



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:38 PM UTC

PDB ID : 7PDW / pdb_00007pdw
Title : Crystal structure of parent TCR (728) complexed to HLA-A*02:01 presenting MAGE-A10 9-mer peptide
Authors : Simister, P.C.; Border, E.C.; Vieira, J.F.; Pumphrey, N.J.
Deposited on : 2021-08-09
Resolution : 1.82 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

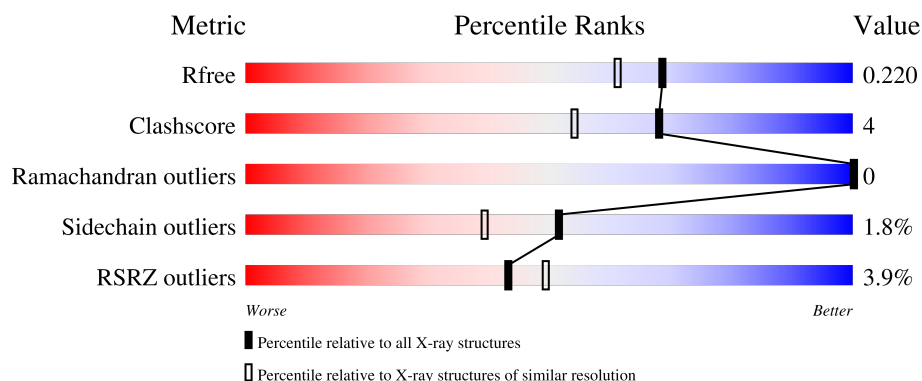
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	AAA	206	6% 92% 5%
1	FFF	206	10% 90% 7%
2	BBB	241	2% 93% 5%
2	GGG	241	3% 90% 9%
3	DDD	100	2% 94% 6%

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Mol	Chain	Length	Quality of chain
3	III	100	5% 94% 6%
4	EEE	9	78% 22%
4	JJJ	9	89% 11%
5	CCC	277	3% 89% 11%
5	HHH	277	% 88% 10% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26055 atoms, of which 12313 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 T-cell receptor alpha chain (TRAV/TRAC).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	200	Total	C	H	N	O	S	56	1	0
			2980	953	1439	261	319	8			
1	FFF	200	Total	C	H	N	O	S	53	1	0
			2998	956	1452	263	319	8			

- Molecule 2 is a protein called T-cell receptor beta chain (TRBV/TRBC).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	BBB	238	Total	C	H	N	O	S	66	0	0
			3626	1180	1768	316	353	9			
2	GGG	238	Total	C	H	N	O	S	65	0	0
			3643	1184	1776	319	355	9			

- Molecule 3 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	DDD	100	Total	C	H	N	O	S	36	0	0
			1575	518	763	135	155	4			
3	III	100	Total	C	H	N	O	S	37	1	0
			1569	516	759	135	155	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DDD	1	MET	-	initiating methionine	UNP P61769
III	1	MET	-	initiating methionine	UNP P61769

- Molecule 4 is a protein called Melanoma-associated antigen 10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	EEE	9	Total	C	H	N	O	S	3	0	0
			138	45	66	11	15	1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	JJJ	9	Total	C	H	N	O	S	3	0	0
			138	45	66	11	15	1			

