



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:59 AM UTC

PDB ID : 3FDS / pdb_00003fds
Title : Structural insight into recruitment of translesion DNA polymerase Dpo4 to sliding clamp PCNA
Authors : Ling, H.
Deposited on : 2008-11-26
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

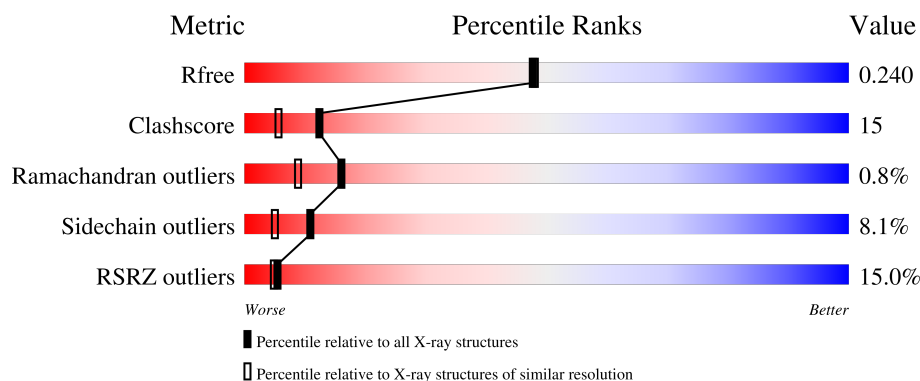
1 Overall quality at a glance

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	352	16% 74% 20% • •
2	C	249	14% 65% 29% 5% •
3	D	245	13% 75% 19% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	358	-	-	X	-
5	PEG	A	369	-	-	X	-
6	1PE	A	370	-	-	X	-
7	GOL	C	260	-	-	X	-
7	GOL	C	261	-	-	X	-
8	PGE	D	247	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7313 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 DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	6	12	0
			2913	1867	506	532	8			

- Molecule 2 is a protein called DNA polymerase sliding clamp B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	249	Total	C	N	O	S	0	10	0
			1991	1272	317	391	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	VAL	PHE	engineered mutation	UNP P57766

- Molecule 3 is a protein called DNA polymerase sliding clamp C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	241	Total	C	N	O	S	0	4	0
			1930	1245	300	379	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP Q97Z84

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



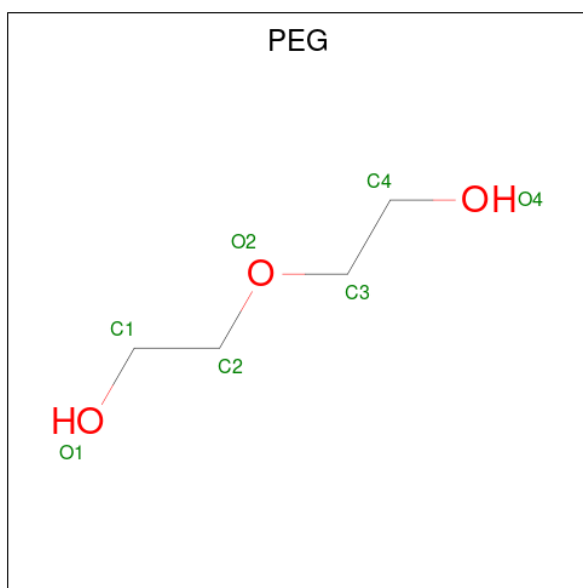
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total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

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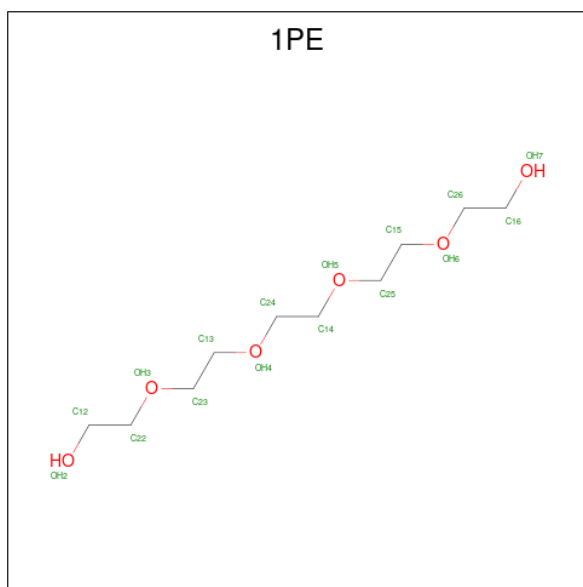
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



