



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:34 am BST

PDB ID : 4OZ3
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 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 : 2.11
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) : 2.11

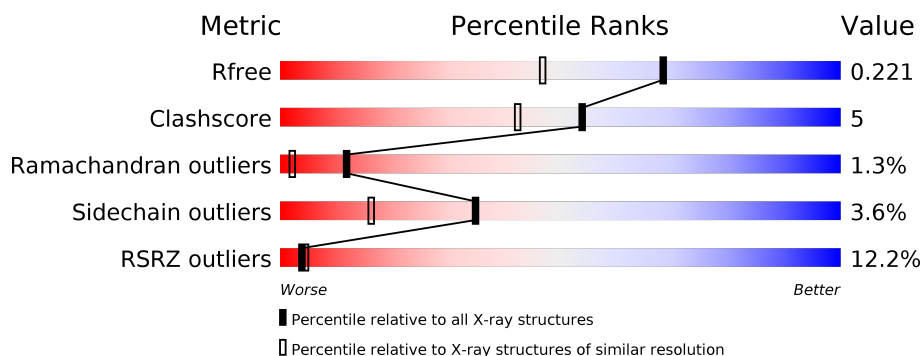
1 Overall quality at a glance

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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 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.

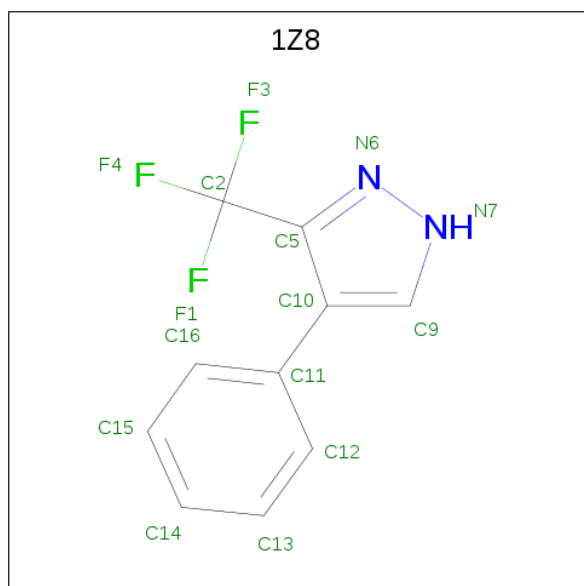
- Molecule 1 is a protein called Adenylate cyclase type 10.

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 (three-letter code: 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 (three-letter code: GOL) (formula: $C_3H_8O_3$).

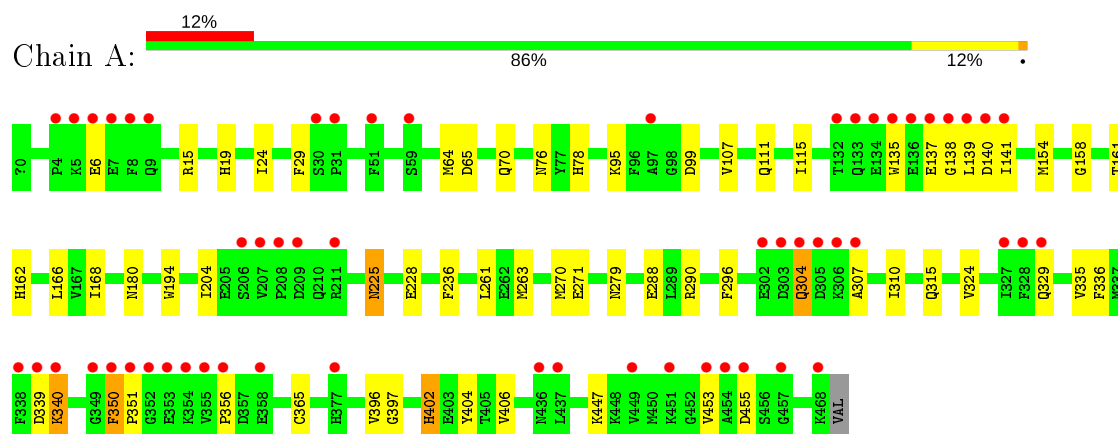


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

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

- 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	99.26 Å 99.26 Å 97.64 Å 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) 94.3 (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 1.70 Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.174 , 0.216 0.184 , 0.221	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)	0.36 , 65.6	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1Z8, GOL, CME, 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	0.66	0/3834	0.72	0/5186

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

There are no bond length outliers.

There are no bond angle outliers.

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 [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	3750	0	3731	39	0
2	A	15	7	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	16	4	0
4	A	633	0	0	8	0
All	All	4410	7	3754	40	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 5.

