Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 05:29 PM JST

PDB ID	:	6JD0
Title	:	Structure of mutant human cathepsin L, engineered for GAG binding
Authors	:	Choudhury, D.; Biswas, S.
Deposited on	:	2019-01-30
Resolution	:	1.80 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 (1)) were used in the production of this report:

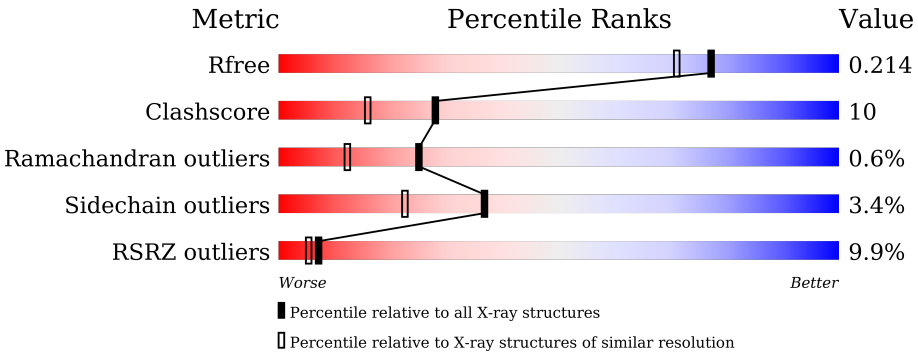
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	360	9% 74% 12% • 13%

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
6	POL	A	439	-	-	X	-
7	PGE	A	445	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	EOH	A	449	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 5600 atoms, of which 2659 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 L1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	314	4890	1600	2354	430	483	23	0	6	0

There are 52 discrepancies between the modelled and reference sequences:

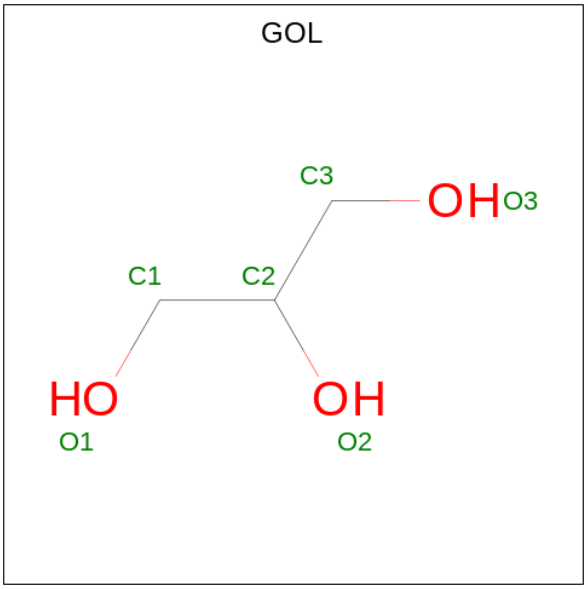
Chain	Residue	Modelled	Actual	Comment	Reference
A	-43	MET	-	initiating methionine	UNP P07711
A	-42	HIS	-	expression tag	UNP P07711
A	-41	HIS	-	expression tag	UNP P07711
A	-40	HIS	-	expression tag	UNP P07711
A	-39	HIS	-	expression tag	UNP P07711
A	-38	HIS	-	expression tag	UNP P07711
A	-37	HIS	-	expression tag	UNP P07711
A	-36	SER	-	expression tag	UNP P07711
A	-35	SER	-	expression tag	UNP P07711
A	-34	GLY	-	expression tag	UNP P07711
A	-33	LEU	-	expression tag	UNP P07711
A	-32	VAL	-	expression tag	UNP P07711
A	-31	PRO	-	expression tag	UNP P07711
A	-30	ARG	-	expression tag	UNP P07711
A	-29	GLY	-	expression tag	UNP P07711
A	-28	SER	-	expression tag	UNP P07711
A	-27	GLY	-	expression tag	UNP P07711
A	-26	MET	-	expression tag	UNP P07711
A	-25	LYS	-	expression tag	UNP P07711
A	-24	GLU	-	expression tag	UNP P07711
A	-23	THR	-	expression tag	UNP P07711
A	-22	ALA	-	expression tag	UNP P07711
A	-21	ALA	-	expression tag	UNP P07711
A	-20	ALA	-	expression tag	UNP P07711
A	-19	LYS	-	expression tag	UNP P07711
A	-18	PHE	-	expression tag	UNP P07711
A	-17	GLU	-	expression tag	UNP P07711

