



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:08 PM UTC

PDB ID : 6H6H / pdb_00006h6h
Title : Crystal structures of the murine class I major histocompatibility complex H-2Dbm13 in complex with adenovirus-derived peptide Ad10
Authors : Achour, A.; Sandalova, T.; Han, X.
Deposited on : 2018-07-27
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

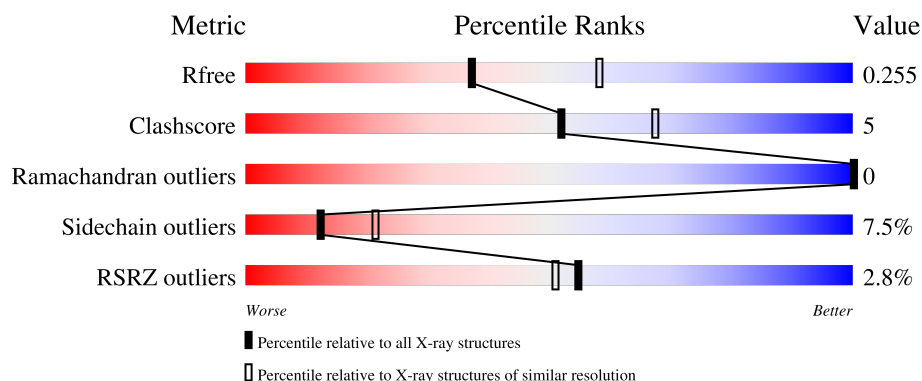
1 Overall quality at a glance

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)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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	338	2% 67% 12% • 20%
1	D	338	4% 64% 15% • 19%
2	B	99	88% 11% •
2	E	99	87% 12% •
3	C	10	80% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	10	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6551 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 H-2D cell surface glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2237	1409	397	422	9			
1	D	273	Total	C	N	O	S	0	0	0
			2245	1415	398	423	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q31167
D	1	GLY	-	expression tag	UNP Q31167

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	E	99	Total	C	N	O	S	0	1	0
			826	528	138	152	8			

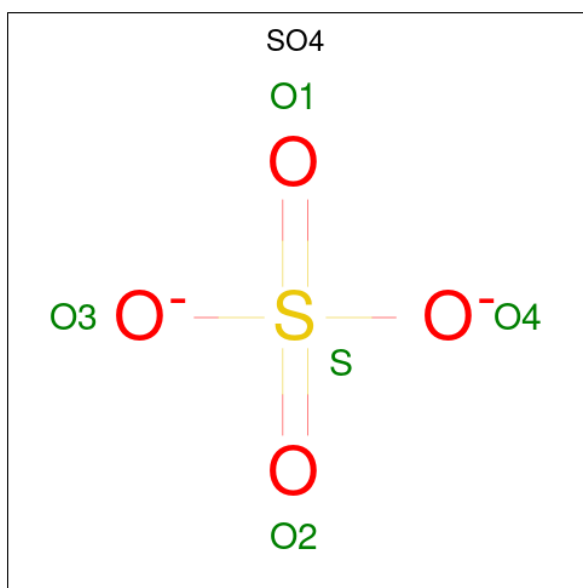
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ASP	ALA	conflict	UNP P01887
E	85	ASP	ALA	conflict	UNP P01887

- Molecule 3 is a protein called SER-GLY-PRO-SER-ASN-THR-PRO-PRO-GLU-ILE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			70	42	11	17			
3	F	10	Total	C	N	O	0	0	0
			70	42	11	17			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



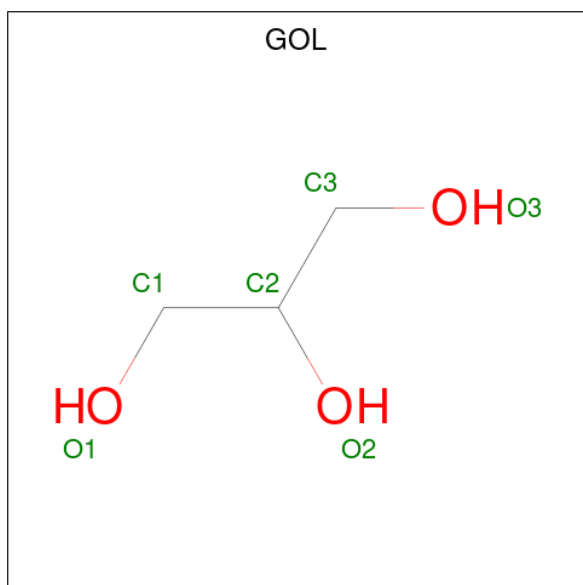
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

