



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:15 PM UTC

PDB ID : 5BS0 / pdb_00005bs0
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

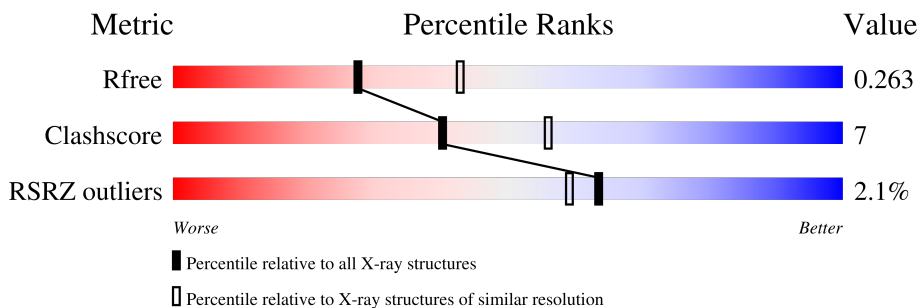
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	275	<div> <div>85%</div> <div>14%</div> <div>.</div> </div>
2	B	100	<div> <div>86%</div> <div>14%</div> </div>
3	C	9	<div> <div>89%</div> <div>11%</div> </div>
4	D	197	<div> <div>4%</div> <div>82%</div> <div>18%</div> </div>
5	E	241	<div> <div>2%</div> <div>87%</div> <div>13%</div> </div>

2 Entry composition

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
1	A	275	Total	C	N	O	S	0	0	0
			2235	1388	409	428	10			

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
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

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
3	C	9	Total	C	N	O	0	0	0
			72	45	10	17			

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

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

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
5	E	241	Total	C	N	O	S	0	0	0
			1914	1202	337	368	7			

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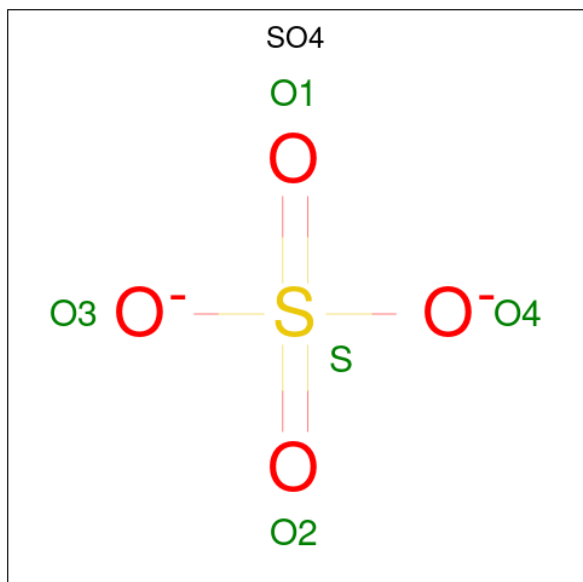
Chain	Residue	Modelled	Actual	Comment	Reference
E	100	THR	-	linker	UNP A0A578
E	101	GLY	-	linker	UNP A0A578
E	202	ASP	ASN	conflict	UNP K7N5M4

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

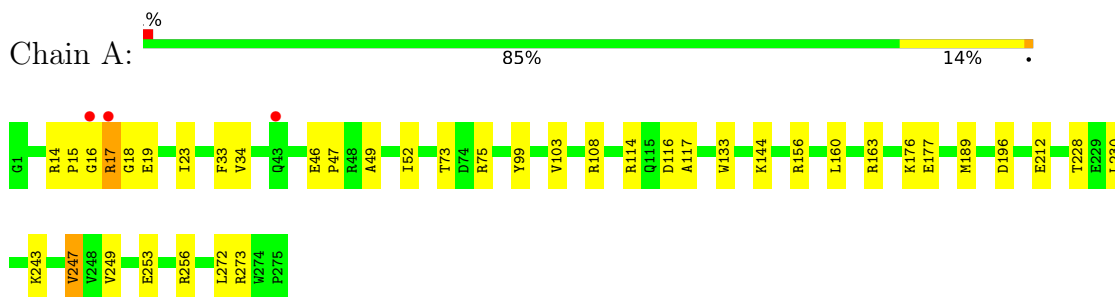
- Molecule 8 is water.

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

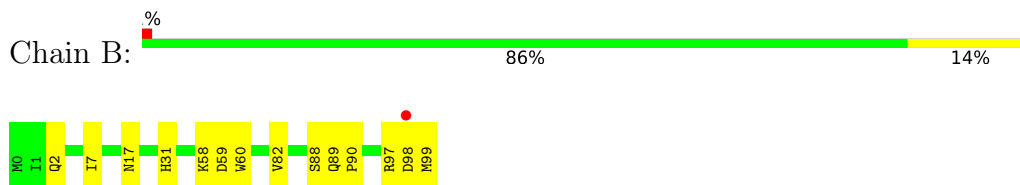
3 Residue-property plots

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.

