Full wwPDB X-ray Structure Validation Report (i)

Feb 10, 2024 – 10:51 PM EST

PDB ID	:	2ILP
Title	:	Clostridium botulinum Serotype A Light Chain inhibited by 4-chlorocinnamic hydroxamate
Authors	:	Silvaggi, N.R.; Allen, K.N.
Deposited on	:	2006-10-03
Resolution	:	1.90 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

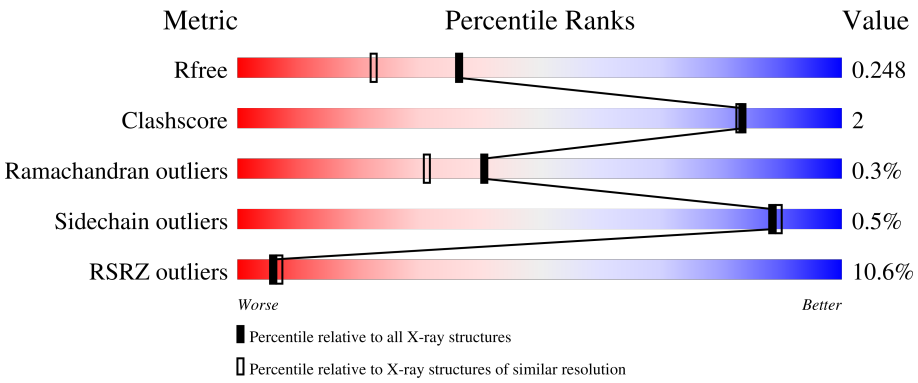
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	444	10% 86% 5% • 8%
1	B	444	10% 87% • 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7294 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 Botulinum neurotoxin A light-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	407	3308	2133	548	619	8	0	1	0
1	B	407	3338	2149	553	628	8	0	5	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	cloning artifact	UNP Q7B8V4
A	-18	GLY	-	cloning artifact	UNP Q7B8V4
A	-17	SER	-	cloning artifact	UNP Q7B8V4
A	-16	SER	-	cloning artifact	UNP Q7B8V4
A	-15	HIS	-	cloning artifact	UNP Q7B8V4
A	-14	HIS	-	cloning artifact	UNP Q7B8V4
A	-13	HIS	-	cloning artifact	UNP Q7B8V4
A	-12	HIS	-	cloning artifact	UNP Q7B8V4
A	-11	HIS	-	cloning artifact	UNP Q7B8V4
A	-10	HIS	-	cloning artifact	UNP Q7B8V4
A	-9	SER	-	cloning artifact	UNP Q7B8V4
A	-8	SER	-	cloning artifact	UNP Q7B8V4
A	-7	GLY	-	cloning artifact	UNP Q7B8V4
A	-6	LEU	-	cloning artifact	UNP Q7B8V4
A	-5	VAL	-	cloning artifact	UNP Q7B8V4
A	-4	PRO	-	cloning artifact	UNP Q7B8V4
A	-3	ARG	-	cloning artifact	UNP Q7B8V4
A	-2	GLY	-	cloning artifact	UNP Q7B8V4
A	-1	SER	-	cloning artifact	UNP Q7B8V4
A	0	HIS	-	cloning artifact	UNP Q7B8V4
A	2	GLN	PRO	conflict	UNP Q7B8V4
B	-19	MET	-	cloning artifact	UNP Q7B8V4
B	-18	GLY	-	cloning artifact	UNP Q7B8V4
B	-17	SER	-	cloning artifact	UNP Q7B8V4
B	-16	SER	-	cloning artifact	UNP Q7B8V4

