Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2023 – 10:04 AM EDT

PDB ID	:	3TWI
Title	:	Variable Lymphocyte Receptor Recognition of the Immunodominant Glycoprotein of Bacillus anthracis Spores
Authors	:	Kirchdoerfer, R.N.; Herrin, B.R.; Han, B.W.; Turnbough Jr., C.L.; Cooper, M.D.; Wilson, I.A.
Deposited on	:	2011-09-21
Resolution	:	2.55 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:

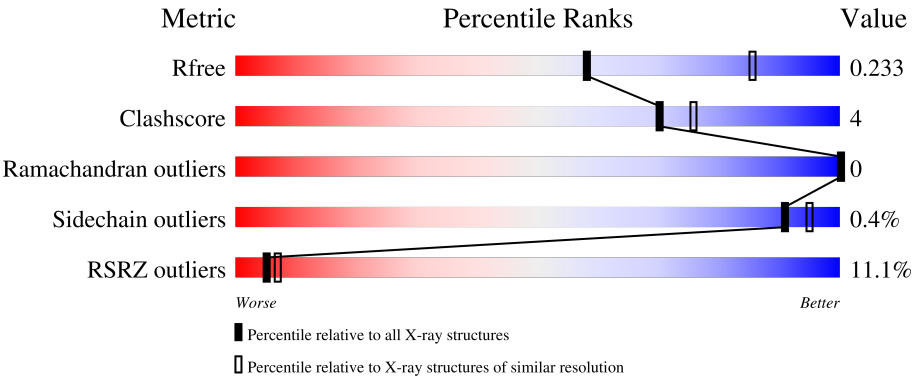
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	160	83% · 15%
1	B	160	% 77% 8% 15%
1	C	160	81% · · 15%
2	D	179	4% 94% 6%
2	E	179	3% 84% 8% 7%

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Mol	Chain	Length	Quality of chain
2	F	179	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6690 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 BclA protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	136	Total 956	C 617	N 149	O 190	0	0	0
1	B	136	Total 956	C 617	N 149	O 190	0	0	0
1	C	136	Total 956	C 617	N 149	O 190	0	0	0