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	ARG	-	expression tag	UNP P07711
A	-15	GLN	-	expression tag	UNP P07711
A	-14	HIS	-	expression tag	UNP P07711
A	-13	MET	-	expression tag	UNP P07711
A	-12	ASP	-	expression tag	UNP P07711
A	-11	SER	-	expression tag	UNP P07711
A	-10	PRO	-	expression tag	UNP P07711
A	-9	ASP	-	expression tag	UNP P07711
A	-8	LEU	-	expression tag	UNP P07711
A	-7	GLY	-	expression tag	UNP P07711
A	-6	THR	-	expression tag	UNP P07711
A	-5	ASP	-	expression tag	UNP P07711
A	-4	ASP	-	expression tag	UNP P07711
A	-3	ASP	-	expression tag	UNP P07711
A	-2	ASP	-	expression tag	UNP P07711
A	-1	LYS	-	expression tag	UNP P07711
A	0	MET	-	expression tag	UNP P07711
A	105	LYS	GLU	engineered mutation	UNP P07711
A	121	SER	CYS	engineered mutation	UNP P07711
A	165	TYR	LEU	engineered mutation	UNP P07711
A	257	LEU	MET	engineered mutation	UNP P07711
A	260	ALA	GLY	engineered mutation	UNP P07711
A	291	ASN	MET	engineered mutation	UNP P07711
A	292	LYS	GLY	engineered mutation	UNP P07711
A	310	LEU	ALA	engineered mutation	UNP P07711

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 13 3 7 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0

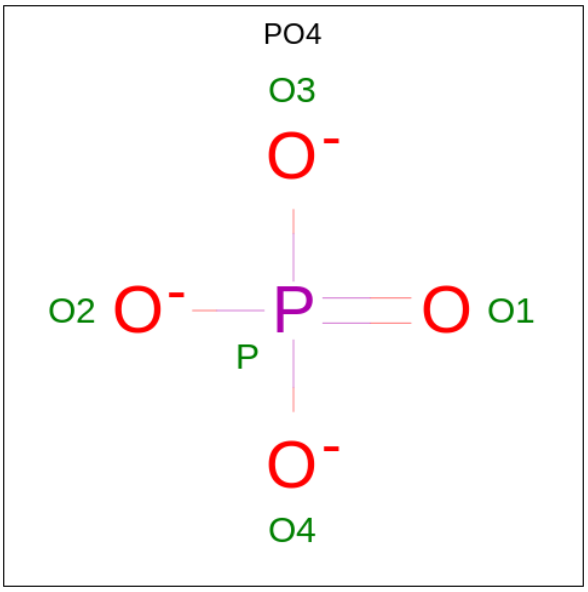
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Cl 3 3	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

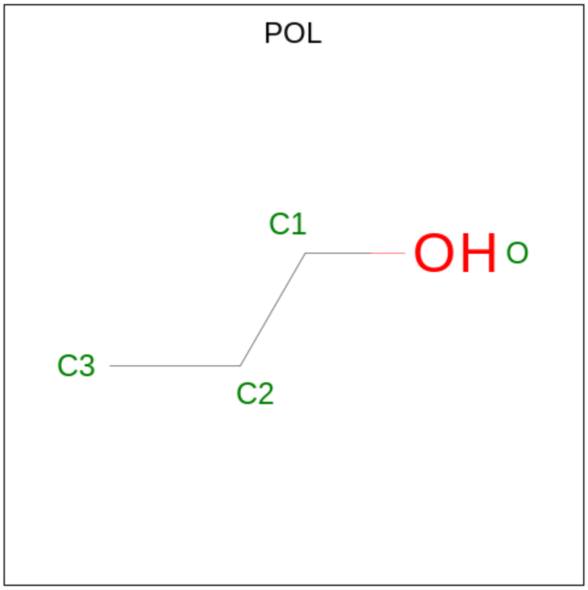
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total Na 5 5	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



