Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 04:55 AM EDT

PDB ID	:	5BS0
Title	:	MAGE-A3 Reactive TCR in complex with Titin Epitope in HLA-A1
Authors	:	Raman, M.C.C.; Rizkallah, P.J.; Simmons, R.; Donellan, Z.; Dukes, J.; Bossi, G.; LeProvost, G.; Mahon, T.; Hickman, E.; Lomax, M.; Oates, J.; Hassan, N.; Vuidepot, A.; Sami, M.; Cole, D.K.; Jakobsen, B.K.
Deposited on	:	2015-06-01
Resolution	:	2.40 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

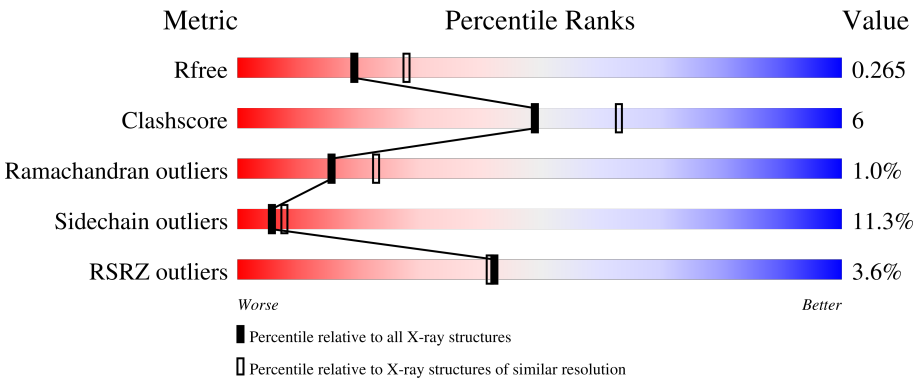
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	275	.% 82% 14% •
2	B	100	79% 18% •
3	C	9	89% 11%
4	D	197	11% 74% 22% •
5	E	241	2% 80% 17% •

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6635 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 I histocompatibility antigen, A-1 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	2235	1388	409	428	10	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	PRO	-	expression tag	UNP P30443

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	837	533	141	159	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Titin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	72	45	10	17	0	0	0

- Molecule 4 is a protein called Protein TRAV21,T-cell receptor alpha chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	197	1506	942	256	301	7	0	0	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	2	ALA	-	expression tag	UNP A0A0B4J279
D	50	TYR	LEU	conflict	UNP A0A0B4J279
D	51	VAL	ILE	conflict	UNP A0A0B4J279
D	52	ARG	GLN	conflict	UNP A0A0B4J279
D	53	PRO	SER	conflict	UNP A0A0B4J279
D	54	TYR	SER	conflict	UNP A0A0B4J279
D	95	PRO	-	linker	UNP A0A0B4J279
D	96	GLY	-	linker	UNP A0A0B4J279
D	97	GLY	-	linker	UNP A0A0B4J279
D	98	ALA	-	linker	UNP A0A0B4J279
D	99	GLY	-	linker	UNP A0A0B4J279
D	100	PRO	-	linker	UNP A0A0B4J279
D	101	PHE	-	linker	UNP A0A0B4J279
D	102	PHE	-	linker	UNP A0A0B4J279
D	103	VAL	-	linker	UNP A0A0B4J279
D	104	VAL	-	linker	UNP A0A0B4J279
D	105	PHE	-	linker	UNP A0A0B4J279
D	106	GLY	-	linker	UNP A0A0B4J279
D	107	LYS	-	linker	UNP A0A0B4J279
D	108	GLY	-	linker	UNP A0A0B4J279
D	109	THR	-	linker	UNP A0A0B4J279
D	110	LYS	-	linker	UNP A0A0B4J279
D	111	LEU	-	linker	UNP A0A0B4J279
D	112	SER	-	linker	UNP A0A0B4J279
D	113	VAL	-	linker	UNP A0A0B4J279
D	114	ILE	-	linker	UNP A0A0B4J279
D	115	PRO	-	linker	UNP A0A0B4J279
D	116	ASN	-	linker	UNP A0A0B4J279
D	163	CYS	THR	conflict	UNP P01848

- Molecule 5 is a protein called Protein TRBV5-1,Human nkt tcr beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	241	1914	1202	337	368	7	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	96	PHE	-	linker	UNP A0A578
E	97	ASN	-	linker	UNP A0A578
E	98	MET	-	linker	UNP A0A578
E	99	ALA	-	linker	UNP A0A578

