



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:37 AM UTC

PDB ID : 7AZK / pdb_00007azk
Title : DNA polymerase sliding clamp from Escherichia coli with peptide 35 bound
Authors : Monsarrat, C.; Compain, G.; Andre, C.; Martiel, I.; Engilberge, S.; Olieric, V.;
Wolff, P.; Brillet, K.; Landolfo, M.; Silva da Veiga, C.; Wagner, J.; Guichard,
G.; Burnouf, D.Y.
Deposited on : 2020-11-16
Resolution : 2.05 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

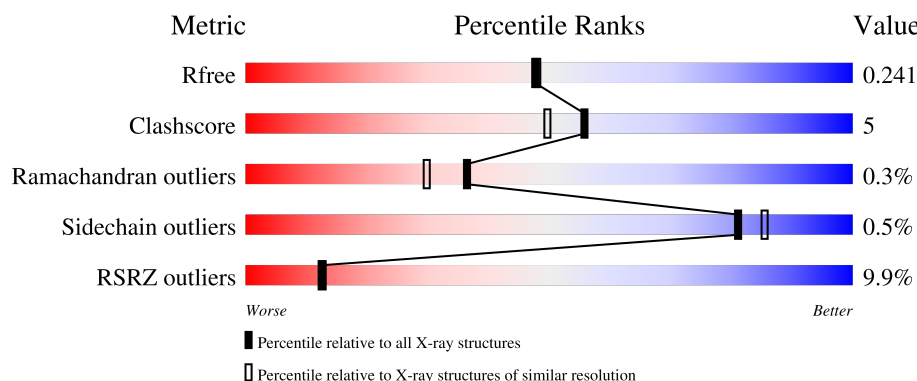
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	386	7% 83% 12% 5%
1	B	386	12% 85% 10% 5%
1	C	386	9% 85% 9% 5%
1	D	386	10% 84% 10% 6%
2	H	6	83% 17%

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Mol	Chain	Length	Quality of chain
2	I	6	 50%50%
2	J	6	 50%50%
2	K	6	 67%33%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12789 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 Beta sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	4	0
			2887	1811	510	547	19			
1	B	365	Total	C	N	O	S	0	5	0
			2844	1792	496	536	20			
1	C	365	Total	C	N	O	S	0	2	0
			2851	1791	503	538	19			
1	D	364	Total	C	N	O	S	0	3	0
			2850	1793	501	537	19			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A073FMV0
A	-18	GLY	-	expression tag	UNP A0A073FMV0
A	-17	SER	-	expression tag	UNP A0A073FMV0
A	-16	SER	-	expression tag	UNP A0A073FMV0
A	-15	HIS	-	expression tag	UNP A0A073FMV0
A	-14	HIS	-	expression tag	UNP A0A073FMV0
A	-13	HIS	-	expression tag	UNP A0A073FMV0
A	-12	HIS	-	expression tag	UNP A0A073FMV0
A	-11	HIS	-	expression tag	UNP A0A073FMV0
A	-10	HIS	-	expression tag	UNP A0A073FMV0
A	-9	SER	-	expression tag	UNP A0A073FMV0
A	-8	SER	-	expression tag	UNP A0A073FMV0
A	-7	GLY	-	expression tag	UNP A0A073FMV0
A	-6	LEU	-	expression tag	UNP A0A073FMV0
A	-5	VAL	-	expression tag	UNP A0A073FMV0
A	-4	PRO	-	expression tag	UNP A0A073FMV0
A	-3	ARG	-	expression tag	UNP A0A073FMV0
A	-2	GLY	-	expression tag	UNP A0A073FMV0
A	-1	SER	-	expression tag	UNP A0A073FMV0
A	0	HIS	-	expression tag	UNP A0A073FMV0
B	-19	MET	-	initiating methionine	UNP A0A073FMV0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A0A073FMV0
B	-17	SER	-	expression tag	UNP A0A073FMV0
B	-16	SER	-	expression tag	UNP A0A073FMV0
B	-15	HIS	-	expression tag	UNP A0A073FMV0
B	-14	HIS	-	expression tag	UNP A0A073FMV0
B	-13	HIS	-	expression tag	UNP A0A073FMV0
B	-12	HIS	-	expression tag	UNP A0A073FMV0
B	-11	HIS	-	expression tag	UNP A0A073FMV0
B	-10	HIS	-	expression tag	UNP A0A073FMV0
B	-9	SER	-	expression tag	UNP A0A073FMV0
B	-8	SER	-	expression tag	UNP A0A073FMV0
B	-7	GLY	-	expression tag	UNP A0A073FMV0
B	-6	LEU	-	expression tag	UNP A0A073FMV0
B	-5	VAL	-	expression tag	UNP A0A073FMV0
B	-4	PRO	-	expression tag	UNP A0A073FMV0
B	-3	ARG	-	expression tag	UNP A0A073FMV0
B	-2	GLY	-	expression tag	UNP A0A073FMV0
B	-1	SER	-	expression tag	UNP A0A073FMV0
B	0	HIS	-	expression tag	UNP A0A073FMV0
C	-19	MET	-	initiating methionine	UNP A0A073FMV0
C	-18	GLY	-	expression tag	UNP A0A073FMV0
C	-17	SER	-	expression tag	UNP A0A073FMV0
C	-16	SER	-	expression tag	UNP A0A073FMV0
C	-15	HIS	-	expression tag	UNP A0A073FMV0
C	-14	HIS	-	expression tag	UNP A0A073FMV0
C	-13	HIS	-	expression tag	UNP A0A073FMV0
C	-12	HIS	-	expression tag	UNP A0A073FMV0
C	-11	HIS	-	expression tag	UNP A0A073FMV0
C	-10	HIS	-	expression tag	UNP A0A073FMV0
C	-9	SER	-	expression tag	UNP A0A073FMV0
C	-8	SER	-	expression tag	UNP A0A073FMV0
C	-7	GLY	-	expression tag	UNP A0A073FMV0
C	-6	LEU	-	expression tag	UNP A0A073FMV0
C	-5	VAL	-	expression tag	UNP A0A073FMV0
C	-4	PRO	-	expression tag	UNP A0A073FMV0
C	-3	ARG	-	expression tag	UNP A0A073FMV0
C	-2	GLY	-	expression tag	UNP A0A073FMV0
C	-1	SER	-	expression tag	UNP A0A073FMV0
C	0	HIS	-	expression tag	UNP A0A073FMV0
D	-19	MET	-	initiating methionine	UNP A0A073FMV0
D	-18	GLY	-	expression tag	UNP A0A073FMV0
D	-17	SER	-	expression tag	UNP A0A073FMV0

