



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:56 PM UTC

PDB ID : 4I04 / pdb_00004i04
Title : Structure of zymogen of cathepsin B1 from *Schistosoma mansoni*
Authors : Rezacova, P.; Jilkova, A.; Brynda, J.; Horn, M.; Mares, M.
Deposited on : 2012-11-16
Resolution : 1.95 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:

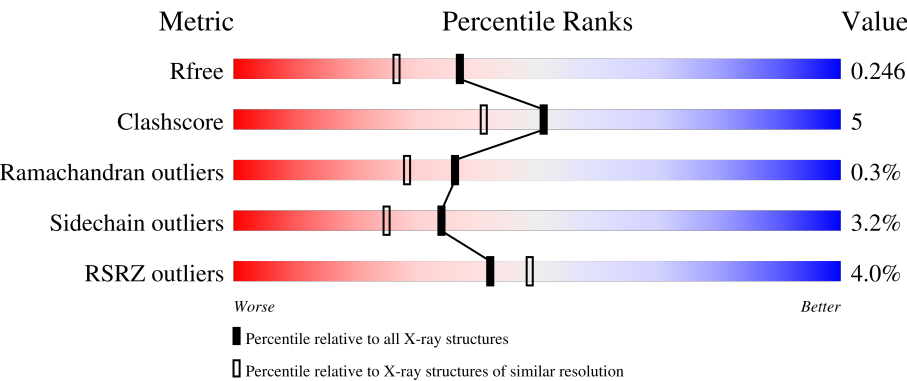
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	323	10% 80% 11% 6%
1	B	323	2% 88% 7%
1	C	323	% 85% 9% 5%
1	D	323	3% 83% 12% 5%

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	EDO	D	401	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10371 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 Cathepsin B-like peptidase (C01 family).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	1	0
			2428	1515	437	461	15			
1	B	310	Total	C	N	O	S	0	2	0
			2482	1547	446	473	16			
1	C	306	Total	C	N	O	S	0	3	0
			2455	1531	441	468	15			
1	D	308	Total	C	N	O	S	0	1	0
			2463	1535	443	470	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	SER	CYS	engineered mutation	UNP Q8MNY2
A	168	ALA	THR	engineered mutation	UNP Q8MNY2
A	283	ALA	THR	engineered mutation	UNP Q8MNY2
B	100	SER	CYS	engineered mutation	UNP Q8MNY2
B	168	ALA	THR	engineered mutation	UNP Q8MNY2
B	283	ALA	THR	engineered mutation	UNP Q8MNY2
C	100	SER	CYS	engineered mutation	UNP Q8MNY2
C	168	ALA	THR	engineered mutation	UNP Q8MNY2
C	283	ALA	THR	engineered mutation	UNP Q8MNY2
D	100	SER	CYS	engineered mutation	UNP Q8MNY2
D	168	ALA	THR	engineered mutation	UNP Q8MNY2
D	283	ALA	THR	engineered mutation	UNP Q8MNY2

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

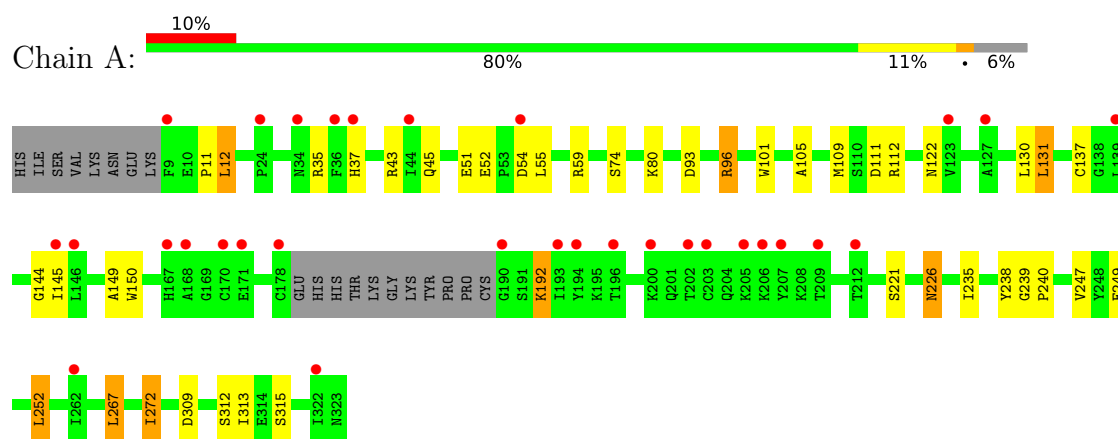
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	84	Total O 84 84	0	0
3	B	137	Total O 137 137	0	0
3	C	172	Total O 172 172	0	0
3	D	126	Total O 126 126	0	0