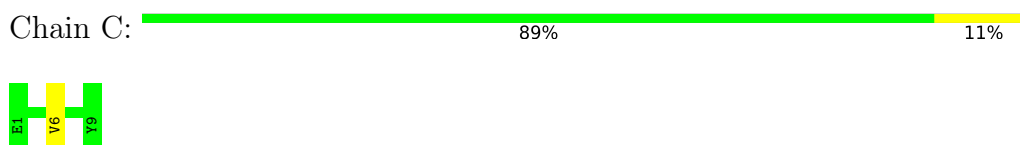
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



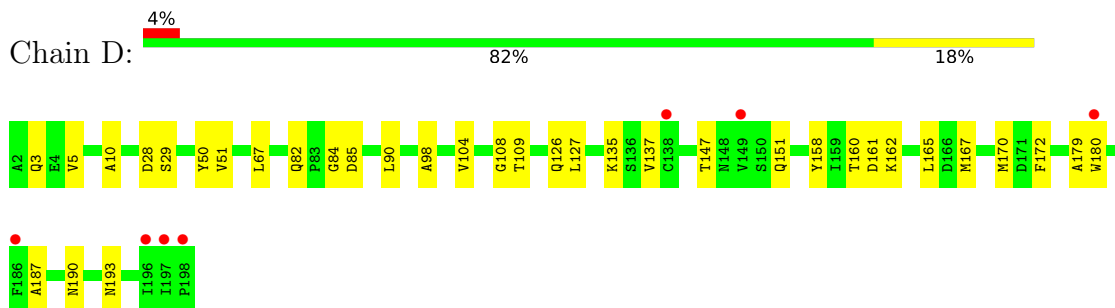
- Molecule 2: Beta-2-microglobulin



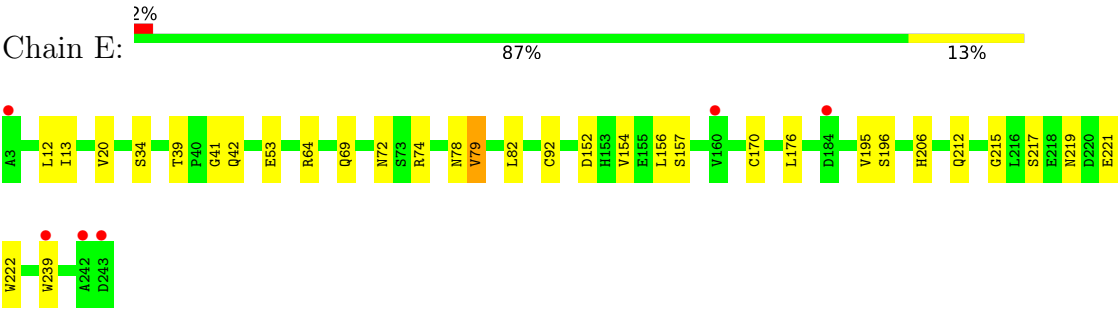
- Molecule 3: Titin



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



- Molecule 5: Protein TRBV5-1,Human nkt 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	173.81Å 47.48Å 119.53Å 90.00° 109.36° 90.00°	Depositor
Resolution (Å)	81.82 – 2.40 81.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (81.82-2.40) 94.8 (81.82-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.203 , 0.262 (Not available) , 0.263	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)	0.32 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

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: GOL, SO4

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	0.99	0/2296	1.07	6/3113 (0.2%)
2	B	0.97	0/860	1.00	0/1162
3	C	0.96	0/73	1.10	0/98
4	D	0.93	0/1537	1.08	5/2088 (0.2%)
5	E	0.95	0/1966	0.98	1/2672 (0.0%)
All	All	0.96	0/6732	1.04	12/9133 (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 (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	GLY	N-CA-C	-6.30	98.24	113.18
1	A	17	ARG	N-CA-C	6.19	116.02	107.73
4	D	98	ALA	N-CA-C	5.99	117.60	111.14
1	A	249	VAL	N-CA-C	5.77	113.92	109.19
4	D	50	TYR	CA-C-N	-5.75	115.60	123.14
4	D	50	TYR	C-N-CA	-5.75	115.60	123.14
4	D	135	LYS	N-CA-C	-5.72	102.01	110.48
1	A	163	ARG	N-CA-C	5.52	117.30	111.28
4	D	29	SER	N-CA-C	5.45	117.97	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	VAL	CB-CA-C	-5.30	102.66	110.82
5	E	79	VAL	CB-CA-C	5.14	118.06	110.77
1	A	23	ILE	N-CA-C	5.08	115.97	108.45

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

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	26	0
2	B	837	0	803	11	0
3	C	72	0	66	2	0
4	D	1506	0	1457	23	0
5	E	1914	0	1811	27	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	85	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 7.

