



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2020 – 02:40 PM EST

PDB ID : 6V1A
Title : immune receptor complex
Authors : Lim, J.J.; Rossjohn, J.
Deposited on : 2019-11-20
Resolution : 2.29 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 : 2.14.6
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

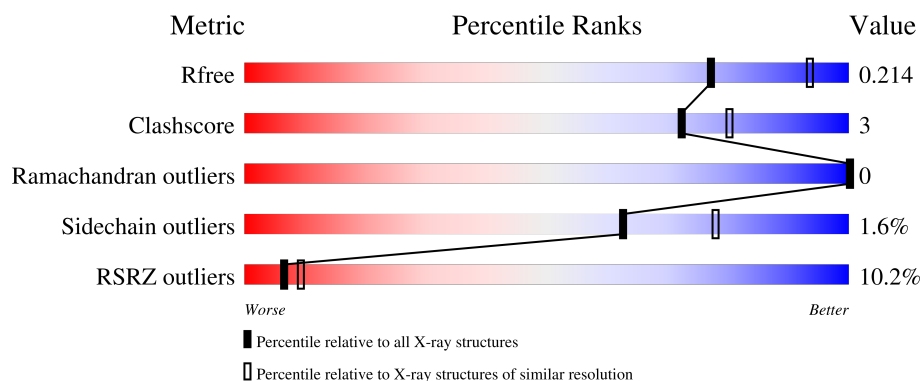
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	189	<div> <div>16%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>• 5%</div> </div> </div>
2	B	198	<div> <div>16%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>13%</div> </div> </div>
3	C	13	<div> <div></div> <div> <div></div> <div>85%</div> <div>15%</div> </div> </div>
4	D	209	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>• •</div> </div> </div>
5	E	242	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>11%</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	202	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6902 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	180	Total	C	N	O	S	0	0	0
			1438	934	235	264	5			

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
2	B	173	Total	C	N	O	S	0	0	0
			1402	890	243	265	4			

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 74cit69-81.

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

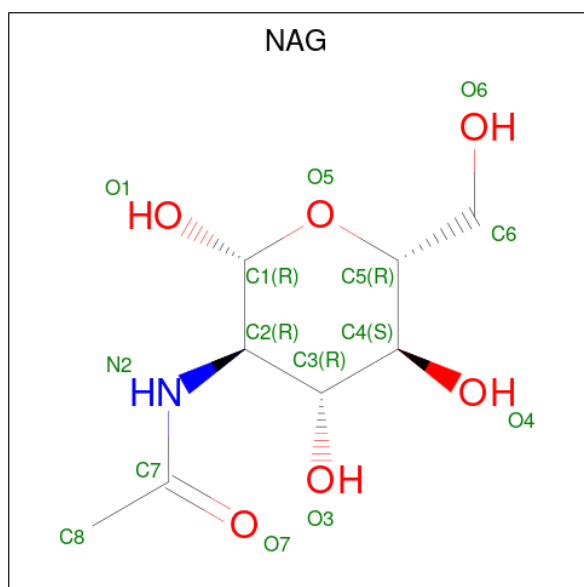
- Molecule 4 is a protein called M134 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	205	Total	C	N	O	S	0	0	0
			1571	985	255	324	7			

- Molecule 5 is a protein called M134 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	1	0
			1949	1234	338	370	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	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	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		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Na	0	0
			1	1		