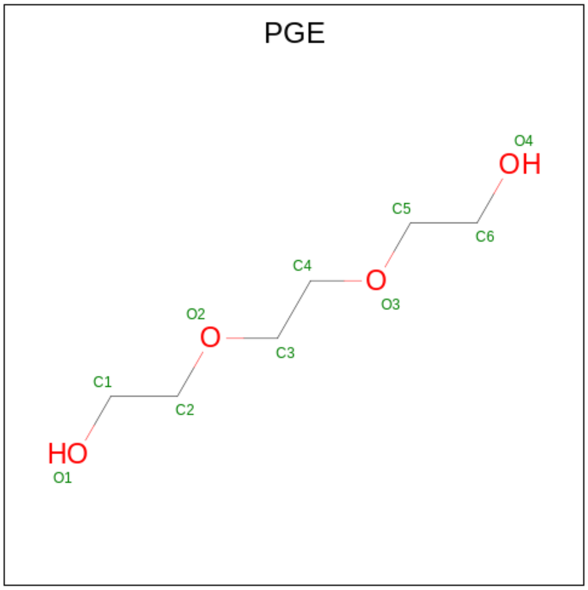
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0

- Molecule 6 is N-PROPANOL (three-letter code: POL) (formula: C_3H_8O).



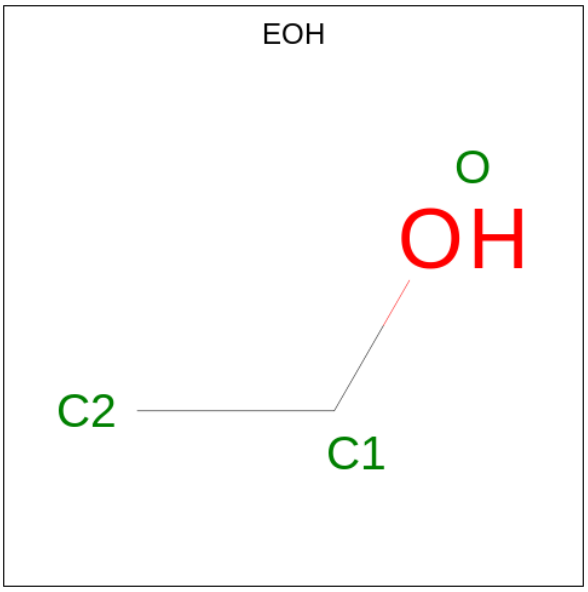
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 12 3 8 1	0	0
6	A	1	Total C H O 12 3 8 1	0	0
6	A	1	Total C H O 12 3 8 1	0	0
6	A	1	Total C H O 12 3 8 1	0	0
6	A	1	Total C H O 12 3 8 1	0	0
6	A	1	Total C H O 12 3 8 1	0	0
6	A	1	Total C H O 12 3 8 1	0	0
6	A	1	Total C H O 12 3 8 1	0	0
6	A	1	Total C H O 12 3 8 1	0	0
6	A	1	Total C H O 12 3 8 1	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



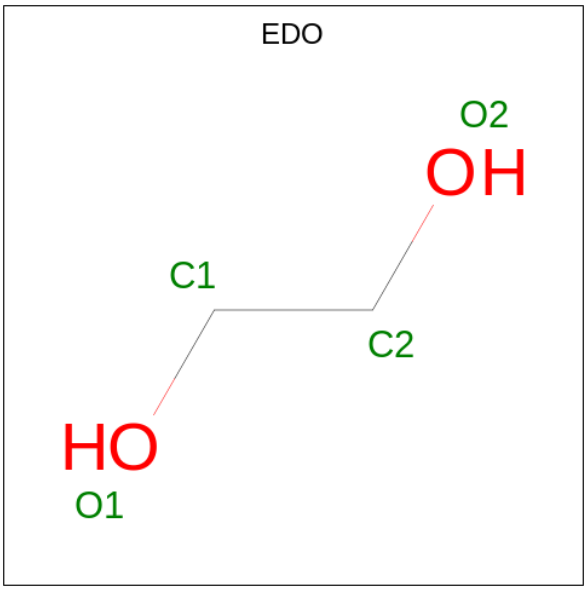
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H O 24 6 14 4	0	0
7	A	1	Total C H O 24 6 14 4	0	0
7	A	1	Total C H O 24 6 14 4	0	0
7	A	1	Total C H O 24 6 14 4	0	0
7	A	1	Total C H O 24 6 14 4	0	0
7	A	1	Total C H O 24 6 14 4	0	0

