



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 05:32 AM UTC

PDB ID : 7AO3 / pdb_00007ao3
Title : Crystal structure of CotB2 variant F149L in complex with alendronate
Authors : Dimos, N.; Driller, R.; Loll, B.
Deposited on : 2020-10-13
Resolution : 1.45 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

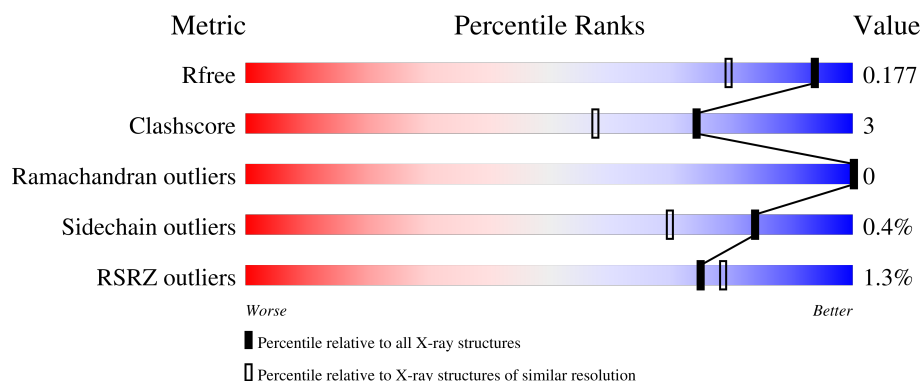
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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 $\leq 5\%$. 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	
1	B	318	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5620 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.

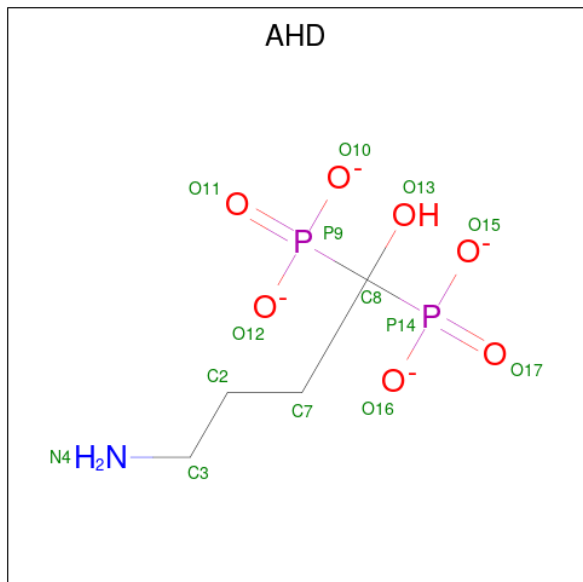
- Molecule 1 is a protein called Cyclooctat-9-en-7-ol synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	16	0
			2618	1652	456	493	17			
1	B	292	Total	C	N	O	S	0	7	0
			2442	1551	410	464	17			

There are 24 discrepancies between the modelled and reference sequences:

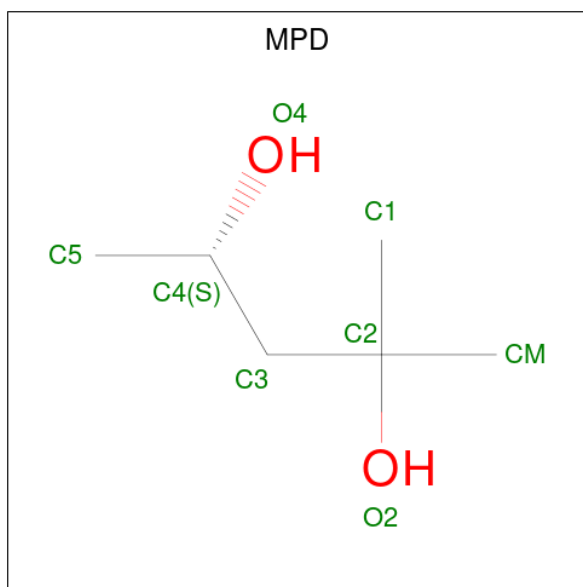
Chain	Residue	Modelled	Actual	Comment	Reference
A	149	LEU	PHE	engineered mutation	UNP C9K1X5
A	308	ALA	-	expression tag	UNP C9K1X5
A	309	ALA	-	expression tag	UNP C9K1X5
A	310	ALA	-	expression tag	UNP C9K1X5
A	311	LEU	-	expression tag	UNP C9K1X5
A	312	GLU	-	expression tag	UNP C9K1X5
A	313	HIS	-	expression 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	149	LEU	PHE	engineered mutation	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 (CCD ID: AHD) (formula: $C_4H_9NO_7P_2$).