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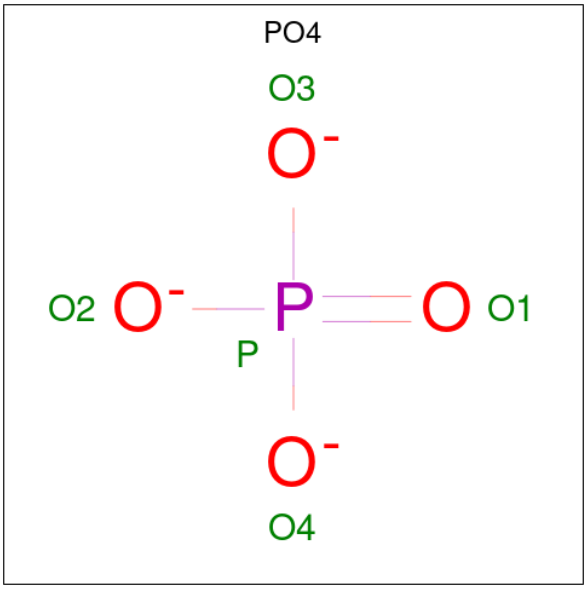
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	cloning artifact	UNP Q7B8V4
B	-14	HIS	-	cloning artifact	UNP Q7B8V4
B	-13	HIS	-	cloning artifact	UNP Q7B8V4
B	-12	HIS	-	cloning artifact	UNP Q7B8V4
B	-11	HIS	-	cloning artifact	UNP Q7B8V4
B	-10	HIS	-	cloning artifact	UNP Q7B8V4
B	-9	SER	-	cloning artifact	UNP Q7B8V4
B	-8	SER	-	cloning artifact	UNP Q7B8V4
B	-7	GLY	-	cloning artifact	UNP Q7B8V4
B	-6	LEU	-	cloning artifact	UNP Q7B8V4
B	-5	VAL	-	cloning artifact	UNP Q7B8V4
B	-4	PRO	-	cloning artifact	UNP Q7B8V4
B	-3	ARG	-	cloning artifact	UNP Q7B8V4
B	-2	GLY	-	cloning artifact	UNP Q7B8V4
B	-1	SER	-	cloning artifact	UNP Q7B8V4
B	0	HIS	-	cloning artifact	UNP Q7B8V4
B	2	GLN	PRO	conflict	UNP Q7B8V4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

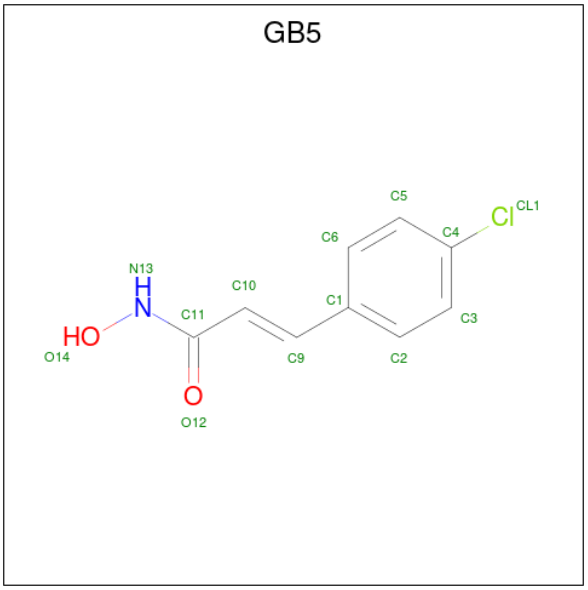
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0
			Total	Zn		
2	B	1	1	1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	A	1	5	4	1	0	0

- Molecule 4 is (2E)-3-(4-CHLOROPHENYL)-N-HYDROXYACRYLAMIDE (three-letter code: GB5) (formula: $C_9H_8ClNO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
4	A	1	13	9	1	1	2	0	0
			Total	C	Cl	N	O		
4	B	1	13	9	1	1	2	0	0

- Molecule 5 is water.

