



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2017 – 10:39 AM EDT

PDB ID : 5UZS
Title : Crystal Structure of Inosine 5'-monophosphate Dehydrogenase from *Clostridium perfringens* Complexed with IMP and P200
Authors : Maltseva, N.; Kim, Y.; Mulligan, R.; Makowska-Grzyska, M.; Gu, M.; Gollapalli, D.R.; Hedstrom, L.; Joachimiak, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : unknown
Resolution : 2.37 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

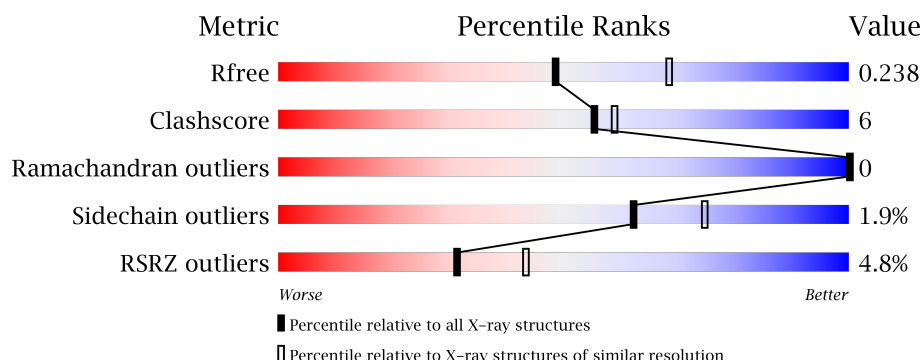
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	363	<div> <div>7%</div> <div>81%</div> <div>14%</div> <div>• •</div> </div>
1	B	363	<div> <div>5%</div> <div>80%</div> <div>14%</div> <div>• 5%</div> </div>
1	C	363	<div> <div>3%</div> <div>85%</div> <div>10%</div> <div>• •</div> </div>
1	D	363	<div> <div>2%</div> <div>84%</div> <div>11%</div> <div>•</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PGE	B	504	-	-	-	X
5	PEG	C	502	-	-	-	X
5	PEG	D	503	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 10821 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 Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	3	0
			2585	1623	449	491	22			
1	B	345	Total	C	N	O	S	0	2	0
			2559	1606	443	490	20			
1	C	347	Total	C	N	O	S	0	4	0
			2594	1627	449	498	20			
1	D	347	Total	C	N	O	S	0	8	0
			2632	1650	459	502	21			

There are 24 discrepancies between the modelled and reference sequences:

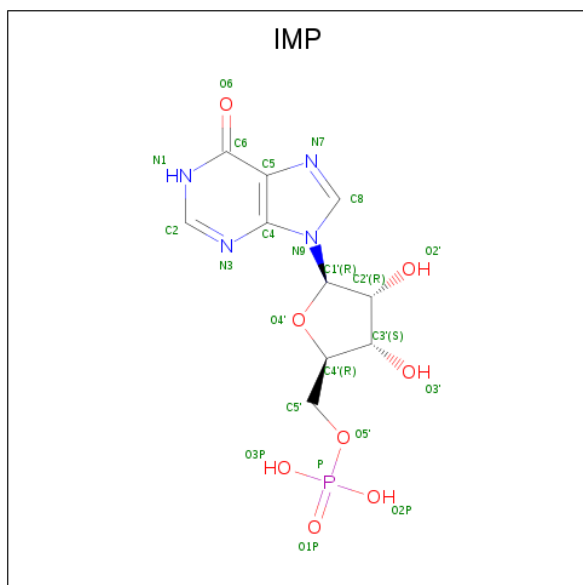
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0A0H2YRZ7
A	-1	ASN	-	expression tag	UNP A0A0H2YRZ7
A	0	ALA	-	expression tag	UNP A0A0H2YRZ7
A	89	SER	-	linker	UNP A0A0H2YRZ7
A	90	GLY	-	linker	UNP A0A0H2YRZ7
A	91	GLY	-	linker	UNP A0A0H2YRZ7
B	-2	SER	-	expression tag	UNP A0A0H2YRZ7
B	-1	ASN	-	expression tag	UNP A0A0H2YRZ7
B	0	ALA	-	expression tag	UNP A0A0H2YRZ7
B	89	SER	-	linker	UNP A0A0H2YRZ7
B	90	GLY	-	linker	UNP A0A0H2YRZ7
B	91	GLY	-	linker	UNP A0A0H2YRZ7
C	-2	SER	-	expression tag	UNP A0A0H2YRZ7
C	-1	ASN	-	expression tag	UNP A0A0H2YRZ7
C	0	ALA	-	expression tag	UNP A0A0H2YRZ7
C	89	SER	-	linker	UNP A0A0H2YRZ7
C	90	GLY	-	linker	UNP A0A0H2YRZ7
C	91	GLY	-	linker	UNP A0A0H2YRZ7
D	-2	SER	-	expression tag	UNP A0A0H2YRZ7
D	-1	ASN	-	expression tag	UNP A0A0H2YRZ7
D	0	ALA	-	expression tag	UNP A0A0H2YRZ7

