



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 09:07 pm BST

PDB ID : 6PUG  
Title : Structure of human MAIT A-F7 TCR in complex with human MR1-2'OH-Et  
hyl-5-OP-U  
Authors : Awad, W.; Rossjohn, J.  
Deposited on : 2019-07-18  
Resolution : 1.80 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.

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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)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

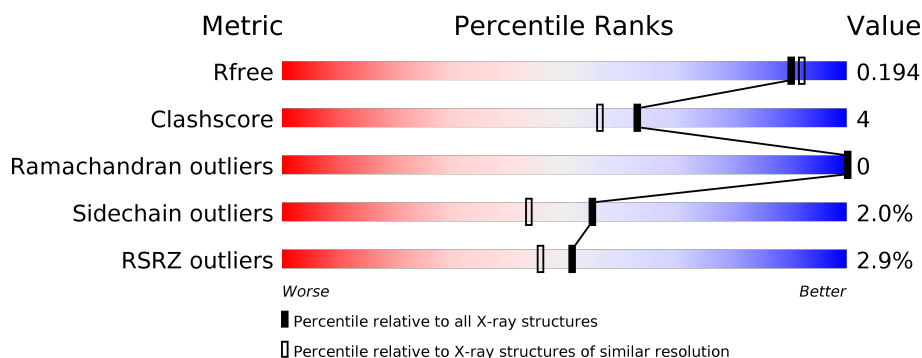
## 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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.



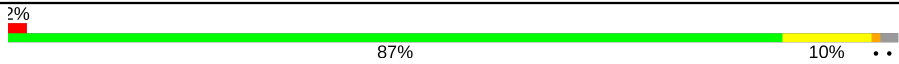

<b>Metric</b>	<b>Whole archive (#Entries)</b>	<b>Similar resolution (#Entries, resolution range(Å))</b>
R <sub>free</sub>	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on 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	<div> <div></div> <div>87%</div> <div>10%</div> <div>• •</div> </div>
1	C	271	<div> <div></div> <div>87%</div> <div>10%</div> <div>• •</div> </div>
2	B	100	<div> <div>17%</div> <div></div> <div>90%</div> <div>7%</div> <div>• •</div> </div>
2	F	100	<div> <div></div> <div>98%</div> <div></div> <div>•</div> </div>
3	D	204	<div> <div>8%</div> <div></div> <div>89%</div> <div>6%</div> <div>• •</div> </div>
3	G	204	<div> <div></div> <div>88%</div> <div>10%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	246	 2% 87% 10% ..
4	H	246	 87% 11% ..

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15466 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	13	0
			2234	1430	384	407	13			
1	C	267	Total	C	N	O	S	0	17	0
			2297	1479	393	413	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q95460
A	261	SER	CYS	conflict	UNP Q95460
C	0	MET	-	initiating methionine	UNP Q95460
C	261	SER	CYS	conflict	UNP Q95460

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	1	0
			799	514	134	148	3			
2	F	100	Total	C	N	O	S	0	2	0
			825	533	139	149	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
F	0	MET	-	initiating methionine	UNP P61769

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	196	Total	C	N	O	S	0	8	0
			1523	973	237	303	10			

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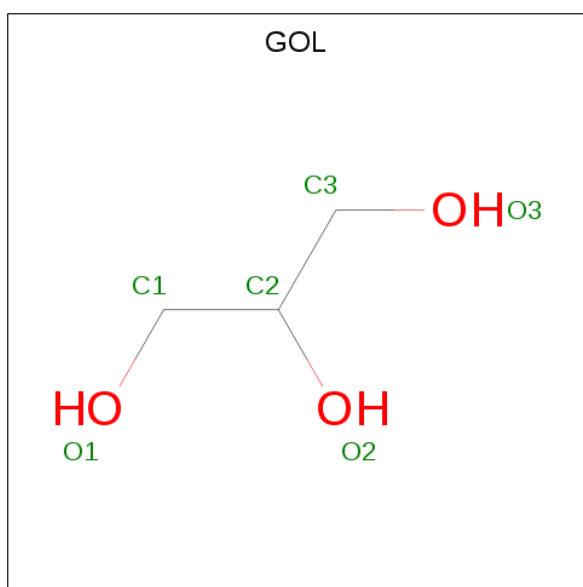
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	200	Total	C	N	O	S	0	20	0
			1655	1053	257	334	11			

