



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:59 AM UTC

PDB ID : 7Q9A / pdb_00007q9a
Title : MHC Class I A02 Allele presenting LLLGIGILVL, in complex with Mel5 TCR
Authors : Rizkallah, P.J.; Sewell, A.K.; Wall, A.; Fuller, A.
Deposited on : 2021-11-12
Resolution : 2.10 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

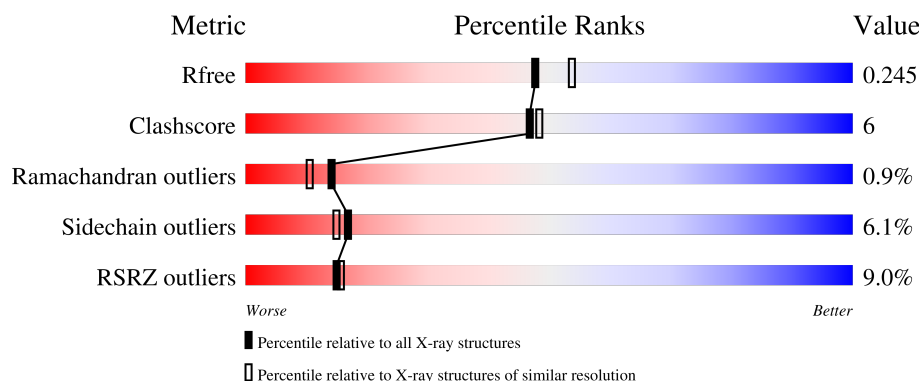
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	276	13% 79% 19% .
2	B	100	2% 83% 15% .
3	C	10	80% 20%
4	D	199	13% 77% 19% .
5	E	244	5% 82% 16% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6911 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	1	0
			2265	1414	414	428	9			

- 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
			837	533	141	159	4			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called LEU-LEU-LEU-GLY-ILE-GLY-ILE-LEU-VAL-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			72	51	10	11			

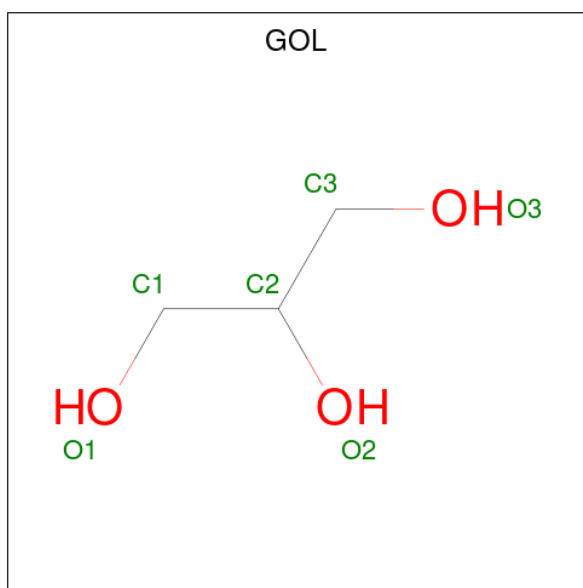
- Molecule 4 is a protein called Human Mel5 T Cell Receptor, Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	199	Total	C	N	O	S	0	1	0
			1549	963	255	323	8			

- Molecule 5 is a protein called Human Mel5 T Cell Receptor, Beta Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	244	Total	C	N	O	S	0	1	0
			1936	1227	333	371	5			