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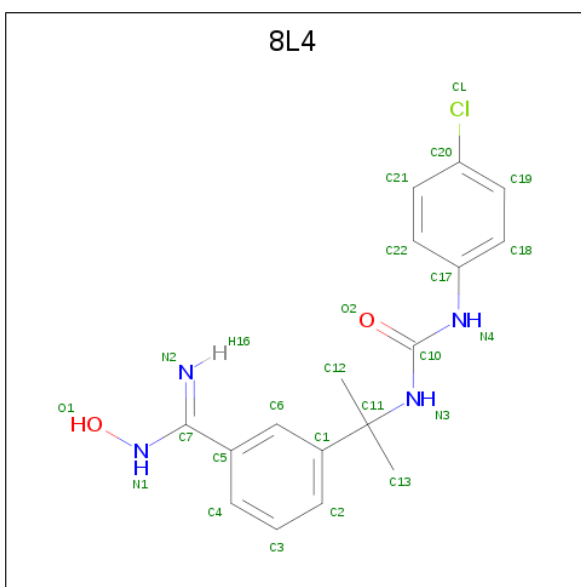
Chain	Residue	Modelled	Actual	Comment	Reference
D	89	SER	-	linker	UNP A0A0H2YRZ7
D	90	GLY	-	linker	UNP A0A0H2YRZ7
D	91	GLY	-	linker	UNP A0A0H2YRZ7

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: C₁₀H₁₃N₄O₈P).



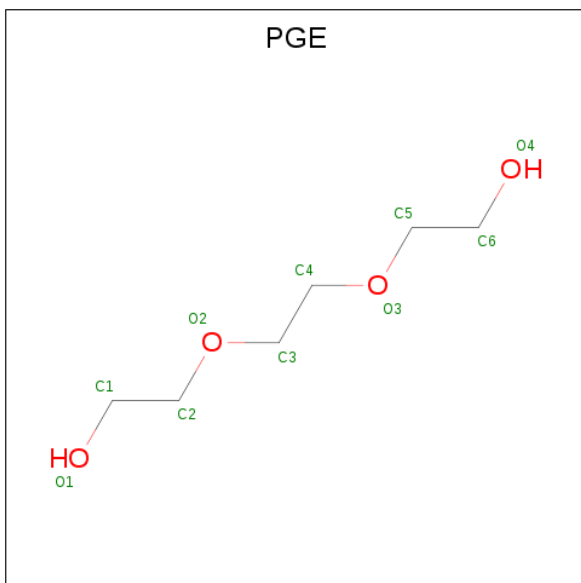
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is 3-(2-[[[(4-chlorophenyl)carbamoyl]amino]propan-2-yl]-N-hydroxybenzene-1-carboximidamide (three-letter code: 8L4) (formula: C₁₇H₁₉ClN₄O₂).



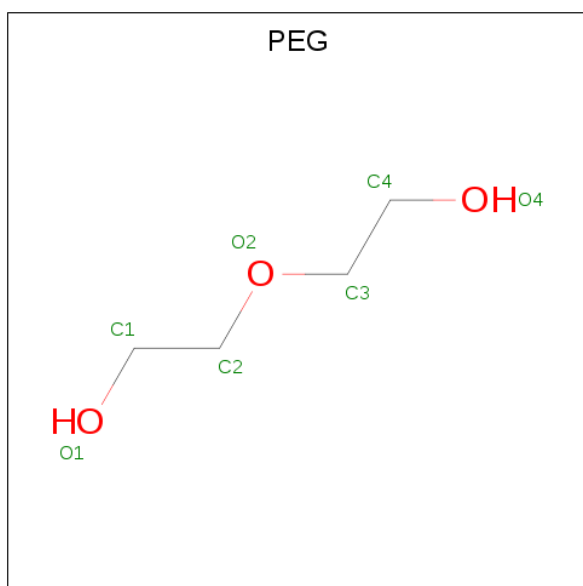
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			24	17	1	4	2		
3	B	1	Total	C	Cl	N	O	0	0
			24	17	1	4	2		
3	C	1	Total	C	Cl	N	O	0	0
			24	17	1	4	2		
3	D	1	Total	C	Cl	N	O	0	0
			24	17	1	4	2		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



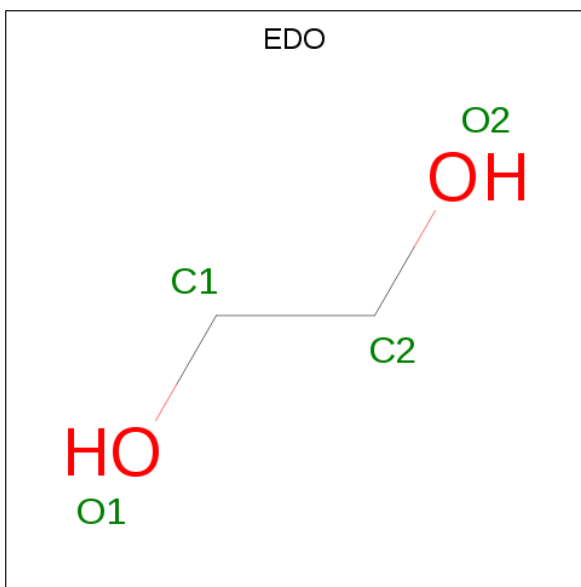
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 10 6 4	0	0
4	B	1	Total C O 10 6 4	0	0
4	C	1	Total C O 10 6 4	0	0
4	C	1	Total C O 10 6 4	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

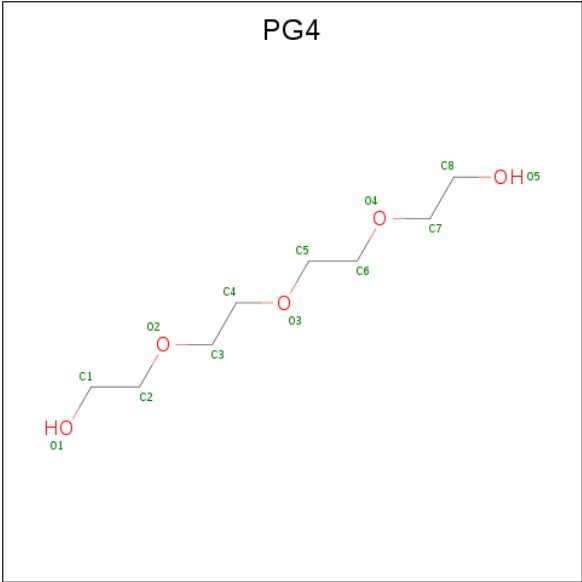
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	K	0	0
			1	1		
8	C	1	Total	K	0	0
			1	1		

