



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:33 PM UTC

PDB ID : 3D36 / pdb_00003d36
Title : How to Switch Off a Histidine Kinase: Crystal Structure of Geobacillus stearothermophilus KinB with the Inhibitor Sda
Authors : Bick, M.J.; Lamour, V.; Rajashankar, K.R.; Gordiyenko, Y.; Robinson, C.V.; Darst, S.A.
Deposited on : 2008-05-09
Resolution : 2.03 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:

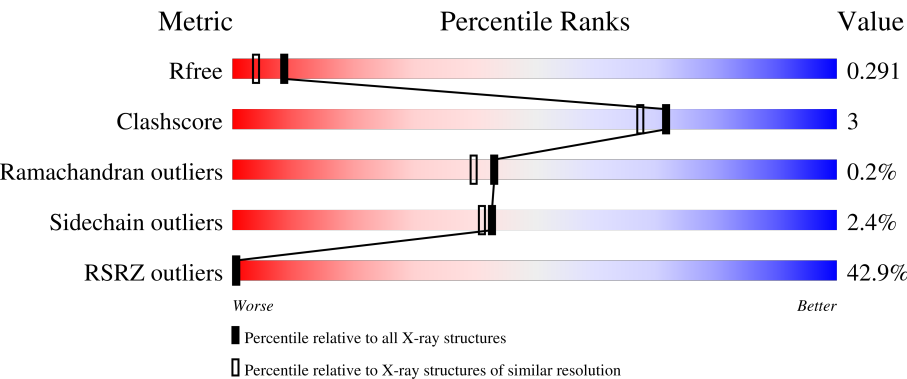
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	244	44% 84% 5% 11%
1	B	244	34% 81% 9% 9%
2	C	46	37% 74% 17% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4224 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 Sporulation kinase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1687	1068	296	313	10			
1	B	221	Total	C	N	O	S	0	0	0
			1720	1088	303	319	10			

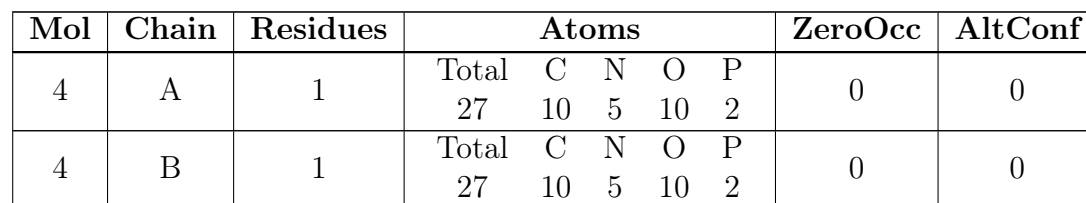
- Molecule 2 is a protein called Sporulation kinase inhibitor Sda.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	42	Total	C	N	O	S	0	0	0
			356	230	59	66	1			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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- The chemical structure of 2-methylpentane-2,4-diol (MPD) is shown. The molecule consists of a five-carbon chain. The second carbon (C2) is bonded to a methyl group (CM) and a hydroxyl group (OH, labeled O2). The fourth carbon (C4) is bonded to a hydroxyl group (OH, labeled O4) and a methyl group (C5). The third carbon (C3) is bonded to the second and fourth carbons. The labels C1, C2, C3, C4(S), and C5 are in green, while the labels CM, O2, O4, and the OH groups are in red.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			8	6	2		
5	C	1	Total	C	O	0	0
			8	6	2		

