



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2022 – 01:11 pm BST

PDB ID : 7PC7
Title : The PDZ domain of SNTG1 complexed with the acetylated PDZ-binding motif of PTEN
Authors : Cousido-Siah, A.; Trave, G.; Gogl, G.
Deposited on : 2021-08-03
Resolution : 2.10 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

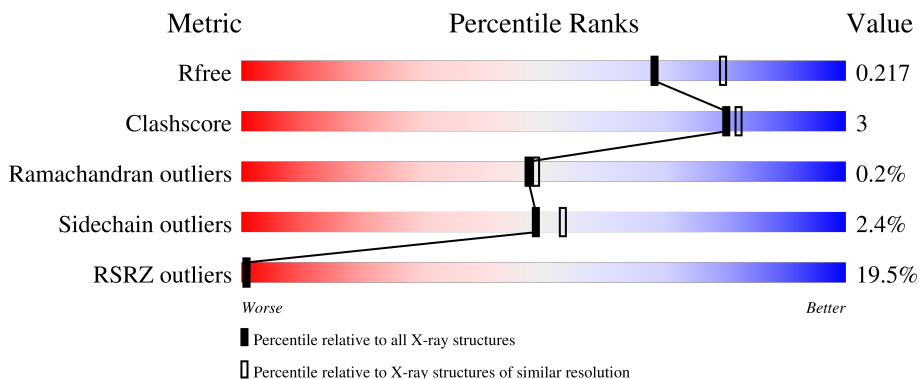
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	414	
1	B	414	
2	E	10	
2	F	10	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 6965 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 Gamma-1-syntrophin,Annexin A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	398	3187	1998	558	619	12	0	3	0
1	B	404	3215	2016	561	626	12	0	2	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	GLY	-	expression tag	UNP Q9NSN8
A	50	SER	-	expression tag	UNP Q9NSN8
A	51	HIS	-	expression tag	UNP Q9NSN8
A	52	MET	-	expression tag	UNP Q9NSN8
A	53	GLY	-	expression tag	UNP Q9NSN8
A	140D	GLY	-	linker	UNP Q9NSN8
A	188	GLU	ALA	conflict	UNP P07355
B	49	GLY	-	expression tag	UNP Q9NSN8
B	50	SER	-	expression tag	UNP Q9NSN8
B	51	HIS	-	expression tag	UNP Q9NSN8
B	52	MET	-	expression tag	UNP Q9NSN8
B	53	GLY	-	expression tag	UNP Q9NSN8
B	139E	GLY	-	linker	UNP Q9NSN8
B	188	GLU	ALA	conflict	UNP P07355

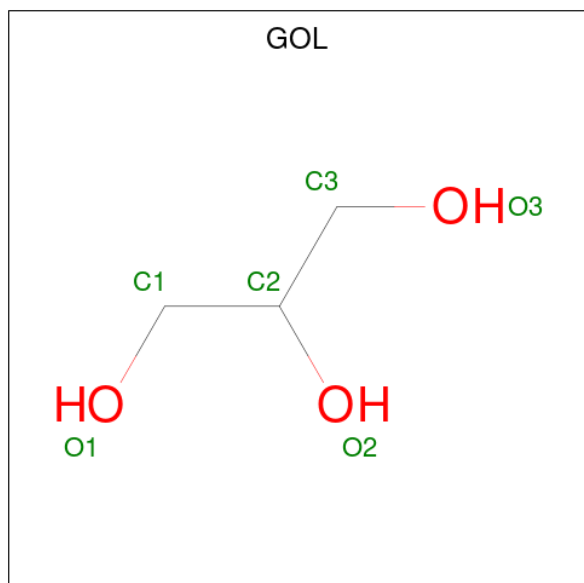
- Molecule 2 is a protein called Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	10	87	52	15	20	0	0	0
2	F	4	35	23	5	7	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total Ca 6 6	0	0
3	B	6	Total Ca 6 6	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