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			13	8	5		

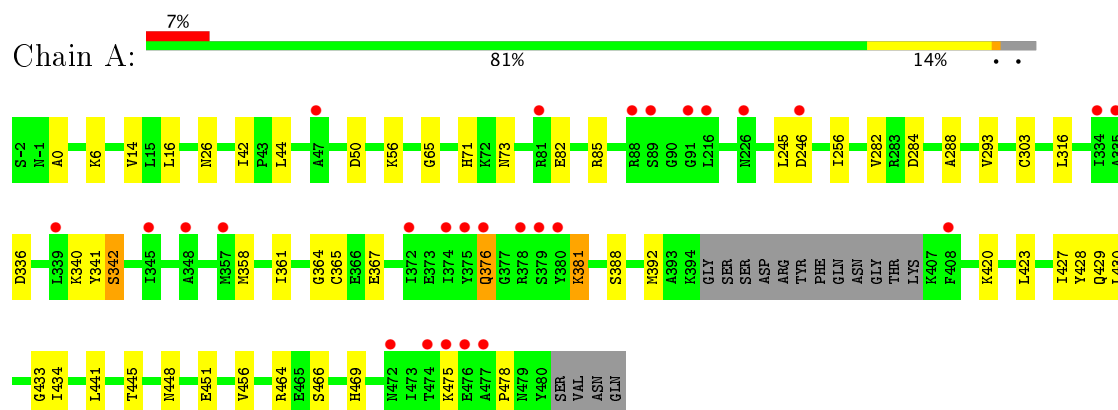
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	15	Total	O	0	0
			15	15		
10	B	30	Total	O	0	0
			30	30		
10	C	48	Total	O	0	0
			48	48		
10	D	54	Total	O	0	0
			54	54		

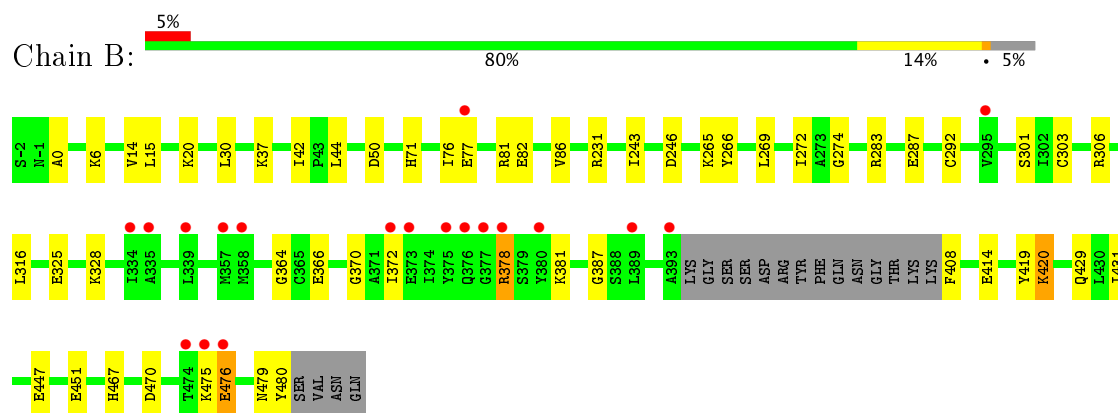
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

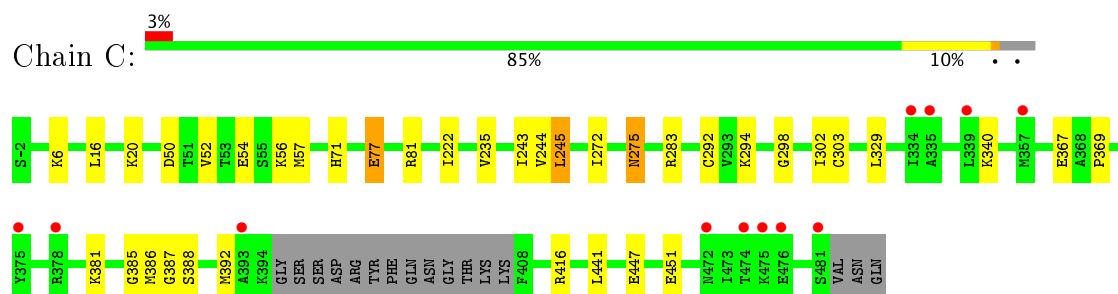
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



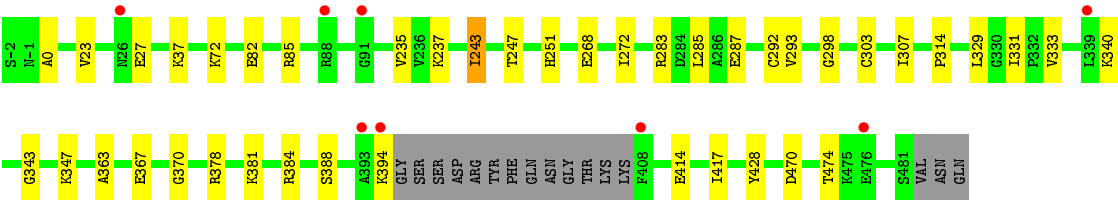
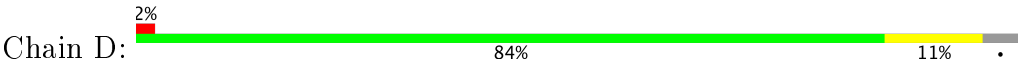
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