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		

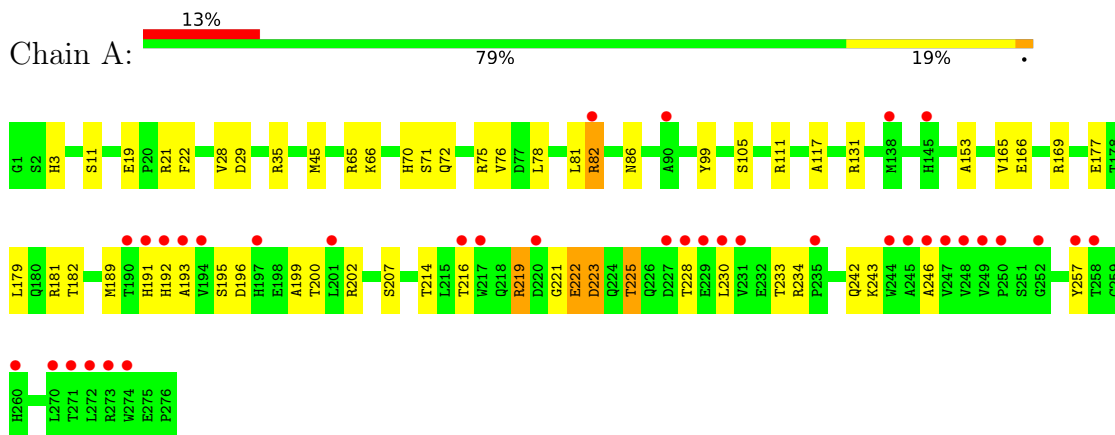
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	84	Total	O	0	0
			84	84		
7	B	23	Total	O	0	0
			23	23		
7	C	3	Total	O	0	0
			3	3		
7	D	51	Total	O	0	0
			51	51		
7	E	67	Total	O	0	0
			67	67		

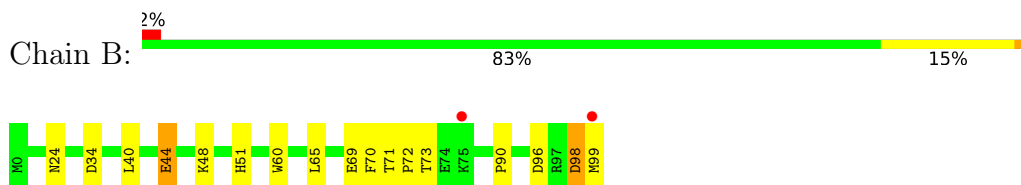
3 Residue-property plots [i](#)

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.

