Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:07 AM GMT

PDB ID	:	3H9S
Title	:	The complex between TCR A6 and human Class I MHC HLA-A2 with the bound Tel1p peptide
Authors	:	Borbulevych, O.Y.; Baker, B.M.
Deposited on	:	2009-04-30
Resolution	:	2.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

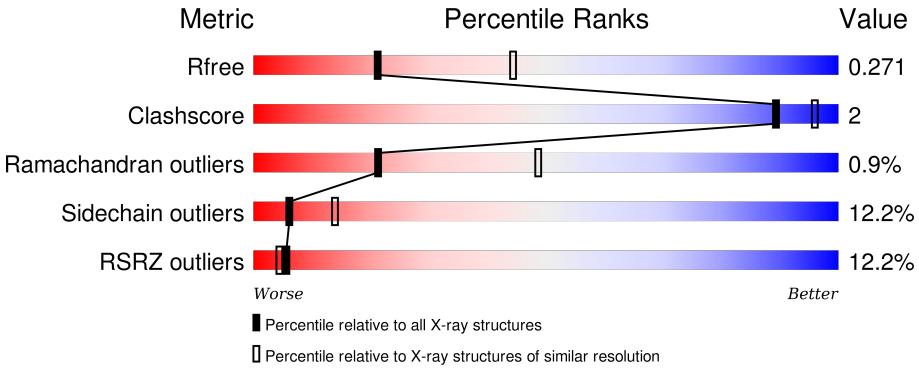
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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. 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	A	275	14% 86% 13% •
2	B	100	5% 85% 13% •
3	C	9	44% 44% 11%
4	D	200	20% 81% 17% ••
5	E	245	7% 83% 15% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	276	-	-	-	X
6	GOL	B	100	-	-	-	X
6	GOL	E	247	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6723 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called Tel1p peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			83	58	11	13	1			

- Molecule 4 is a protein called A6 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	200	Total	C	N	O	S	0	0	0
			1552	965	255	325	7			

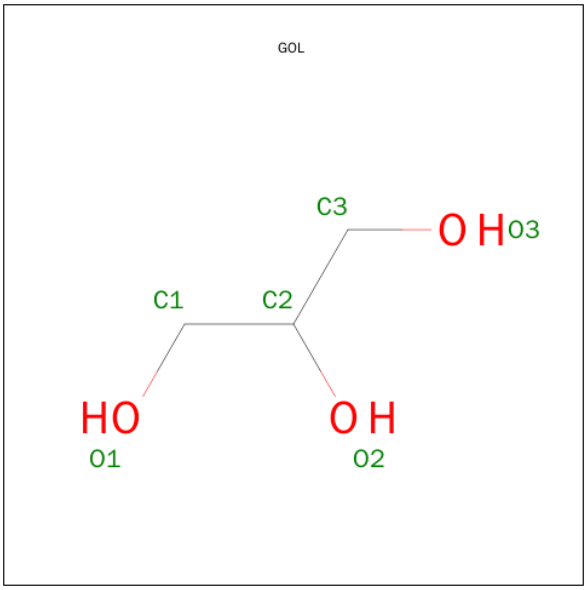
- Molecule 5 is a protein called TRBV6-5 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	245	Total	C	N	O	S	0	0	0
			1928	1209	338	373	8			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	SER	DELETION	UNP Q2YDB4
E	98	LEU	-	INSERTION	UNP Q2YDB4
E	99	ALA	-	INSERTION	UNP Q2YDB4
E	100	GLY	GLN	CONFLICT	UNP Q2YDB4
E	102	ARG	THR	CONFLICT	UNP Q2YDB4
E	103	PRO	GLU	CONFLICT	UNP Q2YDB4
E	105	GLU	THR	CONFLICT	UNP Q2YDB4
E	115	THR	LEU	CONFLICT	UNP Q2YDB4
E	116A	THR	LEU	CONFLICT	UNP Q2YDB4
E	191	ALA	CYS	CONFLICT	UNP Q2YDB4
E	205	ASP	ASN	CONFLICT	UNP Q2YDB4

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



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

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

- Molecule 7 is water.