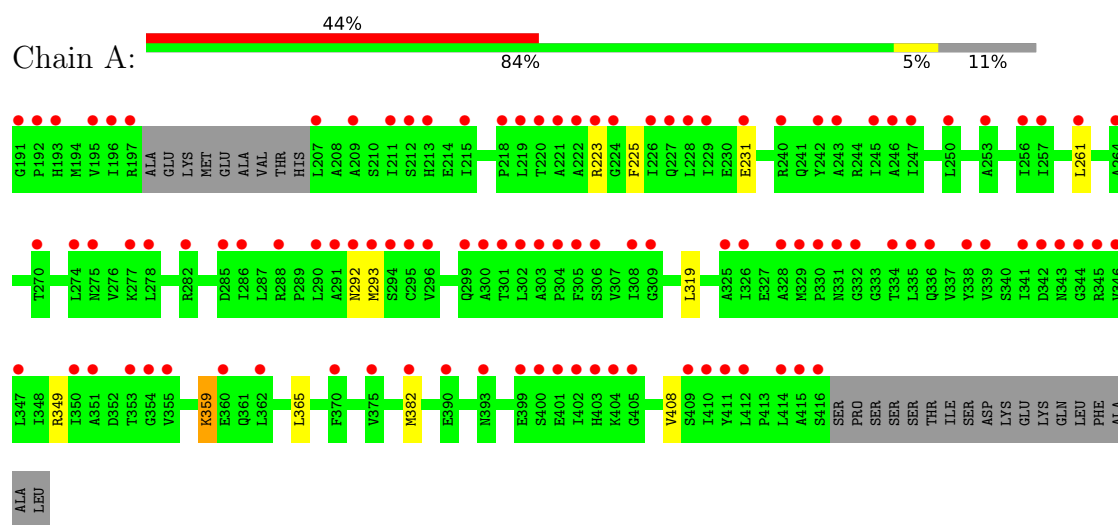
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	123	Total	O	0	0
			123	123		
6	B	209	Total	O	0	0
			209	209		
6	C	41	Total	O	0	0
			41	41		

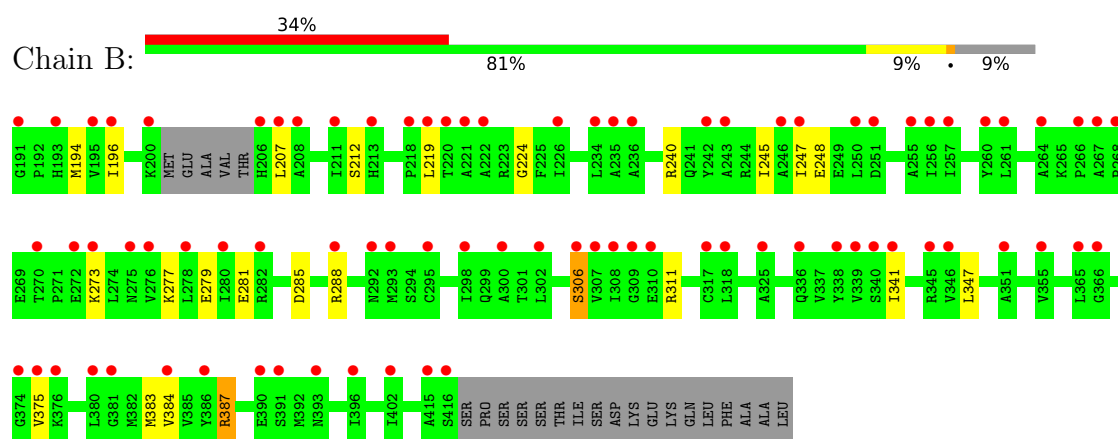
3 Residue-property plots [i](#)

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.

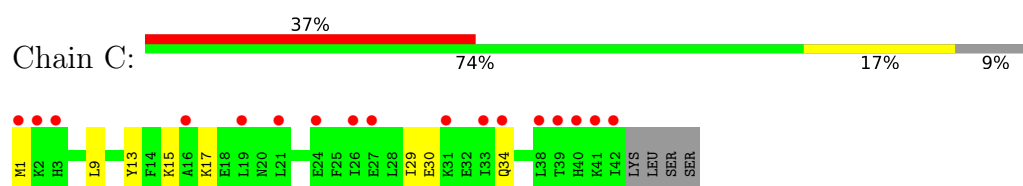
• Molecule 1: Sporulation kinase B



• Molecule 1: Sporulation kinase B



• Molecule 2: Sporulation kinase inhibitor Sda



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	66.11Å 66.11Å 315.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.41 – 2.03 42.41 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.9 (42.41-2.03) 98.8 (42.41-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.215 0.282 , 0.291	Depositor DCC
R_{free} test set	2649 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4224	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: MPD, MG, ADP

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	0.50	1/1710 (0.1%)	0.76	0/2310
1	B	0.52	0/1744	0.78	0/2355
2	C	0.47	0/361	0.78	0/481
All	All	0.51	1/3815 (0.0%)	0.77	0/5146

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	LYS	CE-NZ	7.14	1.70	1.49

There are no bond angle outliers.