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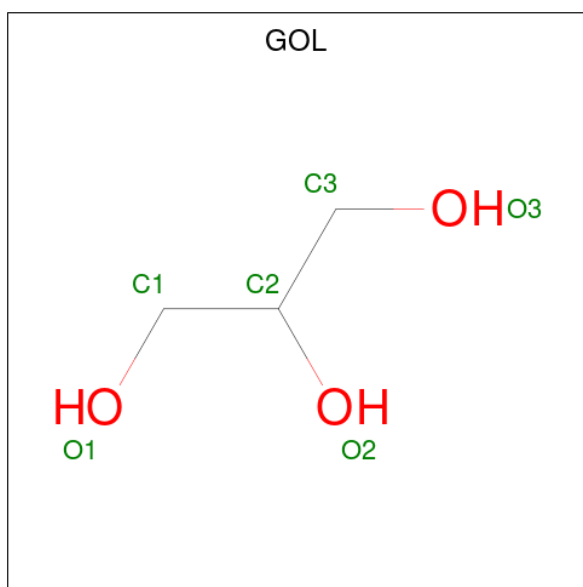
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A0A073FMV0
D	-15	HIS	-	expression tag	UNP A0A073FMV0
D	-14	HIS	-	expression tag	UNP A0A073FMV0
D	-13	HIS	-	expression tag	UNP A0A073FMV0
D	-12	HIS	-	expression tag	UNP A0A073FMV0
D	-11	HIS	-	expression tag	UNP A0A073FMV0
D	-10	HIS	-	expression tag	UNP A0A073FMV0
D	-9	SER	-	expression tag	UNP A0A073FMV0
D	-8	SER	-	expression tag	UNP A0A073FMV0
D	-7	GLY	-	expression tag	UNP A0A073FMV0
D	-6	LEU	-	expression tag	UNP A0A073FMV0
D	-5	VAL	-	expression tag	UNP A0A073FMV0
D	-4	PRO	-	expression tag	UNP A0A073FMV0
D	-3	ARG	-	expression tag	UNP A0A073FMV0
D	-2	GLY	-	expression tag	UNP A0A073FMV0
D	-1	SER	-	expression tag	UNP A0A073FMV0
D	0	HIS	-	expression tag	UNP A0A073FMV0

- Molecule 2 is a protein called Peptide 35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	6	Total	C	Cl	N	O	0	0	0
			54	36	2	6	10			
2	I	6	Total	C	Cl	N	O	0	0	0
			54	36	2	6	10			
2	J	6	Total	C	Cl	N	O	0	0	0
			54	36	2	6	10			
2	K	6	Total	C	Cl	N	O	0	0	0
			54	36	2	6	10			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

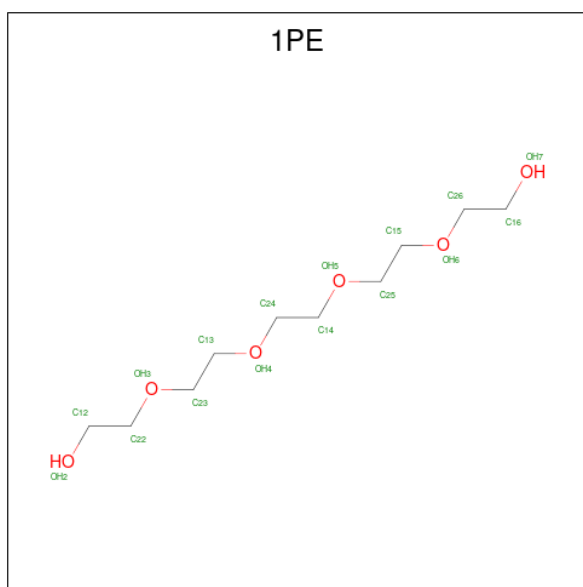


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).

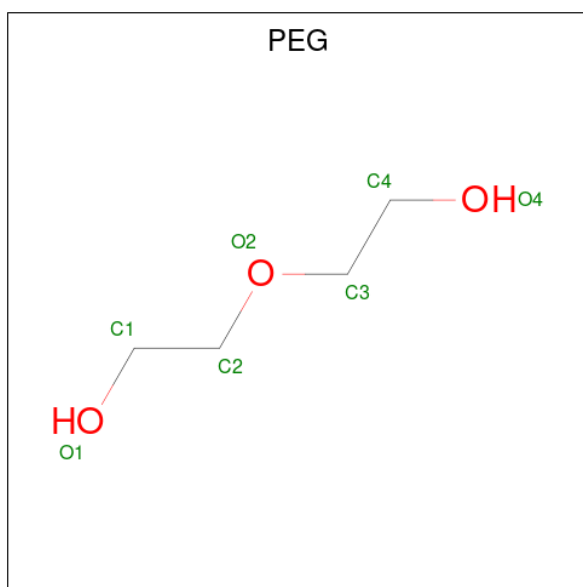


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	10	6		
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			11	7	4		
5	B	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			16	10	6		
5	C	1	Total	C	O	0	0
			5	3	2		
5	C	1	Total	C	O	0	0
			11	7	4		
5	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		
6	D	1	Total	Cl	0	0
			1	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

