Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 04:10 PM EST

PDB ID	:	6V18
Title	:	immune receptor complex
Authors	:	Lim, J.J.; Rossjohn, J.
Deposited on	:	2019-11-20
Resolution	:	2.35 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

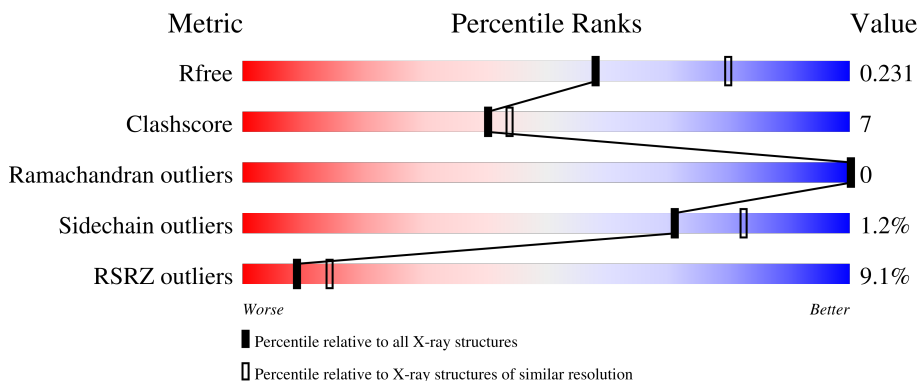|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	Percentile Ranks	Value
Rfree		0.231
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		1.2%
RSRZ outliers		9.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	7% 80% 14% 5%
2	B	198	23% 70% 19% • 10%
3	C	13	8% 92% 8%
4	D	209	4% 86% 11% ••
5	E	242	2% 88% 12%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 6722 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	179	Total 1425	C 927	N 234	O 259	S 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
2	B	178	Total 1403	C 888	N 248	O 262	S 5	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.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	206	Total 1580	C 991	N 257	O 324	S 8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total 1944	C 1231	N 338	O 368	S 7	0	0	0

• Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
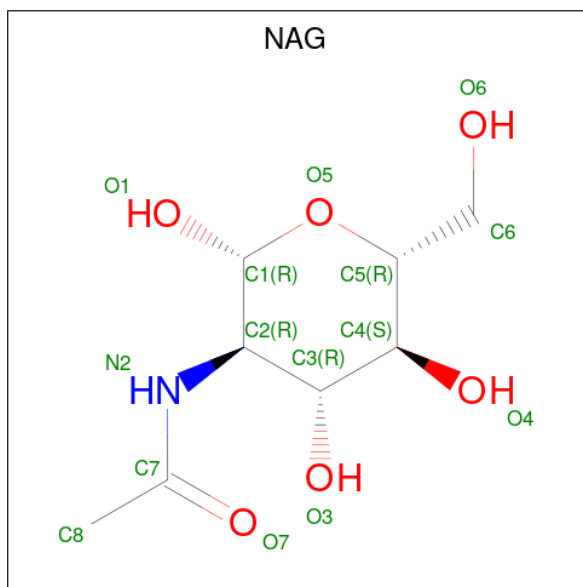
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 14	C 8	N 1	O 5	0	0
6	B	1	Total 14	C 8	N 1	O 5	0	0

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

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GOL

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

- Molecule 8 is water.

