



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:45 am BST

PDB ID : 6G9Q
Title : Ternary complex of P14 TCR with murine MHC class I H-2 Db in complex with self-antigen derived from dopamine monooxygenase.
Authors : Achour, A.; Sandalova, T.; Allerbring, E.
Deposited on : 2018-04-11
Resolution : 1.89 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

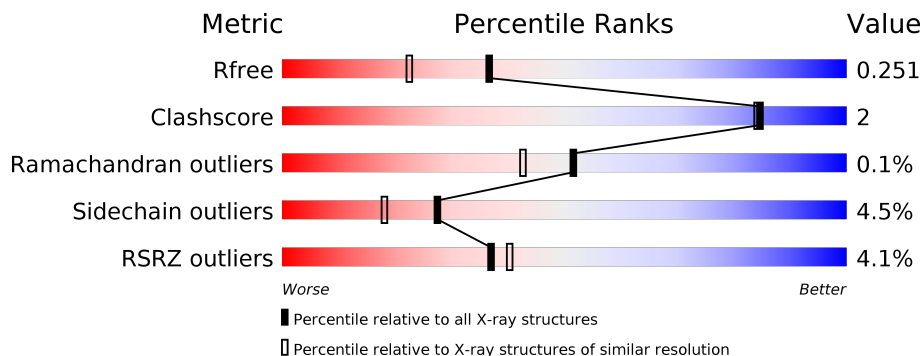
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	 4% 92% 7% ..
2	B	119	 2% 76% 7% 18%
3	G	205	 9% 80% 11% • 8%
4	H	238	 94% 5%
5	P	9	 78% 11% 11%

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 6675 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2261	1427	399	426	9	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	98	813	518	137	151	7	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	TYR	conflict	UNP P01887
B	0	GLY	ALA	conflict	UNP P01887
B	85	ASP	ALA	variant	UNP P01887

- Molecule 3 is a protein called T cell receptor alpha variable 14-1,T-cell receptor alpha chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	188	1473	937	235	293	8	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	100	LEU	-	linker	UNP A0A0G2JF94
G	101	TYR	-	linker	UNP A0A0G2JF94
G	102	GLY	-	linker	UNP A0A0G2JF94
G	103	ASN	-	linker	UNP A0A0G2JF94
G	104	GLU	-	linker	UNP A0A0G2JF94
G	105	LYS	-	linker	UNP A0A0G2JF94

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Chain	Residue	Modelled	Actual	Comment	Reference
G	106	ILE	-	linker	UNP A0A0G2JF94
G	107	THR	-	linker	UNP A0A0G2JF94
G	108	PHE	-	linker	UNP A0A0G2JF94
G	109	GLY	-	linker	UNP A0A0G2JF94
G	110	ALA	-	linker	UNP A0A0G2JF94
G	111	GLY	-	linker	UNP A0A0G2JF94
G	112	THR	-	linker	UNP A0A0G2JF94
G	113	LYS	-	linker	UNP A0A0G2JF94
G	114	LEU	-	linker	UNP A0A0G2JF94
G	115	THR	-	linker	UNP A0A0G2JF94
G	116	ILE	-	linker	UNP A0A0G2JF94
G	117	LYS	-	linker	UNP A0A0G2JF94
G	119	ASN	TYR	conflict	UNP P01849
G	124	ASP	GLU	conflict	UNP P01849
G	134	LYS	ARG	conflict	UNP P01849
G	166	CYS	THR	conflict	UNP P01849

- Molecule 4 is a protein called T-cell receptor beta chain V region C5,T-cell receptor beta-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	237	1873	1176	333	358	6	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	93	ASP	GLY	conflict	UNP P04213
H	94	ALA	THR	conflict	UNP P04213
H	?	-	ALA	deletion	UNP P04213
H	97	ARG	LEU	conflict	UNP P04213
H	98	ASN	ASP	conflict	UNP P04213
H	100	LEU	GLN	conflict	UNP P04213
H	104	ALA	PRO	conflict	UNP P04213
H	109	SER	LEU	conflict	UNP P04213
H	133	SER	ALA	conflict	UNP P01852
H	168	CYS	SER	conflict	UNP P01852
H	182	SER	CYS	conflict	UNP P01852

