



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:13 AM UTC

PDB ID : 7QQL / pdb_00007qq1
Title : The PDZ domain of SNTG2 complexed with the phosphorylated PDZ-binding motif of RSK1
Authors : Cousido-Siah, A.; Trave, G.; Gogl, G.
Deposited on : 2022-01-10
Resolution : 2.44 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:

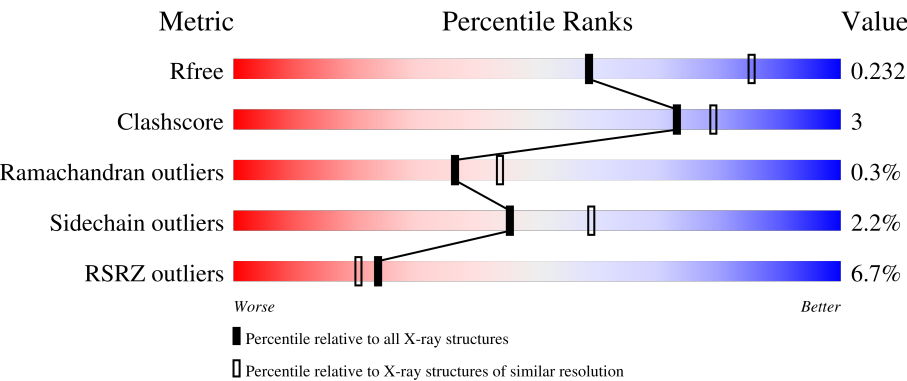
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	408	12% 86% 11% .
1	B	408	3% 87% 10% .
1	C	408	3% 87% 10% .
2	D	11	36% 18% 18% 9% 55%
2	E	11	36% 18% 18% 9% 55%

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Mol	Chain	Length	Quality of chain
2	F	11	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9838 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-2-syntrophin,Annexin A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	396	Total	C	N	O	S	0	0	0
			3154	1975	551	616	12			
1	A	398	Total	C	N	O	S	0	0	0
			3164	1982	553	617	12			
1	B	395	Total	C	N	O	S	0	0	0
			3145	1969	550	614	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	65	GLY	-	expression tag	UNP Q9NY99
C	66	SER	-	expression tag	UNP Q9NY99
C	67	HIS	-	expression tag	UNP Q9NY99
C	68	MET	-	expression tag	UNP Q9NY99
C	69	GLY	-	expression tag	UNP Q9NY99
C	160	GLY	-	linker	UNP Q9NY99
C	161	SER	-	linker	UNP Q9NY99
C	199	GLU	ALA	conflict	UNP P07355
A	65	GLY	-	expression tag	UNP Q9NY99
A	66	SER	-	expression tag	UNP Q9NY99
A	67	HIS	-	expression tag	UNP Q9NY99
A	68	MET	-	expression tag	UNP Q9NY99
A	69	GLY	-	expression tag	UNP Q9NY99
A	160	GLY	-	linker	UNP Q9NY99
A	161	SER	-	linker	UNP Q9NY99
A	199	GLU	ALA	conflict	UNP P07355
B	65	GLY	-	expression tag	UNP Q9NY99
B	66	SER	-	expression tag	UNP Q9NY99
B	67	HIS	-	expression tag	UNP Q9NY99
B	68	MET	-	expression tag	UNP Q9NY99
B	69	GLY	-	expression tag	UNP Q9NY99
B	160	GLY	-	linker	UNP Q9NY99
B	161	SER	-	linker	UNP Q9NY99

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Chain	Residue	Modelled	Actual	Comment	Reference
B	199	GLU	ALA	conflict	UNP P07355