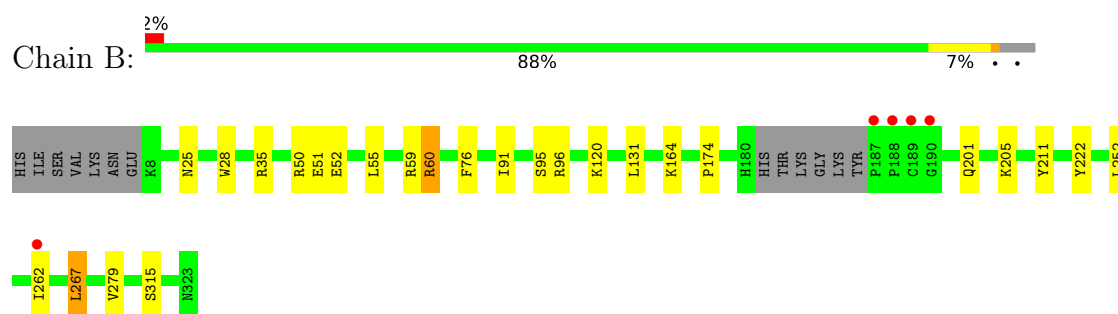
3 Residue-property plots [i](#)

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.

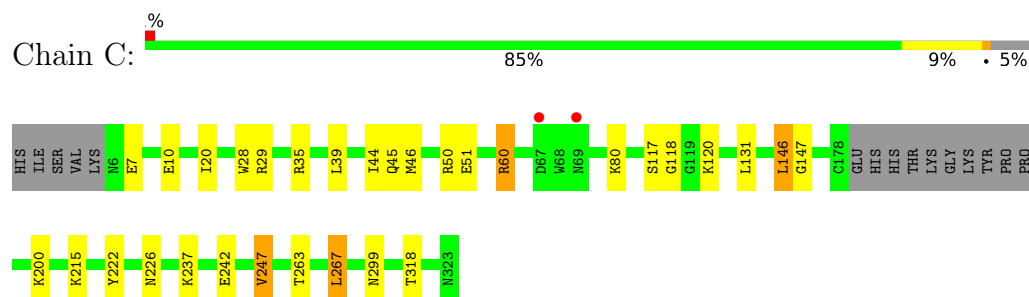
- Molecule 1: Cathepsin B-like peptidase (C01 family)



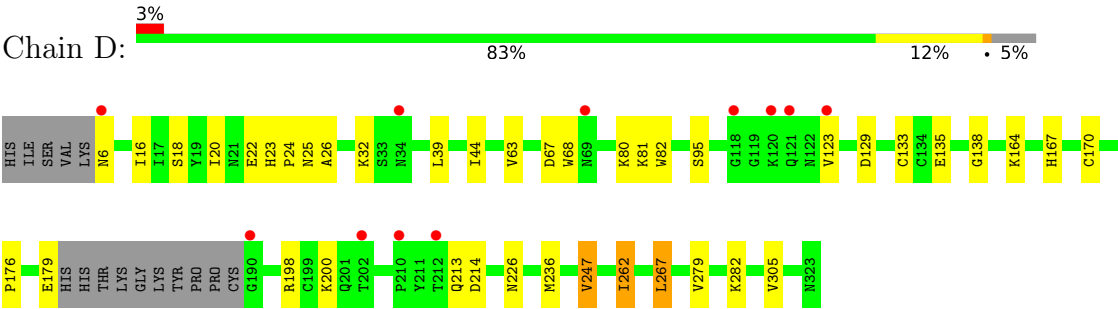
- Molecule 1: Cathepsin B-like peptidase (C01 family)