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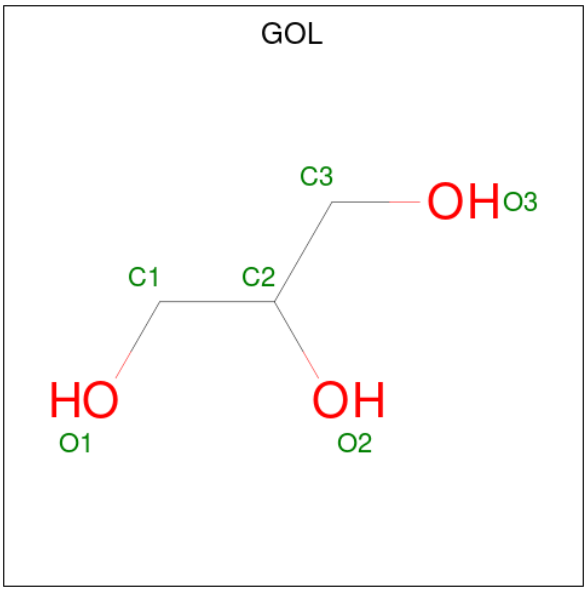
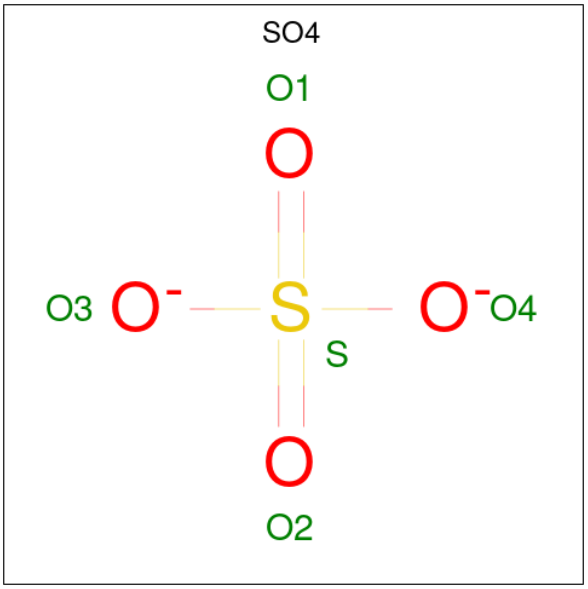
Chain	Residue	Modelled	Actual	Comment	Reference
E	100	THR	-	linker	UNP A0A578
E	101	GLY	-	linker	UNP A0A578
E	202	ASP	ASN	conflict	UNP K7N5M4

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	B	1	5	4	1	0	0
			Total	O	S		
7	D	1	5	4	1	0	0
			Total	O	S		
7	E	1	5	4	1	0	0
			Total	O	S		
7	E	1	5	4	1	0	0
			Total	O	S		
7	E	1	5	4	1	0	0
			Total	O	S		
7	E	1	5	4	1	0	0
			Total	O	S		
7	E	1	5	4	1	0	0
			Total	O	S		
7	E	1	5	4	1	0	0

- Molecule 8 is water.

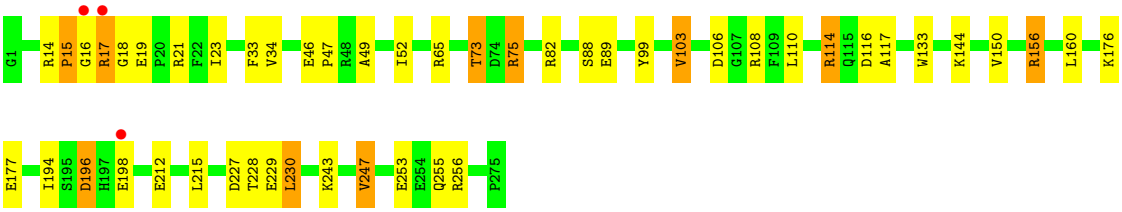
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	5	5	5	0	0
			Total	O		
8	D	1	1	1	0	0
			Total	O		
8	E	4	4	4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

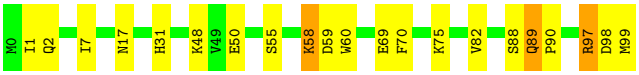
• Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain

Chain A:



• Molecule 2: Beta-2-microglobulin

Chain B:

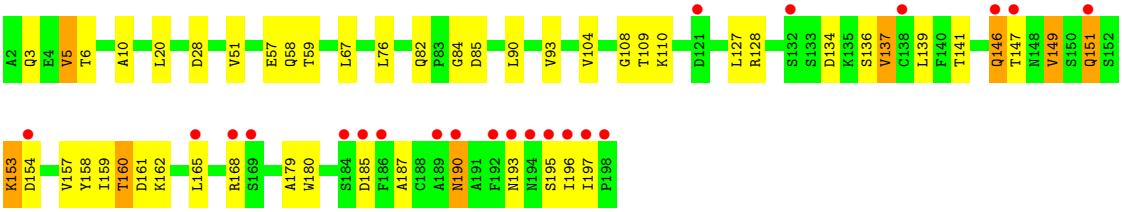


• Molecule 3: Titin

Chain C:

• Molecule 4: Protein TRAV21,T-cell receptor alpha chain C region

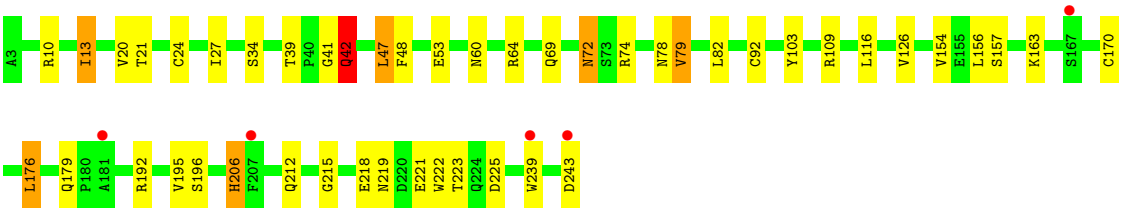
Chain D:



• Molecule 5: Protein TRBV5-1,Human nkt tcr beta chain

Chain E:

2%
80%
17%


A3
R10
I13
V20
T21
C24
I27
S34
T39
P40
G41
Q42
L47
F48
E53
N60
R64
Q69
N72
S73
R74
N78
V79
L82
C92
Y103
R109
L116
V126
V154
E155
L156
S157
K163
S167
C170
L176
Q179
P180
A181
R192
V195
S196
H206
F207
Q212
G215
E218
N219
D220
E221
W222
T223
Q224
D225
W239
D243

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	173.81Å 47.48Å 119.53Å 90.00° 109.36° 90.00°	Depositor
Resolution (Å)	81.82 – 2.40 81.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (81.82-2.40) 99.1 (81.99-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.203 , 0.262 0.208 , 0.265	Depositor DCC
R_{free} test set	1807 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6635	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.77	0/2296	0.92	6/3113 (0.2%)
2	B	0.73	0/860	0.83	0/1162
3	C	0.74	0/73	0.91	0/98
4	D	0.68	0/1537	0.83	0/2088
5	E	0.72	0/1966	0.81	1/2672 (0.0%)
All	All	0.73	0/6732	0.86	7/9133 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
5	E	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	A	114	ARG	NE-CZ-NH2	6.39	123.50	120.30
5	E	47	LEU	CA-CB-CG	5.99	129.07	115.30
1	A	16	GLY	N-CA-C	-5.94	98.24	113.10
1	A	75	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	A	65	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	82	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	84	GLY	Peptide
5	E	222	TRP	Peptide

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	2235	0	2093	23	0
2	B	837	0	803	11	0
3	C	72	0	66	2	0
4	D	1506	0	1457	20	0
5	E	1914	0	1811	24	0
6	A	6	0	8	0	0
7	A	15	0	0	0	1
7	B	5	0	0	0	0
7	D	5	0	0	0	0
7	E	30	0	0	0	0
8	A	5	0	0	0	0
8	D	1	0	0	0	0
8	E	4	0	0	0	0
All	All	6635	0	6238	76	1

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 6.