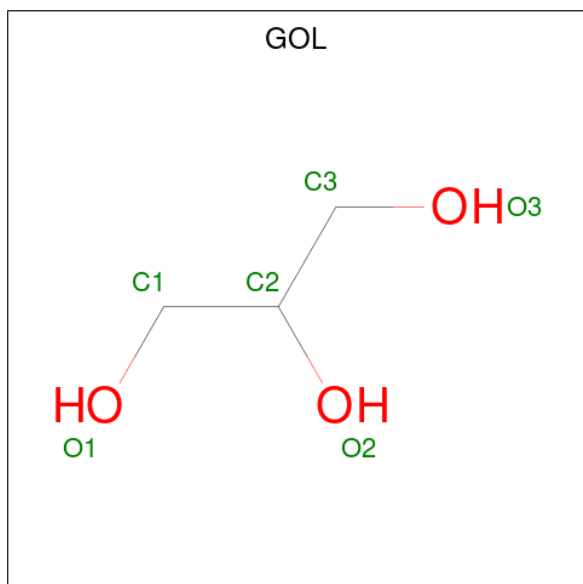
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



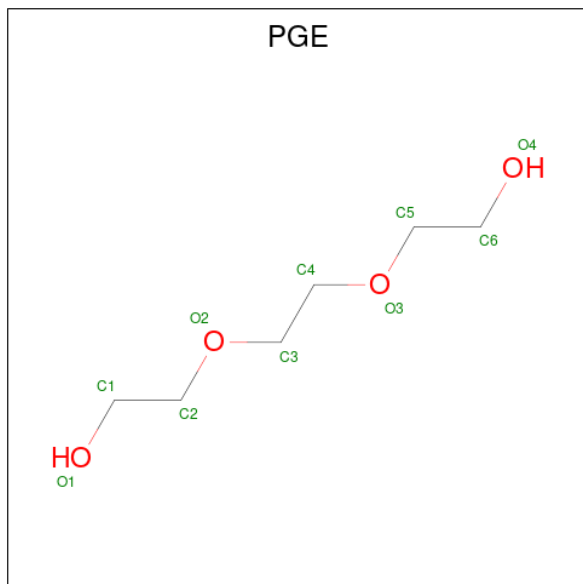
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			10	6	4		

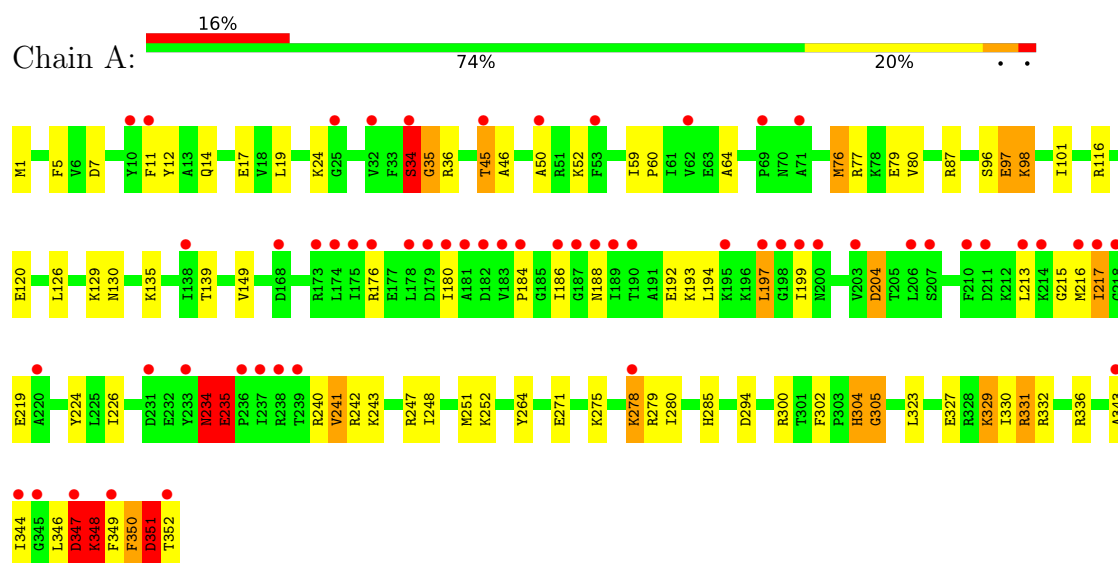
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	160	Total	O	0	0
			160	160		
9	C	99	Total	O	0	0
			99	99		
9	D	58	Total	O	0	0
			58	58		

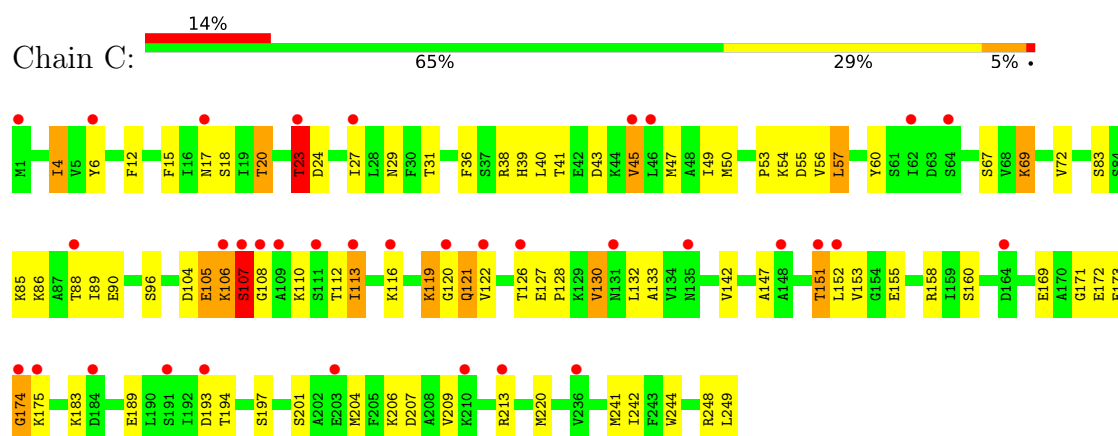
3 Residue-property plots [i](#)