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	1687	0	1754	10	0
1	B	1720	0	1785	11	0
2	C	356	0	374	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	24	0	42	2	0
5	C	8	0	14	0	0
6	A	123	0	0	1	0
6	B	209	0	0	3	0
6	C	41	0	0	0	0
All	All	4224	0	3993	26	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 (26) 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:359:LYS:CE	1:A:359:LYS:NZ	1.70	1.49
5:B:702:MPD:H51	5:B:703:MPD:H51	1.70	0.73
1:A:225:PHE:HZ	2:C:1:MET:HE3	1.54	0.71
1:A:231:GLU:HG2	2:C:15:LYS:HB3	1.82	0.61
2:C:1:MET:HE1	2:C:29:ILE:HG12	1.86	0.58
1:A:365:LEU:HD11	1:A:382:MET:HG3	1.86	0.57
1:B:245:ILE:HG23	6:B:847:HOH:O	2.07	0.55
1:A:292:ASN:O	1:A:293:MET:HB3	2.07	0.54
2:C:1:MET:HE2	2:C:9:LEU:CD1	2.37	0.54
1:B:383:MET:O	1:B:387:ARG:HG3	2.09	0.52
2:C:1:MET:HE2	2:C:9:LEU:HD13	1.95	0.48
1:A:359:LYS:NZ	6:A:616:HOH:O	2.47	0.47
1:B:224:GLY:HA3	5:B:700:MPD:H11	1.97	0.46
1:B:248:GLU:OE2	6:B:847:HOH:O	2.21	0.46
1:A:223:ARG:HG3	1:B:247:ILE:HD12	1.97	0.46
1:B:273:LYS:HG2	1:B:306:SER:OG	2.16	0.45
1:A:292:ASN:O	1:A:293:MET:CB	2.65	0.45
1:A:261:LEU:O	1:B:212:SER:HB3	2.17	0.44
2:C:30:GLU:O	2:C:34:GLN:HG3	2.17	0.44
2:C:13:TYR:HB2	2:C:29:ILE:HG21	2.00	0.43
1:A:349:ARG:HA	1:A:408:VAL:O	2.18	0.43
1:B:285:ASP:OD1	1:B:288:ARG:NH1	2.52	0.41
2:C:13:TYR:CZ	2:C:17:LYS:HD2	2.55	0.41
1:B:277:LYS:HE2	1:B:281:GLU:OE2	2.20	0.41
1:B:240:ARG:NH2	6:B:842:HOH:O	2.53	0.41
1:B:279:GLU:OE2	1:B:311:ARG:NH1	2.54	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	213/244 (87%)	209 (98%)	4 (2%)	0	100	100
1	B	217/244 (89%)	214 (99%)	2 (1%)	1 (0%)	24	17
2	C	40/46 (87%)	40 (100%)	0	0	100	100
All	All	470/534 (88%)	463 (98%)	6 (1%)	1 (0%)	43	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	207	LEU

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	183/206 (89%)	182 (100%)	1 (0%)	81	81
1	B	186/206 (90%)	177 (95%)	9 (5%)	23	15
2	C	41/45 (91%)	41 (100%)	0	100	100
All	All	410/457 (90%)	400 (98%)	10 (2%)	43	41

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	LEU
1	B	194	MET

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Mol	Chain	Res	Type
1	B	196	ILE
1	B	219	LEU
1	B	306	SER
1	B	341	ILE
1	B	347	LEU
1	B	375	VAL
1	B	384	VAL
1	B	387	ARG

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

Mol	Chain	Res	Type
1	A	227	GLN
1	A	241	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
5	MPD	B	700	-	7,7,7	0.29	0	9,10,10	0.28	0
5	MPD	C	701	-	7,7,7	0.30	0	9,10,10	0.48	0
4	ADP	B	500	3	28,29,29	1.42	5 (17%)	43,45,45	1.76	9 (20%)
5	MPD	B	702	-	7,7,7	0.32	0	9,10,10	0.35	0
5	MPD	B	703	-	7,7,7	0.27	0	9,10,10	0.31	0
4	ADP	A	500	3	28,29,29	1.47	5 (17%)	43,45,45	1.79	9 (20%)

