



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:37 PM UTC

PDB ID : 4OZ3 / pdb_00004oz3
Title : Human solAC Complexed with 4-phenyl-3-(trifluoromethyl)-1H-pyrazole
Authors : Vinkovic, M.
Deposited on : 2014-02-13
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

<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

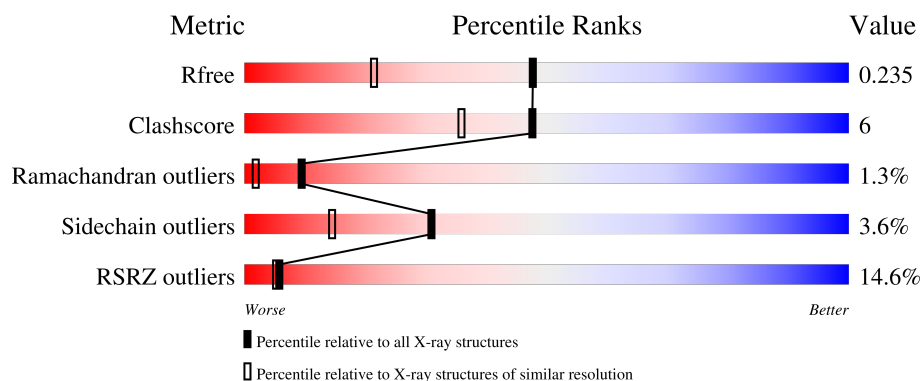
1 Overall quality at a glance

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 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	470	

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
3	GOL	A	502	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4417 atoms, of which 7 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.

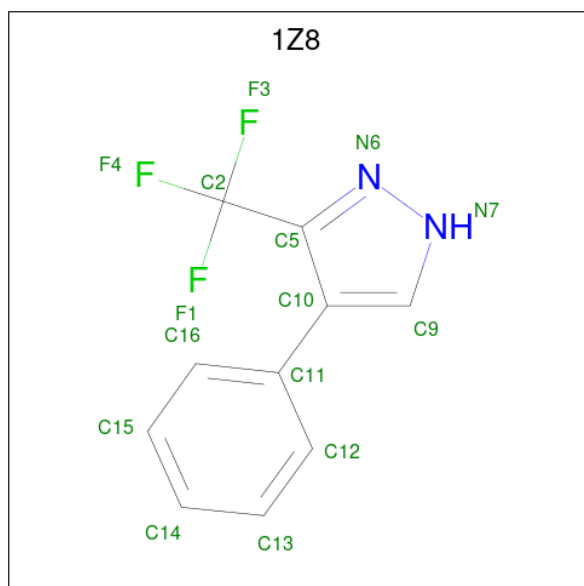
- Molecule 1 is a protein called Adenylate cyclase type 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	469	3750	2427	608	680	35	0	2	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 4-phenyl-3-(trifluoromethyl)-1H-pyrazole (CCD ID: 1Z8) (formula: $C_{10}H_7F_3N_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	H	N		
2	A	1	22	10	3	7	2	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

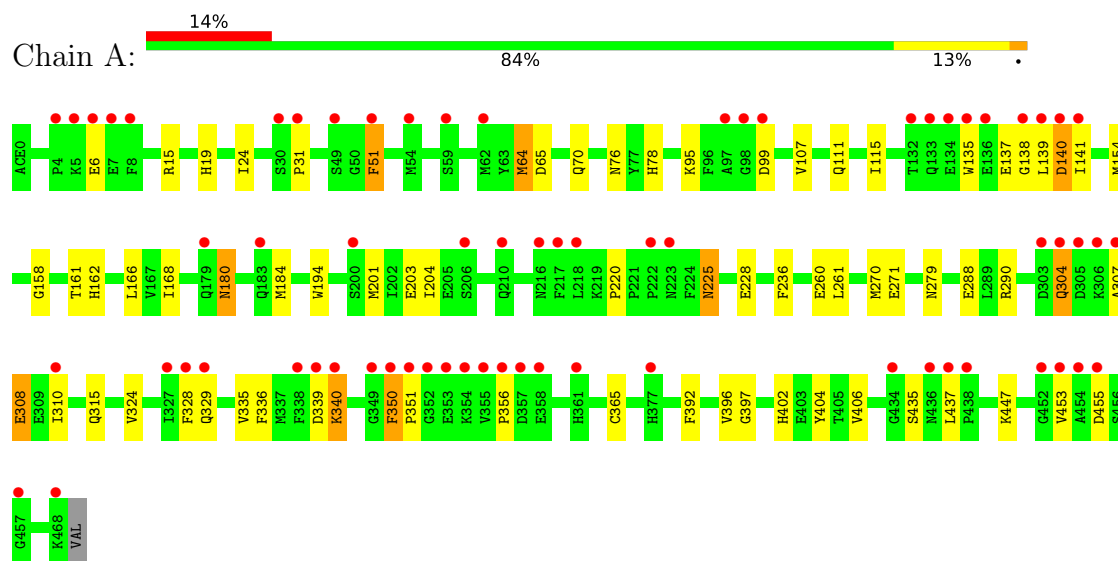
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	618	Total	O	0	15
			633	633		