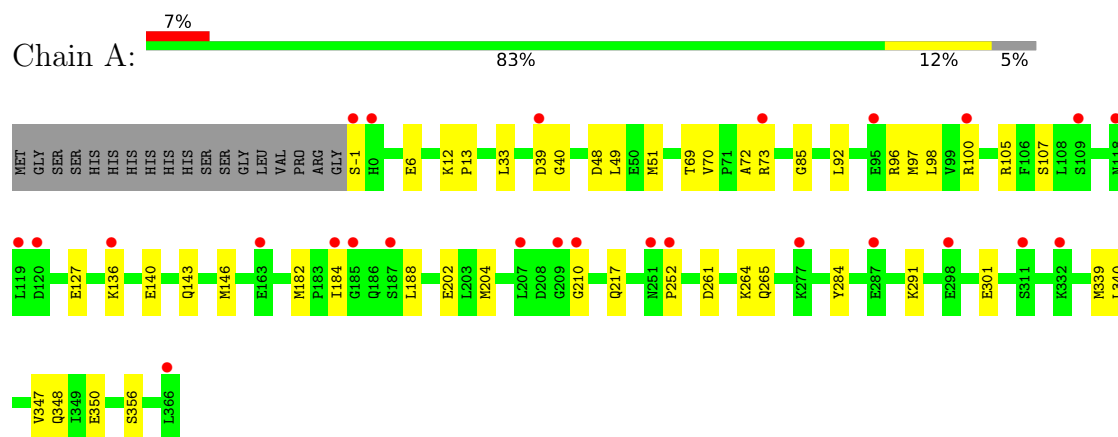
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	296	Total	O	0	10
			306	306		
8	H	12	Total	O	0	0
			12	12		
8	B	203	Total	O	0	2
			205	205		
8	I	8	Total	O	0	0
			8	8		
8	C	249	Total	O	0	3
			252	252		
8	J	13	Total	O	0	0
			13	13		
8	D	208	Total	O	0	5
			213	213		
8	K	8	Total	O	0	1
			9	9		

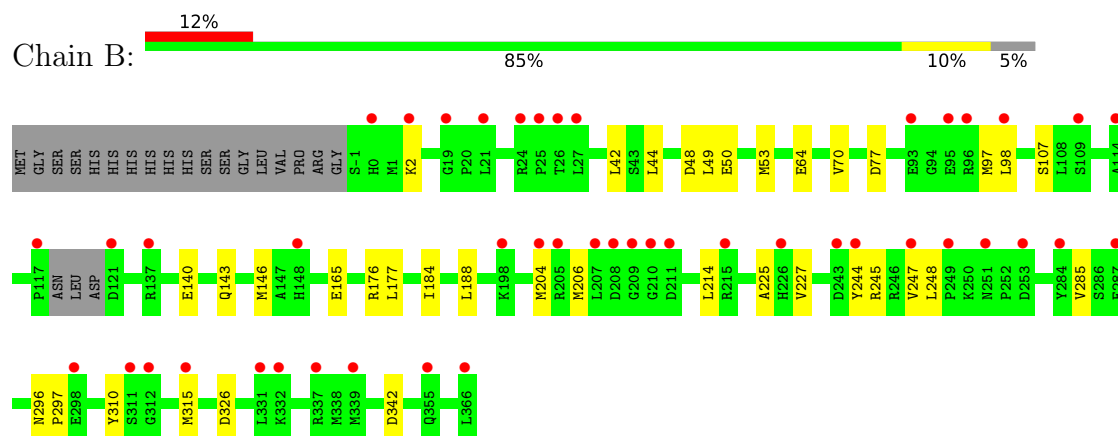
3 Residue-property plots [i](#)

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.