- Molecule 1: Cathepsin B-like peptidase (C01 family)



- Molecule 1: Cathepsin B-like peptidase (C01 family)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.28Å 83.17Å 84.57Å 76.97° 86.60° 71.11°	Depositor
Resolution (Å)	38.40 – 1.95 38.40 – 1.95	Depositor EDS
% Data completeness (in resolution range)	75.3 (38.40-1.95) 75.8 (38.40-1.95)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.29 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.199 , 0.252 0.195 , 0.246	Depositor DCC
R_{free} test set	5001 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.0	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	0.94	EDS
Total number of atoms	10371	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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: 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	0.62	0/2491	0.87	0/3359
1	B	0.68	0/2551	0.88	1/3440 (0.0%)
1	C	0.74	0/2524	0.88	0/3403
1	D	0.67	0/2526	0.90	1/3405 (0.0%)
All	All	0.68	0/10092	0.88	2/13607 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	138	GLY	N-CA-C	5.59	117.03	111.21
1	B	315	SER	N-CA-C	5.24	118.83	112.23

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	2428	0	2323	36	0
1	B	2482	0	2366	20	0
1	C	2455	0	2353	21	0
1	D	2463	0	2354	23	0
2	A	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	18	5	0
2	D	4	0	6	4	0
3	A	84	0	0	2	0
3	B	137	0	0	4	0
3	C	172	0	0	7	0
3	D	126	0	0	6	0
All	All	10371	0	9432	100	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 5.

