



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:32 PM GMT

PDB ID : 1XOM
Title : Catalytic Domain Of Human Phosphodiesterase 4D In Complex With Cilomilast
Authors : Card, G.L.; England, B.P.; Suzuki, Y.; Fong, D.; Powell, B.; Lee, B.; Luu, C.; Tabrizizad, M.; Gillette, S.; Ibrahim, P.N.; Artis, D.R.; Bollag, G.; Milburn, M.V.; Kim, S.-H.; Schlessinger, J.; Zhang, K.Y.J.
Deposited on : 2004-10-06
Resolution : 1.55 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

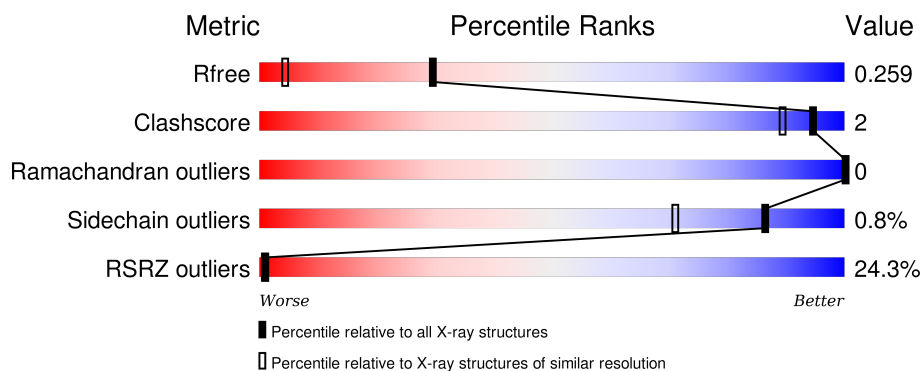
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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}	91344	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

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. 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	349	<div> <div>15%</div> <div>88%</div> <div>5%</div> <div>7%</div> </div>
1	B	349	<div> <div>30%</div> <div>88%</div> <div>•</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	A	1001	-	-	-	X
3	MG	A	1002	-	-	-	X
4	CIO	A	603[A]	-	-	-	X
4	CIO	A	603[B]	-	-	-	X
5	EDO	A	704	-	-	-	X
5	EDO	A	707	-	-	-	X
5	EDO	A	716	-	-	X	-
5	EDO	B	705	-	-	-	X
5	EDO	B	710	-	-	-	X
5	EDO	B	711	-	-	-	X
5	EDO	B	713	-	-	X	X
5	EDO	B	714	-	-	-	X
5	EDO	B	717	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6068 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	4	6	0
			2655	1678	450	511	16			
1	B	321	Total	C	N	O	S	0	9	0
			2633	1668	446	503	16			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	MET	-	INITIATING METHIONINE	UNP Q08499
A	66	GLY	-	CLONING ARTIFACT	UNP Q08499
A	67	SER	-	CLONING ARTIFACT	UNP Q08499
A	68	SER	-	CLONING ARTIFACT	UNP Q08499
A	69	HIS	-	EXPRESSION TAG	UNP Q08499
A	70	HIS	-	EXPRESSION TAG	UNP Q08499
A	71	HIS	-	EXPRESSION TAG	UNP Q08499
A	72	HIS	-	EXPRESSION TAG	UNP Q08499
A	73	HIS	-	EXPRESSION TAG	UNP Q08499
A	74	HIS	-	EXPRESSION TAG	UNP Q08499
A	75	SER	-	CLONING ARTIFACT	UNP Q08499
A	76	SER	-	CLONING ARTIFACT	UNP Q08499
A	77	GLY	-	CLONING ARTIFACT	UNP Q08499
A	78	LEU	-	CLONING ARTIFACT	UNP Q08499
A	79	VAL	-	CLONING ARTIFACT	UNP Q08499
A	80	PRO	-	CLONING ARTIFACT	UNP Q08499
A	81	ARG	-	CLONING ARTIFACT	UNP Q08499
A	82	GLY	-	CLONING ARTIFACT	UNP Q08499
A	83	SER	-	CLONING ARTIFACT	UNP Q08499
A	84	HIS	-	CLONING ARTIFACT	UNP Q08499
A	85	MET	-	CLONING ARTIFACT	UNP Q08499
B	65	MET	-	INITIATING METHIONINE	UNP Q08499
B	66	GLY	-	CLONING ARTIFACT	UNP Q08499
B	67	SER	-	CLONING ARTIFACT	UNP Q08499
B	68	SER	-	CLONING ARTIFACT	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
B	69	HIS	-	EXPRESSION TAG	UNP Q08499
B	70	HIS	-	EXPRESSION TAG	UNP Q08499
B	71	HIS	-	EXPRESSION TAG	UNP Q08499
B	72	HIS	-	EXPRESSION TAG	UNP Q08499
B	73	HIS	-	EXPRESSION TAG	UNP Q08499
B	74	HIS	-	EXPRESSION TAG	UNP Q08499
B	75	SER	-	CLONING ARTIFACT	UNP Q08499
B	76	SER	-	CLONING ARTIFACT	UNP Q08499
B	77	GLY	-	CLONING ARTIFACT	UNP Q08499
B	78	LEU	-	CLONING ARTIFACT	UNP Q08499
B	79	VAL	-	CLONING ARTIFACT	UNP Q08499
B	80	PRO	-	CLONING ARTIFACT	UNP Q08499
B	81	ARG	-	CLONING ARTIFACT	UNP Q08499
B	82	GLY	-	CLONING ARTIFACT	UNP Q08499
B	83	SER	-	CLONING ARTIFACT	UNP Q08499
B	84	HIS	-	CLONING ARTIFACT	UNP Q08499
B	85	MET	-	CLONING ARTIFACT	UNP Q08499