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

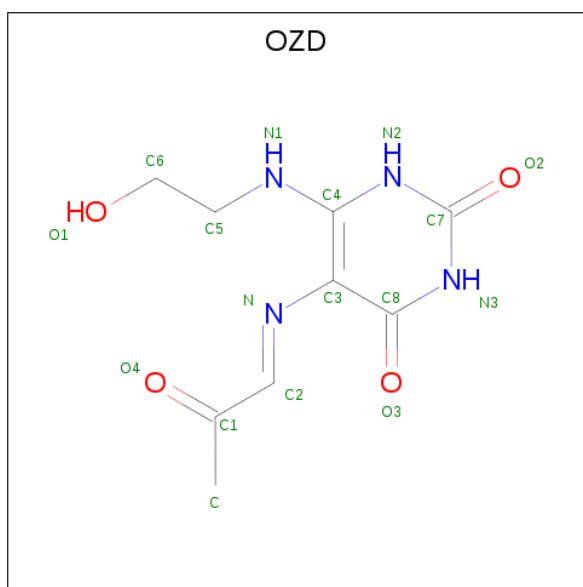
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	242	Total	C	N	O	S	0	12	0
			1930	1224	324	369	13			
4	H	244	Total	C	N	O	S	0	21	0
			2015	1281	340	381	13			

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



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

- Molecule 6 is 6-[(2-hydroxyethyl)amino]-5-[(E)-(2-oxopropylidene)amino]pyrimidine-2,4(1H, 3H)-dione (three-letter code: OZD) (formula:  $C_9H_{12}N_4O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			16	9	4	3		
6	C	1	Total	C	N	O	0	0
			16	9	4	3		

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

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

- Molecule 8 is SODIUM ION (three-letter code: 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	372	Total	O	0	0
			372	372		
9	B	103	Total	O	0	0
			103	103		
9	C	387	Total	O	0	0
			387	387		

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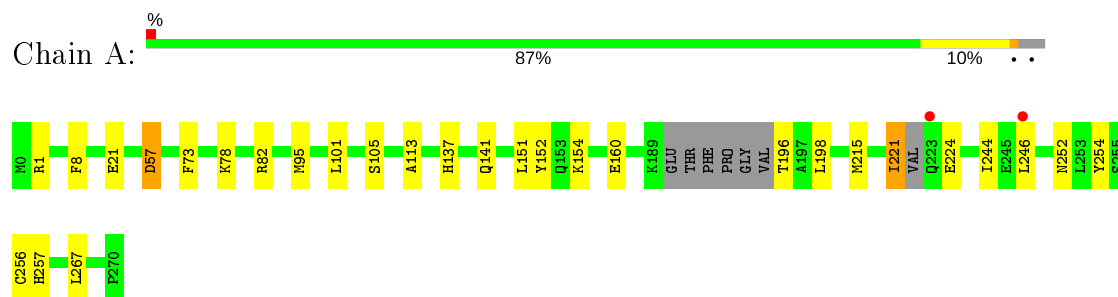
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	192	Total 192	O 192	0	0
9	E	220	Total 220	O 220	0	0
9	F	160	Total 160	O 160	0	0
9	G	329	Total 329	O 329	0	0
9	H	373	Total 373	O 373	0	0

