



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:33 PM GMT

PDB ID : 1PJQ
Title : Structure and function of CysG, the multifunctional methyltransferase/dehydrogenase/ferrochelatase for siroheme synthesis
Authors : Stroupe, M.E.; Leech, H.K.; Daniels, D.S.; Warren, M.J.; Getzoff, E.D.
Deposited on : 2003-06-03
Resolution : 2.21 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

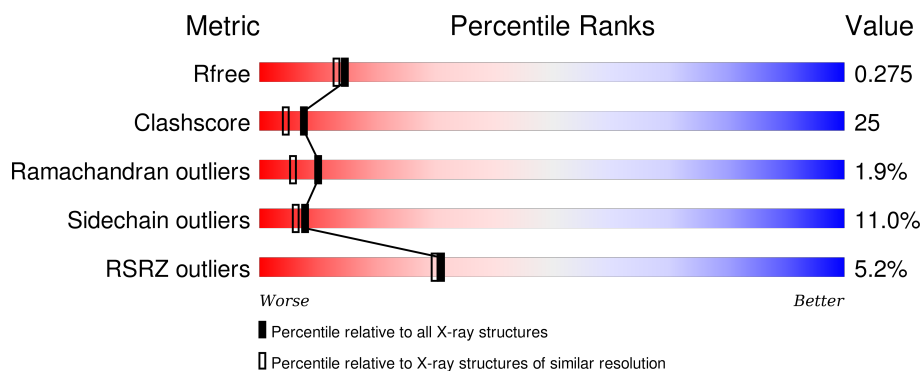
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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}	91344	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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 $\leq 5\%$. 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	457	<div> <div>5%</div> <div>60%</div> <div>31%</div> <div>5% . .</div> </div>
1	B	457	<div> <div>5%</div> <div>65%</div> <div>28%</div> <div>5% .</div> </div>

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
1	SEP	B	128	-	-	X	-
2	ACT	A	504	-	-	X	X
2	ACT	A	505	-	-	X	-
3	PGE	A	502	-	-	X	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7503 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.

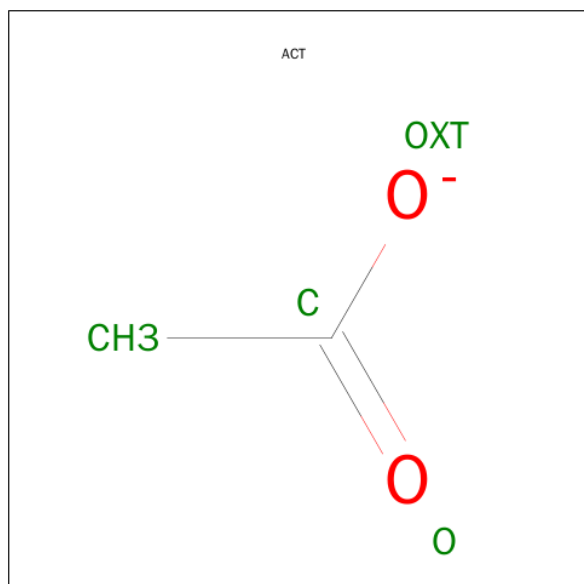
- Molecule 1 is a protein called Siroheme synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	P	S	0	13	0
			3581	2249	650	663	1	18			
1	B	455	Total	C	N	O	P	S	0	4	0
			3548	2228	643	659	1	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	SEP	SER	MODIFIED RESIDUE	UNP P25924
B	128	SEP	SER	MODIFIED RESIDUE	UNP P25924

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



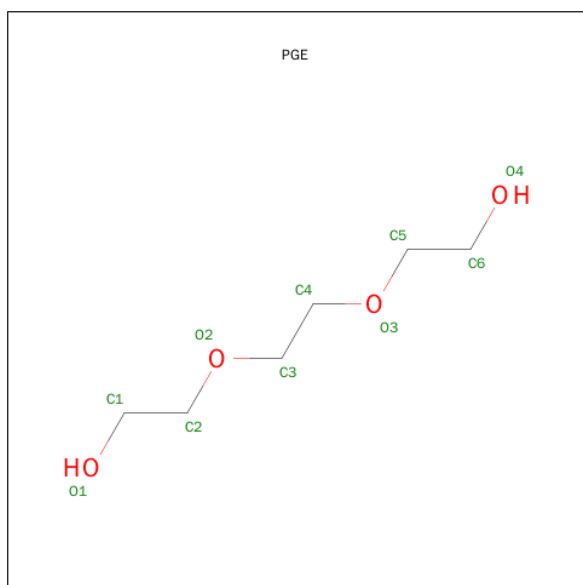
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		