- Molecule 1: Inosine-5'-monophosphate dehydrogenase



● Molecule 1: Inosine-5'-monophosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	111.12Å 144.40Å 87.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.09 – 2.37 31.09 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.5 (31.09-2.37) 98.5 (31.09-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.36Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.170 , 0.238 0.169 , 0.238	Depositor DCC
R_{free} test set	2838 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10821	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: MG, PGE, K, EDO, IMP, PG4, ALY, PEG, 8L4

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	0.36	0/2608	0.56	0/3514
1	B	0.40	0/2580	0.57	0/3480
1	C	0.41	0/2615	0.60	0/3526
1	D	0.43	0/2653	0.60	0/3576
All	All	0.40	0/10456	0.58	0/14096

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 [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	2585	0	2657	34	0
1	B	2559	0	2621	40	0
1	C	2594	0	2654	38	0
1	D	2632	0	2697	30	0
2	A	23	0	11	3	0
2	B	23	0	11	3	0
2	C	23	0	11	3	0
2	D	23	0	11	2	0
3	A	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	0	0	0
3	C	24	0	0	0	0
3	D	24	0	0	0	0
4	A	20	0	28	2	0
4	B	10	0	14	0	0
4	C	20	0	28	3	0
5	A	7	0	10	2	0
5	B	7	0	10	1	0
5	C	7	0	10	0	0
5	D	21	0	30	1	0
6	B	4	0	6	1	0
6	C	4	0	6	0	0
7	B	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	D	13	0	18	0	0
10	A	15	0	0	0	0
10	B	30	0	0	1	0
10	C	48	0	0	1	0
10	D	54	0	0	2	0
All	All	10821	0	10833	127	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 6.

