



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 08:47 PM UTC

PDB ID : 21KB / pdb_000021kb
Title : Cystathionine beta-lyase from *Klebsiella pneumoniae*
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Deposited on : 2025-12-15
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

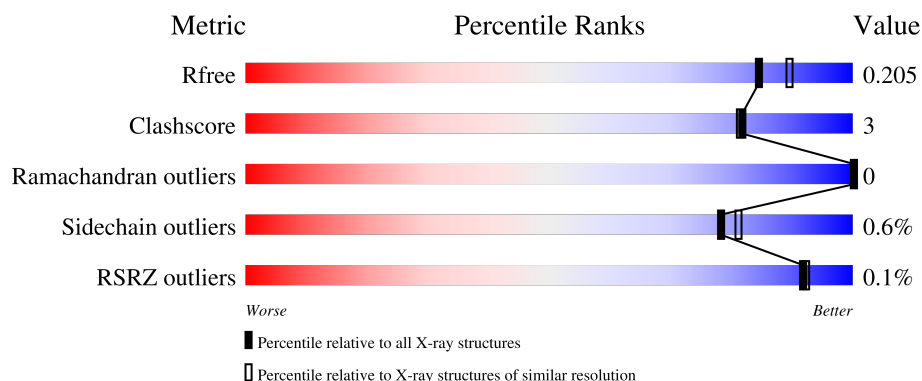
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	395	<div> <div>92%</div> <div>7% ..</div> </div>
1	B	395	<div> <div>91%</div> <div>7% ..</div> </div>
1	C	395	<div> <div>90%</div> <div>8% .</div> </div>
1	D	395	<div> <div>90%</div> <div>8% ..</div> </div>

2 Entry composition [i](#)

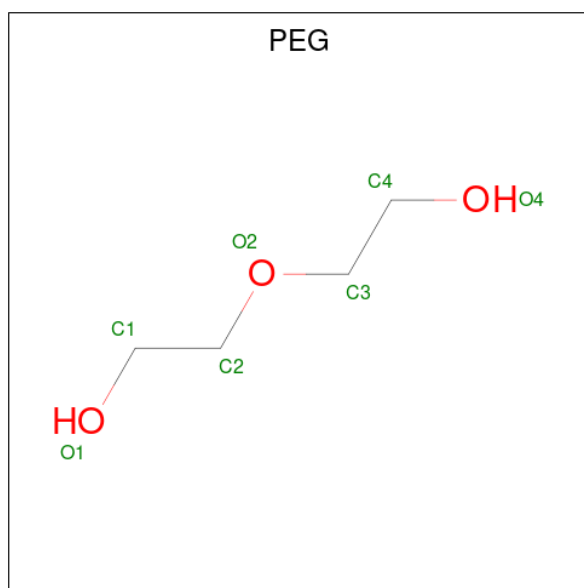
There are 4 unique types of molecules in this entry. The entry contains 13722 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 cysteine-S-conjugate beta-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	P	S	0	5	0
			3044	1922	537	569	1	15			
1	B	391	Total	C	N	O	P	S	0	6	0
			3045	1923	536	569	1	16			
1	C	391	Total	C	N	O	P	S	0	5	0
			3040	1923	534	567	1	15			
1	D	392	Total	C	N	O	P	S	0	2	0
			3032	1917	533	566	1	15			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



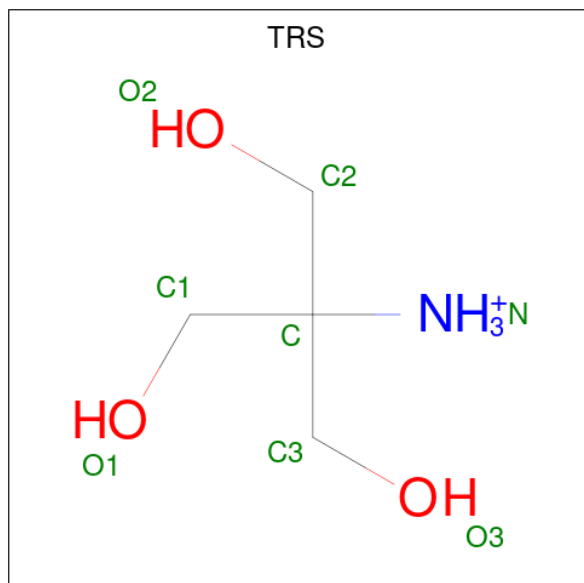
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			5	3	2		
2	B	1	Total	C	O	0	0
			5	3	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			6	4	2		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