All (40) 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: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
1:A:350:PHE:CE2	1:A:406:VAL:HG11	2.46	0.50
1:A:350:PHE:HB2	4:A:815:HOH:O	2.12	0.49
1:A:324:VAL:HG12	1:A:365[B]:CYS:HG	1.78	0.48
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:166:LEU:HD21	1:A:335:VAL:HG12	2.02	0.42
1:A:263:MET:HB3	1:A:263:MET:HE3	1.90	0.41
1:A:288:GLU:CD	1:A:290:ARG:HD2	2.41	0.41
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

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%)	12	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 [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	413/412 (100%)	398 (96%)	15 (4%)	35	16

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

Mol	Chain	Res	Type
1	A	29	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	225	ASN
1	A	296	PHE
1	A	304	GLN
1	A	340	LYS
1	A	350	PHE
1	A	402	HIS
1	A	447	LYS
1	A	453	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	78	HIS
1	A	162	HIS
1	A	210	GLN
1	A	225	ASN
1	A	266	GLN
1	A	279	ASN
1	A	298	ASN
1	A	315	GLN
1	A	333	ASN
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	0.38	0	5,9,11	0.89	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 ⓘ

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
3	GOL	A	503	-	5,5,5	0.13	0	5,5,5	0.44	0
3	GOL	A	502	-	5,5,5	0.30	0	5,5,5	0.53	0
2	1Z8	A	501	-	15,16,16	0.87	1 (6%)	16,23,23	0.56	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
3	GOL	A	503	-	-	2/4/4/4	-
3	GOL	A	502	-	-	4/4/4/4	-
2	1Z8	A	501	-	-	3/10/10/10	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	1Z8	C2-C5	-2.37	1.47	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
2	A	501	1Z8	F3-C2-C5-N6
3	A	503	GOL	O1-C1-C2-C3
3	A	502	GOL	O1-C1-C2-C3
2	A	501	1Z8	F1-C2-C5-N6

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Mol	Chain	Res	Type	Atoms
3	A	502	GOL	O2-C2-C3-O3
3	A	503	GOL	O1-C1-C2-O2
2	A	501	1Z8	F4-C2-C5-N6
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
3	A	502	GOL	4	0
2	A	501	1Z8	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	467/470 (99%)	0.81	57 (12%) 4 4	7, 24, 67, 113	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	LEU	17.2
1	A	135	TRP	11.4
1	A	355	VAL	10.2
1	A	136	GLU	9.0
1	A	354	LYS	8.9
1	A	352	GLY	8.5
1	A	138	GLY	8.0
1	A	304	GLN	7.5
1	A	351	PRO	7.4
1	A	8	PHE	7.3
1	A	356	PRO	6.9
1	A	454	ALA	6.8
1	A	350	PHE	6.8
1	A	338	PHE	5.9
1	A	340	LYS	5.9
1	A	31	PRO	5.3
1	A	455	ASP	5.2
1	A	6	GLU	5.2
1	A	137	GLU	5.1
1	A	141	ILE	4.9
1	A	305	ASP	4.8
1	A	134	GLU	4.7
1	A	453	VAL	4.7
1	A	140	ASP	4.7
1	A	5	LYS	4.6
1	A	468	LYS	4.6
1	A	302	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	133	GLN	4.4
1	A	353	GLU	4.4
1	A	132	THR	4.4
1	A	303	ASP	4.2
1	A	7	GLU	4.1
1	A	208	PRO	4.1
1	A	328	PHE	4.0
1	A	306	LYS	3.8
1	A	9	GLN	3.7
1	A	209	ASP	3.5
1	A	377	HIS	3.5
1	A	97	ALA	3.4
1	A	451	LYS	3.4
1	A	436	ASN	3.1
1	A	339	ASP	3.0
1	A	457	GLY	3.0
1	A	449	VAL	3.0
1	A	30	SER	2.8
1	A	211	ARG	2.6
1	A	307	ALA	2.6
1	A	206	SER	2.6
1	A	329	GLN	2.5
1	A	358	GLU	2.5
1	A	207	VAL	2.5
1	A	437	LEU	2.4
1	A	349	GLY	2.4
1	A	327	ILE	2.2
1	A	4	PRO	2.2
1	A	59	SER	2.2
1	A	51	PHE	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. 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(\AA^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 carbohydrates 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(\AA^2)	Q<0.9
2	1Z8	A	501	15/15	0.82	0.19	30,40,44,46	0
3	GOL	A	503	6/6	0.86	0.15	36,44,47,48	0
3	GOL	A	502	6/6	0.90	0.17	31,32,37,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.