All (100) 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:51:GLU:HG3	1:A:145[A]:ILE:HD11	1.30	1.09
1:B:91:ILE:H	2:B:402:EDO:H11	1.28	0.96
1:A:51:GLU:CG	1:A:145[A]:ILE:HD11	2.08	0.83
1:D:20:ILE:HD12	1:D:262[B]:ILE:HD11	1.59	0.82
1:C:60:ARG:HG3	1:C:222:TYR:HA	1.61	0.82
1:C:29:ARG:HD2	3:C:521:HOH:O	1.81	0.81
1:C:80:LYS:HE3	3:C:500:HOH:O	1.82	0.80
1:A:80:LYS:HB2	2:A:401:EDO:H22	1.63	0.79
1:C:117:SER:O	1:C:120:LYS:HG2	1.84	0.76
1:D:282:LYS:H	2:D:401:EDO:C2	1.98	0.75
1:A:55:LEU:HB3	1:A:59:ARG:HE	1.52	0.74
1:A:137:CYS:O	1:A:145[A]:ILE:HG22	1.88	0.73
1:D:282:LYS:H	2:D:401:EDO:H22	1.52	0.72
1:C:146:LEU:HD13	1:C:242:GLU:HG2	1.69	0.72
1:B:91:ILE:H	2:B:402:EDO:C1	2.04	0.71
1:C:46:MET:SD	1:C:247[B]:VAL:HG11	2.34	0.68
1:C:215:LYS:HE2	3:C:485:HOH:O	1.94	0.66
1:A:43:ARG:HG2	1:A:267:LEU:CD2	2.27	0.64
1:B:205:LYS:HE3	3:B:621:HOH:O	1.97	0.64
1:D:32:LYS:HG3	3:D:560:HOH:O	1.97	0.63
1:B:28:TRP:HE1	1:B:262:ILE:HD12	1.63	0.63
1:A:43:ARG:HG2	1:A:267:LEU:HD22	1.81	0.62
1:C:50:ARG:NH1	3:C:535:HOH:O	2.33	0.62
1:B:91:ILE:N	2:B:402:EDO:H11	2.09	0.61
1:A:192:LYS:HD2	1:A:192:LYS:H	1.66	0.61
1:B:252:LEU:HD11	1:B:267:LEU:HD21	1.83	0.59
1:B:51:GLU:OE1	1:B:60:ARG:NH2	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:LEU:HD22	1:D:267:LEU:HD21	1.85	0.57
1:D:279:VAL:HG12	2:D:401:EDO:H22	1.86	0.57
1:A:35:ARG:NE	1:A:45:GLN:OE1	2.36	0.57
1:D:18:SER:O	1:D:22:GLU:HG2	2.05	0.57
1:A:111:ASP:OD2	1:A:240:PRO:HG2	2.05	0.56
1:A:11:PRO:O	1:A:12:LEU:HD12	2.07	0.55
1:B:60:ARG:HG3	1:B:222:TYR:HA	1.88	0.54
1:B:76:PHE:CE1	2:B:403:EDO:H21	2.42	0.54
1:D:129:ASP:O	1:D:133:CYS:HB2	2.08	0.54
1:B:76:PHE:CD1	2:B:403:EDO:H21	2.42	0.54
1:B:205:LYS:CE	3:B:621:HOH:O	2.53	0.54
1:A:54:ASP:OD1	1:A:55:LEU:N	2.41	0.54
1:D:68:TRP:CD1	3:D:535:HOH:O	2.61	0.53
1:C:46:MET:SD	1:C:247[A]:VAL:HG21	2.49	0.52
1:A:226:ASN:ND2	1:A:315:SER:HA	2.25	0.51
1:A:150:TRP:HB3	1:A:221:SER:HB2	1.91	0.51
1:C:118:GLY:HA2	3:C:458:HOH:O	2.10	0.51
1:C:44:ILE:HD13	1:C:193:ILE:HG12	1.93	0.50
1:D:305:VAL:HG22	3:D:555:HOH:O	2.10	0.50
1:A:35:ARG:NH2	1:A:93:ASP:OD1	2.38	0.50
1:A:101:TRP:CD1	1:A:144:GLY:HA3	2.47	0.50
1:C:39:LEU:HD22	1:C:267:LEU:HD11	1.93	0.50
1:D:170:CYS:HB2	1:D:214:ASP:OD2	2.12	0.49
1:D:23:HIS:ND1	1:D:24:PRO:HD2	2.27	0.49
1:C:299:ASN:HB2	3:C:490:HOH:O	2.13	0.49
1:A:249:GLU:O	1:A:252:LEU:HD13	2.13	0.49
1:D:164:LYS:O	1:D:167:HIS:CE1	2.66	0.48
1:B:28:TRP:NE1	1:B:262:ILE:HD12	2.27	0.48
1:B:279:VAL:HG12	2:D:401:EDO:H12	1.95	0.48
1:D:164:LYS:O	1:D:167:HIS:ND1	2.47	0.48
1:B:164:LYS:HD2	1:B:174:PRO:O	2.14	0.48
1:D:20:ILE:CD1	1:D:262[B]:ILE:HD11	2.37	0.48
1:C:51:GLU:OE1	1:C:60:ARG:NH2	2.41	0.47
1:C:20:ILE:HD13	1:C:28:TRP:CH2	2.48	0.47
1:C:35:ARG:NE	1:C:45:GLN:OE1	2.48	0.47
1:C:147:GLY:HA2	1:C:318:THR:HG21	1.97	0.46
1:D:63:VAL:HA	3:D:533:HOH:O	2.15	0.46
1:D:67:ASP:OD1	1:D:67:ASP:N	2.47	0.46
1:A:43:ARG:CG	1:A:267:LEU:CD2	2.93	0.46
1:A:112:ARG:HG2	1:A:238:TYR:O	2.16	0.45
1:A:96:ARG:NH1	3:A:583:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:MET:CE	1:C:247[B]:VAL:CG1	2.95	0.45
1:A:252:LEU:HD11	1:A:267:LEU:HD12	1.97	0.45
1:A:55:LEU:HD13	1:A:59:ARG:HH21	1.82	0.44
1:B:201:GLN:HA	1:B:211:TYR:CZ	2.52	0.44
1:C:237:LYS:HE2	3:C:447:HOH:O	2.17	0.44
1:B:52:GLU:HB3	1:B:55:LEU:HD12	2.00	0.44
1:D:81:LYS:HD3	1:D:82:TRP:CZ2	2.52	0.44
1:D:6:ASN:HB3	3:D:578:HOH:O	2.17	0.44
1:A:272:ILE:HD11	1:A:313:ILE:HD11	1.99	0.44
1:A:51:GLU:HG3	1:A:145[A]:ILE:CD1	2.22	0.44
1:D:247:VAL:HA	3:D:501:HOH:O	2.17	0.44
1:B:50:ARG:HD2	3:B:576:HOH:O	2.19	0.43
1:A:309:ASP:OD1	1:A:312:SER:HA	2.18	0.43
1:A:130:LEU:HD21	1:A:149:ALA:HB1	2.00	0.43
1:A:101:TRP:CG	1:A:144:GLY:HA3	2.53	0.43
1:A:101:TRP:CZ2	1:A:131:LEU:HA	2.53	0.43
1:C:44:ILE:HG22	1:C:44:ILE:O	2.18	0.43
1:A:105:ALA:O	1:A:109:MET:HG3	2.19	0.42
1:A:235:ILE:HA	1:A:239:GLY:O	2.19	0.42
1:C:7:GLU:O	1:C:263:THR:OG1	2.38	0.42
1:A:252:LEU:HD12	1:A:252:LEU:N	2.35	0.41
1:D:16:ILE:O	1:D:20:ILE:HG12	2.19	0.41
1:D:95:SER:HB3	1:D:176:PRO:O	2.20	0.41
1:A:137:CYS:C	1:A:145[A]:ILE:HG22	2.44	0.41
1:A:101:TRP:CH2	1:A:131:LEU:HA	2.55	0.41
1:B:55:LEU:O	1:B:59:ARG:HB2	2.20	0.41
1:A:52:GLU:HB3	1:A:55:LEU:HD12	2.02	0.41
1:B:25:ASN:HB2	3:B:572:HOH:O	2.21	0.40
1:A:252:LEU:N	1:A:252:LEU:CD1	2.84	0.40
1:A:37:HIS:CD2	3:A:576:HOH:O	2.73	0.40
1:B:95:SER:OG	1:B:96:ARG:N	2.54	0.40
1:D:26:ALA:HB1	1:D:262[A]:ILE:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	301/323 (93%)	287 (95%)	13 (4%)	1 (0%)	36	28
1	B	308/323 (95%)	289 (94%)	19 (6%)	0	100	100
1	C	305/323 (94%)	294 (96%)	10 (3%)	1 (0%)	36	28
1	D	305/323 (94%)	289 (95%)	14 (5%)	2 (1%)	18	10
All	All	1219/1292 (94%)	1159 (95%)	56 (5%)	4 (0%)	36	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	25	ASN
1	A	226	ASN
1	C	226	ASN
1	D	226	ASN