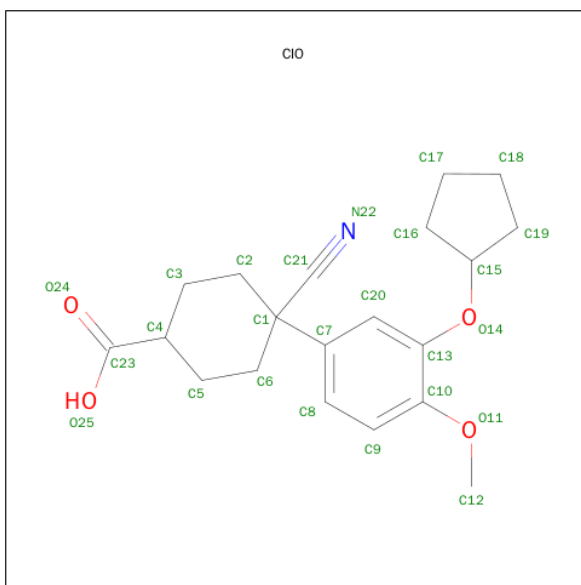
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 4 is CILOMILAST (three-letter code: CIO) (formula: C₂₀H₂₅NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	1
			50	40	2	8		
4	A	1	Total	C	N	O	0	1
			50	40	2	8		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	299	Total 299	O 299	0	0

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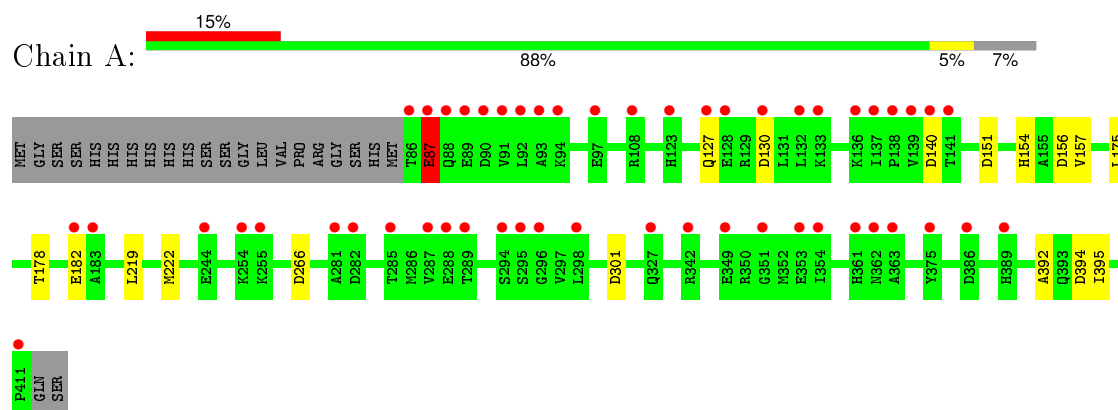
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	297	Total	O	0	0
			297	297		

