Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 05:41 PM EST

PDB ID	:	5V44
Title	:	Crystal structure of the SR1 domain of human sacsin
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Deposited on	:	2017-03-08
Resolution	:	1.56 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:

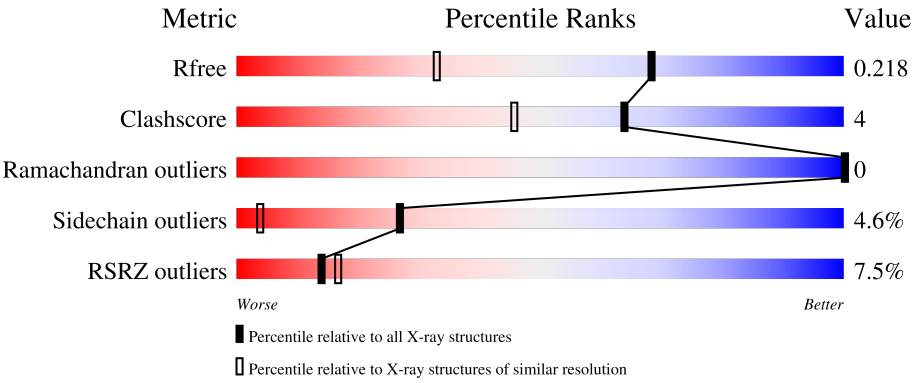
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.56 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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 <=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	253	6% 81% 7% • 11%
1	B	253	7% 78% 12% • 9%
1	C	253	8% 85% 10% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6047 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.

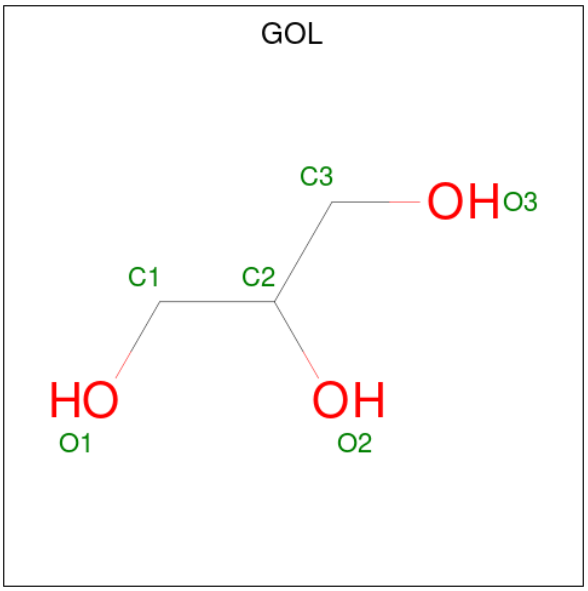
- Molecule 1 is a protein called Sacsin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	Se	0	4	0
			1823	1178	291	349	3	2			
1	B	231	Total	C	N	O	S	Se	0	3	0
			1867	1204	299	360	2	2			
1	C	242	Total	C	N	O	S	Se	0	1	0
			1932	1247	311	370	2	2			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	GLY	-	expression tag	UNP Q9NZJ4
A	85	PRO	-	expression tag	UNP Q9NZJ4
A	86	LEU	-	expression tag	UNP Q9NZJ4
A	87	GLY	-	expression tag	UNP Q9NZJ4
A	88	SER	-	expression tag	UNP Q9NZJ4
B	84	GLY	-	expression tag	UNP Q9NZJ4
B	85	PRO	-	expression tag	UNP Q9NZJ4
B	86	LEU	-	expression tag	UNP Q9NZJ4
B	87	GLY	-	expression tag	UNP Q9NZJ4
B	88	SER	-	expression tag	UNP Q9NZJ4
C	84	GLY	-	expression tag	UNP Q9NZJ4
C	85	PRO	-	expression tag	UNP Q9NZJ4
C	86	LEU	-	expression tag	UNP Q9NZJ4
C	87	GLY	-	expression tag	UNP Q9NZJ4
C	88	SER	-	expression tag	UNP Q9NZJ4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is water.

