



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 06:03 am GMT

PDB ID : 5L2K
Title : Crystal structure of GEM42 TCR-CD1b-GMM complex
Authors : Gras, S.; Shahine, A.; Le Nours, J.; Rossjohn, J.
Deposited on : 2016-08-02
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

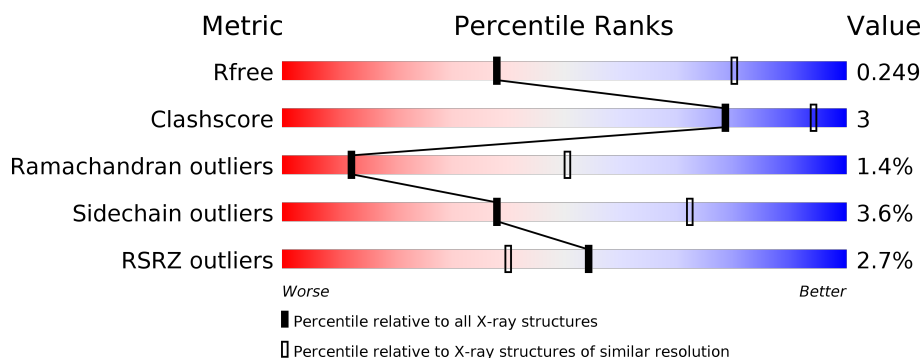
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	111664	1121 (3.22-3.18)
Clashscore	122126	1091 (3.20-3.20)
Ramachandran outliers	120053	1074 (3.20-3.20)
Sidechain outliers	120020	1073 (3.20-3.20)
RSRZ outliers	108989	1083 (3.22-3.18)

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. 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	300	<div> <div></div> <div>85% 7% 8%</div> </div>
2	B	98	<div> <div></div> <div>91% 9%</div> </div>
3	D	204	<div> <div>8%</div> <div>74% 15% 9%</div> </div>
4	E	243	<div> <div></div> <div>85% 13%</div> </div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 6497 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 T-cell surface glycoprotein CD1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	11	1	0
			2163	1386	368	399	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	ALA	ILE	engineered mutation	UNP P29016
A	279	GLY	-	expression tag	UNP P29016
A	280	SER	-	expression tag	UNP P29016
A	281	GLY	-	expression tag	UNP P29016
A	282	LEU	-	expression tag	UNP P29016
A	283	ASN	-	expression tag	UNP P29016
A	284	ASP	-	expression tag	UNP P29016
A	285	ILE	-	expression tag	UNP P29016
A	286	PHE	-	expression tag	UNP P29016
A	287	GLU	-	expression tag	UNP P29016
A	288	ALA	-	expression tag	UNP P29016
A	289	GLN	-	expression tag	UNP P29016
A	290	LYS	-	expression tag	UNP P29016
A	291	ILE	-	expression tag	UNP P29016
A	292	GLU	-	expression tag	UNP P29016
A	293	TRP	-	expression tag	UNP P29016
A	294	HIS	-	expression tag	UNP P29016
A	295	GLU	-	expression tag	UNP P29016
A	296	HIS	-	expression tag	UNP P29016
A	297	HIS	-	expression tag	UNP P29016
A	298	HIS	-	expression tag	UNP P29016
A	299	HIS	-	expression tag	UNP P29016
A	300	HIS	-	expression tag	UNP P29016
A	301	HIS	-	expression tag	UNP P29016

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			820	523	139	156	2			

- Molecule 3 is a protein called GEM42 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	185	Total	C	N	O	S	0	0	0
			1442	903	241	289	9			

- Molecule 4 is a protein called GEM42 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	242	Total	C	N	O	S	0	0	0
			1916	1210	333	364	9			

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

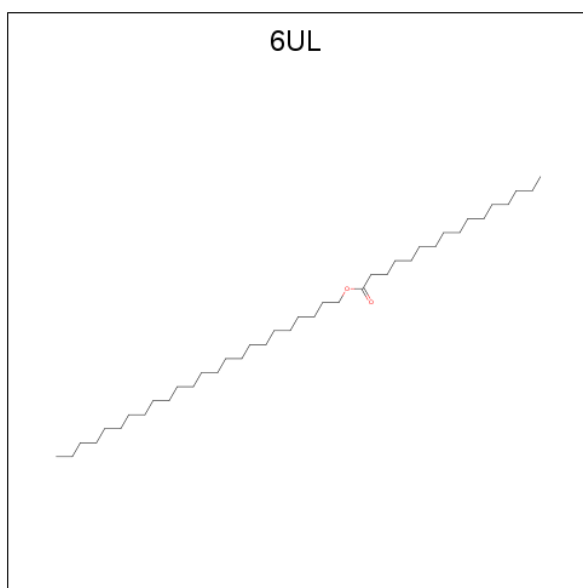
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		
7	A	3	Total	Cl	0	0
			3	3		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Na	0	0
			1	1		
8	E	1	Total	Na	0	0
			1	1		

- Molecule 9 is TETRACOSYL PALMITATE (three-letter code: 6UL) (formula: $C_{40}H_{80}O_2$).

