



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 05:13 pm BST

PDB ID : 3C3O
Title : ALIX Bro1-domain:CHMIP4A co-crystal structure
Authors : McCullough, J.B.; Fisher, R.D.; Whitby, F.G.; Sundquist, W.I.; Hill, C.P.
Deposited on : 2008-01-28
Resolution : 2.15 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

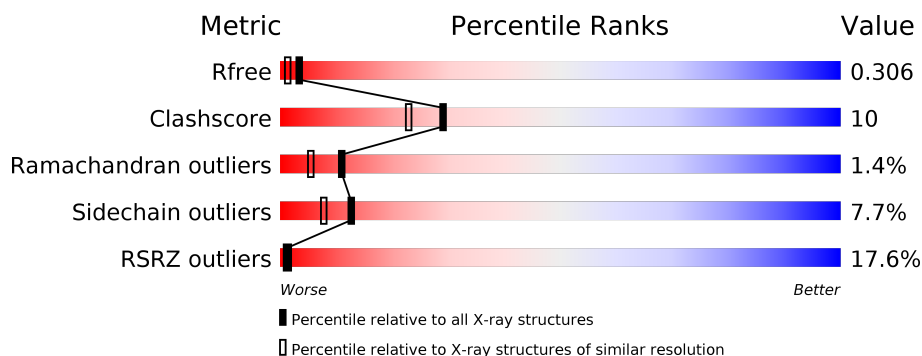
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	380	<div> <div>15%</div> <div>73%</div> <div>18%</div> <div>•• 6%</div> </div>
2	B	13	<div> <div>54%</div> <div>62%</div> <div>38%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3043 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 Programmed cell death 6-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	357	2803	1792	471	529	11	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q8WUM4
A	-19	HIS	-	EXPRESSION TAG	UNP Q8WUM4
A	-18	HIS	-	EXPRESSION TAG	UNP Q8WUM4
A	-17	HIS	-	EXPRESSION TAG	UNP Q8WUM4
A	-16	HIS	-	EXPRESSION TAG	UNP Q8WUM4
A	-15	HIS	-	EXPRESSION TAG	UNP Q8WUM4
A	-14	HIS	-	EXPRESSION TAG	UNP Q8WUM4
A	-13	HIS	-	EXPRESSION TAG	UNP Q8WUM4
A	-12	HIS	-	EXPRESSION TAG	UNP Q8WUM4
A	-11	HIS	-	EXPRESSION TAG	UNP Q8WUM4
A	-10	HIS	-	EXPRESSION TAG	UNP Q8WUM4
A	-9	SER	-	EXPRESSION TAG	UNP Q8WUM4
A	-8	GLY	-	EXPRESSION TAG	UNP Q8WUM4
A	-7	GLN	-	EXPRESSION TAG	UNP Q8WUM4
A	-6	ASN	-	EXPRESSION TAG	UNP Q8WUM4
A	-5	LEU	-	EXPRESSION TAG	UNP Q8WUM4
A	-4	TYR	-	EXPRESSION TAG	UNP Q8WUM4
A	-3	PHE	-	EXPRESSION TAG	UNP Q8WUM4
A	-2	GLN	-	EXPRESSION TAG	UNP Q8WUM4
A	-1	GLY	-	EXPRESSION TAG	UNP Q8WUM4
A	0	HIS	-	EXPRESSION TAG	UNP Q8WUM4

- Molecule 2 is a protein called Charged multivesicular body protein 4a peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	0	0	0
			107	67	16	24			