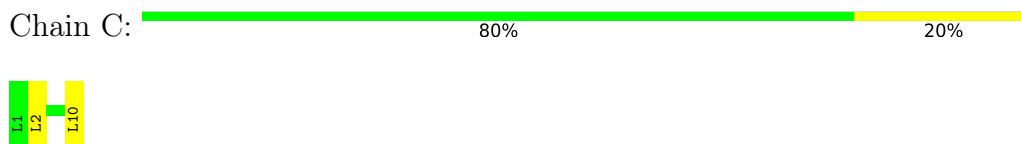
- Molecule 1: MHC class I antigen



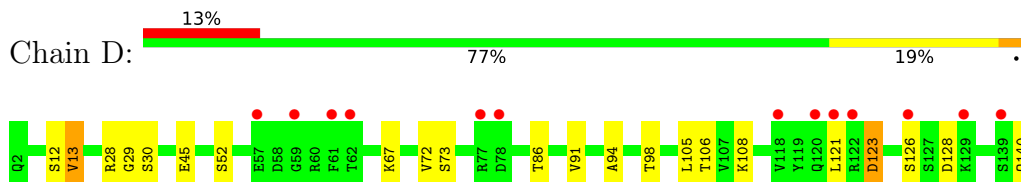
- Molecule 2: Beta-2-microglobulin

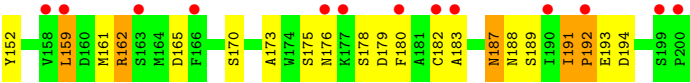


- Molecule 3: LEU-LEU-LEU-GLY-ILE-GLY-ILE-LEU-VAL-LEU

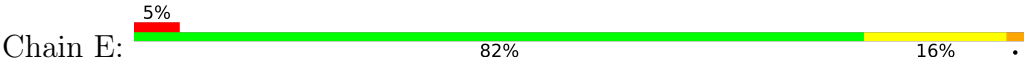


- Molecule 4: Human Mel5 T Cell Receptor, Alpha Chain





● Molecule 5: Human Mel5 T Cell Receptor, Beta Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	122.02Å 122.02Å 82.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.01 – 2.10 61.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (61.01-2.10) 99.8 (61.01-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.204 , 0.243 0.211 , 0.245	Depositor DCC
R_{free} test set	3456 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6911	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.06	0/2331	1.38	7/3163 (0.2%)
2	B	1.09	1/860 (0.1%)	1.33	1/1162 (0.1%)
3	C	1.07	0/71	1.20	0/94
4	D	1.06	0/1582	1.42	8/2146 (0.4%)
5	E	1.04	1/1990 (0.1%)	1.35	4/2713 (0.1%)
All	All	1.06	2/6834 (0.0%)	1.37	20/9278 (0.2%)

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
4	D	0	1
5	E	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	90	PRO	C-O	-7.20	1.14	1.23
5	E	176	PRO	C-O	-5.72	1.17	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	224	THR	CA-CB-OG1	-6.75	99.47	109.60
1	A	111	ARG	CA-C-N	6.68	126.79	122.18
1	A	111	ARG	C-N-CA	6.68	126.79	122.18
5	E	6	GLN	CB-CA-C	6.54	123.20	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	162	ARG	CA-C-N	5.99	128.31	120.28
4	D	162	ARG	C-N-CA	5.99	128.31	120.28
5	E	42	ARG	CG-CD-NE	-5.88	99.06	112.00
4	D	123	ASP	CA-CB-CG	5.83	118.43	112.60
4	D	45	GLU	CB-CA-C	5.80	120.20	109.70
2	B	34	ASP	CB-CA-C	5.79	118.50	110.16
5	E	38	GLN	CB-CA-C	5.69	119.91	110.74
1	A	35	ARG	CG-CD-NE	-5.44	100.04	112.00
4	D	98	THR	CA-CB-OG1	-5.42	101.47	109.60
1	A	76	VAL	O-C-N	5.29	127.09	121.91
4	D	193	GLU	CA-C-N	5.29	127.62	120.38
4	D	193	GLU	C-N-CA	5.29	127.62	120.38
1	A	182	THR	CB-CA-C	5.13	118.51	111.23
4	D	106	THR	CA-CB-OG1	-5.08	101.99	109.60
1	A	219	ARG	CA-C-N	5.00	126.94	120.44
1	A	219	ARG	C-N-CA	5.00	126.94	120.44

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	191	ILE	Peptide
5	E	43	GLY	Peptide

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	2265	0	2115	27	0
2	B	837	0	803	8	0
3	C	72	0	94	2	0
4	D	1549	0	1452	29	0
5	E	1936	0	1851	19	0
6	A	12	0	16	0	0
6	D	6	0	8	1	0
6	E	6	0	8	0	0
7	A	84	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	23	0	0	0	0
7	C	3	0	0	0	0
7	D	51	0	0	1	0
7	E	67	0	0	0	0
All	All	6911	0	6347	74	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 6.

