



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2020 – 10:12 pm BST

PDB ID : 6GGJ
Title : Crystal structure of CotB2 in complex with alendronate
Authors : Driller, R.; Janke, S.; Fuchs, M.; Warner, E.; Mhashal, A.R.; Major, D.T.; Christmann, M.; Brueck, T.; Loll, B.
Deposited on : 2018-05-03
Resolution : 2.10 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

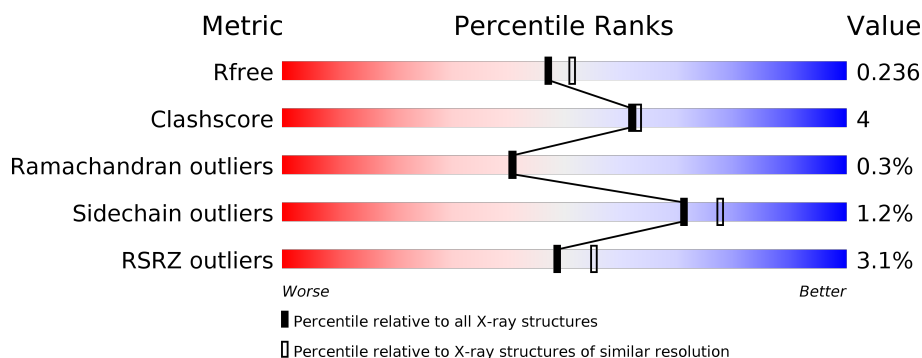
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	318	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>11%</div> </div> </div>
1	B	318	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5015 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.

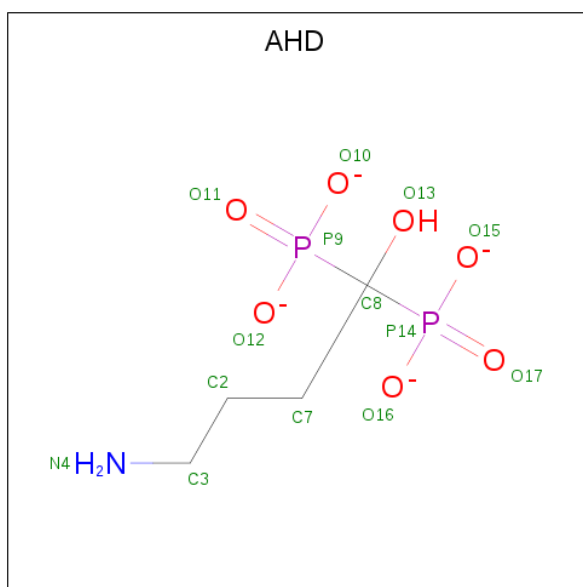
- Molecule 1 is a protein called Cyclooctat-9-en-7-ol synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	1	0
			2320	1480	387	436	17			
1	B	296	Total	C	N	O	S	0	3	0
			2438	1549	414	458	17			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	ALA	-	expression tag	UNP C9K1X5
A	309	ALA	-	expression tag	UNP C9K1X5
A	310	ALA	-	expression tag	UNP C9K1X5
A	311	LEU	-	expression tag	UNP C9K1X5
A	312	GLU	-	expression tag	UNP C9K1X5
A	313	HIS	-	expression tag	UNP C9K1X5
A	314	HIS	-	expression tag	UNP C9K1X5
A	315	HIS	-	expression tag	UNP C9K1X5
A	316	HIS	-	expression tag	UNP C9K1X5
A	317	HIS	-	expression tag	UNP C9K1X5
A	318	HIS	-	expression tag	UNP C9K1X5
B	308	ALA	-	expression tag	UNP C9K1X5
B	309	ALA	-	expression tag	UNP C9K1X5
B	310	ALA	-	expression tag	UNP C9K1X5
B	311	LEU	-	expression tag	UNP C9K1X5
B	312	GLU	-	expression tag	UNP C9K1X5
B	313	HIS	-	expression tag	UNP C9K1X5
B	314	HIS	-	expression tag	UNP C9K1X5
B	315	HIS	-	expression tag	UNP C9K1X5
B	316	HIS	-	expression tag	UNP C9K1X5
B	317	HIS	-	expression tag	UNP C9K1X5
B	318	HIS	-	expression tag	UNP C9K1X5

- Molecule 2 is 4-AMINO-1-HYDROXYBUTANE-1,1-DIYLDIPHOSPHONATE (three-letter code: AHD) (formula: C₄H₉NO₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Mg	0	0
			3	3		
3	A	3	Total	Mg	0	0
			3	3		