All (85) 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	0.70
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
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
4:D:167:MET:HE3	4:D:172:PHE:CD2	2.40	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:156:LEU:C	5:E:156:LEU:HD23	2.33	0.54
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:170:MET:HA	4:D:170:MET:HE3	1.92	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
1:A:176:LYS:O	1:A:177:GLU:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:E:41:GLY:C	5:E:42:GLN:O	2.60	0.45
2:B:59:ASP:O	2:B:60:TRP:HB2	2.17	0.45
5:E:217:SER:C	5:E:219:ASN:H	2.25	0.44
1:A:189:MET:HE2	1:A:272:LEU:HB3	1.99	0.43
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
1:A:189:MET:HE1	1:A:273:ARG:CA	2.49	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:152:ASP:O	5:E:152:ASP:CG	2.61	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
4:D:126:GLN:C	4:D:127:LEU:HD12	2.46	0.40
5:E:12:LEU:C	5:E:13:ILE:HD12	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:VAL:HA	1:A:108:ARG:O	2.21	0.40
1:A:189:MET:HE1	1:A:273:ARG:C	2.46	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](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides 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	$\# Z > 2$
6	GOL	A	301	-	5,5,5	0.96	0	5,5,5	0.86	0
7	SO4	A	304	-	4,4,4	0.44	0	6,6,6	0.38	0
7	SO4	E	301	-	4,4,4	0.57	0	6,6,6	0.41	0
7	SO4	E	306	-	4,4,4	0.45	0	6,6,6	0.77	0
7	SO4	D	201	-	4,4,4	0.67	0	6,6,6	0.54	0
7	SO4	E	303	-	4,4,4	0.48	0	6,6,6	0.44	0
7	SO4	E	305	-	4,4,4	0.43	0	6,6,6	0.29	0
7	SO4	B	101	-	4,4,4	0.48	0	6,6,6	0.37	0
7	SO4	A	303	-	4,4,4	0.45	0	6,6,6	0.35	0
7	SO4	A	302	-	4,4,4	0.63	0	6,6,6	0.36	0
7	SO4	E	304	-	4,4,4	0.46	0	6,6,6	0.08	0
7	SO4	E	302	-	4,4,4	0.45	0	6,6,6	0.21	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
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

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	275/275 (100%)	-0.02	3 (1%) 78 74	24, 47, 92, 109	0
2	B	100/100 (100%)	-0.02	1 (1%) 79 76	29, 47, 74, 91	0
3	C	9/9 (100%)	-0.48	0 100 100	31, 36, 43, 49	0
4	D	197/197 (100%)	0.36	7 (3%) 46 42	30, 64, 116, 147	0
5	E	241/241 (100%)	0.15	6 (2%) 58 54	26, 51, 93, 123	0
All	All	822/822 (100%)	0.12	17 (2%) 63 59	24, 50, 102, 147	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	197	ILE	4.6
4	D	138	CYS	3.7
1	A	16	GLY	3.5
4	D	198	PRO	3.4
5	E	242	ALA	3.0
1	A	17	ARG	2.9
4	D	196	ILE	2.7
5	E	239	TRP	2.6
4	D	149	VAL	2.3
5	E	3	ALA	2.3
5	E	243	ASP	2.2
5	E	160	VAL	2.1
4	D	180	TRP	2.1
2	B	98	ASP	2.1
5	E	184	ASP	2.1
1	A	43	GLN	2.0
4	D	186	PHE	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 oligosaccharides 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(\AA^2)	Q<0.9
7	SO4	E	302	5/5	0.81	0.07	79,92,96,97	0
6	GOL	A	301	6/6	0.83	0.14	53,60,61,61	0
7	SO4	E	305	5/5	0.83	0.09	87,88,92,96	0
7	SO4	E	303	5/5	0.85	0.11	72,75,83,90	0
7	SO4	E	301	5/5	0.85	0.12	76,82,88,91	0
7	SO4	E	304	5/5	0.86	0.17	121,137,139,145	0
7	SO4	A	304	5/5	0.86	0.10	64,85,119,121	2
7	SO4	B	101	5/5	0.88	0.12	76,94,107,108	0
7	SO4	A	303	5/5	0.91	0.11	66,71,74,79	0
7	SO4	A	302	5/5	0.92	0.13	55,65,71,76	0
7	SO4	D	201	5/5	0.93	0.21	50,70,75,82	0
7	SO4	E	306	5/5	0.97	0.08	48,49,55,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.