W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:04 am GMT

PDB ID	:	4OYB
Title	:	Crystal Structure Analysis of the solAC
Authors	:	Vinkovic, M.
Deposited on	:	2014-02-11
Resolution	:	1.70 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
http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 1.70 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.
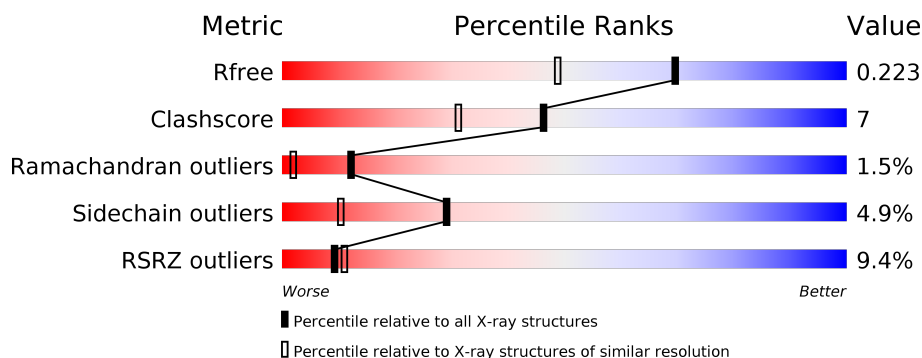
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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 <=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	470	9% / 86% / 12% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	501[A]	-	-	X	X
2	GOL	A	501[B]	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4444 atoms, of which 13 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.
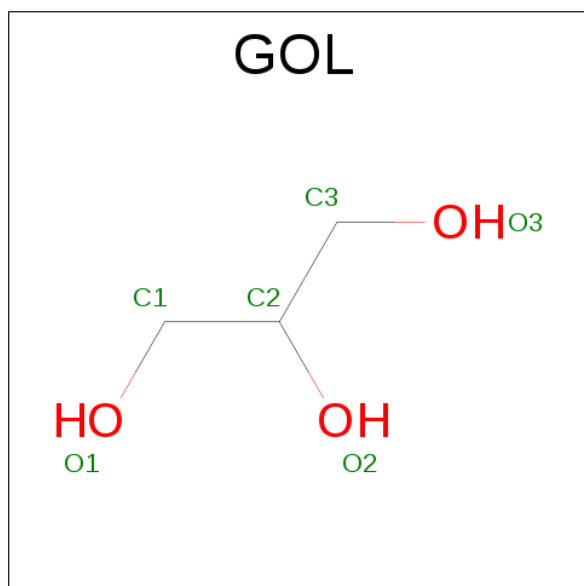
- Molecule 1 is a protein called Adenylate cyclase type 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total 3787	C 2449	N 615	O 688	S 35	0	8	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	acetylation	UNP Q96PN6

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 12	C 6	O 6	0	1

- Molecule 3 is ethyl 2-[3-[(4-azanyl-1,2,5-oxadiazol-3-yl)carbonyl]phenoxy]ethanoate (three-letter code: 1VJ) (formula: $C_{13}H_{13}N_3O_5$).
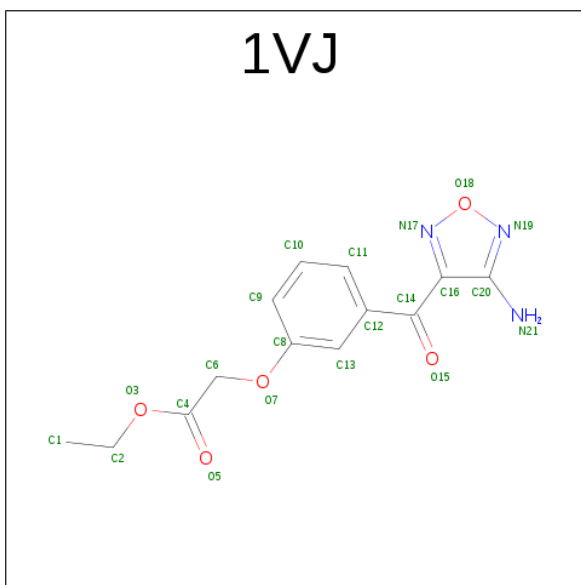
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
3	A	1	34	13	13	3	5	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	606	611	611	0	5

