



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:57 AM UTC

PDB ID : 3NRE / pdb_00003nre
Title : Crystal structure of a Putative aldose 1-epimerase (b2544) from ES-CHERICHIA COLI K12 at 1.59 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2010-06-30
Resolution : 1.59 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

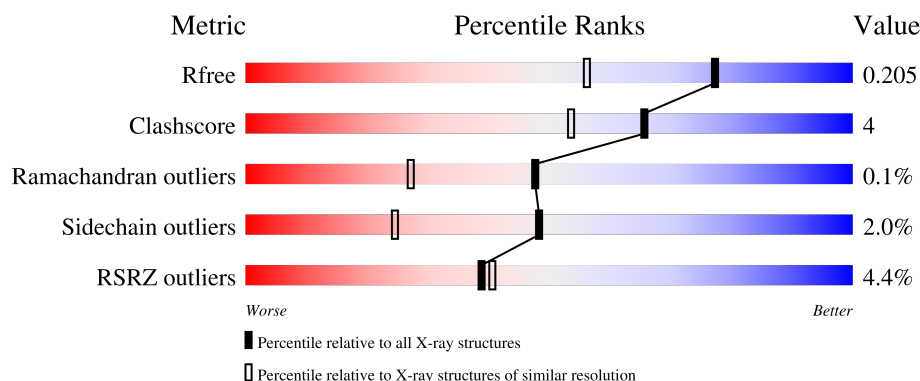
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	291	4% 92% 8%
1	B	291	5% 93% 6%
1	C	291	4% 90% 9%
1	D	291	4% 94% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10985 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.

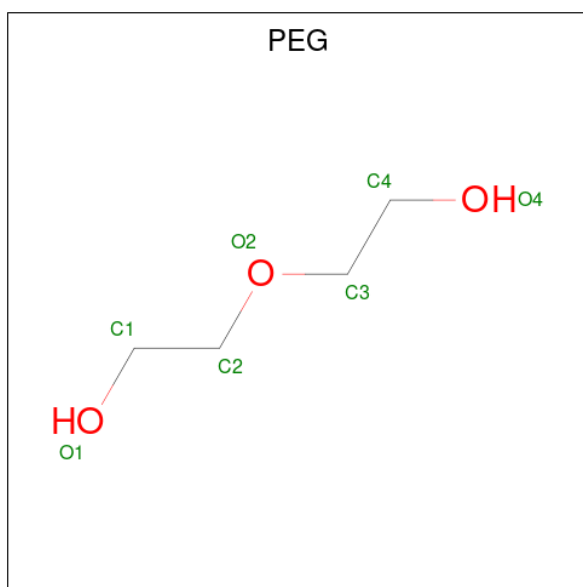
- Molecule 1 is a protein called Aldose 1-epimerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	Se	0	22	0
			2409	1549	404	443	7	6			
1	B	291	Total	C	N	O	S	Se	0	23	0
			2415	1558	402	444	7	4			
1	C	291	Total	C	N	O	S	Se	0	31	0
			2454	1600	403	439	7	5			
1	D	291	Total	C	N	O	S	Se	0	26	0
			2446	1575	406	454	7	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP C9QPM9
B	0	GLY	-	expression tag	UNP C9QPM9
C	0	GLY	-	expression tag	UNP C9QPM9
D	0	GLY	-	expression tag	UNP C9QPM9

- 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
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		

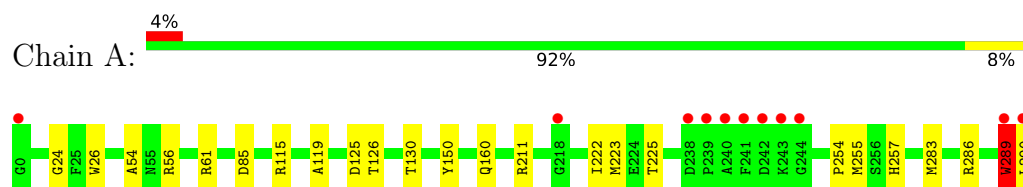
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	237	Total	O	0	13
			248	248		
4	B	259	Total	O	0	11
			268	268		
4	C	319	Total	O	0	12
			330	330		
4	D	279	Total	O	0	9
			288	288		

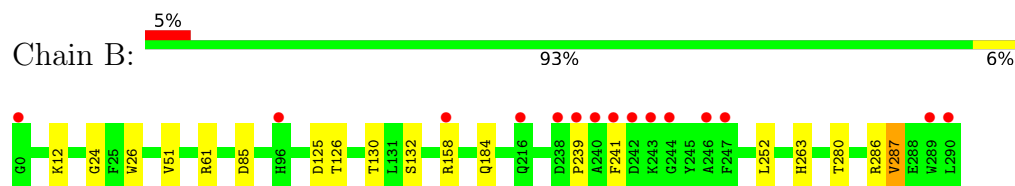
3 Residue-property plots [i](#)

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.