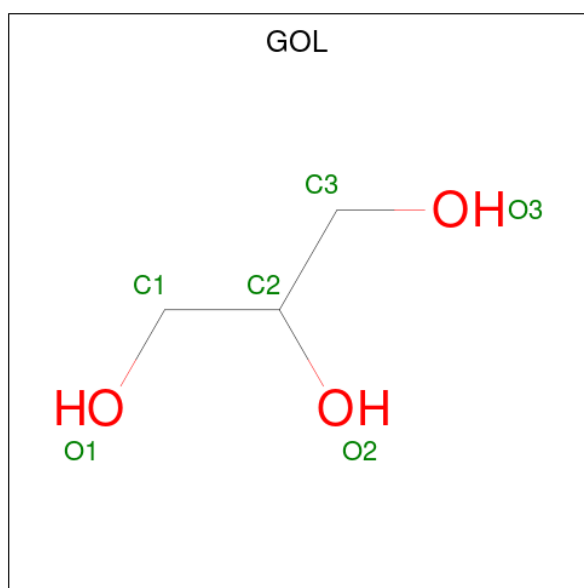
- Molecule 2 is a protein called Ribosomal protein S6 kinase alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	5	Total	C	N	O	P	0	0	0
			40	22	5	12	1			
2	D	5	Total	C	N	O	P	0	0	0
			40	22	5	12	1			
2	E	5	Total	C	N	O	P	0	0	0
			40	22	5	12	1			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	5	Total	Ca	0	0
			5	5		
3	A	4	Total	Ca	0	0
			4	4		
3	B	5	Total	Ca	0	0
			5	5		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	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

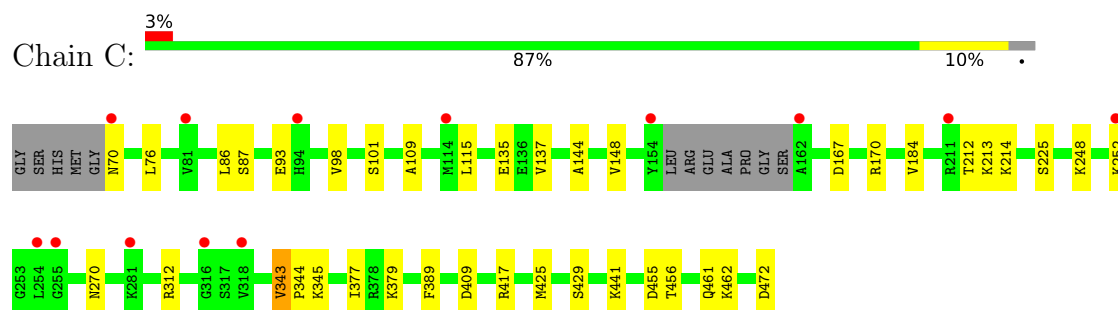
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	54	Total O 54 54	0	0
5	A	92	Total O 92 92	0	0
5	B	77	Total O 77 77	0	0

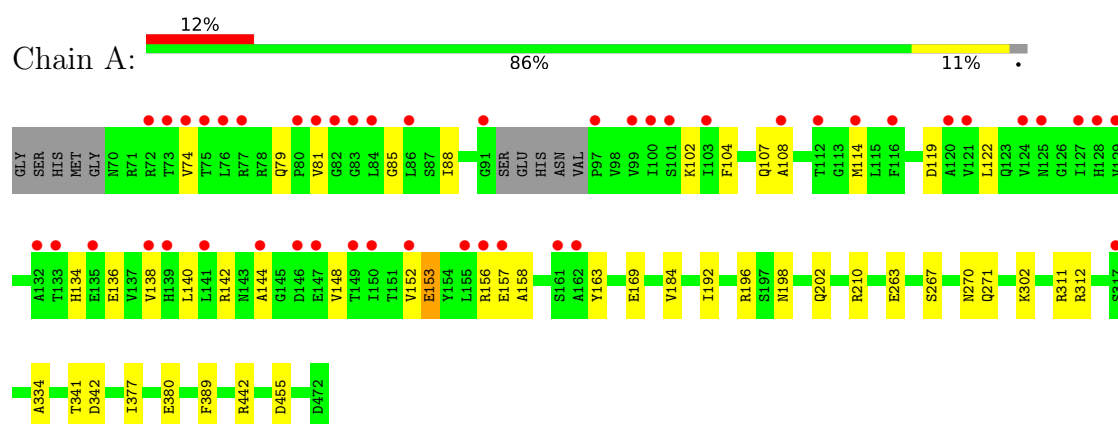
3 Residue-property plots [i](#)

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.