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
5	MPD	B	700	-	-	1/5/5/5	-
5	MPD	C	701	-	-	0/5/5/5	-
4	ADP	B	500	3	-	2/16/32/32	0/3/3/3
5	MPD	B	702	-	-	2/5/5/5	-
5	MPD	B	703	-	-	0/5/5/5	-
4	ADP	A	500	3	-	2/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	ADP	C5-C4	4.79	1.47	1.39
4	B	500	ADP	C5-C4	4.68	1.47	1.39
4	B	500	ADP	C5-C6	2.70	1.48	1.41
4	A	500	ADP	C5-C6	2.67	1.48	1.41
4	A	500	ADP	PA-O3A	2.41	1.62	1.59
4	A	500	ADP	C5-N7	-2.29	1.34	1.39
4	A	500	ADP	C8-N7	2.26	1.36	1.31
4	B	500	ADP	C8-N7	2.18	1.35	1.31
4	B	500	ADP	C5-N7	-2.08	1.35	1.39
4	B	500	ADP	C4-N9	-2.07	1.33	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	500	ADP	C5-C4-N3	-5.69	118.89	126.72
4	B	500	ADP	C5-C4-N3	-5.19	119.57	126.72
4	A	500	ADP	N3-C4-N9	4.64	135.07	127.17
4	B	500	ADP	N3-C4-N9	4.32	134.51	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	500	ADP	N3-C2-N1	-4.01	122.52	128.58
4	B	500	ADP	C2-N3-C4	3.78	121.07	111.83
4	A	500	ADP	C2-N3-C4	3.74	120.97	111.83
4	A	500	ADP	N3-C2-N1	-3.62	123.10	128.58
4	A	500	ADP	C4-C5-N7	-3.35	106.75	110.58
4	B	500	ADP	C4-C5-N7	-2.94	107.22	110.58
4	B	500	ADP	C4-N9-C8	2.82	108.70	105.74
4	A	500	ADP	C4-N9-C8	2.70	108.57	105.74
4	A	500	ADP	C5-N7-C8	2.48	107.35	103.45
4	B	500	ADP	C2-N1-C6	2.33	122.56	118.73
4	B	500	ADP	C6-C5-N7	2.25	136.43	132.09
4	B	500	ADP	C5-N7-C8	2.12	106.78	103.45
4	A	500	ADP	C2-N1-C6	2.08	122.15	118.73
4	A	500	ADP	C6-C5-N7	2.06	136.05	132.09

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	500	ADP	PA-O3A-PB-O2B
4	A	500	ADP	PA-O3A-PB-O3B
4	B	500	ADP	PA-O3A-PB-O2B
4	B	500	ADP	PA-O3A-PB-O3B
5	B	700	MPD	O2-C2-C3-C4
5	B	702	MPD	C1-C2-C3-C4
5	B	702	MPD	CM-C2-C3-C4