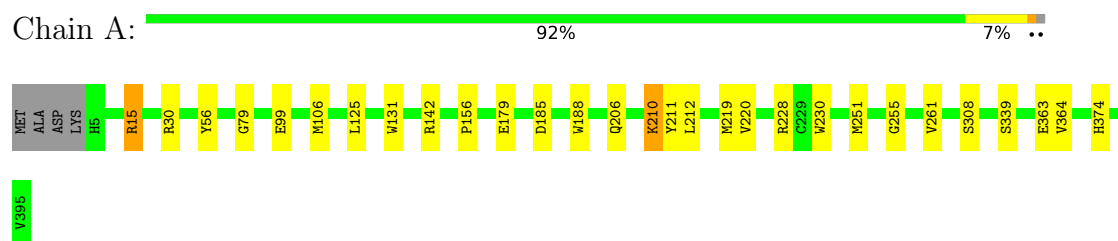
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	407	Total	O	0	0
			407	407		
4	B	388	Total	O	0	0
			388	388		
4	C	385	Total	O	0	0
			385	385		
4	D	353	Total	O	0	0
			353	353		

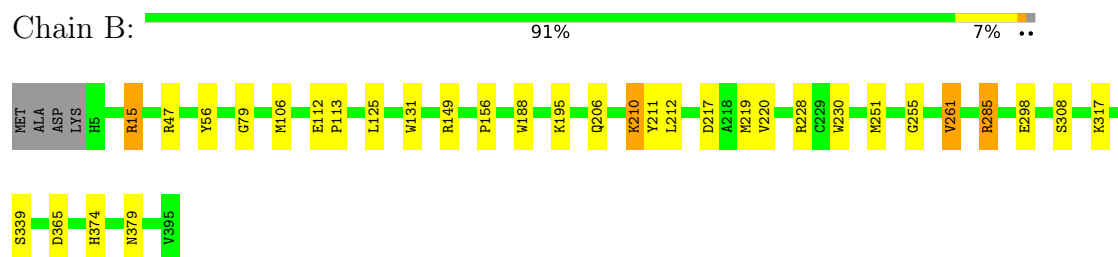
3 Residue-property plots [i](#)

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.

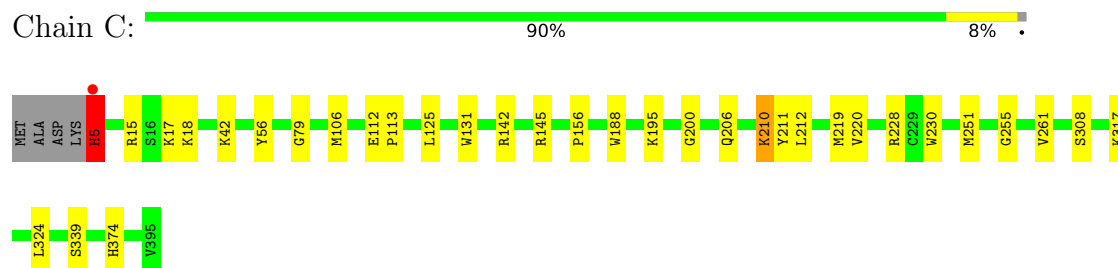
- Molecule 1: cysteine-S-conjugate beta-lyase