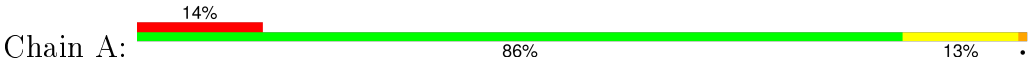
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	14	Total O 14 14	0	0
7	B	8	Total O 8 8	0	0
7	C	1	Total O 1 1	0	0
7	D	5	Total O 5 5	0	0
7	E	12	Total O 12 12	0	0

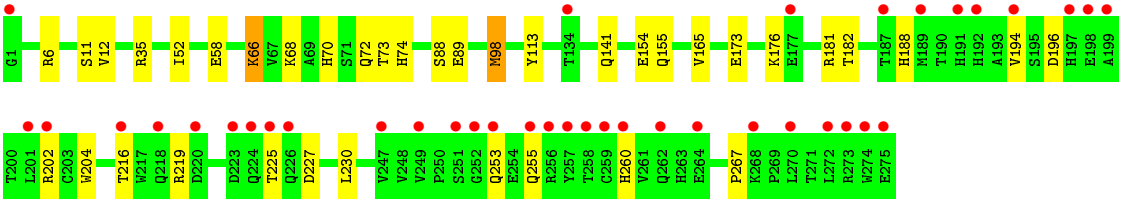
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: HLA class I histocompatibility antigen, A-2 alpha chain

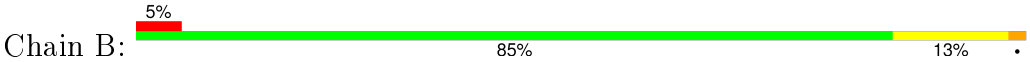
Chain A:

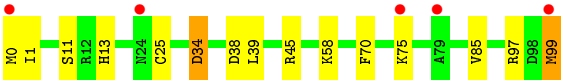




- Molecule 2: Beta-2-microglobulin

Chain B:



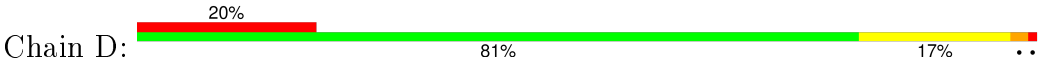


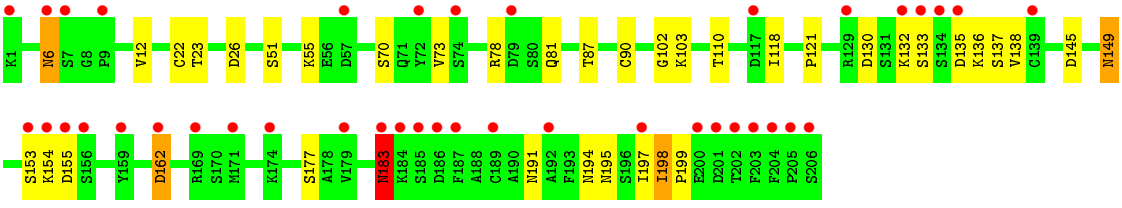
- Molecule 3: Tel1p peptide

Chain C:

- Molecule 4: A6 TCR alpha chain

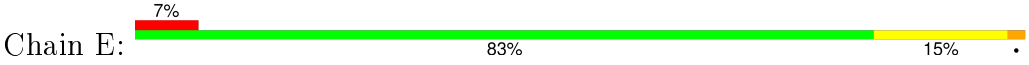
Chain D:

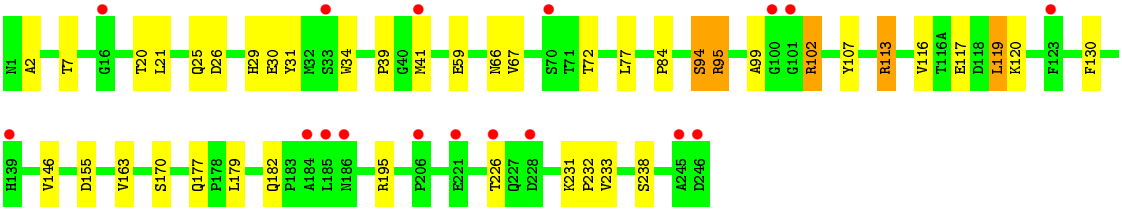




- Molecule 5: TRBV6-5 protein

Chain E:




N1
A2
T7
G16
T20
L21
Q25
D26
H29
E30
Y31
M32
S33
W34
P39
G40
M41
E59
N66
V67
S70
T71
T72
L77
P84
S94
R95
A99
G100
G101
R102
Y107
R113
V116
T116A
E117
D118
L119
K120
F123
F130
H139
V146
D155
V163
S170
Q177
P178
L179
Q182
P183
A184
L185
N186
R195
P206
E221
T226
Q227
D228
K231
P232
V233
S238
A245
D246