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 (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			16	12	4		
3	A	1	Total	C	O	0	1
			16	12	4		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	1
			16	12	4		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	255	Total	O	0	8
			255	255		
6	B	213	Total	O	0	2
			213	213		

- 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	53.58Å 57.21Å 57.63Å 90.80° 116.11° 102.21°	Depositor
Resolution (Å)	38.27 – 1.45 38.27 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.27-1.45) 99.0 (38.27-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.45Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.138 , 0.178 0.138 , 0.177	Depositor DCC
R_{free} test set	5237 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.4	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	0.98	EDS
Total number of atoms	5620	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.74% 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: AHD, CL, MPD, MG

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	0.56	0/2689	0.68	0/3644
1	B	0.57	0/2502	0.68	0/3393
All	All	0.56	0/5191	0.68	0/7037

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2618	0	2509	15	0
1	B	2442	0	2353	13	0
2	A	14	0	9	3	0
2	B	14	0	9	0	0
3	A	32	0	56	11	0
3	B	24	0	42	3	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	255	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	213	0	0	1	0
All	All	5620	0	4978	31	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 (31) 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)
3:A:403[B]:MPD:H52	1:B:175:ARG:HH21	1.46	0.81
2:A:401:AHD:H21	3:A:402[A]:MPD:HM2	1.64	0.80
1:A:24[B]:GLU:OE1	1:A:27[B]:ARG:NH2	2.16	0.77
3:A:403[B]:MPD:H12	1:B:175:ARG:HE	1.56	0.70
1:B:186:TRP:CZ3	3:B:407[A]:MPD:HM2	2.36	0.61
2:A:401:AHD:N4	3:A:402[B]:MPD:H12	2.19	0.58
1:B:186:TRP:CE3	3:B:407[A]:MPD:HM2	2.43	0.53
3:A:402[A]:MPD:O2	3:A:402[A]:MPD:O4	2.16	0.53
1:A:80:VAL:HG11	3:A:402[A]:MPD:H13	1.93	0.50
1:A:113[A]:ASP:OD1	1:A:305:ARG:NE	2.41	0.50
1:A:214:ARG:HD3	3:A:403[A]:MPD:H53	1.95	0.48
1:B:58:CYS:HB3	1:B:74:TRP:CH2	2.49	0.47
1:A:311:LEU:HB3	1:A:314:HIS:HB2	1.97	0.46
1:B:297[A]:THR:HG22	1:B:300:ASN:HD22	1.80	0.46
1:A:214:ARG:HD3	3:A:403[A]:MPD:C5	2.46	0.46
1:A:91:LYS:HB3	1:A:91:LYS:HE2	1.69	0.46
1:A:173:TYR:CE2	1:A:237:CYS:HB3	2.51	0.45
1:A:98:ALA:HB2	1:A:133:TYR:CB	2.47	0.45
1:A:191:TYR:CG	1:A:192:PRO:HD3	2.52	0.44
1:B:225:TYR:O	1:B:229:VAL:HG22	2.17	0.44
1:A:175:ARG:HG3	1:B:210:ARG:HB3	1.99	0.44
1:B:173:TYR:CE2	1:B:237:CYS:HB3	2.52	0.44
1:B:80:VAL:HG21	3:B:407[B]:MPD:C1	2.49	0.43
1:A:206:SER:HA	6:A:645:HOH:O	2.19	0.43
1:A:178:VAL:CG2	3:A:403[A]:MPD:HM2	2.49	0.42
1:A:285:ASN:OD1	3:A:402[B]:MPD:H4	2.20	0.41
2:A:401:AHD:C2	3:A:402[A]:MPD:HM2	2.44	0.41
1:B:42:THR:OG1	1:B:87:PRO:HG2	2.21	0.41
1:A:27[A]:ARG:NH2	1:A:31[A]:GLU:OE1	2.54	0.41
1:B:98:ALA:HB2	1:B:133:TYR:CB	2.51	0.41
1:B:206:SER:HA	6:B:614:HOH:O	2.21	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	317/318 (100%)	313 (99%)	4 (1%)	0	100	100
1	B	297/318 (93%)	295 (99%)	2 (1%)	0	100	100
All	All	614/636 (96%)	608 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	287/281 (102%)	286 (100%)	1 (0%)	86	74
1	B	270/281 (96%)	269 (100%)	1 (0%)	84	70
All	All	557/562 (99%)	555 (100%)	2 (0%)	84	70

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	PHE
1	B	107	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	307	GLN
1	B	30	GLN
1	B	125	GLN
1	B	285	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 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	$\# Z > 2$
3	MPD	A	402[B]	-	7,7,7	0.41	0	9,10,10	0.70	0
3	MPD	A	402[A]	-	7,7,7	0.61	0	9,10,10	0.86	0
2	AHD	A	401	4	13,13,13	1.48	3 (23%)	19,21,21	1.24	1 (5%)
3	MPD	B	407[B]	-	7,7,7	0.42	0	9,10,10	0.99	0
3	MPD	A	403[B]	-	7,7,7	0.41	0	9,10,10	0.67	0
2	AHD	B	406	4	13,13,13	1.36	2 (15%)	19,21,21	1.13	2 (10%)
3	MPD	B	405	-	7,7,7	0.31	0	9,10,10	0.68	0
3	MPD	B	407[A]	-	7,7,7	0.47	0	9,10,10	0.54	0
3	MPD	A	403[A]	-	7,7,7	0.63	0	9,10,10	1.48	2 (22%)