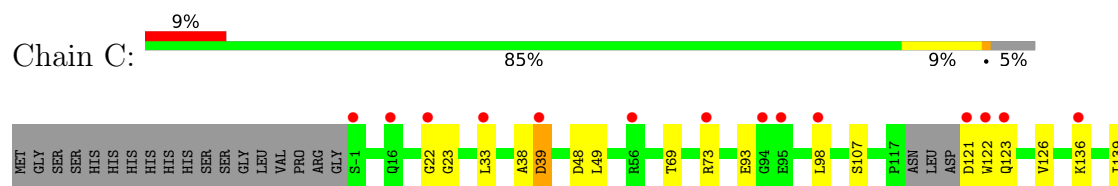
- Molecule 1: Beta sliding clamp

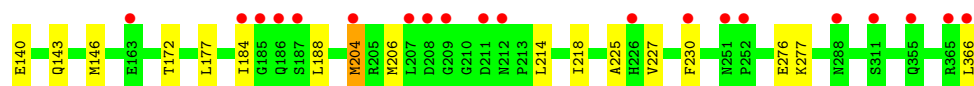


- Molecule 1: Beta sliding clamp

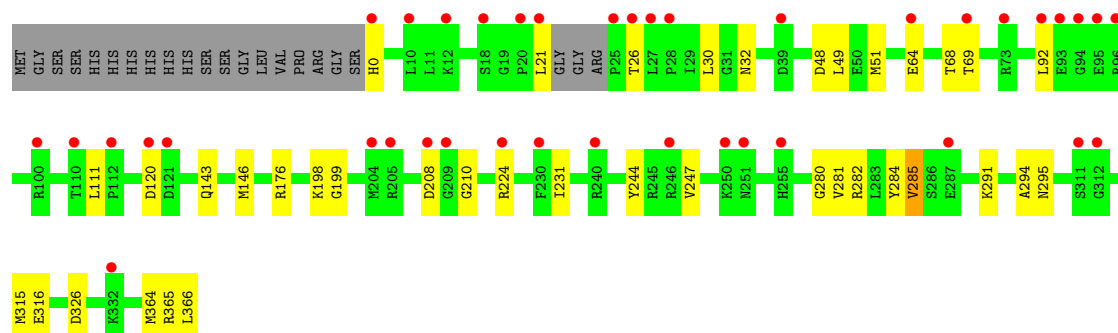
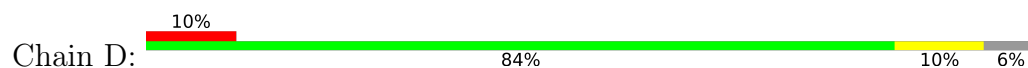


- Molecule 1: Beta sliding clamp

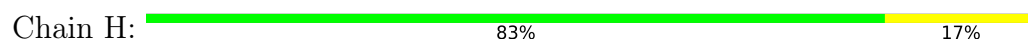




- Molecule 1: Beta sliding clamp



- Molecule 2: Peptide 35



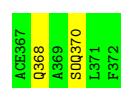
- Molecule 2: Peptide 35



- Molecule 2: Peptide 35



- Molecule 2: Peptide 35



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.81Å 135.83Å 87.54Å 90.00° 106.15° 90.00°	Depositor
Resolution (Å)	84.09 – 2.05 84.09 – 2.05	Depositor EDS
% Data completeness (in resolution range)	78.3 (84.09-2.05) 78.4 (84.09-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.210 , 0.241 0.211 , 0.241	Depositor DCC
R_{free} test set	4327 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12789	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: K, GOL, ALC, PEG, CL, 1PE, SOQ, ZCL, ACE

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	0.15	0/2942	0.40	0/3983
1	B	0.15	0/2906	0.38	0/3933
1	C	0.15	0/2907	0.38	0/3931
1	D	0.17	0/2908	0.40	0/3933
2	H	0.05	0/16	0.12	0/19
2	I	0.08	0/16	0.17	0/19
2	J	0.06	0/16	0.16	0/19
2	K	0.08	0/16	0.18	0/19
All	All	0.15	0/11727	0.39	0/15856

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
2	H	0	1
2	I	0	2
2	J	0	2
2	K	0	2
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	371	LEU	Mainchain

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Mol	Chain	Res	Type	Group
2	I	368	GLN	Mainchain
2	I	371	LEU	Mainchain
2	J	369	ALC	Mainchain
2	J	370	SOQ	Mainchain
2	K	368	GLN	Mainchain
2	K	370	SOQ	Mainchain

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	2887	0	2884	38	0
1	B	2844	0	2853	25	0
1	C	2851	0	2870	25	0
1	D	2850	0	2875	23	0
2	H	54	0	42	0	0
2	I	54	0	42	0	0
2	J	54	0	42	0	0
2	K	54	0	42	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	26	0	35	3	0
5	B	40	0	52	1	0
5	C	16	0	18	0	0
5	D	10	0	13	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	C	7	0	10	0	0
7	D	7	0	10	0	0
8	A	306	0	0	10	0
8	B	205	0	0	1	0
8	C	252	0	0	4	0
8	D	213	0	0	3	0
8	H	12	0	0	0	0
8	I	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	13	0	0	0	0
8	K	9	0	0	0	0
All	All	12789	0	11804	111	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 5.