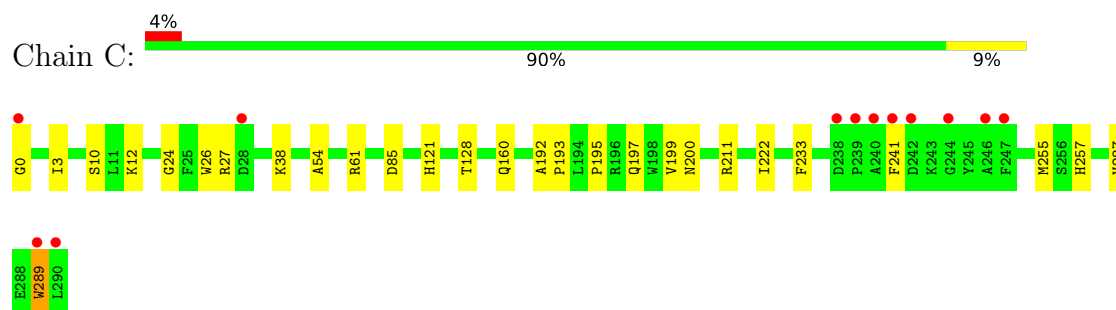
- Molecule 1: Aldose 1-epimerase



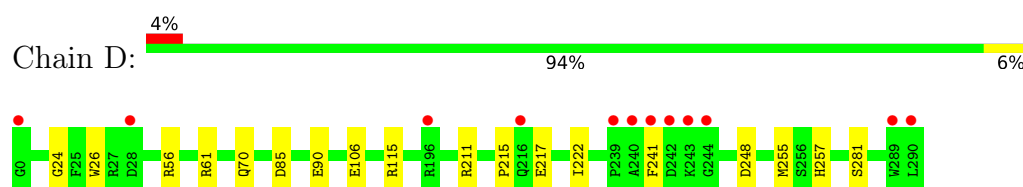
- Molecule 1: Aldose 1-epimerase



- Molecule 1: Aldose 1-epimerase



- Molecule 1: Aldose 1-epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.73Å 72.00Å 272.79Å 90.00° 90.70° 90.00°	Depositor
Resolution (Å)	28.54 – 1.59 28.54 – 1.59	Depositor EDS
% Data completeness (in resolution range)	98.7 (28.54-1.59) 98.7 (28.54-1.59)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.5.0110, PHENIX	Depositor
R, R_{free}	0.161 , 0.190 (Not available) , 0.205	Depositor DCC
R_{free} test set	9534 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.033 for k,h,-l 0.030 for -k,-h,-l 0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10985	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: PEG, MG

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	0.91	0/2549	0.86	1/3472 (0.0%)
1	B	0.93	1/2559 (0.0%)	0.85	0/3488
1	C	1.07	0/2623	0.91	1/3571 (0.0%)
1	D	0.92	0/2595	0.85	0/3535
All	All	0.96	1/10326 (0.0%)	0.87	2/14066 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	51	VAL	CA-CB	5.70	1.61	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	TRP	N-CA-C	-5.70	101.85	110.28
1	C	241	PHE	N-CA-C	-5.34	105.88	112.72

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	2409	0	2285	23	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2415	0	2307	18	0
1	C	2454	0	2376	24	0
1	D	2446	0	2321	9	1
2	A	42	0	60	4	0
2	B	28	0	40	4	0
2	C	21	0	30	1	0
2	D	35	0	50	2	0
3	D	1	0	0	0	0
4	A	248	0	0	1	0
4	B	268	0	0	3	0
4	C	330	0	0	5	0
4	D	288	0	0	3	0
All	All	10985	0	9469	74	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 4.