- Molecule 8 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			9	2	6	1		
8	A	1	Total	C	H	O	0	0
			9	2	6	1		
8	A	1	Total	C	H	O	0	0
			9	2	6	1		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			10	2	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			10	2	6	2		

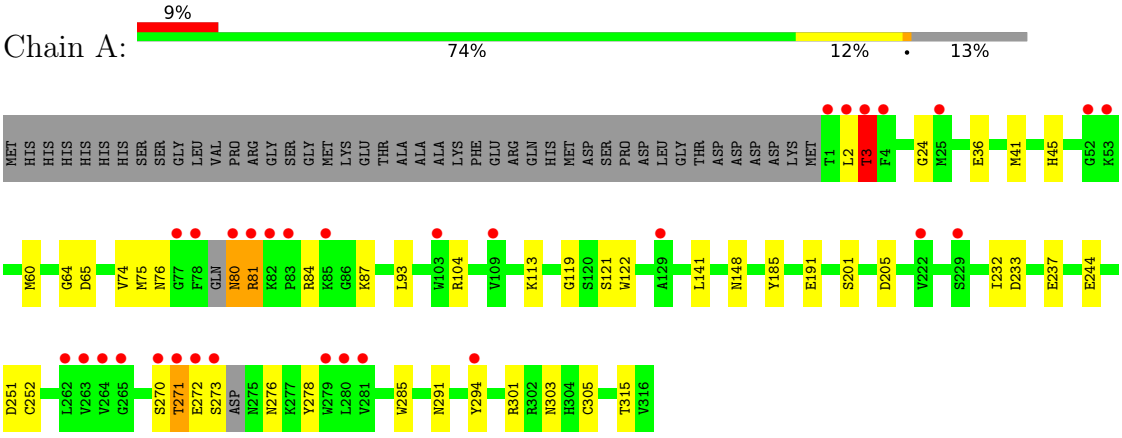
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	156	Total	O	0	0
			156	156		

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 L1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.84Å 64.17Å 92.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.41 – 1.80 32.41 – 1.81	Depositor EDS
% Data completeness (in resolution range)	96.4 (32.41-1.80) 96.4 (32.41-1.81)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.171 , 0.215 0.172 , 0.214	Depositor DCC
R_{free} test set	2016 reflections (5.85%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.804	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5600	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POL, PGE, NA, EOH, CL, PO4, GOL, 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	0.52	0/2619	0.61	0/3525

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2536	2354	2393	53	0
2	A	84	111	112	4	0
3	A	3	0	0	0	0
4	A	5	0	0	0	0
5	A	40	0	0	0	0
6	A	40	80	79	22	0
7	A	60	84	84	2	0
8	A	9	18	18	3	0
9	A	8	12	12	1	0
10	A	156	0	0	9	0
All	All	2941	2659	2698	54	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 10.