3 Residue-property plots ⓘ

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: Adenylate cyclase type 10
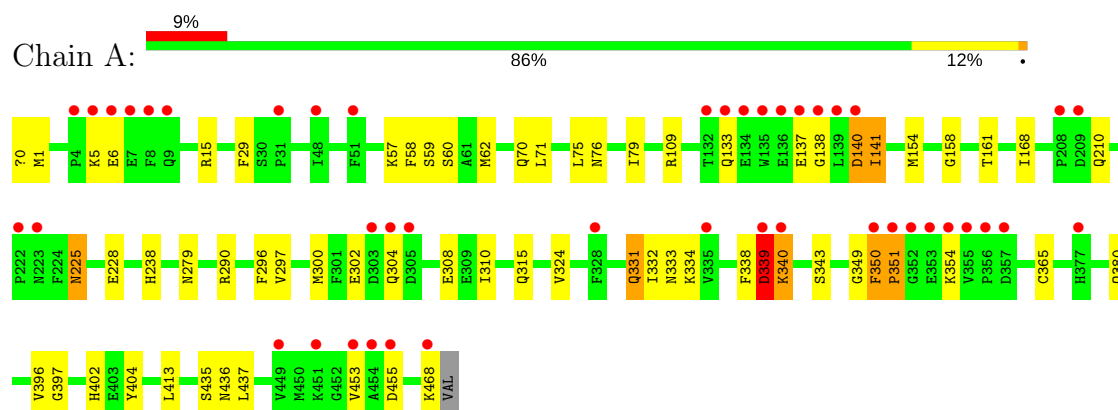
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	99.75Å 99.75Å 98.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.75 – 1.70 28.79 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (28.75-1.70) 99.4 (28.79-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0064	Depositor
R, R_{free}	0.170 , 0.211 0.184 , 0.223	Depositor DCC
R_{free} test set	3036 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.1	EDS
L-test for twinning [2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4444	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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, CME, 1VJ, ACE

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	0.59	1/3881 (0.0%)	0.74	1/5247 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	0	ACE	C-N	7.96	1.52	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	29	PHE	CB-CA-C	-5.14	100.11	110.40

There are no chirality outliers.

There are no planarity outliers.

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	3787	0	3770	55	0
2	A	12	0	16	7	0
3	A	21	13	13	0	0
4	A	611	0	0	7	0
All	All	4431	13	3799	55	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 7.