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.

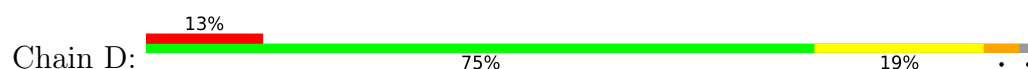
• Molecule 1: DNA polymerase IV

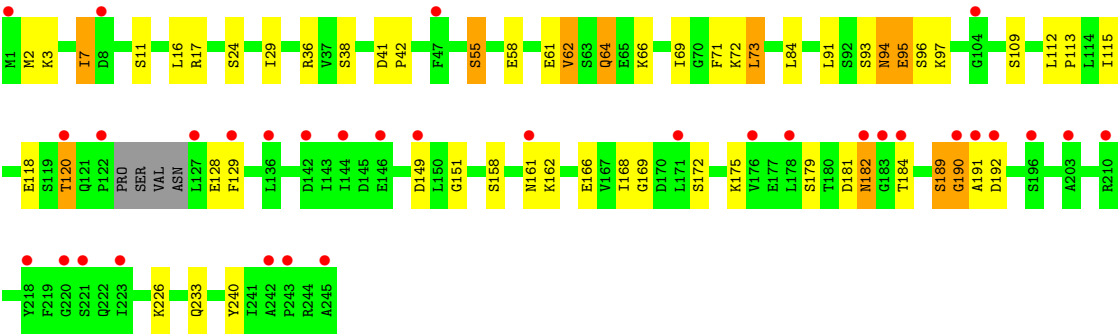


• Molecule 2: DNA polymerase sliding clamp B



• Molecule 3: DNA polymerase sliding clamp C





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.99Å 86.41Å 97.58Å 90.00° 107.30° 90.00°	Depositor
Resolution (Å)	29.88 – 2.05 29.88 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.88-2.05) 98.4 (29.88-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.240 0.193 , 0.240	Depositor DCC
R_{free} test set	1371 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7313	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: PGE, 1PE, PEG, GOL, EDO

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	1.08	8/2975 (0.3%)	1.19	19/3989 (0.5%)
2	C	0.97	2/2036 (0.1%)	1.04	7/2741 (0.3%)
3	D	1.08	5/1969 (0.3%)	1.03	5/2657 (0.2%)
All	All	1.05	15/6980 (0.2%)	1.11	31/9387 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
2	C	0	1
3	D	0	1
All	All	0	7

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	ARG	CZ-NH2	8.48	1.44	1.33
1	A	176	ARG	CD-NE	8.18	1.57	1.46
3	D	189	SER	C-N	8.14	1.45	1.32
1	A	219	GLU	C-O	7.67	1.33	1.24
2	C	112	THR	C-O	-7.35	1.14	1.23
3	D	191	ALA	CA-C	6.87	1.62	1.53
2	C	209	VAL	CA-CB	6.50	1.62	1.54
3	D	190	GLY	C-N	5.95	1.41	1.33
1	A	234	ASN	CA-C	5.83	1.59	1.52
1	A	176	ARG	CZ-NH1	5.61	1.40	1.32
3	D	191	ALA	C-N	5.55	1.41	1.33
1	A	305	GLY	N-CA	5.40	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	VAL	CA-CB	5.11	1.59	1.53
1	A	204	ASP	CG-OD2	5.05	1.34	1.25
3	D	192	ASP	CA-CB	5.03	1.59	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	LYS	N-CA-C	-19.92	88.07	113.17
1	A	35	GLY	N-CA-C	-17.06	88.55	110.38
1	A	97	GLU	N-CA-C	12.97	127.64	111.69
1	A	235	GLU	N-CA-C	-9.11	89.67	109.81
1	A	304	HIS	CA-C-N	-8.40	109.52	121.54
1	A	304	HIS	C-N-CA	-8.40	109.52	121.54
2	C	155	GLU	N-CA-C	-7.76	103.60	113.23
1	A	34[A]	SER	CA-C-N	7.60	134.52	121.97
1	A	34[A]	SER	C-N-CA	7.60	134.52	121.97
1	A	34[B]	SER	CA-C-N	7.60	134.52	121.97
1	A	34[B]	SER	C-N-CA	7.60	134.52	121.97
1	A	97	GLU	CA-C-N	7.28	134.79	121.70
1	A	97	GLU	C-N-CA	7.28	134.79	121.70
2	C	173	GLU	CA-C-N	-6.86	108.95	120.74
2	C	173	GLU	C-N-CA	-6.86	108.95	120.74
2	C	23	THR	CB-CA-C	-6.75	94.57	109.56
2	C	112	THR	O-C-N	6.66	131.85	123.19
3	D	184	THR	N-CA-C	6.64	121.51	113.41
3	D	190	GLY	CA-C-O	-6.42	113.51	121.02
1	A	197	LEU	CA-C-O	6.27	126.87	119.28
3	D	73	LEU	CA-CB-CG	-5.79	96.05	116.30
1	A	176	ARG	NH1-CZ-NH2	5.53	126.49	119.30
1	A	11	PHE	N-CA-C	5.50	117.73	111.02
2	C	113	ILE	CB-CA-C	-5.43	102.14	110.50
2	C	174	GLY	N-CA-C	5.28	120.75	113.99
3	D	64	GLN	N-CA-CB	-5.23	101.79	111.52
1	A	304	HIS	O-C-N	-5.22	115.72	122.20
1	A	219	GLU	N-CA-C	5.14	119.86	111.37
3	D	120	THR	N-CA-C	5.07	117.61	108.48
1	A	347	ASP	CA-C-N	-5.03	114.23	122.54
1	A	347	ASP	C-N-CA	-5.03	114.23	122.54