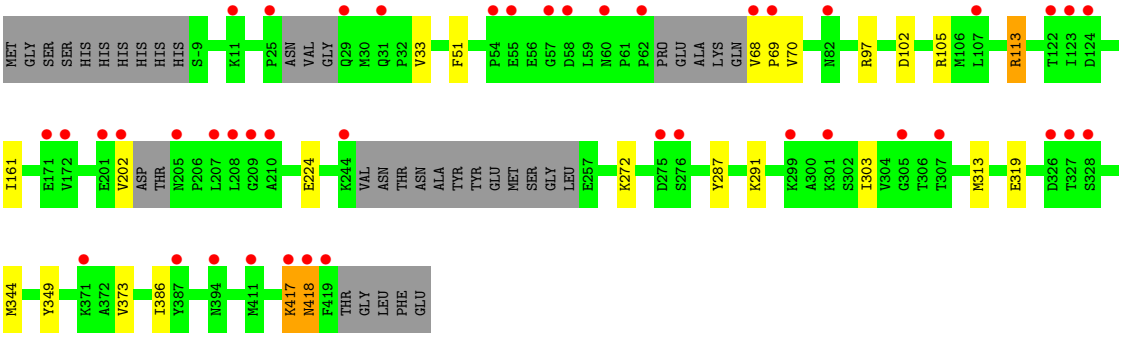
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	313	313	313	0	0
			Total	O		
5	B	302	302	302	0	0

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.

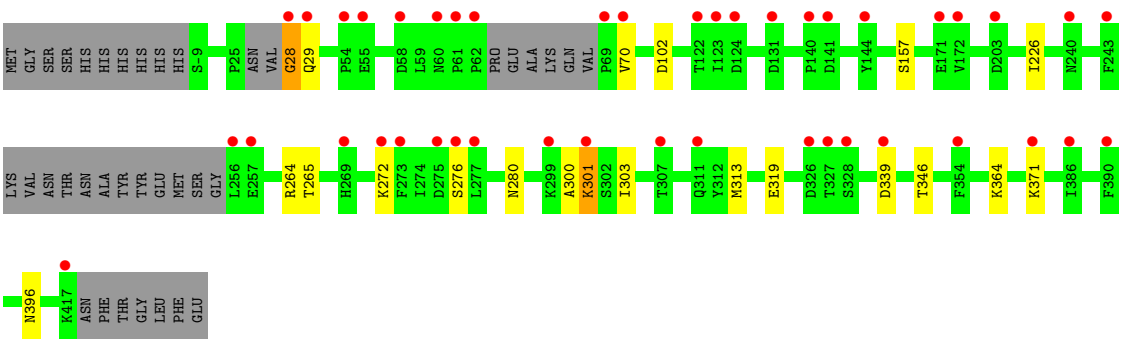
- Molecule 1: Botulinum neurotoxin A light-chain

Chain A:



- Molecule 1: Botulinum neurotoxin A light-chain

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.66Å 67.69Å 98.40Å 90.00° 106.53° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 16.21 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-1.90) 98.0 (16.21-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.173 , 0.216 0.215 , 0.248	Depositor DCC
R_{free} test set	3626 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 56.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7294	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 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ZN, GB5

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	0.54	0/3383	0.67	2/4569 (0.0%)
1	B	0.53	0/3415	0.62	0/4615
All	All	0.54	0/6798	0.64	2/9184 (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	A	0	1
1	B	0	1
All	All	0	2

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	A	113	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	A	113	ARG	NE-CZ-NH1	8.40	124.50	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	417	LYS	Peptide
1	B	28	GLY	Peptide

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	3308	0	3264	19	0
1	B	3338	0	3284	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
4	A	13	0	7	1	0
4	B	13	0	7	0	0
5	A	313	0	0	1	0
5	B	302	0	0	8	0
All	All	7294	0	6562	32	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 2.