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	expression tag	UNP Q81JD7
A	61	GLY	-	expression tag	UNP Q81JD7
A	62	SER	-	expression tag	UNP Q81JD7
A	63	SER	-	expression tag	UNP Q81JD7
A	64	HIS	-	expression tag	UNP Q81JD7
A	65	HIS	-	expression tag	UNP Q81JD7
A	66	HIS	-	expression tag	UNP Q81JD7
A	67	HIS	-	expression tag	UNP Q81JD7
A	68	HIS	-	expression tag	UNP Q81JD7
A	69	HIS	-	expression tag	UNP Q81JD7
A	70	GLU	-	expression tag	UNP Q81JD7
A	71	ASN	-	expression tag	UNP Q81JD7
A	72	LEU	-	expression tag	UNP Q81JD7
A	73	TYR	-	expression tag	UNP Q81JD7
A	74	PHE	-	expression tag	UNP Q81JD7
A	75	GLN	-	expression tag	UNP Q81JD7
A	76	GLY	-	expression tag	UNP Q81JD7
A	185	ASN	THR	engineered mutation	UNP Q81JD7
A	215	PHE	-	expression tag	UNP Q81JD7
A	216	ARG	-	expression tag	UNP Q81JD7
A	217	PHE	-	expression tag	UNP Q81JD7
A	218	ARG	-	expression tag	UNP Q81JD7
A	219	ASN	-	expression tag	UNP Q81JD7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	60	MET	-	expression tag	UNP Q81JD7
B	61	GLY	-	expression tag	UNP Q81JD7
B	62	SER	-	expression tag	UNP Q81JD7
B	63	SER	-	expression tag	UNP Q81JD7
B	64	HIS	-	expression tag	UNP Q81JD7
B	65	HIS	-	expression tag	UNP Q81JD7
B	66	HIS	-	expression tag	UNP Q81JD7
B	67	HIS	-	expression tag	UNP Q81JD7
B	68	HIS	-	expression tag	UNP Q81JD7
B	69	HIS	-	expression tag	UNP Q81JD7
B	70	GLU	-	expression tag	UNP Q81JD7
B	71	ASN	-	expression tag	UNP Q81JD7
B	72	LEU	-	expression tag	UNP Q81JD7
B	73	TYR	-	expression tag	UNP Q81JD7
B	74	PHE	-	expression tag	UNP Q81JD7
B	75	GLN	-	expression tag	UNP Q81JD7
B	76	GLY	-	expression tag	UNP Q81JD7
B	185	ASN	THR	engineered mutation	UNP Q81JD7
B	215	PHE	-	expression tag	UNP Q81JD7
B	216	ARG	-	expression tag	UNP Q81JD7
B	217	PHE	-	expression tag	UNP Q81JD7
B	218	ARG	-	expression tag	UNP Q81JD7
B	219	ASN	-	expression tag	UNP Q81JD7
C	60	MET	-	expression tag	UNP Q81JD7
C	61	GLY	-	expression tag	UNP Q81JD7
C	62	SER	-	expression tag	UNP Q81JD7
C	63	SER	-	expression tag	UNP Q81JD7
C	64	HIS	-	expression tag	UNP Q81JD7
C	65	HIS	-	expression tag	UNP Q81JD7
C	66	HIS	-	expression tag	UNP Q81JD7
C	67	HIS	-	expression tag	UNP Q81JD7
C	68	HIS	-	expression tag	UNP Q81JD7
C	69	HIS	-	expression tag	UNP Q81JD7
C	70	GLU	-	expression tag	UNP Q81JD7
C	71	ASN	-	expression tag	UNP Q81JD7
C	72	LEU	-	expression tag	UNP Q81JD7
C	73	TYR	-	expression tag	UNP Q81JD7
C	74	PHE	-	expression tag	UNP Q81JD7
C	75	GLN	-	expression tag	UNP Q81JD7
C	76	GLY	-	expression tag	UNP Q81JD7
C	185	ASN	THR	engineered mutation	UNP Q81JD7
C	215	PHE	-	expression tag	UNP Q81JD7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	216	ARG	-	expression tag	UNP Q81JD7
C	217	PHE	-	expression tag	UNP Q81JD7
C	218	ARG	-	expression tag	UNP Q81JD7
C	219	ASN	-	expression tag	UNP Q81JD7

- Molecule 2 is a protein called Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	168	Total	C	N	O	S	0	0	0
			1272	805	215	243	9			
2	E	166	Total	C	N	O	S	0	0	0
			1256	794	212	241	9			
2	F	117	Total	C	N	O	S	0	0	0
			893	570	155	162	6			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	10	ALA	-	expression tag	UNP A9Z0I5
D	11	MET	-	expression tag	UNP A9Z0I5
D	12	VAL	-	expression tag	UNP A9Z0I5
D	13	HIS	-	expression tag	UNP A9Z0I5
D	14	HIS	-	expression tag	UNP A9Z0I5
D	15	HIS	-	expression tag	UNP A9Z0I5
D	16	HIS	-	expression tag	UNP A9Z0I5
D	17	HIS	-	expression tag	UNP A9Z0I5
D	18	HIS	-	expression tag	UNP A9Z0I5
D	19	SER	-	expression tag	UNP A9Z0I5
D	20	ALA	-	expression tag	UNP A9Z0I5
E	10	ALA	-	expression tag	UNP A9Z0I5
E	11	MET	-	expression tag	UNP A9Z0I5
E	12	VAL	-	expression tag	UNP A9Z0I5
E	13	HIS	-	expression tag	UNP A9Z0I5
E	14	HIS	-	expression tag	UNP A9Z0I5
E	15	HIS	-	expression tag	UNP A9Z0I5
E	16	HIS	-	expression tag	UNP A9Z0I5
E	17	HIS	-	expression tag	UNP A9Z0I5
E	18	HIS	-	expression tag	UNP A9Z0I5
E	19	SER	-	expression tag	UNP A9Z0I5
E	20	ALA	-	expression tag	UNP A9Z0I5
F	10	ALA	-	expression tag	UNP A9Z0I5
F	11	MET	-	expression tag	UNP A9Z0I5