All (127) 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:272[B]:ILE:HD11	1:C:294:LYS:HB2	1.70	0.71
1:B:364:GLY:HA3	1:B:420:LYS:HD3	1.72	0.70
1:C:303:CYS:SG	2:C:500:IMP:H2	2.32	0.69
1:C:386:MET:HE2	1:C:386:MET:HA	1.73	0.68
1:A:365:CYS:O	1:A:381:LYS:NZ	2.27	0.67
1:A:303:CYS:SG	2:A:500:IMP:H2	2.34	0.67
1:C:272[A]:ILE:HG12	1:C:292:CYS:HB3	1.79	0.65
1:A:429:GLN:HE21	1:A:478:PRO:HB2	1.62	0.64
1:D:329:LEU:HB2	1:D:331[B]:ILE:HG22	1.81	0.62
1:C:54:GLU:HG3	1:C:369:PRO:HG3	1.82	0.62
1:B:303:CYS:SG	2:B:500:IMP:H2	2.42	0.60
1:D:303:CYS:SG	2:D:500:IMP:H2	2.42	0.59
1:B:366:GLU:HG3	1:B:372:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:TYR:CE2	5:A:504:PEG:H31	2.37	0.58
1:A:475:LYS:HB2	1:B:414:GLU:HG3	1.86	0.58
1:B:14:VAL:HG21	1:B:316:LEU:HD22	1.86	0.57
1:B:265:LYS:HD3	1:B:266:TYR:CE2	2.40	0.57
1:D:384:ARG:HH22	1:D:394:LYS:HD3	1.69	0.56
1:C:6:LYS:NZ	4:C:503:PGE:H22	2.21	0.56
1:A:14:VAL:HG21	1:A:316:LEU:HD22	1.87	0.56
1:A:358[B]:MET:HG2	1:A:361:ILE:HD12	1.86	0.56
1:B:6:LYS:HA	6:B:503:EDO:H11	1.89	0.55
1:B:20:LYS:HG3	1:D:251:HIS:CD2	2.41	0.55
1:C:6:LYS:HZ2	4:C:503:PGE:H3	1.72	0.55
1:D:23:VAL:HG23	1:D:27:GLU:HB2	1.89	0.54
1:A:56:LYS:HE2	1:A:367:GLU:HA	1.90	0.54
1:D:235:VAL:HG21	1:D:243[A]:ILE:HD11	1.89	0.54
1:C:56:LYS:HD3	1:C:367:GLU:HA	1.90	0.54
1:C:77[A]:GLU:O	1:C:81:ARG:HG3	2.07	0.54
1:A:303:CYS:SG	2:A:500:IMP:C2	2.97	0.53
1:D:82:GLU:OE1	1:D:85:ARG:NH1	2.41	0.53
1:A:50:ASP:HA	1:A:71:HIS:CD2	2.44	0.53
1:B:246:ASP:HA	1:B:274:GLY:O	2.08	0.53
1:D:370:GLY:O	1:D:381:LYS:NZ	2.42	0.52
1:B:467:HIS:HA	1:D:307:ILE:HD11	1.91	0.52
1:A:82:GLU:OE1	1:A:85:ARG:NH2	2.43	0.52
1:B:30:LEU:HD13	1:B:431:ILE:HD12	1.91	0.52
1:C:303:CYS:SG	2:C:500:IMP:C2	2.97	0.52
1:C:244:VAL:HG22	1:C:272[B]:ILE:HG23	1.92	0.52
1:D:283:ARG:O	1:D:287:GLU:HG2	2.10	0.52
1:A:430:LEU:O	1:A:434:ILE:HG13	2.10	0.52
1:B:50:ASP:HA	1:B:71:HIS:CD2	2.45	0.51
1:C:244:VAL:HG13	1:C:272[B]:ILE:HD13	1.92	0.51
1:C:298:GLY:HA2	1:C:303:CYS:SG	2.51	0.51
1:B:476:GLU:HG2	1:B:476:GLU:O	2.10	0.51
1:B:82:GLU:O	1:B:86:VAL:HG23	2.11	0.50
1:D:247:THR:HG22	10:D:648:HOH:O	2.11	0.50
1:A:423:LEU:HG	1:A:427:ILE:HD13	1.94	0.50
1:B:470:ASP:OD1	1:D:340:LYS:HD2	2.12	0.49
1:A:6:LYS:HD3	4:A:502:PGE:H2	1.94	0.49
1:C:77[B]:GLU:O	1:C:81:ARG:HG3	2.11	0.49
1:B:325:GLU:HA	1:B:328:LYS:HD2	1.95	0.49
1:B:372:ILE:HG12	1:B:381:LYS:HD3	1.95	0.49
1:B:272:ILE:HG12	1:B:292:CYS:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283[B]:ARG:CZ	1:C:329:LEU:HD21	2.43	0.49
1:D:363:ALA:HB3	1:D:417:ILE:HD11	1.94	0.48
1:B:387:GLY:N	2:B:500:IMP:O6	2.37	0.48
1:C:6:LYS:HZ1	4:C:503:PGE:H22	1.79	0.48
1:B:447:GLU:O	1:B:451:GLU:HG3	2.14	0.47
1:C:369:PRO:HD3	10:C:632:HOH:O	2.14	0.47
1:A:282:VAL:HG22	1:A:293:VAL:HG21	1.95	0.47
1:A:429:GLN:NE2	1:A:478:PRO:HB2	2.29	0.47
1:B:303:CYS:SG	2:B:500:IMP:C2	3.02	0.47
1:A:364:GLY:HA3	1:A:420:LYS:HG3	1.97	0.47
1:D:343:GLY:O	1:D:347:LYS:HG3	2.15	0.47
1:C:275:ASN:HD21	1:C:294:LYS:NZ	2.12	0.46
1:D:37:LYS:O	1:D:37:LYS:HG3	2.15	0.46
1:A:336:ASP:OD1	2:A:500:IMP:O3'	2.29	0.46
1:A:376:GLN:HG3	1:A:376:GLN:O	2.16	0.46
1:B:77:GLU:HG3	1:B:81:ARG:CZ	2.46	0.46
1:C:275:ASN:HD21	1:C:294:LYS:HZ1	1.64	0.46
1:A:26:ASN:HD22	1:B:408:PHE:HE1	1.63	0.46
1:B:429:GLN:HE21	1:B:479:ASN:HB3	1.81	0.45
1:B:42:ILE:HD12	1:B:44:LEU:HD12	1.99	0.45
1:C:416:ARG:NE	1:D:474:THR:HG21	2.31	0.45
1:D:298:GLY:HA2	1:D:303:CYS:SG	2.57	0.45
1:B:480:TYR:CE1	1:D:307:ILE:HD13	2.51	0.45
1:D:367:GLU:OE1	1:D:367:GLU:N	2.50	0.44
1:A:256:ILE:HG23	1:A:288:ALA:HB2	2.00	0.44
1:A:451:GLU:HB3	1:B:0:ALA:HB1	1.99	0.44
1:D:428:TYR:CE2	5:D:502:PEG:H42	2.52	0.44
1:B:283:ARG:O	1:B:287:GLU:HG3	2.17	0.44
1:C:283[A]:ARG:CZ	1:C:329:LEU:HD21	2.48	0.44
1:C:52:VAL:O	1:C:57:MET:HG2	2.18	0.44
5:B:502:PEG:O4	10:B:601:HOH:O	2.21	0.44
1:C:244:VAL:HG22	1:C:272[B]:ILE:CG2	2.48	0.44
1:D:285:LEU:HD23	1:D:285:LEU:HA	1.89	0.44
1:A:42:ILE:HD12	1:A:44:LEU:HD12	1.99	0.43
1:B:243:ILE:HG12	1:B:269:LEU:HD21	1.99	0.43
1:B:370:GLY:O	1:B:381:LYS:NZ	2.51	0.43
1:C:388:SER:O	1:C:392:MET:HG3	2.19	0.43
1:A:0:ALA:HB1	1:C:451:GLU:HB3	2.00	0.43
1:C:447:GLU:O	1:C:451:GLU:HG3	2.19	0.43
1:A:388:SER:O	1:A:392:MET:HG3	2.19	0.43
1:A:445:THR:OG1	1:A:448:ASN:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:LYS:HG3	1:D:251:HIS:NE2	2.33	0.43
1:B:378:ARG:HD3	1:B:378:ARG:HA	1.69	0.43
1:C:387:GLY:N	2:C:500:IMP:O6	2.44	0.43
1:C:222:ILE:HG13	1:C:243:ILE:HG23	2.01	0.43
1:A:16:LEU:HD22	1:A:441:LEU:HD21	2.01	0.43
1:D:293:VAL:HG22	1:D:333:VAL:HG12	2.00	0.43
1:C:50:ASP:HA	1:C:71:HIS:CD2	2.54	0.42
1:A:342:SER:OG	1:A:433:GLY:HA3	2.19	0.42
1:B:372:ILE:HD13	1:B:419:TYR:CE1	2.54	0.42
1:D:272:ILE:HG12	1:D:292:CYS:HB3	2.01	0.42
1:D:303:CYS:SG	2:D:500:IMP:C2	3.06	0.42
1:D:388:SER:HB2	1:D:414[B]:GLU:HG2	2.01	0.42
1:C:50:ASP:H	1:C:386:MET:HE3	1.84	0.42
1:C:235:VAL:HG21	1:C:243:ILE:HD11	2.01	0.42
1:C:381:LYS:HE2	1:C:381:LYS:HB3	1.70	0.42
1:C:16:LEU:HD22	1:C:441:LEU:HD21	2.02	0.41
5:A:504:PEG:H11	1:B:408:PHE:HA	2.02	0.41
1:A:469:HIS:O	1:B:301:SER:HB2	2.21	0.41
1:A:466:SER:HA	1:B:306:ARG:HD2	2.03	0.41
1:C:302:ILE:HD13	1:C:385:GLY:HA2	2.02	0.41
1:A:284:ASP:OD2	1:C:20:LYS:HE3	2.21	0.41
1:A:56:LYS:CE	1:A:367:GLU:HA	2.51	0.41
1:C:245:LEU:HD23	1:C:245:LEU:HA	1.82	0.41
1:B:451:GLU:HB3	1:D:0:ALA:HB1	2.03	0.40
1:C:340:LYS:NZ	1:D:470:ASP:OD1	2.26	0.40
1:B:76:ILE:HG23	1:B:231:ARG:HA	2.03	0.40
1:C:56:LYS:CD	1:C:367:GLU:HA	2.50	0.40
1:D:72:LYS:HG2	10:D:622:HOH:O	2.20	0.40
1:B:372:ILE:HD13	1:B:419:TYR:CZ	2.57	0.40
1:A:340:LYS:HE2	1:A:341:TYR:CZ	2.56	0.40
1:A:65:GLY:HA2	4:A:503:PGE:H22	2.02	0.40
1:B:15:LEU:HD12	1:D:314:PRO:HD3	2.03	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	345/363 (95%)	333 (96%)	12 (4%)	0	100	100
1	B	342/363 (94%)	332 (97%)	10 (3%)	0	100	100
1	C	346/363 (95%)	337 (97%)	9 (3%)	0	100	100
1	D	350/363 (96%)	340 (97%)	10 (3%)	0	100	100
All	All	1383/1452 (95%)	1342 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	270/281 (96%)	261 (97%)	9 (3%)	43	54
1	B	267/281 (95%)	262 (98%)	5 (2%)	62	75
1	C	271/281 (96%)	267 (98%)	4 (2%)	70	81
1	D	275/281 (98%)	269 (98%)	6 (2%)	57	70
All	All	1083/1124 (96%)	1059 (98%)	24 (2%)	62	70