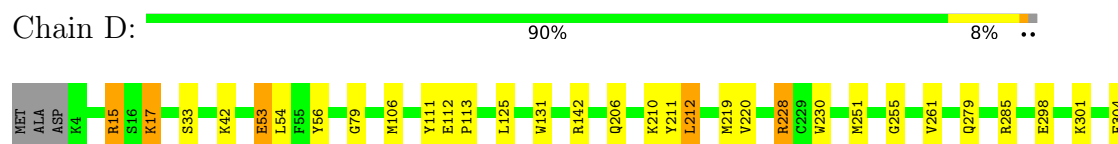
- Molecule 1: cysteine-S-conjugate beta-lyase



- Molecule 1: cysteine-S-conjugate beta-lyase



- Molecule 1: cysteine-S-conjugate beta-lyase



T306	
S308	
K317	
S339	
L348	
E363	
H374	
V395	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.42Å 131.21Å 84.57Å 90.00° 100.46° 90.00°	Depositor
Resolution (Å)	22.89 – 1.90 22.89 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (22.89-1.90) 98.0 (22.89-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.92 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.166 , 0.205 0.166 , 0.205	Depositor DCC
R_{free} test set	6918 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	12.1	Xtriage
Anisotropy	0.744	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13722	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.50% 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: LLP, TRS, PEG

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	0.80	0/3107	1.19	11/4214 (0.3%)
1	B	0.80	0/3114	1.18	12/4222 (0.3%)
1	C	0.74	0/3103	1.16	11/4208 (0.3%)
1	D	0.74	0/3080	1.18	16/4178 (0.4%)
All	All	0.77	0/12404	1.18	50/16822 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	1
1	D	0	2
All	All	0	9

There are no bond length outliers.

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	15	ARG	CD-NE-CZ	12.03	141.24	124.40
1	C	15	ARG	CD-NE-CZ	11.50	140.50	124.40
1	A	15	ARG	CD-NE-CZ	11.43	140.41	124.40
1	B	15	ARG	CD-NE-CZ	11.03	139.84	124.40
1	B	15	ARG	NE-CZ-NH2	-10.25	109.98	119.20

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ARG	Sidechain
1	A	15	ARG	Sidechain
1	B	149[A]	ARG	Sidechain
1	B	149[B]	ARG	Sidechain
1	B	15	ARG	Sidechain

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	3044	0	2990	15	0
1	B	3045	0	2991	19	0
1	C	3040	0	2989	22	0
1	D	3032	0	2978	20	0
2	A	5	0	5	0	0
2	B	5	0	5	0	0
2	C	4	0	5	0	0
2	D	6	0	7	1	0
3	B	8	0	12	0	0
4	A	407	0	0	1	0
4	B	388	0	0	5	0
4	C	385	0	0	4	0
4	D	353	0	0	2	0
All	All	13722	0	11982	61	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 3.

The worst 5 of 61 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:C:195:LYS:HD2	4:C:602:HOH:O	1.80	0.80
1:B:379[B]:ASN:OD1	1:C:5:HIS:HB3	1.94	0.68
1:B:285:ARG:HD2	4:B:836:HOH:O	1.95	0.67
1:B:379[B]:ASN:CG	1:C:5:HIS:HB3	2.25	0.62
1:D:42:LYS:HE2	4:D:789:HOH:O	2.05	0.56

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	393/395 (100%)	382 (97%)	11 (3%)	0	100	100
1	B	394/395 (100%)	383 (97%)	11 (3%)	0	100	100
1	C	393/395 (100%)	382 (97%)	11 (3%)	0	100	100
1	D	391/395 (99%)	381 (97%)	10 (3%)	0	100	100
All	All	1571/1580 (99%)	1528 (97%)	43 (3%)	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	317/315 (101%)	316 (100%)	1 (0%)	86	88
1	B	317/315 (101%)	316 (100%)	1 (0%)	86	88
1	C	316/315 (100%)	313 (99%)	3 (1%)	70	73
1	D	313/315 (99%)	310 (99%)	3 (1%)	68	70
All	All	1263/1260 (100%)	1255 (99%)	8 (1%)	78	81