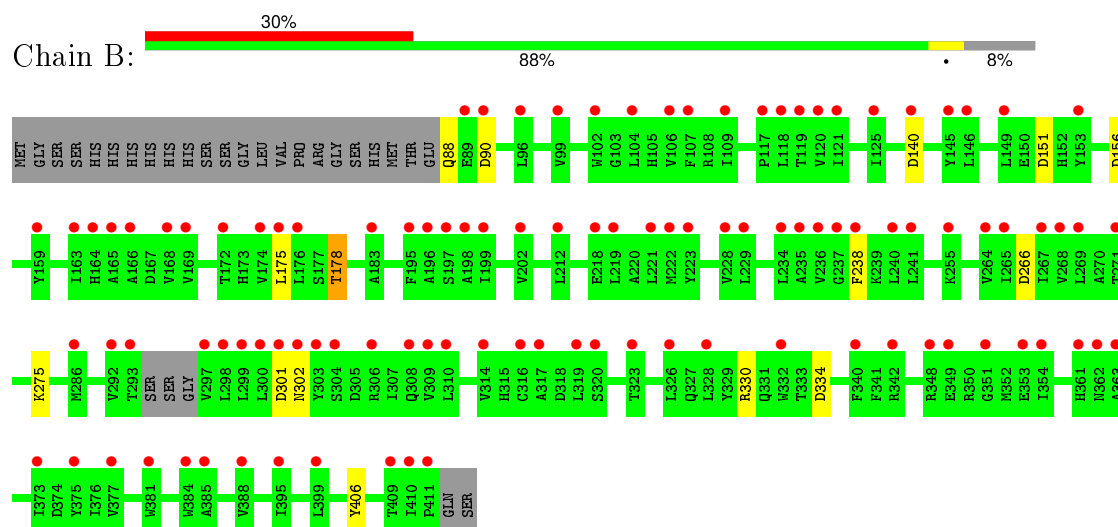
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.49 Å 78.97 Å 164.19 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.65 – 1.55 44.98 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.1 (81.65-1.55) 99.1 (44.98-1.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 1.55 Å)	Xtriage
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.183 , 0.205 0.238 , 0.259	Depositor DCC
R_{free} test set	5683 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 113639 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6068	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, CIO, MG, EDO

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	0.34	1/2735 (0.0%)	0.72	8/3716 (0.2%)
1	B	0.32	0/2728	0.71	6/3704 (0.2%)
All	All	0.33	1/5463 (0.0%)	0.71	14/7420 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	GLU	CB-CG	-9.32	1.34	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	GLU	CA-CB-CG	8.07	131.16	113.40
1	B	151	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	151	ASP	CB-CG-OD2	6.35	124.01	118.30
1	B	266	ASP	CB-CG-OD2	6.34	124.00	118.30
1	A	156	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	301	ASP	CB-CG-OD2	5.94	123.65	118.30
1	B	90	ASP	CB-CG-OD2	5.92	123.62	118.30
1	B	140	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	156	ASP	CB-CG-OD2	5.43	123.18	118.30
1	A	266	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	301	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	130	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	140	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	394	ASP	CB-CG-OD2	5.06	122.85	118.30

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	2655	0	2606	9	2
1	B	2633	0	2589	8	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	50	0	48	0	0
4	B	50	0	48	0	0
5	A	36	0	54	6	0
5	B	44	0	66	7	0
6	A	299	0	0	0	2
6	B	297	0	0	2	0
All	All	6068	0	5411	19	2

