



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2026 – 10:08 AM EDT

PDB ID : 9Y0V / pdb_00009y0v
Title : Crystal Structure of human MAIT A-F7 TCR-MR1*04 complex
Authors : Letoga, V.; Rossjohn, J.; Awad, W.
Deposited on : 2025-08-29
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

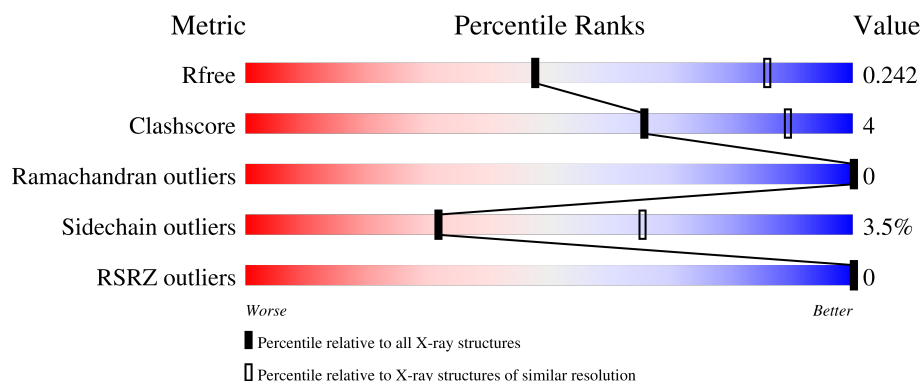
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	271	
1	C	271	
2	B	100	
2	F	100	
3	D	204	

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Mol	Chain	Length	Quality of chain
3	G	204	 90% 7% •
4	E	246	 83% 15% ••
4	H	246	 88% 11% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12912 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 protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	1	0
			2135	1378	370	376	11			
1	C	266	Total	C	N	O	S	0	3	0
			2160	1392	365	392	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q95460
A	9	HIS	ARG	variant	UNP Q95460
A	17	ARG	HIS	variant	UNP Q95460
A	261	SER	CYS	conflict	UNP Q95460
C	0	MET	-	initiating methionine	UNP Q95460
C	9	HIS	ARG	variant	UNP Q95460
C	17	ARG	HIS	variant	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	100	Total	C	N	O	S	0	0	0
			801	513	138	146	4			
2	F	99	Total	C	N	O	S	0	0	0
			779	502	134	141	2			

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

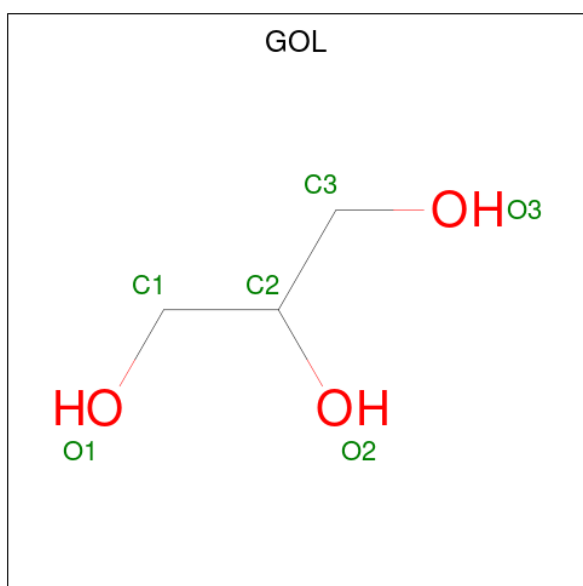
- Molecule 3 is a protein called TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	198	Total	C	N	O	S	0	5	0
			1525	967	244	304	10			
3	G	198	Total	C	N	O	S	0	3	0
			1507	956	240	301	10			

- Molecule 4 is a protein called TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	243	Total	C	N	O	S	0	6	0
			1882	1195	320	355	12			
4	H	243	Total	C	N	O	S	0	3	0
			1862	1180	319	352	11			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

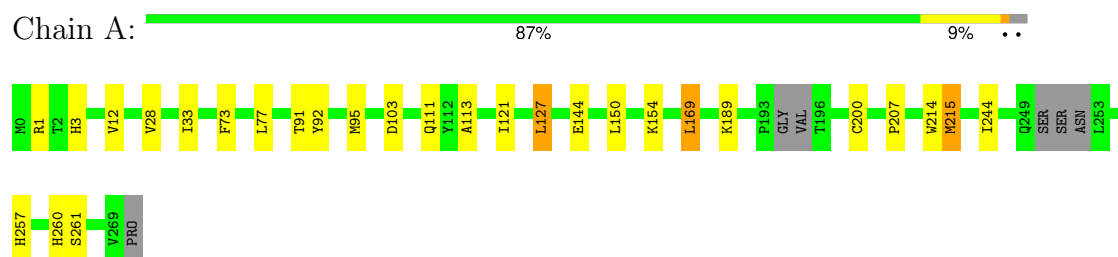
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	46	Total 46	O 46	0	0
6	B	24	Total 24	O 24	0	0
6	C	40	Total 40	O 40	0	0
6	D	31	Total 31	O 31	0	0
6	E	25	Total 25	O 25	0	0
6	F	10	Total 10	O 10	0	0
6	G	31	Total 31	O 31	0	0
6	H	36	Total 36	O 36	0	0