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	223.11Å 48.31Å 92.48Å 90.00° 90.97° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.70) 99.4 (19.96-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.289 0.210 , 0.271	Depositor DCC
R_{free} test set	1387 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	57.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 61.0	EDS
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 27378 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6723	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.65	0/2312	0.77	0/3137
2	B	0.73	0/860	0.83	0/1162
3	C	0.93	0/86	1.41	2/115 (1.7%)
4	D	0.62	2/1585 (0.1%)	0.75	1/2150 (0.0%)
5	E	0.65	0/1981	0.87	4/2699 (0.1%)
All	All	0.66	2/6824 (0.0%)	0.81	7/9263 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	90	CYS	CB-SG	-6.51	1.71	1.82
4	D	22	CYS	CB-SG	-6.29	1.71	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	113	ARG	NE-CZ-NH1	7.15	123.88	120.30
5	E	113	ARG	NE-CZ-NH2	-7.01	116.79	120.30
5	E	119	LEU	CA-CB-CG	6.56	130.39	115.30
5	E	113	ARG	CG-CD-NE	5.86	124.11	111.80
3	C	6	LEU	CA-CB-CG	5.82	128.69	115.30
3	C	3	TRP	CA-CB-CG	5.80	124.71	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	26	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	121	PRO	Peptide

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	A	2247	0	2096	7	0
2	B	837	0	803	5	0
3	C	83	0	81	2	0
4	D	1552	0	1461	11	0
5	E	1928	0	1830	12	0
6	A	18	0	24	0	0
6	B	6	0	8	0	0
6	D	6	0	8	0	0
6	E	6	0	8	0	0
7	A	14	0	0	0	0
7	B	8	0	0	0	0
7	C	1	0	0	0	0
7	D	5	0	0	0	0
7	E	12	0	0	0	0
All	All	6723	0	6319	31	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 (31) 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)
4:D:102:GLY:O	5:E:95:ARG:NH2	2.24	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:153:SER:OG	4:D:154:LYS:N	2.30	0.64
4:D:162:ASP:N	4:D:162:ASP:OD1	2.32	0.60
2:B:38:ASP:OD2	2:B:45:ARG:NE	2.35	0.59
5:E:155:ASP:N	5:E:155:ASP:OD1	2.41	0.54
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.91	0.51
1:A:70:HIS:O	1:A:74:HIS:HD2	1.95	0.50
4:D:118:ILE:HD11	4:D:145:ASP:HA	1.95	0.49
5:E:102:ARG:NH2	5:E:107:TYR:OH	2.46	0.48
3:C:3:TRP:CH2	3:C:5:TYR:HB3	2.49	0.47
5:E:29:HIS:ND1	5:E:94:SER:OG	2.38	0.47
4:D:138:VAL:HG11	5:E:146:VAL:HG21	1.95	0.47
5:E:231:LYS:HA	5:E:232:PRO:HD3	1.75	0.47
2:B:11:SER:OG	2:B:13:HIS:O	2.32	0.46
4:D:149:ASN:N	4:D:149:ASN:OD1	2.49	0.45
1:A:202:ARG:NH1	2:B:99:MET:SD	2.90	0.45
1:A:6:ARG:HD3	1:A:98:MET:HE1	1.98	0.44
5:E:84:PRO:HA	5:E:116:VAL:HB	2.00	0.44
5:E:102:ARG:HH21	5:E:102:ARG:HB2	1.82	0.44
1:A:155:GLN:HB3	3:C:3:TRP:HH2	1.83	0.44
4:D:132:LYS:HB3	4:D:133:SER:H	1.48	0.43
4:D:130:ASP:HA	5:E:130:PHE:HA	2.01	0.43
1:A:154:GLU:OE2	4:D:55:LYS:NZ	2.48	0.43
4:D:198:ILE:HA	4:D:199:PRO:HD2	1.73	0.43
4:D:183:ASN:OD1	4:D:183:ASN:N	2.35	0.43
5:E:34:TRP:CE2	5:E:77:LEU:HB2	2.54	0.42
1:A:188:HIS:HB3	1:A:204:TRP:HB2	2.01	0.42
5:E:30:GLU:HG3	5:E:99:ALA:HB2	2.00	0.42
5:E:231:LYS:HG2	5:E:233:VAL:HG13	2.02	0.41
2:B:34:ASP:N	2:B:34:ASP:OD1	2.51	0.41
1:A:66:LYS:HE3	1:A:66:LYS:HB2	1.77	0.41

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	273/275 (99%)	257 (94%)	15 (6%)	1 (0%)	39 69
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100 100
3	C	7/9 (78%)	7 (100%)	0	0	100 100
4	D	198/200 (99%)	179 (90%)	15 (8%)	4 (2%)	9 24
5	E	243/245 (99%)	230 (95%)	11 (4%)	2 (1%)	24 51
All	All	819/829 (99%)	768 (94%)	44 (5%)	7 (1%)	21 49