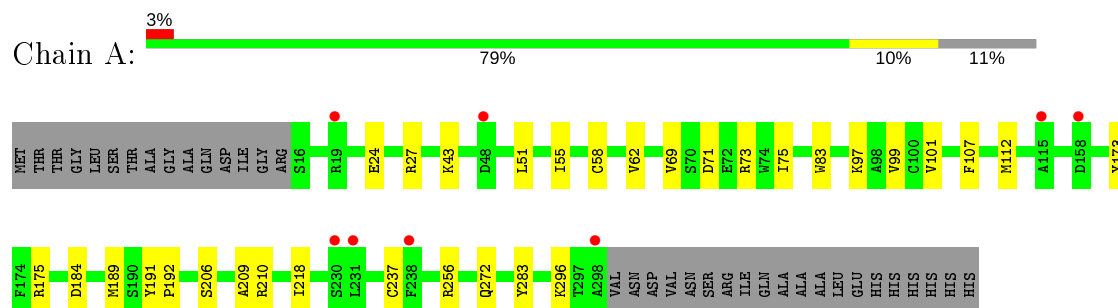
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	114	Total	O	0	0
			114	114		

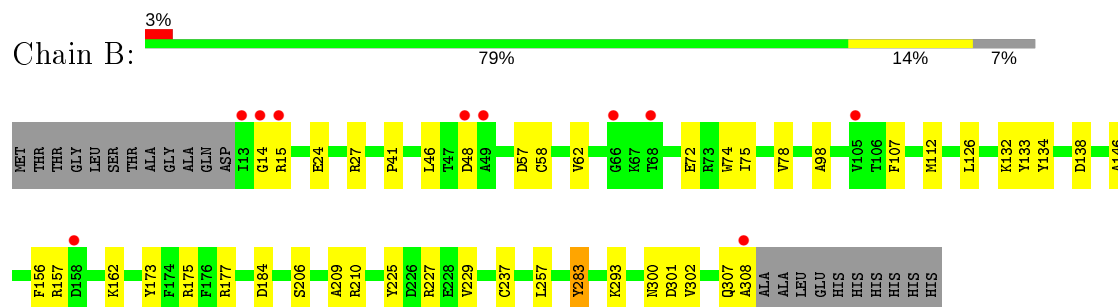
3 Residue-property plots [i](#)

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: Cyclooctat-9-en-7-ol synthase



• Molecule 1: Cyclooctat-9-en-7-ol synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.38 Å 56.46 Å 56.93 Å 91.82° 101.66° 115.93°	Depositor
Resolution (Å)	19.83 – 2.10 19.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.83-2.10) 99.3 (19.83-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.09 Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.183 , 0.237 0.183 , 0.236	Depositor DCC
R_{free} test set	1680 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5015	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.22% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.39	0/2381	0.51	0/3229
1	B	0.42	0/2499	0.57	1/3388 (0.0%)
All	All	0.41	0/4880	0.54	1/6617 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	LEU	CA-CB-CG	5.09	127.00	115.30

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	2320	0	2237	19	0
1	B	2438	0	2358	24	0
2	A	14	0	9	0	0
2	B	14	0	9	2	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	109	0	0	2	0
4	B	114	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5015	0	4613	41	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 4.

All (41) 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:112:MET:O	1:B:157:ARG:NH2	2.28	0.66
1:A:69:VAL:HG13	1:A:73:ARG:HD3	1.79	0.65
1:A:24:GLU:OE2	1:A:27:ARG:NH2	2.31	0.64
1:B:24:GLU:OE1	1:B:27:ARG:NH1	2.34	0.60
1:B:227:ARG:NH2	2:B:401:AHD:O10	2.34	0.60
1:A:218:ILE:HD13	1:A:256:ARG:HB3	1.88	0.56
1:B:227:ARG:HH22	2:B:401:AHD:P9	2.30	0.55
1:A:296:LYS:HA	1:A:296:LYS:HE2	1.89	0.54
1:B:156:PHE:HB3	1:B:162:LYS:HD3	1.88	0.54
1:B:173:TYR:CE2	1:B:237:CYS:HB3	2.42	0.54
1:A:210:ARG:HB3	1:B:175:ARG:HG3	1.91	0.51
1:B:293:LYS:NZ	1:B:301:ASP:OD1	2.36	0.51
1:B:225:TYR:O	1:B:229:VAL:HG22	2.11	0.50
1:B:307:GLN:HG2	1:B:308:ALA:H	1.77	0.49
1:A:272:GLN:NE2	4:A:505:HOH:O	2.46	0.49
1:B:41:PRO:HD3	1:B:283:TYR:CD2	2.50	0.47
1:A:173:TYR:CE2	1:A:237:CYS:HB3	2.49	0.46
1:A:58:CYS:O	1:A:62:VAL:HG12	2.16	0.46
1:B:184:ASP:HA	1:B:209:ALA:HB2	1.97	0.46
1:A:112:MET:HB3	1:A:112:MET:HE2	1.62	0.46
1:B:98:ALA:HB2	1:B:133:TYR:CB	2.46	0.46
1:B:134:TYR:HB3	1:B:138:ASP:HB2	1.97	0.45
1:B:72:GLU:OE1	1:B:293:LYS:NZ	2.49	0.45
1:B:46:LEU:HD23	1:B:46:LEU:HA	1.82	0.45
1:B:75:ILE:HA	1:B:78:VAL:HG12	1.99	0.45
1:A:191:TYR:CG	1:A:192:PRO:HD3	2.52	0.44
1:B:206:SER:HA	4:B:572:HOH:O	2.18	0.44
1:A:191:TYR:CD2	1:A:192:PRO:HD3	2.53	0.44
1:B:126:LEU:HD13	1:B:146:ALA:HB1	2.00	0.44
1:A:184:ASP:HA	1:A:209:ALA:HB2	1.99	0.43
1:A:97:LYS:O	1:A:101:VAL:HG23	2.17	0.43
1:B:58:CYS:O	1:B:62:VAL:HG22	2.18	0.43
1:B:300:ASN:OD1	1:B:302:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ASP:OD2	1:B:132:LYS:NZ	2.52	0.42
1:A:43:LYS:HD2	1:A:83:TRP:NE1	2.34	0.42
1:A:71:ASP:O	1:A:75:ILE:HG13	2.21	0.41
1:B:58:CYS:HB3	1:B:74:TRP:CH2	2.55	0.41
1:A:51:LEU:O	1:A:55:ILE:HG13	2.20	0.41
1:A:175:ARG:HG3	1:B:210:ARG:HB3	2.03	0.40
1:A:206:SER:HA	4:A:545:HOH:O	2.21	0.40
1:A:99:VAL:HG22	1:A:189:MET:HG3	2.02	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	282/318 (89%)	278 (99%)	4 (1%)	0	100	100
1	B	297/318 (93%)	292 (98%)	3 (1%)	2 (1%)	22	18
All	All	579/636 (91%)	570 (98%)	7 (1%)	2 (0%)	41	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	48	ASP
1	B	14	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	255/281 (91%)	253 (99%)	2 (1%)	81	86
1	B	268/281 (95%)	264 (98%)	4 (2%)	65	71
All	All	523/562 (93%)	517 (99%)	6 (1%)	71	79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	PHE
1	A	283	TYR
1	B	15	ARG
1	B	107	PHE
1	B	177	ARG
1	B	283	TYR