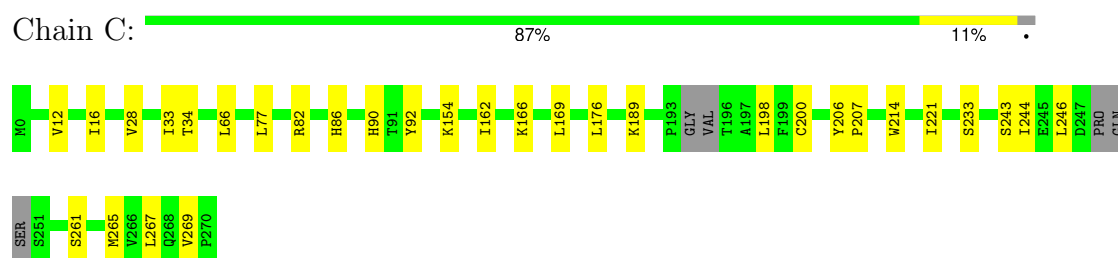
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

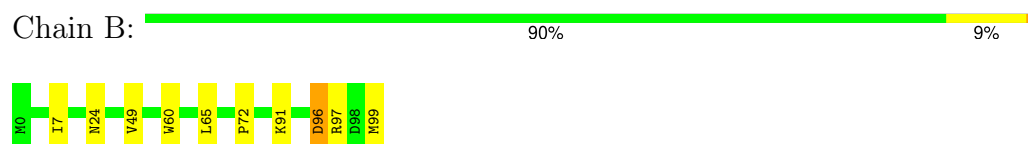
- Molecule 1: Major histocompatibility complex class I-related protein 1



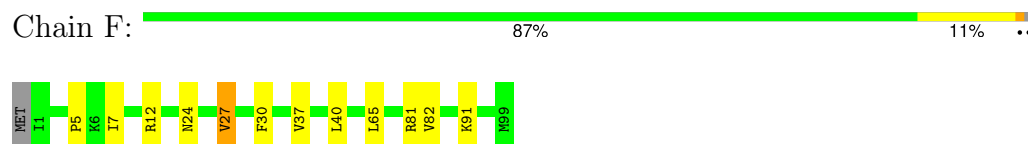
- Molecule 1: Major histocompatibility complex class I-related protein 1



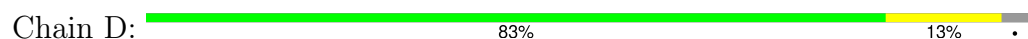
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

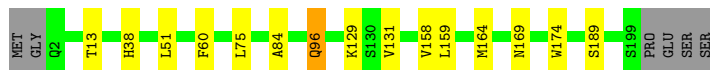
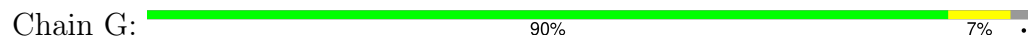


- Molecule 3: TCR alpha chain

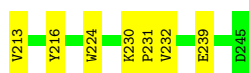
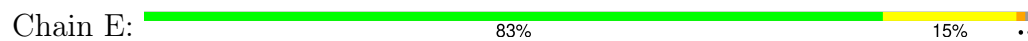




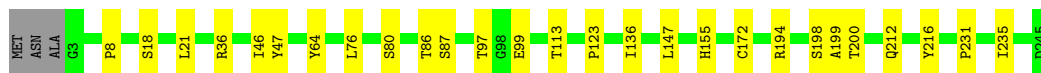
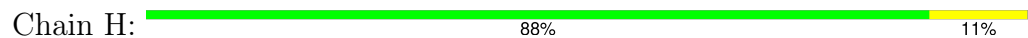
- Molecule 3: TCR alpha chain



