Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2022 – 04:08 pm BST

PDB ID	:	7PBC
Title	:	Crystal structure of engineered TCR (796) 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	:	2021-08-02
Resolution	:	2.04 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:

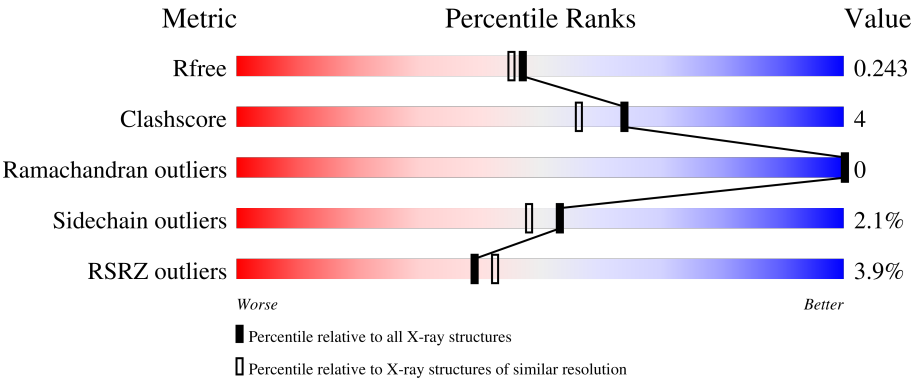
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	CCC	277	5% 90% 9%
2	DDD	100	6% 87% 12%
3	AAA	206	2% 87% 9%
4	BBB	241	2% 86% 13%
5	EEE	9	100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12927 atoms, of which 6101 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
			Total	C	H	N	O	S			
1	CCC	276	4258	1383	2056	394	416	9	92	2	1

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	DDD	99	1538	507	748	134	146	3	40	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called T-cell receptor (TRAV/TRAC).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	AAA	201	2970	953	1437	257	315	8	58	1	0

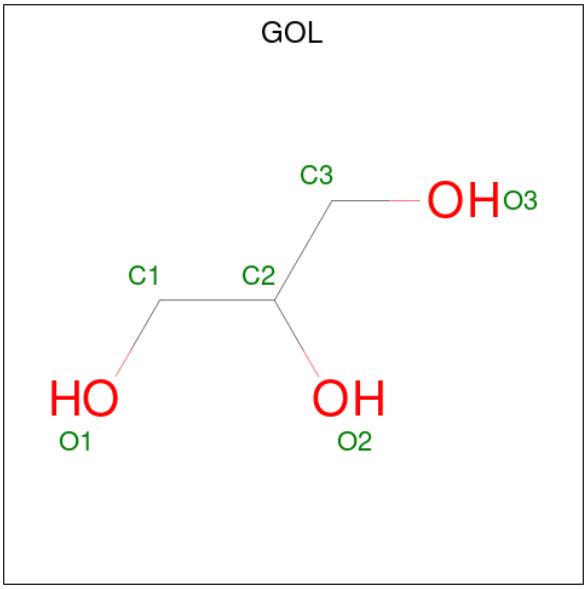
- Molecule 4 is a protein called T-cell receptor (TRBV/TRBC).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	BBB	240	3634	1182	1770	318	355	9	68	0	0

- Molecule 5 is a protein called Melanoma-associated antigen 10.

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	CCC	118	Total	O	0	0
			118	118		
8	DDD	26	Total	O	0	0
			26	26		

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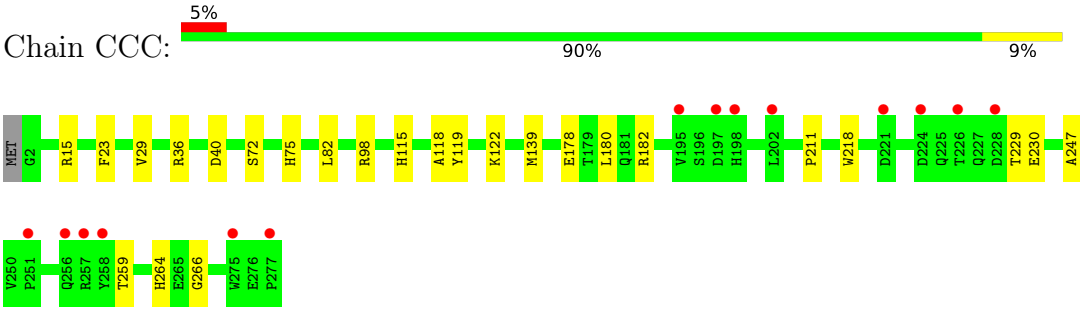
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	95	Total O 95 95	0	0
8	BBB	100	Total O 100 100	0	0
8	EEE	7	Total O 7 7	0	0

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.