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	ASN	Peptide
1	A	347	ASP	Peptide
1	A	350	PHE	Peptide
1	A	351	ASP	Peptide
1	A	97	GLU	Peptide
2	C	119	LYS	Peptide
3	D	190	GLY	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	2913	0	3062	92	1
2	C	1991	0	2071	82	0
3	D	1930	0	1943	47	1
4	A	64	0	96	11	0
4	C	36	0	54	7	0
4	D	4	0	6	3	0
5	A	7	0	10	4	0
5	C	7	0	10	2	0
6	A	16	0	22	7	0
7	A	6	0	8	1	0
7	C	12	0	16	19	0
8	D	10	0	14	17	0
9	A	160	0	0	10	1
9	C	99	0	0	5	1
9	D	58	0	0	0	0
All	All	7313	0	7312	221	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (221) 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)
2:C:171:GLY:O	7:C:260:GOL:H32	1.46	1.15
1:A:304:HIS:H	4:A:358:EDO:H12	1.10	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:72:LYS:H	8:D:247:PGE:H2	1.13	1.09
7:C:260:GOL:H2	9:C:618:HOH:O	1.54	1.07
2:C:147:ALA:O	2:C:151[B]:THR:HG22	1.53	1.07
1:A:351:ASP:HB3	1:A:352:THR:CA	1.83	1.06
3:D:113:PRO:HD2	8:D:247:PGE:H5	1.41	1.02
1:A:14:GLN:HE22	1:A:139:THR:H	0.99	0.98
1:A:351:ASP:HB3	1:A:352:THR:HA	1.43	0.96
2:C:174:GLY:HA3	3:D:113:PRO:CG	1.95	0.96
2:C:175:LYS:HE2	8:D:247:PGE:H4	1.47	0.96
1:A:188:ASN:H	1:A:352:THR:C	1.73	0.96
1:A:304:HIS:N	4:A:358:EDO:H12	1.84	0.91
1:A:34[A]:SER:OG	1:A:35:GLY:HA3	1.72	0.90
5:A:369:PEG:H42	9:A:435:HOH:O	1.71	0.89
1:A:45:THR:HG21	7:A:371:GOL:O3	1.71	0.89
1:A:193:LYS:NZ	1:A:216:MET:O	2.05	0.89
2:C:174:GLY:HA3	3:D:113:PRO:HG3	1.53	0.87
1:A:302:PHE:HB3	4:A:358:EDO:H21	1.57	0.87
3:D:72:LYS:N	8:D:247:PGE:H2	1.92	0.85
1:A:130:ASN:HD21	6:A:370:1PE:C13	1.90	0.84
1:A:96:SER:OG	1:A:98:LYS:HB3	1.77	0.83
1:A:351:ASP:HB3	1:A:352:THR:CB	2.07	0.83
3:D:113:PRO:CD	8:D:247:PGE:H5	2.09	0.82
3:D:151:GLY:HA2	4:D:246:EDO:H21	1.63	0.81
2:C:175:LYS:HE2	8:D:247:PGE:C4	2.12	0.80
2:C:45:VAL:HG21	7:C:261:GOL:H31	1.62	0.79
2:C:153:VAL:HG22	5:C:259:PEG:H11	1.63	0.79
1:A:135:LYS:HE2	9:A:470:HOH:O	1.84	0.78
2:C:133:ALA:HB1	2:C:194:THR:HG22	1.67	0.76
1:A:350:PHE:O	1:A:351:ASP:O	2.04	0.76
2:C:171:GLY:O	7:C:260:GOL:H12	1.86	0.76
3:D:2:MET:HE3	3:D:93:SER:HB3	1.69	0.75
1:A:101:ILE:H	1:A:240:ARG:NH2	1.83	0.75
2:C:172:GLU:HB2	4:C:250:EDO:H12	1.69	0.75
1:A:247[A]:ARG:NH1	1:A:248:ILE:O	2.19	0.74
2:C:175:LYS:HE2	8:D:247:PGE:H52	1.69	0.74
2:C:175:LYS:HB3	5:C:259:PEG:H12	1.68	0.74
3:D:95:GLU:CD	3:D:95:GLU:H	1.96	0.74
2:C:45:VAL:HG21	7:C:261:GOL:C1	2.18	0.74
2:C:174:GLY:HA3	3:D:113:PRO:HG2	1.69	0.73
2:C:248:ARG:HE	7:C:261:GOL:H2	1.53	0.73
2:C:147:ALA:O	2:C:151[A]:THR:HB	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLN:NE2	1:A:139:THR:H	1.82	0.71
