



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:04 AM UTC

PDB ID : 6JD8 / pdb_00006jd8
Title : Structure of a proline specific mutant of human cathepsin L
Authors : Choudhury, D.; Biswas, S.
Deposited on : 2019-01-31
Resolution : 1.46 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

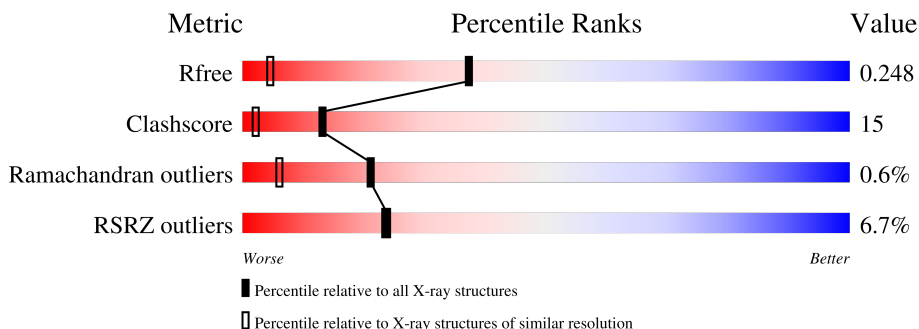
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.46 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	360	

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
3	EOH	A	408	-	-	X	-
3	EOH	A	410	-	-	X	-
3	EOH	A	412	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EOH	A	413	-	-	X	-
5	EDO	A	415	-	-	X	-
6	PGE	A	416	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5415 atoms, of which 2537 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	5014	1640	2429	427	491	27	0	17	0

There are 49 discrepancies between the modelled and reference sequences:

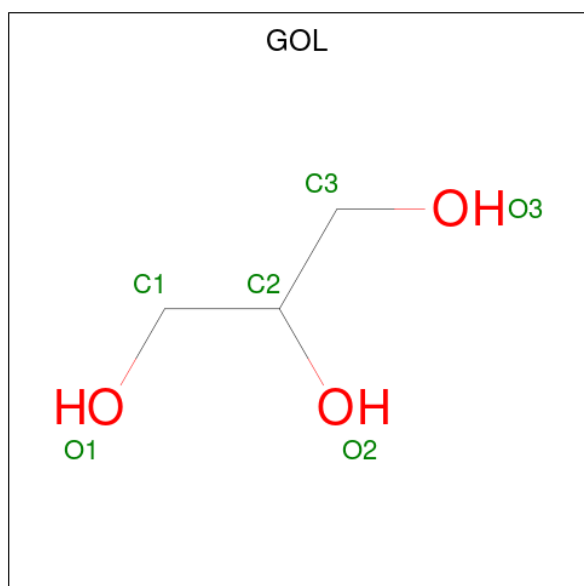
Chain	Residue	Modelled	Actual	Comment	Reference
A	-43	MET	-	expression tag	UNP P07711
A	-42	HIS	-	expression tag	UNP P07711
A	-41	HIS	-	expression tag	UNP P07711
A	-40	HIS	-	expression tag	UNP P07711
A	-39	HIS	-	expression tag	UNP P07711
A	-38	HIS	-	expression tag	UNP P07711
A	-37	HIS	-	expression tag	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

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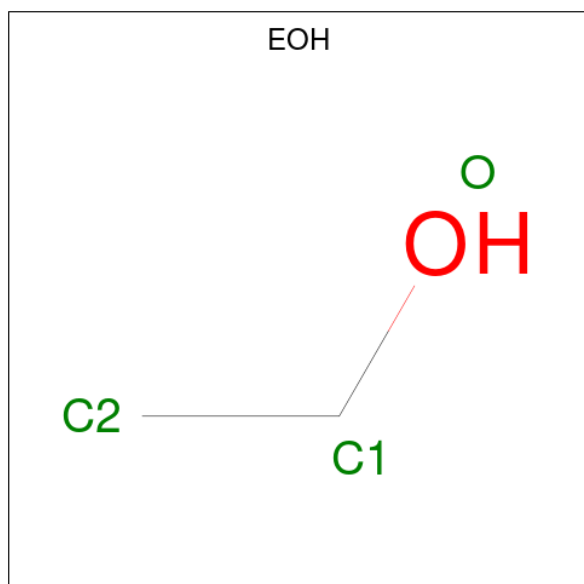
Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	ARG	-	expression tag	UNP P07711
A	-15	GLN	-	expression tag	UNP P07711
A	-14	HIS	-	expression tag	UNP P07711
A	-13	MET	-	expression tag	UNP P07711
A	-12	ASP	-	expression tag	UNP P07711
A	-11	SER	-	expression tag	UNP P07711
A	-10	PRO	-	expression tag	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	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	310	LEU	ALA	engineered mutation	UNP P07711