- 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		

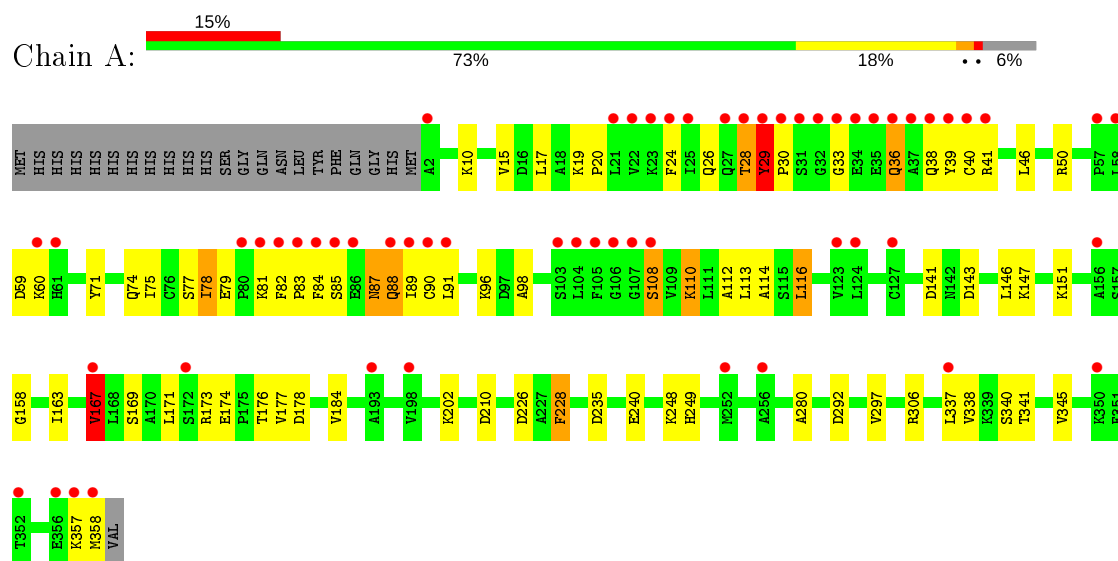
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	126	Total	O	0	0
			126	126		
4	B	1	Total	O	0	0
			1	1		

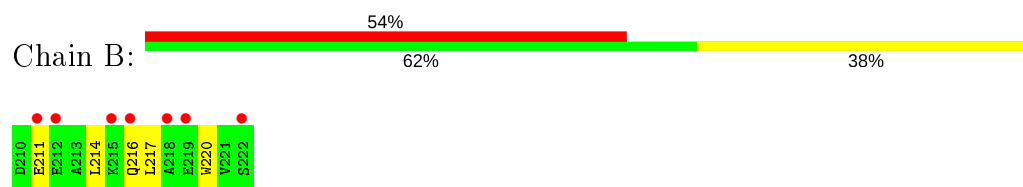
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Programmed cell death 6-interacting protein



- Molecule 2: Charged multivesicular body protein 4a peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.67Å 62.68Å 76.12Å 90.00° 122.13° 90.00°	Depositor
Resolution (Å)	32.22 – 2.15 31.78 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.9 (32.22-2.15) 94.9 (31.78-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.214 , 0.284 0.233 , 0.306	Depositor DCC
R_{free} test set	1799 reflections (7.19%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3043	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.22% 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