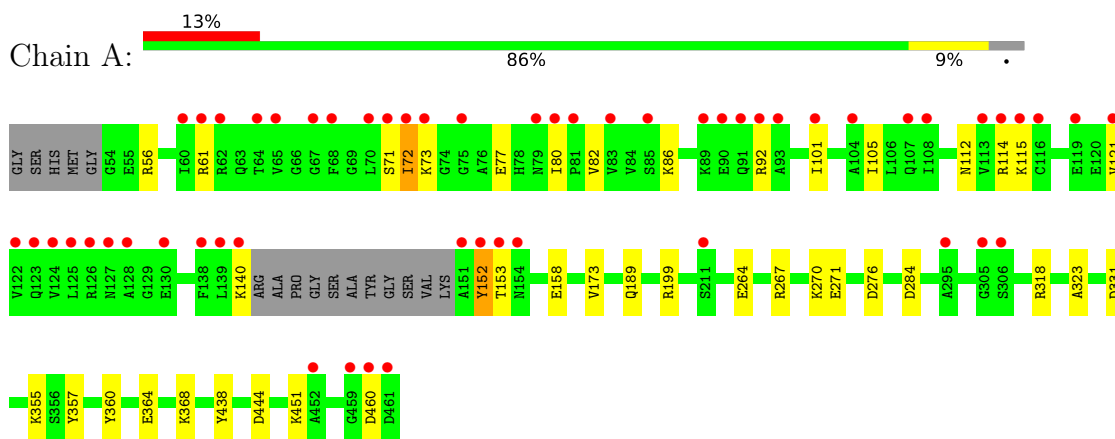
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	289	Total O 289 289	0	0
5	B	115	Total O 115 115	0	0
5	F	1	Total O 1 1	0	0

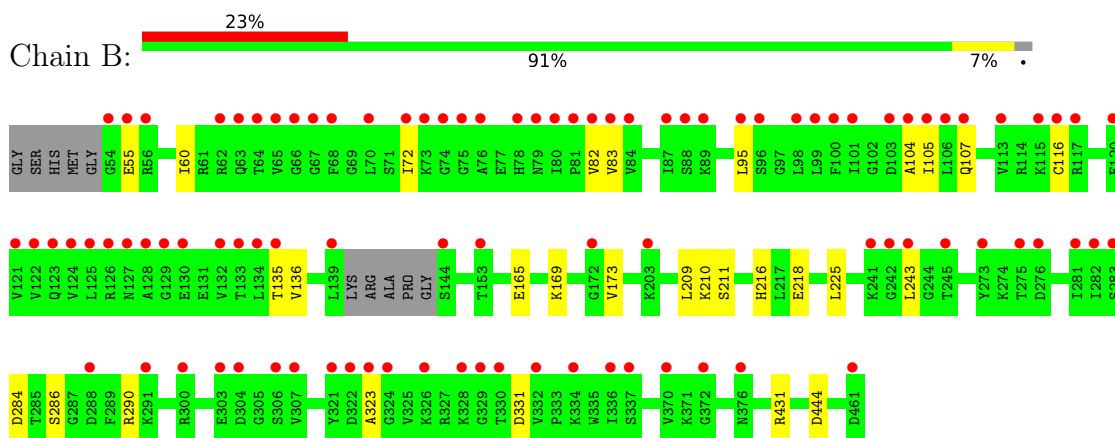
3 Residue-property plots [i](#)

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.

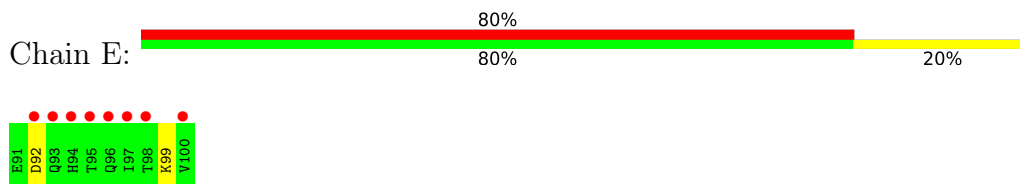
- Molecule 1: Gamma-1-syntrophin,Annexin A2



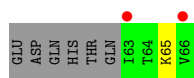
- Molecule 1: Gamma-1-syntrophin,Annexin A2



- Molecule 2: Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN



- Molecule 2: Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.31Å 61.74Å 285.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.69 – 2.10 47.56 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.69-2.10) 100.0 (47.56-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.14 3260	Depositor
R, R_{free}	0.185 , 0.218 0.185 , 0.217	Depositor DCC
R_{free} test set	3176 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtrriage
Anisotropy	0.109	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.031 for k,h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6965	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: CA, GOL, ALY

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	0.39	0/3231	0.52	0/4338
1	B	0.29	0/3260	0.45	0/4379
2	E	0.22	0/74	0.44	0/97
2	F	0.23	0/21	0.54	0/25
All	All	0.34	0/6586	0.49	0/8839

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	3187	0	3239	21	0
1	B	3215	0	3259	13	0
2	E	87	0	80	1	0
2	F	35	0	39	1	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
4	A	12	0	16	0	0
4	B	12	0	16	0	0
5	A	289	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	115	0	0	2	0
5	F	1	0	0	0	0
All	All	6965	0	6649	36	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.