3 Residue-property plots

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: 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	99.26Å 99.26Å 97.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.22 – 1.70 27.22 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.3 (27.22-1.70) 94.2 (27.22-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 1.70Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.174 , 0.216 (Not available) , 0.235	Depositor DCC
R_{free} test set	2817 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 65.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4417	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 3.74% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACE, CME, 1Z8

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	1.00	1/3834 (0.0%)	1.15	8/5186 (0.2%)

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	GLU	CA-C	5.61	1.60	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ASN	CA-CB-CG	7.13	119.73	112.60
1	A	31	PRO	CA-C-N	6.41	129.94	120.90
1	A	31	PRO	C-N-CA	6.41	129.94	120.90
1	A	51	PHE	CA-CB-CG	5.87	119.67	113.80
1	A	64	MET	CA-C-N	-5.43	115.46	125.02
1	A	64	MET	C-N-CA	-5.43	115.46	125.02
1	A	392	PHE	CA-CB-CG	-5.43	108.37	113.80
1	A	328	PHE	CA-CB-CG	-5.03	108.78	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	ASP	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	3750	0	3731	41	0
2	A	15	7	7	1	0
3	A	12	0	16	4	0
4	A	633	0	0	8	0
All	All	4410	7	3754	42	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 6.

All (42) 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:324:VAL:HG12	1:A:365[B]:CYS:SG	2.18	0.83
1:A:158:GLY:H	1:A:315:GLN:HE22	1.32	0.77
1:A:162:HIS:HD2	4:A:883:HOH:O	1.71	0.72
1:A:76:ASN:HD21	1:A:396:VAL:HA	1.58	0.69
1:A:76:ASN:ND2	1:A:397:GLY:H	1.94	0.66
1:A:304:GLN:HB3	1:A:340:LYS:HB2	1.78	0.65
1:A:261:LEU:CD1	3:A:502:GOL:H32	2.28	0.63
1:A:201:MET:HE1	1:A:220:PRO:HB3	1.82	0.61
1:A:351:PRO:HG2	4:A:1132:HOH:O	2.00	0.61
1:A:15:ARG:HH22	1:A:279:ASN:HD21	1.47	0.61
1:A:261:LEU:HD11	3:A:502:GOL:H32	1.83	0.60
1:A:162:HIS:HE1	1:A:271:GLU:OE2	1.87	0.56
1:A:324:VAL:CG1	1:A:365[B]:CYS:SG	2.91	0.56
3:A:502:GOL:H12	4:A:803:HOH:O	2.06	0.56
1:A:107:VAL:HG11	1:A:115:ILE:HG13	1.87	0.56
1:A:168:ILE:HD13	1:A:310:ILE:HD11	1.88	0.55
1:A:351:PRO:HG3	4:A:798:HOH:O	2.07	0.53
1:A:270:MET:HG2	4:A:826:HOH:O	2.09	0.53
1:A:24:ILE:O	3:A:502:GOL:H31	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:PHE:CE2	1:A:406:VAL:HG11	2.46	0.50
1:A:140:ASP:HB3	1:A:184:MET:HE3	1.94	0.49
1:A:350:PHE:HB2	4:A:815:HOH:O	2.12	0.49
1:A:64:MET:O	1:A:65:ASP:HB2	2.14	0.48
1:A:329:GLN:HA	4:A:873:HOH:O	2.14	0.48
1:A:194:TRP:CH2	1:A:204:ILE:HG12	2.49	0.47
1:A:350:PHE:CZ	1:A:404:TYR:HE2	2.32	0.47
1:A:15:ARG:HH22	1:A:279:ASN:ND2	2.12	0.47
1:A:288:GLU:CD	1:A:290:ARG:HD2	2.41	0.46
1:A:78:HIS:HE1	1:A:135:TRP:HE1	1.63	0.46
1:A:225:ASN:HD22	1:A:228:GLU:H	1.64	0.45
1:A:95:LYS:HD2	2:A:501:1Z8:F4	2.08	0.44
1:A:288:GLU:OE1	1:A:351:PRO:HB3	2.18	0.44
1:A:350:PHE:CE2	1:A:406:VAL:CG1	3.01	0.44
1:A:19:HIS:HA	1:A:402:HIS:O	2.19	0.43
1:A:166:LEU:CD2	1:A:336:PHE:HA	2.49	0.42
1:A:161:THR:HG23	4:A:730:HOH:O	2.19	0.42
1:A:435:SER:C	1:A:437:LEU:H	2.28	0.42
1:A:166:LEU:HD21	1:A:335:VAL:HG12	2.02	0.42
1:A:168:ILE:HD11	1:A:307:ALA:HB2	2.03	0.41
1:A:350:PHE:HE2	1:A:406:VAL:CG1	2.33	0.41
1:A:111:GLN:HG3	1:A:236:PHE:CG	2.56	0.40
1:A:308:GLU:CD	1:A:308:GLU:H	2.29	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	468/470 (100%)	447 (96%)	15 (3%)	6 (1%)	9 2