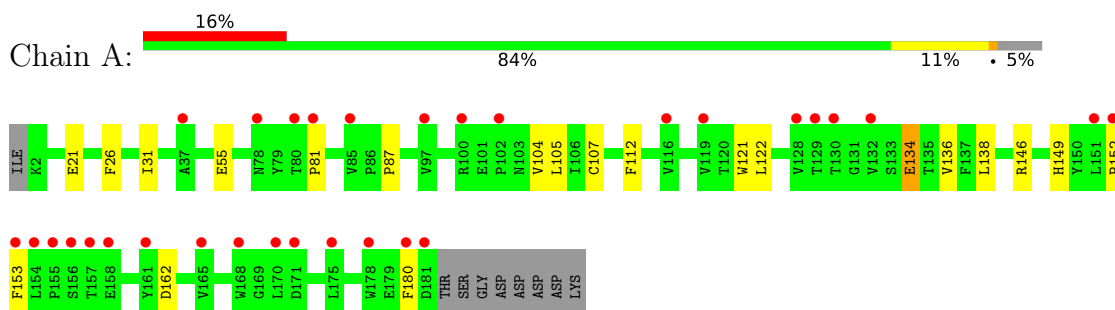
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	31	Total	O	0	0
			31	31		
9	B	31	Total	O	0	0
			31	31		
9	C	8	Total	O	0	0
			8	8		
9	D	101	Total	O	0	0
			101	101		
9	E	118	Total	O	0	0
			118	118		

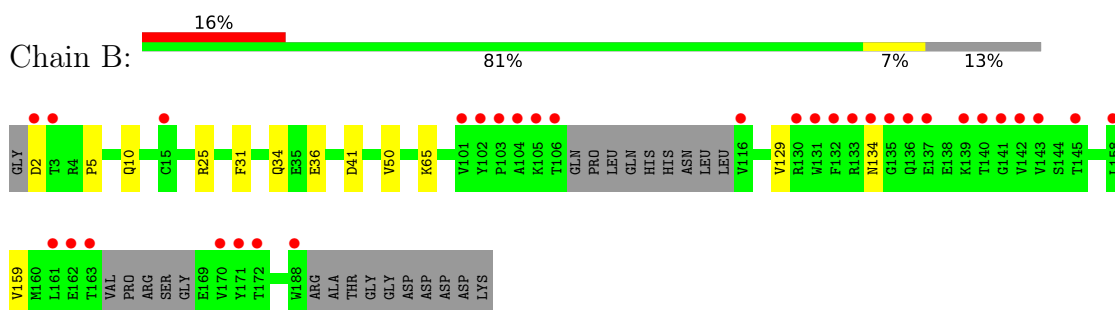
3 Residue-property plots

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.

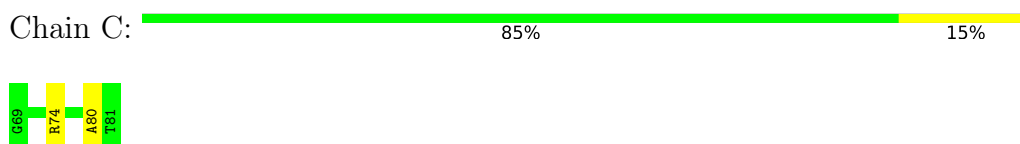
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



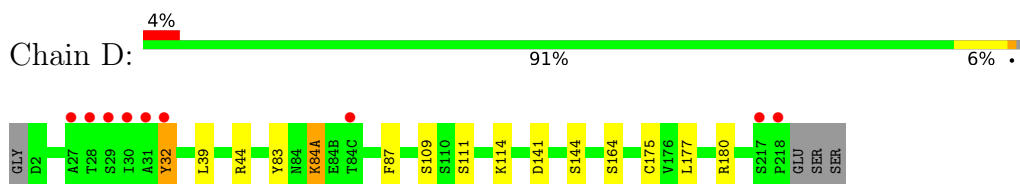
- Molecule 2: HLA class II histocompatibility antigen, DRB1-4 beta chain