All (74) 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:166:GLU:OE2	4:D:28:ARG:NH1	2.19	0.76
1:A:193:ALA:HB1	1:A:199:ALA:HA	1.76	0.66
1:A:72:GLN:NE2	7:A:401:HOH:O	2.29	0.65
4:D:86:THR:HG21	5:E:42:ARG:HG2	1.78	0.64
4:D:123:ASP:HB3	4:D:126:SER:O	1.98	0.64
4:D:191:ILE:HG22	4:D:194:ASP:HB3	1.80	0.63
5:E:219:GLU:O	5:E:229:LYS:NZ	2.34	0.61
4:D:191:ILE:HD12	4:D:191:ILE:N	2.16	0.60
4:D:140:GLN:N	4:D:140:GLN:OE1	2.35	0.59
4:D:159:LEU:C	4:D:159:LEU:HD23	2.29	0.58
4:D:159:LEU:HD11	5:E:195:ARG:HB2	1.85	0.58
1:A:233:THR:OG1	1:A:243:LYS:HE2	2.06	0.56
1:A:78:LEU:O	1:A:82[B]:ARG:HG3	2.06	0.55
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.42	0.55
1:A:169:ARG:HD2	7:A:478:HOH:O	2.07	0.55
4:D:121:LEU:HB3	5:E:129:GLU:O	2.08	0.54
4:D:150:ASP:O	4:D:175:SER:OG	2.24	0.53
1:A:131:ARG:HA	1:A:153:ALA:HB1	1.88	0.53
1:A:66:LYS:O	1:A:70:HIS:HD2	1.92	0.52
5:E:139:GLN:HG3	5:E:139:GLN:O	2.09	0.52
1:A:81:LEU:HD11	3:C:10:LEU:CD1	2.40	0.51
5:E:135:ILE:HG23	5:E:198:ALA:HB1	1.92	0.51
1:A:202:ARG:HG2	1:A:246:ALA:HB2	1.93	0.51
5:E:112:THR:HG1	5:E:154[B]:HIS:CE1	2.27	0.50
1:A:3:HIS:HA	1:A:29:ASP:OD1	2.11	0.50
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.58	0.50
1:A:22:PHE:CD2	1:A:71:SER:HB2	2.47	0.50
1:A:45:MET:CE	3:C:2:LEU:HD11	2.43	0.49
1:A:221:GLY:O	1:A:223:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:33:LEU:HD13	5:E:74:PHE:HB2	1.95	0.48
5:E:177:LEU:C	5:E:177:LEU:HD12	2.38	0.48
4:D:12:SER:OG	4:D:108:LYS:HE2	2.13	0.48
2:B:96:ASP:HB3	2:B:99:MET:HB2	1.95	0.48
1:A:234:ARG:HE	1:A:242:GLN:NE2	2.12	0.48
1:A:166:GLU:CD	4:D:28:ARG:HH12	2.21	0.48
4:D:52:SER:HA	7:D:446:HOH:O	2.14	0.47
4:D:30:SER:HB3	4:D:91:VAL:HG13	1.97	0.47
4:D:191:ILE:HD12	4:D:191:ILE:H	1.78	0.47
4:D:152:TYR:O	4:D:173:ALA:HA	2.14	0.47
1:A:202:ARG:NH2	2:B:98:ASP:O	2.36	0.47
4:D:28:ARG:NH2	4:D:67:LYS:O	2.48	0.47
5:E:30:ASN:N	5:E:31:PRO:CD	2.78	0.47
1:A:65:ARG:HH21	4:D:94:ALA:HB1	1.80	0.46
4:D:191:ILE:O	4:D:192:PRO:O	2.34	0.46
5:E:220:ASN:ND2	5:E:220:ASN:H	2.13	0.46
4:D:182:CYS:O	4:D:183:ALA:C	2.58	0.46
4:D:187:ASN:CG	4:D:187:ASN:O	2.58	0.46
5:E:38:GLN:HB2	5:E:44:LEU:HD23	1.98	0.46
1:A:19:GLU:OE1	1:A:75:ARG:HD3	2.16	0.46
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.98	0.45
1:A:219:ARG:HG3	1:A:257:TYR:CE2	2.52	0.45
4:D:12:SER:OG	4:D:108:LYS:CE	2.65	0.45
4:D:29:GLY:HA3	6:D:301:GOL:O2	2.18	0.43
5:E:155:VAL:HA	5:E:213:GLN:O	2.19	0.43
5:E:25:VAL:O	5:E:72:ARG:HB3	2.18	0.43
5:E:32:ASN:O	5:E:93:TRP:HA	2.19	0.43
1:A:225:THR:O	1:A:228:THR:HG23	2.19	0.43
2:B:51:HIS:HA	2:B:65:LEU:O	2.19	0.42
4:D:161:MET:HE2	5:E:195:ARG:HD3	2.01	0.42
4:D:13:VAL:HG13	4:D:105:LEU:HD11	2.02	0.42
1:A:28:VAL:HG11	1:A:179:LEU:HD13	2.02	0.42
2:B:40:LEU:HA	2:B:44:GLU:O	2.20	0.42
4:D:144:SER:HB2	4:D:188:ASN:HB3	2.00	0.42
5:E:11:LEU:N	5:E:11:LEU:HD12	2.35	0.42
4:D:178:SER:C	4:D:180:PHE:H	2.28	0.42
5:E:153:ASP:HB3	5:E:188:TYR:CE2	2.56	0.41
1:A:70:HIS:HE1	1:A:99:TYR:OH	2.03	0.41
1:A:11:SER:HA	1:A:21:ARG:O	2.21	0.41
4:D:161:MET:O	4:D:162:ARG:C	2.64	0.41
1:A:222:GLU:O	1:A:223:ASP:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:THR:HA	2:B:72:PRO:HD2	1.96	0.41
2:B:98:ASP:N	2:B:98:ASP:OD1	2.54	0.40
4:D:176:ASN:HD22	4:D:176:ASN:HA	1.78	0.40
5:E:83:LEU:HA	5:E:83:LEU:HD23	1.84	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	275/276 (100%)	255 (93%)	17 (6%)	3 (1%)	11	8
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
4	D	198/199 (100%)	184 (93%)	10 (5%)	4 (2%)	6	2
5	E	243/244 (100%)	231 (95%)	12 (5%)	0	100	100
All	All	822/829 (99%)	773 (94%)	42 (5%)	7 (1%)	14	10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	HIS
1	A	222	GLU
4	D	192	PRO
1	A	223	ASP
4	D	128	ASP
4	D	165	ASP
4	D	179	ASP