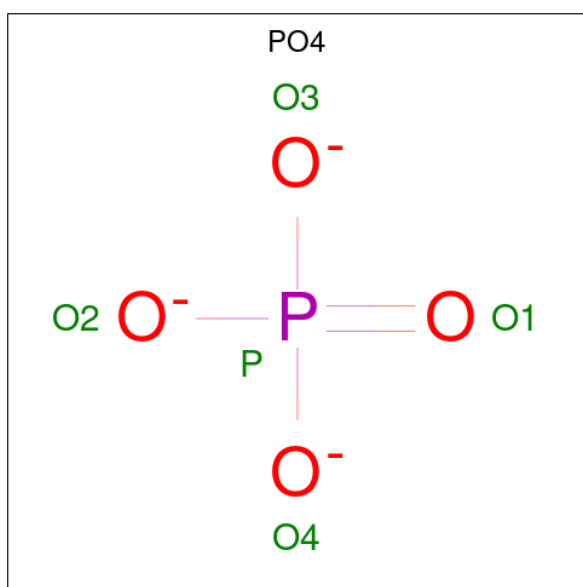
- Molecule 5 is a protein called MHC class I antigen.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	CCC	276	Total 4335	C 1403	H 2095	N 403	O 425	S 9	88	5	1
5	HHH	276	Total 4376	C 1415	H 2113	N 405	O 434	S 9	86	7	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	1	MET	-	initiating methionine	UNP Q861F7
HHH	1	MET	-	initiating methionine	UNP Q861F7

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	III	1	Total	O P	0	0
			5	4 1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	CCC	1	Total	C	H	O	2	0
			14	3	8	3		
7	CCC	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	70	Total	O	0	0
			70	70		
8	BBB	70	Total	O	0	0
			70	70		
8	DDD	40	Total	O	0	0
			40	40		
8	EEE	9	Total	O	0	0
			9	9		
8	FFF	52	Total	O	0	0
			52	52		
8	GGG	90	Total	O	0	0
			90	90		
8	III	31	Total	O	0	0
			31	31		
8	JJJ	6	Total	O	0	0
			6	6		
8	CCC	129	Total	O	0	0
			129	129		
8	HHH	147	Total	O	0	0
			147	147		

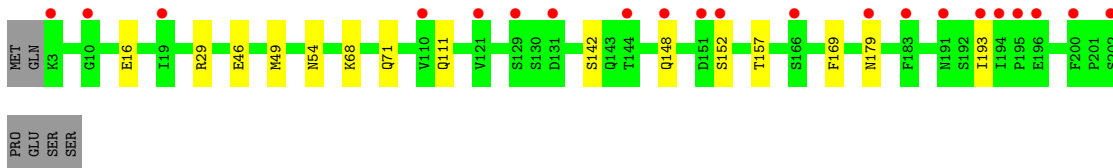
3 Residue-property plots [i](#)

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: T-cell receptor alpha chain (TRAV/TRAC)



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- Molecule 2: T-cell receptor beta chain (TRBV/TRBC)



- Molecule 2: T-cell receptor beta chain (TRBV/TRBC)



- Molecule 3: Beta-2-microglobulin

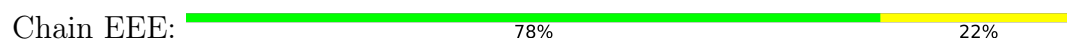




- Molecule 3: Beta-2-microglobulin



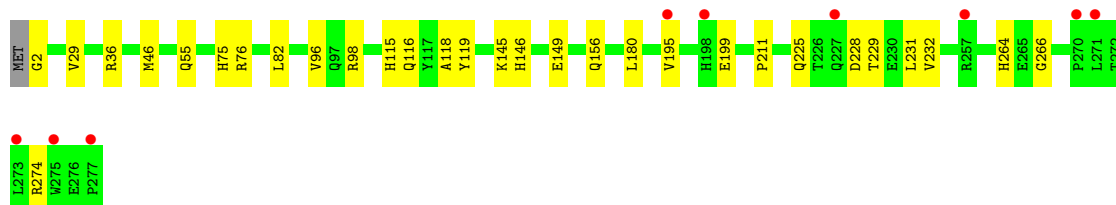
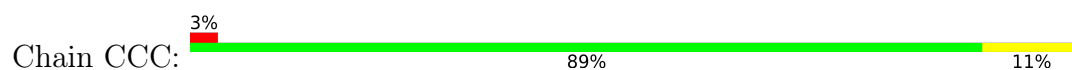
- Molecule 4: Melanoma-associated antigen 10