All (54) 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:65:ASP:OD2	10:A:501:HOH:O	1.79	0.96
1:A:84:ARG:O	10:A:502:HOH:O	1.84	0.95
1:A:80:ASN:O	1:A:80:ASN:ND2	2.02	0.92
1:A:191:GLU:OE2	8:A:449:EOH:O	1.90	0.88
1:A:121:SER:H	6:A:439:POL:C2	2.00	0.73
1:A:75:MET:C	6:A:439:POL:H12	2.10	0.71
1:A:121:SER:H	6:A:439:POL:H21	1.57	0.70
1:A:121:SER:CB	6:A:439:POL:H21	2.26	0.65
1:A:76:ASN:HB2	6:A:439:POL:H33	1.79	0.65
1:A:87:LYS:NZ	10:A:508:HOH:O	2.33	0.60
1:A:233:ASP:O	1:A:305[B]:CYS:SG	2.60	0.60
1:A:81:ARG:NH1	10:A:509:HOH:O	2.34	0.59
1:A:36:GLU:OE2	10:A:503:HOH:O	2.17	0.59
1:A:273:SER:HB3	1:A:276:ASN:OD1	2.04	0.58
1:A:271:THR:OG1	1:A:272:GLU:N	2.37	0.58
1:A:119:GLY:HA2	6:A:439:POL:H22	1.87	0.57
1:A:41[B]:MET:SD	1:A:237:GLU:OE1	2.65	0.54
1:A:76:ASN:CB	6:A:439:POL:H33	2.36	0.54
1:A:121:SER:HB3	6:A:439:POL:H21	1.89	0.54
1:A:65:ASP:OD1	10:A:504:HOH:O	2.18	0.52
1:A:81:ARG:O	1:A:81:ARG:HG3	2.10	0.51
1:A:244:GLU:HB3	7:A:443:PGE:H42	1.92	0.51
1:A:232:ILE:HB	1:A:305[B]:CYS:SG	2.51	0.51
1:A:303:ASN:HD22	6:A:433:POL:H32	1.75	0.51
1:A:251:ASP:O	8:A:447:EOH:H22	2.11	0.51
1:A:80:ASN:HB3	10:A:619:HOH:O	2.09	0.51
1:A:45:HIS:CE1	2:A:401:GOL:HO1	2.21	0.49
1:A:93:LEU:HB2	2:A:414:GOL:H2	1.96	0.47
1:A:104:ARG:HD3	1:A:294:TYR:CZ	2.50	0.46
1:A:60:MET:H	6:A:431:POL:C2	2.28	0.46
1:A:75:MET:CA	6:A:439:POL:H12	2.46	0.45
1:A:74:VAL:C	6:A:439:POL:H11	2.37	0.45
1:A:74:VAL:HG12	1:A:285:TRP:HE1	1.82	0.45
1:A:141:LEU:H	6:A:438:POL:H12	1.82	0.44
1:A:60:MET:SD	1:A:64:GLY:HA3	2.58	0.44
1:A:119:GLY:C	6:A:439:POL:H22	2.37	0.44
1:A:205:ASP:HB2	1:A:315:THR:O	2.18	0.43
1:A:3:THR:O	1:A:3:THR:CG2	2.67	0.42
1:A:113:LYS:HA	6:A:435:POL:H21	2.01	0.42
6:A:432:POL:H33	10:A:592:HOH:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASN:HD21	1:A:122:TRP:HB3	1.84	0.42
1:A:278:TYR:OH	9:A:450:EDO:H22	2.19	0.42
1:A:80:ASN:CB	10:A:619:HOH:O	2.65	0.42
1:A:24:GLY:HA3	2:A:412:GOL:H31	2.02	0.42
1:A:119:GLY:CA	6:A:439:POL:H22	2.48	0.42
1:A:201:SER:OG	2:A:410:GOL:H32	2.19	0.42
1:A:74:VAL:O	6:A:439:POL:H11	2.20	0.41
1:A:121:SER:OG	6:A:439:POL:H21	2.20	0.41
1:A:301:ARG:HD2	7:A:442:PGE:H6	2.01	0.41
1:A:76:ASN:N	6:A:439:POL:H12	2.34	0.41
1:A:76:ASN:HA	6:A:439:POL:H32	2.02	0.41
1:A:104:ARG:HD3	1:A:294:TYR:CE2	2.56	0.41
1:A:191:GLU:OE2	8:A:449:EOH:C1	2.68	0.41
1:A:121:SER:H	6:A:439:POL:C3	2.33	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	314/360 (87%)	303 (96%)	9 (3%)	2 (1%)	25 12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	THR
1	A	3	THR

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	269/303 (89%)	260 (97%)	9 (3%)	38 23