3:D:179:SER:O	3:D:182:ASN:ND2	2.23	0.71
3:D:151:GLY:CA	4:D:246:EDO:H21	2.22	0.70
1:A:329:LYS:HE3	9:A:377:HOH:O	1.92	0.70
2:C:220:MET:HE3	9:C:507:HOH:O	1.91	0.69
1:A:87:ARG:HH22	4:A:360:EDO:H21	1.57	0.69
2:C:248:ARG:HE	7:C:261:GOL:C2	2.05	0.69
3:D:169:GLY:HA2	4:D:246:EDO:H22	1.74	0.69
1:A:344:ILE:HD13	2:C:249:LEU:HD12	1.76	0.68
1:A:304:HIS:HB2	4:A:358:EDO:H11	1.74	0.68
1:A:101:ILE:H	1:A:240:ARG:HH22	1.42	0.67
1:A:304:HIS:H	4:A:358:EDO:C1	1.99	0.67
1:A:130:ASN:HD21	6:A:370:1PE:H132	1.59	0.67
1:A:216:MET:N	1:A:217:ILE:CA	2.58	0.67
3:D:179:SER:H	3:D:182:ASN:HD21	1.43	0.66
1:A:278:LYS:H	1:A:278:LYS:CD	2.08	0.66
1:A:34[B]:SER:HB3	1:A:35:GLY:CA	2.25	0.66
2:C:45:VAL:HG11	7:C:261:GOL:H32	1.77	0.66
2:C:15:PHE:HD2	2:C:241[A]:MET:HE2	1.61	0.66
2:C:248:ARG:NE	7:C:261:GOL:H2	2.11	0.65
2:C:160:SER:HB3	2:C:197:SER:HB3	1.78	0.65
2:C:171:GLY:O	7:C:260:GOL:C3	2.37	0.65
1:A:77:ARG:HD2	1:A:80:VAL:HG21	1.76	0.65
5:A:369:PEG:H12	5:A:369:PEG:H41	1.79	0.64
6:A:370:1PE:H242	9:A:559:HOH:O	1.97	0.63
1:A:304:HIS:HB2	4:A:358:EDO:C1	2.28	0.63
1:A:278:LYS:H	1:A:278:LYS:HD3	1.63	0.62
2:C:45:VAL:CG2	7:C:261:GOL:H12	2.28	0.62
3:D:118:GLU:OE2	3:D:118:GLU:HA	1.99	0.62
1:A:331:ARG:HD3	1:A:331:ARG:O	2.00	0.62
2:C:45:VAL:HG11	7:C:261:GOL:C3	2.30	0.62
3:D:94:ASN:ND2	3:D:96:SER:H	1.97	0.61
2:C:45:VAL:HG21	7:C:261:GOL:H12	1.81	0.61
1:A:336[A]:ARG:NH1	9:A:398:HOH:O	2.34	0.61
1:A:347:ASP:HB2	1:A:348:LYS:HD3	1.83	0.60
2:C:106:LYS:O	2:C:107:SER:C	2.44	0.60
1:A:347:ASP:HB3	1:A:348:LYS:HD2	1.82	0.60
1:A:34[A]:SER:OG	1:A:35:GLY:CA	2.49	0.59
1:A:130:ASN:HD21	6:A:370:1PE:H131	1.67	0.59
1:A:193:LYS:HD3	1:A:216:MET:HB3	1.85	0.59
3:D:113:PRO:HD2	8:D:247:PGE:C5	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:226:LYS:HE3	3:D:240:TYR:CZ	2.38	0.59
1:A:213:LEU:O	1:A:215:GLY:HA3	2.02	0.58
3:D:36:ARG:NH1	3:D:36:ARG:HB2	2.18	0.58
2:C:120:GLY:O	2:C:121:GLN:HB2	2.03	0.57
3:D:94:ASN:HD22	3:D:94:ASN:C	2.13	0.57
2:C:40:LEU:HD11	2:C:47[A]:MET:HE2	1.86	0.57
1:A:347:ASP:HB3	1:A:348:LYS:CD	2.33	0.57
3:D:113:PRO:CG	8:D:247:PGE:H5	2.34	0.56
3:D:36:ARG:HB2	3:D:36:ARG:HH11	1.70	0.56
2:C:39:HIS:HA	4:C:251:EDO:H11	1.88	0.56
3:D:112:LEU:HD13	8:D:247:PGE:H22	1.88	0.56
1:A:327:GLU:H	1:A:327:GLU:CD	2.13	0.56
1:A:129:LYS:HB3	4:A:366:EDO:H11	1.88	0.56
1:A:188:ASN:O	1:A:192:GLU:HB2	2.06	0.56
1:A:87:ARG:NH2	4:A:360:EDO:H21	2.21	0.55
1:A:327:GLU:CD	1:A:327:GLU:N	2.64	0.55
1:A:194:LEU:HB3	1:A:199:ILE:HB	1.88	0.55
2:C:86:LYS:HB3	2:C:105:GLU:HG2	1.90	0.54