All (76) 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:17:ASN:OD1	2:B:97:ARG:NH2	2.01	0.93
5:E:72:ASN:HD22	5:E:72:ASN:C	1.97	0.68
4:D:187:ALA:HB1	4:D:190:ASN:HB3	1.78	0.66
1:A:228:THR:HG22	1:A:247:VAL:HG13	1.78	0.66
4:D:160:THR:HG23	4:D:161:ASP:O	1.97	0.65
1:A:73:THR:HG21	3:C:6:VAL:HG21	1.79	0.65
4:D:165:LEU:HD13	5:E:170:CYS:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:51:VAL:CG2	4:D:67:LEU:HD22	2.31	0.60
1:A:49:ALA:O	1:A:52:ILE:HG22	2.05	0.57
4:D:3:GLN:HE22	4:D:28:ASP:H	1.52	0.56
4:D:137:VAL:HG12	4:D:180:TRP:HB3	1.88	0.56
2:B:88:SER:O	2:B:89:GLN:NE2	2.38	0.55
1:A:99:TYR:HB3	1:A:114:ARG:HG2	1.88	0.55
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.41	0.55
5:E:20:VAL:O	5:E:78:ASN:ND2	2.41	0.53
5:E:20:VAL:HG13	5:E:82:LEU:HD11	1.91	0.53
1:A:230:LEU:HD21	1:A:243:LYS:HE3	1.91	0.53
5:E:53:GLU:H	5:E:69:GLN:HE21	1.56	0.53
1:A:114:ARG:NH2	1:A:116:ASP:OD2	2.41	0.53
4:D:160:THR:HG23	4:D:161:ASP:N	2.25	0.52
4:D:5:VAL:HG13	4:D:104:VAL:HG12	1.91	0.52
4:D:158:TYR:O	4:D:179:ALA:HA	2.10	0.51
4:D:151:GLN:HE21	4:D:151:GLN:HA	1.75	0.51
5:E:72:ASN:HD22	5:E:74:ARG:H	1.59	0.51
1:A:230:LEU:CD2	1:A:243:LYS:HE3	2.41	0.51
4:D:187:ALA:HB1	4:D:190:ASN:CB	2.41	0.51
5:E:206:HIS:HB3	5:E:239:TRP:CE3	2.46	0.50
5:E:64:ARG:O	5:E:79:VAL:HA	2.11	0.50
1:A:73:THR:HG21	3:C:6:VAL:CG2	2.41	0.50
5:E:221:GLU:HA	5:E:221:GLU:OE2	2.12	0.49
4:D:82:GLN:O	4:D:85:ASP:OD1	2.30	0.49
5:E:13:ILE:HD13	5:E:215:GLY:O	2.12	0.49
5:E:156:LEU:C	5:E:156:LEU:HD23	2.33	0.49
4:D:51:VAL:HG21	4:D:67:LEU:HD22	1.94	0.48
4:D:10:ALA:O	4:D:109:THR:HA	2.13	0.48
4:D:190:ASN:HA	4:D:193:ASN:HB2	1.95	0.48
2:B:89:GLN:HG3	2:B:90:PRO:HD2	1.94	0.48
5:E:72:ASN:ND2	5:E:74:ARG:H	2.11	0.48
2:B:7:ILE:HD13	2:B:82:VAL:HG21	1.95	0.48
1:A:19:GLU:OE1	1:A:75:ARG:HD2	2.14	0.48
2:B:2:GLN:HA	2:B:31:HIS:O	2.14	0.48
1:A:228:THR:CG2	1:A:247:VAL:HG13	2.44	0.47
1:A:133:TRP:HB2	1:A:144:LYS:HD2	1.96	0.47
1:A:17:ARG:CG	1:A:18:GLY:H	2.26	0.47
5:E:195:VAL:HG12	5:E:196:SER:H	1.79	0.47
2:B:98:ASP:O	2:B:99:MET:HG2	2.14	0.47
5:E:39:THR:O	5:E:42:GLN:O	2.33	0.46
1:A:196:ASP:OD1	1:A:196:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:147:THR:HG21	4:D:162:LYS:CE	2.46	0.46
5:E:206:HIS:HB3	5:E:239:TRP:CZ3	2.51	0.46
1:A:46:GLU:HB2	1:A:47:PRO:HD2	1.98	0.45
5:E:156:LEU:HD23	5:E:157:SER:N	2.30	0.45
1:A:46:GLU:HB2	1:A:47:PRO:CD	2.47	0.45
2:B:59:ASP:O	2:B:60:TRP:HB2	2.17	0.45
1:A:176:LYS:O	1:A:177:GLU:C	2.56	0.44
4:D:127:LEU:HD12	4:D:127:LEU:N	2.32	0.43
5:E:34:SER:O	5:E:92:CYS:HA	2.18	0.43
5:E:72:ASN:HD21	5:E:74:ARG:HB3	1.83	0.43
2:B:58:LYS:CD	2:B:58:LYS:H	2.32	0.42
5:E:154:VAL:HA	5:E:212:GLN:O	2.19	0.42
1:A:156:ARG:O	1:A:160:LEU:HG	2.19	0.42
4:D:147:THR:HG21	4:D:162:LYS:HE2	2.01	0.42
4:D:90:LEU:HD23	4:D:108:GLY:HA3	2.02	0.42
5:E:13:ILE:HD12	5:E:13:ILE:N	2.34	0.42
5:E:176:LEU:HD12	5:E:176:LEU:H	1.85	0.42
5:E:42:GLN:HE21	5:E:42:GLN:HB3	1.66	0.42
5:E:53:GLU:H	5:E:69:GLN:NE2	2.18	0.42
1:A:14:ARG:HA	1:A:15:PRO:HD2	1.87	0.41
2:B:89:GLN:HG3	2:B:90:PRO:CD	2.50	0.41
2:B:98:ASP:O	2:B:99:MET:CG	2.69	0.41
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.56	0.41
4:D:151:GLN:HE21	4:D:151:GLN:CA	2.33	0.41
1:A:253:GLU:OE1	1:A:256:ARG:HD2	2.20	0.41
1:A:212:GLU:HA	1:A:212:GLU:OE1	2.21	0.40
1:A:103:VAL:HA	1:A:108:ARG:O	2.21	0.40
5:E:41:GLY:C	5:E:42:GLN:O	2.60	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:304:SO4:O2	7:A:304:SO4:O2[2_7510]	1.60	0.60