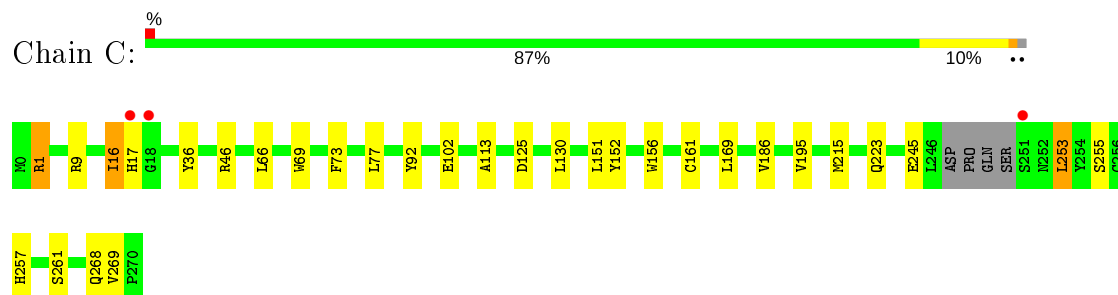
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

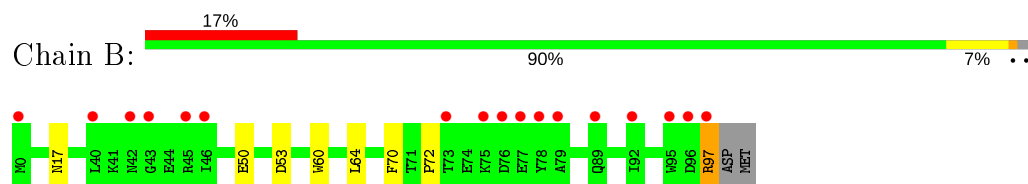
- Molecule 1: Major histocompatibility complex class I-related gene protein



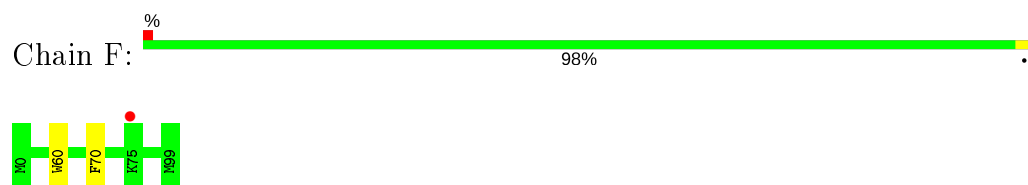
- Molecule 1: Major histocompatibility complex class I-related gene protein



- Molecule 2: Beta-2-microglobulin

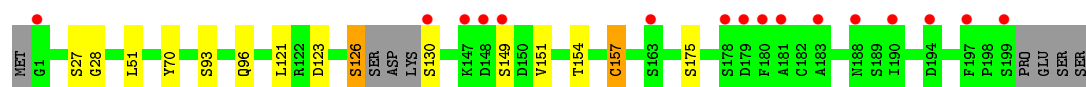


- Molecule 2: Beta-2-microglobulin



- Molecule 3: Human TCR alpha chain

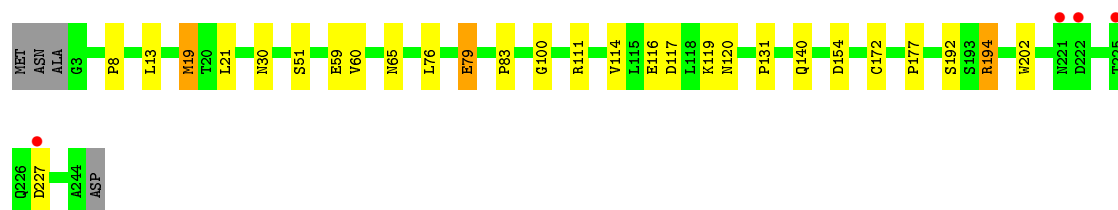




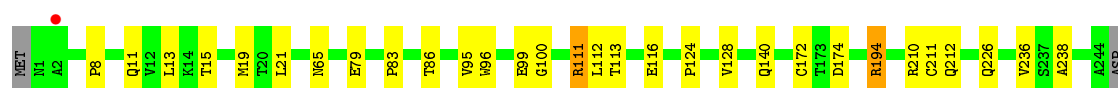
- Molecule 3: Human TCR alpha chain



- Molecule 4: Human TCR beta chain



- Molecule 4: Human TCR beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.62 Å   69.27 Å   142.06 Å 90.00°   103.68°   90.00°	Depositor
Resolution (Å)	47.03 – 1.80 47.03 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.03-1.80) 99.9 (47.03-1.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 1.79 Å)	Xtriage
Refinement program	PHENIX 1.16_3549-000, PHENIX 1.16_3549-000	Depositor
R, $R_{free}$	0.160 , 0.194 0.161 , 0.194	Depositor DCC
$R_{free}$ test set	9337 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15466	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: GOL, OZD, CL, NA

