Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 12:29 pm BST

PDB ID	:	4CC9
Title	:	Crystal structure of human SAMHD1 (amino acid residues 582-626) bound to Vpx isolated from sooty mangabey and human DCAF1 (amino acid residues 1058-1396)
Authors	:	Schwefel, D.; Groom, H.C.T.; Boucherit, V.C.; Christodoulou, E.; Walker, P.A.; Stoye, J.P.; Bishop, K.N.; Taylor, I.A.
Deposited on	:	2013-10-19
Resolution	:	2.47 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 (i) 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 (i)) were used in the production of this report:

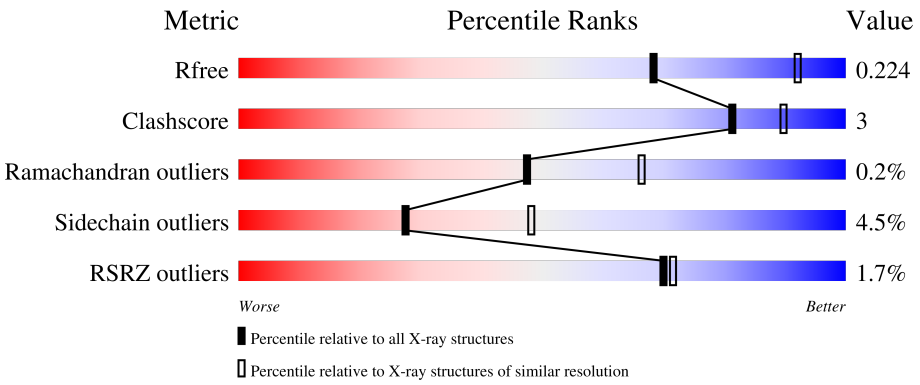
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.47 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	361	.% 77% 7% • 15%
2	B	119	3% 74% 8% • 18%
3	C	71	.% 21% 6% 73%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3459 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 PROTEIN VPRBP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	307	2448	1547	424	460	17	54	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1057	MET	-	expression tag	UNP Q9Y4B6
A	1397	GLU	-	expression tag	UNP Q9Y4B6
A	1398	LEU	-	expression tag	UNP Q9Y4B6
A	1399	ALA	-	expression tag	UNP Q9Y4B6
A	1400	LEU	-	expression tag	UNP Q9Y4B6
A	1401	VAL	-	expression tag	UNP Q9Y4B6
A	1402	PRO	-	expression tag	UNP Q9Y4B6
A	1403	ARG	-	expression tag	UNP Q9Y4B6
A	1404	GLY	-	expression tag	UNP Q9Y4B6
A	1405	SER	-	expression tag	UNP Q9Y4B6
A	1406	SER	-	expression tag	UNP Q9Y4B6
A	1407	ALA	-	expression tag	UNP Q9Y4B6
A	1408	HIS	-	expression tag	UNP Q9Y4B6
A	1409	HIS	-	expression tag	UNP Q9Y4B6
A	1410	HIS	-	expression tag	UNP Q9Y4B6
A	1411	HIS	-	expression tag	UNP Q9Y4B6
A	1412	HIS	-	expression tag	UNP Q9Y4B6
A	1413	HIS	-	expression tag	UNP Q9Y4B6
A	1414	HIS	-	expression tag	UNP Q9Y4B6
A	1415	HIS	-	expression tag	UNP Q9Y4B6
A	1416	HIS	-	expression tag	UNP Q9Y4B6
A	1417	HIS	-	expression tag	UNP Q9Y4B6

- Molecule 2 is a protein called PROTEIN VPX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	98	801	511	144	138	8	20	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	GLY	-	expression tag	UNP P19508
B	-5	PRO	-	expression tag	UNP P19508
B	-4	GLY	-	expression tag	UNP P19508
B	-3	TYR	-	expression tag	UNP P19508
B	-2	GLN	-	expression tag	UNP P19508
B	-1	ASP	-	expression tag	UNP P19508
B	0	PRO	-	expression tag	UNP P19508

- Molecule 3 is a protein called DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	19	158	96	32	30	4	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	556	MET	-	expression tag	UNP Q9Y3Z3
C	557	ALA	-	expression tag	UNP Q9Y3Z3
C	558	SER	-	expression tag	UNP Q9Y3Z3
C	559	TRP	-	expression tag	UNP Q9Y3Z3
C	560	SER	-	expression tag	UNP Q9Y3Z3
C	561	HIS	-	expression tag	UNP Q9Y3Z3
C	562	PRO	-	expression tag	UNP Q9Y3Z3
C	563	GLN	-	expression tag	UNP Q9Y3Z3
C	564	PHE	-	expression tag	UNP Q9Y3Z3
C	565	GLU	-	expression tag	UNP Q9Y3Z3
C	566	LYS	-	expression tag	UNP Q9Y3Z3
C	567	GLY	-	expression tag	UNP Q9Y3Z3
C	568	ALA	-	expression tag	UNP Q9Y3Z3
C	569	LEU	-	expression tag	UNP Q9Y3Z3
C	570	GLU	-	expression tag	UNP Q9Y3Z3
C	571	VAL	-	expression tag	UNP Q9Y3Z3
C	572	LEU	-	expression tag	UNP Q9Y3Z3
C	573	PHE	-	expression tag	UNP Q9Y3Z3
C	574	GLN	-	expression tag	UNP Q9Y3Z3