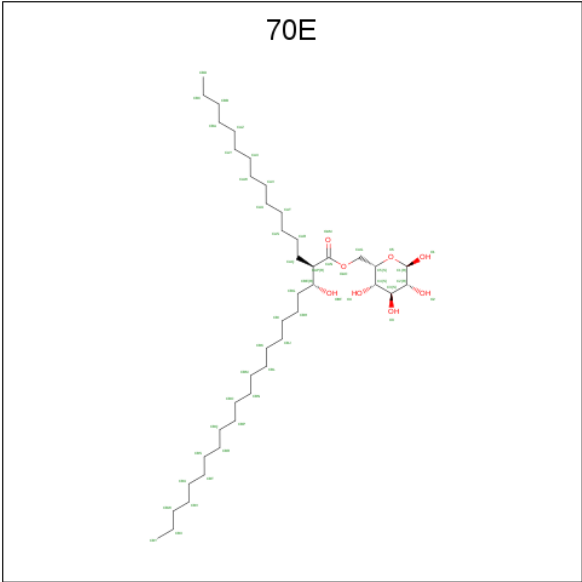


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			26	24	2		

- Molecule 10 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	1	Total	Cs	0	0
			1	1		

- Molecule 11 is 6-O-[(2R,3R)-3-hydroxy-2-tetradecyldocosanoyl]-alpha-L-idopyranose (three-letter code: 70E) (formula: $C_{42}H_{82}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	E	1	Total	C	O	0	0
			50	42	8		

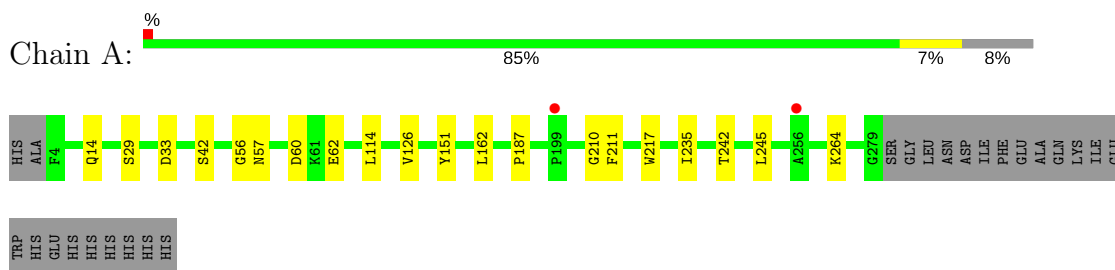
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	2	Total	O	0	0
			2	2		
12	B	3	Total	O	0	0
			3	3		
12	D	1	Total	O	0	0
			1	1		

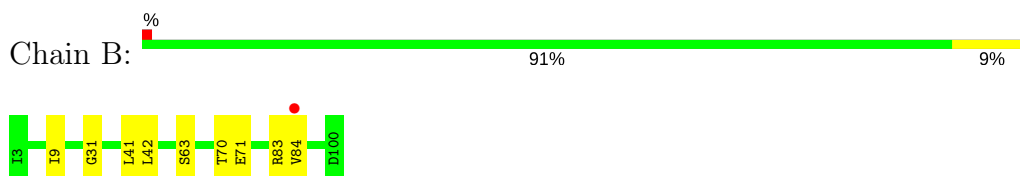
3 Residue-property plots [i](#)

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.

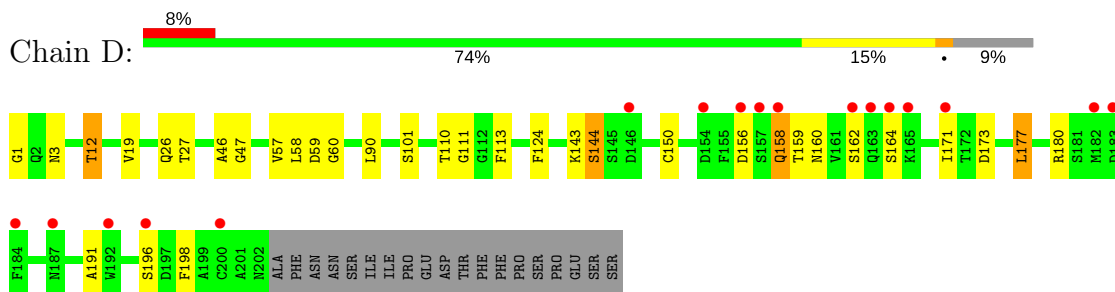
- Molecule 1: T-cell surface glycoprotein CD1b