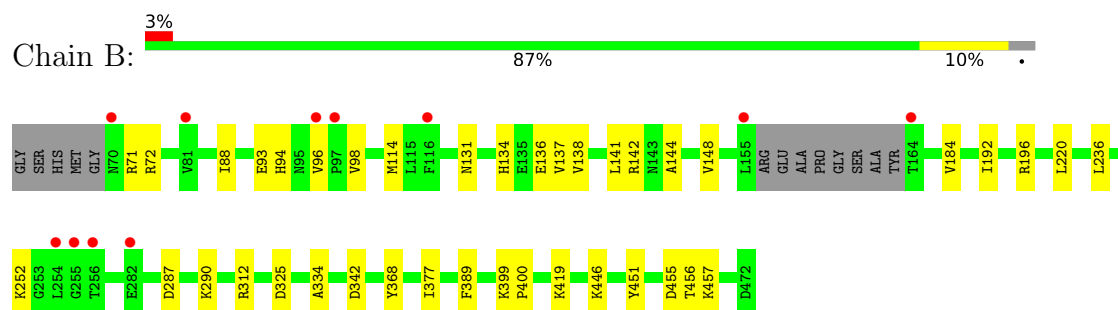
- Molecule 1: Gamma-2-syntrophin,Annexin A2



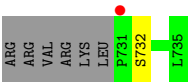
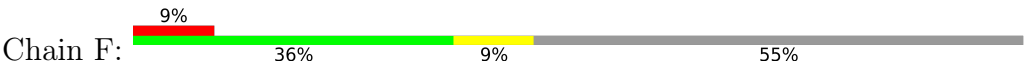
- Molecule 1: Gamma-2-syntrophin,Annexin A2



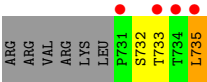
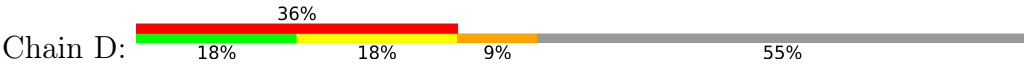
- Molecule 1: Gamma-2-syntrophin,Annexin A2



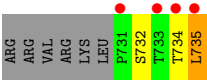
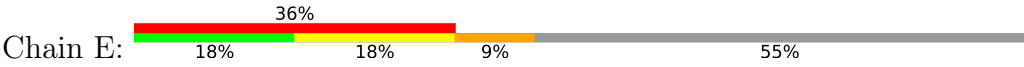
- Molecule 2: Ribosomal protein S6 kinase alpha-1



● Molecule 2: Ribosomal protein S6 kinase alpha-1



● Molecule 2: Ribosomal protein S6 kinase alpha-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.46Å 60.55Å 135.21Å 90.00° 92.42° 90.00°	Depositor
Resolution (Å)	48.42 – 2.44 48.42 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.42-2.44) 99.9 (48.42-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.195 , 0.230 0.196 , 0.232	Depositor DCC
R_{free} test set	2958 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9838	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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, SEP

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	0.19	0/3205	0.34	0/4309
1	B	0.10	0/3185	0.28	0/4283
1	C	0.10	0/3195	0.27	0/4297
2	D	0.14	0/29	0.22	0/36
2	E	0.13	0/29	0.24	0/36
2	F	0.16	0/29	0.23	0/36
All	All	0.14	0/9672	0.30	0/12997