- Molecule 4: TCR beta chain



- Molecule 4: TCR beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.39Å 140.99Å 114.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.50 – 3.00 43.50 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.50-3.00) 99.8 (43.50-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.195 , 0.244 0.195 , 0.242	Depositor DCC
R_{free} test set	1979 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.427 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12912	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.09	0/2204	0.26	0/2999
1	C	0.08	0/2235	0.24	0/3043
2	B	0.07	0/824	0.26	0/1120
2	F	0.08	0/802	0.27	0/1093
3	D	0.08	0/1571	0.26	0/2137
3	G	0.07	0/1547	0.25	0/2105
4	E	0.09	0/1951	0.26	0/2659
4	H	0.10	0/1922	0.27	0/2622
All	All	0.08	0/13056	0.26	0/17778

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2135	0	2004	15	0
1	C	2160	0	2030	14	0
2	B	801	0	745	5	0
2	F	779	0	716	8	0
3	D	1525	0	1400	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1507	0	1377	10	0
4	E	1882	0	1753	20	0
4	H	1862	0	1721	14	0
5	A	6	0	8	1	0
5	B	6	0	8	0	0
5	G	6	0	8	1	0
6	A	46	0	0	1	0
6	B	24	0	0	0	0
6	C	40	0	0	0	0
6	D	31	0	0	0	0
6	E	25	0	0	0	0
6	F	10	0	0	0	0
6	G	31	0	0	0	0
6	H	36	0	0	0	0
All	All	12912	0	11770	92	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 4.