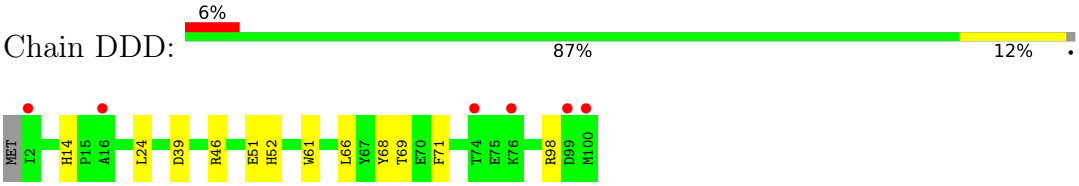
• Molecule 1: MHC class I antigen

Chain CCC:



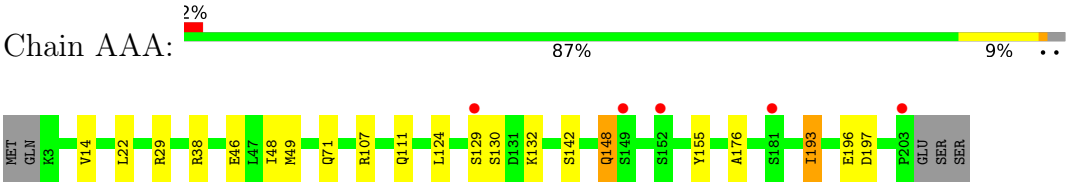
• Molecule 2: Beta-2-microglobulin

Chain DDD:



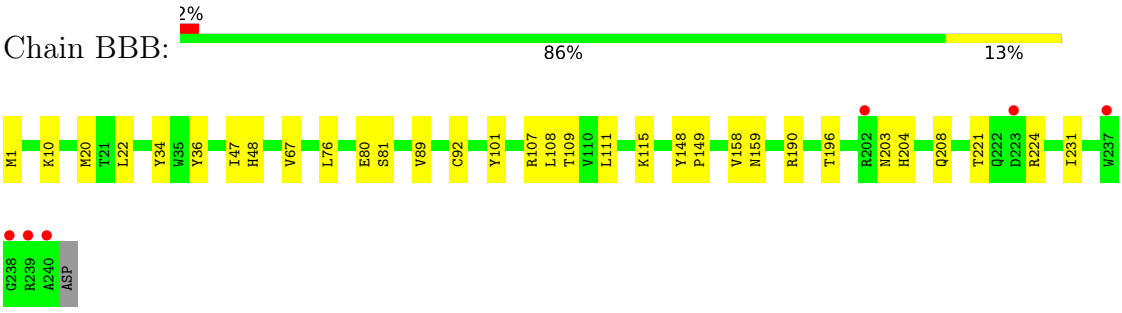
• Molecule 3: T-cell receptor (TRAV/TRAC)

Chain AAA:

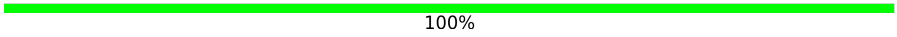


• Molecule 4: T-cell receptor (TRBV/TRBC)

Chain BBB:



• Molecule 5: Melanoma-associated antigen 10

Chain EEE: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.33Å 77.50Å 115.12Å 90.00° 102.88° 90.00°	Depositor
Resolution (Å)	63.85 – 2.04 63.77 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.3 (63.85-2.04) 92.4 (63.77-2.04)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.186 , 0.236 0.193 , 0.243	Depositor DCC
R_{free} test set	2618 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	27.9	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12927	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: CL, 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	CCC	0.69	0/2276	0.85	0/3097
2	DDD	0.64	0/813	0.77	0/1107
3	AAA	0.69	0/1568	0.85	0/2130
4	BBB	0.66	0/1916	0.83	0/2616
5	EEE	0.85	0/73	0.94	0/95
All	All	0.68	0/6646	0.83	0/9045

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

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	CCC	2202	2056	2013	13	1
2	DDD	790	748	719	6	0
3	AAA	1533	1437	1417	14	0
4	BBB	1864	1770	1743	20	1
5	EEE	72	66	65	0	0
6	CCC	18	24	24	0	0
7	BBB	1	0	0	0	0
8	AAA	95	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	BBB	100	0	0	3	0
8	CCC	118	0	0	1	0
8	DDD	26	0	0	1	0
8	EEE	7	0	0	0	0
All	All	6826	6101	5981	52	1