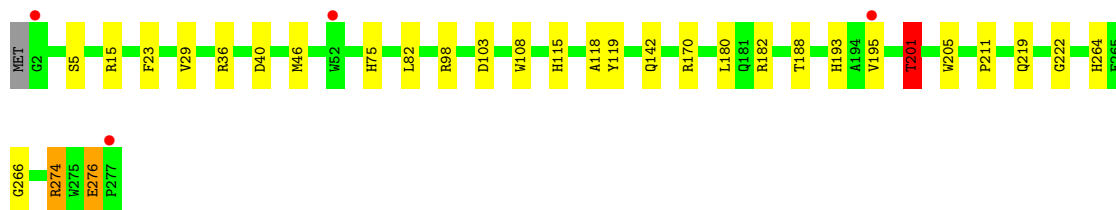
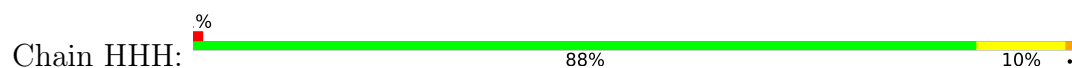
- Molecule 4: Melanoma-associated antigen 10



- Molecule 5: MHC class I antigen



- Molecule 5: MHC class I antigen



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.08Å 95.83Å 106.26Å 109.17° 96.51° 99.70°	Depositor
Resolution (Å)	81.94 – 1.82 81.94 – 1.82	Depositor EDS
% Data completeness (in resolution range)	90.2 (81.94-1.82) 66.6 (81.94-1.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.201 , 0.229 0.194 , 0.220	Depositor DCC
R_{free} test set	8036 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26055	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.32% 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: PO4, 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	AAA	1.01	0/1572	1.29	0/2133
1	FFF	0.98	0/1580	1.29	0/2143
2	BBB	1.00	0/1910	1.19	0/2606
2	GGG	0.99	0/1919	1.21	1/2617 (0.0%)
3	DDD	0.98	0/835	1.20	0/1135
3	III	0.97	0/837	1.20	0/1139
4	EEE	1.18	0/73	1.43	0/95
4	JJJ	1.12	0/73	1.41	0/95
5	CCC	1.03	0/2327	1.26	1/3163 (0.0%)
5	HHH	1.01	0/2356	1.27	1/3200 (0.0%)
All	All	1.00	0/13482	1.25	3/18326 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	HHH	201	THR	CB-CA-C	6.53	121.03	109.72
5	CCC	55	GLN	CB-CA-C	-5.70	100.09	110.63
2	GGG	98	ASP	CA-CB-CG	5.60	118.20	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	AAA	1541	1439	1423	11	0
1	FFF	1546	1452	1444	8	0
2	BBB	1858	1768	1744	12	0
2	GGG	1867	1776	1754	17	0
3	DDD	812	763	743	4	0
3	III	810	759	735	3	0
4	EEE	72	66	65	1	0
4	JJJ	72	66	65	1	0
5	CCC	2240	2095	2065	18	0
5	HHH	2263	2113	2089	26	0
6	III	5	0	0	0	0
7	CCC	12	16	16	1	0
8	AAA	70	0	0	3	0
8	BBB	70	0	0	3	0
8	CCC	129	0	0	7	0
8	DDD	40	0	0	1	0
8	EEE	9	0	0	0	0
8	FFF	52	0	0	0	0
8	GGG	90	0	0	1	0
8	HHH	147	0	0	6	0
8	III	31	0	0	1	0
8	JJJ	6	0	0	0	0