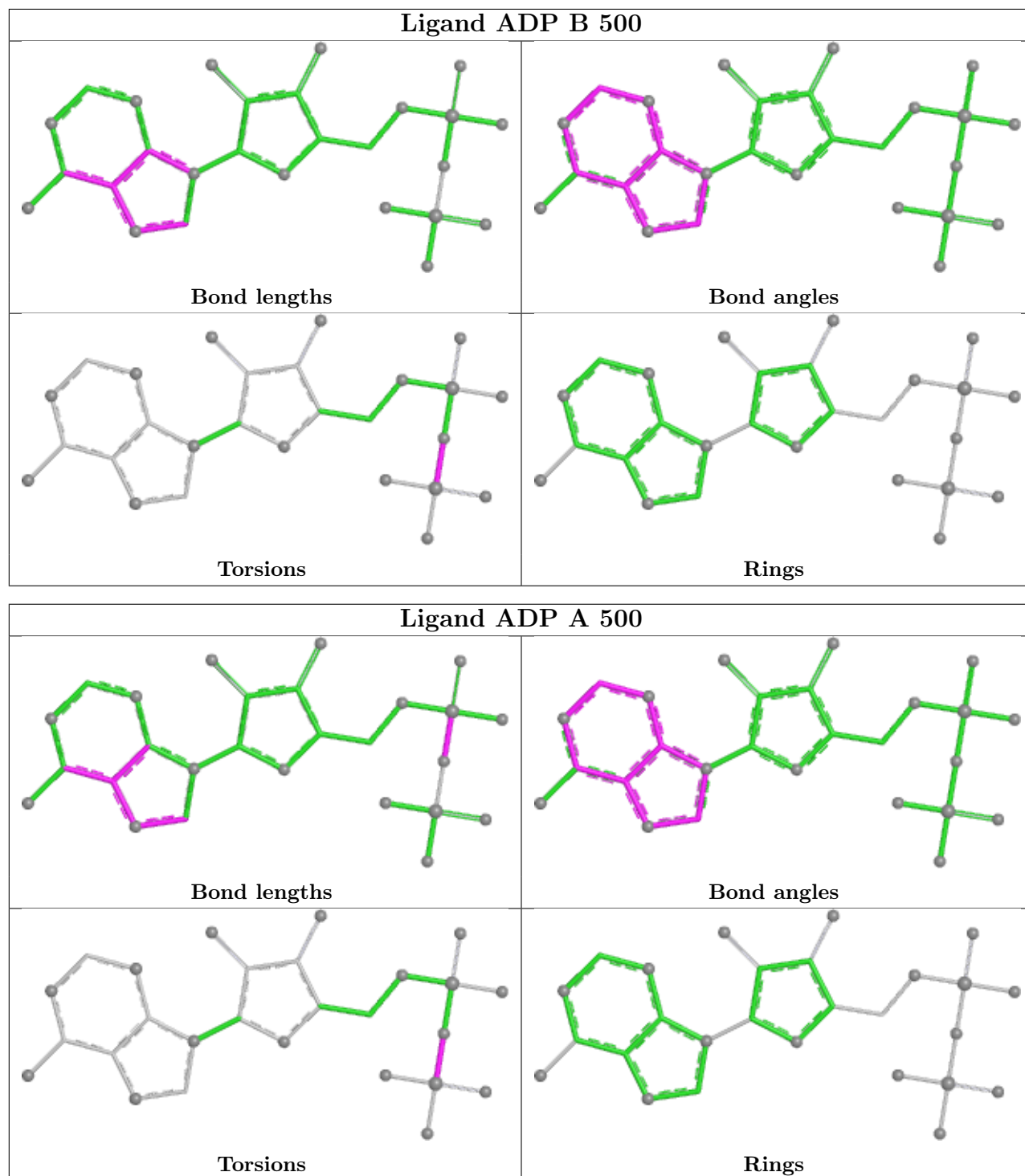
There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	700	MPD	1	0
5	B	702	MPD	1	0
5	B	703	MPD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	217/244 (88%)	2.10	107 (49%) 0 0	34, 39, 46, 50	0
1	B	221/244 (90%)	1.83	82 (37%) 1 1	35, 40, 44, 54	0
2	C	42/46 (91%)	1.86	17 (40%) 0 1	36, 39, 48, 54	0
All	All	480/534 (89%)	1.96	206 (42%) 0 0	34, 39, 46, 54	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338	TYR	6.4
1	A	303	ALA	5.6
2	C	42	ILE	5.5
1	A	191	GLY	5.1
2	C	34	GLN	5.0
1	A	405	GLY	4.8
1	A	293	MET	4.8
1	B	207	LEU	4.8
2	C	3	HIS	4.6
1	A	338	TYR	4.5
1	A	296	VAL	4.5
1	B	416	SER	4.3
1	A	292	ASN	4.2
1	B	317	CYS	4.2
1	A	415	ALA	4.2
1	A	282	ARG	4.1
1	A	207	LEU	4.1
1	A	402	ILE	3.9
1	A	401	GLU	3.9
1	A	331	ASN	3.8
1	A	404	LYS	3.8
1	A	345	ARG	3.8
1	B	206	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	270	THR	3.7
1	A	218	PRO	3.7
1	B	306	SER	3.6
1	A	339	VAL	3.6
1	B	193	HIS	3.6
1	B	390	GLU	3.6
1	A	196	ILE	3.6
2	C	40	HIS	3.6
1	A	344	GLY	3.5
1	A	288	ARG	3.5
1	A	275	ASN	3.5
1	A	416	SER	3.4
1	B	341	ILE	3.4
1	B	415	ALA	3.4
1	A	346	VAL	3.4
1	A	400	SER	3.4
1	A	334	THR	3.3
1	A	360	GLU	3.3
1	A	300	ALA	3.3
1	A	306	SER	3.2
1	A	399	GLU	3.2
1	A	295	CYS	3.2
1	A	326	ILE	3.2
1	B	346	VAL	3.2
1	B	336	GLN	3.2
1	A	247	ILE	3.2
1	A	341	ILE	3.2
1	A	245	ILE	3.1
1	B	220	THR	3.1
1	A	299	GLN	3.1
1	A	274	LEU	3.1
1	A	332	GLY	3.1
1	A	343	ASN	3.1
1	A	257	ILE	3.1
1	A	336	GLN	3.1
1	A	213	HIS	3.0
1	B	200	LYS	3.0
1	A	304	PRO	3.0
1	A	221	ALA	3.0
1	B	247	ILE	3.0
1	B	309	GLY	3.0
2	C	39	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	193	HIS	3.0
1	A	243	ALA	3.0
1	B	255	ALA	3.0
1	A	219	LEU	3.0
1	A	229	ILE	3.0
1	B	191	GLY	2.9
1	A	250	LEU	2.9
1	A	226	ILE	2.9
1	B	292	ASN	2.9
1	A	325	ALA	2.9
1	B	267	ALA	2.9
2	C	38	LEU	2.9
1	B	276	VAL	2.9
1	A	411	TYR	2.9
1	B	351	ALA	2.9
1	A	228	LEU	2.8
1	A	256	ILE	2.8
1	B	221	ALA	2.8
1	B	381	GLY	2.8
1	A	305	PHE	2.8
1	A	246	ALA	2.8
1	A	302	LEU	2.8
1	B	256	ILE	2.8
1	B	366	GLY	2.8
1	A	362	LEU	2.8
1	A	353	THR	2.8
1	A	215	ILE	2.8