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are 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	$\# Z > 2$
2	AHD	A	401	3	13,13,13	1.34	1 (7%)	19,21,21	1.82	4 (21%)
2	AHD	B	401	3	13,13,13	1.56	4 (30%)	19,21,21	1.68	5 (26%)

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
2	AHD	A	401	3	-	4/23/23/23	-
2	AHD	B	401	3	-	1/23/23/23	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	AHD	O13-C8	-3.23	1.40	1.44
2	A	401	AHD	O13-C8	-2.82	1.41	1.44
2	B	401	AHD	P9-O12	-2.23	1.50	1.54
2	B	401	AHD	P14-O15	-2.02	1.51	1.54
2	B	401	AHD	P14-O16	-2.01	1.51	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	AHD	C2-C7-C8	-5.15	106.61	116.07
2	B	401	AHD	C2-C7-C8	-4.12	108.50	116.07
2	B	401	AHD	O16-P14-C8	2.97	112.83	106.17
2	A	401	AHD	C7-C2-C3	-2.54	107.79	112.35
2	A	401	AHD	O10-P9-O11	-2.49	107.47	113.06
2	B	401	AHD	O16-P14-O17	-2.43	107.61	113.06
2	B	401	AHD	P14-C8-P9	-2.27	108.75	112.81
2	B	401	AHD	C7-C2-C3	-2.17	108.46	112.35
2	A	401	AHD	O10-P9-C8	2.09	110.86	106.17

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	AHD	C2-C7-C8-P9
2	A	401	AHD	C2-C7-C8-P14
2	A	401	AHD	C2-C7-C8-O13
2	B	401	AHD	C2-C7-C8-O13
2	A	401	AHD	O13-C8-P14-O17

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	AHD	2	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	283/318 (88%)	0.02	8 (2%) 53 59	20, 34, 53, 69	0
1	B	296/318 (93%)	-0.11	10 (3%) 45 51	18, 32, 52, 71	0
All	All	579/636 (91%)	-0.04	18 (3%) 49 55	18, 33, 53, 71	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	ILE	5.3
1	A	298	ALA	4.0
1	B	308	ALA	3.6
1	B	15	ARG	3.1
1	B	48	ASP	3.1
1	B	14	GLY	3.0
1	B	105	VAL	3.0
1	A	48	ASP	2.9
1	A	158	ASP	2.6
1	A	19	ARG	2.5
1	A	238	PHE	2.4
1	A	231	LEU	2.3
1	B	158	ASP	2.2
1	A	230	SER	2.2
1	A	115	ALA	2.2
1	B	66	GLY	2.1
1	B	49	ALA	2.0
1	B	68	THR	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 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	MG	A	402	1/1	0.93	0.08	38,38,38,38	0
3	MG	A	404	1/1	0.93	0.04	34,34,34,34	0
3	MG	B	402	1/1	0.95	0.11	31,31,31,31	0
3	MG	A	403	1/1	0.96	0.08	37,37,37,37	0
3	MG	B	403	1/1	0.98	0.05	29,29,29,29	0
2	AHD	A	401	14/14	0.98	0.08	29,34,42,43	0
3	MG	B	404	1/1	0.98	0.04	26,26,26,26	0
2	AHD	B	401	14/14	0.99	0.07	20,25,29,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.