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is ETHANOL (CCD ID: EOH) (formula: C_2H_6O).



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

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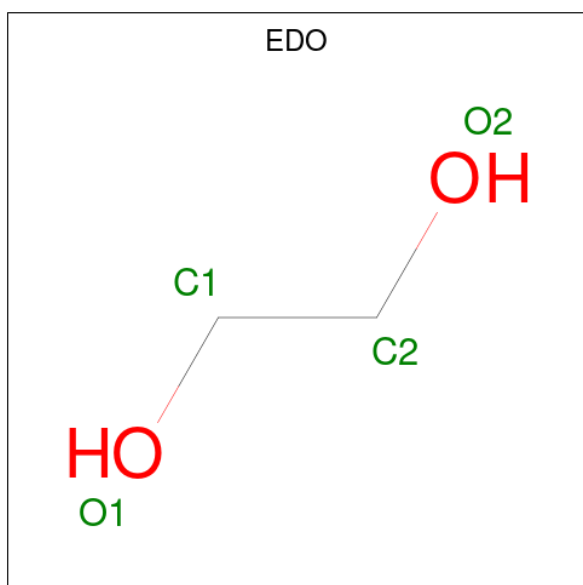
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			9	2	6	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



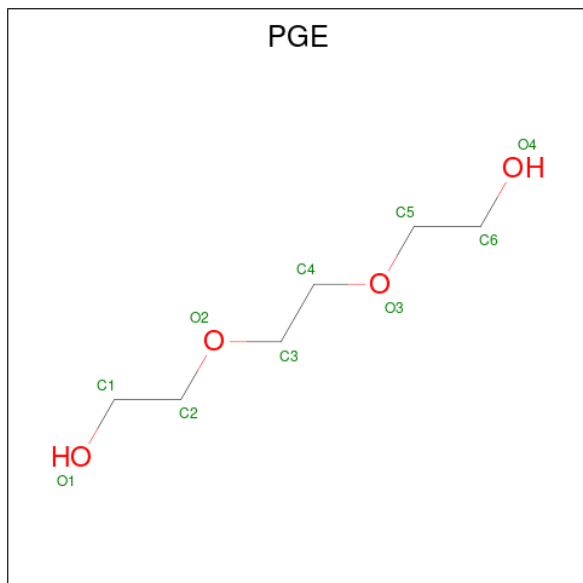
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

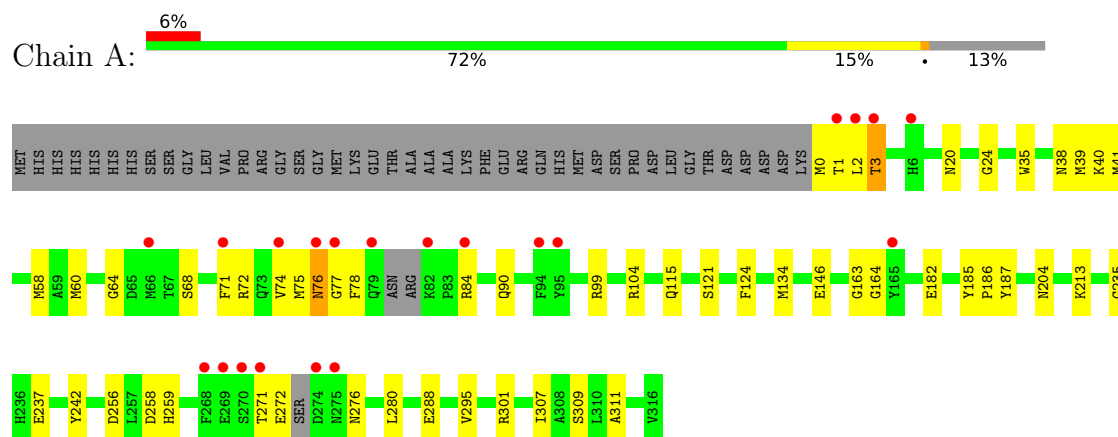
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	225	Total	O	0	5
			230	230		

