



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2020 – 02:38 PM EST

PDB ID : 6V13  
Title : immune receptor complex  
Authors : Lim, J.J.; Rossjohn, J.  
Deposited on : 2019-11-19  
Resolution : 2.75 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](mailto: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.

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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 : 2.14.6  
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) : 2.14.6

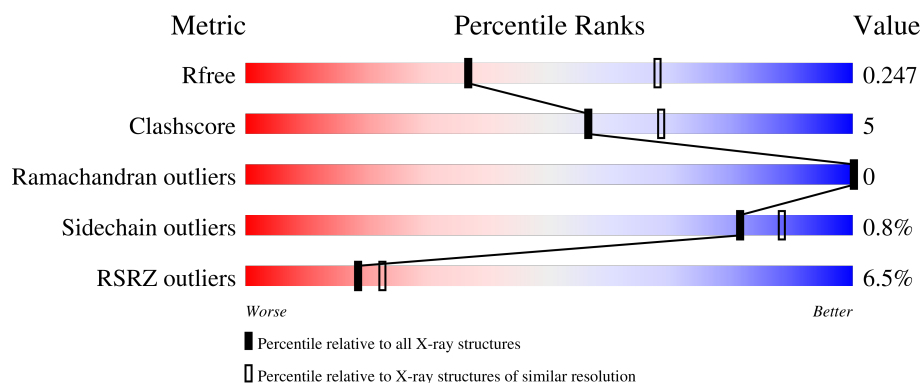
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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  $\geq 3$ , 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	189	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>
2	B	198	<div> <div>15%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>9%</div> </div> </div>
3	C	13	<div> <div></div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
4	D	206	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div></div> </div> </div>
5	E	241	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>

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
3	CIR	C	74	-	X	-	-
6	NAG	A	201	-	-	-	X
6	NAG	B	201	-	-	-	X
7	GOL	B	202	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6640 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
1	A	178	Total	C	N	O	S	0	0	0
			1447	940	234	268	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ILE	-	expression tag	UNP P01903
A	2	LYS	-	expression tag	UNP P01903
A	3	GLU	-	expression tag	UNP P01903
A	4	GLU	-	expression tag	UNP P01903
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
2	B	180	Total	C	N	O	S	0	0	0
			1453	924	251	273	5			

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 74cit69-81.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			90	55	19	16			

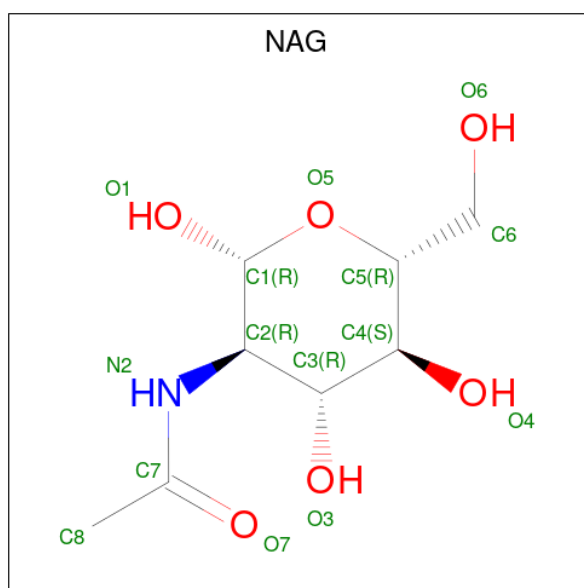
- Molecule 4 is a protein called G08 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	203	Total	C	N	O	S	0	0	0
			1573	986	257	323	7			

- Molecule 5 is a protein called G08 TCR beta chain.