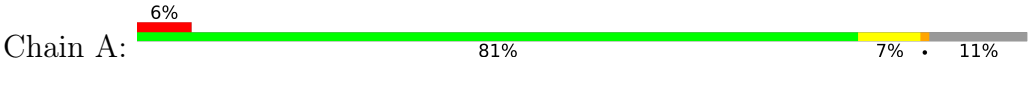
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	152	Total O 152 152	0	0
3	B	103	Total O 103 103	0	0
3	C	134	Total O 134 134	0	0

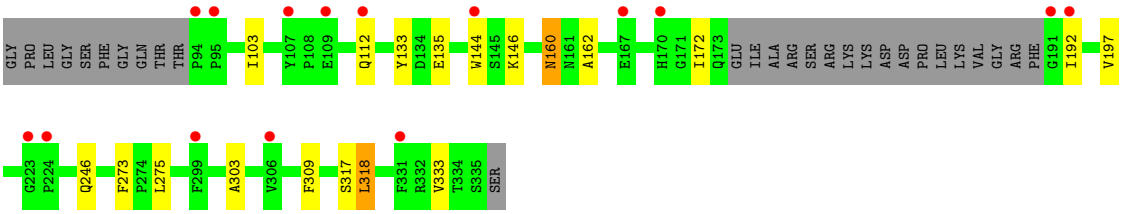
3 Residue-property plots (i)

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: Sacsin

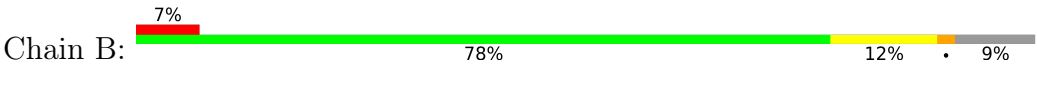
Chain A:

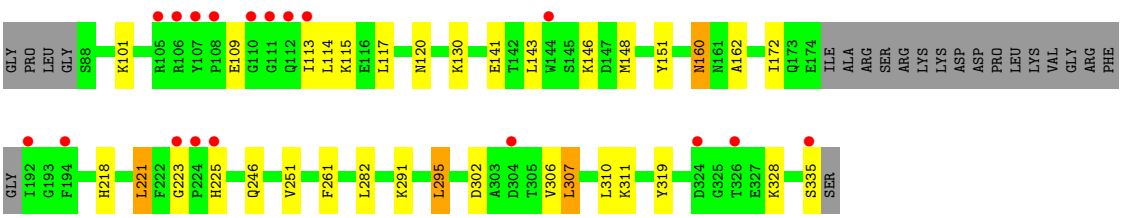




- Molecule 1: Sacsin

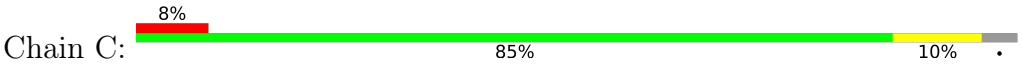
Chain B:

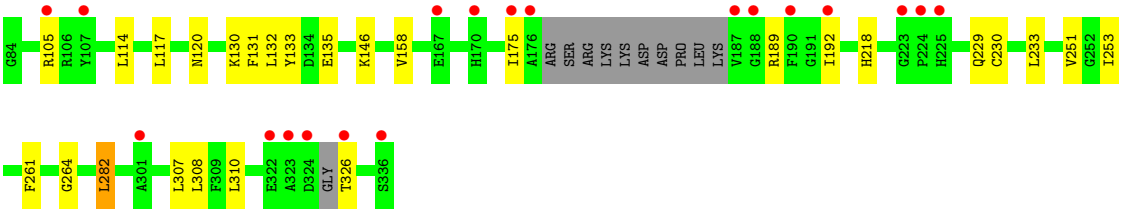




- Molecule 1: Sacsin

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	41.07Å 41.72Å 105.89Å 97.86° 95.76° 107.20°	Depositor
Resolution (Å)	50.00 – 1.56 38.79 – 1.56	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-1.56) 96.3 (38.79-1.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	4.19 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.182 , 0.214 0.184 , 0.218	Depositor DCC
R_{free} test set	4459 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for k,h,-h-k-l 0.015 for -k,-h,-l 0.000 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6047	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% 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: 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	0.40	0/1881	0.60	0/2549
1	B	0.39	0/1923	0.59	0/2606
1	C	0.38	0/1983	0.58	0/2687
All	All	0.39	0/5787	0.59	0/7842

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	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	223	GLY	Peptide
1	C	175	ILE	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	1823	0	1760	11	0
1	B	1867	0	1797	24	0
1	C	1932	0	1860	12	0
2	A	18	0	24	0	0
2	B	12	0	16	3	0
2	C	6	0	8	0	0
3	A	152	0	0	1	0
3	B	103	0	0	4	0
3	C	134	0	0	2	0
All	All	6047	0	5465	47	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 4.