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	245	LEU
1	A	246	ASP
1	A	342	SER
1	A	376	GLN
1	A	381	LYS
1	A	456	VAL
1	A	464[A]	ARG

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Mol	Chain	Res	Type
1	A	464[B]	ARG
1	B	37	LYS
1	B	378	ARG
1	B	420	LYS
1	B	475	LYS
1	B	476	GLU
1	C	77[A]	GLU
1	C	77[B]	GLU
1	C	245	LEU
1	C	275	ASN
1	D	237	LYS
1	D	243[A]	ILE
1	D	243[B]	ILE
1	D	268[A]	GLU
1	D	268[B]	GLU
1	D	378	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	41	ASN
1	A	73	ASN
1	B	73	ASN
1	B	429	GLN
1	B	452	ASN
1	C	41	ASN
1	C	275	ASN

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	ALY	A	327	1	8,8,12	0.99	1 (12%)	5,8,14	1.01	1 (20%)
1	ALY	B	327	1	10,10,12	0.64	0	6,10,14	0.96	1 (16%)
1	ALY	C	327	1	10,10,12	0.92	1 (10%)	6,10,14	0.91	1 (16%)
1	ALY	D	327	1	10,10,12	0.91	1 (10%)	6,10,14	1.27	1 (16%)

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	ALY	A	327	1	-	0/5/7/12	0/0/0/0
1	ALY	B	327	1	-	0/7/9/12	0/0/0/0
1	ALY	C	327	1	-	0/7/9/12	0/0/0/0
1	ALY	D	327	1	-	1/7/9/12	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	ALY	CA-C	2.11	1.53	1.50
1	C	327	ALY	CA-C	2.16	1.53	1.50
1	D	327	ALY	CA-C	2.16	1.53	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	327	ALY	O-C-CA	-2.29	118.71	125.02
1	B	327	ALY	O-C-CA	-2.19	118.98	125.02
1	A	327	ALY	O-C-CA	-2.12	119.16	125.02
1	C	327	ALY	O-C-CA	-2.05	119.35	125.02