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	0.49	0/2332	0.62	0/3165
1	C	0.48	0/2410	0.64	1/3272 (0.0%)
2	B	0.39	0/825	0.56	0/1123
2	F	0.45	0/854	0.60	0/1157
3	D	0.44	0/1574	0.60	0/2139
3	G	0.50	0/1742	0.69	1/2364 (0.0%)
4	E	0.42	0/2014	0.58	0/2742
4	H	0.52	0/2121	0.66	0/2886
All	All	0.47	0/13872	0.62	2/18848 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	ARG	NE-CZ-NH2	-6.10	117.25	120.30
3	G	159	LEU	CA-CB-CG	5.24	127.36	115.30

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	2234	0	2131	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2297	0	2230	26	0
2	B	799	0	746	5	0
2	F	825	0	795	1	0
3	D	1523	0	1423	10	0
3	G	1655	0	1604	18	0
4	E	1930	0	1819	18	0
4	H	2015	0	1941	27	0
5	A	6	0	8	0	0
5	F	12	0	16	0	0
6	A	16	0	0	0	0
6	C	16	0	0	0	0
7	E	1	0	0	0	0
8	H	1	0	0	0	0
9	A	372	0	0	6	4
9	B	103	0	0	1	0
9	C	387	0	0	6	1
9	D	192	0	0	3	0
9	E	220	0	0	3	0
9	F	160	0	0	0	1
9	G	329	0	0	10	2
9	H	373	0	0	7	4
All	All	15466	0	12713	113	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (113) 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)
1:A:160[B]:GLU:OE2	9:A:401:HOH:O	1.91	0.86
1:A:221:ILE:HG21	1:A:244:ILE:HD11	1.59	0.83
4:H:140[B]:GLN:OE1	9:H:401:HOH:O	2.01	0.77
1:A:21:GLU:OE2	9:A:402:HOH:O	2.05	0.75
1:C:125:ASP:OD2	9:C:901:HOH:O	2.04	0.74
1:C:46[B]:ARG:NH1	9:C:903:HOH:O	2.20	0.73
3:G:138[B]:ASP:OD1	9:G:302:HOH:O	2.06	0.73
3:G:3[A]:ASN:ND2	9:G:305:HOH:O	2.23	0.71
4:E:13:LEU:HD21	4:E:19[B]:MET:HG3	1.71	0.70
3:G:188[B]:ASN:OD1	9:G:301:HOH:O	2.06	0.70
3:G:41[B]:GLU:OE1	9:G:303:HOH:O	2.08	0.70
4:E:140:GLN:NE2	9:E:403:HOH:O	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:172[A]:CYS:HB3	4:H:194[A]:ARG:HD3	1.76	0.68
4:H:99[B]:GLU:OE1	9:H:403:HOH:O	2.13	0.67
1:A:57[B]:ASP:OD2	9:A:403:HOH:O	2.12	0.67
4:H:100:GLY:O	9:H:404:HOH:O	2.13	0.66
3:D:28:GLY:HA3	3:D:93:SER:HB3	1.78	0.65
2:B:53:ASP:OD2	9:B:101:HOH:O	2.14	0.65
4:E:65[A]:ASN:ND2	4:E:79:GLU:OE2	2.30	0.64
4:H:99[B]:GLU:HG2	4:H:100:GLY:H	1.64	0.62
1:C:1:ARG:HA	1:C:102:GLU:HG2	1.81	0.62
9:G:518:HOH:O	4:H:99[B]:GLU:HB3	2.00	0.61
3:G:28:GLY:HA3	3:G:93[B]:SER:OG	2.00	0.61