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	273/275 (99%)	261 (96%)	10 (4%)	2 (1%)	22	32
2	B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	D	195/197 (99%)	173 (89%)	18 (9%)	4 (2%)	7	8
5	E	239/241 (99%)	226 (95%)	11 (5%)	2 (1%)	19	29
All	All	812/822 (99%)	761 (94%)	43 (5%)	8 (1%)	15	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	42	GLN
1	A	15	PRO
1	A	88	SER
4	D	149	VAL
4	D	153	LYS
4	D	146	GLN
5	E	218	GLU
4	D	196	ILE

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	232/232 (100%)	213 (92%)	19 (8%)	11	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	95/95 (100%)	85 (90%)	10 (10%)	7 9
3	C	8/8 (100%)	8 (100%)	0	100 100
4	D	170/170 (100%)	142 (84%)	28 (16%)	2 2
5	E	209/209 (100%)	185 (88%)	24 (12%)	5 7
All	All	714/714 (100%)	633 (89%)	81 (11%)	6 8

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	21	ARG
1	A	23	ILE
1	A	73	THR
1	A	89	GLU
1	A	103	VAL
1	A	106	ASP
1	A	110	LEU
1	A	150	VAL
1	A	156	ARG
1	A	194	ILE
1	A	196	ASP
1	A	198	GLU
1	A	215	LEU
1	A	227	ASP
1	A	229	GLU
1	A	230	LEU
1	A	247	VAL
1	A	255	GLN
2	B	1	ILE
2	B	48	LYS
2	B	50	GLU
2	B	55	SER
2	B	58	LYS
2	B	69	GLU
2	B	70	PHE
2	B	75	LYS
2	B	89	GLN
2	B	97	ARG
4	D	5	VAL
4	D	6	THR
4	D	20	LEU

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Mol	Chain	Res	Type
4	D	57	GLU
4	D	58	GLN
4	D	59	THR
4	D	76	LEU
4	D	93	VAL
4	D	110	LYS
4	D	128	ARG
4	D	134	ASP
4	D	136	SER
4	D	137	VAL
4	D	139	LEU
4	D	141	THR
4	D	146	GLN
4	D	149	VAL
4	D	151	GLN
4	D	153	LYS
4	D	154	ASP
4	D	157	VAL
4	D	159	ILE
4	D	160	THR
4	D	168	ARG
4	D	185	ASP
4	D	190	ASN
4	D	195	SER
4	D	197	ILE
5	E	10	ARG
5	E	13	ILE
5	E	21	THR
5	E	24	CYS
5	E	27	ILE
5	E	42	GLN
5	E	47	LEU
5	E	48	PHE
5	E	60	ASN
5	E	72	ASN
5	E	79	VAL
5	E	103	TYR
5	E	109	ARG
5	E	116	LEU
5	E	126	VAL
5	E	163	LYS
5	E	176	LEU