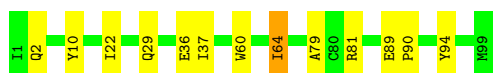
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	78	Total	O	0	0
			78	78		
6	D	53	Total	O	0	0
			53	53		
6	B	28	Total	O	0	0
			28	28		
6	E	29	Total	O	0	0
			29	29		
6	C	4	Total	O	0	0
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	3	Total	O	0	0
			3	3		



- Molecule 3: SER-GLY-PRO-SER-ASN-THR-PRO-PRO-GLU-ILE

Chain C: 80% 20%



- Molecule 3: SER-GLY-PRO-SER-ASN-THR-PRO-PRO-GLU-ILE

Chain F: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.41Å 70.27Å 87.05Å 83.98° 86.90° 81.75°	Depositor
Resolution (Å)	19.94 – 2.40 19.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.94-2.40) 97.0 (19.94-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.200 , 0.249 0.206 , 0.255	Depositor DCC
R_{free} test set	2133 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.1	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	0.95	EDS
Total number of atoms	6551	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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: 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	0.90	4/2303 (0.2%)	0.92	6/3126 (0.2%)
1	D	0.88	2/2311 (0.1%)	0.88	2/3137 (0.1%)
2	B	0.67	0/847	0.78	0/1148
2	E	0.64	0/855	0.74	0/1158
3	C	1.86	3/72 (4.2%)	1.49	2/98 (2.0%)
3	F	1.31	0/72	0.89	0/98
All	All	0.86	9/6460 (0.1%)	0.87	10/8765 (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
1	A	0	1
1	D	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	6	THR	C-N	6.21	1.40	1.33
3	C	7	PRO	C-O	-5.70	1.18	1.24
1	A	116	TYR	C-O	-5.62	1.16	1.23
1	A	14	ARG	C-N	5.33	1.40	1.33
1	D	14	ARG	C-N	5.28	1.40	1.33
1	A	234	ARG	C-N	5.27	1.40	1.33
1	D	15	PRO	N-CD	5.26	1.55	1.47
3	C	7	PRO	N-CD	5.04	1.54	1.47
1	A	34	VAL	C-O	-5.02	1.18	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	GLY	N-CA-C	7.43	121.70	112.79
3	C	6	THR	CA-C-N	-7.28	112.89	120.38
3	C	6	THR	C-N-CA	-7.28	112.89	120.38
1	D	14	ARG	CA-C-N	-6.53	113.25	119.85
1	D	14	ARG	C-N-CA	-6.53	113.25	119.85
1	A	14	ARG	CA-C-N	-6.31	113.48	119.85
1	A	14	ARG	C-N-CA	-6.31	113.48	119.85
1	A	234	ARG	CA-C-N	-6.01	113.50	119.99
1	A	234	ARG	C-N-CA	-6.01	113.50	119.99
1	A	145	ARG	NE-CZ-NH2	5.51	124.16	119.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	ALA	Peptide
1	D	136	ALA	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	2237	0	2096	25	0
1	D	2245	0	2107	35	0
2	B	821	0	796	6	0
2	E	826	0	805	8	0
3	C	70	0	66	0	0
3	F	70	0	66	0	0
4	A	25	0	0	0	0
4	B	25	0	0	0	0
4	D	15	0	0	0	0
4	E	10	0	0	1	0
5	A	12	0	16	1	0
6	A	78	0	0	0	0
6	B	28	0	0	0	0
6	C	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	53	0	0	0	0
6	E	29	0	0	0	0
6	F	3	0	0	0	0
All	All	6551	0	5952	63	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 5.