All	All	13742	12313	12143	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:AAA:32[A]:GLN:NE2	8:AAA:301:HOH:O	1.99	0.96
1:AAA:32[B]:GLN:HG2	8:AAA:334:HOH:O	1.67	0.94
5:CCC:2:GLY:C	8:CCC:409:HOH:O	2.12	0.91
5:HHH:274:ARG:HB3	8:HHH:303:HOH:O	1.72	0.89
5:HHH:98:ARG:HE	5:HHH:115:HIS:HE1	1.23	0.87
3:III:4:ARG:HD2	8:III:324:HOH:O	1.76	0.86
5:CCC:98:ARG:HE	5:CCC:115:HIS:HE1	1.25	0.83
2:BBB:20:MET:CE	2:BBB:108:LEU:HD22	2.13	0.78
2:GGG:20:MET:CE	2:GGG:108:LEU:HD22	2.17	0.74
2:BBB:20:MET:HE1	2:BBB:108:LEU:HD13	1.73	0.70
2:GGG:20:MET:HE1	2:GGG:108:LEU:HD13	1.76	0.68
5:HHH:5[B]:SER:OG	5:HHH:103:ASP:OD1	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CCC:75:HIS:CD2	8:CCC:462:HOH:O	2.52	0.62
5:CCC:225:GLN:O	5:CCC:229:THR:HG23	2.01	0.60
2:GGG:20:MET:CE	2:GGG:108:LEU:HD13	2.33	0.59
5:CCC:264:HIS:CD2	5:CCC:266:GLY:H	2.22	0.58
1:AAA:29:ARG:HH21	1:AAA:71:GLN:HE21	1.52	0.58
2:BBB:20:MET:CE	2:BBB:108:LEU:HD13	2.34	0.58
1:FFF:29:ARG:HH21	1:FFF:71:GLN:HE21	1.51	0.58
5:HHH:264:HIS:CD2	5:HHH:266:GLY:H	2.22	0.58
1:FFF:193:ILE:O	1:FFF:193:ILE:HG23	2.05	0.57
5:HHH:195:VAL:CG2	5:HHH:201:THR:HG22	2.35	0.57
2:BBB:29:ASN:HB2	8:BBB:318:HOH:O	2.04	0.56
5:HHH:276:GLU:OE2	5:HHH:276:GLU:HA	2.04	0.56
1:AAA:193:ILE:O	1:AAA:193:ILE:HG23	2.06	0.56
2:GGG:20:MET:HE3	2:GGG:108:LEU:HD22	1.87	0.56
5:HHH:15:ARG:NH2	5:HHH:40:ASP:OD2	2.40	0.55
2:GGG:111:LEU:CD2	2:GGG:148:TYR:HE2	2.20	0.55
1:AAA:32[B]:GLN:HE21	5:CCC:156:GLN:HE21	1.54	0.54
2:BBB:20:MET:HE3	2:BBB:108:LEU:HD22	1.87	0.54
1:AAA:157:THR:HG21	2:BBB:188:SER:OG	2.07	0.54
3:DDD:32:HIS:ND1	8:DDD:201:HOH:O	2.30	0.54
5:CCC:76:ARG:CD	8:CCC:415:HOH:O	2.55	0.54
5:CCC:146[B]:HIS:HD2	8:CCC:523:HOH:O	1.90	0.53
2:GGG:16:THR:HG22	2:GGG:84:PRO:HD3	1.90	0.53
1:FFF:111:GLN:HB3	1:FFF:142:SER:HB3	1.92	0.52
5:CCC:82:LEU:HD13	5:CCC:119:TYR:CD1	2.45	0.51