1:C:36:TYR:HB2	1:C:66[B]:LEU:HD23	1.83	0.61
1:C:9:ARG:NH1	9:C:912:HOH:O	2.33	0.61
1:C:66[B]:LEU:HD12	1:C:69:TRP:CE3	2.36	0.60
4:H:65[B]:ASN:ND2	4:H:79:GLU:OE2	2.35	0.60
3:G:122:ARG:NH1	9:G:310:HOH:O	2.34	0.60
1:C:215[A]:MET:HG3	1:C:257:HIS:CD2	2.36	0.59
1:A:252:ASN:HB2	1:A:254:TYR:CE1	2.37	0.59
3:G:96[A]:GLN:OE1	9:G:304:HOH:O	2.17	0.59
4:E:154[B]:ASP:OD2	9:E:401:HOH:O	2.17	0.59
1:A:196:THR:HG23	1:A:246:LEU:HB2	1.85	0.58
4:H:11:GLN:HB3	4:H:112[A]:LEU:HD22	1.84	0.58
4:H:128[B]:VAL:HG23	4:H:238:ALA:HB3	1.85	0.58
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.40	0.56
3:G:150:ASP:HB2	3:G:177:LYS:HD2	1.87	0.56
1:A:152:TYR:CD1	4:H:100:GLY:HA3	2.41	0.56
1:A:151:LEU:HD22	3:G:51:LEU:HD12	1.86	0.55
3:D:149:SER:OG	9:D:301:HOH:O	2.18	0.55
4:H:128[B]:VAL:HG22	4:H:211[B]:CYS:SG	2.48	0.54
1:C:36:TYR:CB	1:C:66[B]:LEU:HD23	2.38	0.54
4:E:120:ASN:HB2	9:E:445:HOH:O	2.08	0.54
1:C:195:VAL:HG13	1:C:245[B]:GLU:HG3	1.91	0.53
2:B:72:PRO:HB2	2:B:97:ARG:NH1	2.25	0.52
4:H:15[B]:THR:HG21	4:H:116:GLU:OE2	2.10	0.52
1:A:215:MET:HG3	1:A:257:HIS:CD2	2.45	0.51
1:C:255[B]:SER:OG	1:C:268:GLN:HG2	2.11	0.51
3:D:121:LEU:O	3:D:130:SER:HB2	2.11	0.51
4:E:172[B]:CYS:SG	4:E:194:ARG:HD3	2.50	0.51
1:C:151:LEU:HD22	3:D:51:LEU:HD12	1.93	0.51
2:B:17:ASN:OD1	2:B:97:ARG:NH1	2.45	0.50
1:C:113:ALA:HB2	2:F:60:TRP:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256[B]:CYS:HB2	1:A:267:LEU:HB2	1.94	0.50
4:H:15[B]:THR:HG22	4:H:83:PRO:HD3	1.93	0.49
3:G:13[B]:THR:HG23	9:G:438:HOH:O	2.14	0.48
3:D:123:ASP:HB3	3:D:126:SER:HA	1.96	0.48
4:H:95:VAL:HG12	4:H:96:TRP:CD1	2.48	0.48
4:H:8:PRO:HD2	4:H:21[B]:LEU:CD2	2.44	0.48
4:H:124:PRO:HG2	4:H:236[B]:VAL:HG11	1.95	0.48
1:C:130[B]:LEU:HD23	3:G:125:LYS:O	2.12	0.47
1:A:198:LEU:HB2	1:A:244:ILE:HG22	1.95	0.47
3:G:148:ASP:OD2	3:G:177:LYS:NZ	2.32	0.47
4:H:174:ASP:OD1	4:H:194[B]:ARG:NH2	2.33	0.46
1:C:156:TRP:CZ3	1:C:161:CYS:HB2	2.51	0.46
3:D:157:CYS:SG	4:E:172[B]:CYS:HB2	2.55	0.46
1:A:154:LYS:HD3	3:G:51:LEU:HD11	1.97	0.46
4:H:13:LEU:HD11	4:H:19[A]:MET:SD	2.56	0.46
1:C:152:TYR:CD1	4:E:100:GLY:HA3	2.51	0.46
4:E:8:PRO:HD2	4:E:21[B]:LEU:HD22	1.98	0.46
1:C:46[B]:ARG:NH2	9:C:926:HOH:O	2.49	0.45