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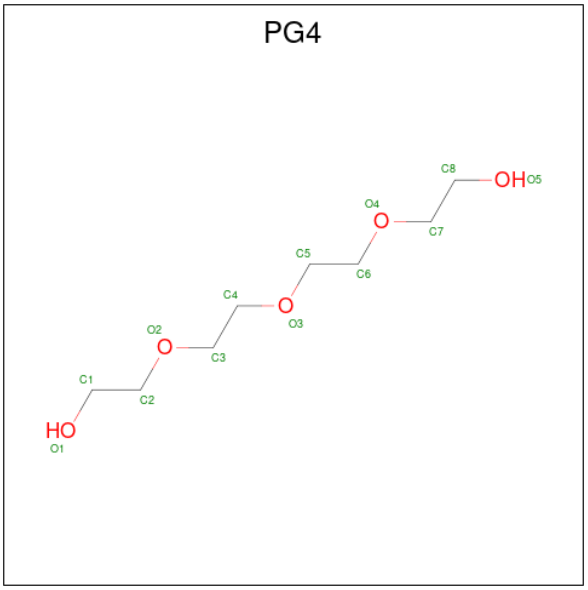
Chain	Residue	Modelled	Actual	Comment	Reference
C	575	GLY	-	expression tag	UNP Q9Y3Z3
C	576	PRO	-	expression tag	UNP Q9Y3Z3
C	577	GLY	-	expression tag	UNP Q9Y3Z3
C	578	TYR	-	expression tag	UNP Q9Y3Z3
C	579	GLN	-	expression tag	UNP Q9Y3Z3
C	580	ASP	-	expression tag	UNP Q9Y3Z3
C	581	PRO	-	expression tag	UNP Q9Y3Z3

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	13	8	5	0	0
			Total	C	O		
4	A	1	13	8	5	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	B	1	1	1	0	0

- Molecule 6 is water.

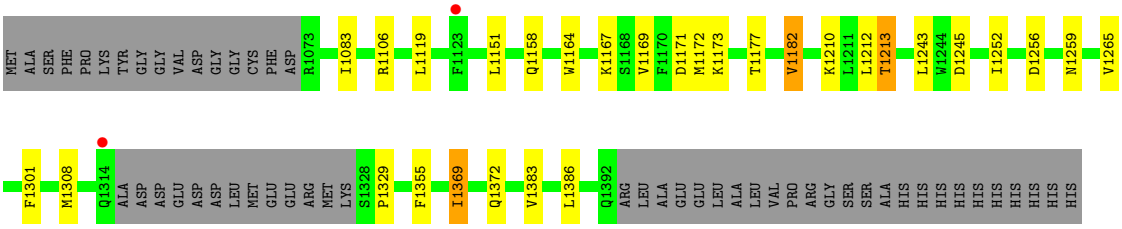
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	21	21	21	0	0
			Total	O		
6	B	3	3	3	0	0
			Total	O		
6	C	1	1	1	0	0

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: PROTEIN VPRBP

Chain A:

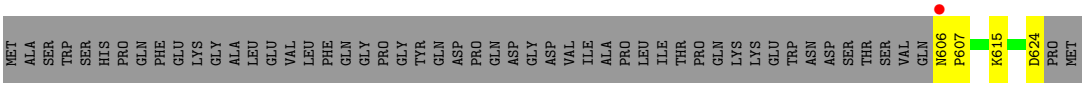


• Molecule 2: PROTEIN VPX

Chain B:

• Molecule 3: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.25Å 82.88Å 115.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.23 – 2.47 29.23 – 2.47	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.23-2.47) 97.8 (29.23-2.47)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.176 , 0.216 0.189 , 0.224	Depositor DCC
R_{free} test set	1303 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 62.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3459	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 5.21% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, ZN

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	0.42	0/2505	0.60	1/3394 (0.0%)
2	B	0.42	0/828	0.52	0/1123
3	C	0.39	0/159	0.59	0/211
All	All	0.42	0/3492	0.58	1/4728 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1369	ILE	CG1-CB-CG2	-5.28	99.79	111.40

There are no chirality outliers.

There are no planarity outliers.