5.3.2 Protein sidechains ⓘ

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	260/277 (94%)	250 (96%)	10 (4%)	29	19
1	B	267/277 (96%)	262 (98%)	5 (2%)	50	45
1	C	265/277 (96%)	257 (97%)	8 (3%)	36	27
1	D	264/277 (95%)	251 (95%)	13 (5%)	22	11
All	All	1056/1108 (95%)	1020 (97%)	36 (3%)	34	23

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	74	SER

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Mol	Chain	Res	Type
1	A	96	ARG
1	A	122	ASN
1	A	131	LEU
1	A	192	LYS
1	A	247	VAL
1	A	252	LEU
1	A	267	LEU
1	A	272	ILE
1	B	35	ARG
1	B	60	ARG
1	B	120	LYS
1	B	131	LEU
1	B	267	LEU
1	C	10	GLU
1	C	60	ARG
1	C	131	LEU
1	C	146	LEU
1	C	200	LYS
1	C	247[A]	VAL
1	C	247[B]	VAL
1	C	267	LEU
1	D	44	ILE
1	D	80	LYS
1	D	123	VAL
1	D	135	GLU
1	D	179	GLU
1	D	198	ARG
1	D	200	LYS
1	D	213	GLN
1	D	236	MET
1	D	247	VAL
1	D	262[A]	ILE
1	D	262[B]	ILE
1	D	267	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	216	HIS
1	B	37	HIS
1	B	121	GLN

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Mol	Chain	Res	Type
1	C	121	GLN
1	D	121	GLN

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 ⓘ

6 ligands are modelled in this entry.