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	2	ALA
4	D	135	ASP
4	D	183	ASN
1	A	267	PRO
4	D	6	ASN
4	D	191	ASN
5	E	39	PRO

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	231/231 (100%)	202 (87%)	29 (13%)	5 13
2	B	95/95 (100%)	86 (90%)	9 (10%)	11 24
3	C	8/8 (100%)	6 (75%)	2 (25%)	1 2
4	D	178/178 (100%)	156 (88%)	22 (12%)	6 13
5	E	209/209 (100%)	183 (88%)	26 (12%)	6 13
All	All	721/721 (100%)	633 (88%)	88 (12%)	6 14

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	12	VAL
1	A	35	ARG
1	A	52	ILE
1	A	58	GLU
1	A	66	LYS
1	A	68	LYS
1	A	72	GLN
1	A	73	THR
1	A	88	SER
1	A	89	GLU
1	A	98	MET
1	A	113	TYR
1	A	141	GLN
1	A	165	VAL
1	A	173	GLU
1	A	176	LYS
1	A	181	ARG
1	A	182	THR
1	A	194	VAL
1	A	196	ASP
1	A	216	THR
1	A	219	ARG
1	A	225	THR
1	A	227	ASP
1	A	230	LEU
1	A	253	GLN
1	A	255	GLN
1	A	260	HIS
2	B	0	MET
2	B	1	ILE
2	B	34	ASP
2	B	58	LYS
2	B	70	PHE
2	B	75	LYS
2	B	85	VAL
2	B	97	ARG
2	B	99	MET
3	C	7	GLN
3	C	9	VAL
4	D	6	ASN
4	D	12	VAL
4	D	23	THR

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Mol	Chain	Res	Type
4	D	51	SER
4	D	70	SER
4	D	73	VAL
4	D	78	ARG
4	D	81	GLN
4	D	87	THR
4	D	103	LYS
4	D	110	THR
4	D	136	LYS
4	D	137	SER
4	D	149	ASN
4	D	155	ASP
4	D	162	ASP
4	D	177	SER
4	D	183	ASN
4	D	194	ASN
4	D	195	ASN
4	D	197	ILE
4	D	198	ILE
5	E	7	THR
5	E	20	THR
5	E	21	LEU
5	E	25	GLN
5	E	26	ASP
5	E	31	TYR
5	E	41	MET
5	E	59	GLU
5	E	66	ASN
5	E	67	VAL
5	E	72	THR
5	E	94	SER
5	E	95	ARG
5	E	102	ARG
5	E	113	ARG
5	E	117	GLU
5	E	119	LEU
5	E	120	LYS
5	E	163	VAL
5	E	170	SER
5	E	177	GLN
5	E	179	LEU
5	E	182	GLN