4:H:111:ARG:NE	9:H:407:HOH:O	2.23	0.45
1:A:101[B]:LEU:HD12	1:A:105:SER:OG	2.17	0.45
1:C:186:VAL:HG11	1:C:269:VAL:HG22	1.99	0.45
4:E:21[B]:LEU:HD12	4:E:76:LEU:HD23	1.98	0.45
3:D:154:THR:HG21	4:E:192:SER:OG	2.16	0.45
1:C:1:ARG:HA	1:C:102:GLU:CG	2.46	0.45
1:C:223:GLN:N	1:C:223:GLN:OE1	2.50	0.45
4:H:99[B]:GLU:OE1	9:H:405:HOH:O	2.21	0.44
4:E:59:GLU:HG2	4:E:60:VAL:HG13	1.98	0.44
4:H:99[A]:GLU:OE1	9:H:406:HOH:O	2.21	0.44
3:D:151:VAL:HG22	3:D:175:SER:HB2	2.00	0.44
1:A:8:PHE:CE2	1:A:95[B]:MET:HG3	2.53	0.43
4:E:117:ASP:OD2	4:E:119:LYS:HB2	2.18	0.43
2:B:64[B]:LEU:HD12	2:B:64[B]:LEU:HA	1.83	0.43
1:C:130[B]:LEU:HD12	9:C:1055:HOH:O	2.18	0.43
4:H:210:ARG:NH1	4:H:212:GLN:HB2	2.34	0.43
1:A:141:GLN:HG3	9:A:654:HOH:O	2.19	0.43
3:D:96:GLN:HG3	9:D:422:HOH:O	2.19	0.43
1:C:36:TYR:CG	1:C:66[B]:LEU:HD23	2.54	0.42
4:E:131:PRO:HD2	4:E:202:TRP:CZ2	2.54	0.42
4:E:8:PRO:HD2	4:E:21[B]:LEU:CD2	2.49	0.42
3:G:34:TRP:CG	3:G:73[B]:LEU:HG	2.54	0.42
1:A:152:TYR:CG	4:H:100:GLY:HA3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130[B]:LEU:HD11	9:C:1241:HOH:O	2.19	0.42
3:G:96[A]:GLN:NE2	9:G:308:HOH:O	2.26	0.42
4:H:86:THR:HG23	4:H:113:THR:HA	2.01	0.41
4:E:83:PRO:HA	4:E:114:VAL:HB	2.02	0.41
1:C:253:LEU:HA	1:C:253:LEU:HD12	1.88	0.41
1:C:169[B]:LEU:HA	1:C:169[B]:LEU:HD12	1.90	0.41
3:G:157:CYS:SG	4:H:172[B]:CYS:SG	3.17	0.41
3:D:70:TYR:OH	9:D:302:HOH:O	2.20	0.41
1:C:77:LEU:HD13	1:C:92:TYR:HB2	2.02	0.41
4:E:30:ASN:O	4:E:51:SER:HA	2.20	0.41
4:H:226:GLN:NE2	9:H:402:HOH:O	2.10	0.41
1:A:141:GLN:OE1	9:A:404:HOH:O	2.22	0.41
4:E:154[A]:ASP:OD1	4:E:177:PRO:HG3	2.21	0.41
1:A:1[A]:ARG:HH11	1:A:1[A]:ARG:HD3	1.75	0.40
1:C:16[A]:ILE:H	1:C:16[A]:ILE:HG12	1.60	0.40
3:G:96[A]:GLN:NE2	9:G:314:HOH:O	2.39	0.40
1:A:137:HIS:HD2	9:A:681:HOH:O	2.03	0.40
3:G:70[B]:TYR:OH	3:G:72:TYR:HD2	2.04	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:571:HOH:O	9:H:625:HOH:O[4_548]	2.01	0.19
9:C:1133:HOH:O	9:G:307:HOH:O[4_558]	2.11	0.09
9:A:634:HOH:O	9:H:531:HOH:O[2_658]	2.12	0.08
9:A:686:HOH:O	9:F:224:HOH:O[4_558]	2.17	0.03
9:A:666:HOH:O	9:H:705:HOH:O[2_658]	2.18	0.02
9:A:636:HOH:O	9:H:563:HOH:O[2_658]	2.19	0.01

