Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2022 – 04:08 pm BST

PDB ID	:	7PDW
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:

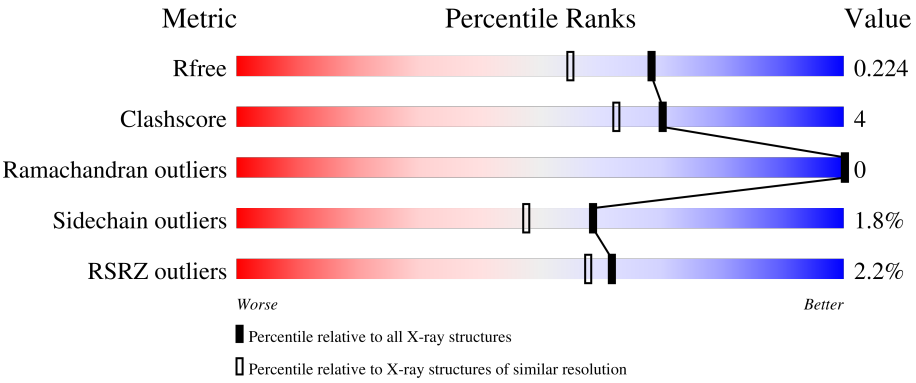
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

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}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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 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 <=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	7% 93%
1	FFF	206	5% 90% 7%
2	BBB	241	2% 93% 6%
2	GGG	241	91% 8%
3	DDD	100	94% 6%

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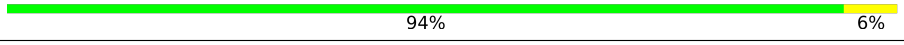
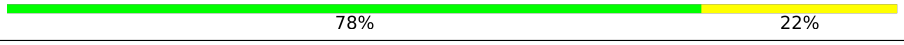
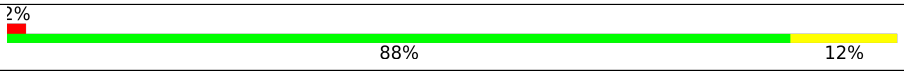
Mol	Chain	Length	Quality of chain
3	III	100	
4	EEE	9	
4	JJJ	9	
5	CCC	277	
5	HHH	277	

2 Entry composition (i)

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			

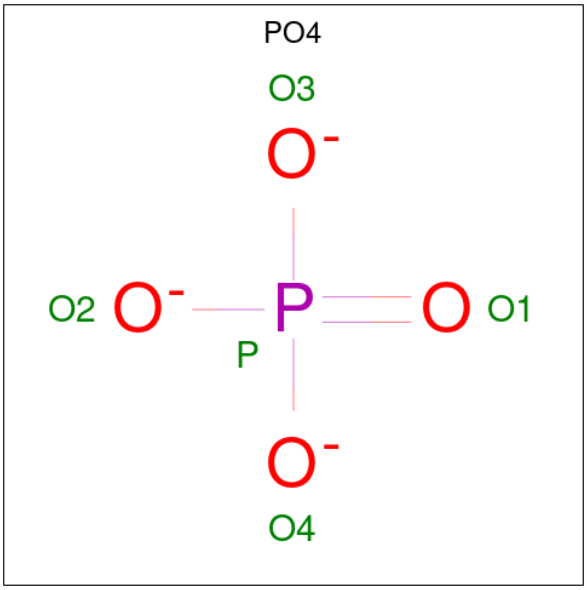
- Molecule 5 is a protein called MHC class I antigen.