All (111) 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:73:ARG:NH1	8:A:501:HOH:O	2.00	0.94
1:B:50:GLU:OE1	8:B:501:HOH:O	1.97	0.82
1:B:184:ILE:HD11	1:B:188:LEU:HD11	1.64	0.80
1:C:276:GLU:OE1	8:C:601:HOH:O	2.00	0.78
1:B:140:GLU:CG	1:B:204[A]:MET:HE1	2.18	0.74
1:A:301:GLU:OE1	8:A:502:HOH:O	2.07	0.72
1:D:120:ASP:OD1	1:D:224:ARG:NH2	2.22	0.72
1:A:39:ASP:OD1	1:A:40:GLY:N	2.24	0.69
1:C:93:GLU:CD	1:C:98:LEU:HD12	2.18	0.68
1:A:73:ARG:NH1	8:A:503:HOH:O	2.11	0.68
1:A:51:MET:SD	8:A:749:HOH:O	2.52	0.66
1:A:73:ARG:CZ	8:A:501:HOH:O	2.43	0.62
1:C:206:MET:HE3	1:C:230:PHE:CD2	2.35	0.62
1:C:139:ILE:HG21	1:C:204:MET:HG3	1.82	0.62
1:B:140:GLU:HG2	1:B:204[A]:MET:HE1	1.82	0.61
1:C:184:ILE:HD11	1:C:188:LEU:HD11	1.81	0.61
1:B:98:LEU:HD23	1:B:107:SER:HA	1.83	0.61
1:A:105:ARG:NH1	8:A:507:HOH:O	2.26	0.61
1:B:214:LEU:HD11	1:B:225:ALA:HB1	1.85	0.58
1:A:184:ILE:HD11	1:A:188:LEU:HD11	1.85	0.57
1:D:280:GLY:HA2	1:D:364:MET:HE1	1.86	0.57
1:A:348:GLN:NE2	1:A:350:GLU:OE1	2.32	0.57
1:B:227:VAL:HG13	1:B:227:VAL:O	2.04	0.56
1:D:68:THR:HG21	1:D:92:LEU:HD21	1.88	0.56
1:D:21:LEU:HD12	1:D:21:LEU:N	2.20	0.56
1:A:140:GLU:HG3	1:A:204:MET:HE1	1.88	0.55
1:B:140:GLU:HG3	1:B:204[A]:MET:HE1	1.88	0.55
1:D:365:ARG:NH1	8:D:509:HOH:O	2.40	0.55
1:C:73:ARG:NH2	8:C:607:HOH:O	2.40	0.54
1:B:70:VAL:HG11	1:B:97:MET:SD	2.48	0.54
1:C:126:VAL:CG1	1:C:218:ILE:HB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:GLN:HG3	1:D:146:MET:HE2	1.90	0.53
1:C:98:LEU:HD23	1:C:107:SER:HA	1.91	0.52
1:A:182:MET:HE3	1:A:356:SER:OG	2.10	0.52
1:C:206:MET:HE3	1:C:230:PHE:HD2	1.72	0.51
1:C:143:GLN:HG3	1:C:146:MET:HE2	1.91	0.51
1:D:280:GLY:CA	1:D:364:MET:HE1	2.41	0.50
1:C:214:LEU:HD11	1:C:225:ALA:HB1	1.92	0.50
1:D:282:ARG:HD3	1:D:316:GLU:OE1	2.12	0.50
1:C:206:MET:HE2	1:C:227:VAL:HG12	1.93	0.50
1:D:32:ASN:HB3	1:D:69:THR:HG23	1.93	0.50
1:A:202:GLU:OE1	8:A:504:HOH:O	2.20	0.49
1:A:291:LYS:HE3	5:A:403:1PE:H131	1.94	0.49
1:B:315:MET:HE1	1:B:342:ASP:C	2.38	0.49
1:C:22:GLY:N	1:C:23:GLY:HA3	2.27	0.49
1:B:206:MET:HE2	1:B:227:VAL:HG12	1.94	0.49
1:C:126:VAL:HG12	1:C:218:ILE:HB	1.95	0.49
1:A:184:ILE:HD11	1:A:188:LEU:CD1	2.44	0.48
1:D:366:LEU:OXT	8:D:501:HOH:O	2.20	0.47
1:B:227:VAL:O	1:B:227:VAL:CG1	2.61	0.47
1:B:42:LEU:HG	1:B:44:LEU:CD1	2.44	0.47
1:B:48:ASP:O	1:B:49:LEU:HB2	2.13	0.47
1:B:176:ARG:NH1	1:B:326:ASP:OD2	2.38	0.47
1:B:244:TYR:O	1:B:247:VAL:HG22	2.15	0.47