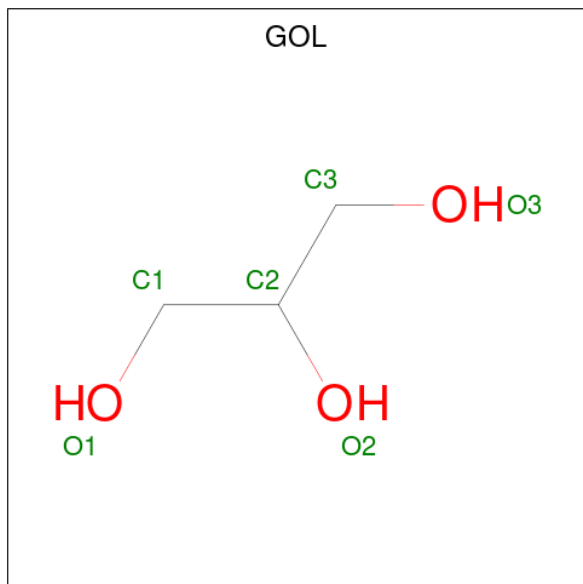
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	241	Total	C	N	O	S	0	0	0
			1934	1227	336	364	7			

- 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
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	8	Total	O	0	0
			8	8		
8	B	10	Total	O	0	0
			10	10		

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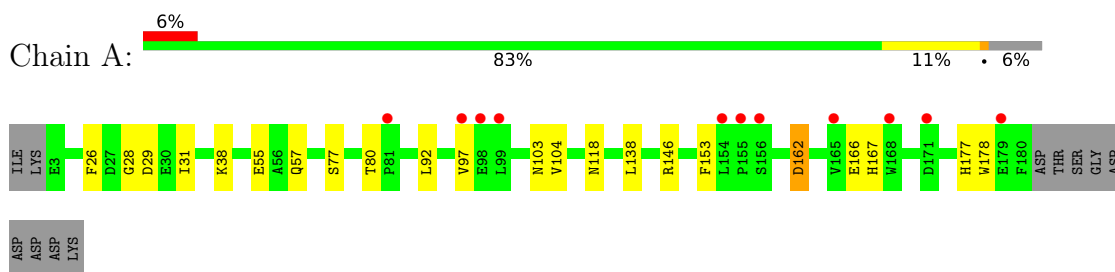
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	5	Total 5	O 5	0	0
8	D	23	Total 23	O 23	0	0
8	E	25	Total 25	O 25	0	0

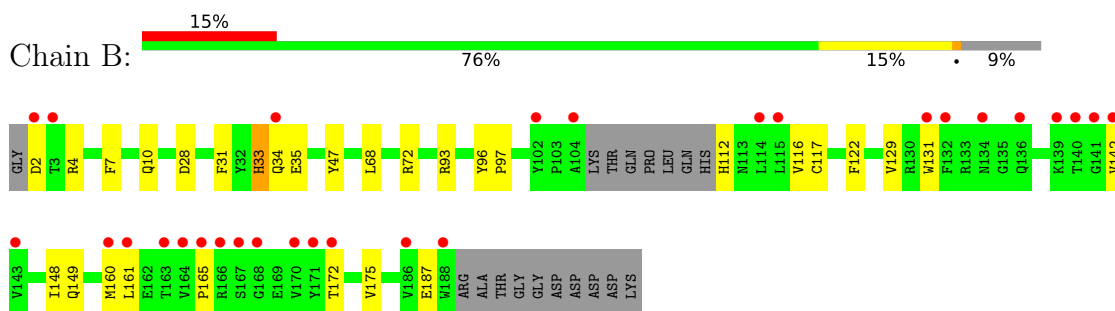
### 3 Residue-property plots

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.