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	3164	0	3198	23	0
1	B	3145	0	3177	22	0
1	C	3154	0	3180	17	0
2	D	40	0	35	4	0
2	E	40	0	36	2	0
2	F	40	0	35	0	0
3	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	1	0
4	C	6	0	8	0	0
5	A	92	0	0	1	0
5	B	77	0	0	0	0
5	C	54	0	0	2	0
All	All	9838	0	9685	62	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 (62) 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:C:379:LYS:NZ	5:C:604:HOH:O	2.27	0.68
1:A:119:ASP:HB3	1:A:152:VAL:HB	1.81	0.63
1:B:287:ASP:HB2	1:B:290:LYS:HD2	1.82	0.62
1:B:88:ILE:HG12	2:D:735:LEU:HD11	1.82	0.61
1:B:94:HIS:HB2	1:B:96:VAL:HG22	1.85	0.57
1:C:76:LEU:HD11	1:C:115:LEU:HD11	1.87	0.56
1:A:74:VAL:HG22	1:A:114:MET:HE2	1.86	0.56
1:B:312:ARG:HE	4:B:506:GOL:H12	1.69	0.56
1:A:142:ARG:HD3	2:E:735:LEU:HB3	1.88	0.55
1:C:212:THR:HB	1:C:214:LYS:HZ3	1.73	0.54
1:A:302:LYS:NZ	5:A:608:HOH:O	2.42	0.53
1:B:334:ALA:HB1	1:B:342:ASP:HB3	1.92	0.52
1:C:248:LYS:HG3	1:C:252:LYS:HE3	1.92	0.52
1:C:98:VAL:HG21	1:C:137:VAL:HG21	1.91	0.52
1:A:271:GLN:H	1:A:271:GLN:CD	2.18	0.52
1:C:225:SER:N	5:C:601:HOH:O	2.20	0.51
1:B:377:ILE:HD13	1:B:389:PHE:HB3	1.93	0.51
1:A:88:ILE:HG13	1:A:134:HIS:CE1	2.46	0.51
1:A:377:ILE:HD13	1:A:389:PHE:HB3	1.94	0.50
1:C:456:THR:O	1:C:461:GLN:NE2	2.40	0.50
1:C:377:ILE:HD13	1:C:389:PHE:HB3	1.95	0.49
1:C:441:LYS:NZ	1:C:472:ASP:OD2	2.41	0.49
1:A:144:ALA:HB3	1:A:148:VAL:HG22	1.94	0.49
1:B:72:ARG:NH1	1:B:114:MET:O	2.47	0.48
1:B:134:HIS:HE1	2:D:733:THR:HB	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HD11	1:A:153:GLU:HB2	1.95	0.48
1:B:220:LEU:HD12	1:B:236:LEU:HD11	1.96	0.47
1:A:169:GLU:OE2	1:A:210:ARG:NH2	2.46	0.47
1:C:343:VAL:HG22	1:C:344:PRO:HD3	1.97	0.47
1:A:334:ALA:HB1	1:A:342:ASP:HB3	1.96	0.47
1:C:167:ASP:OD2	1:C:170:ARG:NH2	2.48	0.46
1:B:192:ILE:O	1:B:196:ARG:HG2	2.16	0.46
1:A:85:GLY:HA2	1:A:107:GLN:OE1	2.15	0.46
1:C:86:LEU:HD23	1:C:109:ALA:HB2	1.98	0.45
1:B:446:LYS:HB2	1:B:451:TYR:HE1	1.81	0.45
1:A:198:ASN:O	1:A:202:GLN:HG2	2.16	0.45
1:A:158:ALA:O	1:A:163:TYR:HB3	2.17	0.45
1:A:136:GLU:O	1:A:140:LEU:HG	2.17	0.44
1:C:270:ASN:ND2	1:C:312:ARG:O	2.45	0.44
1:A:138:VAL:HG22	2:E:735:LEU:HD21	2.00	0.44
1:A:192:ILE:O	1:A:196:ARG:HG2	2.18	0.43
1:B:399:LYS:HB3	1:B:400:PRO:HD3	2.00	0.43
1:A:341:THR:OG1	1:A:380:GLU:OE1	2.33	0.43
1:B:325:ASP:OD1	1:B:368:TYR:OH	2.25	0.43
1:C:144:ALA:HB3	1:C:148:VAL:HG22	2.01	0.43
1:B:144:ALA:HB3	1:B:148:VAL:HG22	2.01	0.43
1:A:270:ASN:ND2	1:A:312:ARG:O	2.50	0.42
1:B:98:VAL:HG21	1:B:137:VAL:HG21	2.01	0.42
1:A:79:GLN:HG2	1:A:108:ALA:HB2	2.01	0.42
1:B:138:VAL:HG22	2:D:735:LEU:HD21	2.01	0.42
1:B:456:THR:C	1:B:457:LYS:HD2	2.45	0.42
1:C:425:MET:O	1:C:429:SER:HB2	2.20	0.42
1:A:104:PHE:HB2	1:A:107:GLN:CD	2.45	0.42
1:A:442:ARG:HE	1:A:442:ARG:HB3	1.70	0.41
1:B:138:VAL:O	1:B:142:ARG:HG2	2.20	0.41
1:B:141:LEU:HB2	2:D:735:LEU:HD22	2.02	0.41
1:B:252:LYS:HE2	1:B:252:LYS:HB3	1.91	0.41
1:A:263:GLU:O	1:A:267:SER:OG	2.28	0.41
1:B:456:THR:O	1:B:457:LYS:HD2	2.21	0.41
1:B:419:LYS:HE2	1:B:419:LYS:HB3	1.84	0.40
1:C:87:SER:O	1:C:101:SER:N	2.41	0.40
1:C:409:ASP:HB3	1:C:417:ARG:HH12	1.87	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	394/408 (97%)	383 (97%)	10 (2%)	1 (0%)	36	44
1	B	391/408 (96%)	379 (97%)	11 (3%)	1 (0%)	36	44
1	C	392/408 (96%)	381 (97%)	10 (3%)	1 (0%)	36	44
2	D	2/11 (18%)	2 (100%)	0	0	100	100
2	E	2/11 (18%)	2 (100%)	0	0	100	100
2	F	2/11 (18%)	2 (100%)	0	0	100	100
All	All	1183/1257 (94%)	1149 (97%)	31 (3%)	3 (0%)	36	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	VAL
1	C	184	VAL
1	A	184	VAL