1:A:182:MET:HA	1:A:182:MET:HE2	1.97	0.46
1:B:53:MET:HE1	1:B:206:MET:HE3	1.97	0.46
1:C:277:LYS:NZ	8:C:608:HOH:O	2.42	0.46
1:A:100:ARG:NH1	8:A:514:HOH:O	2.48	0.46
1:D:69:THR:HB	1:D:111:LEU:O	2.16	0.46
1:D:284:TYR:HB2	1:D:291:LYS:HB3	1.97	0.46
1:A:48:ASP:O	1:A:49:LEU:HB2	2.15	0.46
1:C:121:ASP:OD1	1:C:122:TRP:N	2.48	0.46
1:A:33:LEU:HG	1:A:72:ALA:CB	2.46	0.46
1:D:48:ASP:O	1:D:49:LEU:HB2	2.16	0.45
1:A:284:TYR:HB2	1:A:291:LYS:HB3	1.99	0.45
1:A:136:LYS:HD2	1:A:204:MET:CE	2.46	0.45
1:A:261:ASP:OD2	1:A:265[B]:GLN:NE2	2.50	0.45
1:A:291:LYS:HZ2	5:A:403:1PE:H131	1.82	0.45
1:B:245:ARG:HA	1:B:248:LEU:HD23	1.98	0.45
1:C:22:GLY:H	1:C:23:GLY:HA3	1.82	0.44
1:C:93:GLU:OE2	1:C:98:LEU:HD12	2.16	0.44
1:A:252:PRO:HB2	1:A:339:MET:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ARG:HD3	1:D:231:ILE:CG2	2.48	0.44
1:D:26:THR:OG1	1:D:30:LEU:HD12	2.18	0.44
1:B:177:LEU:HD11	1:B:244:TYR:HB2	1.99	0.44
1:C:172:THR:HB	1:C:177:LEU:HD12	2.00	0.44
1:D:51:MET:HE1	1:D:199:GLY:N	2.32	0.44
1:C:136:LYS:HE3	1:C:140:GLU:OE2	2.18	0.44
1:C:48:ASP:O	1:C:49:LEU:HB2	2.18	0.44
1:A:202:GLU:OE2	8:A:505:HOH:O	2.21	0.43
1:A:33:LEU:O	1:A:69:THR:HA	2.17	0.43
1:B:77:ASP:HB3	5:B:403:1PE:H142	2.00	0.43
1:D:21:LEU:N	1:D:21:LEU:CD1	2.81	0.43
1:D:0:HIS:O	1:D:64:GLU:OE1	2.37	0.43
1:A:340:LEU:HG	1:A:347:VAL:HG23	2.00	0.43
1:D:291:LYS:NZ	8:D:514:HOH:O	2.51	0.43
1:A:98:LEU:HD13	1:A:100:ARG:NH2	2.34	0.43
1:C:136:LYS:HD2	1:C:204:MET:SD	2.58	0.42
1:C:73:ARG:CZ	8:C:607:HOH:O	2.66	0.42
1:A:12:LYS:HB3	1:A:13:PRO:HD3	2.02	0.42
1:C:38:ALA:O	1:C:39:ASP:C	2.62	0.42
1:D:285:VAL:CG2	1:D:315:MET:HG2	2.50	0.42
1:A:-1:SER:HA	1:A:92:LEU:HD23	2.02	0.41
1:A:136:LYS:NZ	1:A:204:MET:HE3	2.34	0.41
1:A:96:ARG:HD2	1:A:107:SER:OG	2.20	0.41
1:D:281:VAL:HG12	1:D:294:ALA:HB2	2.03	0.41
1:B:2:LYS:HE2	1:B:64:GLU:HG3	2.01	0.41
1:D:176:ARG:NH1	1:D:326:ASP:OD2	2.43	0.41
1:A:143:GLN:HG3	1:A:146:MET:HE2	2.03	0.41
1:A:264:LYS:NZ	8:A:519:HOH:O	2.53	0.41
1:B:143:GLN:HG3	1:B:146:MET:HE2	2.02	0.41
1:C:33:LEU:O	1:C:69:THR:HA	2.21	0.41
1:A:291:LYS:HE3	5:A:403:1PE:C13	2.51	0.41
1:A:127:GLU:HG2	1:A:217:GLN:HG2	2.03	0.41
1:D:244:TYR:O	1:D:247:VAL:HG22	2.21	0.41
1:A:136:LYS:HD2	1:A:204:MET:HE1	2.03	0.41
1:B:285:VAL:HG22	1:B:310:TYR:CD2	2.55	0.40
1:A:6:GLU:OE2	1:A:85:GLY:HA2	2.21	0.40
1:B:296:ASN:HB2	1:B:297:PRO:HD2	2.04	0.40
1:A:70:VAL:HG11	1:A:97:MET:SD	2.61	0.40