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	42.22Å 67.58Å 103.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.56 – 1.46 25.56 – 1.46	Depositor EDS
% Data completeness (in resolution range)	94.3 (25.56-1.46) 94.3 (25.56-1.46)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 1.46Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.192 , 0.237 (Not available) , 0.248	Depositor DCC
R_{free} test set	2000 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.999	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5415	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EOH, PEG, EDO, PGE, GOL

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	0.39	0/2702	0.60	0/3635

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	2585	2429	2468	71	1
2	A	6	6	8	0	0
3	A	36	72	72	16	0
4	A	7	10	10	1	0
5	A	4	6	6	4	0
6	A	10	14	14	24	0
7	A	230	0	0	13	0
All	All	2878	2537	2578	78	1

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 15.

All (78) 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:84:ARG:NH1	7:A:501:HOH:O	2.02	0.90
1:A:0:MET:HE2	1:A:1:THR:HG22	1.52	0.89
1:A:77:GLY:O	6:A:416:PGE:O4	2.00	0.77
1:A:74:VAL:O	6:A:416:PGE:H12	1.86	0.76
1:A:76:ASN:HB2	6:A:416:PGE:H42	1.66	0.76
1:A:182:GLU:OE1	3:A:413:EOH:H22	1.91	0.69
1:A:0:MET:HE3	1:A:0:MET:HA	1.75	0.69
3:A:413:EOH:H21	7:A:602:HOH:O	1.93	0.66
1:A:41[B]:MET:SD	1:A:58:MET:HE1	2.35	0.66
1:A:77:GLY:HA2	1:A:258:ASP:HA	1.78	0.66
1:A:307:ILE:O	7:A:528[B]:HOH:O	2.15	0.65
1:A:276:ASN:OD1	7:A:502:HOH:O	2.14	0.64
1:A:0:MET:HE2	1:A:1:THR:H	1.64	0.62
1:A:134[B]:MET:HE3	1:A:204:ASN:H	1.63	0.61
1:A:74:VAL:O	6:A:416:PGE:H22	1.99	0.61
1:A:213:LYS:HD2	1:A:213:LYS:N	2.15	0.61
1:A:182:GLU:OE1	3:A:413:EOH:C2	2.49	0.60
1:A:90:GLN:OE1	7:A:503:HOH:O	2.16	0.59
3:A:412:EOH:H12	7:A:559:HOH:O	2.02	0.59
1:A:115:GLN:HE22	6:A:416:PGE:C2	2.16	0.58
1:A:24:GLY:O	7:A:504:HOH:O	2.18	0.56
1:A:39:MET:HE2	1:A:60:MET:HE3	1.88	0.55
1:A:182:GLU:HG2	3:A:412:EOH:O	2.06	0.55
1:A:74:VAL:O	6:A:416:PGE:C1	2.55	0.54
1:A:121:SER:H	6:A:416:PGE:H2	1.73	0.54
1:A:1:THR:HG23	3:A:410:EOH:H11	1.90	0.53
1:A:187:TYR:O	5:A:415:EDO:H22	2.08	0.53
1:A:0:MET:HG3	1:A:1:THR:N	2.25	0.52
1:A:40[B]:LYS:CE	7:A:512:HOH:O	2.58	0.52