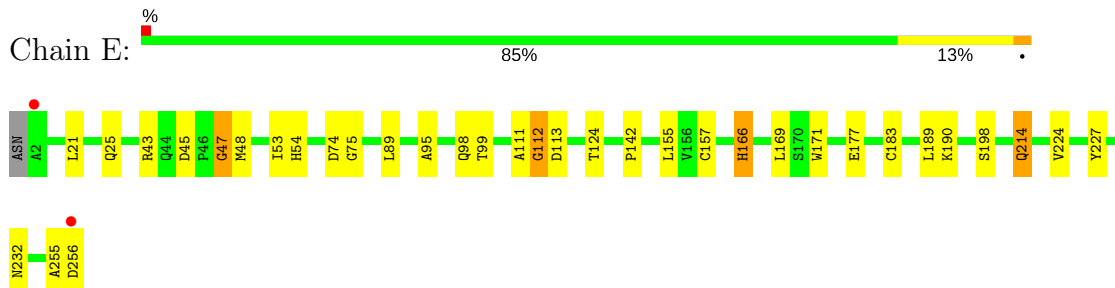
- Molecule 2: Beta-2-microglobulin



- Molecule 3: GEM42 TCR alpha chain



- Molecule 4: GEM42 TCR beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	175.00Å 175.00Å 170.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.73 – 3.20 47.73 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.73-3.20) 100.0 (47.73-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.218 , 0.239 0.227 , 0.249	Depositor DCC
R_{free} test set	1259 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	78.1	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6497	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, NA, 6UL, SO4, CS, 70E

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	0.36	0/2223	0.55	0/3017
2	B	0.36	0/843	0.53	0/1142
3	D	0.37	0/1470	0.60	0/1984
4	E	0.34	0/1968	0.58	0/2676
All	All	0.36	0/6504	0.57	0/8819

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2163	0	2079	8	0
2	B	820	0	782	4	0
3	D	1442	0	1378	11	0
4	E	1916	0	1833	18	0
5	A	42	0	39	0	0
6	A	15	0	0	0	0
6	D	5	0	0	0	0
6	E	5	0	0	0	0
7	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
8	A	1	0	0	0	0
8	E	1	0	0	0	0
9	A	26	0	42	1	0
10	D	1	0	0	0	0
11	E	50	0	0	0	0
12	A	2	0	0	0	0
12	B	3	0	0	0	0
12	D	1	0	0	0	0
All	All	6497	0	6153	39	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 3.

The worst 5 of 39 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:A:187:PRO:HB3	1:A:211:PHE:HB3	1.77	0.66
3:D:1:GLY:CA	3:D:27:THR:HG22	2.32	0.58
1:A:217:TRP:HB3	1:A:264:LYS:HB2	1.84	0.58
3:D:3:ASN:HB2	3:D:26:GLN:HB2	1.86	0.57
2:B:31:GLY:HA2	2:B:63:SER:HB3	1.86	0.57

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	275/300 (92%)	266 (97%)	7 (2%)	2 (1%)	24	66
2	B	96/98 (98%)	93 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	183/204 (90%)	160 (87%)	16 (9%)	7 (4%)	3	24
4	E	240/243 (99%)	224 (93%)	14 (6%)	2 (1%)	21	62
All	All	794/845 (94%)	743 (94%)	40 (5%)	11 (1%)	12	50

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	196	SER
4	E	47	GLY
1	A	56	GLY
3	D	144	SER
3	D	160	ASN

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	226/246 (92%)	221 (98%)	5 (2%)	55	82
2	B	93/93 (100%)	92 (99%)	1 (1%)	76	90
3	D	160/178 (90%)	148 (92%)	12 (8%)	15	49
4	E	207/208 (100%)	200 (97%)	7 (3%)	40	73
All	All	686/725 (95%)	661 (96%)	25 (4%)	38	72

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	113	PHE
3	D	144	SER
4	E	232	ASN
3	D	143	LYS
3	D	156	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	25	GLN
4	E	237	GLN
4	E	54	HIS
3	D	108	ASN
4	E	29	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 for Mogul analysis.