There are no symmetry-related clashes.

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	370/386 (96%)	363 (98%)	6 (2%)	1 (0%)	36	30
1	B	366/386 (95%)	360 (98%)	6 (2%)	0	100	100
1	C	363/386 (94%)	357 (98%)	5 (1%)	1 (0%)	36	30
1	D	363/386 (94%)	354 (98%)	7 (2%)	2 (1%)	21	13
2	H	2/6 (33%)	2 (100%)	0	0	100	100
2	I	2/6 (33%)	2 (100%)	0	0	100	100
2	J	2/6 (33%)	2 (100%)	0	0	100	100
2	K	2/6 (33%)	2 (100%)	0	0	100	100
All	All	1470/1568 (94%)	1442 (98%)	24 (2%)	4 (0%)	36	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	GLY
1	C	39	ASP
1	D	208	ASP
1	D	210	GLY

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	317/330 (96%)	317 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	311/330 (94%)	311 (100%)	0	100	100
1	C	314/330 (95%)	311 (99%)	3 (1%)	68	72
1	D	314/330 (95%)	311 (99%)	3 (1%)	68	72
2	H	2/2 (100%)	2 (100%)	0	100	100
2	I	2/2 (100%)	2 (100%)	0	100	100
2	J	2/2 (100%)	2 (100%)	0	100	100
2	K	2/2 (100%)	2 (100%)	0	100	100
All	All	1264/1328 (95%)	1258 (100%)	6 (0%)	81	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	123	GLN
1	C	204	MET
1	C	366	LEU
1	D	198	LYS
1	D	285	VAL
1	D	295	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	15	GLN
1	A	16	GLN
1	A	149	GLN
1	A	295	ASN
1	B	148	HIS
1	B	221	ASN
1	C	15	GLN
1	C	175	HIS
2	J	368	GLN
1	D	175	HIS
1	D	335	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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
2	ZCL	I	372	2	13,14,14	1.15	2 (15%)	15,19,19	0.23	0
2	ALC	J	369	2	9,11,12	0.17	0	11,13,15	0.43	0
2	ALC	H	369	2	9,11,12	0.17	0	11,13,15	0.42	0
2	ALC	K	369	2	9,11,12	0.16	0	11,13,15	0.36	0
2	ZCL	H	372	2	13,14,14	0.13	0	15,19,19	0.27	0
2	ZCL	J	372	2	13,14,14	1.11	2 (15%)	15,19,19	0.20	0
2	ZCL	K	372	2	13,14,14	0.12	0	15,19,19	0.17	0
2	ALC	I	369	2	9,11,12	0.16	0	11,13,15	0.51	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	ZCL	I	372	2	-	6/8/8/8	0/1/1/1
2	ALC	J	369	2	-	0/5/14/16	0/1/1/1
2	ALC	H	369	2	-	0/5/14/16	0/1/1/1
2	ALC	K	369	2	-	0/5/14/16	0/1/1/1
2	ZCL	H	372	2	-	1/8/8/8	0/1/1/1
2	ZCL	J	372	2	-	2/8/8/8	0/1/1/1
2	ZCL	K	372	2	-	4/8/8/8	0/1/1/1
2	ALC	I	369	2	-	0/5/14/16	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	372	ZCL	O-C	3.03	1.31	1.22
2	J	372	ZCL	O-C	2.95	1.30	1.22
2	I	372	ZCL	OXT-C	-2.78	1.21	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	372	ZCL	OXT-C	-2.68	1.22	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	372	ZCL	N-CA-CB-CG
2	I	372	ZCL	O-C-CA-N
2	J	372	ZCL	N-CA-CB-CG
2	J	372	ZCL	C-CA-CB-CG
2	K	372	ZCL	N-CA-CB-CG
2	K	372	ZCL	C-CA-CB-CG
2	I	372	ZCL	OXT-C-CA-N
2	K	372	ZCL	OXT-C-CA-N
2	I	372	ZCL	O-C-CA-CB
2	I	372	ZCL	OXT-C-CA-CB
2	I	372	ZCL	C-CA-CB-CG
2	H	372	ZCL	OXT-C-CA-N
2	K	372	ZCL	O-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 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
3	GOL	A	401	-	5,5,5	0.82	0	5,5,5	0.99	0
5	1PE	B	403	-	12,12,15	0.17	0	11,11,14	0.21	0
7	PEG	C	501	-	6,6,6	0.27	0	5,5,5	0.15	0
5	1PE	A	404	-	9,9,15	0.24	0	8,8,14	0.21	0
5	1PE	A	403	-	15,15,15	0.26	0	14,14,14	0.15	0
7	PEG	D	401	-	6,6,6	0.28	0	5,5,5	0.15	0
5	1PE	B	404	-	15,15,15	0.22	0	14,14,14	0.11	0
5	1PE	D	402	-	9,9,15	0.23	0	8,8,14	0.14	0
3	GOL	B	401	-	5,5,5	0.82	0	5,5,5	0.94	0
5	1PE	C	504	-	10,10,15	0.23	0	9,9,14	0.11	0
5	1PE	C	503	-	4,4,15	0.31	0	3,3,14	0.16	0
5	1PE	B	402	-	10,10,15	0.22	0	9,9,14	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
3	GOL	A	401	-	-	0/4/4/4	-
5	1PE	B	403	-	-	3/10/10/13	-
7	PEG	C	501	-	-	0/4/4/4	-
5	1PE	A	404	-	-	2/7/7/13	-
5	1PE	A	403	-	-	5/13/13/13	-
7	PEG	D	401	-	-	2/4/4/4	-
5	1PE	B	404	-	-	8/13/13/13	-
5	1PE	D	402	-	-	3/7/7/13	-
3	GOL	B	401	-	-	2/4/4/4	-
5	1PE	C	504	-	-	4/8/8/13	-
5	1PE	C	503	-	-	0/2/2/13	-
5	1PE	B	402	-	-	5/8/8/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	A	403	1PE	OH5-C14-C24-OH4
5	B	403	1PE	OH5-C14-C24-OH4
5	A	404	1PE	OH7-C16-C26-OH6
3	B	401	GOL	O2-C2-C3-O3
5	C	504	1PE	C14-C24-OH4-C13
5	C	504	1PE	OH5-C14-C24-OH4
5	A	403	1PE	OH6-C15-C25-OH5
5	B	402	1PE	C25-C15-OH6-C26
5	B	403	1PE	C14-C24-OH4-C13
5	A	403	1PE	OH4-C13-C23-OH3
5	A	403	1PE	C24-C14-OH5-C25
5	B	402	1PE	C15-C25-OH5-C14
5	B	404	1PE	C13-C23-OH3-C22
5	B	403	1PE	C25-C15-OH6-C26
5	D	402	1PE	C24-C14-OH5-C25
7	D	401	PEG	C4-C3-O2-C2
5	B	404	1PE	C23-C13-OH4-C24
5	B	404	1PE	C25-C15-OH6-C26
5	B	402	1PE	OH7-C16-C26-OH6
7	D	401	PEG	C1-C2-O2-C3
5	A	404	1PE	OH6-C15-C25-OH5
5	D	402	1PE	C25-C15-OH6-C26
5	B	404	1PE	C15-C25-OH5-C14
5	C	504	1PE	C16-C26-OH6-C15
5	A	403	1PE	C16-C26-OH6-C15
5	C	504	1PE	C25-C15-OH6-C26
5	B	404	1PE	C12-C22-OH3-C23
5	B	404	1PE	OH5-C14-C24-OH4
5	D	402	1PE	OH7-C16-C26-OH6
5	B	402	1PE	OH5-C14-C24-OH4
5	B	404	1PE	OH2-C12-C22-OH3
5	B	404	1PE	OH6-C15-C25-OH5
5	B	402	1PE	OH6-C15-C25-OH5

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	403	1PE	1	0
5	A	403	1PE	3	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	368/386 (95%)	0.36	26 (7%)	22	22	13, 27, 49, 108	4 (1%)
1	B	365/386 (94%)	0.67	46 (12%)	8	7	18, 34, 65, 114	5 (1%)
1	C	365/386 (94%)	0.53	34 (9%)	14	14	18, 32, 58, 127	2 (0%)
1	D	364/386 (94%)	0.74	39 (10%)	11	10	16, 35, 64, 97	3 (0%)
2	H	2/6 (33%)	-0.04	0	100	100	29, 29, 29, 30	0
2	I	2/6 (33%)	0.28	0	100	100	27, 27, 27, 37	0
2	J	2/6 (33%)	-0.46	0	100	100	26, 26, 26, 29	0
2	K	2/6 (33%)	0.21	0	100	100	26, 26, 26, 35	0
All	All	1470/1568 (93%)	0.57	145 (9%)	13	12	13, 32, 61, 127	14 (0%)