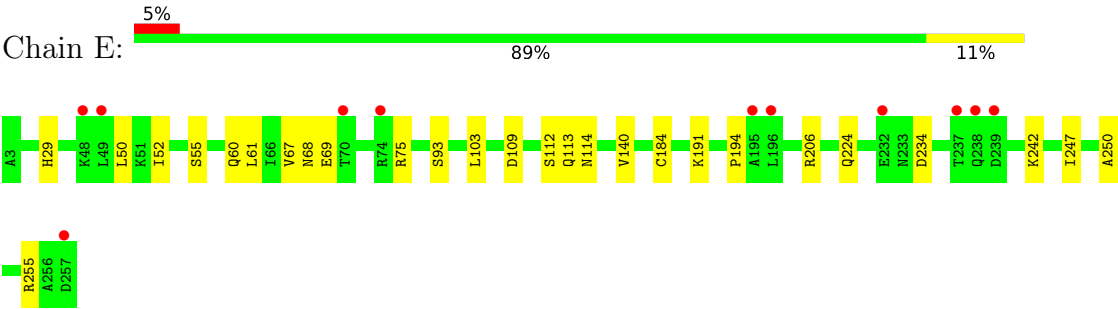
- Molecule 3: Fibrinogen beta 74cit69-81



- Molecule 4: M134 TCR alpha chain



- Molecule 5: M134 TCR beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.34Å 56.99Å 131.18Å 90.00° 90.87° 90.00°	Depositor
Resolution (Å)	43.72 – 2.29 43.72 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.72-2.29) 99.0 (43.72-2.29)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.187 , 0.214 0.187 , 0.214	Depositor DCC
R_{free} test set	2456 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6902	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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

5.1 Standard geometry

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

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	0.28	0/1483	0.44	0/2029
2	B	0.30	0/1440	0.45	0/1961
3	C	0.56	0/79	0.64	0/103
4	D	0.28	0/1604	0.49	0/2179
5	E	0.35	2/2005 (0.1%)	0.47	0/2731
All	All	0.31	2/6611 (0.0%)	0.47	0/9003

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	60[A]	GLN	C-O	7.10	1.36	1.23
5	E	60[B]	GLN	C-O	7.10	1.36	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1438	0	1343	11	0
2	B	1402	0	1275	6	0
3	C	90	0	89	1	0
4	D	1571	0	1484	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1949	0	1862	16	0
6	A	28	0	26	0	0
6	B	14	0	13	0	0
7	B	24	0	32	0	0
7	C	6	0	8	1	0
7	D	54	0	72	1	0
7	E	36	0	48	3	0
8	D	1	0	0	0	0
9	A	31	0	0	0	0
9	B	31	0	0	0	0
9	C	8	0	0	0	0
9	D	101	0	0	1	0
9	E	118	0	0	1	0
All	All	6902	0	6252	44	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 3.