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	3	THR
1	A	80	ASN
1	A	81	ARG
1	A	148	ASN
1	A	185	TYR
1	A	252	CYS
1	A	270	SER
1	A	291	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 51 ligands modelled in this entry, 8 are monoatomic - leaving 43 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	$\#\|Z\| > 2$
2	GOL	A	405	-	5,5,5	0.79	0	5,5,5	1.16	1 (20%)
9	EDO	A	451	-	3,3,3	0.46	0	2,2,2	0.22	0
7	PGE	A	442	-	9,9,9	0.33	0	8,8,8	0.34	0
8	EOH	A	448	-	2,2,2	0.47	0	1,1,1	0.01	0
5	PO4	A	428	4	4,4,4	1.18	0	6,6,6	0.44	0
5	PO4	A	427	-	4,4,4	0.83	0	6,6,6	0.55	0
8	EOH	A	449	-	2,2,2	0.46	0	1,1,1	0.07	0
2	GOL	A	402	-	5,5,5	1.15	0	5,5,5	1.05	0
7	PGE	A	444	-	9,9,9	0.31	0	8,8,8	0.30	0
5	PO4	A	426	-	4,4,4	0.83	0	6,6,6	0.34	0
5	PO4	A	425	-	4,4,4	0.86	0	6,6,6	0.56	0
2	GOL	A	407	-	5,5,5	0.80	0	5,5,5	1.15	0
5	PO4	A	423	4	4,4,4	0.78	0	6,6,6	0.54	0
8	EOH	A	447	-	2,2,2	0.40	0	1,1,1	0.32	0
7	PGE	A	441	-	9,9,9	0.31	0	8,8,8	0.41	0
2	GOL	A	404	-	5,5,5	1.07	0	5,5,5	0.81	0
2	GOL	A	411	-	5,5,5	1.09	0	5,5,5	1.01	0
6	POL	A	436	-	3,3,3	0.42	0	2,2,2	0.33	0
2	GOL	A	412	-	5,5,5	1.28	0	5,5,5	0.75	0
6	POL	A	433	-	3,3,3	0.40	0	2,2,2	0.35	0
2	GOL	A	401	-	5,5,5	0.93	0	5,5,5	0.84	0
6	POL	A	438	-	3,3,3	0.46	0	2,2,2	0.19	0
5	PO4	A	424	4	4,4,4	0.84	0	6,6,6	0.38	0
2	GOL	A	410	-	5,5,5	1.06	0	5,5,5	1.00	0
2	GOL	A	406	-	5,5,5	1.07	0	5,5,5	0.93	0
6	POL	A	434	-	3,3,3	0.43	0	2,2,2	0.34	0
7	PGE	A	443	-	9,9,9	0.39	0	8,8,8	0.30	0
6	POL	A	432	-	3,3,3	0.36	0	2,2,2	0.45	0
2	GOL	A	413	-	5,5,5	0.83	0	5,5,5	1.08	0
5	PO4	A	430	-	4,4,4	0.76	0	6,6,6	0.50	0
7	PGE	A	445	-	9,9,9	0.35	0	8,8,8	0.27	0
2	GOL	A	414	-	5,5,5	0.96	0	5,5,5	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	POL	A	437	-	3,3,3	0.43	0	2,2,2	0.26	0
9	EDO	A	450	-	3,3,3	0.75	0	2,2,2	0.35	0
6	POL	A	435	4	3,3,3	0.34	0	2,2,2	0.25	0
5	PO4	A	429	-	4,4,4	0.92	0	6,6,6	0.44	0
7	PGE	A	446	-	9,9,9	0.38	0	8,8,8	0.52	0
6	POL	A	431	-	3,3,3	0.43	0	2,2,2	0.36	0
2	GOL	A	403	-	5,5,5	1.23	0	5,5,5	0.84	0
6	POL	A	439	-	3,3,3	0.29	0	2,2,2	0.30	0
6	POL	A	440	-	3,3,3	0.38	0	2,2,2	0.27	0
2	GOL	A	409	-	5,5,5	1.20	0	5,5,5	0.76	0
2	GOL	A	408	-	5,5,5	0.89	0	5,5,5	1.04	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	GOL	A	405	-	-	0/4/4/4	-
9	EDO	A	451	-	-	1/1/1/1	-
7	PGE	A	442	-	-	3/7/7/7	-
2	GOL	A	402	-	-	0/4/4/4	-
7	PGE	A	444	-	-	2/7/7/7	-
2	GOL	A	407	-	-	2/4/4/4	-
7	PGE	A	441	-	-	1/7/7/7	-
2	GOL	A	404	-	-	3/4/4/4	-
2	GOL	A	411	-	-	2/4/4/4	-
6	POL	A	436	-	-	0/1/1/1	-
2	GOL	A	412	-	-	4/4/4/4	-
6	POL	A	433	-	-	0/1/1/1	-
2	GOL	A	401	-	-	4/4/4/4	-
6	POL	A	438	-	-	0/1/1/1	-
2	GOL	A	410	-	-	0/4/4/4	-
2	GOL	A	406	-	-	2/4/4/4	-
6	POL	A	434	-	-	1/1/1/1	-
7	PGE	A	443	-	-	5/7/7/7	-
6	POL	A	432	-	-	0/1/1/1	-
2	GOL	A	413	-	-	2/4/4/4	-
7	PGE	A	445	-	-	2/7/7/7	-
2	GOL	A	414	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	POL	A	437	-	-	0/1/1/1	-
9	EDO	A	450	-	-	1/1/1/1	-
6	POL	A	435	4	-	0/1/1/1	-
7	PGE	A	446	-	-	5/7/7/7	-
6	POL	A	431	-	-	0/1/1/1	-
2	GOL	A	403	-	-	0/4/4/4	-
6	POL	A	439	-	-	0/1/1/1	-
6	POL	A	440	-	-	0/1/1/1	-
2	GOL	A	409	-	-	2/4/4/4	-
2	GOL	A	408	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	405	GOL	C3-C2-C1	-2.18	103.23	111.70