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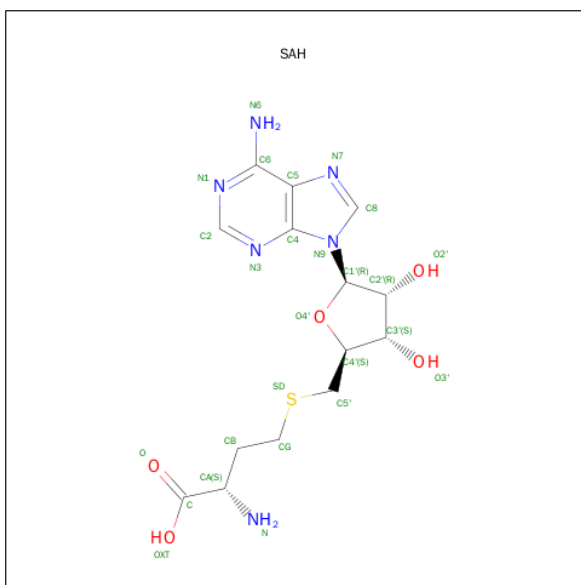
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

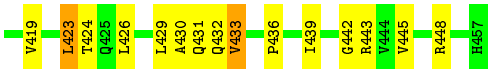
- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	147	Total O 147 147	0	0
5	B	179	Total O 179 179	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.73Å 121.49Å 130.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.21 19.97 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.97-2.21) 98.9 (19.97-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.21Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.273 0.239 , 0.275	Depositor DCC
R_{free} test set	4891 reflections (10.01%)	DCC
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 48911 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7503	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ACT, SAH, PGE, 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	0.53	4/3627 (0.1%)	0.84	13/4903 (0.3%)
1	B	0.46	0/3594	0.85	12/4861 (0.2%)
All	All	0.49	4/7221 (0.1%)	0.85	25/9764 (0.3%)

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	3
1	B	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	LYS	CA-CB	-7.08	1.38	1.53
1	A	375	LYS	N-CA	6.88	1.60	1.46
1	A	276	CYS	N-CA	-6.62	1.33	1.46
1	A	375	LYS	CA-C	6.57	1.70	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	CYS	N-CA-CB	-12.98	87.23	110.60
1	A	375	LYS	CB-CA-C	10.45	131.30	110.40
1	B	350	ALA	N-CA-C	9.13	135.66	111.00
1	A	400	GLN	CB-CA-C	-9.13	92.14	110.40
1	B	375	LYS	N-CA-C	8.63	134.30	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	HIS	Mainchain
1	A	374[A]	GLU	Mainchain
1	A	374[B]	GLU	Mainchain
1	B	374	GLU	Mainchain

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	3581	0	3611	232	0
1	B	3548	0	3584	157	0
2	A	8	0	6	14	0
2	B	4	0	3	1	0
3	A	10	0	13	8	0
4	B	26	0	19	0	0
5	A	147	0	0	9	0
5	B	179	0	0	4	0
All	All	7503	0	7236	367	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 25.

The worst 5 of 367 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:127:SER:C	1:B:128:SEP:N	1.67	1.43
1:A:374[A]:GLU:HG2	1:A:375:LYS:N	1.36	1.33
1:B:128:SEP:CB	1:B:128:SEP:OG	1.83	1.27
1:A:302:GLY:HA3	2:A:505:ACT:H2	1.25	1.13
1:A:374[B]:GLU:HG2	1:A:375:LYS:N	1.68	1.07

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	454/457 (99%)	419 (92%)	23 (5%)	12 (3%)	7	3
1	B	454/457 (99%)	428 (94%)	20 (4%)	6 (1%)	15	11
All	All	908/914 (99%)	847 (93%)	43 (5%)	18 (2%)	10	5

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	LYS
1	A	279	GLN
1	A	347	ARG
1	A	375	LYS
1	A	382[A]	MET

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	379/372 (102%)	341 (90%)	38 (10%)	9	8
1	B	375/372 (101%)	329 (88%)	46 (12%)	6	4
All	All	754/744 (101%)	670 (89%)	84 (11%)	8	6