All (63) 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)
1:D:111:ARG:HG2	1:D:111:ARG:HH11	1.47	0.78
1:D:129:ASP:HB3	1:D:131:LYS:H	1.53	0.74
1:D:129:ASP:O	1:D:130:LEU:HB2	1.93	0.69
1:D:111:ARG:NH1	1:D:112:GLY:O	2.26	0.69
1:D:111:ARG:HD3	1:D:113:TYR:CZ	2.26	0.69
1:A:35:ARG:NH2	2:B:54:MET:O	2.26	0.64
1:A:52:MET:HE1	1:A:171:TYR:CD1	2.37	0.59
1:D:28:VAL:HG23	1:D:33:PHE:CE1	2.37	0.59
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.39	0.58
1:A:268:GLU:HG3	1:D:169:HIS:HE1	1.66	0.58
1:D:126:LEU:HB2	1:D:133:TRP:CZ3	2.39	0.58
1:D:52:MET:HE1	1:D:171:TYR:CD1	2.41	0.56
1:D:15:PRO:HG3	1:D:91:GLY:O	2.06	0.55
1:A:129:ASP:O	1:A:130:LEU:HB2	2.06	0.54
1:A:268:GLU:HG3	1:D:169:HIS:CE1	2.43	0.53
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.44	0.52
1:A:191:HIS:NE2	1:A:199:VAL:HG11	2.24	0.51
1:D:129:ASP:OD2	1:D:132:THR:HG23	2.11	0.51
1:D:234:ARG:HD3	2:E:10:TYR:CZ	2.46	0.50
1:D:189:VAL:HG22	1:D:274:TRP:HA	1.94	0.50
1:A:52:MET:HE1	1:A:171:TYR:CE1	2.47	0.50
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.47	0.49
2:E:81:ARG:NH1	4:E:101:SO4:S	2.85	0.49
2:B:54:MET:HE2	2:B:64:ILE:HD13	1.93	0.49
1:D:111:ARG:HG2	1:D:111:ARG:NH1	2.22	0.49
1:A:111:ARG:HG2	1:A:113:TYR:CZ	2.47	0.49
1:A:189:VAL:HG22	1:A:274:TRP:HA	1.96	0.48
1:A:129:ASP:OD2	1:A:130:LEU:N	2.48	0.47
1:D:111:ARG:HH11	1:D:111:ARG:CG	2.17	0.47
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:HIS:CE1	1:D:199:VAL:HG11	2.50	0.46
1:D:234:ARG:HD3	2:E:10:TYR:CE2	2.51	0.46
1:D:52:MET:HE1	1:D:171:TYR:CE1	2.51	0.46
1:D:111:ARG:NH1	1:D:111:ARG:CG	2.75	0.46
1:A:11:ALA:HA	1:A:21:ARG:O	2.16	0.45
1:A:202:ARG:HG2	1:A:204:TRP:NE1	2.32	0.45
1:A:191:HIS:CD2	1:A:199:VAL:HG11	2.52	0.45
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.52	0.45
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.53	0.44
1:A:23:ILE:HD12	5:A:407:GOL:H2	1.99	0.44
1:D:11:ALA:HA	1:D:21:ARG:O	2.18	0.44
1:A:85:TYR:OH	1:A:137:ASP:OD1	2.29	0.44
1:D:228:MET:HE3	1:D:230:LEU:HD13	2.00	0.43
1:A:111:ARG:HG3	1:A:112:GLY:N	2.34	0.43
1:D:28:VAL:HG23	1:D:33:PHE:CD1	2.53	0.43
1:A:228:MET:HE3	1:A:230:LEU:HD13	2.00	0.42
1:D:9:GLU:OE1	1:D:22:TYR:OH	2.34	0.42
1:D:189:VAL:HA	1:D:202:ARG:O	2.20	0.42
1:A:169:HIS:CE1	1:D:268:GLU:HB3	2.55	0.42
1:A:189:VAL:HA	1:A:202:ARG:O	2.20	0.41
1:A:9:GLU:O	1:A:96:GLN:HA	2.20	0.41
2:E:79:ALA:HB2	2:E:94:TYR:CD2	2.55	0.41
1:D:85:TYR:OH	1:D:137:ASP:OD1	2.27	0.41
1:D:98:MET:HE2	2:E:60:TRP:CH2	2.56	0.41
2:E:89:GLU:HB2	2:E:90:PRO:CD	2.51	0.41
1:A:187:ALA:HA	1:A:204:TRP:O	2.21	0.41
1:D:194:ARG:HB2	1:D:198:GLU:O	2.20	0.41
1:D:51:TRP:CZ3	1:D:52:MET:HE3	2.57	0.40
2:E:37:ILE:HD11	2:E:64:ILE:HG21	2.02	0.40
1:D:130:LEU:C	1:D:131:LYS:HG2	2.45	0.40
2:B:37:ILE:HD11	2:B:64:ILE:HG21	2.03	0.40
1:D:8:PHE:CE2	1:D:98:MET:HG2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	268/338 (79%)	260 (97%)	8 (3%)	0	100	100
1	D	269/338 (80%)	257 (96%)	12 (4%)	0	100	100
2	B	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	E	98/99 (99%)	96 (98%)	2 (2%)	0	100	100
3	C	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	F	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
All	All	748/894 (84%)	722 (96%)	26 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/280 (82%)	217 (94%)	14 (6%)	17	30
1	D	232/280 (83%)	209 (90%)	23 (10%)	7	11
2	B	94/94 (100%)	86 (92%)	8 (8%)	10	16
2	E	95/94 (101%)	90 (95%)	5 (5%)	20	36
3	C	9/9 (100%)	9 (100%)	0	100	100
3	F	9/9 (100%)	9 (100%)	0	100	100
All	All	670/766 (88%)	620 (92%)	50 (8%)	12	21