All (44) 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)
2:B:10:GLN:HB2	2:B:31:PHE:HB2	1.73	0.71
1:A:87:PRO:HB3	1:A:112:PHE:HB3	1.82	0.61
5:E:52:ILE:HG23	5:E:69:GLU:HG3	1.83	0.61
5:E:67:VAL:HA	7:E:304:GOL:H32	1.84	0.60
1:A:138:LEU:HB2	1:A:146:ARG:HG3	1.84	0.58
5:E:109:ASP:OD1	5:E:114:ASN:ND2	2.35	0.57
5:E:55:SER:HB3	5:E:67:VAL:HB	1.87	0.56
5:E:255:ARG:HB3	7:E:303:GOL:H32	1.87	0.56
4:D:141:ASP:HB3	4:D:144:SER:O	2.07	0.55
4:D:177:LEU:HB3	5:E:184:CYS:HB2	1.89	0.55
3:C:80:ALA:HA	7:C:101:GOL:H11	1.91	0.53
5:E:75:ARG:HD2	5:E:93:SER:O	2.08	0.53
4:D:39:LEU:HD13	4:D:87:PHE:HB2	1.91	0.53
1:A:55:GLU:HG3	4:D:111:SER:HB3	1.91	0.52
4:D:32:TYR:HD1	4:D:32:TYR:O	1.93	0.52
4:D:84(A):LYS:H	4:D:84(A):LYS:CD	2.23	0.51
1:A:21:GLU:OE1	1:A:136:VAL:HB	2.12	0.50
4:D:84(A):LYS:H	4:D:84(A):LYS:HD3	1.77	0.49
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.94	0.49
2:B:129:VAL:HG11	2:B:159:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HB2	1:A:162:ASP:HB2	1.95	0.49
4:D:44:ARG:NE	9:E:401:HOH:O	2.48	0.47
5:E:140:VAL:HG23	5:E:250:ALA:HB3	1.97	0.47
1:A:104:VAL:HA	1:A:152:PRO:HA	1.97	0.46
4:D:114:LYS:HG3	5:E:52:ILE:HG21	1.97	0.46
2:B:65:LYS:HB3	5:E:29:HIS:HE2	1.80	0.46
5:E:234:ASP:O	5:E:242:LYS:NZ	2.40	0.46
5:E:50:LEU:HD11	5:E:103:LEU:HD12	1.97	0.45
4:D:109:SER:HA	5:E:112:SER:OG	2.16	0.45
4:D:180:ARG:NH2	9:D:404:HOH:O	2.48	0.45
1:A:81:PRO:HB3	2:B:5:PRO:HB2	1.99	0.44
4:D:32:TYR:O	4:D:32:TYR:CD1	2.70	0.44
7:E:301:GOL:H32	7:E:302:GOL:H2	2.00	0.44
4:D:84(A):LYS:HB2	4:D:84(A):LYS:HE2	1.79	0.43
2:B:25:ARG:NH2	2:B:41:ASP:OD2	2.51	0.43
1:A:105:LEU:HG	1:A:153:PHE:CE1	2.54	0.43
5:E:191:LYS:HE3	5:E:194:PRO:HA	1.99	0.43
4:D:32:TYR:C	4:D:32:TYR:CD1	2.93	0.42
5:E:224:GLN:HG3	5:E:247:ILE:HG23	2.02	0.42
5:E:61:LEU:HD21	5:E:68:ASN:HB2	2.01	0.42
1:A:107:CYS:HB2	1:A:121:TRP:CH2	2.56	0.41
1:A:134:GLU:HB2	1:A:149:HIS:CE1	2.56	0.41
4:D:164:SER:HA	7:D:309:GOL:H11	2.03	0.40
2:B:36:GLU:HG2	2:B:50:VAL:HG21	2.02	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	178/189 (94%)	175 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	167/198 (84%)	162 (97%)	5 (3%)	0	100	100
3	C	8/13 (62%)	8 (100%)	0	0	100	100
4	D	203/209 (97%)	198 (98%)	5 (2%)	0	100	100
5	E	241/242 (100%)	237 (98%)	4 (2%)	0	100	100
All	All	797/851 (94%)	780 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	154/173 (89%)	152 (99%)	2 (1%)	69	82
2	B	147/177 (83%)	144 (98%)	3 (2%)	55	72
3	C	5/5 (100%)	5 (100%)	0	100	100
4	D	180/187 (96%)	176 (98%)	4 (2%)	52	69
5	E	216/216 (100%)	214 (99%)	2 (1%)	78	89
All	All	702/758 (93%)	691 (98%)	11 (2%)	62	78

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	GLU
1	A	180	PHE
2	B	2	ASP
2	B	34	GLN
2	B	134	ASN
4	D	32	TYR
4	D	83	TYR
4	D	84(A)	LYS
4	D	175	CYS
5	E	113	GLN

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Mol	Chain	Res	Type
5	E	206	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	34	GLN
5	E	113	GLN

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	2.22	4 (44%)	6,11,13	2.12	3 (50%)

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	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	74	CIR	C7-N6	-4.32	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	74	CIR	O7-C7	-3.34	1.19	1.24
3	C	74	CIR	C3-C2	-2.39	1.50	1.53
3	C	74	CIR	C5-N6	-2.26	1.41	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	74	CIR	C5-N6-C7	-3.91	118.08	122.73
3	C	74	CIR	C3-C4-C5	-2.29	105.20	112.05
3	C	74	CIR	O7-C7-N6	-2.16	120.14	121.74

There are no chirality outliers.