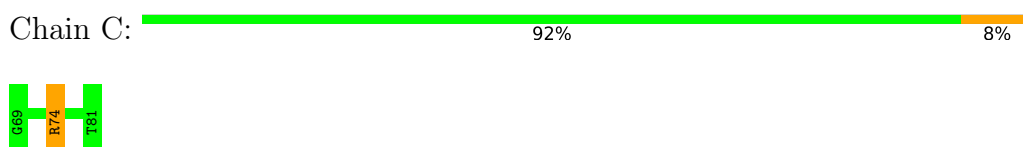
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



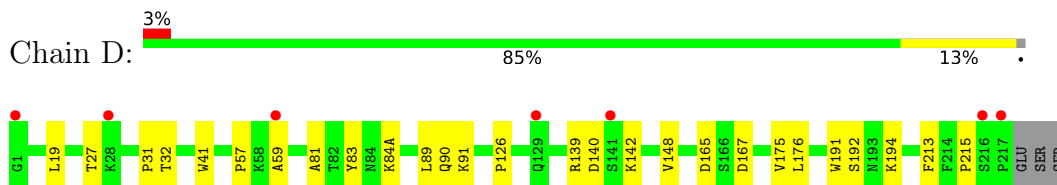
- Molecule 2: HLA class II histocompatibility antigen, DRB1-4 beta chain



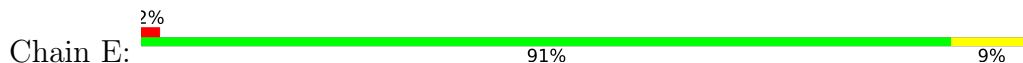
- Molecule 3: Fibrinogen beta 74cit69-81



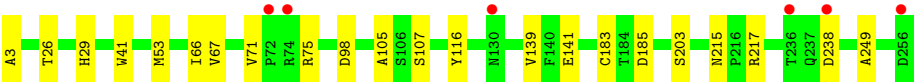
- Molecule 4: G08 TCR alpha chain



- Molecule 5: G08 TCR beta chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.46Å 56.77Å 136.25Å 90.00° 92.42° 90.00°	Depositor
Resolution (Å)	45.38 – 2.75 45.38 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.38-2.75) 99.9 (45.38-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.210 , 0.247 0.210 , 0.247	Depositor DCC
$R_{free}$ test set	1528 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.2	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6640	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CIR, NAG, 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	0.46	0/1492	0.51	0/2038
2	B	0.53	0/1493	0.61	4/2035 (0.2%)
3	C	0.82	0/79	0.74	0/103
4	D	0.60	0/1610	0.60	0/2191
5	E	0.61	0/1987	0.55	0/2706
All	All	0.56	0/6661	0.57	4/9073 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	93	ARG	O-C-N	-8.09	109.76	122.70
2	B	93	ARG	C-N-CA	7.44	140.31	121.70
2	B	93	ARG	CA-C-N	5.50	129.29	117.20
2	B	33	HIS	N-CA-C	-5.09	97.27	111.00

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	1447	0	1371	17	0
2	B	1453	0	1336	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	90	0	89	1	0
4	D	1573	0	1488	19	0
5	E	1934	0	1855	14	0
6	A	28	0	26	2	0
6	B	14	0	13	0	0
7	A	12	0	16	2	0
7	B	6	0	8	0	0
7	C	6	0	8	0	0
7	D	6	0	8	1	0
8	A	8	0	0	1	0
8	B	10	0	0	0	0
8	C	5	0	0	0	0
8	D	23	0	0	1	0
8	E	25	0	0	0	0
All	All	6640	0	6218	64	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.