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 (19) 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:406:TYR:OH	5:B:713:EDO:H22	1.77	0.84
1:A:395:ILE:HD12	5:A:716:EDO:H22	1.68	0.74
1:A:178[B]:THR:HG23	5:A:716:EDO:H11	1.78	0.64
1:B:88:GLN:N	6:B:2066:HOH:O	2.38	0.56
1:A:219:LEU:HD23	1:A:222[B]:MET:CE	2.39	0.53
1:A:392:ALA:CA	5:A:716:EDO:H12	2.43	0.49
1:A:175:LEU:O	1:A:178[A]:THR:HG23	2.13	0.47
1:B:330:ARG:HB3	5:B:713:EDO:H11	1.98	0.45
1:B:175:LEU:O	1:B:178[B]:THR:HG23	2.17	0.45
5:B:701:EDO:H22	5:B:713:EDO:H21	1.99	0.45
1:B:334:ASP:OD1	5:B:713:EDO:H12	2.17	0.45
1:A:392:ALA:HB2	5:A:716:EDO:H12	1.98	0.44
1:A:154:HIS:O	1:A:157:VAL:HG22	2.16	0.44
1:B:238:PHE:CD1	5:B:717:EDO:H22	2.53	0.44
1:A:178[B]:THR:CG2	5:A:716:EDO:H11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275[A]:LYS:NZ	6:B:2268:HOH:O	2.29	0.40
1:B:330:ARG:CB	5:B:713:EDO:H11	2.50	0.40
1:A:395:ILE:CD1	5:A:716:EDO:H22	2.46	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLU:OE1	6:A:1133:HOH:O[4_455]	1.24	0.96
1:A:87:GLU:CD	6:A:1133:HOH:O[4_455]	1.99	0.21

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	330/349 (95%)	326 (99%)	4 (1%)	0	100	100
1	B	326/349 (93%)	322 (99%)	4 (1%)	0	100	100
All	All	656/698 (94%)	648 (99%)	8 (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	304/318 (96%)	301 (99%)	3 (1%)	82	62
1	B	303/318 (95%)	300 (99%)	3 (1%)	82	62
All	All	607/636 (95%)	601 (99%)	6 (1%)	86	62

