wwPDB X-ray Structure Validation Summary Report (i)

Nov 7, 2023 – 02:46 AM EST

PDB ID	:	6V0Y
Title	:	immune receptor complex
Authors	:	Lim, J.J.; Rossjohn, J.
Deposited on	:	2019-11-19
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

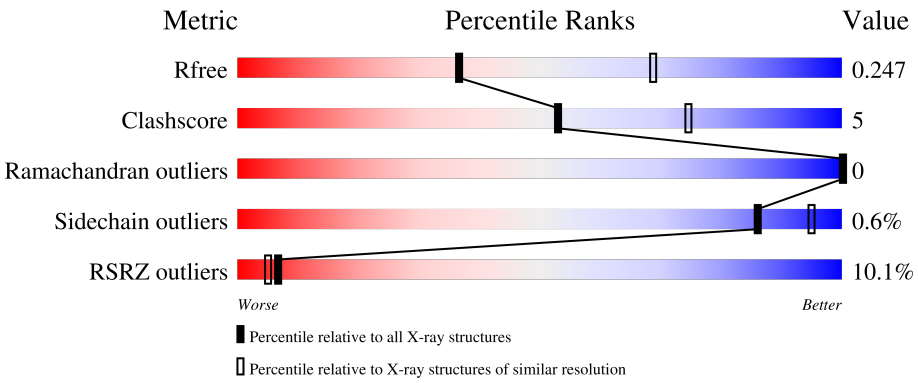
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 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	A	189	23%, 81%, 12%, 7%
2	B	198	12%, 77%, 13%, •, 10%
3	C	13	69%, 23%, 8%
4	D	209	3%, 85%, 12%, • •
5	E	242	3%, 90%, 10%

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	NAG	A	201	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6505 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 II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	175	1374	890	226	253	5	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	THR	-	expression tag	UNP P01903
A	183	SER	-	expression tag	UNP P01903
A	184	GLY	-	expression tag	UNP P01903
A	185	ASP	-	expression tag	UNP P01903
A	186	ASP	-	expression tag	UNP P01903
A	187	ASP	-	expression tag	UNP P01903
A	188	ASP	-	expression tag	UNP P01903
A	189	LYS	-	expression tag	UNP P01903

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1-4 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	179	1407	891	243	269	4	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	191	THR	-	expression tag	UNP P13760
B	192	GLY	-	expression tag	UNP P13760
B	193	GLY	-	expression tag	UNP P13760
B	194	ASP	-	expression tag	UNP P13760
B	195	ASP	-	expression tag	UNP P13760
B	196	ASP	-	expression tag	UNP P13760
B	197	ASP	-	expression tag	UNP P13760
B	198	LYS	-	expression tag	UNP P13760

- Molecule 3 is a protein called Fibrinogen beta 72,74cit69-81.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	13	89	55	18	16	0	0	0

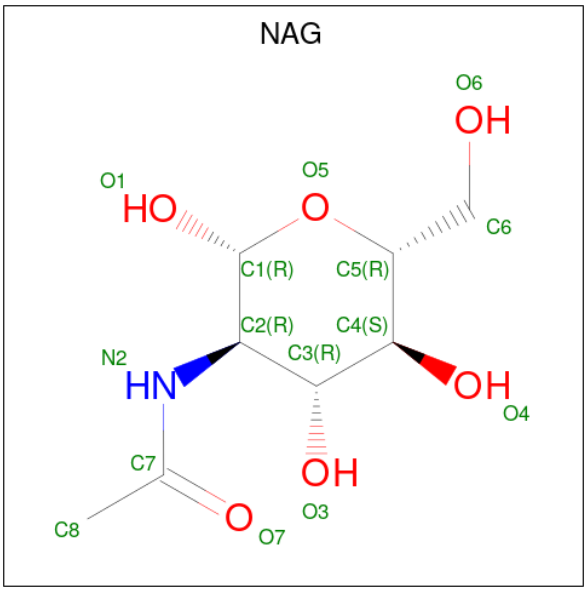
- Molecule 4 is a protein called M141 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	205	1576	989	256	323	8	0	0	0

- Molecule 5 is a protein called M141 TCR beta chain.