## 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	271/271 (100%)	266 (98%)	5 (2%)	0	100	100
1	C	280/271 (103%)	274 (98%)	6 (2%)	0	100	100
2	B	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
2	F	100/100 (100%)	99 (99%)	1 (1%)	0	100	100
3	D	200/204 (98%)	194 (97%)	6 (3%)	0	100	100
3	G	218/204 (107%)	214 (98%)	4 (2%)	0	100	100
4	E	252/246 (102%)	246 (98%)	6 (2%)	0	100	100
4	H	263/246 (107%)	257 (98%)	6 (2%)	0	100	100
All	All	1681/1642 (102%)	1646 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	241/241 (100%)	234 (97%)	7 (3%)	42	29
1	C	251/241 (104%)	244 (97%)	7 (3%)	43	30
2	B	86/95 (90%)	83 (96%)	3 (4%)	36	21
2	F	90/95 (95%)	89 (99%)	1 (1%)	73	68
3	D	165/181 (91%)	161 (98%)	4 (2%)	49	36
3	G	194/181 (107%)	193 (100%)	1 (0%)	88	87
4	E	209/212 (99%)	202 (97%)	7 (3%)	38	23
4	H	222/212 (105%)	219 (99%)	3 (1%)	67	59
All	All	1458/1458 (100%)	1425 (98%)	33 (2%)	55	37