All (74) 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:255[B]:MSE:HE1	4:C:410:HOH:O	1.61	1.00
1:B:287[B]:VAL:HG22	2:B:304:PEG:H22	1.52	0.90
1:C:211[B]:ARG:NH1	1:C:222[B]:ILE:HD11	1.91	0.85
1:A:223[B]:MSE:HE1	1:A:254:PRO:HG3	1.65	0.79
1:D:106[B]:GLU:OE1	1:D:115[B]:ARG:NH1	2.18	0.75
1:A:119:ALA:HB3	1:A:130[B]:THR:HG22	1.75	0.67
1:C:211[B]:ARG:NH1	1:C:222[B]:ILE:CD1	2.57	0.67
1:C:200:ASN:OD1	1:C:233[B]:PHE:HE2	1.79	0.66
1:D:255:MSE:HE2	1:D:257:HIS:O	1.95	0.66
1:A:119:ALA:HB3	1:A:130[B]:THR:CG2	2.26	0.65
1:A:223[B]:MSE:HE1	1:A:254:PRO:CG	2.27	0.65
1:B:125:ASP:OD1	1:B:126[A]:THR:HG23	1.97	0.65
1:B:158[B]:ARG:HH11	1:B:158[B]:ARG:CG	2.10	0.64
1:C:54:ALA:HB1	1:C:255[B]:MSE:HE2	1.81	0.63
1:A:56:ARG:HH22	2:A:310:PEG:C3	2.14	0.61
1:C:0[B]:GLY:N	4:C:1336[B]:HOH:O	2.33	0.61
1:C:200:ASN:OD1	1:C:233[B]:PHE:CE2	2.53	0.61
1:C:24:GLY:HA3	1:C:26:TRP:CH2	2.36	0.60
1:B:130[B]:THR:HG23	4:B:494:HOH:O	2.03	0.59
1:A:150:TYR:OH	2:A:316:PEG:H41	2.02	0.58
1:C:211[B]:ARG:HH12	1:C:222[B]:ILE:HD11	1.64	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158[B]:ARG:HH11	1:B:158[B]:ARG:HG2	1.66	0.58
1:C:193[B]:PRO:HB3	4:C:664:HOH:O	2.04	0.57
1:B:132[A]:SER:HB2	1:B:280[A]:THR:HG22	1.87	0.56
1:C:211[B]:ARG:HH11	1:C:222[B]:ILE:CD1	2.18	0.56
1:B:132[A]:SER:CB	1:B:280[A]:THR:HG22	2.36	0.56
1:C:121:HIS:HB3	1:C:128[B]:THR:HG22	1.88	0.56
1:A:56:ARG:HH22	2:A:310:PEG:H31	1.70	0.55
1:A:223[B]:MSE:CE	1:A:254:PRO:HG3	2.36	0.55
1:A:223[B]:MSE:HE1	1:A:254:PRO:CB	2.36	0.55
1:B:126[A]:THR:HG22	1:B:286:ARG:CB	2.37	0.55
1:D:90[A]:GLU:OE2	4:D:1335:HOH:O	2.18	0.54
1:C:192:ALA:HB1	1:C:193[A]:PRO:HD2	1.90	0.54
1:D:24:GLY:HA3	1:D:26:TRP:CH2	2.44	0.53
1:A:24:GLY:HA3	1:A:26:TRP:CH2	2.44	0.53
1:C:255[B]:MSE:HG3	1:C:257:HIS:O	2.09	0.52