All (64) 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:55:GLU:HG3	1:A:57:GLN:OE1	1.54	1.07
1:A:55:GLU:CG	1:A:57:GLN:OE1	2.23	0.87
7:A:204:GOL:O3	7:A:204:GOL:O1	2.01	0.74
1:A:28:GLY:HA2	7:A:204:GOL:H32	1.72	0.71
4:D:148:VAL:HG12	4:D:191:TRP:HB3	1.74	0.68
4:D:176:LEU:HB3	5:E:183:CYS:HB2	1.79	0.65
4:D:167:ASP:O	8:D:401:HOH:O	2.14	0.65
6:A:201:NAG:O4	8:A:301:HOH:O	2.15	0.64
1:A:97:VAL:HG11	1:A:178:TRP:HZ2	1.62	0.63
4:D:126:PRO:HG3	4:D:175:VAL:HG21	1.80	0.62
2:B:172:THR:HG22	2:B:187:GLU:HG3	1.82	0.62
5:E:41:TRP:HB3	5:E:53:MET:HE2	1.82	0.61
2:B:10:GLN:HB2	2:B:31:PHE:HB2	1.84	0.59
1:A:162:ASP:OD1	1:A:177:HIS:ND1	2.35	0.59
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.87	0.57
2:B:142:VAL:HG22	2:B:161:LEU:HD13	1.86	0.57
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.87	0.56
5:E:238:ASP:OD1	5:E:238:ASP:N	2.39	0.55
5:E:66:ILE:HG22	5:E:67:VAL:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:81:ALA:HA	7:D:301:GOL:H11	1.89	0.55
4:D:139:ARG:O	5:E:141:GLU:N	2.33	0.54
1:A:138:LEU:HB2	1:A:146:ARG:HG3	1.88	0.54
2:B:2:ASP:OD1	2:B:4:ARG:HG2	2.09	0.52
5:E:3:ALA:N	5:E:26:THR:HG1	2.08	0.52
4:D:192:SER:OG	4:D:194:LYS:HG2	2.12	0.49
1:A:92:LEU:CD1	2:B:148:ILE:HD13	2.42	0.49
2:B:112:HIS:O	2:B:165:PRO:HG3	2.13	0.49
5:E:185:ASP:OD2	5:E:203:SER:OG	2.25	0.49
2:B:7:PHE:HA	2:B:33:HIS:HE1	1.78	0.48
2:B:116:VAL:HB	2:B:160:MET:HG2	1.96	0.48
1:A:97:VAL:HG11	1:A:178:TRP:CZ2	2.47	0.48
5:E:29:HIS:HB3	5:E:107:SER:O	2.13	0.48
4:D:165:ASP:OD2	4:D:194:LYS:NZ	2.47	0.47
1:A:167:HIS:HA	6:A:202:NAG:H81	1.95	0.47
1:A:77:SER:O	1:A:80:THR:HG23	2.14	0.47
2:B:28:ASP:OD2	2:B:47:TYR:OH	2.29	0.47
4:D:41:TRP:CE2	4:D:89:LEU:HB2	2.50	0.47
2:B:142:VAL:CG2	2:B:161:LEU:HD13	2.45	0.47
4:D:84(A):LYS:HE3	4:D:84(A):LYS:HB2	1.58	0.47
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.50	0.46
5:E:75:ARG:NH1	5:E:98:ASP:OD2	2.46	0.46
5:E:71:VAL:HG21	5:E:75:ARG:HD3	1.98	0.46
4:D:19:LEU:O	4:D:90:GLN:HA	2.15	0.46
4:D:19:LEU:N	4:D:91:LYS:O	2.48	0.46
1:A:55:GLU:HG2	1:A:57:GLN:HB2	1.99	0.45
1:A:92:LEU:HD11	2:B:148:ILE:HD13	1.98	0.45
4:D:27:THR:HG21	4:D:31:PRO:HG3	1.99	0.45