1:A:35:GLY:HA2	2:C:193:ASP:HB3	1.90	0.54
2:C:12:PHE:CD2	2:C:89:ILE:HD12	2.42	0.54
1:A:34[A]:SER:CB	1:A:35:GLY:CA	2.85	0.54
2:C:18:SER:HB3	2:C:241[A]:MET:HE3	1.89	0.54
1:A:216:MET:H	1:A:217:ILE:CA	2.20	0.54
1:A:278:LYS:HD3	1:A:278:LYS:N	2.23	0.53
3:D:7:ILE:HG22	3:D:58:GLU:HG3	1.91	0.53
2:C:38:ARG:HG3	2:C:49:ILE:HG12	1.91	0.53
1:A:285:HIS:HB2	1:A:336[A]:ARG:HG2	1.90	0.53
1:A:347:ASP:CB	1:A:348:LYS:HD3	2.38	0.53
2:C:53:PRO:O	2:C:56:VAL:HG22	2.09	0.53
3:D:72:LYS:H	8:D:247:PGE:C2	2.04	0.52
1:A:347:ASP:C	1:A:349:PHE:H	2.00	0.52
1:A:213:LEU:C	1:A:215:GLY:HA3	2.35	0.52
1:A:194:LEU:HA	1:A:197:LEU:HB2	1.92	0.52
1:A:12:TYR:HB2	1:A:45:THR:HG23	1.92	0.52
2:C:54:LYS:HA	2:C:57:LEU:HD23	1.92	0.52
1:A:344:ILE:HD13	2:C:249:LEU:CD1	2.40	0.51
2:C:31:THR:HG22	2:C:122[A]:VAL:HG21	1.93	0.51
2:C:45:VAL:CG2	7:C:261:GOL:C1	2.88	0.51
1:A:275:LYS:O	1:A:279[A]:ARG:NH2	2.43	0.51
1:A:351:ASP:CB	1:A:352:THR:CB	2.87	0.51
3:D:94:ASN:ND2	3:D:97:LYS:H	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:ASN:O	2:C:20:THR:HB	2.11	0.50
1:A:116:ARG:HD2	1:A:120:GLU:OE1	2.11	0.50
1:A:280:ILE:CG2	1:A:305:GLY:HA3	2.41	0.50
2:C:133:ALA:CB	2:C:194:THR:HG22	2.40	0.50
1:A:188:ASN:N	1:A:352:THR:C	2.56	0.50
2:C:207:ASP:OD2	4:C:253:EDO:H11	2.11	0.50
1:A:347:ASP:C	1:A:349:PHE:N	2.59	0.49
2:C:158:ARG:HB3	2:C:169[B]:GLU:CG	2.43	0.49
2:C:220:MET:HE2	4:C:257:EDO:H11	1.95	0.49
3:D:2:MET:HE2	3:D:69:ILE:CD1	2.42	0.49
2:C:24:ASP:HB3	2:C:72:VAL:HG22	1.94	0.49
2:C:27:ILE:HG12	2:C:69:LYS:HG2	1.94	0.49
2:C:242:ILE:HD11	4:C:255:EDO:H11	1.93	0.49
2:C:54:LYS:HA	2:C:57:LEU:CD2	2.42	0.49
1:A:347:ASP:CB	1:A:348:LYS:CD	2.91	0.48
1:A:235:GLU:CA	9:A:666:HOH:O	2.61	0.48
1:A:351:ASP:CB	1:A:352:THR:CA	2.71	0.48
2:C:29:ASN:HB3	2:C:122[A]:VAL:HG23	1.93	0.48
1:A:60:PRO:HB3	4:A:354:EDO:H21	1.95	0.48
1:A:126:LEU:HB2	6:A:370:1PE:H121	1.94	0.48
2:C:142:VAL:HG21	4:C:256:EDO:H12	1.96	0.48
3:D:115[A]:ILE:HG12	8:D:247:PGE:H12	1.94	0.48
1:A:46:ALA:HB1	1:A:50:ALA:HB3	1.96	0.48
2:C:158:ARG:HB3	2:C:169[B]:GLU:HG3	1.96	0.48
2:C:45:VAL:CG2	2:C:204:MET:HG3	2.44	0.48
3:D:94:ASN:HD22	3:D:96:SER:H	1.61	0.48
2:C:67:SER:O	2:C:120:GLY:N	2.48	0.47
3:D:158:SER:HA	3:D:162:LYS:O	2.15	0.47
3:D:182:ASN:C	3:D:182:ASN:HD22	2.22	0.47
1:A:14:GLN:HE22	1:A:139:THR:N	1.85	0.47
2:C:4:ILE:HD13	2:C:60:TYR:CE1	2.49	0.47
5:A:369:PEG:H12	5:A:369:PEG:C4	2.42	0.46
1:A:199:ILE:HG23	1:A:204:ASP:HB2	1.97	0.46
2:C:96:SER:HB2	2:C:116:LYS:HD3	1.97	0.46
1:A:304:HIS:CA	4:A:358:EDO:H12	2.45	0.46
1:A:343:ALA:CB	7:C:261:GOL:H32	2.46	0.46