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 (52) 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)
3:AAA:38:ARG:HB2	3:AAA:48:ILE:HD11	1.71	0.73
4:BBB:36:TYR:OH	8:BBB:401:HOH:O	2.05	0.69
3:AAA:29:ARG:HH21	3:AAA:71:GLN:HE21	1.45	0.65
1:CCC:98:ARG:HE	1:CCC:115:HIS:HE1	1.47	0.62
3:AAA:48:ILE:HG22	3:AAA:49:MET:HG2	1.81	0.61
1:CCC:82:LEU:HD13	1:CCC:119:TYR:CD1	2.36	0.60
4:BBB:20:MET:CE	4:BBB:108:LEU:HD22	2.31	0.60
4:BBB:221:THR:HG22	8:BBB:405:HOH:O	2.02	0.60
3:AAA:107:ARG:CD	8:AAA:329:HOH:O	2.52	0.57
1:CCC:264:HIS:CD2	1:CCC:266:GLY:H	2.23	0.57
2:DDD:51:GLU:HB2	2:DDD:68:TYR:CZ	2.41	0.56
2:DDD:39:ASP:OD1	2:DDD:46:ARG:NH1	2.39	0.55
4:BBB:20:MET:HE2	4:BBB:108:LEU:HD22	1.90	0.54
3:AAA:193:ILE:HG23	8:AAA:356:HOH:O	2.08	0.52
4:BBB:67:VAL:HA	4:BBB:76:LEU:O	2.11	0.50
4:BBB:111:LEU:HD21	4:BBB:148:TYR:HE2	1.76	0.49
4:BBB:80:GLU:HA	4:BBB:80:GLU:OE1	2.12	0.49
3:AAA:155:TYR:O	3:AAA:176:ALA:HA	2.11	0.49
4:BBB:115:LYS:O	4:BBB:224:ARG:NH2	2.45	0.49
4:BBB:1:MET:CB	4:BBB:101:TYR:CD1	2.95	0.48
3:AAA:196:GLU:O	3:AAA:197:ASP:CB	2.62	0.48
3:AAA:193:ILE:HG13	3:AAA:193:ILE:O	2.14	0.48
1:CCC:15:ARG:NH2	1:CCC:40:ASP:OD2	2.46	0.48
3:AAA:22:LEU:HD22	3:AAA:22:LEU:N	2.29	0.47
1:CCC:23:PHE:HE1	1:CCC:75:HIS:HD1	1.62	0.47
4:BBB:196:THR:HG23	8:BBB:422:HOH:O	2.15	0.47
1:CCC:230:GLU:HG3	1:CCC:247:ALA:HB3	1.98	0.46
4:BBB:158:VAL:HA	4:BBB:204:HIS:O	2.16	0.46
3:AAA:124:LEU:HD12	3:AAA:124:LEU:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BBB:111:LEU:HD21	4:BBB:148:TYR:CE2	2.51	0.45
2:DDD:14:HIS:HE1	8:DDD:219:HOH:O	1.99	0.45
3:AAA:111:GLN:HB3	3:AAA:142:SER:HB3	1.97	0.45
2:DDD:52:HIS:HA	2:DDD:66:LEU:O	2.17	0.45
2:DDD:24:LEU:O	2:DDD:68:TYR:HA	2.16	0.44
4:BBB:47:ILE:HG22	4:BBB:48:HIS:CD2	2.52	0.44
4:BBB:89:VAL:HG22	4:BBB:107:ARG:HD2	2.00	0.43
4:BBB:208:GLN:HG3	4:BBB:231:ILE:HG23	2.01	0.43
1:CCC:218:TRP:HB2	1:CCC:229:THR:CG2	2.49	0.43
1:CCC:118:ALA:HB2	2:DDD:61:TRP:CE2	2.53	0.43
4:BBB:34:TYR:O	4:BBB:92:CYS:HA	2.19	0.43
1:CCC:211:PRO:O	1:CCC:264:HIS:HE1	2.01	0.42
1:CCC:229:THR:HG22	1:CCC:248:VAL:HG13	2.00	0.42
1:CCC:23:PHE:CD2	1:CCC:72:SER:HB3	2.54	0.42
4:BBB:159:ASN:OD1	4:BBB:203:ASN:HA	2.19	0.42
1:CCC:29:VAL:HG11	1:CCC:180:LEU:HD13	2.02	0.42
3:AAA:148:GLN:HE21	3:AAA:148:GLN:HA	1.83	0.42
4:BBB:20:MET:HE3	4:BBB:22:LEU:HD11	2.00	0.42
3:AAA:129:SER:O	3:AAA:130:SER:HB2	2.20	0.41
4:BBB:148:TYR:CD1	4:BBB:149:PRO:HA	2.55	0.41
4:BBB:109:THR:HG21	4:BBB:149:PRO:HB3	2.03	0.41
1:CCC:139:MET:HE3	8:CCC:475:HOH:O	2.20	0.41
3:AAA:130:SER:HB3	3:AAA:132:LYS:HB2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:122:LYS:HZ1	4:BBB:81:SER:HG[2_856]	1.10	0.50