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	LEU	6.2
1	C	22	GLY	5.3
1	B	209	GLY	5.0
1	D	94	GLY	4.5
1	D	25	PRO	4.4
1	A	209	GLY	4.4
1	B	121	ASP	4.3
1	D	20	PRO	4.2
1	D	26	THR	4.1
1	B	93	GLU	4.0
1	B	0	HIS	4.0
1	D	73	ARG	4.0
1	C	187	SER	3.9
1	A	332	LYS	3.9
1	C	136	LYS	3.9
1	D	21	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	209	GLY	3.8
1	D	332	LYS	3.7
1	C	-1	SER	3.7
1	B	332	LYS	3.7
1	B	27	LEU	3.7
1	A	-1	SER	3.6
1	D	0	HIS	3.6
1	B	26	THR	3.6
1	D	204	MET	3.6
1	D	27	LEU	3.6
1	C	366	LEU	3.5
1	D	287	GLU	3.4
1	A	73	ARG	3.4
1	B	287	GLU	3.4
1	C	365	ARG	3.4
1	C	251	ASN	3.3
1	C	208	ASP	3.3
1	B	137	ARG	3.3
1	D	93	GLU	3.3
1	D	250	LYS	3.3
1	A	366	LEU	3.3
1	A	120	ASP	3.3
1	C	186	GLN	3.1
1	D	64	GLU	3.1
1	D	208	ASP	3.1
1	B	198	LYS	3.1
1	D	311	SER	3.0
1	C	94	GLY	3.0
1	B	205[A]	ARG	3.0
1	C	204	MET	3.0
1	D	205[A]	ARG	3.0
1	C	121	ASP	3.0
1	B	96	ARG	2.9
1	B	21	LEU	2.9
1	C	185	GLY	2.9
1	C	95	GLU	2.9
1	D	209	GLY	2.9
1	A	252	PRO	2.9
1	B	366	LEU	2.8
1	C	230	PHE	2.8
1	B	215	ARG	2.8
1	C	211	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	98	LEU	2.7
1	C	207	LEU	2.7
1	D	246	ARG	2.7
1	B	249	PRO	2.7
1	D	251	ASN	2.7
1	A	0	HIS	2.7
1	D	95	GLU	2.7
1	B	210	GLY	2.7
1	B	312	GLY	2.7
1	D	92	LEU	2.7
1	B	298	GLU	2.7
1	D	112	PRO	2.7
1	B	284	TYR	2.7
1	D	240	ARG	2.7
1	B	226[A]	HIS	2.6
1	A	184	ILE	2.6
1	B	95	GLU	2.6
1	C	39	ASP	2.6
1	D	224	ARG	2.6
1	B	204[A]	MET	2.6
1	C	252	PRO	2.6
1	C	184	ILE	2.5
1	B	148	HIS	2.5
1	A	100	ARG	2.5
1	D	120	ASP	2.5
1	A	163	GLU	2.5
1	B	24	ARG	2.5
1	D	96	ARG	2.5
1	A	210	GLY	2.5
1	A	298	GLU	2.4
1	D	69	THR	2.4
1	C	33	LEU	2.4
1	C	98	LEU	2.4
1	B	253	ASP	2.4
1	B	244	TYR	2.4
1	D	100	ARG	2.4
1	D	312	GLY	2.4
1	D	12	LYS	2.4
1	D	18	SER	2.4
1	C	226	HIS	2.4
1	C	288	ASN	2.3
1	A	277	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	230	PHE	2.3
1	D	28	PRO	2.3
1	B	211	ASP	2.3
1	D	255	HIS	2.3
1	A	39	ASP	2.3
1	B	243	ASP	2.3
1	C	122	TRP	2.3
1	C	163	GLU	2.3
1	B	25	PRO	2.3
1	D	110	THR	2.3
1	B	2	LYS	2.3
1	B	207	LEU	2.3
1	A	311	SER	2.2
1	A	118	ASN	2.2
1	C	73	ARG	2.2
1	B	208	ASP	2.2
1	B	19	GLY	2.2
1	A	207	LEU	2.2
1	C	355	GLN	2.2
1	C	311	SER	2.2
1	C	123	GLN	2.2
1	B	109	SER	2.2
1	B	117	PRO	2.2
1	A	95	GLU	2.2
1	A	109	SER	2.2
1	B	315	MET	2.2
1	D	121	ASP	2.2
1	B	331	LEU	2.1
1	C	212	ASN	2.1
1	B	247	VAL	2.1
1	A	136	LYS	2.1
1	C	16	GLN	2.1
1	A	185	GLY	2.1
1	A	287	GLU	2.1
1	B	355	GLN	2.1
1	D	10	LEU	2.0
1	B	251	ASN	2.0
1	B	337	ARG	2.0
1	A	187	SER	2.0
1	B	311	SER	2.0
1	B	339	MET	2.0
1	B	114	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	251	ASN	2.0
1	D	39	ASP	2.0
1	C	56[A]	ARG	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. 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	ZCL	K	372	14/14	0.75	0.18	59,60,62,63	0
2	ZCL	I	372	14/14	0.77	0.19	59,62,64,64	0
2	ZCL	H	372	14/14	0.89	0.12	33,34,36,36	0
2	ZCL	J	372	14/14	0.90	0.11	34,35,37,37	0
2	ALC	I	369	11/12	0.91	0.09	22,23,25,27	0
2	ALC	K	369	11/12	0.92	0.08	27,28,28,29	0
2	ALC	H	369	11/12	0.93	0.08	26,27,29,29	0
2	ALC	J	369	11/12	0.94	0.08	25,25,27,28	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
5	1PE	C	503	5/16	0.65	0.31	67,67,69,70	0
3	GOL	B	401	6/6	0.69	0.21	66,66,67,67	0
5	1PE	C	504	11/16	0.70	0.23	63,65,65,66	0
5	1PE	B	403	13/16	0.71	0.27	81,82,86,87	0
5	1PE	A	403	16/16	0.74	0.24	71,72,74,74	0
5	1PE	B	404	16/16	0.76	0.23	75,77,80,80	0
5	1PE	D	402	10/16	0.76	0.19	60,61,62,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PEG	D	401	7/7	0.76	0.24	64,64,65,65	0
5	1PE	A	404	10/16	0.78	0.20	58,59,59,61	0
5	1PE	B	402	11/16	0.78	0.23	70,71,72,74	0
3	GOL	A	401	6/6	0.82	0.23	67,67,67,67	6
7	PEG	C	501	7/7	0.87	0.17	63,63,63,64	0
6	CL	B	405	1/1	0.96	0.06	36,36,36,36	0
6	CL	A	405	1/1	0.98	0.04	30,30,30,30	0
6	CL	D	403	1/1	0.98	0.06	38,38,38,38	0
4	K	A	402	1/1	0.99	0.03	24,24,24,24	0
4	K	C	502	1/1	1.00	0.02	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.