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	GLY
1	A	6	GLU
1	A	455	ASP
1	A	99	ASP
1	A	339	ASP
1	A	356	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	413/412 (100%)	398 (96%)	15 (4%)	31	14

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	PHE
1	A	70	GLN
1	A	137	GLU
1	A	139	LEU
1	A	141	ILE
1	A	154	MET
1	A	180	ASN
1	A	203	GLU
1	A	225	ASN
1	A	304	GLN
1	A	308	GLU
1	A	340	LYS
1	A	350	PHE
1	A	447	LYS
1	A	453	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN

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Mol	Chain	Res	Type
1	A	78	HIS
1	A	162	HIS
1	A	170	GLN
1	A	192	ASN
1	A	225	ASN
1	A	245	HIS
1	A	279	ASN
1	A	298	ASN
1	A	315	GLN
1	A	333	ASN
1	A	377	HIS
1	A	461	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	8,9,10	0.41	0	6,9,11	0.91	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	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	253	CME	CZ-CE-SD-SG

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](#)

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	1Z8	A	501	-	16,16,16	0.65	0	21,23,23	0.41	0
3	GOL	A	503	-	5,5,5	0.13	0	5,5,5	0.44	0
3	GOL	A	502	-	5,5,5	0.31	0	5,5,5	0.58	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	1Z8	A	501	-	-	0/10/10/10	0/2/2/2
3	GOL	A	503	-	-	2/4/4/4	-
3	GOL	A	502	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	A	502	GOL	O1-C1-C2-C3
3	A	503	GOL	O1-C1-C2-C3
3	A	502	GOL	O2-C2-C3-O3
3	A	503	GOL	O1-C1-C2-O2
3	A	502	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	1Z8	1	0
3	A	502	GOL	4	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	467/470 (99%)	0.54	68 (14%) 6 5	7, 24, 67, 113	2 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	TRP	7.4
1	A	355	VAL	6.5
1	A	139	LEU	5.9
1	A	338	PHE	5.5
1	A	350	PHE	5.1
1	A	351	PRO	5.1
1	A	97	ALA	5.0
1	A	304	GLN	4.9
1	A	453	VAL	4.3
1	A	305	ASP	4.3
1	A	141	ILE	4.3
1	A	8	PHE	4.0
1	A	31	PRO	4.0
1	A	468	LYS	3.9
1	A	328	PHE	3.7
1	A	354	LYS	3.6
1	A	138	GLY	3.6
1	A	307	ALA	3.5
1	A	306	LYS	3.5
1	A	51	PHE	3.4
1	A	349	GLY	3.4
1	A	340	LYS	3.4
1	A	357	ASP	3.4
1	A	356	PRO	3.4
1	A	437	LEU	3.3
1	A	454	ALA	3.2
1	A	217	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	452	GLY	3.1
1	A	99	ASP	2.9
1	A	136	GLU	2.9
1	A	133	GLN	2.8
1	A	98	GLY	2.8
1	A	140	ASP	2.8
1	A	455	ASP	2.7
1	A	457	GLY	2.6
1	A	438	PRO	2.6
1	A	132	THR	2.5
1	A	49	SER	2.5
1	A	361	HIS	2.4
1	A	223	ASN	2.4
1	A	206	SER	2.4
1	A	216	ASN	2.4
1	A	352	GLY	2.4
1	A	210	GLN	2.4
1	A	329	GLN	2.4
1	A	339	ASP	2.4
1	A	434	GLY	2.3
1	A	353	GLU	2.2
1	A	218	LEU	2.2
1	A	7	GLU	2.2
1	A	200	SER	2.2
1	A	54	MET	2.2
1	A	62	MET	2.2
1	A	327	ILE	2.2
1	A	30	SER	2.2
1	A	134	GLU	2.1
1	A	436	ASN	2.1
1	A	310	ILE	2.1
1	A	377	HIS	2.1
1	A	5	LYS	2.1
1	A	6	GLU	2.1
1	A	179	GLN	2.1
1	A	222	PRO	2.1
1	A	183	GLN	2.1
1	A	59	SER	2.1
1	A	4	PRO	2.1
1	A	303	ASP	2.0
1	A	358	GLU	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
1	CME	A	253	10/11	0.97	0.08	11,15,23,24	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
2	1Z8	A	501	15/15	0.83	0.14	30,40,44,46	0
3	GOL	A	503	6/6	0.83	0.14	36,44,47,48	0
3	GOL	A	502	6/6	0.89	0.11	31,32,37,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.