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.99	0.44
4:D:213:PHE:CE2	4:D:215:PRO:HG3	2.51	0.44
5:E:41:TRP:HB3	5:E:53:MET:CE	2.48	0.44
5:E:105:ALA:HA	5:E:116:TYR:O	2.17	0.44
4:D:142:LYS:HA	4:D:142:LYS:HD2	1.89	0.43
1:A:103:ASN:OD1	1:A:104:VAL:N	2.45	0.43
4:D:140:ASP:N	4:D:140:ASP:OD1	2.52	0.43
4:D:148:VAL:HG12	4:D:191:TRP:CB	2.47	0.42
1:A:38:LYS:HB3	1:A:38:LYS:HE2	1.86	0.42
1:A:29:ASP:OD1	2:B:149:GLN:NE2	2.53	0.42
2:B:68:LEU:O	2:B:72:ARG:HG3	2.20	0.42
2:B:129:VAL:HG22	2:B:175:VAL:HG12	2.02	0.41
4:D:32:THR:HB	4:D:57:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:74:CIR:H52	3:C:74:CIR:H2	1.68	0.41
5:E:139:VAL:HG13	5:E:249:ALA:HB3	2.01	0.41
5:E:215:ASN:HD21	5:E:217:ARG:CZ	2.34	0.40
4:D:59:ALA:HB1	4:D:84(A):LYS:HD2	2.03	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	176/189 (93%)	172 (98%)	4 (2%)	0	100	100
2	B	176/198 (89%)	168 (96%)	8 (4%)	0	100	100
3	C	8/13 (62%)	8 (100%)	0	0	100	100
4	D	201/206 (98%)	190 (94%)	11 (6%)	0	100	100
5	E	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
All	All	800/847 (94%)	773 (97%)	27 (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	A	159/173 (92%)	157 (99%)	2 (1%)	69	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	154/177 (87%)	151 (98%)	3 (2%)	57	73
3	C	5/5 (100%)	5 (100%)	0	100	100
4	D	181/185 (98%)	180 (99%)	1 (1%)	86	90
5	E	214/215 (100%)	214 (100%)	0	100	100
All	All	713/755 (94%)	707 (99%)	6 (1%)	81	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	PHE
1	A	162	ASP
2	B	34	GLN
2	B	35	GLU
2	B	96	TYR
4	D	83	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	34	GLN
5	E	22	ASN
5	E	215	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue 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
3	CIR	C	74	3	9,10,11	2.36	4 (44%)	6,11,13	2.38	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	-	6/8/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	74	CIR	C7-N6	-4.17	1.29	1.34
3	C	74	CIR	O7-C7	-3.82	1.18	1.24
3	C	74	CIR	C3-C2	-3.11	1.49	1.53
3	C	74	CIR	C5-N6	-2.29	1.40	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	74	CIR	O7-C7-N6	-4.39	118.48	121.74
3	C	74	CIR	N8-C7-N6	2.89	119.90	116.85