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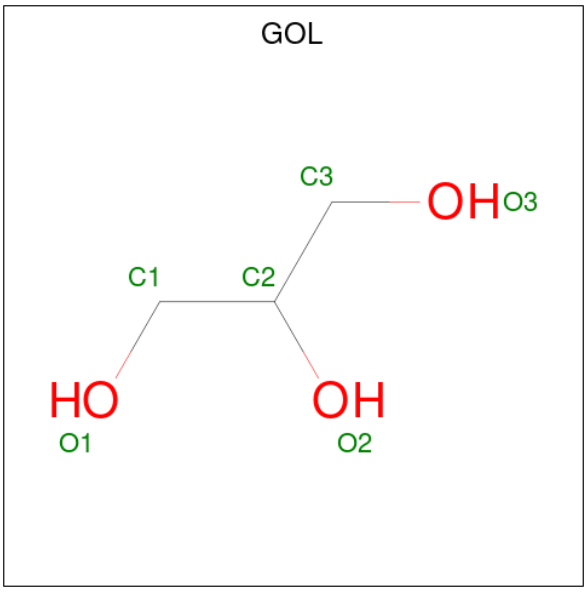
Chain	Residue	Modelled	Actual	Comment	Reference
F	12	VAL	-	expression tag	UNP A9Z0I5
F	13	HIS	-	expression tag	UNP A9Z0I5
F	14	HIS	-	expression tag	UNP A9Z0I5
F	15	HIS	-	expression tag	UNP A9Z0I5
F	16	HIS	-	expression tag	UNP A9Z0I5
F	17	HIS	-	expression tag	UNP A9Z0I5
F	18	HIS	-	expression tag	UNP A9Z0I5
F	19	SER	-	expression tag	UNP A9Z0I5
F	20	ALA	-	expression tag	UNP A9Z0I5

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	78	Total O 78 78	0	0
4	B	86	Total O 86 86	0	0

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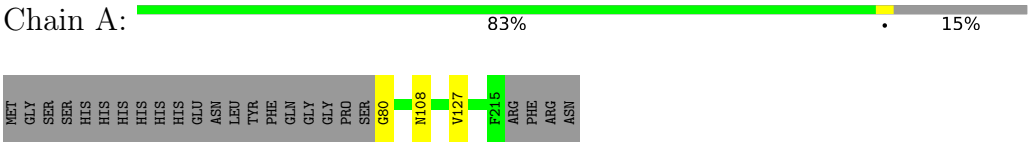
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	83	Total O 83 83	0	0
4	D	91	Total O 91 91	0	0
4	E	40	Total O 40 40	0	0
4	F	5	Total O 5 5	0	0

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.

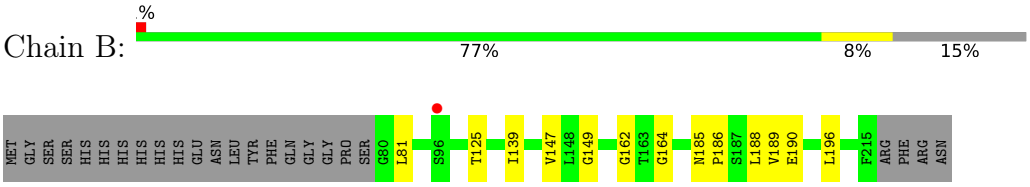
• Molecule 1: BclA protein

Chain A:



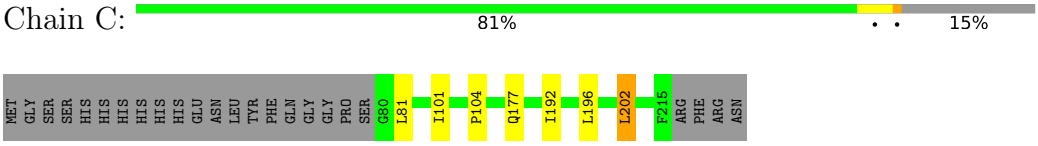
• Molecule 1: BclA protein

Chain B:



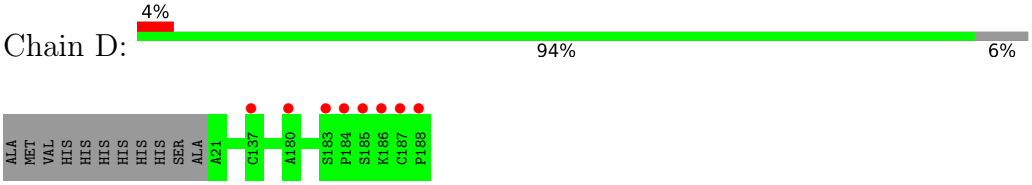
• Molecule 1: BclA protein

Chain C:



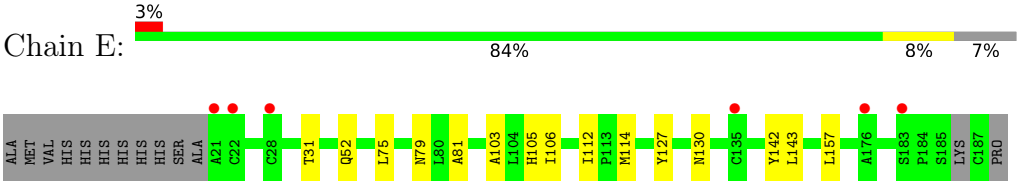
• Molecule 2: Variable lymphocyte receptor B

Chain D:



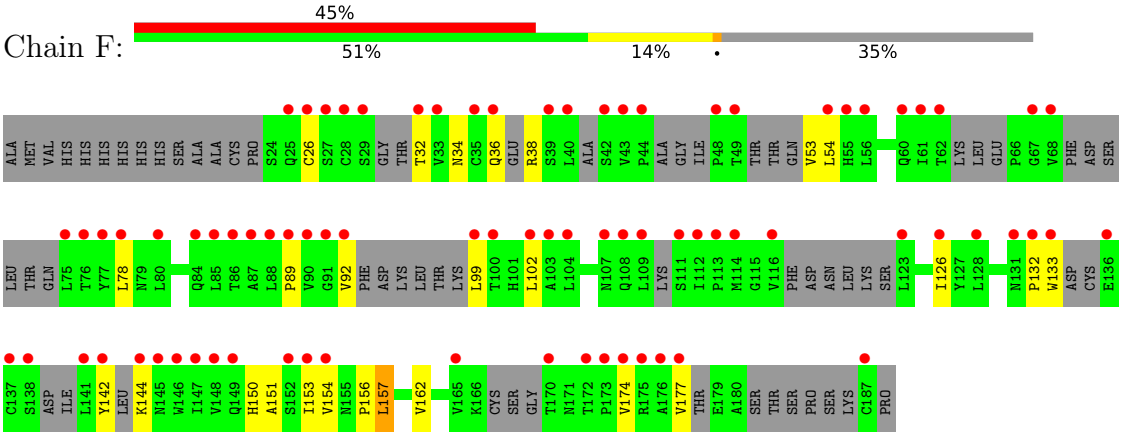
• Molecule 2: Variable lymphocyte receptor B

Chain E:



• Molecule 2: Variable lymphocyte receptor B

Chain F:


45%
51%
14%
35%
ALA MET VAL HIS HIS HIS HIS HIS HIS SER ALA ALA CYS PRO S24 Q25 C26 S27 C28 S29 GLY THR T32 V33 N34 C35 Q36 GLU R38 S39 L40 ALA S42 V43 P44 ALA GLY ILE P48 T49 THR THR GLN V53 L54 H55 L56 Q60 I61 T62 LYS LEU GLU P66 G67 V68 PHE ASP SER
LEU THR GLN L75 T76 Y77 L78 N79 L80 Q84 L85 T86 A87 L88 P89 V90 G91 V92 PHE ASP LYS LEU THR LYS L99 T100 H101 L102 A103 L104 N107 Q108 L109 LYS S111 I112 P113 M114 G115 V116 PHE ASP ASN LEU LYS SER L123 I126 Y127 L128 N131 P132 W133 ASP CYS E136
C137 S138 ASP ILE L141 Y142 LEU K144 N145 W146 I147 V148 Q149 H150 A151 S152 I153 V154 N155 P156 L157 V162 V165 K166 CYS SER GLY T170 N171 T172 P173 V174 R175 A176 V177 THR E179 A180 SER THR SER PRO SER LYS C187 PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	74.81Å 146.53Å 209.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.88 – 2.55 41.88 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.7 (41.88-2.55) 96.7 (41.88-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.189 , 0.233 0.191 , 0.233	Depositor DCC
R_{free} test set	1878 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6690	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.57	0/970	0.63	0/1330
1	B	0.50	0/970	0.61	0/1330
1	C	0.54	0/970	0.64	0/1330
2	D	0.52	0/1299	0.59	0/1779
2	E	0.43	0/1281	0.56	0/1753
2	F	0.38	0/896	0.50	0/1204
All	All	0.49	0/6386	0.59	0/8726

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	956	0	991	3	0
1	B	956	0	991	13	0
1	C	956	0	991	5	0
2	D	1272	0	1274	0	0
2	E	1256	0	1253	11	0
2	F	893	0	887	17	0
3	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	3	0
3	D	6	0	8	0	0
4	A	78	0	0	3	0
4	B	86	0	0	1	0
4	C	83	0	0	1	0
4	D	91	0	0	0	0
4	E	40	0	0	0	0
4	F	5	0	0	0	0
All	All	6690	0	6411	46	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 4.