7:CCC:301:GOL:O3	8:CCC:401:HOH:O	2.19	0.51
2:GGG:12:ARG:NE	8:GGG:301:HOH:O	2.43	0.50
5:HHH:108:TRP:O	5:HHH:170:ARG:NH1	2.38	0.50
5:HHH:82:LEU:HD13	5:HHH:119:TYR:CD1	2.46	0.49
5:CCC:211:PRO:O	5:CCC:264:HIS:HE1	1.95	0.49
2:GGG:111:LEU:HD21	2:GGG:148:TYR:CE2	2.48	0.49
5:HHH:211:PRO:O	5:HHH:264:HIS:HE1	1.96	0.49
2:BBB:29:ASN:CB	8:BBB:318:HOH:O	2.59	0.49
2:GGG:111:LEU:CD2	2:GGG:148:TYR:CE2	2.96	0.49
1:FFF:169:PHE:CD1	2:GGG:137:LYS:HE2	2.49	0.48
2:BBB:67:VAL:HA	2:BBB:76:LEU:O	2.14	0.48
2:BBB:151:HIS:HB3	2:BBB:212:TYR:HB2	1.96	0.47
2:GGG:67:VAL:HA	2:GGG:76:LEU:O	2.14	0.47
5:HHH:219:GLN:HE21	5:HHH:222:GLY:HA2	1.79	0.47
8:AAA:334:HOH:O	5:CCC:156:GLN:HG3	2.15	0.46
5:CCC:145:LYS:HE3	5:CCC:149:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:49:MET:HE3	1:FFF:49:MET:HB3	1.90	0.45
5:CCC:75:HIS:CG	8:CCC:462:HOH:O	2.70	0.45
5:CCC:96:VAL:HB	8:CCC:468:HOH:O	2.16	0.45
1:AAA:49:MET:HE3	1:AAA:49:MET:HB3	1.92	0.45
2:BBB:29:ASN:CG	8:BBB:318:HOH:O	2.59	0.44
1:AAA:111:GLN:HB3	1:AAA:142:SER:HB3	1.99	0.44
5:HHH:23:PHE:HE1	5:HHH:75:HIS:HD1	1.65	0.44
5:HHH:142:GLN:HG2	8:HHH:434:HOH:O	2.16	0.44
3:DDD:61:TRP:CE2	5:CCC:118:ALA:HB2	2.53	0.44
1:AAA:169:PHE:CD2	2:BBB:137:LYS:HE2	2.53	0.44
1:FFF:193:ILE:O	1:FFF:193:ILE:CG2	2.66	0.44
1:AAA:193:ILE:O	1:AAA:193:ILE:CG2	2.65	0.44
1:FFF:157:THR:HG21	2:GGG:188:SER:OG	2.18	0.43
2:GGG:177:GLN:O	2:GGG:183:SER:HB2	2.18	0.43
5:HHH:264:HIS:HD2	5:HHH:266:GLY:H	1.66	0.43
1:AAA:104:SER:HA	2:BBB:43:GLY:HA3	2.01	0.42
5:HHH:195:VAL:HG22	5:HHH:201:THR:HG22	2.01	0.42
5:HHH:188:THR:HA	5:HHH:205:TRP:O	2.19	0.42
3:DDD:25:ASN:HB3	3:DDD:66:LEU:HD11	2.02	0.42
4:JJJ:2:LEU:HD11	5:HHH:46:MET:CE	2.50	0.42
2:GGG:16:THR:HG21	2:GGG:112:GLU:CD	2.44	0.42
3:III:61:TRP:CE2	5:HHH:118:ALA:HB2	2.55	0.42
5:HHH:274:ARG:CB	8:HHH:303:HOH:O	2.49	0.42