All (36) 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:56:ARG:HG3	1:A:460:ASP:HB2	1.64	0.80
1:B:72:ILE:HD11	1:B:82:VAL:HB	1.75	0.69
1:A:270:LYS:NZ	5:A:608:HOH:O	2.31	0.64
1:A:264:GLU:OE1	1:A:267:ARG:NH2	2.23	0.63
1:B:82:VAL:HG23	1:B:105:ILE:HB	1.86	0.56
1:B:107:GLN:HB2	1:B:135:THR:HB	1.87	0.55
1:B:216:HIS:ND1	5:B:606:HOH:O	2.33	0.54
1:B:209:LEU:HD12	1:B:225:LEU:HD11	1.93	0.51
1:A:158:GLU:OE2	1:A:199:ARG:NH2	2.44	0.51
1:B:210:LYS:HG3	1:B:218:GLU:OE2	2.12	0.49
1:B:105:ILE:HA	1:B:136:VAL:HG12	1.95	0.49
1:A:360:TYR:HB3	1:A:364[B]:GLU:HB3	1.94	0.49
1:A:270:LYS:HG3	1:A:276:ASP:HA	1.96	0.48
1:A:355:LYS:NZ	5:A:619:HOH:O	2.46	0.47
1:B:60:ILE:HG12	1:B:95:LEU:HD11	1.97	0.47
1:A:71:SER:HB2	1:A:86:LYS:HB3	1.97	0.46
1:A:112:ASN:OD1	1:A:114:ARG:HB2	2.16	0.46
1:A:152:TYR:H	1:A:189:GLN:HE22	1.65	0.45
1:A:82:VAL:HG21	1:A:121:VAL:HG21	1.98	0.45
1:B:323:ALA:HB1	1:B:331:ASP:HB3	1.98	0.45
1:A:72:ILE:HD11	1:A:105:ILE:HD11	1.98	0.44
1:B:286:SER:HA	1:B:290:ARG:HH21	1.82	0.44
1:A:56:ARG:HG2	1:A:438:TYR:CZ	2.53	0.44
2:F:65:ALY:HE3	2:F:65:ALY:HH31	1.65	0.43
1:A:73:LYS:HB3	1:A:73:LYS:HE2	1.81	0.43
1:A:92:ARG:HH22	1:A:101:ILE:HD11	1.83	0.43
1:A:318:ARG:HG3	1:A:357:TYR:CZ	2.53	0.43
1:A:323:ALA:HB1	1:A:331:ASP:HB3	2.00	0.43
1:A:115:LYS:HD3	1:A:115:LYS:HA	1.75	0.42
2:E:99:ALY:HH31	2:E:99:ALY:HE3	1.69	0.42
1:A:360:TYR:CE1	1:A:368:LYS:HE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ILE:HD12	1:A:72:ILE:HA	1.88	0.42
1:B:165:GLU:OE2	1:B:169:LYS:NZ	2.41	0.41
1:A:267:ARG:NH1	1:A:271:GLU:OE1	2.54	0.41
1:B:83:VAL:HG12	1:B:104:ALA:HA	2.03	0.41
1:B:431:ARG:NH1	5:B:601:HOH:O	2.26	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	397/414 (96%)	387 (98%)	9 (2%)	1 (0%)	41	41
1	B	402/414 (97%)	394 (98%)	7 (2%)	1 (0%)	47	49
2	E	7/10 (70%)	7 (100%)	0	0	100	100
2	F	1/10 (10%)	1 (100%)	0	0	100	100
All	All	807/848 (95%)	789 (98%)	16 (2%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	VAL
1	B	173	VAL

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	349/357 (98%)	339 (97%)	10 (3%)	42	46
1	B	351/357 (98%)	345 (98%)	6 (2%)	60	67
2	E	9/9 (100%)	8 (89%)	1 (11%)	6	3
2	F	3/9 (33%)	3 (100%)	0	100	100
All	All	712/732 (97%)	695 (98%)	17 (2%)	49	53