1	B	393	ASN	2.7
1	B	293	MET	2.7
1	B	273	LYS	2.7
1	B	282	ARG	2.7
1	A	330	PRO	2.7
1	B	213	HIS	2.7
1	B	234	LEU	2.7
2	C	21	LEU	2.7
1	A	328	ALA	2.6
1	B	300	ALA	2.6
1	A	347	LEU	2.6
1	A	192	PRO	2.6
1	A	212	SER	2.6
1	B	219	LEU	2.6
1	A	285	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	250	LEU	2.6
1	A	224	GLY	2.5
1	A	342	ASP	2.5
1	A	291	ALA	2.5
1	B	222	ALA	2.5
2	C	1	MET	2.5
1	A	410	ILE	2.5
1	A	294	SER	2.5
2	C	27	GLU	2.5
1	A	335	LEU	2.5
1	A	403	HIS	2.5
1	B	339	VAL	2.5
1	B	375	VAL	2.5
1	A	290	LEU	2.5
2	C	19	LEU	2.5
1	A	277	LYS	2.5
1	B	345	ARG	2.5
1	B	402	ILE	2.5
1	A	220	THR	2.4
1	B	266	PRO	2.4
1	A	264	ALA	2.4
1	A	278	LEU	2.4
1	A	412	LEU	2.4
1	B	318	LEU	2.4
1	B	211	ILE	2.4
1	B	226	ILE	2.4
1	B	295	CYS	2.4
1	A	351	ALA	2.4
1	B	236	ALA	2.4
1	B	251	ASP	2.4
1	A	286	ILE	2.4
1	B	307	VAL	2.4
1	A	253	ALA	2.4
1	B	380	LEU	2.4
1	B	374	GLY	2.4
1	B	260	TYR	2.3
1	A	222	ALA	2.3
1	B	261	LEU	2.3
1	B	278	LEU	2.3
1	A	370	PHE	2.3
1	A	308	ILE	2.3
1	B	196	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	257	ILE	2.3
1	B	340	SER	2.3
1	A	409	SER	2.3
1	B	308	ILE	2.3
1	A	309	GLY	2.3
1	B	302	LEU	2.3
1	B	310	GLU	2.3
1	B	280	ILE	2.3
2	C	26	ILE	2.3
1	B	218	PRO	2.3
2	C	31	LYS	2.3
1	A	261	LEU	2.3
1	B	365	LEU	2.3
1	B	235	ALA	2.2
1	B	272	GLU	2.2
1	B	298	ILE	2.2
1	A	355	VAL	2.2
1	A	382	MET	2.2
1	B	208	ALA	2.2
1	B	243	ALA	2.2
2	C	16	ALA	2.2
1	A	242	TYR	2.2
1	B	275	ASN	2.2
1	A	211	ILE	2.2
1	B	355	VAL	2.2
1	A	231	GLU	2.2
2	C	24	GLU	2.2
1	A	223	ARG	2.2
1	A	240	ARG	2.2
1	B	288	ARG	2.2
1	B	391	SER	2.2
1	A	393	ASN	2.2
1	A	329	MET	2.2
1	A	195	VAL	2.1
1	B	246	ALA	2.1
1	B	325	ALA	2.1
1	A	390	GLU	2.1
1	A	301	THR	2.1
1	B	268	PRO	2.1
1	A	227	GLN	2.1
1	A	350	ILE	2.1
1	B	396	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	195	VAL	2.1
1	B	264	ALA	2.1
2	C	2	LYS	2.1
2	C	41	LYS	2.1
1	B	242	TYR	2.1
1	A	270	THR	2.1
2	C	33	ILE	2.1
1	A	375	VAL	2.1
1	B	376	LYS	2.0
1	B	386	TYR	2.0
1	B	384	VAL	2.0
1	A	209	ALA	2.0
1	A	414	LEU	2.0
1	A	197	ARG	2.0
1	A	354	GLY	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](#)