All (47) 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:B:113:ILE:O	1:B:117:LEU:HD23	1.68	0.94
1:A:144:TRP:H	1:A:246:GLN:HE21	1.27	0.81
1:B:160:ASN:HD22	1:B:162:ALA:H	1.32	0.78
1:C:229:GLN:HE21	1:C:230:CYS:H	1.34	0.76
1:A:160:ASN:HD22	1:A:162:ALA:H	1.31	0.76
1:C:307:LEU:HD23	1:C:310:LEU:HD12	1.71	0.73
1:B:295:LEU:HG	3:B:593:HOH:O	1.95	0.65
1:C:133:TYR:HE2	1:C:135:GLU:HG2	1.62	0.65
1:B:148:MSE:HG3	3:B:545:HOH:O	2.00	0.61
1:C:133:TYR:CE2	1:C:135:GLU:HG2	2.36	0.60
1:B:307:LEU:HD22	1:B:310:LEU:HD12	1.84	0.59
1:B:114:LEU:HG	1:B:295:LEU:HD12	1.84	0.58
1:B:113:ILE:O	1:B:117:LEU:CD2	2.49	0.57
1:A:144:TRP:H	1:A:246:GLN:NE2	2.01	0.56
1:B:218:HIS:HD2	3:B:507:HOH:O	1.88	0.55
1:B:130[B]:LYS:HE3	1:B:319:TYR:CD1	2.42	0.54
1:C:120:ASN:HB3	3:C:609:HOH:O	2.07	0.54
1:C:132:LEU:HD22	1:C:253:ILE:HD11	1.90	0.54
1:A:317:SER:C	1:A:318:LEU:HD12	2.28	0.53
1:B:148:MSE:CE	1:B:221:LEU:HG	2.40	0.52
1:C:218:HIS:CE1	1:C:282:LEU:HB2	2.46	0.50
1:A:309:PHE:HB2	3:A:505:HOH:O	2.13	0.48
1:B:148:MSE:HG2	1:B:246:GLN:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:HG23	1:A:192:ILE:HG21	1.94	0.48
1:B:151:TYR:OH	2:B:401:GOL:C2	2.62	0.48
1:B:151:TYR:OH	2:B:401:GOL:H2	2.14	0.48
1:B:148:MSE:HE2	1:B:221:LEU:HG	1.96	0.47
1:C:114:LEU:HD22	1:C:131:PHE:CE2	2.51	0.46
1:C:233:LEU:HB3	1:C:264:GLY:HA2	1.97	0.45
1:A:133:TYR:HE1	1:A:275:LEU:CD1	2.29	0.45
1:B:148:MSE:SE	3:B:545:HOH:O	2.85	0.44
1:A:160:ASN:ND2	1:A:162:ALA:H	2.06	0.44
1:B:117:LEU:HD22	1:B:117:LEU:N	2.32	0.44
1:B:218:HIS:CG	2:B:401:GOL:H31	2.52	0.44
1:B:251:VAL:HG12	1:B:261:PHE:CE1	2.53	0.43
1:C:117:LEU:HD13	1:C:158:VAL:HG21	2.00	0.43
1:A:197:VAL:HG21	1:A:273:PHE:CE1	2.53	0.43
1:A:303:ALA:HB1	1:A:333:VAL:HG11	2.01	0.43
1:B:160:ASN:ND2	1:B:162:ALA:H	2.08	0.43
1:B:148:MSE:CG	1:B:246:GLN:HE22	2.32	0.42
1:B:143:LEU:HD13	1:B:148:MSE:HB3	2.00	0.42
1:B:218:HIS:HE1	1:B:282:LEU:H	1.68	0.42
1:C:251[A]:VAL:HG12	1:C:261:PHE:CE1	2.55	0.42
1:A:133:TYR:CE2	1:A:135:GLU:HG2	2.55	0.41
1:B:115:LYS:HE2	1:B:306:VAL:CG2	2.50	0.41
1:B:148:MSE:SE	1:B:246:GLN:HE22	2.54	0.41
1:C:130:LYS:HD3	3:C:552:HOH:O	2.21	0.41

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	225/253 (89%)	223 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	230/253 (91%)	226 (98%)	4 (2%)	0	100 100
1	C	237/253 (94%)	232 (98%)	5 (2%)	0	100 100
All	All	692/759 (91%)	681 (98%)	11 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	202/219 (92%)	196 (97%)	6 (3%)	41 12
1	B	207/219 (94%)	190 (92%)	17 (8%)	11 1
1	C	212/219 (97%)	205 (97%)	7 (3%)	38 10
All	All	621/657 (94%)	591 (95%)	30 (5%)	27 3