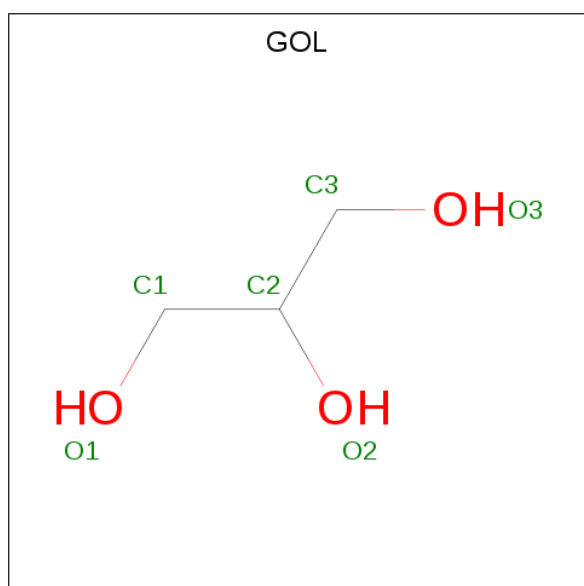
- Molecule 5 is a protein called Dopamine beta-hydroxylase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	P	9	74	50	10	14	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	3	PRO	LEU	engineered mutation	UNP Q64237

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



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

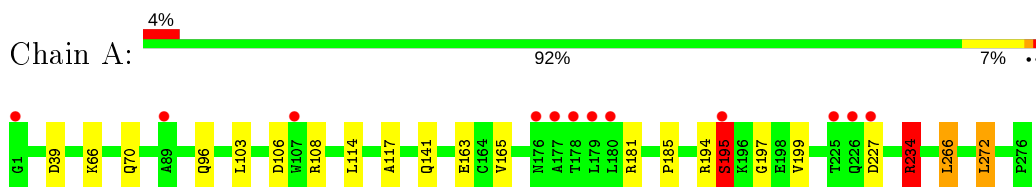
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	66	Total	O	0	0
			66	66		
7	B	19	Total	O	0	0
			19	19		
7	G	24	Total	O	0	0
			24	24		
7	H	63	Total	O	0	0
			63	63		
7	P	3	Total	O	0	0
			3	3		

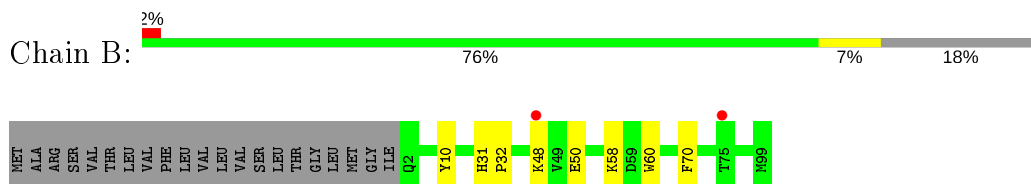
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

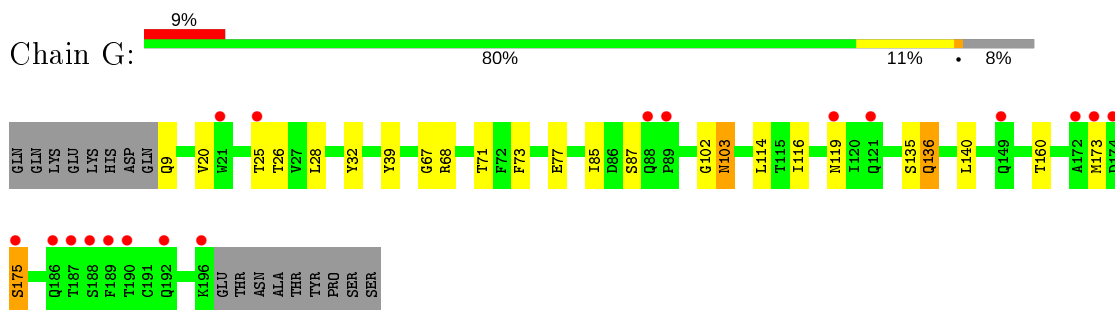
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



