Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 03:40 PM EDT

PDB ID	:	2GCL
Title	:	Structure of the Pob3 Middle domain
Authors	:	VanDemark, A.P.
Deposited on	:	2006-03-14
Resolution	:	2.21 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 following versions of software and data (see references (1)) were used in the production of this report:

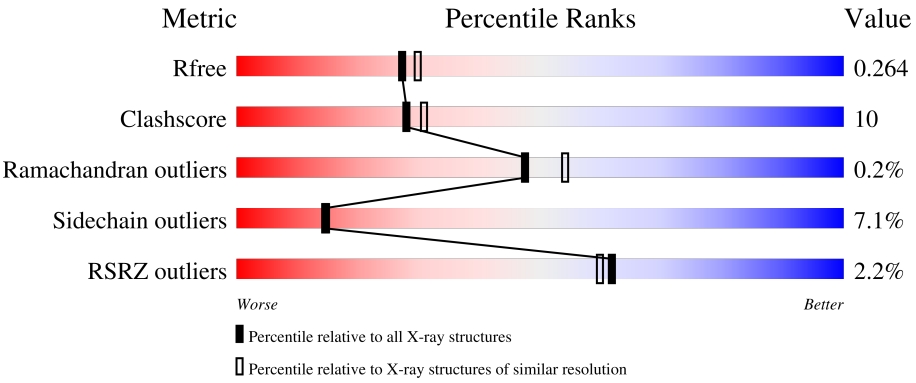
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.21 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}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (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 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	261	2% 69% 16% · 12%
1	B	261	2% 67% 17% 5% 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4050 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 Hypothetical 63.0 kDa protein in DAK1-ORC1 intergenic region.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	Se	0	0	0
			1895	1211	322	356	2	4			
1	B	231	Total	C	N	O	S	Se	0	0	0
			1908	1217	326	359	2	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	GLY	-	cloning artifact	UNP Q04636
A	219	HIS	-	cloning artifact	UNP Q04636
A	220	MSE	MET	modified residue	UNP Q04636
A	297	MSE	LEU	engineered mutation	UNP Q04636
A	298	MSE	LEU	engineered mutation	UNP Q04636
A	300	MSE	LEU	engineered mutation	UNP Q04636
A	419	MSE	MET	modified residue	UNP Q04636
B	218	GLY	-	cloning artifact	UNP Q04636
B	219	HIS	-	cloning artifact	UNP Q04636
B	220	MSE	MET	modified residue	UNP Q04636
B	297	MSE	LEU	engineered mutation	UNP Q04636
B	298	MSE	LEU	engineered mutation	UNP Q04636
B	300	MSE	LEU	engineered mutation	UNP Q04636
B	419	MSE	MET	modified residue	UNP Q04636

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cl	0	0
			4	4		

- Molecule 3 is water.

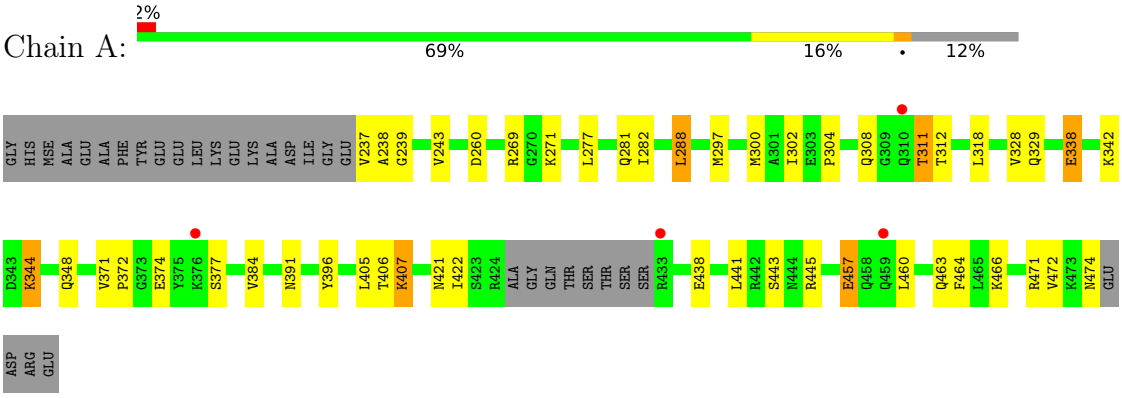
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	137	Total O 137 137	0	0
3	B	106	Total O 106 106	0	0

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.