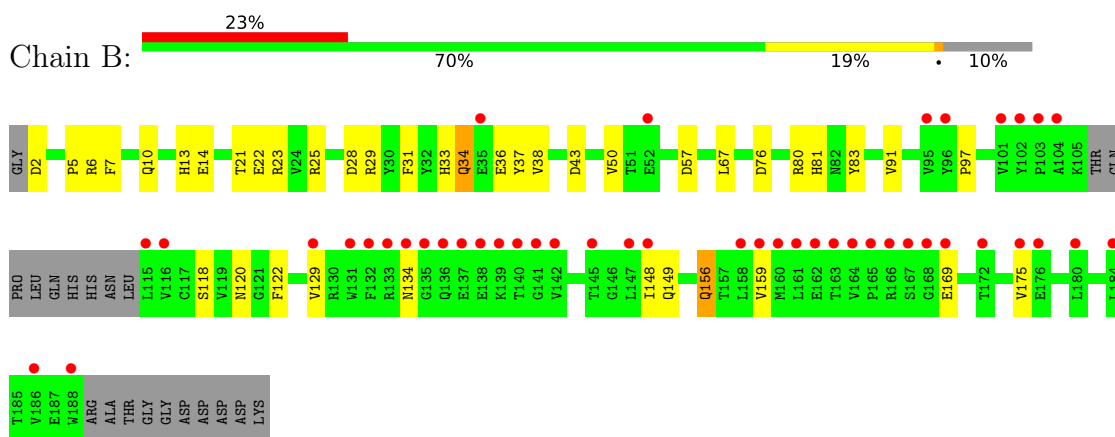| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	16	Total O 16 16		0	0
8	B	19	Total O 19 19		0	0
8	C	7	Total O 7 7		0	0
8	D	66	Total O 66 66		0	0
8	E	66	Total O 66 66		0	0

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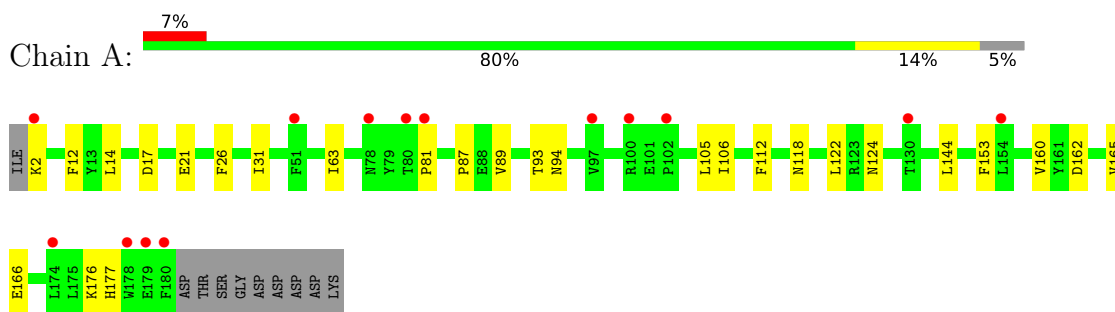
• Molecule 2: HLA class II histocompatibility antigen, DRB1-4 beta chain

• Molecule 3: Fibrinogen beta
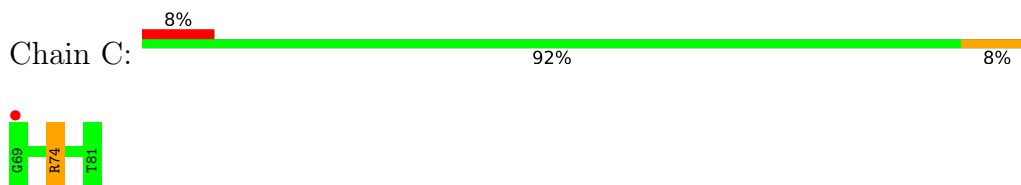
• Molecule 4: M141 TCR alpha chain

G1 I20 I21 A27 I30 A31 Y32 P33 N34 L39 K55 A59 Y83 N84 T84C T85 S86 F87 H88 L89 R122 D141 S144 S145 Y170 V176 L177 M182 D183 F184 N187 A191 W192 S193 F198 A199 C200 S217 P218 GLU SER SER
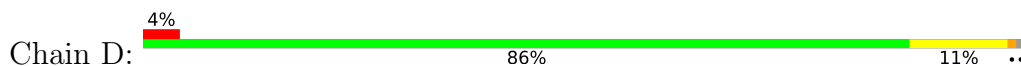
• Molecule 5: M141 TCR beta chain