1:A:251:MET:HE1	1:A:330[A]:ILE:HG13	1.97	0.46
3:D:71:PHE:HA	8:D:247:PGE:C1	2.46	0.46
3:D:161:ASN:ND2	3:D:189:SER:HA	2.30	0.46
1:A:1:MET:HE1	9:A:629:HOH:O	2.16	0.46
2:C:23:THR:HG23	9:C:616:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:45:VAL:HG21	7:C:261:GOL:H11	1.93	0.46
3:D:55:SER:HB2	3:D:233:GLN:HG3	1.97	0.46
1:A:17:GLU:HB3	1:A:24:LYS:HG2	1.98	0.45
2:C:130:VAL:CG1	2:C:132:LEU:HD21	2.47	0.45
1:A:234:ASN:ND2	1:A:235:GLU:N	2.64	0.45
1:A:346:LEU:O	1:A:347:ASP:C	2.59	0.45
1:A:348:LYS:HD2	1:A:348:LYS:HA	1.86	0.45
2:C:106:LYS:O	2:C:107:SER:O	2.35	0.45
2:C:174:GLY:CA	3:D:113:PRO:HG3	2.36	0.45
3:D:41:ASP:HB2	3:D:42:PRO:HD2	1.99	0.45
1:A:251:MET:HG2	1:A:264:TYR:CG	2.52	0.45
2:C:36:PHE:HA	2:C:50:MET:O	2.17	0.44
3:D:128:GLU:CD	3:D:129:PHE:H	2.25	0.44
1:A:126:LEU:HB2	6:A:370:IPE:C12	2.48	0.44
2:C:160:SER:CB	2:C:197:SER:HB3	2.47	0.44
2:C:183:LYS:NZ	2:C:189:GLU:HA	2.31	0.44
2:C:175:LYS:CE	8:D:247:PGE:H4	2.33	0.44
2:C:158:ARG:NH1	2:C:169[B]:GLU:OE2	2.45	0.43
3:D:2:MET:HE3	3:D:93:SER:CB	2.41	0.43
2:C:6:TYR:HB3	9:C:622:HOH:O	2.17	0.43
2:C:105:GLU:HG3	2:C:106:LYS:N	2.34	0.43
5:A:369:PEG:C4	9:A:435:HOH:O	2.46	0.43
3:D:166:GLU:HG2	3:D:175:LYS:HG3	2.00	0.43
2:C:43:ASP:CG	2:C:45:VAL:HG13	2.44	0.43
2:C:201:SER:HB3	7:C:261:GOL:H11	2.01	0.42
1:A:343:ALA:HB2	7:C:261:GOL:H32	2.02	0.42
2:C:41:THR:CG2	4:C:253:EDO:H21	2.49	0.42
1:A:300[A]:ARG:HG2	1:A:302:PHE:CE1	2.54	0.42
2:C:45:VAL:HG22	2:C:204:MET:HG3	2.01	0.42
3:D:71:PHE:HA	8:D:247:PGE:H2	2.02	0.42
3:D:29:ILE:CG2	3:D:66:LYS:HD2	2.50	0.42
1:A:251:MET:HG2	1:A:264:TYR:CD2	2.55	0.41
2:C:83:SER:OG	2:C:85:LYS:HG3	2.20	0.41
1:A:186:ILE:HD13	1:A:224:TYR:HE2	1.85	0.41
1:A:149:VAL:HG13	1:A:184:PRO:HD2	2.02	0.41
1:A:331:ARG:HD3	1:A:331:ARG:C	2.42	0.41
3:D:71:PHE:HA	8:D:247:PGE:H12	2.01	0.41
3:D:3:LYS:HB3	3:D:61:GLU:HG2	2.02	0.41
1:A:188:ASN:O	1:A:192:GLU:CB	2.69	0.41
2:C:47[B]:MET:HE1	2:C:128:PRO:HD3	2.03	0.41
6:A:370:IPE:C24	9:A:559:HOH:O	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:107:SER:HA	2:C:108:GLY:HA3	1.67	0.41
1:A:5:PHE:CE2	1:A:7:ASP:HB2	2.56	0.41
2:C:45:VAL:HG21	7:C:261:GOL:C3	2.43	0.41
1:A:59:ILE:HD11	1:A:64:ALA:HB2	2.03	0.40
1:A:76:MET:HE3	1:A:76:MET:HB3	1.87	0.40
2:C:49:ILE:CD1	2:C:127:GLU:HG2	2.51	0.40
3:D:2:MET:HG3	3:D:93:SER:OG	2.21	0.40
3:D:62[A]:VAL:HG13	3:D:64:GLN:O	2.21	0.40
3:D:71:PHE:CA	8:D:247:PGE:H2	2.51	0.40
2:C:47[B]:MET:HE3	2:C:244:TRP:CD1	2.56	0.40
2:C:152:LEU:O	9:C:382:HOH:O	2.22	0.40
2:C:160:SER:HB3	2:C:197:SER:CB	2.50	0.40
1:A:285:HIS:HD2	9:A:466:HOH:O	2.04	0.40