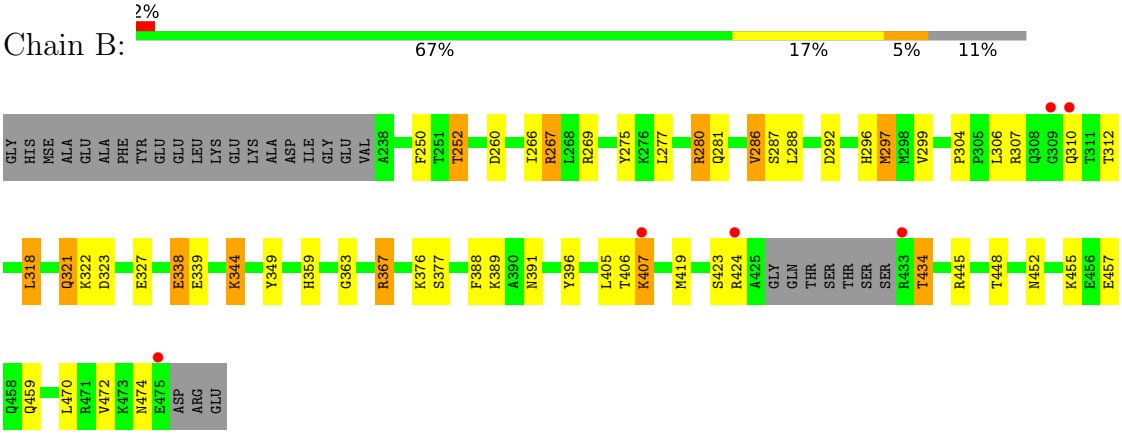
• Molecule 1: Hypothetical 63.0 kDa protein in DAK1-ORC1 intergenic region

Chain A:



• Molecule 1: Hypothetical 63.0 kDa protein in DAK1-ORC1 intergenic region

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.11Å 57.77Å 156.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.21 46.14 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-2.21) 98.7 (46.14-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.207 , 0.264 0.210 , 0.264	Depositor DCC
R_{free} test set	1337 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.034 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4050	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6069e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CL

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	0.60	0/1929	0.68	0/2595
1	B	0.54	0/1942	0.70	2/2611 (0.1%)
All	All	0.57	0/3871	0.69	2/5206 (0.0%)

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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	267	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	B	267	ARG	NE-CZ-NH1	6.60	123.60	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	407	LYS	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	1895	0	1888	29	0
1	B	1908	0	1901	46	0
2	A	4	0	0	0	0
3	A	137	0	0	4	0
3	B	106	0	0	7	0
All	All	4050	0	3789	75	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 10.