All (92) 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:28:VAL:HG23	1:A:33:ILE:HD13	1.73	0.70
1:A:77:LEU:HD13	1:A:92:TYR:HB2	1.77	0.67
1:C:77:LEU:HD13	1:C:92:TYR:HB2	1.76	0.67
4:E:123:PRO:HD3	4:E:231:PRO:HB3	1.80	0.64
1:C:28:VAL:HG23	1:C:33:ILE:HD13	1.80	0.63
4:E:8:PRO:HD2	4:E:21:LEU:HD23	1.82	0.62
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.84	0.59
3:G:164:MET:HE1	4:H:198:SER:HB3	1.85	0.58
1:A:111:GLN:HG2	1:A:121:ILE:HG23	1.86	0.57
2:F:24:ASN:HB3	2:F:65:LEU:HD11	1.86	0.57
1:A:144:GLU:HA	1:A:150:LEU:HD11	1.85	0.57
4:H:21:LEU:HD12	4:H:76:LEU:HD23	1.86	0.57
2:B:7:ILE:HD12	2:B:91:LYS:HD2	1.88	0.56
4:E:230:LYS:HG2	4:E:232:VAL:HG13	1.86	0.56
4:H:123:PRO:HD3	4:H:231:PRO:HB3	1.87	0.55
4:H:8:PRO:HD2	4:H:21:LEU:HD23	1.87	0.55
1:C:154:LYS:HD3	3:G:51:LEU:HD11	1.87	0.55
4:E:21:LEU:HD12	4:E:76:LEU:HD23	1.88	0.55
2:F:40:LEU:HD11	2:F:81:ARG:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:VAL:HG12	1:A:91:THR:HG22	1.90	0.53
4:H:172[B]:CYS:SG	4:H:194:ARG:HD2	2.49	0.52
1:A:154:LYS:HD3	3:D:51:LEU:HD21	1.91	0.52
4:H:155:HIS:HB3	4:H:216:TYR:HB2	1.91	0.52
4:E:155:HIS:HB3	4:E:216:TYR:HB2	1.92	0.52
1:C:169[B]:LEU:HD12	1:C:176:LEU:HD13	1.91	0.51
1:C:33:ILE:HG13	1:C:34:THR:HG23	1.92	0.51
4:E:208:HIS:CE1	4:E:210:ARG:HB2	2.46	0.51
2:F:7:ILE:HG12	2:F:82:VAL:HG21	1.92	0.51
4:H:86:THR:HG23	4:H:113:THR:HA	1.93	0.50
1:A:1:ARG:HD2	6:A:416:HOH:O	2.10	0.50
4:E:224:TRP:HB2	4:E:230:LYS:HD3	1.94	0.49
1:C:233:SER:HB3	2:F:12:ARG:HG3	1.95	0.48
4:E:172[B]:CYS:SG	4:E:194:ARG:HD2	2.53	0.48
3:D:116:PRO:HB2	3:D:195:THR:HA	1.96	0.48
2:F:27:VAL:HG21	2:F:37:VAL:HG21	1.96	0.47
3:D:131:VAL:HG12	3:D:174:TRP:HB3	1.96	0.47
4:E:36:ARG:HH21	4:E:87:SER:HB2	1.79	0.47
1:C:86:HIS:HB3	1:C:90:HIS:NE2	2.30	0.47
1:A:207:PRO:HD2	1:A:260:HIS:CE1	2.49	0.47
4:H:46:ILE:HG22	4:H:47:TYR:HD1	1.80	0.46
4:H:64:TYR:HB3	4:H:76:LEU:HD11	1.98	0.46
4:E:19[B]:MET:HE3	4:E:19[B]:MET:HB2	1.88	0.46
1:C:265:MET:HE2	1:C:267:LEU:HD21	1.97	0.46
2:F:37:VAL:HG22	2:F:82:VAL:HG22	1.98	0.46
1:C:162:ILE:HG22	1:C:166:LYS:HE2	1.98	0.46
3:D:2:GLN:HG2	3:D:26:THR:HA	1.98	0.46
1:A:127:LEU:HD12	1:A:127:LEU:HA	1.83	0.46
3:D:156:LYS:HD3	3:D:169:ASN:ND2	2.31	0.45
3:G:159:LEU:HB3	4:H:172[A]:CYS:HB2	1.99	0.45
3:D:164:MET:H	3:D:164:MET:HG2	1.62	0.45
1:A:215:MET:HG3	1:A:257:HIS:CD2	2.51	0.45
4:H:136:ILE:HG23	4:H:199:ALA:HB1	1.97	0.45
4:E:46:ILE:HG22	4:E:47:TYR:HD1	1.82	0.45
4:E:94:SER:HB3	4:E:104:LEU:HD12	1.98	0.45
1:A:189:LYS:HD2	1:A:189:LYS:HA	1.72	0.44
4:H:36:ARG:HH21	4:H:87:SER:HB2	1.82	0.44
3:G:96:GLN:HA	5:G:301:GOL:H2	2.00	0.44
4:H:212:GLN:HG3	4:H:235:ILE:HG23	2.00	0.44
4:E:45:LEU:HD21	4:E:48:TYR:HB3	2.00	0.44
3:D:156:LYS:HD3	3:D:169:ASN:HD22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:196:PHE:CE2	3:D:198:PRO:HG3	2.53	0.43
3:G:159:LEU:HB3	4:H:172[B]:CYS:HB3	1.99	0.43
1:C:198:LEU:HD13	1:C:269:VAL:HG21	2.00	0.43
1:A:3:HIS:CD2	1:A:169:LEU:HD21	2.53	0.43
4:E:230:LYS:HA	4:E:231:PRO:HD3	1.87	0.43
3:G:60:PHE:CE1	3:G:75:LEU:HD23	2.54	0.43
2:B:96:ASP:O	2:B:99:MET:HG2	2.19	0.42
3:D:38:HIS:CD2	3:D:84:ALA:HB2	2.54	0.42
4:E:11:GLN:HG2	4:E:19[A]:MET:HE2	1.99	0.42
4:E:20:THR:HG23	4:E:77:ARG:HG3	2.01	0.42
3:D:164:MET:HE2	4:E:141:LYS:NZ	2.35	0.42
3:G:129:LYS:HD2	3:G:129:LYS:HA	1.94	0.42
5:A:301:GOL:H2	3:D:96:GLN:HA	2.02	0.41
4:E:46:ILE:HG22	4:E:47:TYR:CD1	2.54	0.41
3:D:108:LYS:HB3	3:D:139:SER:HB3	2.02	0.41
1:C:206:TYR:CD1	1:C:207:PRO:HA	2.56	0.41
3:D:60:PHE:CE1	3:D:75:LEU:HD23	2.56	0.41
1:C:244:ILE:HG13	1:C:246:LEU:HD21	2.02	0.41
2:F:7:ILE:HD12	2:F:91:LYS:HD2	2.03	0.41
3:G:158:VAL:HG22	3:G:169:ASN:OD1	2.21	0.41
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.56	0.41
1:A:200:CYS:HB2	1:A:214:TRP:CZ2	2.56	0.41
2:F:5:PRO:HB3	2:F:30:PHE:HB3	2.02	0.40
1:A:215:MET:HE3	1:A:215:MET:HB3	1.80	0.40
2:B:72:PRO:HB2	2:B:97:ARG:HH12	1.85	0.40
3:D:48:TYR:CZ	3:D:50:VAL:HB	2.56	0.40
4:E:148:ALA:HB2	4:E:213:VAL:HG21	2.03	0.40
1:C:169[A]:LEU:HD23	1:C:176:LEU:HD13	2.02	0.40
1:C:200:CYS:HB2	1:C:214:TRP:CZ2	2.57	0.40
4:E:177:PRO:HB2	4:E:189:TYR:HB3	2.03	0.40
3:G:38:HIS:CD2	3:G:84:ALA:HB2	2.57	0.40
3:G:131:VAL:HG12	3:G:174:TRP:HB3	2.03	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	260/271 (96%)	250 (96%)	10 (4%)	0	100	100
1	C	263/271 (97%)	254 (97%)	9 (3%)	0	100	100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	F	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
3	D	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
3	G	199/204 (98%)	189 (95%)	10 (5%)	0	100	100
4	E	247/246 (100%)	240 (97%)	7 (3%)	0	100	100
4	H	244/246 (99%)	238 (98%)	6 (2%)	0	100	100
All	All	1609/1642 (98%)	1555 (97%)	54 (3%)	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	217/241 (90%)	209 (96%)	8 (4%)	30	64
1	C	225/241 (93%)	217 (96%)	8 (4%)	31	65
2	B	85/95 (90%)	83 (98%)	2 (2%)	43	73
2	F	80/95 (84%)	79 (99%)	1 (1%)	61	81
3	D	163/181 (90%)	155 (95%)	8 (5%)	22	56
3	G	160/181 (88%)	157 (98%)	3 (2%)	50	76
4	E	196/212 (92%)	184 (94%)	12 (6%)	17	49
4	H	193/212 (91%)	187 (97%)	6 (3%)	35	68
All	All	1319/1458 (90%)	1271 (96%)	48 (4%)	32	65

