Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:31 pm BST

PDB ID	:	5BRZ
Title	:	MAGE-A3 reactive TCR in complex with MAGE-A3 in HLA-A1
Authors	:	Raman, M.C.C.; Rizkallah, P.J.; Simmons, R.; Donnellan, 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	:	2.62 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

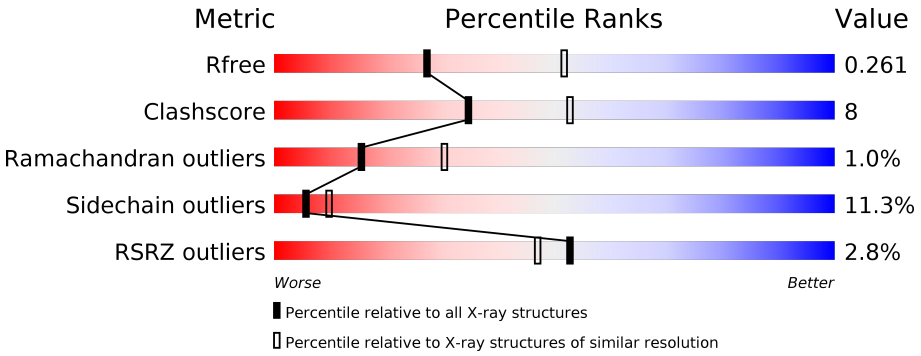
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	83% 16%
2	B	100	76% 21%
3	C	9	44% 44% 11%
4	D	197	11% 66% 26% 8%
5	E	241	73% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	A	302	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6618 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 GLU-VAL-ASP-PRO-ILE-GLY-HIS-LEU-TYR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			74	48	11	15			

- 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 30 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	117	ILE	-	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 8 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

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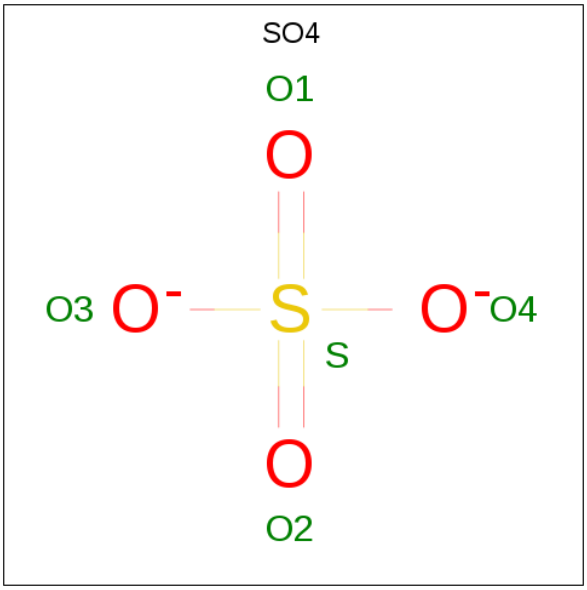
Chain	Residue	Modelled	Actual	Comment	Reference
E	99	ALA	-	linker	UNP A0A578
E	100	THR	-	linker	UNP A0A578
E	101	GLY	-	linker	UNP A0A578
E	202	ASP	ASN	conflict	UNP K7N5M4
E	243	ASP	-	expression tag	UNP K7N5M4

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is water.

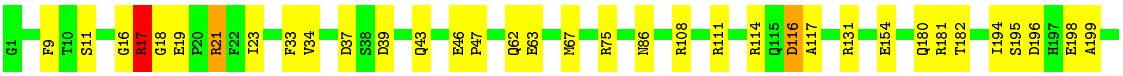
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	9	Total O 9 9	0	0
7	B	1	Total O 1 1	0	0
7	C	1	Total O 1 1	0	0
7	E	6	Total O 6 6	0	0

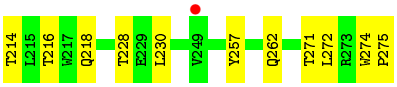
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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:



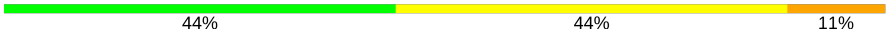


- Molecule 2: Beta-2-microglobulin

Chain B:

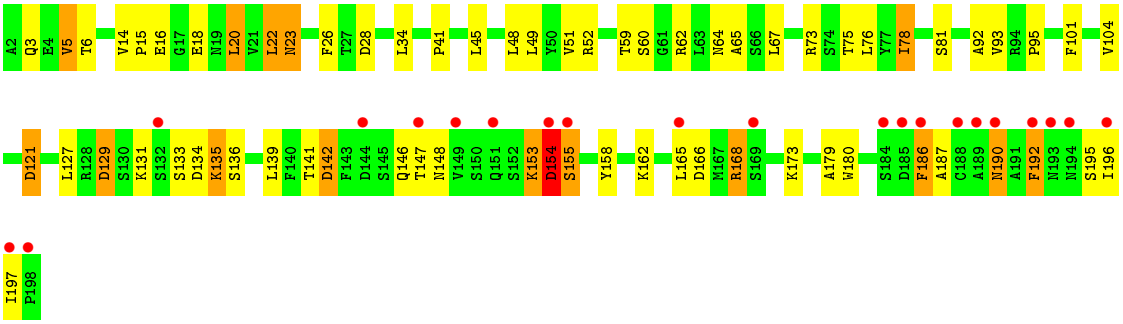
- Molecule 3: GLU-VAL-ASP-PRO-ILE-GLY-HIS-LEU-TYR

Chain C:



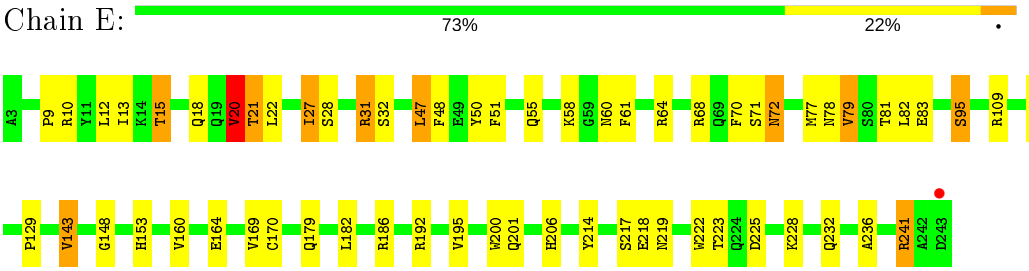
- Molecule 4: Protein TRAV21,T-cell receptor alpha chain C region

Chain D:



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

Chain E:


73%
22%
A3
P9
R10
Y11
L12
I13
K14
T15
Q18
Q19
V20
T21
L22
I27
S28
R31
S32
L47
F48
E49
Y50
F51
Q55
K58
G59
N60
F61
R64
R68
Q69
F70
S71
N72
N77
N78
V79
S80
T81
L82
E83
S95
R109
L116
E123
V126
P129
V143
G148
H153
V160
E164
V169
C170
Q179
L182
R186
R192
V195
W200
Q201
H206
Y214
S217
E218
N219
W222
T223
Q224
D225
K228
Q232
A236
R241
A242
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	173.59Å 47.50Å 119.25Å 90.00° 109.12° 90.00°	Depositor
Resolution (Å)	82.01 – 2.62 82.01 – 2.62	Depositor EDS
% Data completeness (in resolution range)	98.9 (82.01-2.62) 98.9 (82.01-2.62)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.193 , 0.268 0.199 , 0.261	Depositor DCC
R_{free} test set	1399 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	57.7	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6618	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: 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	0.67	0/2296	0.79	0/3113
2	B	0.67	0/860	0.77	1/1162 (0.1%)
3	C	0.70	0/76	0.86	0/102
4	D	0.59	0/1537	0.78	0/2088
5	E	0.63	0/1966	0.80	2/2672 (0.1%)
All	All	0.64	0/6735	0.79	3/9137 (0.0%)