1:A:223[B]:MSE:HE1	1:A:254:PRO:HB3	1.91	0.52
1:D:56:ARG:HH22	2:D:313:PEG:H31	1.75	0.52
1:C:54:ALA:CB	1:C:255[B]:MSE:HE2	2.40	0.52
1:B:126[A]:THR:HG22	1:B:286:ARG:HB2	1.92	0.51
1:A:160[B]:GLN:OE1	4:A:1194:HOH:O	2.19	0.51
1:D:211:ARG:NH1	4:D:1299:HOH:O	2.35	0.50
1:A:223[B]:MSE:HE2	1:A:225:THR:HG23	1.94	0.50
1:B:287[B]:VAL:HG21	2:B:304:PEG:O1	2.12	0.49
1:B:12[B]:LYS:NZ	2:B:303:PEG:O1	2.42	0.49
1:A:289:TRP:N	1:A:289:TRP:HE3	2.11	0.49
1:C:255[A]:MSE:HE2	1:C:257:HIS:O	2.13	0.49
1:A:126[A]:THR:HG22	1:A:286:ARG:CB	2.42	0.49
1:B:287[B]:VAL:HG13	2:B:304:PEG:H32	1.95	0.48
1:C:12[A]:LYS:NZ	2:C:311:PEG:H31	2.29	0.48
1:A:126[A]:THR:HG22	1:A:286:ARG:HB2	1.95	0.48
1:C:128[B]:THR:HG23	4:C:348:HOH:O	2.13	0.48
1:A:211[A]:ARG:HH11	1:A:222:ILE:HD11	1.80	0.46
1:B:24:GLY:HA3	1:B:26:TRP:CH2	2.50	0.46
1:D:70[B]:GLN:NE2	4:D:579:HOH:O	2.48	0.46
1:A:223[B]:MSE:HE3	1:A:283:MSE:HG3	1.97	0.46
1:A:223[B]:MSE:HE3	1:A:283:MSE:SE	2.66	0.46
1:C:287[B]:VAL:HG13	1:C:289:TRP:CZ3	2.51	0.45
1:B:158[B]:ARG:HG2	1:B:158[B]:ARG:NH1	2.32	0.45
1:D:211:ARG:NH1	1:D:222[B]:ILE:HD11	2.31	0.45
1:B:158[B]:ARG:CG	1:B:158[B]:ARG:NH1	2.75	0.45
1:C:10:SER:OG	1:C:27[B]:ARG:NE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LEU:HD23	1:B:252:LEU:C	2.42	0.44
1:C:3[B]:ILE:HD12	1:C:38:LYS:HD3	1.98	0.44
1:C:12[B]:LYS:HE3	1:C:26:TRP:CZ3	2.53	0.44
1:A:125:ASP:OD1	1:A:126[A]:THR:HG23	2.17	0.44
1:C:160[B]:GLN:NE2	4:C:1069:HOH:O	2.50	0.44
1:A:255:MSE:HE2	1:A:257:HIS:O	2.18	0.43
1:B:263[B]:HIS:ND1	4:B:431[B]:HOH:O	2.36	0.42
1:D:56:ARG:HH22	2:D:313:PEG:C3	2.33	0.42
1:C:195:PRO:HG2	1:C:199:VAL:HG21	2.01	0.41
1:A:54:ALA:HB3	1:A:255:MSE:HE3	2.01	0.41
1:A:56:ARG:HH22	2:A:310:PEG:H32	1.85	0.41
1:B:280[A]:THR:HG23	4:B:1181:HOH:O	2.19	0.41