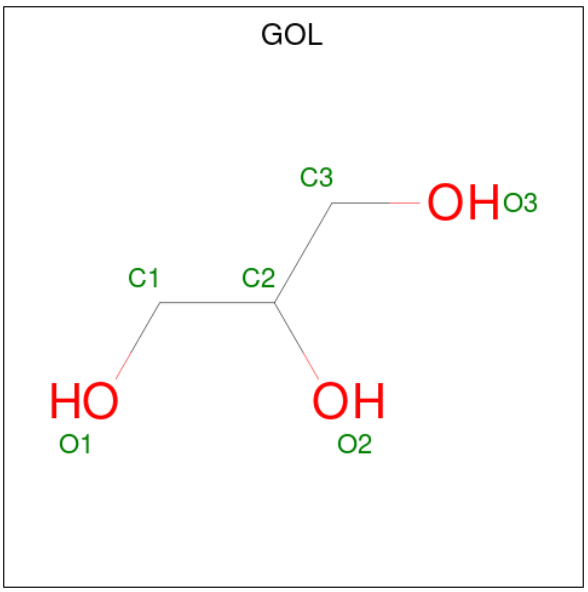
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	242	1936	1225	336	368	7	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
6	A	1	14	8	1	5	0	0
6	B	1	14	8	1	5	0	0

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



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

- Molecule 8 is water.

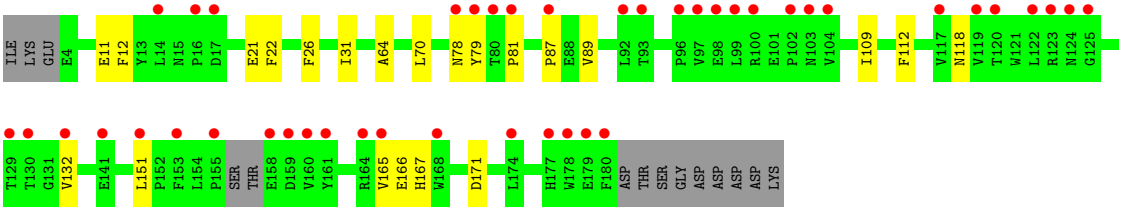
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	3	3	3	0	0
			Total	O		
8	B	10	10	10	0	0
			Total	O		
8	C	1	1	1	0	0
			Total	O		
8	D	18	18	18	0	0
			Total	O		
8	E	25	25	25	0	0

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.

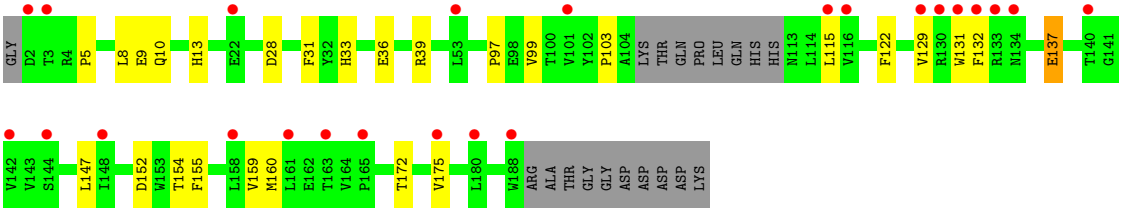
• Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain A:



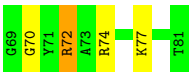
• Molecule 2: HLA class II histocompatibility antigen, DRB1-4 beta chain

Chain B:



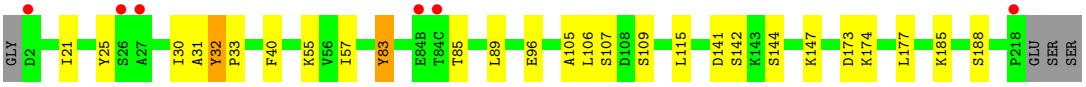
• Molecule 3: Fibrinogen beta 72,74cit69-81