All (55) 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:332:ILE:H	2:A:501[A]:GOL:H32	1.37	0.90
1:A:340[B]:LYS:NZ	1:A:340[B]:LYS:HB3	1.87	0.90
1:A:340[B]:LYS:HZ3	1:A:340[B]:LYS:HB3	1.48	0.79
1:A:339[B]:ASP:O	1:A:340[B]:LYS:HB3	1.84	0.76
1:A:158:GLY:H	1:A:315:GLN:HE22	1.35	0.75
1:A:332:ILE:H	2:A:501[A]:GOL:C3	2.03	0.70
1:A:324:VAL:HG12	1:A:365[A]:CYS:SG	2.31	0.70
1:A:340[A]:LYS:HZ2	1:A:340[A]:LYS:HB2	1.60	0.67
1:A:76:ASN:HD21	1:A:396:VAL:HA	1.62	0.64
1:A:141:ILE:HA	4:A:1189:HOH:O	1.99	0.62
1:A:76:ASN:ND2	1:A:397:GLY:H	2.00	0.60
1:A:350:PHE:CB	1:A:351:PRO:HD2	2.31	0.60
1:A:168:ILE:HD13	1:A:310:ILE:HD11	1.84	0.60
1:A:350:PHE:HB2	4:A:784:HOH:O	2.01	0.59
1:A:340[A]:LYS:NZ	1:A:340[A]:LYS:HB2	2.17	0.58
1:A:332:ILE:N	2:A:501[A]:GOL:H32	2.13	0.58
1:A:331:GLN:HA	2:A:501[B]:GOL:H32	1.85	0.57
1:A:350:PHE:CG	1:A:351:PRO:HD2	2.40	0.57
1:A:57:LYS:NZ	4:A:1058:HOH:O	2.39	0.56
1:A:308:GLU:H	1:A:308:GLU:CD	2.10	0.55
1:A:340[B]:LYS:HZ2	1:A:340[B]:LYS:HB3	1.72	0.55
1:A:304:GLN:HE21	1:A:340[B]:LYS:HB2	1.72	0.54
1:A:304:GLN:HB2	1:A:340[B]:LYS:HB2	1.89	0.53
1:A:331:GLN:HA	2:A:501[A]:GOL:H32	1.91	0.52
1:A:210:GLN:NE2	4:A:1196:HOH:O	2.41	0.52
1:A:15:ARG:HH22	1:A:279:ASN:HD21	1.58	0.51
1:A:350:PHE:CD2	1:A:351:PRO:HD2	2.45	0.51
1:A:297:VAL:O	1:A:343[A]:SER:HA	2.12	0.50
1:A:339[B]:ASP:O	1:A:340[B]:LYS:NZ	2.46	0.49
1:A:331:GLN:HA	2:A:501[B]:GOL:C3	2.42	0.49
1:A:290:ARG:NE	1:A:349:GLY:O	2.37	0.48
1:A:350:PHE:HB3	1:A:351:PRO:HD2	1.95	0.47
1:A:168:ILE:CD1	1:A:310:ILE:HD11	2.45	0.47
1:A:300:MET:CG	1:A:340[B]:LYS:HE2	2.45	0.46
1:A:297:VAL:O	1:A:343[B]:SER:HA	2.15	0.46
1:A:333:ASN:ND2	4:A:1172:HOH:O	2.44	0.46
1:A:225:ASN:HD22	1:A:228:GLU:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:VAL:CG1	1:A:365[A]:CYS:SG	3.01	0.45
1:A:338:PHE:O	1:A:340[B]:LYS:N	2.50	0.45
1:A:133:GLN:O	1:A:140:ASP:O	2.35	0.45
1:A:75:LEU:HG	1:A:79:ILE:HD12	1.99	0.45
1:A:58:PHE:CD1	1:A:71:LEU:HD13	2.52	0.44
1:A:161:THR:HG23	4:A:687:HOH:O	2.17	0.44
1:A:350:PHE:CZ	1:A:404:TYR:HE2	2.34	0.44
1:A:57:LYS:O	1:A:60:SER:HB3	2.18	0.44
1:A:302:GLU:OE1	1:A:380:GLN:NE2	2.51	0.44
1:A:109:ARG:NH1	4:A:1163:HOH:O	2.51	0.43
1:A:300:MET:HG2	1:A:340[B]:LYS:HE2	1.99	0.43
1:A:435:SER:C	1:A:437:LEU:H	2.22	0.43
1:A:15:ARG:HH22	1:A:279:ASN:ND2	2.17	0.42
1:A:350:PHE:HB3	1:A:351:PRO:CD	2.49	0.42
1:A:332:ILE:H	2:A:501[B]:GOL:C3	2.33	0.42
1:A:333:ASN:ND2	1:A:334:LYS:HG2	2.35	0.41
1:A:75:LEU:HD11	1:A:79:ILE:HD11	2.02	0.41
1:A:340[B]:LYS:NZ	1:A:340[B]:LYS:CB	2.69	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	474/470 (101%)	450 (95%)	16 (3%)	8 (2%)	11 1

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339[A]	ASP
1	A	339[B]	ASP
1	A	436	ASN