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:115[B]:ARG:NH2	1:D:215:PRO:O[3_455]	2.15	0.05

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	310/291 (106%)	299 (96%)	11 (4%)	0	100	100
1	B	311/291 (107%)	298 (96%)	12 (4%)	1 (0%)	36	20
1	C	319/291 (110%)	311 (98%)	8 (2%)	0	100	100
1	D	314/291 (108%)	306 (98%)	8 (2%)	0	100	100
All	All	1254/1164 (108%)	1214 (97%)	39 (3%)	1 (0%)	48	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	239	PRO

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	258/241 (107%)	254 (98%)	4 (2%)	55	33
1	B	262/241 (109%)	256 (98%)	6 (2%)	44	20
1	C	265/241 (110%)	260 (98%)	5 (2%)	50	27
1	D	265/241 (110%)	259 (98%)	6 (2%)	44	20
All	All	1050/964 (109%)	1029 (98%)	21 (2%)	48	24

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	85	ASP
1	A	289	TRP
1	A	290	LEU
1	B	61	ARG
1	B	85	ASP
1	B	184	GLN
1	B	241	PHE
1	B	287[A]	VAL
1	B	287[B]	VAL
1	C	61	ARG
1	C	85	ASP
1	C	197[A]	GLN
1	C	197[B]	GLN
1	C	289	TRP
1	D	61	ARG
1	D	85	ASP
1	D	217	GLU
1	D	241	PHE
1	D	248	ASP
1	D	281	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	201	ASN
1	C	201	ASN
1	D	136	GLN
1	D	197	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	PEG	D	302	-	6,6,6	0.53	0	5,5,5	0.43	0
2	PEG	B	312	-	6,6,6	0.58	0	5,5,5	0.57	0
2	PEG	A	307	-	6,6,6	0.71	0	5,5,5	0.55	0
2	PEG	A	308	-	6,6,6	0.61	0	5,5,5	0.50	0
2	PEG	A	318	-	6,6,6	0.70	0	5,5,5	0.49	0
2	PEG	B	303	-	6,6,6	0.66	0	5,5,5	0.95	0
2	PEG	B	305	-	6,6,6	0.40	0	5,5,5	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEG	D	306	-	6,6,6	0.91	0	5,5,5	0.98	0
2	PEG	D	314	-	6,6,6	0.66	0	5,5,5	0.44	0
2	PEG	D	317	-	6,6,6	0.71	0	5,5,5	0.56	0
2	PEG	C	315	-	6,6,6	0.76	0	5,5,5	0.12	0
2	PEG	C	311	-	6,6,6	0.44	0	5,5,5	0.66	0
2	PEG	B	304	-	6,6,6	0.67	0	5,5,5	0.61	0
2	PEG	A	310	-	6,6,6	0.96	0	5,5,5	1.06	1 (20%)
2	PEG	A	309	-	6,6,6	0.52	0	5,5,5	0.62	0
2	PEG	D	313	-	6,6,6	0.99	0	5,5,5	0.91	0
2	PEG	C	301	-	6,6,6	0.48	0	5,5,5	0.71	0
2	PEG	A	316	-	6,6,6	0.98	0	5,5,5	1.05	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	PEG	D	302	-	-	1/4/4/4	-
2	PEG	B	312	-	-	0/4/4/4	-
2	PEG	A	307	-	-	1/4/4/4	-
2	PEG	A	308	-	-	3/4/4/4	-
2	PEG	A	318	-	-	3/4/4/4	-
2	PEG	B	303	-	-	1/4/4/4	-
2	PEG	B	305	-	-	1/4/4/4	-
2	PEG	D	306	-	-	2/4/4/4	-
2	PEG	D	314	-	-	2/4/4/4	-
2	PEG	D	317	-	-	0/4/4/4	-
2	PEG	C	315	-	-	0/4/4/4	-
2	PEG	C	311	-	-	3/4/4/4	-
2	PEG	B	304	-	-	3/4/4/4	-
2	PEG	A	310	-	-	4/4/4/4	-
2	PEG	A	309	-	-	1/4/4/4	-
2	PEG	D	313	-	-	4/4/4/4	-
2	PEG	C	301	-	-	3/4/4/4	-
2	PEG	A	316	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	310	PEG	O2-C3-C4	2.22	119.89	110.11

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	308	PEG	O2-C3-C4-O4
2	D	313	PEG	O1-C1-C2-O2
2	A	307	PEG	O2-C3-C4-O4
2	A	310	PEG	O2-C3-C4-O4
2	A	316	PEG	O2-C3-C4-O4
2	A	318	PEG	O2-C3-C4-O4
2	C	311	PEG	O1-C1-C2-O2
2	B	304	PEG	O1-C1-C2-O2
2	B	304	PEG	O2-C3-C4-O4
2	C	301	PEG	O2-C3-C4-O4
2	D	306	PEG	O2-C3-C4-O4
2	B	305	PEG	O2-C3-C4-O4
2	C	301	PEG	O1-C1-C2-O2
2	C	311	PEG	O2-C3-C4-O4
2	D	314	PEG	O2-C3-C4-O4
2	B	303	PEG	O2-C3-C4-O4
2	D	302	PEG	O1-C1-C2-O2
2	D	314	PEG	O1-C1-C2-O2
2	D	313	PEG	C4-C3-O2-C2
2	A	308	PEG	O1-C1-C2-O2
2	A	310	PEG	C4-C3-O2-C2
2	B	304	PEG	C1-C2-O2-C3
2	A	309	PEG	O2-C3-C4-O4
2	A	316	PEG	C4-C3-O2-C2
2	A	310	PEG	O1-C1-C2-O2
2	A	318	PEG	C1-C2-O2-C3
2	A	310	PEG	C1-C2-O2-C3
2	A	308	PEG	C4-C3-O2-C2
2	A	318	PEG	C4-C3-O2-C2
2	D	313	PEG	O2-C3-C4-O4
2	D	313	PEG	C1-C2-O2-C3
2	C	311	PEG	C1-C2-O2-C3
2	C	301	PEG	C1-C2-O2-C3
2	D	306	PEG	C4-C3-O2-C2