All (75) 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:286:VAL:HG23	1:B:288:LEU:HD13	1.49	0.93
1:B:287:SER:O	1:B:288:LEU:HD12	1.76	0.85
1:B:318:LEU:N	1:B:318:LEU:HD23	1.97	0.80
1:B:287:SER:C	1:B:288:LEU:HD12	2.03	0.79
1:B:349:TYR:OH	1:B:359:HIS:HD2	1.70	0.74
1:B:275:TYR:HE1	1:B:307:ARG:O	1.76	0.68
1:B:391:ASN:HB3	1:B:407:LYS:HB2	1.79	0.64
1:B:288:LEU:HD23	1:B:396:TYR:CD2	2.33	0.64
1:B:252:THR:HG21	3:B:570:HOH:O	1.97	0.63
1:B:286:VAL:HG13	1:B:299:VAL:HB	1.82	0.62
1:A:281:GLN:HG2	1:A:304:PRO:HD2	1.83	0.61
1:A:288:LEU:HD13	1:A:297:MSE:HE3	1.83	0.60
1:B:321:GLN:HE22	1:B:323:ASP:HB2	1.67	0.60
1:B:287:SER:OG	1:B:296:HIS:HE1	1.85	0.59
1:A:384:VAL:HG11	1:A:457:GLU:HG2	1.84	0.58
1:B:286:VAL:CG2	1:B:288:LEU:HD13	2.28	0.58
1:B:318:LEU:HD23	1:B:318:LEU:H	1.68	0.58
1:B:286:VAL:HG23	1:B:288:LEU:CD1	2.28	0.58
1:B:424:ARG:HH12	1:B:455:LYS:HD3	1.70	0.57
3:A:613:HOH:O	1:B:470:LEU:HD23	2.06	0.56
1:B:376:LYS:HD3	3:B:566:HOH:O	2.04	0.56
1:A:421:ASN:HB2	1:A:438:GLU:HB3	1.89	0.55
1:B:297:MSE:HE2	1:B:405:LEU:HD13	1.88	0.55
1:B:376:LYS:CD	3:B:566:HOH:O	2.56	0.54
1:A:374:GLU:HG3	1:A:464:PHE:HE2	1.73	0.54
1:A:460:LEU:HA	1:A:463:GLN:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ASP:OD2	1:B:269:ARG:HD3	2.09	0.53
1:B:269:ARG:NH1	3:B:543:HOH:O	2.41	0.53
1:B:267:ARG:NH2	3:B:517:HOH:O	2.42	0.52
1:A:384:VAL:CG1	1:A:457:GLU:HG2	2.38	0.52
1:A:237:VAL:HG12	1:A:239:GLY:H	1.75	0.52
1:B:349:TYR:OH	1:B:359:HIS:CD2	2.58	0.51
1:B:367:ARG:HH11	1:B:367:ARG:CG	2.24	0.51
1:B:318:LEU:N	1:B:318:LEU:CD2	2.69	0.51
1:B:252:THR:CG2	3:B:576:HOH:O	2.59	0.50
1:A:371:VAL:HB	1:A:372:PRO:HD2	1.93	0.49
1:B:252:THR:HG23	3:B:576:HOH:O	2.12	0.49
1:A:329:GLN:HG2	1:A:348:GLN:HG2	1.96	0.48
1:B:275:TYR:CE1	1:B:307:ARG:O	2.62	0.47
1:A:271:LYS:HE2	3:A:522:HOH:O	2.16	0.46
1:A:374:GLU:HG3	1:A:464:PHE:CE2	2.51	0.46
1:B:287:SER:C	1:B:288:LEU:CD1	2.80	0.45
1:A:260:ASP:OD2	1:A:269:ARG:NE	2.28	0.45
1:A:282:ILE:HD13	1:A:300:MSE:HE1	1.98	0.45
1:A:391:ASN:HB3	1:A:407:LYS:O	2.17	0.45
1:B:424:ARG:NH1	1:B:455:LYS:HD3	2.32	0.44
1:B:250:PHE:CE2	1:B:318:LEU:HD22	2.52	0.44
1:B:306:LEU:HD23	1:B:306:LEU:HA	1.78	0.44
1:B:367:ARG:HH11	1:B:367:ARG:HG3	1.81	0.44
1:B:306:LEU:O	1:B:312:THR:HA	2.17	0.44
1:B:280:ARG:HD3	1:B:280:ARG:C	2.38	0.44
1:B:281:GLN:HG2	1:B:304:PRO:HD2	2.00	0.44
1:B:388:PHE:CE1	1:B:448:THR:HG23	2.52	0.44
1:A:237:VAL:HG12	1:A:238:ALA:N	2.33	0.43
1:A:308:GLN:O	1:A:311:THR:HG23	2.18	0.43
1:A:308:GLN:NE2	3:A:559:HOH:O	2.50	0.43
1:A:338:GLU:HG3	1:A:342:LYS:HE3	2.00	0.43
1:B:266:ILE:HD11	1:B:277:LEU:HD12	2.01	0.42
1:A:277:LEU:HD11	1:A:302:ILE:HD12	2.01	0.42
1:A:288:LEU:HD22	1:A:396:TYR:CE2	2.55	0.42
1:A:405:LEU:HA	1:A:406:THR:HA	1.81	0.42
1:A:443:SER:HB2	1:A:445:ARG:HD3	2.02	0.42
1:A:466:LYS:HE3	1:A:472:VAL:HB	2.00	0.42
1:B:344:LYS:HD3	1:B:363:GLY:O	2.19	0.42
1:B:377:SER:HB2	1:B:457:GLU:OE1	2.19	0.42
1:B:405:LEU:HA	1:B:406:THR:HA	1.79	0.42
1:B:434:THR:HG23	1:B:452:ASN:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ASN:HB3	1:B:407:LYS:CB	2.49	0.41
1:A:288:LEU:CD1	1:A:297:MSE:HE3	2.49	0.41
1:A:243:VAL:HG23	1:A:328:VAL:HG21	2.02	0.41
1:B:338:GLU:HG3	1:B:339:GLU:N	2.36	0.41
1:B:419:MSE:HE3	1:B:419:MSE:HB2	1.92	0.41
1:A:282:ILE:HD13	1:A:300:MSE:CE	2.51	0.41
1:A:344:LYS:HE3	3:A:542:HOH:O	2.21	0.41
1:A:422:ILE:HB	1:A:474:ASN:CB	2.52	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	226/261 (87%)	220 (97%)	5 (2%)	1 (0%)	34 37
1	B	227/261 (87%)	217 (96%)	10 (4%)	0	100 100
All	All	453/522 (87%)	437 (96%)	15 (3%)	1 (0%)	47 54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	SER