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	MPD	A	402[B]	-	-	2/5/5/5	-
3	MPD	A	402[A]	-	-	0/5/5/5	-
2	AHD	A	401	4	-	0/23/23/23	-
3	MPD	B	407[B]	-	-	4/5/5/5	-
3	MPD	A	403[B]	-	-	5/5/5/5	-
2	AHD	B	406	4	-	0/23/23/23	-
3	MPD	B	405	-	-	3/5/5/5	-
3	MPD	B	407[A]	-	-	3/5/5/5	-
3	MPD	A	403[A]	-	-	2/5/5/5	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	AHD	P14-O17	2.95	1.55	1.50
2	A	401	AHD	P9-C8	2.56	1.87	1.85
2	B	406	AHD	P9-C8	2.25	1.86	1.85
2	A	401	AHD	O13-C8	-2.18	1.42	1.44
2	B	406	AHD	P14-C8	2.16	1.86	1.85

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	406	AHD	P14-C8-P9	-2.73	107.84	112.72
3	A	403[A]	MPD	CM-C2-C3	-2.55	99.19	110.20
2	B	406	AHD	O16-P14-C8	2.41	111.50	106.19
2	A	401	AHD	P14-C8-P9	-2.13	108.91	112.72
3	A	403[A]	MPD	O2-C2-C1	2.11	114.56	107.99

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402[B]	MPD	C2-C3-C4-C5
3	A	403[A]	MPD	C2-C3-C4-C5
3	A	403[B]	MPD	C2-C3-C4-O4
3	A	403[B]	MPD	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	407[B]	MPD	C2-C3-C4-C5
3	B	405	MPD	O2-C2-C3-C4
3	B	405	MPD	C2-C3-C4-O4
3	A	403[B]	MPD	CM-C2-C3-C4
3	B	405	MPD	C2-C3-C4-C5
3	A	403[B]	MPD	O2-C2-C3-C4
3	B	407[A]	MPD	O2-C2-C3-C4
3	B	407[B]	MPD	O2-C2-C3-C4
3	A	402[B]	MPD	C2-C3-C4-O4
3	A	403[A]	MPD	C2-C3-C4-O4
3	B	407[A]	MPD	C2-C3-C4-O4
3	B	407[B]	MPD	C2-C3-C4-O4
3	A	403[B]	MPD	C1-C2-C3-C4
3	B	407[A]	MPD	C1-C2-C3-C4
3	B	407[B]	MPD	C1-C2-C3-C4

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402[B]	MPD	2	0
3	A	402[A]	MPD	4	0
2	A	401	AHD	3	0
3	B	407[B]	MPD	1	0
3	A	403[B]	MPD	2	0
3	B	407[A]	MPD	2	0
3	A	403[A]	MPD	3	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	303/318 (95%)	-0.40	7 (2%) 61 63	9, 22, 38, 82	16 (5%)
1	B	292/318 (91%)	-0.31	1 (0%) 90 92	10, 26, 45, 60	7 (2%)
All	All	595/636 (93%)	-0.36	8 (1%) 75 78	9, 24, 44, 82	23 (3%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	310	ALA	3.2
1	A	314	HIS	2.9
1	A	309	ALA	2.5
1	A	317	HIS	2.4
1	A	316	HIS	2.3
1	A	158	ASP	2.2
1	A	313	HIS	2.1
1	B	305	ARG	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 oligosaccharides 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
3	MPD	B	407[A]	8/8	0.83	0.18	35,42,42,44	8
3	MPD	B	407[B]	8/8	0.83	0.18	36,37,38,39	8
3	MPD	B	405	8/8	0.85	0.16	46,48,55,56	0
3	MPD	A	402[A]	8/8	0.85	0.20	37,42,42,42	8
3	MPD	A	402[B]	8/8	0.85	0.20	26,30,33,33	8
3	MPD	A	403[B]	8/8	0.86	0.17	27,30,31,32	8
3	MPD	A	403[A]	8/8	0.86	0.17	18,30,33,35	8
2	AHD	B	406	14/14	0.99	0.04	18,20,23,24	0
2	AHD	A	401	14/14	0.99	0.03	16,17,19,22	0
4	MG	A	405	1/1	0.99	0.02	20,20,20,20	0
4	MG	B	401	1/1	0.99	0.03	23,23,23,23	0
4	MG	A	406	1/1	1.00	0.02	20,20,20,20	0
4	MG	A	404	1/1	1.00	0.02	18,18,18,18	0
4	MG	B	402	1/1	1.00	0.01	19,19,19,19	0
4	MG	B	403	1/1	1.00	0.02	20,20,20,20	0
5	CL	A	407	1/1	1.00	0.05	24,24,24,24	0
5	CL	B	404	1/1	1.00	0.06	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.