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	233/232 (100%)	216 (93%)	17 (7%)	13	10
2	B	95/95 (100%)	89 (94%)	6 (6%)	16	14
3	C	8/8 (100%)	8 (100%)	0	100	100
4	D	178/177 (101%)	171 (96%)	7 (4%)	28	31
5	E	212/211 (100%)	197 (93%)	15 (7%)	13	11
All	All	726/723 (100%)	681 (94%)	45 (6%)	17	14

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82[A]	ARG
1	A	82[B]	ARG
1	A	86	ASN
1	A	105	SER
1	A	165	VAL
1	A	177	GLU
1	A	181	ARG
1	A	189	MET
1	A	191	HIS
1	A	195	SER
1	A	196	ASP
1	A	200	THR
1	A	207	SER
1	A	214	THR
1	A	216	THR
1	A	225	THR
1	A	230	LEU
2	B	44	GLU
2	B	48	LYS
2	B	69	GLU
2	B	70	PHE
2	B	73	THR
2	B	98	ASP

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Mol	Chain	Res	Type
4	D	13	VAL
4	D	72	VAL
4	D	73	SER
4	D	159	LEU
4	D	170	SER
4	D	187	ASN
4	D	189	SER
5	E	3	THR
5	E	4	ILE
5	E	25	VAL
5	E	80	LYS
5	E	115	GLU
5	E	132	GLU
5	E	146	LEU
5	E	161	VAL
5	E	168	SER
5	E	171	CYS
5	E	193	ARG
5	E	220	ASN
5	E	224	THR
5	E	226	ASP
5	E	244	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	70	HIS
1	A	72	GLN
1	A	141	GLN
1	A	174	ASN
1	A	180	GLN
1	A	188	HIS
1	A	242	GLN
1	A	260	HIS
2	B	51	HIS
2	B	89	GLN
4	D	22	ASN
4	D	38	GLN
4	D	120	GLN
4	D	176	ASN
5	E	2	GLN