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	72	ILE
1	A	77	GLU
1	A	80	ILE
1	A	140	LYS
1	A	152	TYR
1	A	153	THR
1	A	284	ASP
1	A	444	ASP
1	A	451	LYS
1	B	55	GLU
1	B	116	CYS
1	B	211	SER
1	B	243	LEU
1	B	284	ASP
1	B	444	ASP
2	E	92	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
2	ALY	E	99	2	10,11,12	0.90	0	7,12,14	0.84	0
2	ALY	F	65	2	10,11,12	0.87	0	7,12,14	0.68	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
2	ALY	E	99	2	-	4/9/10/12	-
2	ALY	F	65	2	-	4/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	99	ALY	OH-CH-NZ-CE
2	E	99	ALY	CH3-CH-NZ-CE
2	F	65	ALY	OH-CH-NZ-CE
2	F	65	ALY	CH3-CH-NZ-CE
2	E	99	ALY	CG-CD-CE-NZ
2	E	99	ALY	CA-CB-CG-CD
2	F	65	ALY	CE-CD-CG-CB
2	F	65	ALY	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	99	ALY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	65	ALY	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	$\# Z > 2$
4	GOL	A	507	-	5,5,5	1.06	0	5,5,5	1.54	1 (20%)
4	GOL	A	506	-	5,5,5	1.10	0	5,5,5	0.86	0
4	GOL	B	506	-	5,5,5	1.08	0	5,5,5	1.13	0
4	GOL	B	507	-	5,5,5	1.01	0	5,5,5	1.14	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
4	GOL	A	507	-	-	4/4/4/4	-
4	GOL	A	506	-	-	2/4/4/4	-
4	GOL	B	506	-	-	2/4/4/4	-
4	GOL	B	507	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	507	GOL	O2-C2-C3	2.48	120.06	109.12