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	79	ARG
1	A	86	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	111	ARG
1	A	130	LEU
1	A	131	LYS
1	A	170	ARG
1	A	189	VAL
1	A	218	GLN
1	A	226	GLN
1	A	234	ARG
1	A	251	LEU
1	A	258	THR
1	A	266	LEU
1	D	17	LEU
1	D	41	GLU
1	D	58	GLU
1	D	79	ARG
1	D	86	ASN
1	D	92	SER
1	D	110	LEU
1	D	129	ASP
1	D	131	LYS
1	D	138	MET
1	D	170	ARG
1	D	180	LEU
1	D	181	ARG
1	D	189	VAL
1	D	194	ARG
1	D	196	LYS
1	D	218	GLN
1	D	226	GLN
1	D	234	ARG
1	D	251	LEU
1	D	258	THR
1	D	266	LEU
1	D	268	GLU
2	B	2	GLN
2	B	22	ILE
2	B	29	GLN
2	B	36	GLU
2	B	44	LYS
2	B	64	ILE
2	B	87	MET
2	B	91	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	2	GLN
2	E	22	ILE
2	E	29	GLN
2	E	36	GLU
2	E	64	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	97	GLN
1	A	114	GLN
1	A	127	ASN
1	A	218	GLN
1	A	255	GLN
1	D	30	ASN
1	D	54	GLN
1	D	87	GLN
1	D	93	HIS
1	D	127	ASN
1	D	169	HIS
1	D	191	HIS
1	D	218	GLN
1	D	255	GLN
2	E	13	HIS
2	E	31	HIS
3	C	5	ASN