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	0.89	1/2856 (0.0%)	0.94	7/3854 (0.2%)
2	B	0.69	0/108	0.86	0/144
All	All	0.88	1/2964 (0.0%)	0.94	7/3998 (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	280	ALA	CA-CB	5.87	1.64	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	ASP	CB-CG-OD2	7.95	125.45	118.30
1	A	210	ASP	CB-CG-OD2	6.75	124.38	118.30
1	A	235	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	292	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	59	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	141	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	167	VAL	CB-CA-C	-5.40	101.14	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	THR	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	2803	0	2828	56	0
2	B	107	0	98	3	0
3	A	6	0	8	1	0
4	A	126	0	0	4	0
4	B	1	0	0	0	0
All	All	3043	0	2934	56	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 (56) 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:19:LYS:HB3	1:A:20:PRO:HD3	1.51	0.92
1:A:163:ILE:O	1:A:167:VAL:HG22	1.75	0.85
1:A:46:LEU:HD22	1:A:78:ILE:HD11	1.70	0.71
1:A:28:THR:O	1:A:29:TYR:HB2	1.92	0.68
1:A:176:THR:HG23	1:A:178:ASP:OD1	1.94	0.67
1:A:29:TYR:H	1:A:30:PRO:HD3	1.60	0.67
1:A:39:TYR:HE2	1:A:358:MET:HB2	1.61	0.65
1:A:89:ILE:HG22	1:A:90:CYS:H	1.62	0.65
1:A:46:LEU:HD13	1:A:74:GLN:CG	2.30	0.61
1:A:112:ALA:O	1:A:113:LEU:HD23	1.99	0.61
1:A:46:LEU:HD13	1:A:74:GLN:HG2	1.83	0.60
1:A:87:ASN:HA	1:A:88:GLN:HB2	1.83	0.59
1:A:84:PHE:O	1:A:87:ASN:HB2	2.05	0.56
1:A:158:GLY:HA3	1:A:341:THR:O	2.06	0.56
1:A:24:PHE:HE2	1:A:83:PRO:HG2	1.70	0.56
1:A:306:ARG:NH1	4:A:431:HOH:O	2.39	0.56
1:A:39:TYR:CE2	1:A:358:MET:HB2	2.40	0.56
1:A:87:ASN:CA	1:A:88:GLN:HB2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:CD2	1:A:78:ILE:HD11	2.38	0.54
1:A:177:VAL:HG22	4:A:433:HOH:O	2.08	0.54
1:A:337:LEU:CD1	2:B:217:LEU:HD13	2.41	0.50
1:A:89:ILE:HG22	1:A:90:CYS:N	2.27	0.50
1:A:176:THR:HG21	4:A:372:HOH:O	2.11	0.50
1:A:151:LYS:HG2	3:A:360:GOL:O1	2.12	0.49
1:A:158:GLY:HA2	1:A:340:SER:HB3	1.95	0.48
1:A:91:LEU:O	1:A:114:ALA:HA	2.13	0.48
1:A:26:GLN:HA	1:A:36:GLN:OE1	2.14	0.48
1:A:19:LYS:HB3	1:A:20:PRO:CD	2.35	0.47
1:A:46:LEU:CD2	1:A:78:ILE:CD1	2.92	0.47
1:A:78:ILE:HG22	1:A:116:LEU:HD21	1.96	0.47
1:A:173:ARG:CG	1:A:174:GLU:N	2.77	0.47
1:A:113:LEU:HD21	1:A:173:ARG:HD3	1.96	0.47
1:A:147:LYS:CD	2:B:220:TRP:O	2.63	0.46
1:A:10:LYS:NZ	1:A:96:LYS:O	2.47	0.46
1:A:38:GLN:C	1:A:40:CYS:H	2.18	0.46
1:A:82:PHE:HA	1:A:83:PRO:HD3	1.78	0.46
1:A:50:ARG:HD2	1:A:71:TYR:OH	2.17	0.45
1:A:147:LYS:HD3	2:B:220:TRP:O	2.16	0.45
1:A:173:ARG:CG	1:A:174:GLU:H	2.29	0.44
1:A:46:LEU:HD13	1:A:74:GLN:HG3	1.97	0.44
1:A:17:LEU:HA	1:A:91:LEU:HD21	1.99	0.44
1:A:98:ALA:N	1:A:178:ASP:OD2	2.36	0.44
1:A:108:SER:HB2	1:A:110:LYS:HG3	2.00	0.44
1:A:10:LYS:HG3	1:A:98:ALA:HB2	1.99	0.44
1:A:15:VAL:HG12	1:A:17:LEU:HD23	1.99	0.43
1:A:71:TYR:CZ	1:A:75:ILE:HD11	2.53	0.43
1:A:83:PRO:HB2	1:A:88:GLN:HB3	1.99	0.43
1:A:143:ASP:OD1	1:A:202:LYS:NZ	2.43	0.43
1:A:84:PHE:HZ	1:A:91:LEU:HD12	1.84	0.43
1:A:87:ASN:N	1:A:88:GLN:HB2	2.34	0.42
1:A:228:PHE:HE2	1:A:249:HIS:CD2	2.37	0.42
1:A:46:LEU:CD1	1:A:74:GLN:HG2	2.47	0.42
1:A:29:TYR:N	1:A:30:PRO:HD3	2.32	0.42
1:A:248:LYS:NZ	4:A:472:HOH:O	2.34	0.40
1:A:240:GLU:CD	1:A:240:GLU:H	2.23	0.40
1:A:173:ARG:HG3	1:A:174:GLU:H	1.86	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	355/380 (93%)	330 (93%)	20 (6%)	5 (1%)	11	5
2	B	11/13 (85%)	8 (73%)	3 (27%)	0	100	100
All	All	366/393 (93%)	338 (92%)	23 (6%)	5 (1%)	11	5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	TYR
1	A	88	GLN
1	A	87	ASN
1	A	108	SER
1	A	33	GLY