Chain E:

2%

88%   12%

A3 T7 E18 N22 H29 V67 N68 R75 R90 I91 K92 S93 L103 S107 L108 Q113 R123 N131 V140 P143 K153 L156 H167 C184 P189 D198 V209 N216 N219 Q224 S231 K242 I247

A250 D257
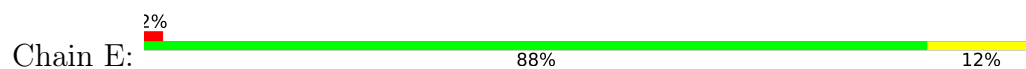
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	147.88Å 56.27Å 128.91Å 90.00° 91.35° 90.00°	Depositor
Resolution (Å)	48.83 – 2.35 48.83 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.83-2.35) 99.2 (48.83-2.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.193 , 0.231 0.193 , 0.231	Depositor DCC
R_{free} test set	2250 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	43.5	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6722	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CIR, 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	0.33	0/1470	0.48	0/2012
2	B	0.36	0/1441	0.54	0/1964
3	C	0.66	0/79	0.73	0/103
4	D	0.41	0/1614	0.60	0/2193
5	E	0.44	0/1997	0.58	0/2718
All	All	0.39	0/6601	0.56	0/8990

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 ⓘ

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	1425	0	1334	23	0
2	B	1403	0	1260	39	0
3	C	90	0	86	1	0
4	D	1580	0	1497	26	0
5	E	1944	0	1861	21	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
7	A	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	12	0	16	4	0
7	D	30	0	40	0	0
7	E	24	0	32	4	0
8	A	16	0	0	0	0
8	B	19	0	0	0	0
8	C	7	0	0	0	0
8	D	66	0	0	0	0
8	E	66	0	0	1	0
All	All	6722	0	6168	91	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 7.