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	279	GLN
1	D	220	VAL
1	C	220	VAL
1	C	17	LYS
1	D	53	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	384	GLN
1	D	226	ASN
1	D	357	HIS
1	D	242	GLN
1	B	242	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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
1	LLP	B	210	1	23,24,25	0.71	1 (4%)	25,32,34	1.21	4 (16%)
1	LLP	A	210	1	23,24,25	0.82	1 (4%)	25,32,34	1.27	3 (12%)
1	LLP	D	210	1	23,24,25	0.79	0	25,32,34	0.92	0
1	LLP	C	210	1	23,24,25	0.68	0	25,32,34	1.26	3 (12%)

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
1	LLP	B	210	1	-	2/16/17/19	0/1/1/1
1	LLP	A	210	1	-	2/16/17/19	0/1/1/1
1	LLP	D	210	1	-	2/16/17/19	0/1/1/1
1	LLP	C	210	1	-	2/16/17/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	LLP	P-OP1	2.39	1.57	1.50
1	B	210	LLP	P-OP1	2.31	1.57	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	210	LLP	C4-C3-C2	-3.92	117.94	120.14
1	A	210	LLP	C4-C3-C2	-2.82	118.55	120.14
1	A	210	LLP	CG-CD-CE	2.71	122.80	113.38
1	B	210	LLP	C4-C3-C2	-2.54	118.72	120.14
1	C	210	LLP	CG-CD-CE	2.32	121.44	113.38

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	210	LLP	O-C-CA-CB
1	B	210	LLP	O-C-CA-CB
1	C	210	LLP	O-C-CA-CB
1	D	210	LLP	O-C-CA-CB
1	A	210	LLP	CA-CB-CG-CD

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	210	LLP	1	0
1	A	210	LLP	2	0
1	D	210	LLP	1	0
1	C	210	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	PEG	D	401	-	5,5,6	0.41	0	4,4,5	0.33	0
2	PEG	C	401	-	3,3,6	0.21	0	2,2,5	0.38	0
2	PEG	A	401	-	4,4,6	0.21	0	3,3,5	0.22	0
2	PEG	B	401	-	4,4,6	0.37	0	3,3,5	0.33	0
3	TRS	B	402	-	7,7,7	0.38	0	9,9,9	1.36	2 (22%)

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	PEG	D	401	-	-	1/3/3/4	-
2	PEG	C	401	-	-	1/1/1/4	-
2	PEG	A	401	-	-	2/2/2/4	-
2	PEG	B	401	-	-	1/2/2/4	-
3	TRS	B	402	-	-	6/9/9/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	TRS	O2-C2-C	-2.38	104.24	110.88
3	B	402	TRS	C2-C-C1	-2.27	104.60	110.66

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	TRS	N-C-C1-O1
3	B	402	TRS	N-C-C2-O2
3	B	402	TRS	C2-C-C1-O1
3	B	402	TRS	C1-C-C2-O2
2	A	401	PEG	O2-C3-C4-O4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	390/395 (98%)	-0.65	0 100 100	5, 10, 23, 41	5 (1%)
1	B	390/395 (98%)	-0.59	0 100 100	5, 11, 24, 37	7 (1%)
1	C	390/395 (98%)	-0.51	1 (0%) 90 91	6, 13, 25, 50	6 (1%)
1	D	391/395 (98%)	-0.31	0 100 100	6, 16, 29, 45	2 (0%)
All	All	1561/1580 (98%)	-0.51	1 (0%) 92 92	5, 12, 26, 50	20 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	HIS	2.4

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	A	210	24/25	0.98	0.04	6,7,9,9	0
1	LLP	C	210	24/25	0.98	0.04	8,11,15,16	0
1	LLP	D	210	24/25	0.98	0.05	9,11,14,18	0
1	LLP	B	210	24/25	0.99	0.04	6,8,12,14	0

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	PEG	D	401	6/7	0.74	0.28	16,18,19,21	6
2	PEG	C	401	4/7	0.78	0.31	19,20,20,22	4
2	PEG	B	401	5/7	0.80	0.21	16,16,17,18	5
3	TRS	B	402	8/8	0.82	0.21	8,10,11,11	8
2	PEG	A	401	5/7	0.89	0.20	11,12,13,15	5

6.5 Other polymers [i](#)

There are no such residues in this entry.