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	345/353 (98%)	338 (98%)	7 (2%)	48	62
1	B	345/353 (98%)	340 (99%)	5 (1%)	59	70
1	C	345/353 (98%)	337 (98%)	8 (2%)	44	57
2	D	4/10 (40%)	3 (75%)	1 (25%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	4/10 (40%)	2 (50%)	2 (50%)	0	0
2	F	4/10 (40%)	4 (100%)	0	100	100
All	All	1047/1089 (96%)	1024 (98%)	23 (2%)	45	59

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	70	ASN
1	C	93	GLU
1	C	135	GLU
1	C	213	LYS
1	C	343	VAL
1	C	345	LYS
1	C	455	ASP
1	C	462	LYS
1	A	81	VAL
1	A	102	LYS
1	A	153	GLU
1	A	156	ARG
1	A	157	GLU
1	A	311	ARG
1	A	455	ASP
1	B	71	ARG
1	B	93	GLU
1	B	131	ASN
1	B	136	GLU
1	B	455	ASP
2	D	735	LEU
2	E	734	THR
2	E	735	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	195	ASN
1	C	227	HIS
1	A	134	HIS
1	A	143	ASN
1	B	143	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 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	SEP	F	732	2	8,9,10	1.61	1 (12%)	7,12,14	1.38	1 (14%)
2	SEP	E	732	2	8,9,10	1.56	1 (12%)	7,12,14	1.30	1 (14%)
2	SEP	D	732	2	8,9,10	1.55	1 (12%)	7,12,14	1.67	1 (14%)

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	SEP	F	732	2	-	0/6/8/10	-
2	SEP	E	732	2	-	0/6/8/10	-
2	SEP	D	732	2	-	2/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	732	SEP	P-O1P	3.53	1.61	1.50
2	D	732	SEP	P-O1P	3.44	1.61	1.50
2	E	732	SEP	P-O1P	3.39	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	732	SEP	OG-CB-CA	3.95	111.99	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	732	SEP	OG-CB-CA	3.06	111.12	108.14
2	E	732	SEP	OG-CB-CA	2.75	110.82	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	732	SEP	N-CA-CB-OG
2	D	732	SEP	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 14 are monoatomic - leaving 3 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	505	-	5,5,5	0.93	0	5,5,5	1.06	0
4	GOL	B	506	-	5,5,5	0.91	0	5,5,5	1.12	0
4	GOL	C	506	-	5,5,5	0.92	0	5,5,5	1.10	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	505	-	-	0/4/4/4	-
4	GOL	B	506	-	-	0/4/4/4	-
4	GOL	C	506	-	-	0/4/4/4	-