All (5) 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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	B	202	-	5,5,5	0.36	0	5,5,5	0.20	0
6	NAG	A	201	1	14,14,15	0.20	0	17,19,21	0.54	0
7	GOL	E	305	-	5,5,5	0.09	0	5,5,5	0.32	0
7	GOL	D	305	-	5,5,5	0.35	0	5,5,5	0.23	0
7	GOL	E	301	-	5,5,5	0.36	0	5,5,5	0.28	0
7	GOL	D	306	-	5,5,5	0.37	0	5,5,5	0.27	0
7	GOL	B	204	-	5,5,5	0.37	0	5,5,5	0.27	0
7	GOL	D	304	-	5,5,5	0.36	0	5,5,5	0.32	0
6	NAG	B	201	2	14,14,15	0.24	0	17,19,21	0.55	0
7	GOL	D	302	-	5,5,5	0.37	0	5,5,5	0.31	0
7	GOL	B	203	-	5,5,5	0.38	0	5,5,5	0.25	0
7	GOL	D	310	-	5,5,5	0.09	0	5,5,5	0.32	0
7	GOL	E	306	-	5,5,5	0.09	0	5,5,5	0.32	0
7	GOL	C	101	-	5,5,5	0.37	0	5,5,5	0.22	0
7	GOL	D	308	-	5,5,5	0.38	0	5,5,5	0.29	0
6	NAG	A	202	1	14,14,15	0.23	0	17,19,21	0.41	0
7	GOL	E	304	-	5,5,5	0.39	0	5,5,5	0.15	0
7	GOL	D	309	-	5,5,5	0.36	0	5,5,5	0.30	0
7	GOL	E	302	-	5,5,5	0.37	0	5,5,5	0.24	0
7	GOL	B	205	-	5,5,5	0.37	0	5,5,5	0.29	0
7	GOL	D	307	-	5,5,5	0.39	0	5,5,5	0.27	0
7	GOL	E	303	-	5,5,5	0.09	0	5,5,5	0.32	0
7	GOL	D	303	-	5,5,5	0.36	0	5,5,5	0.29	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	B	202	-	-	4/4/4/4	-
6	NAG	A	201	1	-	2/6/23/26	0/1/1/1
7	GOL	E	305	-	-	2/4/4/4	-
7	GOL	D	305	-	-	2/4/4/4	-
7	GOL	E	301	-	-	2/4/4/4	-
7	GOL	D	306	-	-	3/4/4/4	-
7	GOL	B	204	-	-	2/4/4/4	-
7	GOL	D	304	-	-	1/4/4/4	-
6	NAG	B	201	2	-	2/6/23/26	0/1/1/1
7	GOL	D	302	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	203	-	-	3/4/4/4	-
7	GOL	D	310	-	-	2/4/4/4	-
7	GOL	E	306	-	-	2/4/4/4	-
7	GOL	C	101	-	-	4/4/4/4	-
7	GOL	D	308	-	-	2/4/4/4	-
6	NAG	A	202	1	-	2/6/23/26	0/1/1/1
7	GOL	E	304	-	-	3/4/4/4	-
7	GOL	D	309	-	-	2/4/4/4	-
7	GOL	E	302	-	-	2/4/4/4	-
7	GOL	B	205	-	-	2/4/4/4	-
7	GOL	D	307	-	-	2/4/4/4	-
7	GOL	E	303	-	-	2/4/4/4	-
7	GOL	D	303	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	202	GOL	O1-C1-C2-C3
7	D	305	GOL	O1-C1-C2-C3
7	E	301	GOL	O1-C1-C2-C3
7	B	204	GOL	O1-C1-C2-C3
7	D	310	GOL	O1-C1-C2-C3
7	C	101	GOL	O1-C1-C2-C3
7	C	101	GOL	O2-C2-C3-O3
7	E	304	GOL	O1-C1-C2-C3
7	D	309	GOL	O1-C1-C2-C3
7	E	302	GOL	O1-C1-C2-C3
7	B	205	GOL	O1-C1-C2-C3
7	D	307	GOL	O1-C1-C2-C3
7	E	304	GOL	O1-C1-C2-O2
7	B	205	GOL	O1-C1-C2-O2
7	B	202	GOL	C1-C2-C3-O3
7	E	305	GOL	O1-C1-C2-C3
7	D	306	GOL	O1-C1-C2-C3
7	D	306	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	D	304	GOL	O1-C1-C2-C3
7	D	302	GOL	O1-C1-C2-C3
7	B	203	GOL	C1-C2-C3-O3
7	E	306	GOL	O1-C1-C2-C3
7	C	101	GOL	C1-C2-C3-O3
7	D	308	GOL	O1-C1-C2-C3
7	E	303	GOL	C1-C2-C3-O3
6	B	201	NAG	O5-C5-C6-O6
7	B	202	GOL	O1-C1-C2-O2
7	D	305	GOL	O1-C1-C2-O2
7	D	306	GOL	O1-C1-C2-O2
7	B	204	GOL	O1-C1-C2-O2
7	D	302	GOL	O1-C1-C2-O2
7	C	101	GOL	O1-C1-C2-O2
7	E	302	GOL	O1-C1-C2-O2
7	E	301	GOL	O1-C1-C2-O2
7	D	310	GOL	O1-C1-C2-O2
7	D	309	GOL	O1-C1-C2-O2
7	D	307	GOL	O1-C1-C2-O2
6	A	202	NAG	C4-C5-C6-O6
7	B	202	GOL	O2-C2-C3-O3
7	E	305	GOL	O1-C1-C2-O2
7	B	203	GOL	O2-C2-C3-O3
7	D	308	GOL	O1-C1-C2-O2
7	E	303	GOL	O2-C2-C3-O3
6	A	202	NAG	O5-C5-C6-O6
7	E	304	GOL	C1-C2-C3-O3
7	B	203	GOL	O1-C1-C2-O2
6	A	201	NAG	C3-C2-N2-C7
6	B	201	NAG	C3-C2-N2-C7
7	E	306	GOL	O1-C1-C2-O2
6	A	201	NAG	C1-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	301	GOL	1	0
7	C	101	GOL	1	0
7	E	304	GOL	1	0
7	D	309	GOL	1	0
7	E	302	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	303	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 ⓘ