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	327	ALY	OH-CH-NZ-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 3 are monoatomic - leaving 22 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	IMP	A	500	-	21,25,25	0.85	0	22,38,38	2.28	5 (22%)
3	8L4	A	501	-	25,25,25	1.03	3 (12%)	33,35,35	1.01	2 (6%)
4	PGE	A	502	-	9,9,9	0.64	0	8,8,8	0.35	0
4	PGE	A	503	-	9,9,9	0.57	0	8,8,8	0.35	0
5	PEG	A	504	-	6,6,6	0.52	0	5,5,5	0.15	0
2	IMP	B	500	-	21,25,25	0.92	0	22,38,38	2.20	3 (13%)
3	8L4	B	501	-	25,25,25	1.05	2 (8%)	33,35,35	1.06	4 (12%)
5	PEG	B	502	-	6,6,6	0.48	0	5,5,5	0.21	0
6	EDO	B	503	-	3,3,3	0.49	0	2,2,2	0.38	0
4	PGE	B	504	-	9,9,9	0.59	0	8,8,8	0.22	0
2	IMP	C	500	-	21,25,25	0.87	0	22,38,38	2.27	5 (22%)
3	8L4	C	501	-	25,25,25	1.11	2 (8%)	33,35,35	1.10	2 (6%)
5	PEG	C	502	-	6,6,6	0.52	0	5,5,5	0.33	0
4	PGE	C	503	-	9,9,9	0.58	0	8,8,8	0.49	0
6	EDO	C	504	-	3,3,3	0.43	0	2,2,2	0.47	0
4	PGE	C	505	-	9,9,9	0.51	0	8,8,8	0.23	0
2	IMP	D	500	-	21,25,25	1.00	0	22,38,38	2.14	4 (18%)
3	8L4	D	501	-	25,25,25	1.09	3 (12%)	33,35,35	1.03	2 (6%)
5	PEG	D	502	-	6,6,6	0.43	0	5,5,5	0.34	0
5	PEG	D	503	-	6,6,6	0.41	0	5,5,5	0.40	0
5	PEG	D	504	-	6,6,6	0.50	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PG4	D	505	-	12,12,12	0.52	0	11,11,11	0.33	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	IMP	A	500	-	-	0/6/26/26	0/3/3/3
3	8L4	A	501	-	-	0/19/21/21	0/2/2/2
4	PGE	A	502	-	-	0/7/7/7	0/0/0/0
4	PGE	A	503	-	-	0/7/7/7	0/0/0/0
5	PEG	A	504	-	-	0/4/4/4	0/0/0/0
2	IMP	B	500	-	-	0/6/26/26	0/3/3/3
3	8L4	B	501	-	-	0/19/21/21	0/2/2/2
5	PEG	B	502	-	-	0/4/4/4	0/0/0/0
6	EDO	B	503	-	-	0/1/1/1	0/0/0/0
4	PGE	B	504	-	-	0/7/7/7	0/0/0/0
2	IMP	C	500	-	-	0/6/26/26	0/3/3/3
3	8L4	C	501	-	-	0/19/21/21	0/2/2/2
5	PEG	C	502	-	-	0/4/4/4	0/0/0/0
4	PGE	C	503	-	-	0/7/7/7	0/0/0/0
6	EDO	C	504	-	-	0/1/1/1	0/0/0/0
4	PGE	C	505	-	-	0/7/7/7	0/0/0/0
2	IMP	D	500	-	-	0/6/26/26	0/3/3/3
3	8L4	D	501	-	-	0/19/21/21	0/2/2/2
5	PEG	D	502	-	-	0/4/4/4	0/0/0/0
5	PEG	D	503	-	-	0/4/4/4	0/0/0/0
5	PEG	D	504	-	-	0/4/4/4	0/0/0/0
9	PG4	D	505	-	-	0/10/10/10	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	8L4	C11-C1	-2.66	1.49	1.53
3	D	501	8L4	C17-N4	-2.56	1.36	1.41
3	A	501	8L4	C17-N4	-2.45	1.36	1.41
3	C	501	8L4	C17-N4	-2.36	1.37	1.41
3	B	501	8L4	C17-N4	-2.26	1.37	1.41
3	A	501	8L4	C11-C1	-2.26	1.50	1.53
3	D	501	8L4	C20-CL	2.04	1.79	1.74
3	C	501	8L4	C5-C7	2.20	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	8L4	C20-CL	2.28	1.79	1.74
3	A	501	8L4	C20-CL	2.35	1.79	1.74