Chain C:



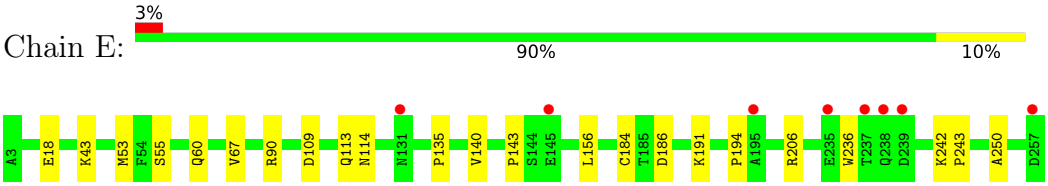
• Molecule 4: M141 TCR alpha chain

Chain D:



• Molecule 5: M141 TCR beta chain

Chain E:


3%
90%
10%
A3
E18
K43
M53
F54
S55
Q60
V67
R90
D109
Q113
N114
N131
P135
V140
P143
S144
E145
L156
C184
T185
D186
K191
P194
A195
R206
E235
W236
T237
Q238
D239
K242
P243
A250
D257

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	149.75Å 57.49Å 128.49Å 90.00° 92.94° 90.00°	Depositor
Resolution (Å)	47.50 – 2.70 47.51 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.50-2.70) 99.9 (47.51-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.220 , 0.247 0.220 , 0.247	Depositor DCC
R_{free} test set	1528 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6505	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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 (i)

5.1 Standard geometry (i)

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

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	0.27	0/1416	0.44	0/1939
2	B	0.27	0/1445	0.48	0/1973
3	C	0.69	0/66	0.75	0/85
4	D	0.26	0/1610	0.45	0/2188
5	E	0.25	0/1989	0.43	0/2710
All	All	0.27	0/6526	0.45	0/8895

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 (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	1374	0	1253	19	0
2	B	1407	0	1261	17	0
3	C	89	0	80	3	0
4	D	1576	0	1491	22	0
5	E	1936	0	1839	16	0
6	A	28	0	26	6	0
6	B	14	0	13	0	0
7	D	12	0	16	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	12	0	16	0	0
8	A	3	0	0	0	0
8	B	10	0	0	0	0
8	C	1	0	0	0	0
8	D	18	0	0	0	0
8	E	25	0	0	0	0
All	All	6505	0	5995	67	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 5.

The worst 5 of 67 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:78:ASN:ND2	6:A:201:NAG:C1	1.99	1.26
1:A:78:ASN:ND2	6:A:201:NAG:O5	1.70	1.25
4:D:188:SER:OG	5:E:206:ARG:HD2	1.64	0.95
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.75	0.69
3:C:70:GLY:HA3	4:D:31:ALA:HB1	1.76	0.68

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	171/189 (90%)	165 (96%)	6 (4%)	0	100	100
2	B	175/198 (88%)	166 (95%)	9 (5%)	0	100	100
3	C	9/13 (69%)	9 (100%)	0	0	100	100
4	D	203/209 (97%)	193 (95%)	10 (5%)	0	100	100
5	E	240/242 (99%)	235 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	798/851 (94%)	768 (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	A	142/173 (82%)	141 (99%)	1 (1%)	84 94
2	B	145/177 (82%)	144 (99%)	1 (1%)	84 94
3	C	4/4 (100%)	4 (100%)	0	100 100
4	D	179/184 (97%)	177 (99%)	2 (1%)	73 90
5	E	213/215 (99%)	213 (100%)	0	100 100
All	All	683/753 (91%)	679 (99%)	4 (1%)	86 95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	ASP
2	B	137	GLU
4	D	32	TYR
4	D	83	TYR

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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
3	CIR	C	74	3	9,10,11	1.84	3 (33%)	6,11,13	1.24	1 (16%)
3	CIR	C	72	3	9,10,11	1.65	2 (22%)	6,11,13	1.95	2 (33%)