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	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	47	LEU	CA-CB-CG	6.86	131.07	115.30
2	B	3	ARG	NE-CZ-NH2	-5.36	117.62	120.30
5	E	20	VAL	CB-CA-C	-5.25	101.42	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	134	ASP	Peptide
4	D	192	PHE	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	28	0
2	B	837	0	803	10	0
3	C	74	0	69	6	0
4	D	1506	0	1457	39	0
5	E	1914	0	1811	30	0
6	A	10	0	0	3	0
6	B	5	0	0	0	0
6	D	10	0	0	0	0
6	E	10	0	0	0	0
7	A	9	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	6	0	0	0	0
All	All	6618	0	6233	106	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 8.

All (106) 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)
5:E:126:VAL:HG23	5:E:236:ALA:HB3	1.55	0.85
1:A:17:ARG:HG2	1:A:17:ARG:O	1.87	0.74
5:E:148:GLY:O	5:E:186:ARG:NE	2.20	0.72
5:E:20:VAL:CG2	5:E:82:LEU:HD11	2.22	0.70
1:A:16:GLY:O	1:A:18:GLY:N	2.25	0.69
5:E:20:VAL:HG22	5:E:82:LEU:HD11	1.74	0.67
4:D:129:ASP:HB2	4:D:135:LYS:O	1.94	0.67
1:A:214:THR:HB	1:A:262:GLN:HB2	1.79	0.65
1:A:154:GLU:OE1	4:D:52:ARG:NE	2.31	0.64
1:A:194:ILE:HD12	1:A:199:ALA:HA	1.81	0.62
4:D:153:LYS:O	4:D:155:SER:N	2.31	0.62
4:D:147:THR:HG23	4:D:162:LYS:HD3	1.82	0.61
2:B:59:ASP:O	2:B:60:TRP:HB2	2.01	0.61
2:B:17:ASN:OD1	2:B:97:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ARG:CG	1:A:17:ARG:O	2.47	0.60
4:D:158:TYR:O	4:D:179:ALA:HA	2.02	0.60
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.37	0.59
4:D:168:ARG:HD3	4:D:168:ARG:N	2.18	0.59
2:B:38:ASP:OD2	2:B:81:ARG:NH2	2.38	0.56
4:D:165:LEU:HD23	4:D:166:ASP:N	2.20	0.56
1:A:274:TRP:CE3	1:A:275:PRO:HD2	2.41	0.56
5:E:64:ARG:NH2	5:E:81:THR:O	2.39	0.56
4:D:127:LEU:N	4:D:127:LEU:HD12	2.21	0.55
1:A:67:MET:CE	3:C:2:VAL:HG21	2.38	0.54
4:D:49:LEU:HD21	4:D:60:SER:HB3	1.89	0.54
4:D:34:LEU:O	4:D:51:VAL:HG12	2.08	0.54
5:E:15:THR:O	5:E:18:GLN:HG3	2.09	0.53
4:D:3:GLN:NE2	4:D:28:ASP:H	2.07	0.53
1:A:114:ARG:NH2	6:A:302:SO4:O4	2.33	0.52
5:E:79:VAL:HG21	5:E:82:LEU:HD23	1.91	0.51
5:E:222:TRP:HB2	5:E:228:LYS:HE2	1.93	0.51
2:B:98:ASP:O	2:B:99:MET:HG2	2.11	0.50
1:A:21:ARG:NH1	1:A:37:ASP:OD1	2.44	0.50
1:A:67:MET:HA	1:A:67:MET:CE	2.42	0.50
4:D:196:ILE:O	4:D:196:ILE:HG23	2.12	0.49
1:A:218:GLN:O	1:A:257:TYR:HA	2.12	0.49
4:D:95:PRO:HG2	4:D:101:PHE:HA	1.93	0.49
5:E:126:VAL:HG23	5:E:236:ALA:CB	2.35	0.49
4:D:5:VAL:HG13	4:D:104:VAL:HG12	1.95	0.49
4:D:20:LEU:HD12	4:D:22:LEU:CD1	2.42	0.49
4:D:18:GLU:O	4:D:81:SER:CB	2.61	0.49
2:B:4:THR:HG22	2:B:5:PRO:HD2	1.95	0.49
4:D:192:PHE:O	4:D:197:ILE:HD13	2.14	0.48
4:D:3:GLN:NE2	4:D:26:PHE:HB2	2.29	0.48
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.48	0.48
2:B:7:ILE:HD13	2:B:82:VAL:HG21	1.96	0.48
5:E:79:VAL:HG21	5:E:82:LEU:CD2	2.44	0.48
5:E:12:LEU:C	5:E:13:ILE:HD12	2.34	0.47
