07	108,108,108,108	0
10	MYR	C	101	15/16	0.95	0.23	17,24,34,37	0
10	MYR	H	101	15/16	0.95	0.26	25,37,50,52	0
11	NA	I	206	1/1	0.95	0.11	22,22,22,22	0
6	IOD	G	101	1/1	0.96	0.05	81,81,81,81	0
7	EDO	G	102	4/4	0.96	0.17	31,38,38,48	0
6	IOD	I	202	1/1	0.97	0.09	103,103,103,103	0
6	IOD	E	302	1/1	0.97	0.07	114,114,114,114	0
6	IOD	E	301	1/1	0.98	0.05	120,120,120,120	0

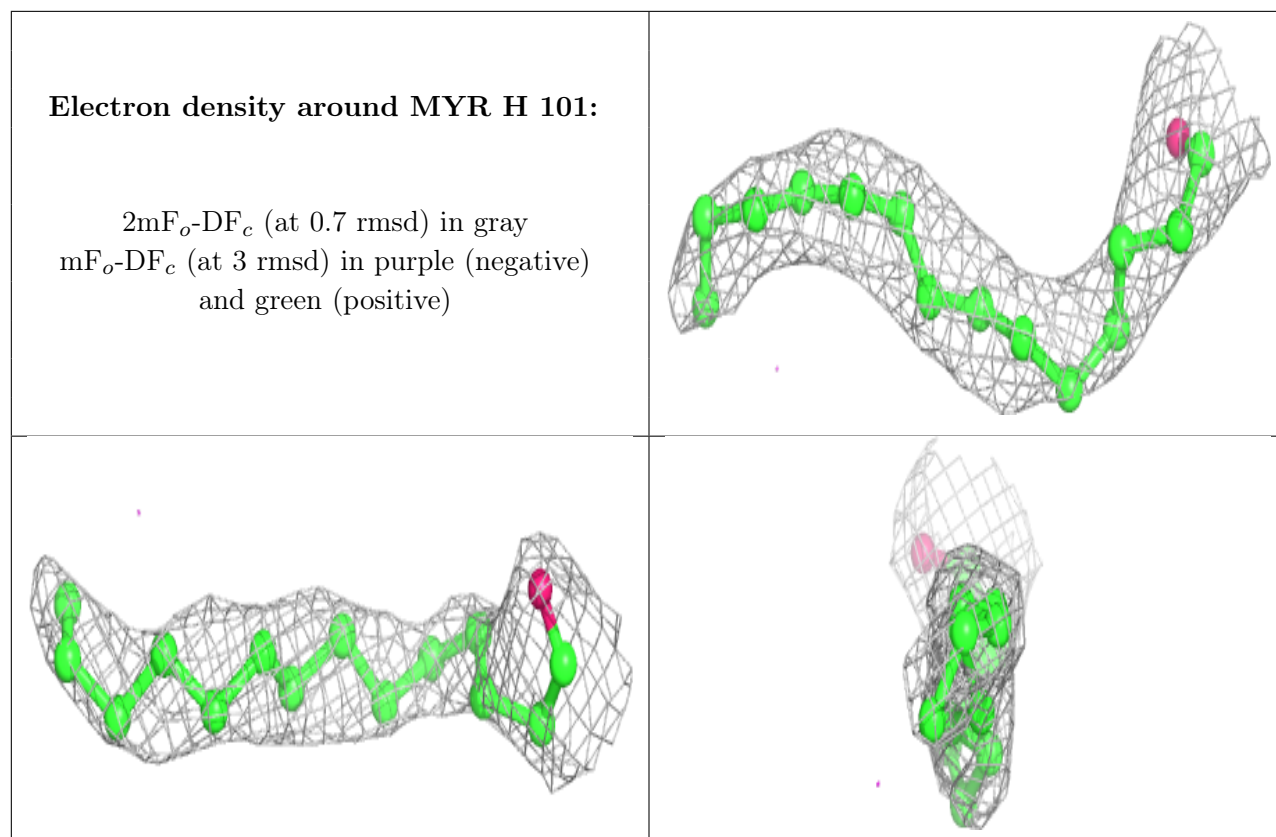
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	IOD	A	302	1/1	0.98	0.06	107,107,107,107	0
6	IOD	J	302	1/1	0.98	0.08	79,79,79,79	0
6	IOD	B	102	1/1	0.98	0.07	62,62,62,62	0
6	IOD	F	301	1/1	0.99	0.08	72,72,72,72	0
6	IOD	A	301	1/1	0.99	0.08	59,59,59,59	0
6	IOD	D	201	1/1	0.99	0.06	85,85,85,85	0
6	IOD	I	201	1/1	0.99	0.06	56,56,56,56	0
6	IOD	A	304	1/1	0.99	0.05	82,82,82,82	0
6	IOD	I	203	1/1	0.99	0.04	77,77,77,77	0
6	IOD	I	204	1/1	0.99	0.07	96,96,96,96	0
6	IOD	J	301	1/1	0.99	0.08	47,47,47,47	0
6	IOD	B	101	1/1	0.99	0.05	73,73,73,73	0
6	IOD	F	302	1/1	1.00	0.06	81,81,81,81	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.