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

Mol	Chain	Res	Type
1	A	87	GLU
1	A	127	GLN
1	A	182	GLU
1	B	178[A]	THR
1	B	178[B]	THR
1	B	302	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	245	ASN
1	A	308	GLN
1	B	88	GLN
1	B	123	HIS
1	B	242	GLN
1	B	245	ASN
1	B	308	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	$\# Z > 2$
4	CIO	A	603[A]	-	22,27,27	0.54	0	26,38,38	0.98	2 (7%)
4	CIO	A	603[B]	-	22,27,27	0.47	0	26,38,38	0.99	2 (7%)
5	EDO	A	702	-	3,3,3	0.26	0	2,2,2	0.50	0
5	EDO	A	703	-	3,3,3	0.29	0	2,2,2	0.48	0
5	EDO	A	704	-	3,3,3	0.29	0	2,2,2	0.37	0
5	EDO	A	707	-	3,3,3	0.29	0	2,2,2	0.62	0
5	EDO	A	712	-	3,3,3	0.29	0	2,2,2	0.40	0
5	EDO	A	715	-	3,3,3	0.26	0	2,2,2	0.48	0
5	EDO	A	716	-	3,3,3	0.29	0	2,2,2	0.24	0
5	EDO	A	719	-	3,3,3	0.27	0	2,2,2	0.53	0
5	EDO	A	720	-	3,3,3	0.28	0	2,2,2	0.50	0
4	CIO	B	601[A]	-	22,27,27	0.59	0	26,38,38	1.12	3 (11%)
4	CIO	B	601[B]	-	22,27,27	0.46	0	26,38,38	0.94	3 (11%)
5	EDO	B	701	-	3,3,3	0.26	0	2,2,2	0.45	0
5	EDO	B	705	-	3,3,3	0.30	0	2,2,2	0.41	0
5	EDO	B	706	-	3,3,3	0.30	0	2,2,2	0.45	0
5	EDO	B	709	-	3,3,3	0.28	0	2,2,2	0.39	0
5	EDO	B	710	-	3,3,3	0.29	0	2,2,2	0.41	0
5	EDO	B	711	-	3,3,3	0.29	0	2,2,2	0.43	0
5	EDO	B	713	-	3,3,3	0.30	0	2,2,2	0.58	0
5	EDO	B	714	-	3,3,3	0.30	0	2,2,2	0.37	0
5	EDO	B	717	-	3,3,3	0.28	0	2,2,2	0.47	0
5	EDO	B	718	-	3,3,3	0.29	0	2,2,2	0.44	0
5	EDO	B	721	-	3,3,3	0.30	0	2,2,2	0.41	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
4	CIO	A	603[A]	-	-	0/12/38/38	0/3/3/3
4	CIO	A	603[B]	-	-	0/12/38/38	0/3/3/3
5	EDO	A	702	-	-	0/1/1/1	0/0/0/0
5	EDO	A	703	-	-	0/1/1/1	0/0/0/0
5	EDO	A	704	-	-	0/1/1/1	0/0/0/0
5	EDO	A	707	-	-	0/1/1/1	0/0/0/0
5	EDO	A	712	-	-	0/1/1/1	0/0/0/0
5	EDO	A	715	-	-	0/1/1/1	0/0/0/0
5	EDO	A	716	-	-	0/1/1/1	0/0/0/0
5	EDO	A	719	-	-	0/1/1/1	0/0/0/0
5	EDO	A	720	-	-	0/1/1/1	0/0/0/0
4	CIO	B	601[A]	-	-	0/12/38/38	0/3/3/3
4	CIO	B	601[B]	-	-	0/12/38/38	0/3/3/3
5	EDO	B	701	-	-	0/1/1/1	0/0/0/0
5	EDO	B	705	-	-	0/1/1/1	0/0/0/0
5	EDO	B	706	-	-	0/1/1/1	0/0/0/0
5	EDO	B	709	-	-	0/1/1/1	0/0/0/0
5	EDO	B	710	-	-	0/1/1/1	0/0/0/0
5	EDO	B	711	-	-	0/1/1/1	0/0/0/0
5	EDO	B	713	-	-	0/1/1/1	0/0/0/0
5	EDO	B	714	-	-	0/1/1/1	0/0/0/0
5	EDO	B	717	-	-	0/1/1/1	0/0/0/0
5	EDO	B	718	-	-	0/1/1/1	0/0/0/0
5	EDO	B	721	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601[B]	CIO	O11-C10-C9	-2.01	120.97	124.35
4	B	601[B]	CIO	C12-O11-C10	2.01	120.60	117.54
4	A	603[B]	CIO	O11-C10-C13	2.33	118.72	115.40
4	A	603[A]	CIO	C8-C7-C1	2.37	124.58	120.80