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

There are 2 discrepancies between the modelled and reference sequences:

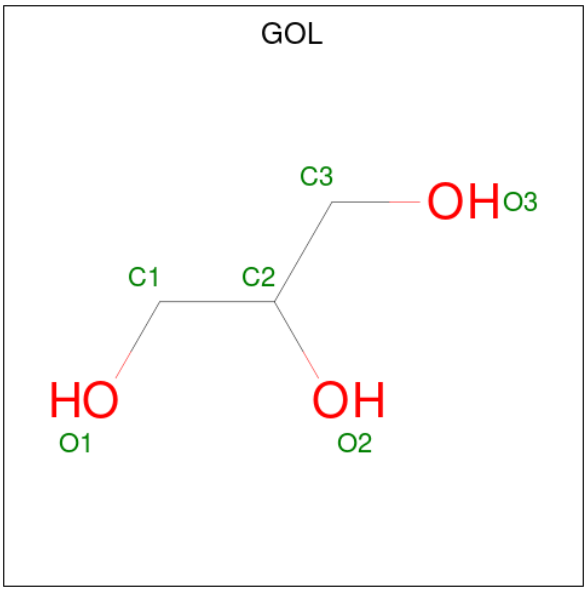
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	1	MET	-	initiating methionine	UNP Q861F7
HHH	1	MET	-	initiating methionine	UNP Q861F7

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

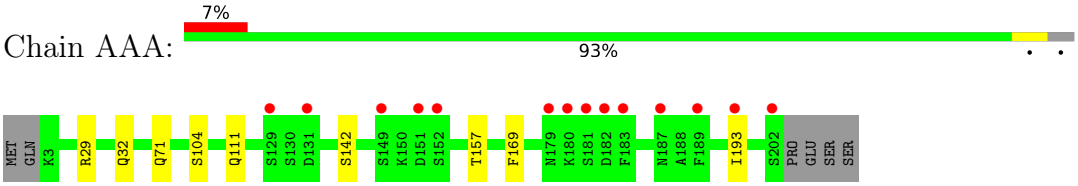
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	70	Total O 70 70	0	0
8	BBB	70	Total O 70 70	0	0
8	DDD	40	Total O 40 40	0	0
8	EEE	9	Total O 9 9	0	0
8	FFF	52	Total O 52 52	0	0
8	GGG	90	Total O 90 90	0	0
8	III	31	Total O 31 31	0	0
8	JJJ	6	Total O 6 6	0	0
8	CCC	129	Total O 129 129	0	0
8	HHH	147	Total O 147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

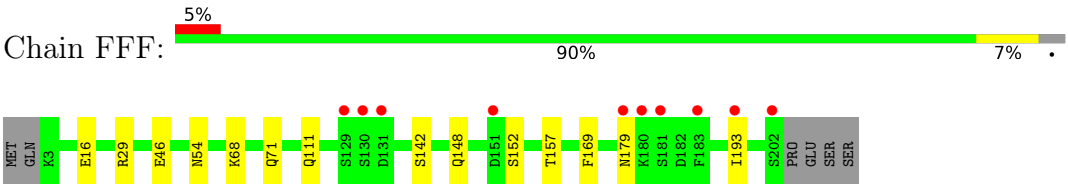
• Molecule 1: T-cell receptor alpha chain (TRAV/TRAC)

Chain AAA:



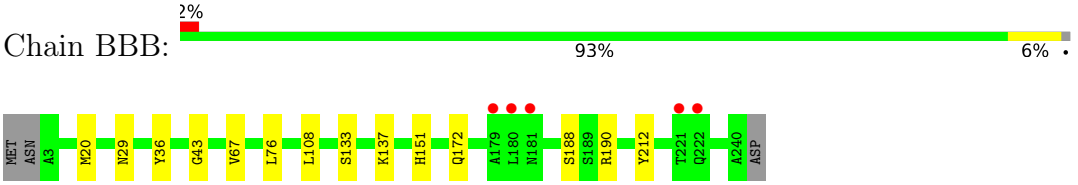
• Molecule 1: T-cell receptor alpha chain (TRAV/TRAC)

Chain FFF:



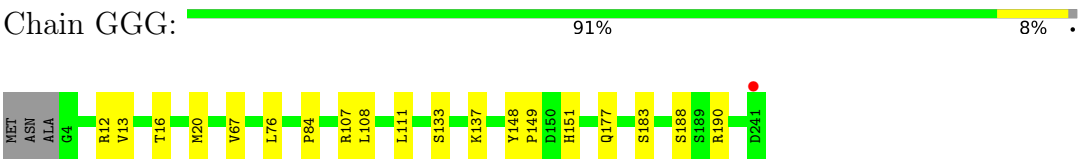
• Molecule 2: T-cell receptor beta chain (TRBV/TRBC)