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, 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	180/189 (95%)	0.94	31 (17%) 1 1	39, 64, 93, 104	0
2	B	173/198 (87%)	1.05	32 (18%) 1 1	39, 59, 110, 131	0
3	C	12/13 (92%)	0.28	0 100 100	36, 40, 51, 62	0
4	D	205/209 (98%)	0.35	9 (4%) 34 41	30, 40, 73, 119	0
5	E	242/242 (100%)	0.44	11 (4%) 33 40	28, 38, 65, 92	0
All	All	812/851 (95%)	0.66	83 (10%) 6 9	28, 48, 92, 131	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	SER	7.0
2	B	106	THR	6.2
4	D	27	ALA	6.1
4	D	29	SER	5.8
4	D	28	THR	5.6
2	B	135	GLY	5.5
2	B	102	TYR	5.4
2	B	3	THR	5.4
2	B	140	THR	4.9
2	B	104	ALA	4.8
2	B	171	TYR	4.7
1	A	102	PRO	4.4
2	B	2	ASP	4.4
2	B	139	LYS	4.3
1	A	78	ASN	4.3
2	B	163	THR	4.3
1	A	180	PHE	4.0
4	D	30	ILE	4.0
2	B	133	ARG	4.0
2	B	131	TRP	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	116	VAL	3.9
4	D	31	ALA	3.8
2	B	142	VAL	3.8
2	B	158	LEU	3.8
1	A	81	PRO	3.8
2	B	134	ASN	3.5
2	B	105	LYS	3.5
2	B	145	THR	3.4
2	B	161	LEU	3.4
2	B	136	GLN	3.4
5	E	239	ASP	3.4
1	A	97	VAL	3.3
4	D	217	SER	3.3
2	B	103	PRO	3.2
2	B	188	TRP	3.2
1	A	157	THR	3.2
1	A	119	VAL	3.2
2	B	101	VAL	3.1
5	E	257	ASP	3.0
1	A	181	ASP	2.9
2	B	141	GLY	2.9
1	A	153	PHE	2.9
1	A	100	ARG	2.8
1	A	129	THR	2.8
2	B	170	VAL	2.8
2	B	132	PHE	2.7
2	B	130	ARG	2.7
1	A	155	PRO	2.6
1	A	130	THR	2.6
4	D	84(C)	THR	2.6
1	A	37	ALA	2.6
5	E	232	GLU	2.6
1	A	80	THR	2.6
2	B	143	VAL	2.6
1	A	132	VAL	2.6
2	B	162	GLU	2.6
5	E	74	ARG	2.6
5	E	238	GLN	2.6
1	A	154	LEU	2.5
1	A	165	VAL	2.5
1	A	171	ASP	2.5
2	B	172	THR	2.5