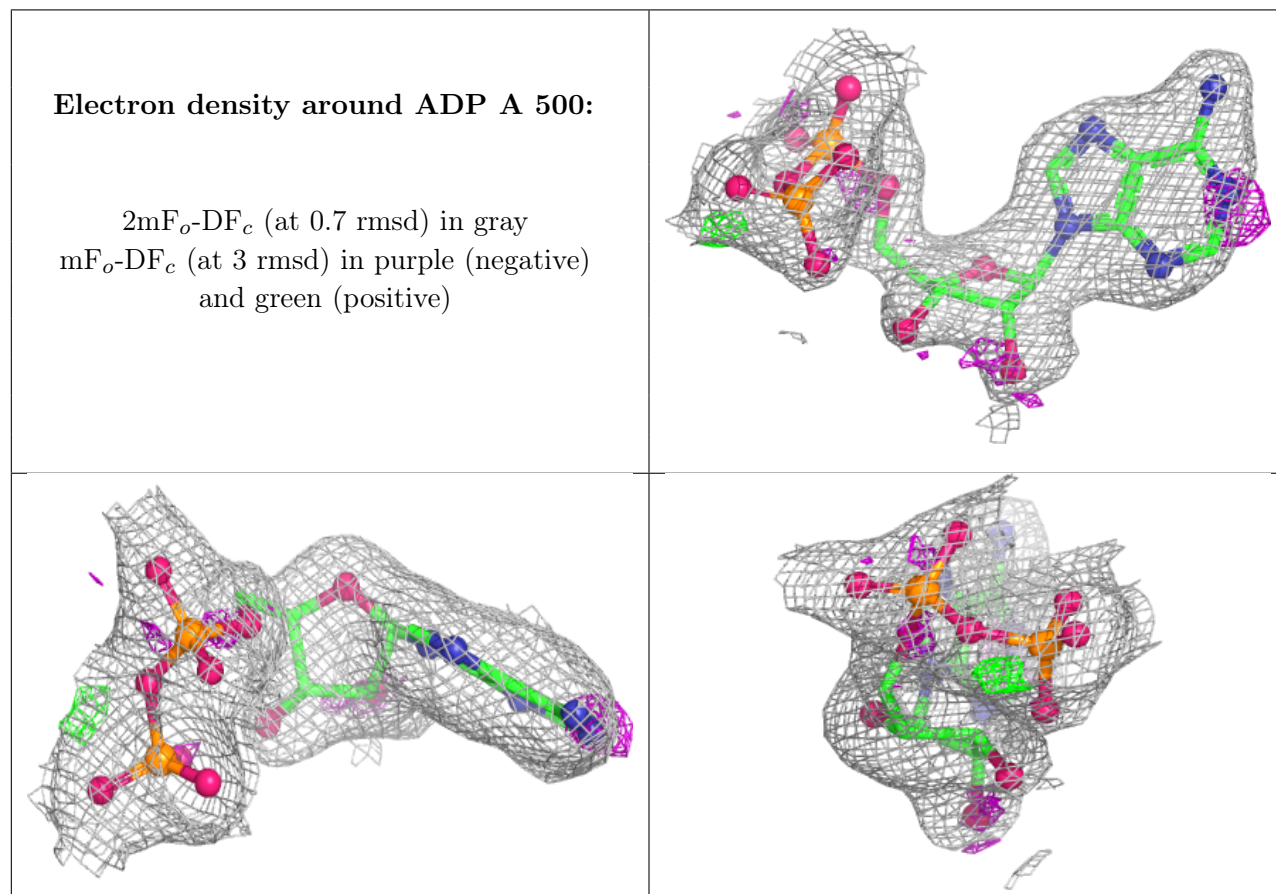
There are no oligosaccharides in this entry.