5:HHH:274:ARG:NH1	8:HHH:303:HOH:O	2.37	0.42
2:GGG:13:VAL:HG22	2:GGG:149:PRO:HG3	2.02	0.41
5:CCC:195:VAL:CG2	5:CCC:199:GLU:HG3	2.50	0.41
5:HHH:142:GLN:CG	8:HHH:434:HOH:O	2.68	0.41
5:HHH:274:ARG:HB3	5:HHH:274:ARG:HH11	1.86	0.41
1:FFF:54:ASN:HD21	1:FFF:68:LYS:HB2	1.86	0.41
2:GGG:107:ARG:HG2	2:GGG:151:HIS:NE2	2.36	0.41
2:GGG:111:LEU:HD21	2:GGG:148:TYR:HE2	1.84	0.41
5:HHH:15:ARG:HH22	5:HHH:40:ASP:CG	2.29	0.41
3:DDD:52:HIS:HA	3:DDD:66:LEU:O	2.21	0.41
4:EEE:2:LEU:HD11	5:CCC:46:MET:CE	2.51	0.41
5:HHH:108:TRP:HB3	5:HHH:170:ARG:HD3	2.02	0.41
3:III:52:HIS:HA	3:III:66:LEU:O	2.22	0.40
5:CCC:29:VAL:HG11	5:CCC:180:LEU:HD13	2.02	0.40
5:HHH:29:VAL:HG11	5:HHH:180:LEU:HD13	2.02	0.40
5:HHH:193:HIS:HD2	8:HHH:420:HOH:O	2.05	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	AAA	199/206 (97%)	190 (96%)	9 (4%)	0	100	100
1	FFF	199/206 (97%)	189 (95%)	10 (5%)	0	100	100
2	BBB	236/241 (98%)	229 (97%)	7 (3%)	0	100	100
2	GGG	236/241 (98%)	229 (97%)	7 (3%)	0	100	100
3	DDD	98/100 (98%)	98 (100%)	0	0	100	100
3	III	99/100 (99%)	99 (100%)	0	0	100	100
4	EEE	7/9 (78%)	7 (100%)	0	0	100	100
4	JJJ	7/9 (78%)	7 (100%)	0	0	100	100
5	CCC	279/277 (101%)	275 (99%)	4 (1%)	0	100	100
5	HHH	281/277 (101%)	275 (98%)	6 (2%)	0	100	100
All	All	1641/1666 (98%)	1598 (97%)	43 (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	AAA	171/183 (93%)	171 (100%)	0	100	100
1	FFF	174/183 (95%)	169 (97%)	5 (3%)	37	19
2	BBB	195/208 (94%)	192 (98%)	3 (2%)	57	46
2	GGG	197/208 (95%)	195 (99%)	2 (1%)	68	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	DDD	87/95 (92%)	86 (99%)	1 (1%)	65	56
3	III	87/95 (92%)	85 (98%)	2 (2%)	44	28
4	EEE	7/7 (100%)	6 (86%)	1 (14%)	3	0
4	JJJ	7/7 (100%)	7 (100%)	0	100	100
5	CCC	230/233 (99%)	224 (97%)	6 (3%)	40	23
5	HHH	235/233 (101%)	230 (98%)	5 (2%)	47	32
All	All	1390/1452 (96%)	1365 (98%)	25 (2%)	51	39