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	CCC	276/277 (100%)	267 (97%)	9 (3%)	0	100	100
2	DDD	97/100 (97%)	92 (95%)	5 (5%)	0	100	100
3	AAA	200/206 (97%)	190 (95%)	10 (5%)	0	100	100
4	BBB	238/241 (99%)	232 (98%)	6 (2%)	0	100	100
5	EEE	7/9 (78%)	7 (100%)	0	0	100	100
All	All	818/833 (98%)	788 (96%)	30 (4%)	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	CCC	220/233 (94%)	215 (98%)	5 (2%)	50	44
2	DDD	82/95 (86%)	79 (96%)	3 (4%)	34	27
3	AAA	169/183 (92%)	165 (98%)	4 (2%)	49	42
4	BBB	195/208 (94%)	193 (99%)	2 (1%)	76	75
5	EEE	7/7 (100%)	7 (100%)	0	100	100
All	All	673/726 (93%)	659 (98%)	14 (2%)	53	48

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	36	ARG
1	CCC	178	GLU
1	CCC	182	ARG
1	CCC	248	VAL
1	CCC	259	THR
2	DDD	69	THR
2	DDD	71	PHE
2	DDD	98	ARG
3	AAA	14	VAL
3	AAA	46	GLU

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Mol	Chain	Res	Type
3	AAA	148	GLN
3	AAA	193	ILE
4	BBB	10	LYS
4	BBB	190	ARG

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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GOL	CCC	303	-	5,5,5	0.11	0	5,5,5	0.33	0
6	GOL	CCC	301	-	5,5,5	0.11	0	5,5,5	0.19	0
6	GOL	CCC	302	-	5,5,5	0.11	0	5,5,5	0.23	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	CCC	303	-	-	4/4/4/4	-
6	GOL	CCC	301	-	-	2/4/4/4	-
6	GOL	CCC	302	-	-	0/4/4/4	-

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
6	CCC	301	GOL	C1-C2-C3-O3
6	CCC	303	GOL	C1-C2-C3-O3
6	CCC	303	GOL	O2-C2-C3-O3
6	CCC	301	GOL	O2-C2-C3-O3
6	CCC	303	GOL	O1-C1-C2-C3
6	CCC	303	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	CCC	276/277 (99%)	0.31	15 (5%) 25 28	20, 31, 74, 89	0
2	DDD	99/100 (99%)	0.27	6 (6%) 21 22	23, 41, 69, 76	0
3	AAA	201/206 (97%)	0.23	5 (2%) 57 61	20, 32, 72, 91	0
4	BBB	240/241 (99%)	0.13	6 (2%) 57 61	19, 33, 66, 82	0
5	EEE	9/9 (100%)	-0.22	0 100 100	21, 21, 23, 24	0
All	All	825/833 (99%)	0.23	32 (3%) 39 42	19, 33, 71, 91	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	277	PRO	6.8
3	AAA	129	SER	5.2
1	CCC	275	TRP	4.5
3	AAA	149	SER	4.2
1	CCC	221	ASP	4.1
4	BBB	202	ARG	4.0
1	CCC	198	HIS	3.6
3	AAA	203	PRO	3.6
1	CCC	224	ASP	3.4
4	BBB	240	ALA	3.3
4	BBB	239	ARG	3.2
1	CCC	226	THR	3.1
4	BBB	237	TRP	3.1
3	AAA	181	SER	3.0
1	CCC	195	VAL	2.9
1	CCC	258	TYR	2.6
1	CCC	249	VAL	2.6
3	AAA	152	SER	2.6
1	CCC	251	PRO	2.5
4	BBB	238	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
4	BBB	223	ASP	2.4
2	DDD	100	MET	2.4
1	CCC	197	ASP	2.4
2	DDD	74	THR	2.2
2	DDD	16	ALA	2.1
2	DDD	99	ASP	2.1
2	DDD	2	ILE	2.1
1	CCC	228	ASP	2.1
1	CCC	257	ARG	2.1
2	DDD	76	LYS	2.0
1	CCC	202	LEU	2.0
1	CCC	256	GLN	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	CCC	301	6/6	0.90	0.10	49,50,55,56	2
6	GOL	CCC	303	6/6	0.92	0.24	56,57,65,66	2
6	GOL	CCC	302	6/6	0.94	0.15	45,53,57,58	2
7	CL	BBB	301	1/1	0.99	0.19	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.