Chain BBB:



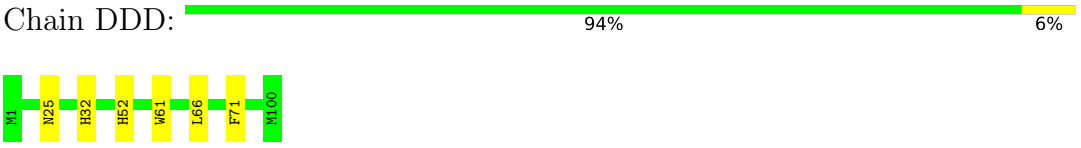
• Molecule 2: T-cell receptor beta chain (TRBV/TRBC)

Chain GGG:



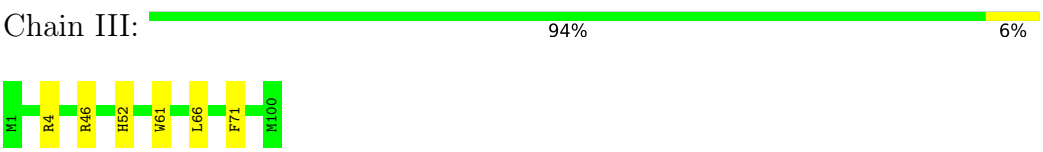
• Molecule 3: Beta-2-microglobulin

Chain DDD:



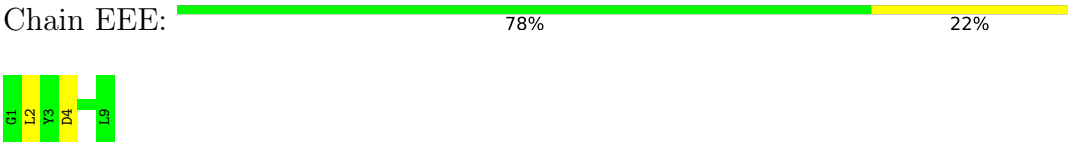
• Molecule 3: Beta-2-microglobulin

Chain III:



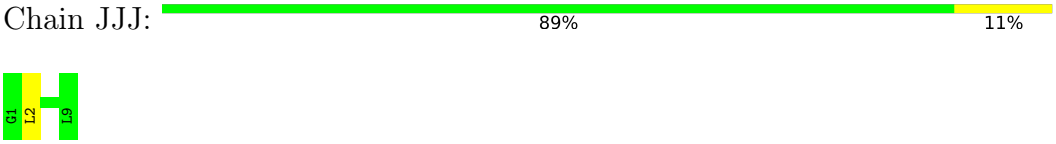
• Molecule 4: Melanoma-associated antigen 10

Chain EEE:



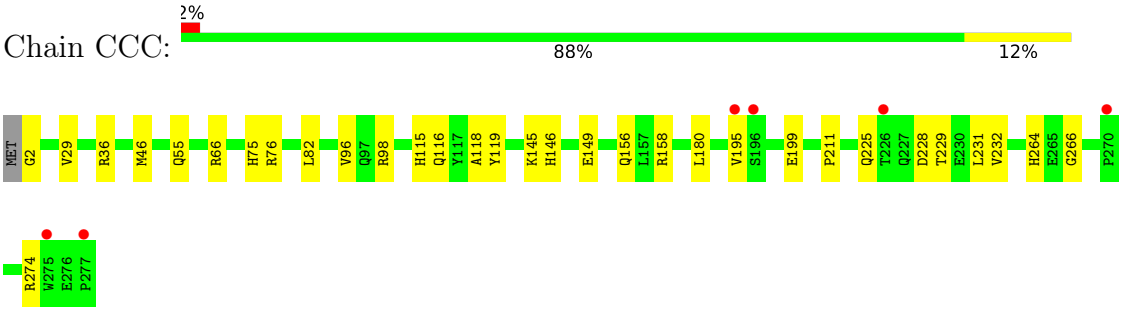
• Molecule 4: Melanoma-associated antigen 10