1:A:3:THR:HA	3:A:410:EOH:C2	2.41	0.50
1:A:121:SER:OG	6:A:416:PGE:H32	2.09	0.50
1:A:74:VAL:O	6:A:416:PGE:C2	2.59	0.50
1:A:38:ASN:OD1	3:A:408:EOH:H23	2.12	0.50
1:A:77:GLY:C	6:A:416:PGE:O4	2.54	0.49
1:A:213:LYS:HE2	1:A:309:SER:O	2.12	0.49
1:A:164:GLY:H	6:A:416:PGE:C5	2.26	0.49
1:A:75[B]:MET:HA	6:A:416:PGE:H12	1.95	0.48
1:A:75[A]:MET:HA	6:A:416:PGE:H12	1.95	0.48
1:A:38:ASN:OD1	3:A:408:EOH:C2	2.62	0.48
1:A:164:GLY:O	6:A:416:PGE:C6	2.62	0.48
1:A:164:GLY:O	6:A:416:PGE:H62	2.14	0.47
1:A:60:MET:SD	1:A:64:GLY:HA3	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:OE1	3:A:413:EOH:O	2.19	0.47
1:A:124:PHE:HE1	3:A:413:EOH:H12	1.79	0.47
1:A:163:GLY:CA	6:A:416:PGE:H5	2.45	0.47
1:A:213:LYS:NZ	1:A:311:ALA:H	2.13	0.46
1:A:35:TRP:CZ2	1:A:39:MET:CE	2.98	0.46
1:A:2:LEU:O	1:A:3:THR:C	2.58	0.46
1:A:237:GLU:HG2	3:A:408:EOH:H22	1.99	0.45
1:A:259:HIS:HA	6:A:416:PGE:HO1	1.82	0.45
1:A:213:LYS:CE	1:A:309:SER:C	2.90	0.45
5:A:415:EDO:H11	7:A:584:HOH:O	2.16	0.45
1:A:71:PHE:HZ	1:A:235:GLY:HA2	1.82	0.45
1:A:213:LYS:HE3	1:A:309:SER:C	2.42	0.45
1:A:259:HIS:ND1	6:A:416:PGE:H1	2.31	0.45
1:A:271:THR:OG1	1:A:272:GLU:N	2.49	0.45
1:A:68:SER:O	1:A:72:ARG:HD3	2.17	0.44
1:A:1:THR:OG1	3:A:410:EOH:O	2.22	0.44
1:A:35:TRP:CZ2	1:A:39:MET:HE3	2.52	0.44
1:A:237:GLU:HG3	7:A:668[A]:HOH:O	2.18	0.43
1:A:104:ARG:NH2	1:A:280[A]:LEU:HD21	2.32	0.43
4:A:414:PEG:H32	7:A:547:HOH:O	2.17	0.43
1:A:164:GLY:H	6:A:416:PGE:H52	1.84	0.43
1:A:78:PHE:CE1	6:A:416:PGE:H62	2.54	0.42
1:A:259:HIS:ND1	6:A:416:PGE:C1	2.83	0.42
1:A:187:TYR:O	5:A:415:EDO:C2	2.67	0.42
1:A:259:HIS:HA	6:A:416:PGE:O1	2.19	0.42
1:A:124:PHE:CE1	3:A:413:EOH:H12	2.55	0.42
1:A:242:TYR:CZ	1:A:295:VAL:HG23	2.55	0.42
1:A:288:GLU:HB3	7:A:539:HOH:O	2.20	0.42
1:A:115:GLN:HE22	6:A:416:PGE:H2	1.85	0.41
3:A:406:EOH:C2	5:A:415:EDO:O1	2.68	0.41
3:A:413:EOH:C2	7:A:692:HOH:O	2.68	0.41
1:A:99:ARG:NH2	1:A:272:GLU:OE1	2.53	0.41
1:A:256:ASP:OD1	1:A:256:ASP:N	2.53	0.40
1:A:35:TRP:CH2	1:A:39:MET:HE3	2.56	0.40
1:A:185:TYR:N	1:A:186[B]:PRO:HD3	2.37	0.40

All (1) 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:20:ASN:OD1	1:A:301:ARG:HE[1_455]	1.57	0.03

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	325/360 (90%)	310 (95%)	13 (4%)	2 (1%)	21 6