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	PHE
1	A	95	MET
1	A	103	ASP
1	A	127	LEU
1	A	169	LEU
1	A	215	MET
1	A	244	ILE
1	A	261	SER
2	B	49	VAL
2	B	96	ASP
1	C	12	VAL
1	C	16	ILE
1	C	66	LEU
1	C	82	ARG
1	C	189	LYS
1	C	221	ILE
1	C	243	SER
1	C	261	SER
3	D	5	ASP
3	D	13	THR
3	D	17	ILE
3	D	111	ILE
3	D	128	ASP
3	D	141	THR
3	D	164	MET
3	D	189	SER
4	E	19[A]	MET
4	E	19[B]	MET
4	E	57	LYS
4	E	71	LYS
4	E	99	GLU
4	E	103[A]	GLU
4	E	103[B]	GLU
4	E	104	LEU
4	E	147	LEU
4	E	188	ARG
4	E	192	SER
4	E	239	GLU
2	F	27	VAL
3	G	13	THR
3	G	96	GLN
3	G	189	SER
4	H	18	SER

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Mol	Chain	Res	Type
4	H	80	SER
4	H	97	THR
4	H	99	GLU
4	H	147	LEU
4	H	200	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
2	B	13	HIS
1	C	71	GLN
1	C	203	HIS
1	C	260	HIS
4	E	30	ASN
2	F	13	HIS
2	F	31	HIS
4	H	29	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	GOL	A	301	-	5,5,5	0.36	0	5,5,5	0.53	0
5	GOL	B	301	-	5,5,5	0.35	0	5,5,5	0.38	0
5	GOL	G	301	-	5,5,5	0.34	0	5,5,5	0.37	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	-	-	2/4/4/4	-
5	GOL	B	301	-	-	2/4/4/4	-
5	GOL	G	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	GOL	O1-C1-C2-O2
5	A	301	GOL	O1-C1-C2-C3
5	B	301	GOL	C1-C2-C3-O3
5	B	301	GOL	O2-C2-C3-O3
5	G	301	GOL	O1-C1-C2-C3
5	G	301	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	301	GOL	1	0
5	G	301	GOL	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	265/271 (97%)	-1.69	0 100 100	24, 36, 61, 93	19 (7%)
1	C	266/271 (98%)	-1.72	0 100 100	18, 37, 71, 91	11 (4%)
2	B	100/100 (100%)	-1.68	0 100 100	27, 40, 65, 73	5 (5%)
2	F	99/100 (99%)	-1.69	0 100 100	22, 39, 62, 78	2 (2%)
3	D	198/204 (97%)	-1.62	0 100 100	15, 42, 75, 89	11 (5%)
3	G	198/204 (97%)	-1.63	0 100 100	15, 39, 70, 90	16 (8%)
4	E	243/246 (98%)	-1.69	0 100 100	20, 42, 63, 93	13 (5%)
4	H	243/246 (98%)	-1.68	0 100 100	20, 40, 62, 84	14 (5%)
All	All	1612/1642 (98%)	-1.68	0 100 100	15, 39, 70, 93	91 (5%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	A	301	6/6	0.99	0.05	36,42,44,47	0
5	GOL	B	301	6/6	0.99	0.05	56,59,61,63	0
5	GOL	G	301	6/6	0.99	0.04	38,46,50,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.