Chain JJJ:



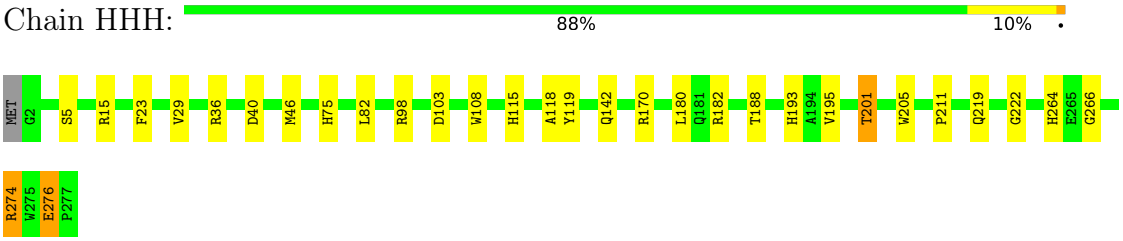
• Molecule 5: MHC class I antigen

Chain CCC:



• Molecule 5: MHC class I antigen

Chain HHH:



4 Data and refinement statistics (i)

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 81.80 – 1.82	Depositor EDS
% Data completeness (in resolution range)	90.2 (81.94-1.82) 66.6 (81.80-1.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 0.201 , 0.224	Depositor DCC
R_{free} test set	5996 reflections (5.14%)	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, PO4

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	0.68	0/1572	0.84	0/2133
1	FFF	0.66	0/1580	0.83	0/2143
2	BBB	0.67	0/1910	0.79	0/2606
2	GGG	0.65	0/1919	0.80	0/2617
3	DDD	0.65	0/835	0.80	0/1135
3	III	0.64	0/837	0.80	0/1139
4	EEE	0.89	0/73	1.06	0/95
4	JJJ	0.80	0/73	1.02	0/95
5	CCC	0.69	0/2327	0.84	3/3163 (0.1%)
5	HHH	0.67	0/2356	0.85	0/3200
All	All	0.67	0/13482	0.82	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(^{o})	Ideal(^{o})
5	CCC	66	ARG	NE-CZ-NH2	-5.89	117.36	120.30
5	CCC	158	ARG	NE-CZ-NH2	-5.19	117.70	120.30
5	CCC	55	GLN	CB-CA-C	-5.16	100.09	110.40

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	10	0
1	FFF	1546	1452	1444	7	0
2	BBB	1858	1768	1744	14	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	25	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	91	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 (91) 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:HHH:274:ARG:HB3	8:HHH:303:HOH:O	1.72	0.89
5:CCC:2:GLY:C	8:CCC:409:HOH:O	2.12	0.87
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
5:HHH:5[B]:SER:OG	5:HHH:103:ASP:OD1	2.14	0.66
3:DDD:32:HIS:ND1	8:DDD:201:HOH:O	2.30	0.64
5:CCC:75:HIS:CD2	8:CCC:462:HOH:O	2.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:36:TYR:OH	8:BBB:301:HOH:O	2.13	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
2:GGG:20:MET:HE3	2:GGG:108:LEU:HD22	1.88	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:BBB:20:MET:HE2	2:BBB:108:LEU:HD13	1.88	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
1:AAA:157:THR:HG21	2:BBB:188:SER:OG	2.07	0.54
2:GGG:20:MET:HE1	2:GGG:108:LEU:HD13	1.90	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
2:BBB:20:MET:HE3	2:BBB:108:LEU:HD22	1.90	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
2:GGG:20:MET:HE2	2:GGG:108:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:BBB:20:MET:HE2	2:BBB:108:LEU:CD1	2.49	0.43
5:HHH:264:HIS:HD2	5:HHH:266:GLY:H	1.66	0.43
2:BBB:20:MET:HE1	2:BBB:108:LEU:HD22	2.00	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
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
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 (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	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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	171/183 (93%)	171 (100%)	0	100	100
1	FFF	174/183 (95%)	169 (97%)	5 (3%)	42	28
2	BBB	195/208 (94%)	192 (98%)	3 (2%)	65	55
2	GGG	197/208 (95%)	195 (99%)	2 (1%)	76	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	DDD	87/95 (92%)	86 (99%)	1 (1%)	73 67
3	III	87/95 (92%)	85 (98%)	2 (2%)	50 37
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%)	46 32
5	HHH	235/233 (101%)	230 (98%)	5 (2%)	53 41
All	All	1390/1452 (96%)	1365 (98%)	25 (2%)	59 48