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	C1-C2-C3-O3
2	A	404	GOL	O1-C1-C2-C3
2	A	406	GOL	O1-C1-C2-O2
2	A	406	GOL	O1-C1-C2-C3
2	A	407	GOL	C1-C2-C3-O3
2	A	409	GOL	C1-C2-C3-O3
2	A	411	GOL	O1-C1-C2-O2
2	A	411	GOL	O1-C1-C2-C3
2	A	412	GOL	O1-C1-C2-O2
2	A	412	GOL	O1-C1-C2-C3
2	A	412	GOL	C1-C2-C3-O3
7	A	441	PGE	O2-C3-C4-O3
7	A	446	PGE	O1-C1-C2-O2
2	A	404	GOL	O1-C1-C2-O2
2	A	413	GOL	O1-C1-C2-O2
7	A	442	PGE	O1-C1-C2-O2
7	A	445	PGE	O1-C1-C2-O2
2	A	404	GOL	C1-C2-C3-O3
2	A	413	GOL	O1-C1-C2-C3
7	A	443	PGE	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	442	PGE	O2-C3-C4-O3
2	A	401	GOL	O2-C2-C3-O3
2	A	407	GOL	O2-C2-C3-O3
9	A	450	EDO	O1-C1-C2-O2
7	A	443	PGE	O3-C5-C6-O4
7	A	443	PGE	O2-C3-C4-O3
7	A	444	PGE	O3-C5-C6-O4
7	A	446	PGE	O3-C5-C6-O4
2	A	401	GOL	O1-C1-C2-O2
2	A	414	GOL	O2-C2-C3-O3
2	A	412	GOL	O2-C2-C3-O3
7	A	443	PGE	C1-C2-O2-C3
6	A	434	POL	O-C1-C2-C3
7	A	446	PGE	C3-C4-O3-C5
2	A	401	GOL	O1-C1-C2-C3
7	A	446	PGE	O2-C3-C4-O3
2	A	409	GOL	O2-C2-C3-O3
7	A	443	PGE	C6-C5-O3-C4
9	A	451	EDO	O1-C1-C2-O2
7	A	442	PGE	C6-C5-O3-C4
7	A	444	PGE	O1-C1-C2-O2
7	A	445	PGE	O2-C3-C4-O3
2	A	414	GOL	O1-C1-C2-C3
7	A	446	PGE	C1-C2-O2-C3

There are no ring outliers.