All (91) 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:84:ASN:ND2	4:D:84(C):THR:CG2	1.87	1.35
1:A:144:LEU:HD21	2:B:34:GLN:NE2	1.56	1.19
4:D:84:ASN:ND2	4:D:84(C):THR:HG22	1.60	1.15
4:D:84:ASN:HD22	4:D:84(C):THR:CG2	1.50	1.13
2:B:134:ASN:HD21	2:B:169:GLU:CB	1.64	1.11
1:A:144:LEU:HD21	2:B:34:GLN:HE22	1.04	1.09
1:A:144:LEU:CD2	2:B:34:GLN:NE2	2.16	1.08
4:D:84:ASN:ND2	4:D:84(C):THR:HG23	1.74	1.02
4:D:84:ASN:HD22	4:D:84(C):THR:HG23	1.27	0.94
4:D:84:ASN:HD21	4:D:84(C):THR:HG22	1.33	0.90
1:A:144:LEU:HD23	2:B:34:GLN:HE21	1.40	0.87
1:A:144:LEU:CD2	2:B:34:GLN:HE21	1.88	0.83
4:D:34:ASN:HD21	5:E:113:GLN:HG2	1.45	0.80
4:D:84:ASN:HD22	4:D:84(C):THR:HG21	1.49	0.76
2:B:37:TYR:CD2	2:B:38:VAL:HG23	2.24	0.72
2:B:134:ASN:ND2	2:B:169:GLU:CB	2.48	0.72
5:E:231:SER:O	5:E:242:LYS:NZ	2.25	0.69
4:D:177:LEU:HB3	5:E:184:CYS:HB2	1.75	0.67
2:B:10:GLN:HB2	2:B:31:PHE:HB2	1.77	0.66
4:D:34:ASN:ND2	5:E:113:GLN:HG2	2.11	0.65
4:D:84(C):THR:OG1	4:D:84(C):THR:O	2.14	0.65
5:E:143:PRO:HD3	5:E:156:LEU:HG	1.80	0.64
1:A:87:PRO:HB3	1:A:112:PHE:HB3	1.79	0.64
1:A:144:LEU:HD23	2:B:34:GLN:NE2	2.01	0.62
4:D:84:ASN:ND2	4:D:84(C):THR:HG21	2.06	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:GLU:HG2	2:B:50:VAL:HG21	1.82	0.61
2:B:2:ASP:OD1	2:B:6:ARG:NH2	2.35	0.60
2:B:13:HIS:ND1	2:B:28:ASP:OD1	2.31	0.59
5:E:18:GLU:OE1	5:E:90:ARG:NH1	2.36	0.59
1:A:122:LEU:HB2	1:A:162:ASP:HB2	1.85	0.59
7:B:203:GOL:H2	4:D:55:LYS:HZ1	1.68	0.58
5:E:68:ASN:H	7:E:301:GOL:H2	1.68	0.58
5:E:75:ARG:HD2	5:E:93:SER:O	2.05	0.57
5:E:22:ASN:ND2	8:E:402:HOH:O	2.29	0.57
1:A:14:LEU:HD11	2:B:6:ARG:HB3	1.87	0.56
4:D:141:ASP:HB3	4:D:144:SER:O	2.04	0.56
5:E:209:VAL:HG12	7:E:304:GOL:H31	1.88	0.56
1:A:89:VAL:HG23	1:A:176:LYS:HG3	1.87	0.55
1:A:17:ASP:OD1	2:B:6:ARG:NH1	2.41	0.54
7:B:203:GOL:H2	4:D:55:LYS:NZ	2.23	0.54
2:B:22:GLU:HG2	2:B:23:ARG:HG3	1.90	0.52
2:B:81:HIS:HE1	4:D:32:TYR:CD2	2.28	0.52
2:B:38:VAL:HG21	2:B:57:ASP:HB2	1.93	0.51
5:E:189:PRO:HG3	7:E:303:GOL:H32	1.91	0.51
4:D:39:LEU:HB3	4:D:87:PHE:CD2	2.46	0.51
2:B:134:ASN:OD1	2:B:169:GLU:HA	2.11	0.50
1:A:12:PHE:CE2	1:A:21:GLU:HB2	2.46	0.50
2:B:14:GLU:OE2	2:B:29:ARG:NH1	2.40	0.49
4:D:176:VAL:HG22	4:D:187:ASN:OD1	2.13	0.49
4:D:85:THR:HG23	4:D:85:THR:O	2.12	0.49
5:E:224:GLN:HG3	5:E:247:ILE:HG23	1.95	0.48
2:B:148:ILE:HA	7:B:202:GOL:H2	1.96	0.48