4	B	601[A]	CIO	C8-C7-C1	2.49	124.78	120.80
4	B	601[A]	CIO	C2-C3-C4	2.62	114.08	111.48
4	B	601[B]	CIO	O11-C10-C13	2.86	119.48	115.40
4	B	601[A]	CIO	C12-O11-C10	2.94	122.00	117.54
4	A	603[B]	CIO	C12-O11-C10	3.03	122.13	117.54
4	A	603[A]	CIO	C12-O11-C10	3.15	122.32	117.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	716	EDO	6	0
5	B	701	EDO	1	0
5	B	709	EDO	1	0
5	B	713	EDO	5	0
5	B	717	EDO	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	326/349 (93%)	0.77	51 (15%) 3 2	3, 9, 20, 33	1 (0%)
1	B	321/349 (91%)	1.68	106 (33%) 0 0	10, 17, 32, 41	0
All	All	647/698 (92%)	1.22	157 (24%) 1 1	3, 13, 28, 41	1 (0%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	293	THR	7.5
1	B	301	ASP	6.6
1	B	299	LEU	6.3
1	A	86	THR	6.1
1	A	289	THR	5.6
1	B	292	VAL	5.3
1	A	139	VAL	5.2
1	B	362	ASN	5.1
1	A	133	LYS	4.8
1	A	375	TYR	4.7
1	B	300	LEU	4.4
1	A	127	GLN	4.3
1	A	130	ASP	4.2
1	B	118	LEU	4.2
1	B	168	VAL	4.1
1	B	199	ILE	4.1
1	A	363	ALA	4.1
1	B	349	GLU	3.9
1	B	236	VAL	3.9
1	B	297	VAL	3.9
1	A	92	LEU	3.9
1	B	314	VAL	3.8
1	B	102	TRP	3.8
1	B	303	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	361	HIS	3.8
1	B	202	VAL	3.8
1	A	90	ASP	3.7
1	B	234	LEU	3.7
1	A	288	GLU	3.7
1	B	268	VAL	3.6
1	A	94	LYS	3.6
1	B	328	LEU	3.5
1	A	93	ALA	3.5
1	B	264	VAL	3.5
1	B	163	ILE	3.5
1	B	149	LEU	3.4
1	B	316	CYS	3.4
1	B	175	LEU	3.3
1	A	183	ALA	3.3
1	A	349	GLU	3.3
1	A	88	GLN	3.3
1	A	295	SER	3.2
1	B	195	PHE	3.2
1	B	165	ALA	3.2
1	A	132	LEU	3.2
1	B	269	LEU	3.2
1	B	121	ILE	3.1
1	B	241	LEU	3.1
1	A	294	SER	3.1
1	A	140	ASP	3.1
1	B	265	ILE	3.1
1	B	410	ILE	3.1
1	B	106	VAL	3.1
1	A	123	HIS	3.1
1	B	96	LEU	3.0
1	B	183	ALA	3.0
1	B	317	ALA	3.0
1	A	97	GLU	3.0
1	B	411	PRO	3.0
1	B	109	ILE	3.0
1	B	146	LEU	3.0
1	B	169	VAL	3.0
1	B	363	ALA	3.0
1	B	153	TYR	3.0
1	B	377	VAL	2.9
1	A	244	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	285	THR	2.9
1	B	271	THR	2.9
1	A	362	ASN	2.9
1	A	298	LEU	2.9
1	A	136	LYS	2.8
1	B	240	LEU	2.8
1	B	166	ALA	2.8
1	A	353	GLU	2.8
1	A	389	HIS	2.8
1	A	137	ILE	2.8
1	B	267	ILE	2.8
1	B	319	LEU	2.8
1	B	399	LEU	2.8
1	B	395	ILE	2.8
1	B	99	VAL	2.7
1	B	237	GLY	2.7
1	B	198	ALA	2.7
1	B	140	ASP	2.7
1	A	351	GLY	2.7
1	A	354	ILE	2.6
1	A	89	GLU	2.6
1	B	221	LEU	2.6
1	B	172	THR	2.6
1	A	282	ASP	2.6
1	B	302	ASN	2.6
1	B	229	LEU	2.6
1	A	254	LYS	2.6
1	B	107	PHE	2.5
1	B	104	LEU	2.5
1	A	342	ARG	2.5
1	B	306	ARG	2.5
1	B	304	SER	2.5
1	B	223	TYR	2.5
1	B	235	ALA	2.5
1	B	381	TRP	2.5
1	B	174	VAL	2.5