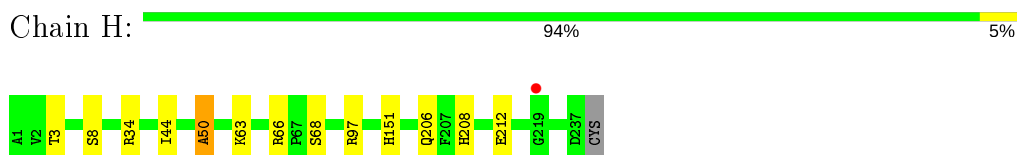
- Molecule 2: Beta-2-microglobulin



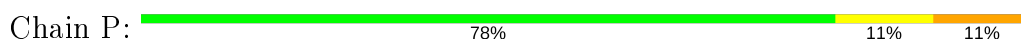
- Molecule 3: T cell receptor alpha variable 14-1, T-cell receptor alpha chain C region

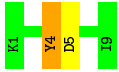


- Molecule 4: T-cell receptor beta chain V region C5, T-cell receptor beta-1 chain C region



- Molecule 5: Dopamine beta-hydroxylase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	256.38Å 46.62Å 90.06Å 90.00° 94.20° 90.00°	Depositor
Resolution (Å)	50.42 – 1.89 50.37 – 1.89	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.42-1.89) 93.7 (50.37-1.89)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.187 , 0.248 0.194 , 0.251	Depositor DCC
R_{free} test set	4052 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtrriage
Anisotropy	0.265	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6675	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/2328	0.63	1/3162 (0.0%)
2	B	0.36	0/839	0.57	0/1137
3	G	0.35	0/1508	0.62	2/2045 (0.1%)
4	H	0.39	0/1925	0.58	0/2616
5	P	1.25	0/77	0.67	0/104
All	All	0.40	0/6677	0.61	3/9064 (0.0%)

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
1	A	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	68	ARG	N-CA-CB	-9.82	92.92	110.60
3	G	67	GLY	N-CA-C	-7.22	95.05	113.10
1	A	234	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	ARG	Peptide
1	A	195	SER	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	2261	0	2125	13	0
2	B	813	0	782	5	0
3	G	1473	0	1418	11	0
4	H	1873	0	1783	6	0
5	P	74	0	72	4	0
6	A	6	0	8	0	0
7	A	66	0	0	0	0
7	B	19	0	0	0	0
7	G	24	0	0	0	0
7	H	63	0	0	0	0
7	P	3	0	0	0	0
All	All	6675	0	6188	29	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 2.

All (29) 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:163:GLU:OE1	5:P:4:TYR:OH	1.93	0.85
1:A:66:LYS:HA	3:G:103:ASN:HD21	1.62	0.65
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.37	0.59
1:A:70:GLN:HE22	5:P:5:ASP:H	1.51	0.58
1:A:106:ASP:OD2	1:A:106:ASP:O	2.20	0.58
1:A:96:GLN:OE1	2:B:31:HIS:HE1	1.87	0.57
4:H:8:SER:HG	4:H:151:HIS:HD1	1.54	0.55
3:G:136:GLN:HE21	3:G:136:GLN:HA	1.73	0.54
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.42	0.54
4:H:151:HIS:HB3	4:H:208:HIS:HB2	1.90	0.52
3:G:26:THR:HG23	3:G:87:SER:OG	2.10	0.51
4:H:212:GLU:HA	4:H:212:GLU:OE1	2.11	0.51
1:A:103:LEU:HD11	1:A:165:VAL:HG22	1.93	0.51
1:A:70:GLN:NE2	5:P:5:ASP:H	2.09	0.50
3:G:102:GLY:HA2	5:P:4:TYR:CE1	2.49	0.47
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:SER:OG	1:A:197:GLY:N	2.44	0.47
2:B:31:HIS:CD2	2:B:32:PRO:HA	2.49	0.47
3:G:39:TYR:CD2	4:H:97:ARG:HG2	2.52	0.45
4:H:50:ALA:O	4:H:66:ARG:O	2.36	0.44
3:G:32:TYR:HH	3:G:73:PHE:HE1	1.64	0.44
3:G:103:ASN:HD22	3:G:103:ASN:C	2.21	0.43
1:A:272:LEU:HD12	1:A:272:LEU:N	2.34	0.43
1:A:185:PRO:HD2	1:A:266:LEU:HD13	2.01	0.42
3:G:25:THR:HG22	3:G:85:ILE:HA	2.02	0.42
3:G:140:LEU:C	3:G:140:LEU:HD12	2.40	0.42
4:H:34:ARG:HB2	4:H:44:ILE:HD11	2.01	0.41
3:G:114:LEU:HD21	3:G:116:ILE:HD11	2.02	0.41
3:G:175:SER:O	3:G:175:SER:OG	2.39	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	274/276 (99%)	266 (97%)	8 (3%)	0	100	100
2	B	96/119 (81%)	94 (98%)	2 (2%)	0	100	100
3	G	186/205 (91%)	179 (96%)	7 (4%)	0	100	100
4	H	235/238 (99%)	228 (97%)	6 (3%)	1 (0%)	34	24
5	P	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	798/847 (94%)	773 (97%)	24 (3%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	50	ALA