1:A:93:THR:HG22	1:A:105:LEU:HD23	1.95	0.47
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.95	0.47
2:B:129:VAL:HG12	2:B:175:VAL:HG22	1.97	0.47
5:E:140:VAL:HG23	5:E:250:ALA:HB3	1.97	0.47
1:A:124:ASN:HA	1:A:160:VAL:HG13	1.97	0.47
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.96	0.46
2:B:21:THR:HB	2:B:80:ARG:HG2	1.97	0.46
5:E:216:ASN:HB3	5:E:219:ASN:ND2	2.29	0.46
5:E:29:HIS:HB3	5:E:107:SER:O	2.16	0.46
2:B:37:TYR:HD2	2:B:38:VAL:HG23	1.75	0.46
2:B:7:PHE:HA	2:B:33:HIS:HE1	1.81	0.45
4:D:27:ALA:HB1	4:D:30:ILE:HD12	1.99	0.45
2:B:118:SER:OG	2:B:120:ASN:OD1	2.30	0.45
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ASN:HB3	1:A:106:ILE:HD11	1.98	0.45
2:B:129:VAL:HG21	2:B:159:VAL:HG21	1.99	0.45
5:E:123:ARG:HD3	5:E:167:HIS:CE1	2.52	0.44
4:D:59:ALA:HA	4:D:83:TYR:CD2	2.52	0.44
1:A:63:ILE:HD13	1:A:63:ILE:HA	1.83	0.44
1:A:144:LEU:CD2	2:B:34:GLN:HE22	1.88	0.44
4:D:184:PHE:CD2	5:E:153:LYS:HE2	2.53	0.44
4:D:170:TYR:O	4:D:191:ALA:HA	2.17	0.43
4:D:21:ILE:HB	4:D:89:LEU:HB3	2.00	0.43
2:B:76:ASP:OD1	2:B:80:ARG:NH1	2.51	0.43
2:B:83:TYR:CZ	2:B:91:VAL:HG21	2.54	0.43
5:E:209:VAL:HB	7:E:304:GOL:H12	2.00	0.43
2:B:13:HIS:ND1	3:C:74:CIR:H42	2.34	0.42
2:B:67:LEU:HA	5:E:108:LEU:HD21	2.01	0.42
2:B:148:ILE:HD11	2:B:156:GLN:HG2	2.02	0.42
2:B:149:GLN:H	7:B:202:GOL:H2	1.84	0.42
4:D:182:MET:SD	5:E:153:LYS:HE3	2.59	0.42
4:D:193:SER:HB3	4:D:198:PHE:CG	2.55	0.41
2:B:25:ARG:HD2	2:B:43:ASP:OD2	2.20	0.41
1:A:89:VAL:HG11	1:A:165:VAL:HG21	2.02	0.41
2:B:129:VAL:CG2	2:B:159:VAL:HG21	2.51	0.41
5:E:18:GLU:HG3	5:E:92:LYS:HA	2.02	0.41
1:A:81:PRO:HB3	2:B:5:PRO:HB2	2.03	0.41
1:A:162:ASP:OD1	1:A:177:HIS:ND1	2.53	0.41
1:A:2:LYS:HA	2:B:91:VAL:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	177/189 (94%)	173 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	174/198 (88%)	166 (95%)	8 (5%)	0	100	100
3	C	10/13 (77%)	10 (100%)	0	0	100	100
4	D	204/209 (98%)	199 (98%)	5 (2%)	0	100	100
5	E	240/242 (99%)	234 (98%)	6 (2%)	0	100	100
All	All	805/851 (95%)	782 (97%)	23 (3%)	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	152/173 (88%)	151 (99%)	1 (1%)	84	91
2	B	142/177 (80%)	140 (99%)	2 (1%)	67	78
3	C	5/5 (100%)	5 (100%)	0	100	100
4	D	179/184 (97%)	175 (98%)	4 (2%)	52	63
5	E	215/215 (100%)	214 (100%)	1 (0%)	88	94
All	All	693/754 (92%)	685 (99%)	8 (1%)	71	82