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Mol	Chain	Res	Type
1	A	455	ASP
1	A	6	GLU
1	A	138	GLY
1	A	141	ILE
1	A	351	PRO

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	418/412 (102%)	396 (95%)	22 (5%)	26	9

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LYS
1	A	59	SER
1	A	62	MET
1	A	70	GLN
1	A	137	GLU
1	A	140	ASP
1	A	154	MET
1	A	225	ASN
1	A	238	HIS
1	A	296	PHE
1	A	331	GLN
1	A	339[A]	ASP
1	A	339[B]	ASP
1	A	340[A]	LYS
1	A	340[B]	LYS
1	A	350	PHE
1	A	354	LYS
1	A	402	HIS
1	A	413	LEU
1	A	453	VAL

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Mol	Chain	Res	Type
1	A	468	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	179	GLN
1	A	180	ASN
1	A	210	GLN
1	A	225	ASN
1	A	266	GLN
1	A	279	ASN
1	A	298	ASN
1	A	304	GLN
1	A	315	GLN
1	A	331	GLN
1	A	333	ASN
1	A	380	GLN
1	A	409	GLN
1	A	461	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	#$|Z| > 2$
1	CME	A	253	1	9,9,10	1.13	1 (11%)	6,9,11	1.04	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
1	CME	A	253	1	-	0/5/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	CME	CA-C	3.19	1.54	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 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	A	501[A]	-	5,5,5	0.27	0	5,5,5	0.98	0
2	GOL	A	501[B]	-	5,5,5	0.31	0	5,5,5	0.61	0
3	1VJ	A	502	-	18,22,22	0.57	0	19,29,29	0.63	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	A	501[A]	-	-	0/4/4/4	0/0/0/0
2	GOL	A	501[B]	-	-	0/4/4/4	0/0/0/0
3	1VJ	A	502	-	-	0/12/16/16	0/1/2/2

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.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501[A]	GOL	4	0
2	A	501[B]	GOL	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	467/470 (99%)	0.40	44 (9%)	9	11	10, 25, 67, 127	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	TRP	9.1
1	A	355	VAL	7.8
1	A	356	PRO	7.5
1	A	137	GLU	5.8
1	A	351	PRO	5.7
1	A	6	GLU	5.5
1	A	8	PHE	5.5
1	A	352	GLY	5.5
1	A	138	GLY	5.4
1	A	350	PHE	5.4
1	A	140	ASP	5.2
1	A	340[A]	LYS	4.9
1	A	304	GLN	4.4
1	A	139	LEU	4.4
1	A	51	PHE	4.3
1	A	454	ALA	4.2
1	A	136	GLU	4.1
1	A	453	VAL	3.7
1	A	455	ASP	3.4
1	A	132	THR	3.4
1	A	209	ASP	3.4
1	A	354	LYS	3.4
1	A	328	PHE	3.4
1	A	305	ASP	3.4
1	A	7	GLU	3.3
1	A	353	GLU	3.2
1	A	31	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	208	PRO	3.1
1	A	4	PRO	3.0
1	A	9	GLN	3.0
1	A	303	ASP	2.9
1	A	449	VAL	2.8
1	A	451	LYS	2.8
1	A	133	GLN	2.7
1	A	5	LYS	2.7
1	A	468	LYS	2.6
1	A	339[A]	ASP	2.4
1	A	357	ASP	2.3
1	A	223	ASN	2.3
1	A	377	HIS	2.2
1	A	48	ILE	2.2
1	A	335	VAL	2.1
1	A	222	PRO	2.1
1	A	134	GLU	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
1	CME	A	253	10/11	0.98	0.06	-	13,19,28,32	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
2	GOL	A	501[B]	6/6	0.75	0.24	5.09	28,37,41,47	6
2	GOL	A	501[A]	6/6	0.75	0.24	5.09	24,34,38,49	6
3	1VJ	A	502	21/21	0.92	0.10	-0.41	24,30,46,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.