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Mol	Chain	Res	Type
5	E	195	ARG
5	E	226	THR
5	E	238	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	GLN
2	B	2	GLN
4	D	37	GLN
4	D	111	GLN
4	D	119	GLN
4	D	152	GLN
5	E	37	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	A	276	-	5,5,5	0.36	0	5,5,5	0.44	0
6	GOL	A	277	-	5,5,5	0.45	0	5,5,5	0.54	0
6	GOL	A	278	-	5,5,5	0.27	0	5,5,5	0.63	0
6	GOL	B	100	-	5,5,5	0.32	0	5,5,5	0.25	0
6	GOL	D	207	-	5,5,5	2.71	3 (60%)	5,5,5	2.27	2 (40%)
6	GOL	E	247	-	5,5,5	0.24	0	5,5,5	0.81	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	276	-	-	0/4/4/4	0/0/0/0
6	GOL	A	277	-	-	0/4/4/4	0/0/0/0
6	GOL	A	278	-	-	0/4/4/4	0/0/0/0
6	GOL	B	100	-	-	0/4/4/4	0/0/0/0
6	GOL	D	207	-	-	0/4/4/4	0/0/0/0
6	GOL	E	247	-	-	0/4/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	207	GOL	C3-C2	2.77	1.62	1.52
6	D	207	GOL	C1-C2	3.63	1.66	1.52
6	D	207	GOL	O2-C2	3.96	1.55	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	207	GOL	O2-C2-C1	-4.00	90.30	108.65
6	D	207	GOL	O3-C3-C2	-2.74	96.89	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	275/275 (100%)	0.74	39 (14%) 4 3	50, 61, 71, 77	0
2	B	100/100 (100%)	0.42	5 (5%) 32 31	49, 62, 71, 86	0
3	C	9/9 (100%)	0.92	0 100 100	61, 66, 73, 73	0
4	D	200/200 (100%)	1.03	40 (20%) 1 1	54, 64, 75, 82	0
5	E	245/245 (100%)	0.46	17 (6%) 20 18	54, 62, 73, 82	0
All	All	829/829 (100%)	0.69	101 (12%) 5 4	49, 62, 73, 86	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	200	GLU	8.5
4	D	205	PRO	7.9
4	D	133	SER	7.0
5	E	245	ALA	6.9
4	D	171	MET	6.7
1	A	273	ARG	6.5
4	D	183	ASN	6.4
5	E	246	ASP	5.5
4	D	203	PHE	5.4
1	A	220	ASP	5.2
4	D	184	LYS	5.1
4	D	206	SER	5.0
2	B	99	MET	5.0
1	A	252	GLY	4.7
5	E	228	ASP	4.6
1	A	251	SER	4.5
4	D	154	LYS	4.5
5	E	123	PHE	4.5
1	A	218	GLN	4.4
4	D	202	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	260	HIS	4.3
1	A	256	ARG	4.2
1	A	198	GLU	4.2
4	D	1	LYS	4.2
1	A	257	TYR	4.1
1	A	258	THR	4.1
1	A	223	ASP	3.8
5	E	226	THR	3.8
4	D	139	CYS	3.8
4	D	134	SER	3.7
1	A	275	GLU	3.7
1	A	255	GLN	3.7
1	A	199	ALA	3.6
1	A	253	GLN	3.6
4	D	153	SER	3.5
4	D	135	ASP	3.5
4	D	156	SER	3.5
4	D	57	ASP	3.5
4	D	79	ASP	3.5
5	E	186	ASN	3.4
4	D	169	ARG	3.2
2	B	0	MET	3.2
1	A	272	LEU	3.2
1	A	247	VAL	3.2
1	A	189	MET	3.1
5	E	185	LEU	3.1
5	E	16	GLY	3.1
4	D	132	LYS	3.1
1	A	177	GLU	3.1
5	E	221	GLU	3.1
5	E	206	PRO	3.0
4	D	129	ARG	3.0
1	A	270	LEU	2.9
1	A	191	HIS	2.9
2	B	75	LYS	2.8
1	A	134	THR	2.8
4	D	162	ASP	2.8
4	D	7	SER	2.8
1	A	274	TRP	2.7
4	D	189	CYS	2.7
1	A	264	GLU	2.7
1	A	226	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	9	PRO	2.7
4	D	185	SER	2.7
1	A	1	GLY	2.6
4	D	201	ASP	2.6
1	A	225	THR	2.6
1	A	192	HIS	2.6
4	D	155	ASP	2.5
1	A	249	VAL	2.5
5	E	41	MET	2.5
4	D	74	SER	2.4
4	D	204	PHE	2.4
4	D	192	ALA	2.4
1	A	201	LEU	2.3
5	E	33	SER	2.3
1	A	216	THR	2.3
4	D	6	ASN	2.3
4	D	179	VAL	2.3
1	A	194	VAL	2.3
1	A	224	GLN	2.3
4	D	174	LYS	2.3
1	A	268	LYS	2.2
1	A	202	ARG	2.2
2	B	79	ALA	2.2
5	E	70	SER	2.2
5	E	100	GLY	2.2
4	D	197	ILE	2.2
4	D	187	PHE	2.2
4	D	117	ASP	2.2
1	A	259	CYS	2.1
4	D	72	TYR	2.1
4	D	159	TYR	2.1
5	E	139	HIS	2.1
5	E	184	ALA	2.1
4	D	186	ASP	2.1
1	A	197	HIS	2.1
1	A	187	THR	2.0
1	A	262	GLN	2.0
2	B	24	ASN	2.0
5	E	101	GLY	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
6	GOL	B	100	6/6	0.83	0.32	8.08	76,76,76,77	0
6	GOL	E	247	6/6	0.81	0.53	5.57	50,51,52,55	0
6	GOL	A	276	6/6	0.89	0.36	2.26	61,62,62,63	0
6	GOL	D	207	6/6	0.88	0.33	0.77	49,49,49,49	6
6	GOL	A	278	6/6	0.94	0.36	-	70,71,71,72	0
6	GOL	A	277	6/6	0.45	0.48	-	78,78,79,79	0

6.5 Other polymers (i)

There are no such residues in this entry.