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	303	PEG	1	0
2	C	311	PEG	1	0
2	B	304	PEG	3	0
2	A	310	PEG	3	0
2	D	313	PEG	2	0
2	A	316	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	287/291 (98%)	0.46	11 (3%)	44 46	15, 28, 47, 78	20 (6%)
1	B	287/291 (98%)	0.19	15 (5%)	33 33	9, 25, 46, 67	23 (8%)
1	C	287/291 (98%)	-0.04	12 (4%)	40 42	9, 19, 33, 57	30 (10%)
1	D	287/291 (98%)	0.15	12 (4%)	40 42	12, 24, 42, 58	26 (9%)
All	All	1148/1164 (98%)	0.19	50 (4%)	39 40	9, 24, 44, 78	99 (8%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	PHE	8.4
1	A	290	LEU	6.7
1	D	241	PHE	6.7
1	A	289	TRP	6.6
1	C	240	ALA	6.5
1	C	241	PHE	6.1
1	B	241	PHE	6.0
1	B	0[A]	GLY	5.8
1	C	289	TRP	5.2
1	A	240	ALA	5.2
1	B	240	ALA	5.1
1	D	240	ALA	4.9
1	B	290	LEU	4.7
1	C	0[A]	GLY	4.3
1	B	239	PRO	3.8
1	B	289	TRP	3.7
1	A	0[A]	GLY	3.6
1	C	239	PRO	3.6
1	C	242	ASP	3.5
1	D	216[A]	GLN	3.4
1	B	242	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	289	TRP	3.1
1	A	239	PRO	3.1
1	B	243	LYS	3.1
1	D	239	PRO	2.9
1	D	290	LEU	2.9
1	A	242	ASP	2.8
1	C	247	PHE	2.8
1	D	244	GLY	2.8
1	C	290	LEU	2.7
1	D	0[A]	GLY	2.6
1	A	218	GLY	2.5
1	C	244	GLY	2.5
1	C	246	ALA	2.5
1	D	28	ASP	2.5
1	D	243	LYS	2.4
1	B	246	ALA	2.4
1	B	244	GLY	2.3
1	C	238	ASP	2.3
1	B	247	PHE	2.3
1	A	238[A]	ASP	2.2
1	D	242	ASP	2.2
1	A	244	GLY	2.2
1	C	28	ASP	2.2
1	B	158[A]	ARG	2.2
1	D	196	ARG	2.1
1	A	243	LYS	2.1
1	B	216	GLN	2.1
1	B	238	ASP	2.0
1	B	96	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

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	313	7/7	0.73	0.17	31,34,46,48	0
2	PEG	B	304	7/7	0.75	0.16	34,40,46,51	0
2	PEG	D	314	7/7	0.80	0.15	37,40,42,44	0
2	PEG	C	301	7/7	0.81	0.14	36,41,45,51	0
2	PEG	D	306	7/7	0.84	0.14	36,41,52,53	0
2	PEG	A	307	7/7	0.84	0.13	36,40,46,47	0
2	PEG	A	318	7/7	0.84	0.14	34,43,47,48	0
2	PEG	D	302	7/7	0.85	0.13	35,38,46,49	0
2	PEG	B	312	7/7	0.85	0.13	33,34,41,42	0
2	PEG	A	308	7/7	0.86	0.14	39,44,45,46	0
2	PEG	C	311	7/7	0.86	0.13	34,38,48,48	0
2	PEG	A	316	7/7	0.87	0.12	30,37,42,43	0
2	PEG	A	309	7/7	0.87	0.12	39,41,43,45	0
2	PEG	A	310	7/7	0.88	0.13	28,34,44,47	0
2	PEG	C	315	7/7	0.88	0.13	29,33,45,45	0
2	PEG	B	305	7/7	0.88	0.12	37,39,45,48	0
2	PEG	B	303	7/7	0.90	0.12	34,37,45,47	0
2	PEG	D	317	7/7	0.92	0.11	30,38,47,49	0
3	MG	D	300	1/1	0.95	0.15	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.