1	B	90	ASP	2.5
1	B	298	LEU	2.5
1	B	409	THR	2.4
1	A	411	PRO	2.4
1	B	354	ILE	2.4
1	A	281	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	238	PHE	2.4
1	B	255	LYS	2.4
1	A	287	VAL	2.4
1	B	197	SER	2.4
1	A	128	GLU	2.4
1	B	196	ALA	2.4
1	B	342	ARG	2.4
1	B	332	TRP	2.3
1	A	91	VAL	2.3
1	B	326	LEU	2.3
1	B	340	PHE	2.3
1	B	218	GLU	2.3
1	B	375	TYR	2.3
1	B	212	LEU	2.3
1	B	320	SER	2.3
1	B	353	GLU	2.3
1	B	89	GLU	2.2
1	A	255	LYS	2.2
1	B	351	GLY	2.2
1	B	219	LEU	2.2
1	B	308	GLN	2.2
1	B	385	ALA	2.2
1	B	119	THR	2.2
1	B	323	THR	2.2
1	B	373	ILE	2.2
1	B	384	TRP	2.2
1	A	386[A]	ASP	2.2
1	A	138	PRO	2.2
1	A	327	GLN	2.2
1	B	117	PRO	2.2
1	A	87	GLU	2.1
1	B	120	VAL	2.1
1	B	348	ARG	2.1
1	B	176	LEU	2.1
1	A	296	GLY	2.1
1	B	228	VAL	2.1
1	B	388	VAL	2.1
1	B	310	LEU	2.1
1	A	141	THR	2.1
1	A	108	ARG	2.1
1	B	145	TYR	2.1
1	B	159	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	286	MET	2.1
1	A	182	GLU	2.0
1	B	125	ILE	2.0
1	A	361	HIS	2.0
1	B	309	VAL	2.0
1	B	164	HIS	2.0
1	B	222[A]	MET	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	MG	A	1002	1/1	0.99	0.25	23.96	8,8,8,8	0
5	EDO	A	704	4/4	0.79	0.20	18.98	36,36,36,36	0
5	EDO	B	717	4/4	0.83	0.28	5.53	42,42,43,43	0
2	ZN	A	1001	1/1	1.00	0.12	5.02	13,13,13,13	0
4	CIO	A	603[A]	25/25	0.89	0.18	4.82	16,20,25,26	25
4	CIO	A	603[B]	25/25	0.89	0.18	4.82	18,19,21,21	25
5	EDO	B	713	4/4	0.91	0.19	3.97	26,27,28,28	0
5	EDO	A	707	4/4	0.92	0.18	3.93	31,31,31,31	0
5	EDO	B	710	4/4	0.50	0.32	3.67	47,47,48,48	0
5	EDO	B	705	4/4	0.66	0.25	3.09	29,31,32,33	0
5	EDO	B	711	4/4	0.68	0.17	3.06	33,34,34,35	0
5	EDO	B	714	4/4	0.60	0.21	2.28	29,31,31,32	0
5	EDO	A	715	4/4	0.79	0.20	2.00	34,35,35,36	0
5	EDO	B	706	4/4	0.60	0.18	1.84	33,33,33,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	EDO	A	720	4/4	0.84	0.15	1.74	36,36,36,37	0
4	CIO	B	601[A]	25/25	0.88	0.19	1.73	13,19,23,26	25
4	CIO	B	601[B]	25/25	0.88	0.19	1.70	17,18,21,21	25
5	EDO	A	716	4/4	0.83	0.18	1.70	33,35,36,38	0
5	EDO	A	719	4/4	0.81	0.17	1.19	32,34,34,35	0
3	MG	B	2002	1/1	1.00	0.19	0.91	7,7,7,7	0
5	EDO	B	709	4/4	0.73	0.17	0.18	42,43,43,43	0
5	EDO	A	702	4/4	0.84	0.13	0.12	26,27,27,27	0
5	EDO	B	721	4/4	0.78	0.18	0.12	41,41,42,42	0
5	EDO	A	712	4/4	0.77	0.16	-0.17	39,40,40,40	0
5	EDO	B	701	4/4	0.88	0.13	-0.48	26,28,30,32	0
2	ZN	B	2001	1/1	1.00	0.13	-1.78	12,12,12,12	0
5	EDO	B	718	4/4	0.90	0.21	-	38,39,39,39	0
5	EDO	A	703	4/4	0.66	0.17	-	39,39,39,39	0

6.5 Other polymers

There are no such residues in this entry.