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57[A]	ASP
1	A	57[B]	ASP

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Mol	Chain	Res	Type
1	A	73	PHE
1	A	78	LYS
1	A	82	ARG
1	A	221	ILE
1	A	224	GLU
2	B	50	GLU
2	B	70	PHE
2	B	97	ARG
1	C	16[A]	ILE
1	C	16[B]	ILE
1	C	17	HIS
1	C	73	PHE
1	C	253	LEU
1	C	261[A]	SER
1	C	261[B]	SER
3	D	27[A]	SER
3	D	27[B]	SER
3	D	126	SER
3	D	157	CYS
4	E	19[A]	MET
4	E	19[B]	MET
4	E	79	GLU
4	E	111	ARG
4	E	116	GLU
4	E	194	ARG
4	E	227	ASP
2	F	70	PHE
3	G	25	GLN
4	H	111	ARG
4	H	194[A]	ARG
4	H	194[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	GOL	A	301	-	5,5,5	1.23	1 (20%)	5,5,5	0.97	0
5	GOL	F	102	-	5,5,5	0.98	0	5,5,5	0.96	0
6	OZD	C	801	1	14,16,17	1.51	2 (14%)	13,20,22	5.27	5 (38%)
6	OZD	A	302	1	14,16,17	1.30	2 (14%)	13,20,22	5.37	6 (46%)
5	GOL	F	101	-	5,5,5	0.93	0	5,5,5	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	301	-	-	0/4/4/4	-
5	GOL	F	102	-	-	0/4/4/4	-
6	OZD	C	801	1	-	3/7/8/9	0/1/1/1
6	OZD	A	302	1	-	3/7/8/9	0/1/1/1
5	GOL	F	101	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	801	OZD	C1-C2	4.05	1.53	1.49
6	C	801	OZD	C8-N3	3.19	1.38	1.33
6	A	302	OZD	C8-N3	3.19	1.38	1.33
5	A	301	GOL	C3-C2	2.08	1.60	1.51
6	A	302	OZD	C3-N	-2.04	1.39	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	801	OZD	C8-N3-C7	14.35	127.26	115.14
6	A	302	OZD	C8-N3-C7	14.03	126.99	115.14
6	A	302	OZD	C8-C3-C4	9.62	120.82	114.53
6	C	801	OZD	C8-C3-C4	8.82	120.30	114.53
6	A	302	OZD	C3-C8-N3	-7.25	113.52	123.43
6	C	801	OZD	C3-C8-N3	-7.13	113.68	123.43
6	A	302	OZD	C7-N2-C4	4.49	124.09	113.80
6	C	801	OZD	C7-N2-C4	4.13	123.26	113.80
6	A	302	OZD	C4-C3-N	-2.25	112.98	125.02
6	A	302	OZD	N1-C4-N2	2.16	121.25	118.50
6	C	801	OZD	C4-C3-N	-2.14	113.61	125.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	801	OZD	C4-C3-N-C2
6	A	302	OZD	C4-C3-N-C2
6	C	801	OZD	C6-C5-N1-C4
6	A	302	OZD	C6-C5-N1-C4
6	C	801	OZD	C8-C3-N-C2
6	A	302	OZD	C8-C3-N-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	264/271 (97%)	-0.48	2 (0%) 86 84	11, 23, 55, 68	8 (3%)
1	C	267/271 (98%)	-0.49	3 (1%) 80 78	14, 23, 43, 66	9 (3%)
2	B	98/100 (98%)	0.63	17 (17%) 1 1	17, 40, 64, 68	6 (6%)
2	F	100/100 (100%)	-0.56	1 (1%) 82 80	15, 25, 44, 53	0
3	D	196/204 (96%)	-0.06	16 (8%) 11 9	17, 31, 65, 78	4 (2%)
3	G	200/204 (98%)	-0.65	2 (1%) 82 80	12, 21, 42, 58	5 (2%)
4	E	242/246 (98%)	-0.45	4 (1%) 70 66	20, 33, 56, 74	4 (1%)
4	H	244/246 (99%)	-0.41	1 (0%) 92 90	14, 22, 39, 65	9 (3%)
All	All	1611/1642 (98%)	-0.37	46 (2%) 51 46	11, 25, 55, 78	45 (2%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	1	GLY	4.8
2	B	0	MET	4.1
3	D	148	ASP	4.0
1	C	17	HIS	3.9
3	D	1	GLY	3.9
2	B	73	THR	3.8
2	B	92	ILE	3.8
3	D	188	ASN	3.6
2	B	96	ASP	3.5
4	E	221	ASN	3.3
3	D	163	SER	3.3
2	B	77	GLU	3.1
2	B	45	ARG	3.0
3	D	180	PHE	3.0
1	C	251	SER	2.9
1	C	18	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	76	ASP	2.9
3	D	181	ALA	2.9
3	D	183	ALA	2.8
2	B	43	GLY	2.8
2	B	75	LYS	2.8
2	B	42	ASN	2.7
4	H	2	ALA	2.6
3	D	197	PHE	2.6
2	B	78	TYR	2.6
3	D	179	ASP	2.6
3	D	149	SER	2.6
3	D	199	SER	2.6
3	D	190	ILE	2.5
2	F	75	LYS	2.5
2	B	89	GLN	2.5
3	D	147	LYS	2.4
3	G	179	ASP	2.4
4	E	222	ASP	2.4
1	A	246	LEU	2.4
2	B	46	ILE	2.3
3	D	194	ASP	2.3
2	B	40	LEU	2.2
2	B	79	ALA	2.2
2	B	97	ARG	2.1
4	E	225	THR	2.1
3	D	178	SER	2.1
2	B	95	TRP	2.1
1	A	223	GLN	2.1
4	E	227	ASP	2.1
3	D	130	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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	OZD	C	801	16/17	0.95	0.10	21,21,27,31	0
6	OZD	A	302	16/17	0.95	0.10	19,19,27,32	0
5	GOL	A	301	6/6	0.96	0.07	24,30,32,34	0
5	GOL	F	102	6/6	0.98	0.06	19,22,26,27	0
7	CL	E	301	1/1	0.98	0.04	37,37,37,37	0
5	GOL	F	101	6/6	0.99	0.07	17,18,21,24	0
8	NA	H	301	1/1	1.00	0.04	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.