All (46) 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:F:132:PRO:CA	2:F:133:TRP:N	2.43	0.81
2:E:31:THR:HG21	2:E:52:GLN:HE21	1.54	0.72
1:B:125:THR:HB	1:B:188:LEU:HD21	1.71	0.71
2:F:132:PRO:O	2:F:133:TRP:N	2.26	0.69
2:F:132:PRO:CA	2:F:132:PRO:O	2.41	0.68
2:F:142:TYR:O	2:F:144:LYS:N	2.31	0.64
1:B:162:GLY:H	3:B:1:GOL:H31	1.65	0.61
2:F:36:GLN:HG2	2:F:38:ARG:NH1	2.16	0.60
1:A:127:VAL:HG13	4:A:245:HOH:O	2.04	0.57
1:B:188:LEU:HD12	2:E:106:ILE:HG12	1.86	0.57
1:A:80:GLY:N	4:A:243:HOH:O	2.38	0.56
2:E:127:TYR:OH	2:E:157:LEU:HD22	2.05	0.55
2:E:52:GLN:O	2:E:75:LEU:HD12	2.06	0.55
2:F:99:LEU:HD21	2:F:102:LEU:HB2	1.87	0.55
2:F:151:ALA:HB1	2:F:162:VAL:HG21	1.90	0.54
2:F:26:CYS:HB2	2:F:34:ASN:O	2.08	0.54
2:F:126:ILE:HG22	2:F:153:ILE:O	2.10	0.51
2:E:31:THR:CG2	2:E:52:GLN:HE21	2.21	0.51
2:F:150:HIS:O	2:F:154:VAL:HG23	2.11	0.50
2:E:112:ILE:CD1	2:E:143:LEU:HD13	2.42	0.48
2:E:114:MET:CE	2:E:142:TYR:HB2	2.44	0.47
1:A:108:ASN:HB2	4:A:20:HOH:O	2.14	0.47
1:B:164:GLY:N	3:B:1:GOL:H11	2.30	0.46
2:F:156:PRO:HB2	2:F:157:LEU:HD13	1.97	0.46
1:B:147:VAL:CG1	1:B:196:LEU:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:112:ILE:HD13	2:E:143:LEU:HD13	1.97	0.46
1:B:164:GLY:H	3:B:1:GOL:H11	1.81	0.46
2:F:36:GLN:HG2	2:F:38:ARG:HH12	1.81	0.46
2:E:81:ALA:HB2	2:E:105:HIS:CE1	2.50	0.46
1:B:149:GLY:HA2	4:B:255:HOH:O	2.15	0.45
1:C:101:ILE:HG22	1:C:196:LEU:HA	1.98	0.45
2:F:174:VAL:HA	2:F:177:VAL:HG23	1.99	0.45
2:F:54:LEU:HD23	2:F:78:LEU:HD13	1.99	0.44
1:B:185:ASN:HA	1:B:186:PRO:HA	1.67	0.44
1:C:202:LEU:HD23	4:C:14:HOH:O	2.17	0.44
2:F:54:LEU:HD23	2:F:78:LEU:CD1	2.48	0.43
1:B:147:VAL:HG11	1:B:196:LEU:HB3	2.00	0.43
1:B:188:LEU:HD23	1:B:189:VAL:N	2.34	0.43
2:E:114:MET:HE2	2:E:142:TYR:HB2	2.01	0.42
1:B:139:ILE:HD12	1:C:177:GLN:HG2	2.01	0.42
2:F:32:THR:HG23	2:F:53:VAL:HB	2.01	0.41
2:E:79:ASN:HA	2:E:103:ALA:HB3	2.01	0.41
1:C:104:PRO:HA	1:C:192:ILE:HD13	2.02	0.41
1:B:125:THR:HG22	1:B:190:GLU:CG	2.51	0.41
2:F:89:PRO:HD2	2:F:92:VAL:HG11	2.03	0.40
1:B:81:LEU:HD12	1:C:81:LEU:HD12	2.04	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	134/160 (84%)	132 (98%)	2 (2%)	0	100	100
1	B	134/160 (84%)	131 (98%)	3 (2%)	0	100	100
1	C	134/160 (84%)	133 (99%)	1 (1%)	0	100	100
2	D	166/179 (93%)	157 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	163/179 (91%)	159 (98%)	4 (2%)	0	100	100
2	F	83/179 (46%)	71 (86%)	12 (14%)	0	100	100
All	All	814/1017 (80%)	783 (96%)	31 (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	106/127 (84%)	106 (100%)	0	100	100
1	B	106/127 (84%)	106 (100%)	0	100	100
1	C	106/127 (84%)	105 (99%)	1 (1%)	78	86
2	D	150/159 (94%)	150 (100%)	0	100	100
2	E	148/159 (93%)	147 (99%)	1 (1%)	84	90
2	F	105/159 (66%)	104 (99%)	1 (1%)	76	84
All	All	721/858 (84%)	718 (100%)	3 (0%)	91	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	202	LEU
2	E	130	ASN
2	F	157	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	52	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