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	$\# Z > 2$
5	NAG	A	401	1	14,14,15	1.91	3 (21%)	17,19,21	1.70	4 (23%)
5	NAG	A	402	1	14,14,15	1.85	4 (28%)	17,19,21	1.57	3 (17%)
5	NAG	A	403	1	14,14,15	1.96	4 (28%)	17,19,21	2.29	7 (41%)
6	SO4	A	404	-	4,4,4	0.18	0	6,6,6	0.10	0
6	SO4	A	405	-	4,4,4	0.19	0	6,6,6	0.11	0
6	SO4	A	406	-	4,4,4	0.20	0	6,6,6	0.12	0
9	6UL	A	411	-	25,25,41	0.63	0	25,25,41	0.68	0
6	SO4	D	301	-	4,4,4	0.18	0	6,6,6	0.09	0
6	SO4	E	301	-	4,4,4	0.17	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	70E	E	303	-	50,50,50	0.72	0	55,58,58	0.93	1 (1%)

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	NAG	A	401	1	-	0/6/23/26	0/1/1/1
5	NAG	A	402	1	-	0/6/23/26	0/1/1/1
5	NAG	A	403	1	-	0/6/23/26	0/1/1/1
6	SO4	A	404	-	-	0/0/0/0	0/0/0/0
6	SO4	A	405	-	-	0/0/0/0	0/0/0/0
6	SO4	A	406	-	-	0/0/0/0	0/0/0/0
9	6UL	A	411	-	-	0/24/24/40	0/0/0/0
6	SO4	D	301	-	-	0/0/0/0	0/0/0/0
6	SO4	E	301	-	-	0/0/0/0	0/0/0/0
11	70E	E	303	-	-	0/46/66/66	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401	NAG	C4-C3	-2.21	1.46	1.52
5	A	403	NAG	C3-C2	-2.19	1.47	1.52
5	A	402	NAG	C4-C3	-2.13	1.46	1.52
5	A	403	NAG	C4-C3	-2.12	1.46	1.52
5	A	402	NAG	C3-C2	-2.04	1.48	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	303	70E	CAR-CAQ-CAP	-2.66	109.42	114.32
5	A	401	NAG	C2-N2-C7	2.08	125.97	122.94
5	A	403	NAG	O6-C6-C5	2.12	118.68	111.29
5	A	402	NAG	C4-C3-C2	2.15	114.16	111.02
5	A	401	NAG	C3-C4-C5	2.52	114.75	110.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	411	6UL	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 [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	276/300 (92%)	-0.10	2 (0%) 87 81	43, 73, 112, 122	3 (1%)
2	B	98/98 (100%)	0.37	1 (1%) 82 73	58, 94, 116, 128	0
3	D	185/204 (90%)	0.38	17 (9%) 9 5	45, 71, 137, 149	9 (4%)
4	E	242/243 (99%)	-0.06	2 (0%) 86 78	51, 73, 105, 123	0
All	All	801/845 (94%)	0.08	22 (2%) 54 40	43, 75, 120, 149	12 (1%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	164	SER	6.2
3	D	156	ASP	4.9
3	D	163	GLN	4.4
1	A	256	ALA	4.0
4	E	2	ALA	3.5

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, 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
6	SO4	D	301	5/5	0.74	0.24	148,148,148,148	0
7	CL	B	201	1/1	0.76	0.27	98,98,98,98	0
6	SO4	E	301	5/5	0.78	0.31	169,169,170,170	0
7	CL	A	408	1/1	0.80	0.14	87,87,87,87	0
7	CL	A	409	1/1	0.81	0.27	93,93,93,93	0
7	CL	A	407	1/1	0.81	0.14	96,96,96,96	0
5	NAG	A	403	14/15	0.83	0.28	97,98,100,101	0
9	6UL	A	411	26/42	0.85	0.47	54,57,67,68	0
6	SO4	A	404	5/5	0.85	0.23	129,129,129,129	0
5	NAG	A	402	14/15	0.88	0.33	108,109,110,110	0
8	NA	A	410	1/1	0.91	0.22	64,64,64,64	0
11	70E	E	303	50/50	0.92	0.39	54,58,67,69	0
6	SO4	A	406	5/5	0.94	0.18	116,116,116,116	0
5	NAG	A	401	14/15	0.94	0.17	61,62,64,64	0
6	SO4	A	405	5/5	0.94	0.17	97,98,98,98	0
8	NA	E	302	1/1	0.94	0.53	43,43,43,43	0
10	CS	D	302	1/1	0.97	0.11	145,145,145,145	0

6.5 Other polymers [i](#)

There are no such residues in this entry.