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	2448	0	2354	11	0
2	B	801	0	765	6	0
3	C	158	0	161	1	0
4	A	26	0	36	0	0
5	B	1	0	0	0	0
6	A	21	0	0	0	0
6	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	1	0	0	0	0
All	All	3459	0	3316	17	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 3.

All (17) 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:1329:PRO:HG3	2:B:85:LYS:HD3	1.69	0.73
2:B:16:GLU:HG3	2:B:20:GLU:HG3	1.73	0.68
1:A:1245:ASP:HB2	1:A:1252:ILE:HD11	1.83	0.60
1:A:1158:GLN:NE2	1:A:1177:THR:OG1	2.35	0.59
2:B:26:ASP:OD1	2:B:68:LYS:NZ	2.38	0.57
2:B:25:LEU:O	2:B:29:VAL:HG12	2.08	0.54
1:A:1171:ASP:OD2	1:A:1173:LYS:NZ	2.40	0.54
1:A:1210:LYS:HD3	1:A:1213:THR:HG22	1.89	0.53
2:B:29:VAL:HG11	2:B:68:LYS:HE2	1.90	0.53
1:A:1151:LEU:HD13	1:A:1182:VAL:HG13	1.92	0.50
1:A:1355:PHE:HB2	1:A:1369:ILE:CG2	2.45	0.46
3:C:606:ASN:HA	3:C:607:PRO:HD3	1.83	0.45
1:A:1355:PHE:HB2	1:A:1369:ILE:HG22	2.00	0.43
1:A:1083:ILE:HD11	1:A:1386:LEU:HD12	2.02	0.42
1:A:1301:PHE:CE1	1:A:1308:MET:HG2	2.55	0.42
1:A:1164:TRP:CZ3	1:A:1172:MET:HB2	2.56	0.40
2:B:100:ARG:NH1	2:B:100:ARG:HB3	2.37	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	303/361 (84%)	294 (97%)	8 (3%)	1 (0%)	41	59
2	B	94/119 (79%)	91 (97%)	3 (3%)	0	100	100
3	C	17/71 (24%)	17 (100%)	0	0	100	100
All	All	414/551 (75%)	402 (97%)	11 (3%)	1 (0%)	47	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1167	LYS

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	271/316 (86%)	259 (96%)	12 (4%)	28	49
2	B	85/99 (86%)	82 (96%)	3 (4%)	36	59
3	C	18/63 (29%)	16 (89%)	2 (11%)	6	10
All	All	374/478 (78%)	357 (96%)	17 (4%)	27	48

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1106	ARG
1	A	1119	LEU
1	A	1169	VAL
1	A	1182	VAL
1	A	1212	LEU
1	A	1213	THR
1	A	1243	LEU
1	A	1256	ASP
1	A	1259	ASN
1	A	1265	VAL
1	A	1372	GLN
1	A	1383	VAL

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Mol	Chain	Res	Type
2	B	7	ARG
2	B	64	VAL
2	B	100	ARG
3	C	615	LYS
3	C	624	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
4	PG4	A	2393	-	12,12,12	0.54	0	11,11,11	0.33	0
4	PG4	A	2394	-	12,12,12	0.57	0	11,11,11	0.43	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
4	PG4	A	2393	-	-	6/10/10/10	-
4	PG4	A	2394	-	-	5/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2393	PG4	O1-C1-C2-O2
4	A	2394	PG4	O3-C5-C6-O4
4	A	2393	PG4	O4-C7-C8-O5
4	A	2394	PG4	C5-C6-O4-C7
4	A	2394	PG4	C8-C7-O4-C6
4	A	2393	PG4	C6-C5-O3-C4
4	A	2394	PG4	O4-C7-C8-O5
4	A	2393	PG4	C8-C7-O4-C6
4	A	2394	PG4	C3-C4-O3-C5
4	A	2393	PG4	C3-C4-O3-C5
4	A	2393	PG4	O2-C3-C4-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	307/361 (85%)	-0.50	2 (0%)	87	89	13, 30, 54, 62	13 (4%)
2	B	98/119 (82%)	-0.33	4 (4%)	37	39	14, 27, 68, 84	5 (5%)
3	C	19/71 (26%)	0.11	1 (5%)	26	27	25, 40, 65, 80	1 (5%)
All	All	424/551 (76%)	-0.43	7 (1%)	70	71	13, 30, 55, 84	19 (4%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	89	CYS	4.0
1	A	1314	GLN	2.9
2	B	88	ARG	2.8
2	B	90	LEU	2.4
3	C	606	ASN	2.2
2	B	101	PRO	2.2
1	A	1123	PHE	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 (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
4	PG4	A	2394	13/13	0.69	0.30	49,68,71,75	0
4	PG4	A	2393	13/13	0.86	0.17	47,54,66,68	0
5	ZN	B	1112	1/1	0.99	0.03	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.