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	PHE
2	B	34	GLN
2	B	156	GLN
4	D	83	TYR
4	D	84(C)	THR
4	D	85	THR
4	D	122	ARG
5	E	7	THR

Sometimes 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
4	D	34	ASN
4	D	84	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	1.95	2 (22%)	6,11,13	1.21	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
3	CIR	C	74	3	-	2/8/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	74	CIR	C7-N6	-3.70	1.30	1.34
3	C	74	CIR	O7-C7	-3.53	1.18	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	74	CIR	CA-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)

15 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	305	-	5,5,5	0.36	0	5,5,5	0.61	0
7	GOL	E	302	-	5,5,5	0.40	0	5,5,5	0.39	0
7	GOL	B	203	-	5,5,5	0.37	0	5,5,5	0.35	0
7	GOL	D	301	-	5,5,5	0.50	0	5,5,5	0.29	0
7	GOL	B	202	-	5,5,5	0.37	0	5,5,5	0.28	0
7	GOL	D	303	-	5,5,5	0.37	0	5,5,5	0.28	0
6	NAG	B	201	2	14,14,15	0.33	0	17,19,21	0.53	0
7	GOL	A	202	-	5,5,5	0.35	0	5,5,5	0.41	0
7	GOL	A	203	-	5,5,5	0.33	0	5,5,5	0.31	0
7	GOL	E	304	-	5,5,5	0.39	0	5,5,5	0.64	0
7	GOL	D	302	-	5,5,5	0.41	0	5,5,5	0.39	0
6	NAG	A	201	1	14,14,15	0.43	0	17,19,21	0.49	0
7	GOL	E	301	-	5,5,5	0.37	0	5,5,5	0.33	0
7	GOL	D	304	-	5,5,5	0.40	0	5,5,5	0.42	0
7	GOL	E	303	-	5,5,5	0.35	0	5,5,5	0.27	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	305	-	-	1/4/4/4	-
7	GOL	E	302	-	-	0/4/4/4	-
7	GOL	B	203	-	-	2/4/4/4	-
7	GOL	D	301	-	-	2/4/4/4	-
7	GOL	B	202	-	-	2/4/4/4	-
7	GOL	D	303	-	-	2/4/4/4	-
6	NAG	B	201	2	-	4/6/23/26	0/1/1/1
7	GOL	A	202	-	-	2/4/4/4	-
7	GOL	A	203	-	-	2/4/4/4	-
7	GOL	E	304	-	-	2/4/4/4	-
7	GOL	D	302	-	-	2/4/4/4	-
6	NAG	A	201	1	-	1/6/23/26	0/1/1/1
7	GOL	E	301	-	-	3/4/4/4	-
7	GOL	D	304	-	-	1/4/4/4	-
7	GOL	E	303	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	301	GOL	O1-C1-C2-C3
7	D	302	GOL	O1-C1-C2-C3
7	D	303	GOL	O1-C1-C2-O2
7	D	303	GOL	O1-C1-C2-C3
7	E	301	GOL	O1-C1-C2-C3
7	E	304	GOL	C1-C2-C3-O3
6	B	201	NAG	C4-C5-C6-O6
6	B	201	NAG	O5-C5-C6-O6
7	A	202	GOL	O1-C1-C2-C3
7	A	203	GOL	O1-C1-C2-C3
7	B	202	GOL	O1-C1-C2-C3
7	B	203	GOL	O1-C1-C2-C3
7	D	304	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	E	301	GOL	C1-C2-C3-O3
7	E	303	GOL	C1-C2-C3-O3
6	A	201	NAG	O5-C5-C6-O6
7	A	202	GOL	O1-C1-C2-O2
7	D	302	GOL	O1-C1-C2-O2
7	E	301	GOL	O1-C1-C2-O2
7	A	203	GOL	O1-C1-C2-O2
7	D	301	GOL	O1-C1-C2-O2
7	E	304	GOL	O2-C2-C3-O3
7	B	202	GOL	O1-C1-C2-O2
7	B	203	GOL	O1-C1-C2-O2
7	E	303	GOL	O2-C2-C3-O3
6	B	201	NAG	C3-C2-N2-C7
7	D	305	GOL	O1-C1-C2-C3
6	B	201	NAG	C1-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	203	GOL	2	0
7	B	202	GOL	2	0
7	E	304	GOL	2	0
7	E	301	GOL	1	0
7	E	303	GOL	1	0