5:E:27:ILE:HD12	5:E:28:SER:N	2.30	0.47
4:D:154:ASP:N	4:D:154:ASP:OD1	2.47	0.47
1:A:63:GLU:O	1:A:67:MET:HG2	2.14	0.47
4:D:147:THR:HG22	4:D:148:ASN:H	1.80	0.46
5:E:21:THR:HA	5:E:77:MET:O	2.15	0.46
5:E:13:ILE:N	5:E:13:ILE:HD12	2.31	0.46
5:E:153:HIS:HB3	5:E:214:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:164:GLU:H	5:E:164:GLU:CD	2.19	0.46
4:D:121:ASP:CG	4:D:121:ASP:O	2.53	0.46
4:D:168:ARG:CD	4:D:168:ARG:N	2.78	0.46
2:B:10:TYR:O	2:B:24:ASN:HB2	2.16	0.46
4:D:78:ILE:HD11	4:D:81:SER:HA	1.98	0.46
5:E:71:SER:C	5:E:72:ASN:O	2.53	0.45
4:D:18:GLU:O	4:D:81:SER:HB2	2.16	0.45
5:E:21:THR:HB	5:E:78:ASN:HD22	1.81	0.45
1:A:21:ARG:CZ	1:A:39:ASP:OD2	2.65	0.45
1:A:19:GLU:OE1	1:A:75:ARG:NH2	2.50	0.45
5:E:201:GLN:HA	5:E:241:ARG:O	2.16	0.45
1:A:180:GLN:C	1:A:181:ARG:HD2	2.38	0.44
4:D:45:LEU:HD12	4:D:45:LEU:N	2.32	0.44
3:C:4:PRO:HG2	3:C:5:ILE:HD13	2.00	0.44
2:B:75:LYS:HE3	2:B:75:LYS:HB3	1.68	0.44
4:D:179:ALA:O	4:D:180:TRP:HB3	2.18	0.44
1:A:195:SER:OG	1:A:196:ASP:N	2.51	0.44
4:D:23:ASN:HD22	4:D:23:ASN:C	2.21	0.44
1:A:21:ARG:NH1	1:A:39:ASP:OD2	2.52	0.43
5:E:129:PRO:HD2	5:E:200:TRP:CZ2	2.52	0.43
4:D:34:LEU:HB3	4:D:51:VAL:CG1	2.48	0.43
4:D:92:ALA:HA	4:D:104:VAL:O	2.18	0.43
1:A:67:MET:HE2	1:A:67:MET:HA	2.01	0.43
4:D:14:VAL:HG12	4:D:15:PRO:O	2.19	0.43
4:D:3:GLN:HE22	4:D:28:ASP:H	1.64	0.43
5:E:68:ARG:HH12	5:E:78:ASN:HB2	1.84	0.43
5:E:9:PRO:HG2	5:E:12:LEU:HD22	2.01	0.42
1:A:116:ASP:OD2	6:A:302:SO4:O4	2.36	0.42
1:A:67:MET:HE1	3:C:2:VAL:HG21	2.01	0.42
4:D:127:LEU:HD22	5:E:143:VAL:CG1	2.50	0.42
1:A:182:THR:OG1	1:A:182:THR:O	2.37	0.42
6:A:302:SO4:O1	3:C:7:HIS:O	2.38	0.42
1:A:271:THR:O	1:A:272:LEU:HD13	2.20	0.42
4:D:186:PHE:O	4:D:186:PHE:CD2	2.73	0.42
1:A:67:MET:HE3	3:C:2:VAL:HG21	2.00	0.42
4:D:187:ALA:HB3	4:D:190:ASN:CB	2.51	0.41
5:E:50:TYR:CE2	5:E:55:GLN:HB2	2.55	0.41
4:D:147:THR:HG23	4:D:162:LYS:CD	2.49	0.41
5:E:169:VAL:HG12	5:E:170:CYS:N	2.34	0.41
5:E:32:SER:HB3	5:E:95:SER:HB3	2.03	0.41
1:A:46:GLU:HB2	1:A:47:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:141:THR:OG1	4:D:142:ASP:N	2.52	0.41
4:D:65:ALA:HA	4:D:75:THR:O	2.20	0.41
5:E:47:LEU:HD13	5:E:61:PHE:CD1	2.56	0.41
4:D:16:GLU:OE2	4:D:173:LYS:HE2	2.21	0.40
3:C:8:LEU:HD11	5:E:31:ARG:HH22	1.86	0.40
5:E:70:PHE:O	5:E:72:ASN:O	2.38	0.40
1:A:9:PHE:HE2	1:A:67:MET:CE	2.35	0.40
2:B:75:LYS:HG2	2:B:76:ASP:N	2.35	0.40
5:E:31:ARG:HB2	5:E:51:PHE:CE1	2.55	0.40
4:D:34:LEU:HD13	4:D:67:LEU:CD1	2.52	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	273/275 (99%)	259 (95%)	12 (4%)	2 (1%)	22 41
2	B	98/100 (98%)	92 (94%)	6 (6%)	0	100 100
3	C	7/9 (78%)	7 (100%)	0	0	100 100
4	D	195/197 (99%)	174 (89%)	15 (8%)	6 (3%)	4 6
5	E	239/241 (99%)	226 (95%)	13 (5%)	0	100 100
All	All	812/822 (99%)	758 (93%)	46 (6%)	8 (1%)	15 30