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Mol	Chain	Res	Type
5	E	5	HIS
5	E	13	GLN
5	E	32	ASN
5	E	38	GLN
5	E	70	GLN
5	E	119	ASN
5	E	207	HIS
5	E	213	GLN
5	E	220	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
6	GOL	A	302	-	5,5,5	0.07	0	5,5,5	0.25	0
6	GOL	E	301	-	5,5,5	0.11	0	5,5,5	0.31	0
6	GOL	D	301	-	5,5,5	0.19	0	5,5,5	0.46	0
6	GOL	A	301	-	5,5,5	0.10	0	5,5,5	0.28	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
6	GOL	A	302	-	-	2/4/4/4	-
6	GOL	E	301	-	-	2/4/4/4	-
6	GOL	D	301	-	-	2/4/4/4	-
6	GOL	A	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	GOL	O1-C1-C2-C3
6	A	302	GOL	O1-C1-C2-O2
6	A	302	GOL	O1-C1-C2-C3
6	D	301	GOL	C1-C2-C3-O3
6	D	301	GOL	O2-C2-C3-O3
6	E	301	GOL	C1-C2-C3-O3
6	A	301	GOL	O1-C1-C2-O2
6	E	301	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/276 (100%)	0.62	36 (13%) 7 7	26, 60, 133, 149	1 (0%)
2	B	100/100 (100%)	0.33	2 (2%) 65 67	37, 68, 117, 131	0
3	C	10/10 (100%)	-0.16	0 100 100	37, 41, 46, 46	0
4	D	199/199 (100%)	0.69	26 (13%) 7 7	24, 59, 117, 131	1 (0%)
5	E	244/244 (100%)	0.30	11 (4%) 38 40	28, 57, 100, 117	1 (0%)
All	All	829/829 (100%)	0.50	75 (9%) 15 16	24, 59, 120, 149	3 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228	THR	7.5
1	A	194	VAL	6.5
1	A	230	LEU	5.7
1	A	245	ALA	5.6
4	D	200	PRO	5.2
1	A	229	GLU	4.4
1	A	258	THR	4.0
1	A	248	VAL	3.8
1	A	244	TRP	3.8
1	A	247	VAL	3.7
5	E	154[A]	HIS	3.6
1	A	201	LEU	3.6
4	D	121	LEU	3.5
1	A	227	ASP	3.4
4	D	163	SER	3.4
1	A	217	TRP	3.3
1	A	273	ARG	3.3
5	E	7	TRP	3.2
1	A	231	VAL	3.2
1	A	260	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	193	ALA	3.1
1	A	246	ALA	3.1
4	D	192	PRO	3.0
4	D	190	ILE	3.0
1	A	82[A]	ARG	3.0
4	D	59	GLY	3.0
1	A	190	THR	3.0
4	D	78	ASP	2.9
4	D	77	ARG	2.9
1	A	274	TRP	2.9
4	D	183	ALA	2.8
5	E	43	GLY	2.8
4	D	126	SER	2.7
1	A	250	PRO	2.7
5	E	5	HIS	2.6
1	A	220	ASP	2.6
5	E	182	ALA	2.6
4	D	139	SER	2.6
1	A	252	GLY	2.6
5	E	241	GLY	2.6
1	A	191	HIS	2.6
5	E	243	ALA	2.6
5	E	60	VAL	2.5
1	A	197	HIS	2.5
1	A	272	LEU	2.5
1	A	249	VAL	2.4
1	A	257	TYR	2.4
5	E	61	PRO	2.4
4	D	57	GLU	2.4
1	A	138	MET	2.4
4	D	129	LYS	2.4
5	E	183	LEU	2.4
4	D	177	LYS	2.4
1	A	192	HIS	2.3
4	D	120	GLN	2.3
4	D	182	CYS	2.3
1	A	270	LEU	2.3
1	A	145	HIS	2.3
4	D	62	THR	2.3
4	D	159	LEU	2.3
1	A	235	PRO	2.2
1	A	271	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	75	LYS	2.2
4	D	158	VAL	2.2
4	D	122	ARG	2.2
4	D	166	PHE	2.2
1	A	90	ALA	2.2
5	E	240	TRP	2.1
4	D	176	ASN	2.1
1	A	216	THR	2.1
4	D	61	PHE	2.1
4	D	118	VAL	2.1
4	D	180	PHE	2.1
2	B	99	MET	2.0
4	D	199	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	D	301	6/6	0.74	0.23	77,79,83,88	0
6	GOL	A	301	6/6	0.88	0.12	83,86,90,96	0
6	GOL	A	302	6/6	0.90	0.12	75,76,79,80	0
6	GOL	E	301	6/6	0.91	0.13	61,75,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.