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	BBB	133	SER
2	BBB	172	GLN
2	BBB	190	ARG
3	DDD	71	PHE
4	EEE	4	ASP
1	FFF	16	GLU
1	FFF	46	GLU
1	FFF	148	GLN
1	FFF	152	SER
1	FFF	179	ASN
2	GGG	133	SER
2	GGG	190	ARG
3	III	46	ARG
3	III	71	PHE
5	CCC	36	ARG
5	CCC	116	GLN
5	CCC	228	ASP
5	CCC	231	LEU
5	CCC	232	VAL
5	CCC	274	ARG
5	HHH	36	ARG
5	HHH	182	ARG
5	HHH	201	THR
5	HHH	274	ARG
5	HHH	276	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
7	GOL	CCC	302	-	5,5,5	0.10	0	5,5,5	0.22	0
7	GOL	CCC	301	-	5,5,5	0.15	0	5,5,5	0.41	0
6	PO4	III	201	-	4,4,4	0.89	0	6,6,6	0.45	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	GOL	CCC	302	-	-	2/4/4/4	-
7	GOL	CCC	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	CCC	302	GOL	C1-C2-C3-O3
7	CCC	302	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
7	CCC	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	AAA	200/206 (97%)	0.44	12 (6%) 27 31	10, 39, 87, 105	1 (0%)
1	FFF	200/206 (97%)	0.69	21 (10%) 11 12	21, 46, 89, 107	1 (0%)
2	BBB	238/241 (98%)	0.40	5 (2%) 63 70	17, 42, 72, 101	0
2	GGG	238/241 (98%)	0.24	7 (2%) 53 60	21, 35, 57, 92	0
3	DDD	100/100 (100%)	0.23	2 (2%) 65 71	21, 39, 64, 71	0
3	III	100/100 (100%)	0.70	5 (5%) 34 40	24, 42, 77, 83	1 (1%)
4	EEE	9/9 (100%)	-0.66	0 100 100	19, 20, 21, 24	0
4	JJJ	9/9 (100%)	-0.45	0 100 100	21, 23, 25, 28	0
5	CCC	276/277 (99%)	0.06	9 (3%) 49 56	12, 30, 70, 91	5 (1%)
5	HHH	276/277 (99%)	-0.00	4 (1%) 73 79	14, 30, 50, 79	7 (2%)
All	All	1646/1666 (98%)	0.29	65 (3%) 43 49	10, 36, 73, 107	15 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	FFF	193	ILE	4.4
1	AAA	193	ILE	3.6
5	CCC	277	PRO	3.6
2	BBB	240	ALA	3.5
1	AAA	177	TRP	3.4
2	GGG	201	PRO	3.1
1	FFF	183	PHE	3.1
1	AAA	150	LYS	3.0
3	III	72	THR	2.9
3	DDD	2	ILE	2.9
1	FFF	151	ASP	2.8
1	FFF	152	SER	2.8
1	FFF	200	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	GGG	221	THR	2.7
1	FFF	194	ILE	2.7
3	III	89	SER	2.6
1	AAA	183	PHE	2.6
5	CCC	275	TRP	2.6
2	GGG	143	LEU	2.6
5	CCC	195	VAL	2.6
5	CCC	270	PRO	2.5
1	FFF	148	GLN	2.5
2	BBB	223	ASP	2.5
1	AAA	189	PHE	2.5
1	FFF	202	SER	2.5
1	AAA	188	ALA	2.5
2	BBB	221	THR	2.5
1	AAA	121	VAL	2.5
1	AAA	135	CYS	2.4
3	III	16	ALA	2.4
1	AAA	130	SER	2.4
3	III	76	LYS	2.4
2	GGG	240	ALA	2.4
1	FFF	195	PRO	2.4
5	HHH	52	TRP	2.4
1	FFF	144	THR	2.3
5	CCC	227	GLN	2.3
5	HHH	2	GLY	2.3
2	GGG	196	THR	2.3
1	FFF	3	LYS	2.3
1	FFF	10	GLY	2.3
1	FFF	179	ASN	2.3
2	BBB	179	ALA	2.3
1	FFF	19	ILE	2.3
1	FFF	129	SER	2.3
1	AAA	196	GLU	2.2
1	FFF	121	VAL	2.2
1	FFF	110	VAL	2.2
5	HHH	277	PRO	2.2
1	AAA	132	LYS	2.2
5	CCC	257	ARG	2.2
1	FFF	131	ASP	2.2
1	AAA	128	LYS	2.2
3	DDD	1	MET	2.1
1	FFF	196	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
5	CCC	271	LEU	2.1
2	BBB	113	ASP	2.1
2	GGG	163	VAL	2.1
2	GGG	111	LEU	2.1
1	FFF	166	SER	2.0
5	CCC	198	HIS	2.0
1	FFF	191	ASN	2.0
3	III	73	PRO	2.0
5	HHH	195	VAL	2.0
5	CCC	273	LEU	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($\text{\AA}^2$)	Q<0.9
7	GOL	CCC	301	6/6	0.88	0.13	36,39,47,48	2
6	PO4	III	201	5/5	0.94	0.10	63,66,79,81	0
7	GOL	CCC	302	6/6	0.94	0.12	46,54,62,62	2

6.5 Other polymers [i](#)

There are no such residues in this entry.