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 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	506	GOL	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	398/408 (97%)	0.19	47 (11%) 9 7	34, 49, 163, 201	0
1	B	395/408 (96%)	-0.03	11 (2%) 55 54	39, 56, 98, 136	0
1	C	396/408 (97%)	0.10	13 (3%) 49 48	42, 64, 95, 134	0
2	D	4/11 (36%)	4.25	4 (100%) 0 0	153, 154, 160, 165	0
2	E	4/11 (36%)	3.55	4 (100%) 0 0	130, 145, 165, 196	0
2	F	4/11 (36%)	2.03	1 (25%) 2 1	88, 94, 101, 130	0
All	All	1201/1257 (95%)	0.12	80 (6%) 24 20	34, 57, 136, 201	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	731	PRO	7.3
2	F	731	PRO	5.4
2	E	731	PRO	5.4
1	A	157	GLU	4.7
1	A	80	PRO	4.3
1	A	127	ILE	4.2
1	A	86	LEU	4.2
1	A	81	VAL	3.9
1	C	254	LEU	3.9
1	A	149	THR	3.9
1	A	128	HIS	3.8
2	E	735	LEU	3.7
1	A	75	THR	3.7
1	A	77	ARG	3.5
1	A	73	THR	3.5
1	A	82	GLY	3.5
1	A	129	VAL	3.5
1	A	84	LEU	3.5
1	B	155	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	735	LEU	3.5
2	D	734	THR	3.4
1	A	133	THR	3.3
1	A	121	VAL	3.3
1	A	150	ILE	3.2
2	E	734	THR	3.1
1	C	154	TYR	3.0
1	A	161	SER	3.0
1	A	162	ALA	2.9
1	A	76	LEU	2.9
1	A	103	ILE	2.9
2	D	733	THR	2.9
1	A	97	PRO	2.8
1	C	252	LYS	2.8
1	A	125	ASN	2.8
1	A	132	ALA	2.8
1	A	156	ARG	2.8
1	A	146	ASP	2.8
1	A	155	LEU	2.7
1	A	91	GLY	2.6
1	C	211	ARG	2.6
1	A	114	MET	2.6
1	A	116	PHE	2.5
1	B	254	LEU	2.5
1	B	255	GLY	2.5
1	A	120	ALA	2.5
1	A	112	THR	2.5
1	B	164	THR	2.5
1	A	147	GLU	2.5
1	A	152	VAL	2.5
1	B	81	VAL	2.5
1	C	114	MET	2.4
1	B	116	PHE	2.4
1	C	318	VAL	2.3
1	C	316	GLY	2.3
1	A	139	HIS	2.3
1	B	282	GLU	2.3
1	B	96	VAL	2.3
1	C	70	ASN	2.2
1	A	72	ARG	2.3
1	C	94	HIS	2.2
1	A	83	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	97	PRO	2.2
1	A	99	VAL	2.2
1	A	124	VAL	2.2
1	A	101	SER	2.1
1	A	138	VAL	2.1
1	A	108	ALA	2.1
1	A	144	ALA	2.1
1	C	255	GLY	2.1
1	B	256	THR	2.1
1	A	317	SER	2.1
1	C	162	ALA	2.0
1	B	70	ASN	2.0
1	A	135	GLU	2.0
1	C	281	LYS	2.0
2	E	733	THR	2.0
1	C	81	VAL	2.0
1	A	74	VAL	2.0
1	A	141	LEU	2.0
1	A	100	ILE	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	SEP	E	732	10/11	0.45	0.12	134,143,152,153	0
2	SEP	D	732	10/11	0.61	0.15	165,172,174,175	0
2	SEP	F	732	10/11	0.74	0.14	107,132,155,158	0

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
3	CA	C	503	1/1	0.81	0.09	126,126,126,126	0
3	CA	B	502	1/1	0.85	0.10	103,103,103,103	0
3	CA	C	502	1/1	0.88	0.08	96,96,96,96	0
4	GOL	B	506	6/6	0.91	0.13	46,49,54,54	0
3	CA	B	503	1/1	0.93	0.05	113,113,113,113	0
4	GOL	C	506	6/6	0.93	0.12	54,62,64,71	0
4	GOL	A	505	6/6	0.93	0.12	50,54,57,62	0
3	CA	A	502	1/1	0.93	0.07	93,93,93,93	0
3	CA	A	501	1/1	0.96	0.05	74,74,74,74	0
3	CA	C	505	1/1	0.97	0.04	60,60,60,60	0
3	CA	C	504	1/1	0.97	0.05	88,88,88,88	0
3	CA	C	501	1/1	0.98	0.05	76,76,76,76	0
3	CA	A	503	1/1	0.98	0.04	53,53,53,53	0
3	CA	B	504	1/1	0.98	0.04	71,71,71,71	0
3	CA	B	501	1/1	0.99	0.03	73,73,73,73	0
3	CA	B	505	1/1	1.00	0.04	50,50,50,50	0
3	CA	A	504	1/1	1.00	0.02	46,46,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.