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Mol	Chain	Res	Type	RSRZ
5	E	237	THR	2.5
4	D	218	PRO	2.5
5	E	196	LEU	2.4
1	A	116	VAL	2.4
2	B	137	GLU	2.4
1	A	128	VAL	2.4
1	A	85	VAL	2.2
5	E	70	THR	2.2
1	A	151	LEU	2.2
1	A	168	TRP	2.2
1	A	175	LEU	2.2
5	E	49	LEU	2.2
1	A	178	TRP	2.1
1	A	158	GLU	2.1
1	A	170	LEU	2.1
5	E	195	ALA	2.1
2	B	15	CYS	2.1
1	A	161	TYR	2.0
4	D	32	TYR	2.0
1	A	152	PRO	2.0
5	E	48	LYS	2.0

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(\AA^2)	Q<0.9
3	CIR	C	74	11/12	0.87	0.24	47,49,60,62	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
6	NAG	A	202	14/15	0.49	0.51	124,130,135,136	0
7	GOL	D	306	6/6	0.68	0.31	84,90,91,99	0
7	GOL	E	303	6/6	0.68	0.32	81,87,90,99	0
7	GOL	D	310	6/6	0.70	0.28	82,100,101,102	0
7	GOL	E	301	6/6	0.71	0.29	84,86,89,98	0
7	GOL	E	304	6/6	0.72	0.15	71,75,82,87	0
7	GOL	E	305	6/6	0.74	0.29	81,85,94,98	0
6	NAG	B	201	14/15	0.77	0.27	96,109,115,118	0
7	GOL	B	205	6/6	0.79	0.29	82,85,88,90	0
7	GOL	D	305	6/6	0.81	0.20	58,73,78,82	0
7	GOL	B	204	6/6	0.82	0.19	82,102,104,109	0
7	GOL	C	101	6/6	0.82	0.27	75,81,83,92	0
6	NAG	A	201	14/15	0.82	0.35	107,117,135,140	0
7	GOL	E	306	6/6	0.83	0.27	50,63,65,66	0
7	GOL	B	202	6/6	0.83	0.34	65,75,81,85	0
7	GOL	D	309	6/6	0.86	0.27	80,82,84,88	0
7	GOL	E	302	6/6	0.86	0.28	72,86,93,98	0
7	GOL	D	302	6/6	0.87	0.25	63,69,70,71	0
7	GOL	D	307	6/6	0.88	0.24	85,88,96,101	0
7	GOL	B	203	6/6	0.88	0.14	65,76,84,84	0
8	NA	D	301	1/1	0.89	0.16	30,30,30,30	0
7	GOL	D	304	6/6	0.90	0.23	63,65,69,71	0
7	GOL	D	308	6/6	0.91	0.20	55,59,62,71	0
7	GOL	D	303	6/6	0.93	0.22	39,51,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.