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Mol	Chain	Res	Type
5	E	179	GLN
5	E	192	ARG
5	E	206	HIS
5	E	219	ASN
5	E	223	THR
5	E	225	ASP
5	E	243	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	70	HIS
1	A	86	ASN
1	A	87	GLN
1	A	174	ASN
1	A	224	GLN
2	B	89	GLN
4	D	3	GLN
4	D	58	GLN
4	D	64	ASN
4	D	118	GLN
4	D	148	ASN
4	D	151	GLN
4	D	190	ASN
5	E	42	GLN
5	E	45	GLN
5	E	55	GLN
5	E	57	ASN
5	E	69	GLN
5	E	72	ASN
5	E	102	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	SO4	D	201	-	4,4,4	0.60	0	6,6,6	0.54	0
7	SO4	A	302	-	4,4,4	0.56	0	6,6,6	0.35	0
7	SO4	E	305	-	4,4,4	0.33	0	6,6,6	0.28	0
7	SO4	A	304	-	4,4,4	0.34	0	6,6,6	0.39	0
6	GOL	A	301	-	5,5,5	0.93	0	5,5,5	0.82	0
7	SO4	E	303	-	4,4,4	0.38	0	6,6,6	0.54	0
7	SO4	A	303	-	4,4,4	0.37	0	6,6,6	0.32	0
7	SO4	E	301	-	4,4,4	0.48	0	6,6,6	0.47	0
7	SO4	E	306	-	4,4,4	0.35	0	6,6,6	0.83	0
7	SO4	E	302	-	4,4,4	0.36	0	6,6,6	0.23	0
7	SO4	B	101	-	4,4,4	0.39	0	6,6,6	0.42	0
7	SO4	E	304	-	4,4,4	0.36	0	6,6,6	0.14	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
6	GOL	A	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	GOL	C1-C2-C3-O3
6	A	301	GOL	O2-C2-C3-O3
6	A	301	GOL	O1-C1-C2-C3
6	A	301	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	304	SO4	0	1

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	275/275 (100%)	0.06	3 (1%) 80 79	24, 47, 92, 109	0
2	B	100/100 (100%)	-0.04	0 100 100	29, 47, 74, 91	0
3	C	9/9 (100%)	-0.15	0 100 100	31, 36, 43, 49	0
4	D	197/197 (100%)	0.54	22 (11%) 5 4	30, 64, 116, 147	0
5	E	241/241 (100%)	0.09	5 (2%) 63 61	26, 51, 93, 123	0
All	All	822/822 (100%)	0.17	30 (3%) 42 42	24, 50, 102, 147	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	198	PRO	7.8
4	D	197	ILE	7.7
5	E	243	ASP	6.1
4	D	169	SER	5.5
4	D	168	ARG	4.5
4	D	186	PHE	4.4
4	D	195	SER	4.3
4	D	184	SER	4.0
4	D	196	ILE	3.9
4	D	132	SER	3.7
4	D	194	ASN	3.5
4	D	190	ASN	3.2
4	D	165	LEU	3.2
4	D	138	CYS	2.9
4	D	151	GLN	2.8
4	D	185	ASP	2.7
1	A	16	GLY	2.6
5	E	239	TRP	2.5
5	E	167	SER	2.4
1	A	17	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	181	ALA	2.3
4	D	121	ASP	2.2
4	D	147	THR	2.2
5	E	207	PHE	2.2
4	D	189	ALA	2.2
4	D	193	ASN	2.2
4	D	146	GLN	2.1
4	D	192	PHE	2.0
4	D	154	ASP	2.0
1	A	198	GLU	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, 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	GOL	A	301	6/6	0.77	0.29	53,60,61,61	0
7	SO4	B	101	5/5	0.83	0.34	76,94,107,108	0
7	SO4	E	305	5/5	0.89	0.19	87,88,92,96	0
7	SO4	E	303	5/5	0.90	0.17	72,75,83,90	0
7	SO4	A	304	5/5	0.92	0.33	64,85,119,121	2
7	SO4	E	304	5/5	0.93	0.71	121,137,139,145	0
7	SO4	E	301	5/5	0.93	0.34	76,82,88,91	0
7	SO4	E	302	5/5	0.94	0.31	79,92,96,97	0
7	SO4	A	302	5/5	0.94	0.14	55,65,71,76	0
7	SO4	D	201	5/5	0.96	0.30	50,70,75,82	0
7	SO4	A	303	5/5	0.97	0.13	66,71,74,79	0
7	SO4	E	306	5/5	0.97	0.13	48,49,55,56	0

6.5 Other polymers (i)

There are no such residues in this entry.