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, 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	179/189 (94%)	0.73	14 (7%)	13	19	43, 69, 98, 108	0
2	B	178/198 (89%)	1.29	45 (25%)	0	1	45, 68, 108, 122	0
3	C	12/13 (92%)	0.77	1 (8%)	11	16	45, 52, 65, 67	0
4	D	206/209 (98%)	0.57	9 (4%)	34	46	36, 49, 71, 84	0
5	E	242/242 (100%)	0.66	5 (2%)	63	74	33, 44, 67, 91	0
All	All	817/851 (96%)	0.79	74 (9%)	9	14	33, 54, 95, 122	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	160	MET	6.3
1	A	102	PRO	6.0
2	B	168	GLY	5.9
2	B	165	PRO	5.8
2	B	132	PHE	5.4
2	B	131	TRP	5.3
2	B	147	LEU	5.2
2	B	134	ASN	5.0
2	B	167	SER	5.0
2	B	141	GLY	4.9
2	B	96	TYR	4.9
2	B	140	THR	4.8
2	B	115	LEU	4.8
1	A	2	LYS	4.8
1	A	180	PHE	4.7
2	B	142	VAL	4.7
2	B	161	LEU	4.4
3	C	69	GLY	4.4
2	B	166	ARG	4.3
2	B	164	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	100	ARG	4.3
1	A	154	LEU	4.0
2	B	184	LEU	4.0
2	B	101	VAL	4.0
2	B	129	VAL	3.9
2	B	139	LYS	3.8
2	B	133	ARG	3.8
2	B	136	GLN	3.7
2	B	163	THR	3.5
5	E	257	ASP	3.5
1	A	51	PHE	3.4
2	B	158	LEU	3.4
2	B	104	ALA	3.3
2	B	103	PRO	3.3
4	D	1	GLY	3.2
2	B	188	TRP	3.2
4	D	59	ALA	3.2
2	B	180	LEU	3.2
2	B	159	VAL	3.2
2	B	162	GLU	3.2
4	D	218	PRO	3.1
2	B	116	VAL	3.0
2	B	175	VAL	3.0
1	A	81	PRO	3.0
2	B	102	TYR	2.9
1	A	80	THR	2.9
4	D	200	CYS	2.8
2	B	137	GLU	2.8
4	D	32	TYR	2.8
2	B	145	THR	2.7
2	B	52	GLU	2.7
5	E	67	VAL	2.5
4	D	20	ILE	2.5
4	D	145	SER	2.5
1	A	78	ASN	2.5
1	A	179	GLU	2.4
5	E	131	ASN	2.4
4	D	217	SER	2.4
2	B	135	GLY	2.4
2	B	148	ILE	2.3
2	B	176	GLU	2.3
2	B	95	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	97	VAL	2.2
4	D	31	ALA	2.2
2	B	35	GLU	2.2
1	A	130	THR	2.2
2	B	172	THR	2.2
2	B	186	VAL	2.1
2	B	169	GLU	2.1
1	A	178	TRP	2.1
2	B	138	GLU	2.1
1	A	174	LEU	2.0
5	E	103	LEU	2.0
5	E	198	ASP	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, 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	0.94	0.16	50,55,60,66	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	304	6/6	0.67	0.32	78,82,85,89	0
7	GOL	E	301	6/6	0.69	0.23	77,83,87,89	0
6	NAG	B	201	14/15	0.70	0.25	86,100,105,109	0
7	GOL	D	305	6/6	0.76	0.27	77,78,83,99	0
7	GOL	D	301	6/6	0.78	0.26	72,76,81,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	A	201	14/15	0.78	0.24	85,100,108,109	0
7	GOL	D	304	6/6	0.80	0.24	85,89,93,96	0
7	GOL	A	203	6/6	0.80	0.20	74,79,89,89	0
7	GOL	D	303	6/6	0.82	0.26	65,71,79,86	0
7	GOL	B	202	6/6	0.83	0.18	79,82,86,87	0
7	GOL	E	303	6/6	0.85	0.30	74,76,86,91	0
7	GOL	E	302	6/6	0.90	0.20	79,82,88,95	0
7	GOL	B	203	6/6	0.91	0.19	65,73,81,83	0
7	GOL	D	302	6/6	0.92	0.29	47,62,64,73	0
7	GOL	A	202	6/6	0.92	0.25	64,74,75,76	0

6.5 Other polymers ⓘ

There are no such residues in this entry.