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112[A]	GLN
1	A	112[B]	GLN
1	A	146	LYS
1	A	160	ASN
1	A	172	ILE
1	A	318	LEU
1	B	101	LYS
1	B	109	GLU
1	B	120[A]	ASN
1	B	120[B]	ASN
1	B	141	GLU
1	B	146	LYS
1	B	160	ASN
1	B	172	ILE
1	B	221	LEU
1	B	225	HIS

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Mol	Chain	Res	Type
1	B	291	LYS
1	B	295	LEU
1	B	302	ASP
1	B	307	LEU
1	B	311	LYS
1	B	328	LYS
1	B	335	SER
1	C	105	ARG
1	C	146	LYS
1	C	189	ARG
1	C	192	ILE
1	C	282	LEU
1	C	308	LEU
1	C	326	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	229	GLN
1	A	246	GLN
1	A	278	GLN
1	B	160	ASN
1	B	218	HIS
1	B	281	GLN
1	C	229	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
2	GOL	B	401	-	5,5,5	0.31	0	5,5,5	0.50	0
2	GOL	A	402	-	5,5,5	0.38	0	5,5,5	0.50	0
2	GOL	A	403	-	5,5,5	0.35	0	5,5,5	0.24	0
2	GOL	A	401	-	5,5,5	0.34	0	5,5,5	0.40	0
2	GOL	B	402	-	5,5,5	0.28	0	5,5,5	0.16	0
2	GOL	C	401	-	5,5,5	0.27	0	5,5,5	0.30	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	GOL	B	401	-	-	0/4/4/4	-
2	GOL	A	402	-	-	2/4/4/4	-
2	GOL	A	403	-	-	0/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
2	GOL	B	402	-	-	0/4/4/4	-
2	GOL	C	401	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	GOL	C1-C2-C3-O3
2	A	402	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	GOL	3	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, 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	223/253 (88%)	0.55	15 (6%)	17	21	18, 27, 44, 60	0
1	B	229/253 (90%)	0.50	18 (7%)	12	15	19, 29, 45, 54	0
1	C	240/253 (94%)	0.53	19 (7%)	12	15	19, 30, 52, 67	0
All	All	692/759 (91%)	0.53	52 (7%)	14	17	18, 29, 48, 67	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	GLY	8.2
1	C	187	VAL	7.1
1	A	94	PRO	5.8
1	B	107	TYR	5.7
1	B	224	PRO	4.7
1	C	323	ALA	4.6
1	C	176	ALA	4.4
1	C	326	THR	4.4
1	B	192	ILE	4.1
1	B	223	GLY	3.9
1	A	107	TYR	3.9
1	B	112	GLN	3.8
1	C	170	HIS	3.5
1	B	111	GLY	3.5
1	B	335	SER	3.5
1	C	188	GLY	3.4
1	C	175	ILE	3.4
1	C	301	ALA	3.4
1	C	223	GLY	3.4
1	B	324	ASP	3.3
1	B	144	TRP	3.2
1	A	223	GLY	3.1
1	B	326	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	190	PHE	3.0
1	C	225	HIS	2.8
1	A	331	PHE	2.8
1	B	225	HIS	2.8
1	C	192	ILE	2.7
1	C	322	GLU	2.7
1	A	224	PRO	2.7
1	C	224	PRO	2.7
1	C	324	ASP	2.5
1	C	105	ARG	2.5
1	A	306	VAL	2.3
1	A	167	GLU	2.3
1	B	110	GLY	2.3
1	A	95	PRO	2.3
1	C	107	TYR	2.3
1	B	113	ILE	2.2
1	A	170	HIS	2.2
1	B	304	ASP	2.2
1	B	194	PHE	2.2
1	C	336	SER	2.2
1	B	105	ARG	2.2
1	A	109	GLU	2.2
1	A	299	PHE	2.1
1	A	144	TRP	2.1
1	A	112[A]	GLN	2.1
1	B	108	PRO	2.1
1	A	192	ILE	2.0
1	B	106	ARG	2.0
1	C	167	GLU	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 monosaccharides in this entry.

6.4 Ligands

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
2	GOL	B	401	6/6	0.77	0.20	42,44,47,47	0
2	GOL	B	402	6/6	0.79	0.18	48,52,54,55	0
2	GOL	A	402	6/6	0.86	0.12	31,32,36,37	0
2	GOL	C	401	6/6	0.93	0.11	32,38,41,44	0
2	GOL	A	403	6/6	0.96	0.11	27,29,30,31	0
2	GOL	A	401	6/6	0.96	0.09	24,25,28,31	0

6.5 Other polymers

There are no such residues in this entry.