15 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	442	PGE	1	0
8	A	449	EOH	2	0
8	A	447	EOH	1	0
2	A	412	GOL	1	0
6	A	433	POL	1	0
2	A	401	GOL	1	0
6	A	438	POL	1	0
2	A	410	GOL	1	0
7	A	443	PGE	1	0
6	A	432	POL	1	0
2	A	414	GOL	1	0
9	A	450	EDO	1	0
6	A	435	POL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	431	POL	1	0
6	A	439	POL	17	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, 95^{th} 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	314/360 (87%)	0.40	31 (9%) 7 5	18, 28, 54, 94	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	THR	11.4
1	A	2	LEU	10.0
1	A	273	SER	7.5
1	A	82	LYS	6.0
1	A	83	PRO	5.9
1	A	77	GLY	4.7
1	A	85	LYS	4.7
1	A	80	ASN	4.0
1	A	272	GLU	3.8
1	A	3	THR	3.6
1	A	52	GLY	3.3
1	A	262	LEU	3.1
1	A	81	ARG	3.1
1	A	129	ALA	3.1
1	A	78	PHE	3.0
1	A	270	SER	2.9
1	A	280	LEU	2.9
1	A	109	VAL	2.8
1	A	263	VAL	2.8
1	A	264	VAL	2.7
1	A	103	TRP	2.7
1	A	279	TRP	2.4
1	A	222	VAL	2.4
1	A	53	LYS	2.3
1	A	25	MET	2.3
1	A	294	TYR	2.3
1	A	265	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	271	THR	2.1
1	A	229	SER	2.1
1	A	281	VAL	2.1
1	A	4	PHE	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, 95^{th} 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
7	PGE	A	445	10/10	0.46	0.51	64,100,121,125	0
2	GOL	A	410	6/6	0.65	0.37	53,64,78,81	0
6	POL	A	440	4/4	0.67	0.29	45,56,70,70	0
7	PGE	A	446	10/10	0.69	0.17	49,63,84,88	0
6	POL	A	438	4/4	0.73	0.27	41,49,52,59	0
6	POL	A	433	4/4	0.73	0.27	33,52,64,64	0
2	GOL	A	405	6/6	0.74	0.37	48,64,70,77	0
5	PO4	A	424	5/5	0.75	0.23	56,61,87,91	0
2	GOL	A	411	6/6	0.75	0.24	45,56,66,67	0
2	GOL	A	408	6/6	0.76	0.38	56,68,79,79	0
2	GOL	A	412	6/6	0.80	0.19	38,47,64,66	0
7	PGE	A	442	10/10	0.80	0.26	51,65,86,96	0
8	EOH	A	448	3/3	0.80	0.35	46,55,61,65	0
2	GOL	A	413	6/6	0.81	0.43	70,84,96,100	0
2	GOL	A	414	6/6	0.81	0.41	49,63,75,75	0
2	GOL	A	409	6/6	0.81	0.22	29,49,73,73	0
7	PGE	A	443	10/10	0.81	0.23	33,49,74,85	0
5	PO4	A	425	5/5	0.81	0.23	60,65,104,105	0
2	GOL	A	404	6/6	0.81	0.25	39,52,63,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	POL	A	437	4/4	0.81	0.28	36,51,68,69	0
6	POL	A	435	4/4	0.82	0.26	25,39,61,61	0
9	EDO	A	451	4/4	0.82	0.47	47,60,72,72	0
2	GOL	A	407	6/6	0.83	0.32	52,63,75,76	0
6	POL	A	434	4/4	0.83	0.13	40,48,69,69	0
2	GOL	A	406	6/6	0.83	0.16	29,51,59,62	0
5	PO4	A	427	5/5	0.84	0.43	70,73,91,92	0
7	PGE	A	444	10/10	0.84	0.28	58,72,82,84	0
9	EDO	A	450	4/4	0.84	0.27	29,54,65,65	0
2	GOL	A	402	6/6	0.84	0.20	41,50,55,60	0
8	EOH	A	447	3/3	0.85	0.37	42,51,68,68	0
6	POL	A	432	4/4	0.85	0.43	50,65,72,72	0
5	PO4	A	426	5/5	0.86	0.30	54,62,82,91	0
4	NA	A	420	1/1	0.86	0.20	49,49,49,49	0
6	POL	A	436	4/4	0.86	0.35	44,58,68,70	0
4	NA	A	421	1/1	0.87	0.29	58,58,58,58	0
2	GOL	A	403	6/6	0.87	0.27	42,60,73,75	0
6	POL	A	439	4/4	0.88	0.19	33,46,58,58	0
7	PGE	A	441	10/10	0.89	0.24	46,56,72,74	0
5	PO4	A	430	5/5	0.89	0.25	57,63,89,98	0
3	CL	A	416	1/1	0.91	0.16	47,47,47,47	0
5	PO4	A	423	5/5	0.91	0.16	48,61,82,87	0
3	CL	A	415	1/1	0.92	0.09	46,46,46,46	0
2	GOL	A	401	6/6	0.92	0.27	43,56,72,74	0
8	EOH	A	449	3/3	0.92	0.59	42,51,57,63	0
4	NA	A	422	1/1	0.92	0.19	50,50,50,50	0
3	CL	A	417	1/1	0.92	0.13	53,53,53,53	0
5	PO4	A	428	5/5	0.94	0.12	30,33,49,65	0
5	PO4	A	429	5/5	0.95	0.25	64,73,91,93	0
6	POL	A	431	4/4	0.96	0.12	24,40,77,77	0
4	NA	A	419	1/1	0.98	0.22	35,35,35,35	0
4	NA	A	418	1/1	0.99	0.07	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.