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	212/232 (91%)	202 (95%)	10 (5%)	26 31
1	B	213/232 (92%)	193 (91%)	20 (9%)	8 7
All	All	425/464 (92%)	395 (93%)	30 (7%)	14 15

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	LEU
1	A	311	THR
1	A	312	THR
1	A	318	LEU
1	A	338	GLU
1	A	344	LYS
1	A	407	LYS
1	A	441	LEU
1	A	457	GLU
1	A	471	ARG
1	B	252	THR
1	B	280	ARG
1	B	286	VAL
1	B	292	ASP
1	B	297	MSE
1	B	310	GLN
1	B	318	LEU
1	B	321	GLN
1	B	322	LYS
1	B	327	GLU
1	B	338	GLU
1	B	344	LYS
1	B	367	ARG
1	B	389	LYS
1	B	423	SER
1	B	434	THR
1	B	445	ARG
1	B	459	GLN
1	B	472	VAL
1	B	474	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	GLN
1	A	319	GLN
1	A	321	GLN
1	A	452	ASN
1	B	296	HIS
1	B	321	GLN
1	B	359	HIS
1	B	421	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

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, 95^{th} 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	226/261 (86%)	-0.08	4 (1%)	68	66	15, 34, 68, 97	6 (2%)
1	B	227/261 (86%)	0.05	6 (2%)	56	54	20, 44, 72, 87	4 (1%)
All	All	453/522 (86%)	-0.01	10 (2%)	62	60	15, 39, 72, 97	10 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	GLN	5.5
1	B	475	GLU	4.0
1	B	424	ARG	3.7
1	A	459	GLN	3.0
1	A	310	GLN	2.7
1	B	407	LYS	2.7
1	B	309	GLY	2.5
1	A	376	LYS	2.3
1	B	433	ARG	2.3
1	A	433	ARG	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	CL	A	482	1/1	0.58	0.35	72,72,72,72	0
2	CL	A	479	1/1	0.87	0.20	70,70,70,70	0
2	CL	A	480	1/1	0.99	0.09	27,27,27,27	0
2	CL	A	481	1/1	1.00	0.08	37,37,37,37	0

6.5 Other polymers

There are no such residues in this entry.