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	IMP	N3-C2-N1	-8.75	121.24	128.86
2	C	500	IMP	N3-C2-N1	-8.67	121.31	128.86
2	D	500	IMP	N3-C2-N1	-8.28	121.65	128.86
2	A	500	IMP	N3-C2-N1	-7.96	121.92	128.86
3	C	501	8L4	C1-C11-N3	-3.29	105.40	110.35
2	C	500	IMP	C4-C5-N7	-2.58	106.91	109.41
2	B	500	IMP	C4-C5-N7	-2.51	106.98	109.41
2	A	500	IMP	C4-C5-N7	-2.41	107.08	109.41
3	B	501	8L4	C1-C11-N3	-2.30	106.89	110.35
3	D	501	8L4	C13-C11-C1	-2.15	104.47	110.68
2	C	500	IMP	C6-C5-C4	-2.14	118.72	120.84
3	B	501	8L4	C12-C11-C13	-2.09	106.75	109.73
2	D	500	IMP	C4-C5-N7	-2.02	107.46	109.41
3	A	501	8L4	C12-C11-N3	2.39	114.80	108.02
3	B	501	8L4	C12-C11-N3	2.40	114.83	108.02
2	D	500	IMP	P-O5'-C5'	2.52	125.24	118.30
3	D	501	8L4	C12-C11-N3	2.68	115.60	108.02
3	A	501	8L4	C5-C7-N1	2.72	118.86	114.77
2	B	500	IMP	C2-N1-C6	2.73	120.47	115.91
2	D	500	IMP	C2-N1-C6	2.76	120.52	115.91
2	A	500	IMP	C2-N1-C6	2.80	120.58	115.91
2	C	500	IMP	P-O5'-C5'	2.84	126.12	118.30
3	B	501	8L4	C5-C7-N1	2.85	119.06	114.77
3	C	501	8L4	C12-C11-N3	2.86	116.13	108.02
2	C	500	IMP	C2-N1-C6	2.97	120.86	115.91
2	A	500	IMP	P-O5'-C5'	3.46	127.82	118.30
2	A	500	IMP	O3P-P-O5'	3.47	115.96	106.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	IMP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	PGE	1	0
4	A	503	PGE	1	0
5	A	504	PEG	2	0
2	B	500	IMP	3	0
5	B	502	PEG	1	0
6	B	503	EDO	1	0
2	C	500	IMP	3	0
4	C	503	PGE	3	0
2	D	500	IMP	2	0
5	D	502	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	346/363 (95%)	0.36	27 (7%)	14 20	26, 45, 69, 96	1 (0%)
1	B	344/363 (94%)	0.14	19 (5%)	26 36	22, 37, 61, 102	2 (0%)
1	C	346/363 (95%)	0.04	12 (3%)	44 57	19, 31, 51, 73	0
1	D	346/363 (95%)	-0.03	8 (2%)	61 71	19, 30, 51, 70	2 (0%)
All	All	1382/1452 (95%)	0.13	66 (4%)	31 43	19, 35, 62, 102	5 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	375	TYR	7.5
1	B	375	TYR	4.9
1	A	476	GLU	4.8
1	A	477	ALA	4.6
1	A	376	GLN	4.4
1	B	476	GLU	4.2
1	B	474	THR	4.0
1	C	475	LYS	3.7
1	B	378	ARG	3.7
1	A	380	TYR	3.6
1	B	380	TYR	3.6
1	B	372	ILE	3.6
1	D	91	GLY	3.4
1	A	91	GLY	3.4
1	A	379	SER	3.4
1	A	474	THR	3.4
1	C	375	TYR	3.3
1	A	374	ILE	3.3
1	D	476	GLU	3.1
1	C	335	ALA	2.9
1	A	357	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	88	ARG	2.9
1	A	475	LYS	2.9
1	A	378	ARG	2.9
1	A	408	PHE	2.8
1	A	472	ASN	2.8
1	A	88	ARG	2.8
1	B	377	GLY	2.8
1	A	335	ALA	2.7
1	C	334	ILE	2.7
1	A	339	LEU	2.7
1	C	474	THR	2.7
1	A	226	ASN	2.6
1	B	339	LEU	2.5
1	D	339	LEU	2.5
1	C	393	ALA	2.5
1	D	393	ALA	2.5
1	A	246	ASP	2.5
1	B	376	GLN	2.5
1	A	372	ILE	2.4
1	B	77	GLU	2.4
1	D	26	ASN	2.4
1	A	334	ILE	2.4
1	A	348	ALA	2.4
1	C	378	ARG	2.4
1	A	345	ILE	2.4
1	A	47	ALA	2.3
1	D	408	PHE	2.3
1	D	394	LYS	2.3
1	A	216	LEU	2.3
1	B	475	LYS	2.3
1	C	476	GLU	2.2
1	C	481	SER	2.2
1	B	393	ALA	2.2
1	B	373	GLU	2.2
1	B	295	VAL	2.1
1	B	335	ALA	2.1
1	B	334	ILE	2.1
1	C	339	LEU	2.1
1	A	89	SER	2.1
1	A	81	ARG	2.1
1	C	472	ASN	2.1
1	B	389	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	358	MET	2.0
1	B	357	MET	2.0
1	C	357	MET	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	ALY	A	327	9/13	0.75	0.24	-	42,46,55,59	0
1	ALY	C	327	11/13	0.91	0.13	-	23,38,62,65	0
1	ALY	B	327	11/13	0.90	0.15	-	39,43,58,59	0
1	ALY	D	327	11/13	0.89	0.17	-	24,44,53,55	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	PEG	D	503	7/7	0.90	0.20	5.03	44,48,53,57	0
4	PGE	B	504	10/10	0.78	0.18	2.68	43,47,50,51	0
5	PEG	C	502	7/7	0.89	0.15	2.30	50,53,59,63	0
9	PG4	D	505	13/13	0.92	0.16	1.80	33,41,49,51	0
4	PGE	A	502	10/10	0.78	0.16	1.47	37,48,52,52	0
4	PGE	A	503	10/10	0.76	0.26	0.81	46,52,59,64	0
4	PGE	C	503	10/10	0.86	0.14	0.56	36,44,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	PEG	B	502	7/7	0.91	0.17	0.40	31,38,48,50	0
6	EDO	B	503	4/4	0.86	0.12	0.39	43,44,45,47	0
2	IMP	B	500	23/23	0.97	0.18	0.30	28,35,44,51	0
2	IMP	C	500	23/23	0.97	0.17	0.21	22,30,36,41	0
2	IMP	D	500	23/23	0.97	0.16	0.11	14,23,31,33	0
2	IMP	A	500	23/23	0.95	0.17	0.03	29,37,40,42	0
5	PEG	A	504	7/7	0.88	0.16	0.00	53,62,67,68	0
5	PEG	D	504	7/7	0.90	0.12	-0.04	38,41,45,49	0
3	8L4	A	501	24/24	0.93	0.14	-0.18	31,41,49,63	0
8	K	B	506	1/1	0.94	0.12	-0.30	59,59,59,59	0
4	PGE	C	505	10/10	0.94	0.15	-0.50	41,46,56,57	0
3	8L4	D	501	24/24	0.96	0.11	-0.64	22,29,39,61	0
5	PEG	D	502	7/7	0.92	0.12	-0.67	44,49,53,56	0
3	8L4	C	501	24/24	0.94	0.11	-0.72	24,35,43,45	0
3	8L4	B	501	24/24	0.94	0.12	-0.77	36,49,53,64	0
6	EDO	C	504	4/4	0.94	0.07	-1.47	31,31,33,43	0
8	K	C	506	1/1	0.98	0.06	-3.61	48,48,48,48	0
7	MG	B	505	1/1	0.86	0.17	-	28,28,28,28	1

6.5 Other polymers [i](#)

There are no such residues in this entry.