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	76	ASN

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
3	EOH	A	412	-	2,2,2	0.45	0	1,1,1	0.10	0
3	EOH	A	407	-	2,2,2	0.46	0	1,1,1	0.04	0
4	PEG	A	414	-	6,6,6	0.45	0	5,5,5	0.57	0
5	EDO	A	415	-	3,3,3	0.30	0	2,2,2	0.34	0
3	EOH	A	408	-	2,2,2	0.40	0	1,1,1	0.31	0
3	EOH	A	410	-	2,2,2	0.47	0	1,1,1	0.07	0
3	EOH	A	413	-	2,2,2	0.37	0	1,1,1	0.08	0
3	EOH	A	406	-	2,2,2	0.39	0	1,1,1	0.15	0
3	EOH	A	405	-	2,2,2	0.49	0	1,1,1	0.19	0
3	EOH	A	411	-	2,2,2	0.43	0	1,1,1	0.13	0
3	EOH	A	402	-	2,2,2	0.43	0	1,1,1	0.33	0
3	EOH	A	409	-	2,2,2	0.37	0	1,1,1	0.06	0
6	PGE	A	416	-	9,9,9	0.43	0	8,8,8	1.26	1 (12%)
3	EOH	A	404	-	2,2,2	0.49	0	1,1,1	0.03	0
2	GOL	A	401	-	5,5,5	1.16	0	5,5,5	0.91	0
3	EOH	A	403	-	2,2,2	0.46	0	1,1,1	0.13	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
6	PGE	A	416	-	-	2/7/7/7	-
4	PEG	A	414	-	-	0/4/4/4	-
2	GOL	A	401	-	-	1/4/4/4	-
5	EDO	A	415	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	416	PGE	C5-O3-C4	-2.37	102.91	113.26

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	416	PGE	O2-C3-C4-O3
6	A	416	PGE	O1-C1-C2-O2
2	A	401	GOL	O1-C1-C2-C3
5	A	415	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	412	EOH	2	0
4	A	414	PEG	1	0
5	A	415	EDO	4	0
3	A	408	EOH	3	0
3	A	410	EOH	3	0
3	A	413	EOH	7	0
3	A	406	EOH	1	0
6	A	416	PGE	24	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	314/360 (87%)	0.66	21 (6%) 24 23	10, 25, 64, 88	17 (5%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	LEU	5.2
1	A	271	THR	4.4
1	A	1	THR	4.2
1	A	71	PHE	3.7
1	A	3	THR	3.4
1	A	275	ASN	3.3
1	A	84	ARG	3.1
1	A	95	TYR	2.8
1	A	74	VAL	2.8
1	A	94	PHE	2.8
1	A	270	SER	2.7
1	A	6	HIS	2.6
1	A	268	PHE	2.5
1	A	76	ASN	2.5
1	A	66	MET	2.4
1	A	82	LYS	2.3
1	A	165	TYR	2.3
1	A	77	GLY	2.1
1	A	274	ASP	2.1
1	A	79	GLN	2.1
1	A	269	GLU	2.1

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($\text{\AA}^2$)	Q<0.9
3	EOH	A	412	3/3	0.61	0.19	45,54,62,62	0
3	EOH	A	405	3/3	0.68	0.14	41,51,61,61	0
6	PGE	A	416	10/10	0.69	0.15	33,47,57,71	0
2	GOL	A	401	6/6	0.73	0.12	36,53,63,63	0
3	EOH	A	410	3/3	0.73	0.18	54,65,76,76	0
3	EOH	A	408	3/3	0.74	0.11	37,45,57,69	0
4	PEG	A	414	7/7	0.75	0.14	41,54,73,80	0
3	EOH	A	404	3/3	0.75	0.13	32,38,67,67	0
3	EOH	A	411	3/3	0.78	0.12	46,56,59,59	0
5	EDO	A	415	4/4	0.78	0.12	46,56,69,72	0
3	EOH	A	413	3/3	0.78	0.11	35,42,48,48	0
3	EOH	A	409	3/3	0.83	0.10	38,47,56,56	0
3	EOH	A	403	3/3	0.83	0.12	44,53,57,58	0
3	EOH	A	407	3/3	0.83	0.11	39,46,57,57	0
3	EOH	A	402	3/3	0.83	0.10	32,39,51,51	0
3	EOH	A	406	3/3	0.89	0.11	29,35,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.