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	299/320 (93%)	278 (93%)	21 (7%)	15	10
2	B	11/11 (100%)	8 (73%)	3 (27%)	0	0
All	All	310/331 (94%)	286 (92%)	24 (8%)	13	8

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	TYR

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Mol	Chain	Res	Type
1	A	36	GLN
1	A	41	ARG
1	A	60	LYS
1	A	77	SER
1	A	78	ILE
1	A	79	GLU
1	A	81	LYS
1	A	85	SER
1	A	110	LYS
1	A	116	LEU
1	A	146	LEU
1	A	167	VAL
1	A	169	SER
1	A	171	LEU
1	A	184	VAL
1	A	228	PHE
1	A	297	VAL
1	A	338	VAL
1	A	345	VAL
1	A	357	LYS
2	B	211	GLU
2	B	214	LEU
2	B	216	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	230	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

1 ligand 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	$\# Z > 2$
3	GOL	A	360	-	5,5,5	0.37	0	5,5,5	0.52	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	360	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	360	GOL	C1-C2-C3-O3
3	A	360	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	360	GOL	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	357/380 (93%)	0.87	58 (16%) 1 2	15, 27, 68, 84	0
2	B	13/13 (100%)	1.83	7 (53%) 0 0	37, 50, 60, 62	0
All	All	370/393 (94%)	0.90	65 (17%) 1 1	15, 28, 68, 84	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	ILE	10.8
1	A	29	TYR	9.9
1	A	30	PRO	9.2
1	A	85	SER	7.6
1	A	106	GLY	7.4
1	A	27	GLN	7.1
1	A	33	GLY	6.9
1	A	105	PHE	6.5
1	A	2	ALA	6.1
1	A	28	THR	5.9
1	A	84	PHE	5.6
1	A	88	GLN	5.4
1	A	34	GLU	5.3
1	A	58	LEU	5.3
1	A	357	LYS	5.3
1	A	90	CYS	4.9
1	A	61	HIS	4.9
1	A	91	LEU	4.8
1	A	35	GLU	4.8
1	A	89	ILE	4.4
1	A	107	GLY	4.3
1	A	39	TYR	4.3
1	A	21	LEU	4.2
1	A	57	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	86	GLU	4.0
2	B	222	SER	3.8
1	A	40	CYS	3.4
1	A	172	SER	3.3
2	B	218	ALA	3.3
1	A	82	PHE	3.3
1	A	356	GLU	3.3
1	A	22	VAL	3.3
1	A	36	GLN	3.3
1	A	32	GLY	3.2
1	A	83	PRO	3.2
1	A	24	PHE	3.0
1	A	350	LYS	2.9
1	A	31	SER	2.9
1	A	38	GLN	2.8
1	A	104	LEU	2.8
2	B	211	GLU	2.7
2	B	212	GLU	2.7
1	A	108	SER	2.7
1	A	337	LEU	2.6
1	A	193	ALA	2.6
1	A	103	SER	2.5
1	A	167	VAL	2.5
1	A	80	PRO	2.5
1	A	60	LYS	2.5
1	A	41	ARG	2.4
1	A	124	LEU	2.4
1	A	127	CYS	2.3
1	A	81	LYS	2.3
2	B	219	GLU	2.3
1	A	23	LYS	2.2
1	A	37	ALA	2.1
1	A	256	ALA	2.1
2	B	216	GLN	2.1
2	B	215	LYS	2.1
1	A	252	MET	2.1
1	A	352	THR	2.1
1	A	358	MET	2.1
1	A	123	VAL	2.1
1	A	198	VAL	2.1
1	A	156	ALA	2.1

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 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
3	GOL	A	360	6/6	0.93	0.19	79,82,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.