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
4	D	142	ASP
4	D	154	ASP
4	D	186	PHE

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Mol	Chain	Res	Type
1	A	86	ASN
4	D	129	ASP
4	D	131	LYS
4	D	41	PRO

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	232/232 (100%)	218 (94%)	14 (6%)	19 37
2	B	95/95 (100%)	85 (90%)	10 (10%)	7 12
3	C	8/8 (100%)	7 (88%)	1 (12%)	4 7
4	D	170/170 (100%)	145 (85%)	25 (15%)	3 4
5	E	209/209 (100%)	178 (85%)	31 (15%)	3 4
All	All	714/714 (100%)	633 (89%)	81 (11%)	6 10

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

Mol	Chain	Res	Type
1	A	11	SER
1	A	17	ARG
1	A	21	ARG
1	A	23	ILE
1	A	43	GLN
1	A	62	GLN
1	A	108	ARG
1	A	111	ARG
1	A	116	ASP
1	A	131	ARG
1	A	198	GLU
1	A	216	THR
1	A	228	THR
1	A	230	LEU
2	B	0	MET

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Mol	Chain	Res	Type
2	B	1	ILE
2	B	3	ARG
2	B	4	THR
2	B	20	SER
2	B	45	ARG
2	B	69	GLU
2	B	70	PHE
2	B	74	GLU
2	B	75	LYS
3	C	5	ILE
4	D	5	VAL
4	D	6	THR
4	D	20	LEU
4	D	22	LEU
4	D	23	ASN
4	D	48	LEU
4	D	59	THR
4	D	62	ARG
4	D	64	ASN
4	D	73	ARG
4	D	76	LEU
4	D	78	ILE
4	D	93	VAL
4	D	121	ASP
4	D	133	SER
4	D	135	LYS
4	D	136	SER
4	D	139	LEU
4	D	146	GLN
4	D	153	LYS
4	D	154	ASP
4	D	155	SER
4	D	168	ARG
4	D	190	ASN
4	D	195	SER
5	E	10	ARG
5	E	15	THR
5	E	20	VAL
5	E	21	THR
5	E	22	LEU
5	E	27	ILE
5	E	31	ARG