All (32) 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:339:ASP:HB3	5:B:758:HOH:O	1.90	0.70
1:B:102:ASP:OD1	5:B:821:HOH:O	2.10	0.69
1:A:272:LYS:NZ	5:A:639:HOH:O	2.26	0.67
1:B:319:GLU:OE2	5:B:784:HOH:O	2.11	0.67
1:A:102:ASP:OD1	1:A:105:ARG:NH2	2.29	0.66
1:A:417:LYS:HA	1:A:418:ASN:CB	2.27	0.65
1:B:28:GLY:N	1:B:29:GLN:HA	2.19	0.57
1:A:70:VAL:HG22	1:A:161:ILE:HD11	1.87	0.56
1:A:344:MET:HG3	1:A:349:TYR:CZ	2.42	0.53
1:A:417:LYS:HA	1:A:418:ASN:HB2	1.89	0.53
1:A:68:VAL:N	1:A:69:PRO:CD	2.72	0.52
1:A:113:ARG:HD2	5:B:809:HOH:O	2.11	0.51
1:B:70:VAL:HG22	1:B:371:LYS:HG2	1.93	0.50
1:A:303:ILE:HD11	1:A:313:MET:HG3	1.92	0.49
1:B:396:ASN:HB3	5:B:847:HOH:O	2.13	0.48
1:A:417:LYS:HA	1:A:418:ASN:HB3	1.97	0.46
1:B:70:VAL:HG22	1:B:371:LYS:CG	2.45	0.46
1:B:364:LYS:N	1:B:364:LYS:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLU:HG2	5:B:809:HOH:O	2.17	0.45
1:B:300:ALA:O	1:B:301:LYS:HE3	2.16	0.45
1:B:272:LYS:NZ	5:B:884:HOH:O	2.49	0.45
1:B:226:ILE:CG2	1:B:265:THR:HG23	2.47	0.44
1:A:161:ILE:HD13	1:A:373:VAL:CG2	2.47	0.44
1:A:287:TYR:CE2	1:A:291:LYS:HD2	2.51	0.44
1:A:33:VAL:HG11	1:A:51:PHE:CZ	2.52	0.44
1:A:417:LYS:CA	1:A:418:ASN:CB	2.95	0.43
1:A:319:GLU:CG	5:B:809:HOH:O	2.67	0.42
1:B:303:ILE:HD11	1:B:313:MET:HG3	2.01	0.42
1:B:264[B]:ARG:HD2	1:B:346:THR:HB	2.02	0.42
1:A:161:ILE:HD13	1:A:373:VAL:HG21	2.02	0.41
1:A:224:GLU:OE1	4:A:600:GB5:N13	2.54	0.40
1:A:97:ARG:HA	1:A:386:ILE:HG23	2.03	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	398/444 (90%)	390 (98%)	7 (2%)	1 (0%)	41	31
1	B	404/444 (91%)	397 (98%)	6 (2%)	1 (0%)	47	38
All	All	802/888 (90%)	787 (98%)	13 (2%)	2 (0%)	41	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	418	ASN
1	B	157	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	366/397 (92%)	365 (100%)	1 (0%)	92	93
1	B	370/397 (93%)	367 (99%)	3 (1%)	81	82
All	All	736/794 (93%)	732 (100%)	4 (0%)	88	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	VAL
1	B	276	SER
1	B	280	ASN
1	B	301	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	288	ASN
1	B	29	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	PO4	A	501	-	4,4,4	0.96	0	6,6,6	0.58	0
4	GB5	B	600	2	13,13,13	3.02	1 (7%)	16,16,16	1.46	4 (25%)
4	GB5	A	600	2	13,13,13	2.99	1 (7%)	16,16,16	1.22	1 (6%)

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
4	GB5	B	600	2	-	0/7/7/7	0/1/1/1
4	GB5	A	600	2	-	0/7/7/7	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	GB5	C4-CL1	-10.49	1.51	1.74
4	B	600	GB5	C4-CL1	-10.41	1.51	1.74