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	455	SER

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Mol	Chain	Res	Type
1	B	135	LEU
1	B	385	ASN
1	B	69	LEU
1	B	104[A]	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	400	GLN
1	A	452	ASN
1	B	386	GLN
1	A	416	GLN
1	A	431	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
1	SEP	A	128	1	8,9,10	3.29	3 (37%)	8,12,14	4.14	5 (62%)
1	SEP	B	128	1	8,9,10	4.65	6 (75%)	8,12,14	5.04	4 (50%)

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	SEP	A	128	1	-	0/6/8/10	0/0/0/0
1	SEP	B	128	1	-	0/6/8/10	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	SEP	P-O1P	2.27	1.58	1.51
1	A	128	SEP	P-O1P	2.58	1.59	1.51
1	B	128	SEP	O-C	3.75	1.37	1.19
1	B	128	SEP	CA-N	3.86	1.60	1.47
1	B	128	SEP	CB-CA	4.79	1.66	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	SEP	O3P-P-OG	-3.63	96.10	106.56
1	A	128	SEP	O-C-CA	-2.53	118.91	125.49
1	B	128	SEP	O-C-CA	-2.48	119.03	125.49
1	B	128	SEP	OG-P-O1P	-2.12	101.74	107.14
1	A	128	SEP	O2P-P-OG	2.01	112.36	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	128	SEP	1	0
1	B	128	SEP	9	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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	PGE	A	502	-	9,9,9	2.05	2 (22%)	8,8,8	1.50	3 (37%)
2	ACT	A	504	-	1,3,3	3.25	1 (100%)	0,3,3	0.00	-
2	ACT	A	505	-	1,3,3	2.45	1 (100%)	0,3,3	0.00	-
4	SAH	B	501	-	20,28,28	2.18	2 (10%)	19,40,40	3.16	3 (15%)
2	ACT	B	503	-	1,3,3	3.45	1 (100%)	0,3,3	0.00	-

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	PGE	A	502	-	-	0/7/7/7	0/0/0/0
2	ACT	A	504	-	-	0/0/0/0	0/0/0/0
2	ACT	A	505	-	-	0/0/0/0	0/0/0/0
4	SAH	B	501	-	-	0/7/31/31	0/3/3/3
2	ACT	B	503	-	-	0/0/0/0	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	PGE	O3-C4	-4.30	1.23	1.42
3	A	502	PGE	O4-C6	-3.42	1.23	1.42
2	A	505	ACT	CH3-C	2.45	1.52	1.48
2	A	504	ACT	CH3-C	3.25	1.53	1.48
2	B	503	ACT	CH3-C	3.45	1.53	1.48

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	SAH	N3-C2-N1	-12.99	118.95	128.89
4	B	501	SAH	C2'-C1'-N9	-2.65	110.25	114.29
4	B	501	SAH	C4-C5-N7	-2.29	107.38	109.48
3	A	502	PGE	O3-C5-C6	2.19	120.52	110.43
3	A	502	PGE	O3-C4-C3	2.23	120.29	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	PGE	8	0
2	A	504	ACT	2	0
2	A	505	ACT	12	0
2	B	503	ACT	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	447/457 (97%)	0.22	24 (5%) 29 28	18, 39, 67, 99	0
1	B	454/457 (99%)	0.15	23 (5%) 32 31	15, 34, 65, 95	0
All	All	901/914 (98%)	0.18	47 (5%) 31 30	15, 36, 66, 99	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	360	LEU	10.4
1	B	362	THR	8.4
1	A	276	CYS	8.2
1	B	272	ALA	7.2
1	B	359	HIS	6.8

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. 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	SEP	B	128	10/11	0.89	0.19	-	30,38,52,53	0
1	SEP	A	128	10/11	0.76	0.27	-	31,38,53,54	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. 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	ACT	A	504	4/4	0.64	0.30	3.59	57,59,60,61	0
3	PGE	A	502	10/10	0.89	0.16	3.55	49,54,57,58	0
2	ACT	A	505	4/4	0.96	0.17	0.65	36,39,42,42	0
4	SAH	B	501	26/26	0.95	0.10	-0.59	27,32,35,37	0
2	ACT	B	503	4/4	0.91	0.20	-	57,58,58,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.