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	A	233/234 (100%)	222 (95%)	11 (5%)	26	16
2	B	93/111 (84%)	89 (96%)	4 (4%)	29	19
3	G	167/184 (91%)	155 (93%)	12 (7%)	14	6
4	H	204/205 (100%)	200 (98%)	4 (2%)	55	51
5	P	7/7 (100%)	6 (86%)	1 (14%)	3	1
All	All	704/741 (95%)	672 (96%)	32 (4%)	27	18

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	108	ARG
1	A	114	LEU
1	A	141	GLN
1	A	181	ARG
1	A	195	SER
1	A	199	VAL
1	A	227	ASP
1	A	234	ARG
1	A	266	LEU
1	A	272	LEU
2	B	48	LYS
2	B	50	GLU
2	B	58	LYS
2	B	70	PHE
3	G	9	GLN
3	G	20	VAL
3	G	28	LEU
3	G	71	THR
3	G	77	GLU
3	G	103	ASN
3	G	119	ASN
3	G	135	SER

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Mol	Chain	Res	Type
3	G	136	GLN
3	G	160	THR
3	G	173	MET
3	G	175	SER
4	H	3	THR
4	H	63	LYS
4	H	68	SER
4	H	206	GLN
5	P	4	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	127	ASN
1	A	149	GLN
1	A	263	HIS
2	B	8	GLN
2	B	31	HIS
3	G	13	GLN
3	G	103	ASN
3	G	136	GLN
4	H	69	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	301	-	5,5,5	0.22	0	5,5,5	0.20	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	301	-	-	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
6	A	301	GOL	C1-C2-C3-O3
6	A	301	GOL	O2-C2-C3-O3

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/276 (100%)	0.38	12 (4%) 35 38	22, 39, 65, 99	0
2	B	98/119 (82%)	0.15	2 (2%) 65 68	24, 44, 63, 70	0
3	G	188/205 (91%)	0.66	18 (9%) 8 9	26, 48, 86, 108	0
4	H	237/238 (99%)	0.08	1 (0%) 92 93	28, 37, 53, 72	0
5	P	9/9 (100%)	0.46	0 100 100	22, 29, 32, 37	0
All	All	808/847 (95%)	0.33	33 (4%) 37 40	22, 40, 69, 108	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	172	ALA	17.5
3	G	187	THR	12.0
1	A	180	LEU	8.3
3	G	173	MET	7.6
3	G	188	SER	6.0
3	G	119	ASN	4.9
1	A	178	THR	4.7
1	A	177	ALA	4.7
3	G	121	GLN	4.5
3	G	189	PHE	4.5
1	A	179	LEU	4.4
3	G	186	GLN	3.9
4	H	219	GLY	3.9
1	A	1	GLY	3.9
1	A	226	GLN	3.5
3	G	174	ASP	3.4
1	A	227	ASP	3.4
3	G	175	SER	3.1
3	G	192	GLN	3.1
2	B	48	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	107	TRP	2.7
2	B	75	THR	2.7
1	A	225	THR	2.7
1	A	176	ASN	2.5
1	A	89	ALA	2.4
3	G	21	TRP	2.4
3	G	88	GLN	2.4
3	G	196	LYS	2.3
3	G	25	THR	2.1
3	G	149	GLN	2.1
3	G	190	THR	2.0
1	A	195	SER	2.0
3	G	89	PRO	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 carbohydrates 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	A	301	6/6	0.96	0.12	36,39,42,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.