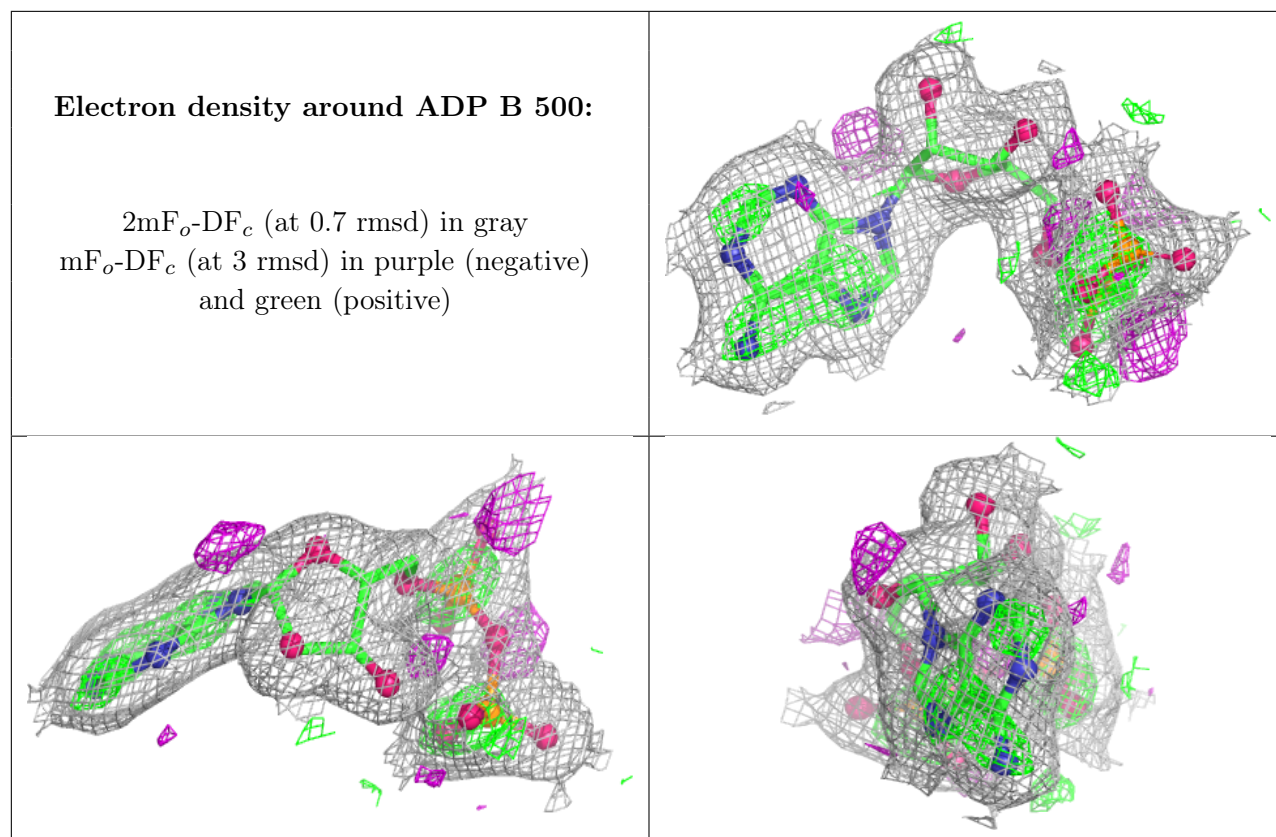
6.4 Ligands [i](#)

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
5	MPD	C	701	8/8	0.70	0.21	62,62,63,64	0
5	MPD	B	700	8/8	0.76	0.20	58,58,59,59	0
5	MPD	B	703	8/8	0.87	0.17	43,45,47,47	0
5	MPD	B	702	8/8	0.89	0.12	38,39,42,42	0
4	ADP	A	500	27/27	0.92	0.11	35,36,37,37	0
3	MG	B	477	1/1	0.94	0.11	40,40,40,40	0
4	ADP	B	500	27/27	0.95	0.14	35,37,39,41	0
3	MG	A	478	1/1	0.97	0.05	41,41,41,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.