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	EDO	B	403	-	3,3,3	0.28	0	2,2,2	0.51	0
2	EDO	B	402	-	3,3,3	0.39	0	2,2,2	0.46	0
2	EDO	A	401	-	3,3,3	0.27	0	2,2,2	0.86	0
2	EDO	D	401	-	3,3,3	0.23	0	2,2,2	0.63	0
2	EDO	A	402	-	3,3,3	0.24	0	2,2,2	0.93	0
2	EDO	B	401	-	3,3,3	0.37	0	2,2,2	0.70	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
2	EDO	B	403	-	-	0/1/1/1	-
2	EDO	B	402	-	-	0/1/1/1	-
2	EDO	A	401	-	-	1/1/1/1	-
2	EDO	D	401	-	-	1/1/1/1	-
2	EDO	A	402	-	-	1/1/1/1	-
2	EDO	B	401	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	EDO	O1-C1-C2-O2
2	D	401	EDO	O1-C1-C2-O2
2	A	401	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	403	EDO	2	0
2	B	402	EDO	3	0
2	A	401	EDO	1	0
2	D	401	EDO	4	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	304/323 (94%)	0.63	31 (10%) 12 13	12, 33, 60, 80	2 (0%)
1	B	310/323 (95%)	-0.07	5 (1%) 70 77	3, 20, 43, 60	2 (0%)
1	C	306/323 (94%)	-0.19	2 (0%) 84 88	4, 17, 36, 54	3 (0%)
1	D	308/323 (95%)	0.16	11 (3%) 46 53	7, 24, 54, 72	1 (0%)
All	All	1228/1292 (95%)	0.13	49 (3%) 42 49	3, 23, 51, 80	8 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	190	GLY	4.2
1	B	188	PRO	3.7
1	B	189	CYS	3.5
1	A	44	ILE	3.5
1	A	193	ILE	3.5
1	A	167	HIS	3.4
1	A	178	CYS	3.2
1	A	202	THR	3.1
1	A	212	THR	3.1
1	D	34	ASN	2.8
1	A	190	GLY	2.8
1	A	171	GLU	2.8
1	A	194	TYR	2.7
1	A	200	LYS	2.7
1	A	262	ILE	2.7
1	A	127	ALA	2.6
1	A	207	TYR	2.6
1	A	170	CYS	2.6
1	A	145[A]	ILE	2.6
1	A	168	ALA	2.6
1	D	69	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	139	LEU	2.6
1	C	69	ASN	2.5
1	A	123	VAL	2.5
1	D	210	PRO	2.5
1	A	146	LEU	2.3
1	D	123	VAL	2.3
1	A	34	ASN	2.3
1	B	190	GLY	2.3
1	D	212	THR	2.3
1	D	6	ASN	2.2
1	B	187	PRO	2.2
1	A	322	ILE	2.2
1	A	203	CYS	2.2
1	D	121	GLN	2.2
1	A	196	THR	2.2
1	A	54	ASP	2.1
1	D	120	LYS	2.1
1	A	37	HIS	2.1
1	A	9	PHE	2.1
1	A	205	LYS	2.1
1	A	36	PHE	2.1
1	B	262	ILE	2.1
1	A	209	THR	2.1
1	D	202	THR	2.1
1	C	67	ASP	2.1
1	D	118	GLY	2.0
1	A	24	PRO	2.0
1	A	206	LYS	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
2	EDO	A	402	4/4	0.80	0.17	28,29,31,32	0
2	EDO	B	402	4/4	0.85	0.15	28,30,31,33	0
2	EDO	D	401	4/4	0.86	0.14	13,16,17,26	0
2	EDO	B	403	4/4	0.88	0.12	13,19,21,29	0
2	EDO	A	401	4/4	0.90	0.08	17,21,21,28	0
2	EDO	B	401	4/4	0.91	0.19	22,25,26,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.