3 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	$\#\|Z\| > 2$
3	GOL	D	2	-	5,5,5	0.45	0	5,5,5	0.25	0
3	GOL	A	3	-	5,5,5	0.50	0	5,5,5	0.39	0
3	GOL	B	1	-	5,5,5	0.37	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
3	GOL	D	2	-	-	0/4/4/4	-
3	GOL	A	3	-	-	0/4/4/4	-
3	GOL	B	1	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1	GOL	O1-C1-C2-C3
3	B	1	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	GOL	3	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	136/160 (85%)	0.03	0 100 100	24, 31, 45, 48	0
1	B	136/160 (85%)	-0.12	1 (0%) 87 90	25, 32, 39, 43	0
1	C	136/160 (85%)	-0.25	0 100 100	25, 33, 41, 44	0
2	D	168/179 (93%)	-0.01	8 (4%) 30 37	24, 36, 65, 86	0
2	E	166/179 (92%)	-0.08	6 (3%) 42 49	32, 50, 83, 106	0
2	F	117/179 (65%)	2.73	80 (68%) 0 0	60, 95, 147, 166	0
All	All	859/1017 (84%)	0.30	95 (11%) 5 7	24, 37, 106, 166	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	35	CYS	6.8
2	F	145	ASN	5.8
2	F	26	CYS	5.7
2	F	90	VAL	5.7
2	F	187	CYS	5.5
2	F	88	LEU	5.5
2	F	86	THR	5.0
2	F	109	LEU	5.0
2	F	137	CYS	5.0
2	F	80	LEU	5.0
2	F	85	LEU	5.0
2	F	112	ILE	4.9
2	F	174	VAL	4.9
2	F	89	PRO	4.8
2	F	114	MET	4.7
2	F	123	LEU	4.6
2	F	147	ILE	4.5
2	F	43	VAL	4.4
2	F	54	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
2	F	113	PRO	4.3
2	F	44	PRO	4.3
2	F	36	GLN	4.2
2	F	99	LEU	4.2
2	F	32	THR	4.1
2	D	188	PRO	4.0
2	F	75	LEU	4.0
2	D	187	CYS	3.9
2	F	42	SER	3.9
2	F	39	SER	3.9
2	F	33	VAL	3.9
2	F	77	TYR	3.8
2	F	92	VAL	3.7
2	F	29	SER	3.7
2	F	84	GLN	3.7
2	F	133	TRP	3.7
2	F	49	THR	3.7
2	F	108	GLN	3.6
2	F	40	LEU	3.6
2	F	48	PRO	3.5
2	D	185	SER	3.5
2	F	56	LEU	3.4
2	F	146	TRP	3.4
2	F	132	PRO	3.4
2	F	116	VAL	3.3
2	F	154	VAL	3.3
2	F	175	ARG	3.3
2	F	128	LEU	3.2
2	F	176	ALA	3.2
2	D	183	SER	3.2
2	F	102	LEU	3.2
2	F	67	GLY	3.2
2	F	87	ALA	3.2
2	F	170	THR	3.1
2	F	173	PRO	3.1
2	F	100	THR	3.1
2	E	183	SER	3.1
2	F	152	SER	3.1
2	F	55	HIS	3.0
2	F	144	LYS	3.0
2	F	27	SER	3.0
2	F	103	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	153	ILE	2.9
2	F	142	TYR	2.9
2	F	76	THR	2.9
2	F	177	VAL	2.8
2	F	62	THR	2.8
2	F	68	VAL	2.8
2	F	149	GLN	2.8
2	F	172	THR	2.7
2	F	148	VAL	2.7
2	E	21	ALA	2.7
2	F	28	CYS	2.7
2	F	61	ILE	2.7
2	F	111	SER	2.7
2	F	60	GLN	2.7
2	F	25	GLN	2.6
2	F	141	LEU	2.6
2	D	180	ALA	2.5
2	F	165	VAL	2.5
2	F	91	GLY	2.5
2	F	107	ASN	2.5
2	D	184	PRO	2.5
2	E	135	CYS	2.4
2	F	126	ILE	2.4
2	E	28	CYS	2.3
2	D	137	CYS	2.3
2	F	104	LEU	2.3
1	B	96	SER	2.3
2	D	186	LYS	2.2
2	E	22	CYS	2.2
2	F	138	SER	2.2
2	F	78	LEU	2.2
2	F	131	ASN	2.0
2	F	136	GLU	2.0
2	E	176	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no 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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	1	6/6	0.90	0.21	36,36,36,36	0
3	GOL	A	3	6/6	0.91	0.18	36,36,36,36	0
3	GOL	D	2	6/6	0.92	0.17	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.