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	506	GOL	O1-C1-C2-C3
4	B	506	GOL	C1-C2-C3-O3
4	B	507	GOL	C1-C2-C3-O3
4	A	506	GOL	O1-C1-C2-O2
4	A	507	GOL	O1-C1-C2-C3
4	A	507	GOL	O1-C1-C2-O2
4	A	507	GOL	O2-C2-C3-O3
4	B	506	GOL	O2-C2-C3-O3
4	B	507	GOL	O2-C2-C3-O3
4	A	507	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	398/414 (96%)	1.06	55 (13%) 2 4	24, 36, 102, 124	0
1	B	404/414 (97%)	1.47	94 (23%) 0 0	37, 58, 113, 139	0
2	E	9/10 (90%)	3.77	8 (88%) 0 0	103, 118, 134, 136	0
2	F	3/10 (30%)	3.07	2 (66%) 0 0	107, 107, 108, 142	0
All	All	814/848 (95%)	1.30	159 (19%) 1 1	24, 50, 108, 142	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	GLY	12.5
1	B	80	ILE	10.3
1	B	134	LEU	10.0
1	B	135	THR	9.7
1	B	121	VAL	9.6
1	B	282	ILE	8.8
1	A	461	ASP	8.8
1	B	76	ALA	8.8
1	B	129	GLY	8.5
1	A	151	ALA	8.4
1	A	139	LEU	7.7
1	B	122	VAL	7.5
1	B	245	THR	7.2
2	E	92	ASP	7.2
1	B	113	VAL	6.9
1	B	79	ASN	6.7
1	B	101	ILE	6.7
1	B	73	LYS	6.7
1	A	79	ASN	6.6
1	B	100	PHE	6.6
1	B	127	ASN	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	67	GLY	6.3
1	A	80	ILE	5.5
2	F	66	VAL	5.4
1	B	288	ASP	5.3
2	E	97	ILE	5.3
1	B	98	LEU	5.2
1	B	128	ALA	5.1
1	B	64	THR	5.1
1	B	70	LEU	5.1
1	A	152	TYR	5.1
1	B	124	VAL	5.0
1	A	130	GLU	5.0
1	B	116	CYS	5.0
1	B	81	PRO	4.9
1	A	460	ASP	4.8
1	B	95	LEU	4.8
2	E	95	THR	4.8
1	A	122	VAL	4.6
1	B	144	SER	4.5
1	B	243	LEU	4.5
1	B	306	SER	4.5
1	B	78	HIS	4.4
1	A	104	ALA	4.4
1	A	153	THR	4.3
1	A	123	GLN	4.3
1	B	321	TYR	4.3
2	E	94	HIS	4.1
1	B	56	ARG	4.1
1	B	304	ASP	4.1
1	B	126	ARG	4.1
1	B	96	SER	4.1
1	B	307	VAL	4.0
1	B	63	GLN	4.0
1	B	275	THR	3.9
1	A	115	LYS	3.9
1	B	104	ALA	3.8
1	B	66	GLY	3.8
1	B	75	GLY	3.8
1	A	72	ILE	3.8
1	A	81	PRO	3.8
1	A	121	VAL	3.8
1	A	119	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	115	LYS	3.7
1	A	113	VAL	3.7
1	B	107	GLN	3.6
1	B	105	ILE	3.6
1	A	154	ASN	3.5
1	A	61	ARG	3.4
1	A	68	PHE	3.4
1	B	82	VAL	3.4
1	B	329	GLY	3.4
1	A	116	CYS	3.4
1	A	89	LYS	3.3
1	B	328	LYS	3.3
1	A	126	ARG	3.3
1	A	114	ARG	3.3
1	B	83	VAL	3.2
1	A	73	LYS	3.2
1	B	72	ILE	3.2
1	A	71	SER	3.1
1	B	303	GLU	3.1
1	B	242	GLY	3.1
2	E	98	THR	3.1
1	A	127	ASN	3.1
1	B	130	GLU	3.1
1	B	332	VAL	3.1
1	B	65	VAL	3.0
1	B	300	ARG	3.0
1	A	101	ILE	2.9
1	B	117	ARG	2.9
1	B	326	LYS	2.9
2	E	93	GLN	2.9
1	B	139	LEU	2.9
1	A	65	VAL	2.9
1	B	123	GLN	2.8
1	B	68	PHE	2.8
1	B	172	GLY	2.8
1	B	106	LEU	2.8
1	B	372	GLY	2.8
1	A	138	PHE	2.8
1	B	330	THR	2.8
1	B	322	ASP	2.8
1	A	70	LEU	2.8
1	B	281	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	203	LYS	2.7
2	F	63	ILE	2.7
1	A	75	GLY	2.6
1	B	55	GLU	2.6
1	B	291	LYS	2.6
2	E	100	VAL	2.6
1	B	133	THR	2.6
2	E	96	GLN	2.6
1	B	283	SER	2.5
1	A	90	GLU	2.5
1	B	323	ALA	2.5
1	B	120	GLU	2.5
1	B	88	SER	2.5
1	B	103	ASP	2.5
1	B	132	VAL	2.5
1	B	336	ILE	2.5
1	A	128	ALA	2.5
1	A	108	ILE	2.4
1	B	461	ASP	2.4
1	A	140	LYS	2.4
1	B	241	LYS	2.4
1	B	74	GLY	2.4
1	B	334	LYS	2.3
1	B	337	SER	2.3
1	A	305	GLY	2.3
1	B	99	LEU	2.3
1	B	87	ILE	2.3
1	A	125	LEU	2.3
1	A	107	GLN	2.3
1	A	67	GLY	2.3
1	A	295	ALA	2.3
1	B	62	ARG	2.2
1	B	370	VAL	2.2
1	B	89	LYS	2.2
1	A	452	ALA	2.2
1	B	324	GLY	2.2
1	A	62	ARG	2.2
1	A	93	ALA	2.2
1	B	153	THR	2.2
1	A	85	SER	2.2
1	B	84	VAL	2.1
1	B	276	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	60	ILE	2.1
1	A	211	SER	2.1
1	A	64	THR	2.1
1	B	125	LEU	2.1
1	A	306	SER	2.1
1	A	83	VAL	2.1
1	B	376	ASN	2.1
1	A	92	ARG	2.1
1	A	124	VAL	2.0
1	B	273	TYR	2.0
1	A	91	GLN	2.0
1	A	459	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	ALY	E	99	12/13	0.36	0.35	112,125,134,134	0
2	ALY	F	65	12/13	0.44	0.35	114,117,124,125	0

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
3	CA	A	508	1/1	0.57	0.18	157,157,157,157	0
3	CA	B	503	1/1	0.64	0.20	117,117,117,117	0
3	CA	B	508	1/1	0.69	0.15	188,188,188,188	0
4	GOL	B	506	6/6	0.75	0.21	49,49,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	507	6/6	0.82	0.19	53,55,56,57	0
4	GOL	A	506	6/6	0.86	0.16	36,42,44,44	0
3	CA	B	502	1/1	0.90	0.10	74,74,74,74	0
3	CA	B	504	1/1	0.90	0.11	75,75,75,75	0
3	CA	A	501	1/1	0.91	0.11	59,59,59,59	0
4	GOL	A	507	6/6	0.91	0.16	29,34,39,40	0
3	CA	B	505	1/1	0.95	0.09	46,46,46,46	0
3	CA	B	501	1/1	0.96	0.04	56,56,56,56	0
3	CA	A	504	1/1	0.97	0.08	40,40,40,40	0
3	CA	A	503	1/1	0.97	0.11	38,38,38,38	0
3	CA	A	502	1/1	0.98	0.15	33,33,33,33	0
3	CA	A	505	1/1	0.99	0.22	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.