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	74	CIR	C1-C2-C3-C4
3	C	74	CIR	O7-C7-N6-C5
3	C	74	CIR	N8-C7-N6-C5
3	C	74	CIR	N2-C2-C3-C4
3	C	74	CIR	C2-C3-C4-C5
3	C	74	CIR	C4-C5-N6-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	74	CIR	1	0



## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	A	203	-	5,5,5	0.42	0	5,5,5	0.47	0
7	GOL	D	301	-	5,5,5	0.41	0	5,5,5	0.32	0
7	GOL	B	202	-	5,5,5	0.36	0	5,5,5	0.46	0
7	GOL	A	204	-	5,5,5	0.47	0	5,5,5	1.00	0
7	GOL	C	300	-	5,5,5	0.41	0	5,5,5	0.58	0
6	NAG	B	201	2	14,14,15	0.68	1 (7%)	17,19,21	0.51	0
6	NAG	A	201	1	14,14,15	0.30	0	17,19,21	0.45	0
6	NAG	A	202	1	14,14,15	0.27	0	17,19,21	0.46	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	A	203	-	-	2/4/4/4	-
7	GOL	D	301	-	-	2/4/4/4	-
7	GOL	B	202	-	-	0/4/4/4	-
7	GOL	A	204	-	-	1/4/4/4	-
7	GOL	C	300	-	-	4/4/4/4	-
6	NAG	B	201	2	-	1/6/23/26	0/1/1/1
6	NAG	A	201	1	-	2/6/23/26	0/1/1/1
6	NAG	A	202	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	201	NAG	C1-C2	2.32	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	301	GOL	O1-C1-C2-O2
7	D	301	GOL	O1-C1-C2-C3
7	C	300	GOL	O1-C1-C2-C3
6	A	201	NAG	O5-C5-C6-O6
6	A	201	NAG	C4-C5-C6-O6
6	B	201	NAG	O5-C5-C6-O6
7	A	204	GOL	O1-C1-C2-C3
7	C	300	GOL	C1-C2-C3-O3
7	C	300	GOL	O1-C1-C2-O2
6	A	202	NAG	C4-C5-C6-O6
7	C	300	GOL	O2-C2-C3-O3
7	A	203	GOL	O1-C1-C2-O2
7	A	203	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	301	GOL	1	0
7	A	204	GOL	2	0
6	A	201	NAG	1	0
6	A	202	NAG	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	178/189 (94%)	0.46	11 (6%) 20 25	35, 54, 75, 84	0
2	B	180/198 (90%)	0.72	29 (16%) 1 1	34, 53, 114, 130	0
3	C	12/13 (92%)	0.35	0 100 100	35, 41, 51, 54	0
4	D	203/206 (98%)	0.20	7 (3%) 45 53	28, 40, 66, 97	0
5	E	241/241 (100%)	0.19	6 (2%) 57 66	26, 39, 62, 79	0
All	All	814/847 (96%)	0.37	53 (6%) 18 22	26, 45, 82, 130	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	142	VAL	5.0
2	B	165	PRO	4.8
2	B	161	LEU	4.6
2	B	167	SER	4.5
2	B	160	MET	4.4
1	A	165	VAL	4.3
2	B	188	TRP	4.1
2	B	164	VAL	4.0
5	E	130	ASN	4.0
2	B	114	LEU	3.8
2	B	136	GLN	3.6
2	B	140	THR	3.5
1	A	168	TRP	3.4
2	B	141	GLY	3.4
2	B	104	ALA	3.4
4	D	141	SER	3.3
4	D	129	GLN	3.3
2	B	2	ASP	3.3
5	E	238	ASP	3.2
1	A	99	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	168	GLY	3.2
2	B	143	VAL	3.0
2	B	3	THR	3.0
2	B	115	LEU	2.8
1	A	81	PRO	2.8
5	E	72	PRO	2.8
1	A	97	VAL	2.8
2	B	34	GLN	2.8
2	B	102	TYR	2.7
5	E	236	THR	2.7
2	B	186	VAL	2.7
1	A	179	GLU	2.6
2	B	132	PHE	2.6
2	B	166	ARG	2.6
1	A	171	ASP	2.6
2	B	172	THR	2.5
2	B	131	TRP	2.4
4	D	28	LYS	2.4
1	A	155	PRO	2.3
5	E	256	ASP	2.3
4	D	217	PRO	2.3
5	E	74	ARG	2.3
1	A	156	SER	2.3
2	B	139	LYS	2.3
2	B	170	VAL	2.3
1	A	98	GLU	2.3
2	B	163	THR	2.2
4	D	1	GLY	2.1
2	B	134	ASN	2.1
1	A	154	LEU	2.1
4	D	216	SER	2.1
4	D	59	ALA	2.1
2	B	171	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	CIR	C	74	11/12	0.94	0.20	32,32,46,46	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
7	GOL	B	202	6/6	0.71	0.43	76,80,84,87	0
6	NAG	A	201	14/15	0.73	0.45	77,81,88,96	0
6	NAG	B	201	14/15	0.76	0.44	70,78,83,87	0
7	GOL	A	203	6/6	0.82	0.30	59,66,70,81	0
7	GOL	C	300	6/6	0.86	0.23	40,51,58,61	0
7	GOL	D	301	6/6	0.88	0.46	49,62,69,71	0
7	GOL	A	204	6/6	0.91	0.20	48,49,52,60	0
6	NAG	A	202	14/15	0.91	0.31	57,68,83,95	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.