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
3	CIR	C	74	3	-	5/8/9/11	-
3	CIR	C	72	3	-	6/8/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	74	CIR	C7-N6	-3.34	1.30	1.34
3	C	74	CIR	O7-C7	-3.23	1.19	1.24
3	C	72	CIR	O7-C7	-3.13	1.19	1.24
3	C	72	CIR	C7-N6	-3.02	1.31	1.34
3	C	74	CIR	C3-CA	-2.14	1.50	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	72	CIR	C5-N6-C7	-3.84	118.16	122.73
3	C	72	CIR	O7-C7-N8	-2.11	119.61	123.22
3	C	74	CIR	O7-C7-N8	-2.04	119.73	123.22

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	72	CIR	C4-C3-CA-C

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Mol	Chain	Res	Type	Atoms
3	C	72	CIR	O7-C7-N6-C5
3	C	72	CIR	N8-C7-N6-C5
3	C	74	CIR	C4-C3-CA-C
3	C	74	CIR	C4-C3-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	72	CIR	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	D	301	-	5,5,5	0.36	0	5,5,5	0.25	0
6	NAG	A	202	1	14,14,15	0.28	0	17,19,21	0.46	0
7	GOL	E	301	-	5,5,5	0.37	0	5,5,5	0.27	0
7	GOL	E	302	-	5,5,5	0.36	0	5,5,5	0.27	0
6	NAG	B	201	2	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	A	201	-	14,14,15	0.29	0	17,19,21	0.61	0
7	GOL	D	302	-	5,5,5	0.37	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
7	GOL	D	301	-	-	0/4/4/4	-
6	NAG	A	202	1	-	2/6/23/26	0/1/1/1
7	GOL	E	301	-	-	0/4/4/4	-
7	GOL	E	302	-	-	2/4/4/4	-
6	NAG	B	201	2	-	0/6/23/26	0/1/1/1
6	NAG	A	201	-	-	3/6/23/26	0/1/1/1
7	GOL	D	302	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	201	NAG	C1-C2-N2-C7
6	A	201	NAG	C8-C7-N2-C2
6	A	201	NAG	O7-C7-N2-C2
6	A	202	NAG	C4-C5-C6-O6
6	A	202	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	301	GOL	2	0
6	A	202	NAG	1	0
6	A	201	NAG	5	0
7	D	302	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 (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	175/189 (92%)	1.20	44 (25%)	0	0	57, 88, 128, 142	0
2	B	179/198 (90%)	0.81	24 (13%)	3	2	54, 82, 118, 128	0
3	C	11/13 (84%)	0.38	0	100	100	57, 62, 71, 77	0
4	D	205/209 (98%)	0.43	6 (2%)	51	52	46, 62, 94, 113	0
5	E	242/242 (100%)	0.41	8 (3%)	46	46	43, 58, 92, 111	0
All	All	812/851 (95%)	0.67	82 (10%)	7	5	43, 69, 115, 142	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	PRO	7.6
1	A	129	THR	5.1
1	A	160	VAL	5.1
1	A	97	VAL	4.8
1	A	153	PHE	4.7

6.2 Non-standard residues in protein, DNA, RNA chains (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
3	CIR	C	74	11/12	0.89	0.24	57,64,74,87	0
3	CIR	C	72	11/12	0.91	0.18	56,61,72,73	0

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, 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
7	GOL	E	301	6/6	0.60	0.32	82,87,92,106	0
6	NAG	A	202	14/15	0.74	0.35	102,116,129,129	0
6	NAG	A	201	14/15	0.76	0.53	105,117,132,136	0
7	GOL	D	302	6/6	0.82	0.26	80,89,93,95	0
7	GOL	E	302	6/6	0.82	0.33	95,99,104,105	0
6	NAG	B	201	14/15	0.90	0.23	89,108,118,129	0
7	GOL	D	301	6/6	0.92	0.19	67,74,88,98	0

6.5 Other polymers (i)

There are no such residues in this entry.