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

17 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	$\# Z > 2$
4	SO4	B	101	-	4,4,4	0.47	0	6,6,6	0.18	0
4	SO4	B	105	-	4,4,4	0.44	0	6,6,6	0.12	0
4	SO4	D	402	-	4,4,4	0.45	0	6,6,6	0.13	0
4	SO4	B	102	-	4,4,4	0.43	0	6,6,6	0.10	0
4	SO4	A	402	-	4,4,4	0.45	0	6,6,6	0.25	0
4	SO4	A	403	-	4,4,4	0.55	0	6,6,6	0.31	0
4	SO4	B	103	-	4,4,4	0.43	0	6,6,6	0.26	0
4	SO4	D	401	-	4,4,4	0.45	0	6,6,6	0.23	0
5	GOL	A	406	-	5,5,5	0.68	0	5,5,5	0.52	0
4	SO4	A	404	-	4,4,4	0.50	0	6,6,6	0.08	0
4	SO4	E	102	-	4,4,4	0.48	0	6,6,6	0.13	0
4	SO4	B	104	-	4,4,4	0.48	0	6,6,6	0.18	0
4	SO4	A	401	-	4,4,4	0.42	0	6,6,6	0.34	0
5	GOL	A	407	-	5,5,5	0.63	0	5,5,5	0.97	0
4	SO4	E	101	-	4,4,4	0.44	0	6,6,6	0.11	0
4	SO4	A	405	-	4,4,4	0.59	0	6,6,6	0.27	0
4	SO4	D	403	-	4,4,4	0.47	0	6,6,6	0.32	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
5	GOL	A	407	-	-	4/4/4/4	-
5	GOL	A	406	-	-	0/4/4/4	-

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
5	A	407	GOL	O1-C1-C2-O2
5	A	407	GOL	O1-C1-C2-C3
5	A	407	GOL	C1-C2-C3-O3
5	A	407	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	407	GOL	1	0
4	E	101	SO4	1	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, 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	272/338 (80%)	0.05	6 (2%) 62 58	30, 48, 84, 107	0
1	D	273/338 (80%)	0.24	15 (5%) 30 27	32, 54, 89, 111	0
2	B	99/99 (100%)	-0.16	0 100 100	31, 49, 74, 84	0
2	E	99/99 (100%)	-0.02	0 100 100	29, 54, 77, 91	1 (1%)
3	C	10/10 (100%)	-0.50	0 100 100	34, 38, 47, 48	0
3	F	10/10 (100%)	-0.41	0 100 100	38, 41, 55, 58	0
All	All	763/894 (85%)	0.07	21 (2%) 55 51	29, 51, 84, 111	1 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	91	GLY	5.2
1	D	90	GLY	4.1
1	D	138	MET	3.4
1	A	1	GLY	3.4
1	A	17	LEU	3.3
1	A	219	LEU	3.3
1	D	2	PRO	3.3
1	D	17	LEU	2.7
1	D	133	TRP	2.5
1	D	149	GLN	2.4
1	D	220	ASN	2.3
1	A	2	PRO	2.3
1	A	220	ASN	2.2
1	D	1	GLY	2.2
1	D	227	ASP	2.2
1	D	89	ALA	2.2
1	D	132	THR	2.2
1	D	142	ILE	2.2
1	D	176	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	88	SER	2.1
1	A	145	ARG	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(Å ²)	Q<0.9
4	SO4	B	104	5/5	0.46	0.12	107,114,116,122	0
4	SO4	A	404	5/5	0.71	0.16	106,111,116,118	0
4	SO4	D	402	5/5	0.75	0.13	103,111,114,119	0
4	SO4	E	101	5/5	0.80	0.08	108,111,116,125	0
4	SO4	D	403	5/5	0.81	0.21	105,114,119,125	0
4	SO4	A	403	5/5	0.82	0.23	85,97,109,112	0
5	GOL	A	407	6/6	0.82	0.18	75,80,87,87	0
4	SO4	B	102	5/5	0.83	0.11	121,122,124,127	0
5	GOL	A	406	6/6	0.84	0.16	50,52,53,59	0
4	SO4	A	402	5/5	0.85	0.14	82,86,87,97	0
4	SO4	B	101	5/5	0.87	0.16	90,90,92,93	0
4	SO4	A	401	5/5	0.87	0.11	111,117,118,119	0
4	SO4	D	401	5/5	0.88	0.14	87,93,103,104	0
4	SO4	E	102	5/5	0.89	0.14	82,85,90,91	0
4	SO4	B	103	5/5	0.90	0.15	98,98,101,109	0
4	SO4	A	405	5/5	0.90	0.16	73,74,82,83	0
4	SO4	B	105	5/5	0.91	0.15	84,84,91,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.