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	600	GB5	C10-C11-N13	2.95	120.26	114.38
4	B	600	GB5	C5-C4-C3	-2.64	117.82	121.24
4	A	600	GB5	C10-C11-N13	2.40	119.15	114.38
4	B	600	GB5	C2-C3-C4	2.13	121.49	119.24
4	B	600	GB5	O12-C11-N13	-2.03	119.14	122.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	GB5	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 (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	407/444 (91%)	0.74	43 (10%)	6	7	22, 32, 44, 56	0
1	B	407/444 (91%)	0.71	43 (10%)	6	7	19, 32, 46, 53	0
All	All	814/888 (91%)	0.73	86 (10%)	6	7	19, 32, 47, 56	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	ASN	8.4
1	B	256	LEU	8.2
1	A	68	VAL	8.0
1	A	202	VAL	7.8
1	B	62	PRO	7.3
1	B	28	GLY	7.2
1	B	277	LEU	6.6
1	A	208	LEU	6.1
1	A	29	GLN	5.8
1	B	54	PRO	5.6
1	B	124	ASP	5.6
1	B	144	TYR	5.5
1	B	69	PRO	5.4
1	A	62	PRO	5.2
1	B	273	PHE	5.1
1	B	327	THR	5.0
1	A	124	ASP	4.9
1	A	305	GLY	4.5
1	A	419	PHE	4.4
1	B	417	LYS	4.3
1	A	417	LYS	4.3
1	A	172	VAL	4.2
1	A	327	THR	4.1
1	B	29	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	69	PRO	4.1
1	B	55	GLU	4.0
1	B	307	THR	3.8
1	B	301	LYS	3.8
1	A	205	ASN	3.8
1	A	201	GLU	3.8
1	A	55	GLU	3.8
1	A	301	LYS	3.6
1	A	209	GLY	3.5
1	B	203	ASP	3.5
1	B	123	ILE	3.4
1	B	60	ASN	3.4
1	A	31	GLN	3.4
1	B	276	SER	3.4
1	A	411	MET	3.4
1	A	387	TYR	3.4
1	B	328	SER	3.3
1	A	60	ASN	3.3
1	A	371	LYS	3.2
1	B	269[A]	HIS	3.2
1	A	54	PRO	3.2
1	B	299	LYS	3.1
1	A	307	THR	3.1
1	A	122	THR	3.1
1	B	243	PHE	3.1
1	B	140	PRO	3.0
1	B	371	LYS	3.0
1	B	354	PHE	2.9
1	A	299	LYS	2.9
1	A	171	GLU	2.9
1	A	25	PRO	2.9
1	A	276	SER	2.9
1	A	328	SER	2.9
1	B	61	PRO	2.9
1	B	172	VAL	2.8
1	B	122	THR	2.8
1	B	257	GLU	2.8
1	A	207	LEU	2.7
1	A	244	LYS	2.7
1	A	57	GLY	2.7
1	A	11	LYS	2.7
1	B	171	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	131	ASP	2.6
1	A	58	ASP	2.6
1	A	107	LEU	2.6
1	B	390	PHE	2.6
1	A	123	ILE	2.6
1	B	275	ASP	2.6
1	A	275	ASP	2.4
1	B	141	ASP	2.4
1	B	386	ILE	2.4
1	B	311	GLN	2.3
1	B	339	ASP	2.3
1	B	70	VAL	2.3
1	A	326	ASP	2.3
1	A	210	ALA	2.2
1	B	272	LYS	2.1
1	B	58	ASP	2.1
1	B	240	ASN	2.1
1	B	326	ASP	2.1
1	A	82	ASN	2.0
1	A	394	ASN	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 monosaccharides 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
4	GB5	A	600	13/13	0.73	0.28	41,46,47,47	0
3	PO4	A	501	5/5	0.78	0.21	35,35,36,37	5
4	GB5	B	600	13/13	0.87	0.18	39,43,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	500	1/1	0.99	0.05	33,33,33,33	0
2	ZN	A	500	1/1	1.00	0.09	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.