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 monosaccharides 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	301	-	5,5,5	0.15	0	5,5,5	0.40	0
7	GOL	CCC	302	-	5,5,5	0.09	0	5,5,5	0.23	0
6	PO4	III	201	-	4,4,4	0.83	0	6,6,6	0.42	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	301	-	-	0/4/4/4	-
7	GOL	CCC	302	-	-	2/4/4/4	-

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, 95^{th} 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%)	0.11	14 (7%) 16 13	18, 40, 94, 112	0
1	FFF	200/206 (97%)	0.16	10 (5%) 28 23	21, 46, 92, 108	0
2	BBB	238/241 (98%)	-0.06	5 (2%) 63 59	18, 42, 73, 101	0
2	GGG	238/241 (98%)	-0.26	1 (0%) 92 91	21, 36, 60, 93	0
3	DDD	100/100 (100%)	-0.41	0 100 100	22, 39, 65, 73	0
3	III	100/100 (100%)	0.01	0 100 100	26, 43, 78, 85	0
4	EEE	9/9 (100%)	-0.13	0 100 100	19, 20, 22, 24	0
4	JJJ	9/9 (100%)	-0.43	0 100 100	21, 23, 26, 28	0
5	CCC	276/277 (99%)	-0.09	6 (2%) 62 58	18, 30, 71, 90	0
5	HHH	276/277 (99%)	-0.43	0 100 100	20, 31, 50, 80	0
All	All	1646/1666 (98%)	-0.13	36 (2%) 62 58	18, 36, 76, 112	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	FFF	129	SER	7.6
1	FFF	181	SER	5.9
5	CCC	277	PRO	5.1
2	BBB	181	ASN	5.0
1	AAA	129	SER	5.0
1	FFF	202	SER	4.3
5	CCC	195	VAL	4.2
1	AAA	131	ASP	4.0
1	FFF	131	ASP	4.0
1	FFF	183	PHE	3.8
1	FFF	179	ASN	3.7
1	FFF	151	ASP	3.5
2	BBB	221	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	FFF	193	ILE	3.4
2	BBB	179	ALA	3.4
5	CCC	226	THR	3.3
1	AAA	182	ASP	3.3
2	BBB	180	LEU	3.3
1	AAA	179	ASN	3.2
5	CCC	275	TRP	3.2
1	AAA	152	SER	3.1
1	AAA	180	LYS	2.9
1	AAA	202	SER	2.9
1	AAA	183	PHE	2.8
5	CCC	270	PRO	2.6
1	AAA	193	ILE	2.6
1	AAA	181	SER	2.5
1	AAA	187	ASN	2.5
1	AAA	151	ASP	2.4
1	FFF	180	LYS	2.4
2	BBB	222	GLN	2.2
5	CCC	196	SER	2.2
1	FFF	130	SER	2.1
1	AAA	189	PHE	2.1
2	GGG	241	ASP	2.0
1	AAA	149	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GOL	CCC	301	6/6	0.85	0.15	36,39,47,48	2
7	GOL	CCC	302	6/6	0.92	0.13	46,54,62,62	2
6	PO4	III	201	5/5	0.94	0.12	63,66,79,81	0

6.5 Other polymers (i)

There are no such residues in this entry.