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Mol	Chain	Res	Type
5	E	48	PHE
5	E	58	LYS
5	E	60	ASN
5	E	72	ASN
5	E	79	VAL
5	E	83	GLU
5	E	95	SER
5	E	109	ARG
5	E	116	LEU
5	E	123	GLU
5	E	143	VAL
5	E	160	VAL
5	E	179	GLN
5	E	182	LEU
5	E	192	ARG
5	E	195	VAL
5	E	206	HIS
5	E	217	SER
5	E	218	GLU
5	E	219	ASN
5	E	223	THR
5	E	225	ASP
5	E	232	GLN
5	E	241	ARG

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

Mol	Chain	Res	Type
1	A	72	GLN
1	A	87	GLN
1	A	174	ASN
4	D	3	GLN
4	D	23	ASN
4	D	39	GLN
4	D	55	GLN
4	D	58	GLN
4	D	82	GLN
4	D	116	ASN
4	D	119	ASN
4	D	190	ASN
5	E	38	GLN
5	E	42	GLN

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Mol	Chain	Res	Type
5	E	45	GLN
5	E	57	ASN
5	E	69	GLN
5	E	72	ASN
5	E	78	ASN
5	E	179	GLN
5	E	205	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

7 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	SO4	A	301	-	4,4,4	0.37	0	6,6,6	0.38	0
6	SO4	E	301	-	4,4,4	0.48	0	6,6,6	0.16	0
6	SO4	A	302	-	4,4,4	0.38	0	6,6,6	0.98	0
6	SO4	E	302	-	4,4,4	0.40	0	6,6,6	0.32	0
6	SO4	D	201	-	4,4,4	0.30	0	6,6,6	0.70	0
6	SO4	D	202	-	4,4,4	0.36	0	6,6,6	0.20	0
6	SO4	B	101	-	4,4,4	0.38	0	6,6,6	0.38	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	302	SO4	3	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, 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	275/275 (100%)	-0.12	1 (0%) 92 91	30, 53, 104, 120	0
2	B	100/100 (100%)	-0.31	0 100 100	32, 51, 81, 108	0
3	C	9/9 (100%)	-0.41	0 100 100	31, 35, 41, 51	0
4	D	197/197 (100%)	0.36	21 (10%) 6 4	33, 71, 130, 162	0
5	E	241/241 (100%)	-0.17	1 (0%) 92 91	33, 60, 97, 133	0
All	All	822/822 (100%)	-0.05	23 (2%) 53 47	30, 58, 110, 162	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	198	PRO	10.8
4	D	186	PHE	7.1
4	D	184	SER	5.8
4	D	196	ILE	5.5
5	E	243	ASP	4.8
4	D	188	CYS	4.2
4	D	154	ASP	3.9
4	D	185	ASP	3.9
4	D	149	VAL	3.6
4	D	197	ILE	3.6
4	D	193	ASN	3.4
1	A	249	VAL	2.9
4	D	165	LEU	2.8
4	D	190	ASN	2.6
4	D	194	ASN	2.6
4	D	151	GLN	2.6
4	D	189	ALA	2.5
4	D	192	PHE	2.5
4	D	132	SER	2.5
4	D	147	THR	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	155	SER	2.2
4	D	169	SER	2.1
4	D	144	ASP	2.1

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 carbohydrates 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
6	SO4	B	101	5/5	0.83	0.47	92,109,126,128	0
6	SO4	A	302	5/5	0.92	0.26	73,82,93,107	0
6	SO4	D	202	5/5	0.93	0.40	96,100,110,117	0
6	SO4	A	301	5/5	0.94	0.43	77,90,99,101	0
6	SO4	E	302	5/5	0.94	0.29	85,90,96,97	0
6	SO4	D	201	5/5	0.96	0.16	62,65,71,79	0
6	SO4	E	301	5/5	0.97	0.10	73,73,76,77	0

6.5 Other polymers (i)

There are no such residues in this entry.