All (2) 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)
9:A:404:HOH:O	9:C:544:HOH:O[1_655]	2.01	0.19
1:A:242:ARG:NH2	3:D:149:ASP:OD1[1_655]	2.08	0.12

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	363/352 (103%)	345 (95%)	12 (3%)	6 (2%)	7	2
2	C	257/249 (103%)	247 (96%)	8 (3%)	2 (1%)	16	9
3	D	240/245 (98%)	234 (98%)	6 (2%)	0	100	100
All	All	860/846 (102%)	826 (96%)	26 (3%)	8 (1%)	16	7

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	ILE
1	A	235	GLU
1	A	347	ASP
1	A	351	ASP
2	C	107	SER
1	A	34[A]	SER
1	A	34[B]	SER
2	C	121	GLN

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	318/309 (103%)	297 (93%)	21 (7%)	15	9
2	C	230/220 (104%)	207 (90%)	23 (10%)	7	3
3	D	219/219 (100%)	200 (91%)	19 (9%)	9	4
All	All	767/748 (102%)	704 (92%)	63 (8%)	11	5

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	36	ARG
1	A	45	THR
1	A	52	LYS
1	A	76	MET
1	A	79	GLU
1	A	98	LYS
1	A	180	ILE
1	A	226	ILE
1	A	234	ASN
1	A	241	VAL
1	A	243	LYS
1	A	252	LYS
1	A	271	GLU
1	A	278	LYS

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Mol	Chain	Res	Type
1	A	294	ASP
1	A	323	LEU
1	A	329	LYS
1	A	331	ARG
1	A	332	ARG
1	A	348	LYS
2	C	4	ILE
2	C	20	THR
2	C	23	THR
2	C	45	VAL
2	C	55	ASP
2	C	57	LEU
2	C	69	LYS
2	C	88	THR
2	C	90	GLU
2	C	104	ASP
2	C	105	GLU
2	C	106	LYS
2	C	107	SER
2	C	110	LYS
2	C	113	ILE
2	C	119	LYS
2	C	126	THR
2	C	130	VAL
2	C	151[A]	THR
2	C	151[B]	THR
2	C	206	LYS
2	C	213[A]	ARG
2	C	213[B]	ARG
3	D	7	ILE
3	D	11	SER
3	D	16	LEU
3	D	24	SER
3	D	38	SER
3	D	55	SER
3	D	62[A]	VAL
3	D	62[B]	VAL
3	D	73	LEU
3	D	84	LEU
3	D	91	LEU
3	D	94	ASN
3	D	95	GLU

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Mol	Chain	Res	Type
3	D	109	SER
3	D	120	THR
3	D	168	ILE
3	D	172	SER
3	D	181	ASP
3	D	182	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	82	GLN
1	A	130	ASN
1	A	188	ASN
1	A	234	ASN
1	A	254	ASN
1	A	285	HIS
2	C	17	ASN
2	C	135	ASN
3	D	27	ASN
3	D	94	ASN
3	D	161	ASN
3	D	182	ASN

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](#)

33 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PEG	A	369	-	6,6,6	0.60	0	5,5,5	0.47	0
7	GOL	A	371	-	5,5,5	0.52	0	5,5,5	0.91	0
4	EDO	C	250	-	3,3,3	0.63	0	2,2,2	0.45	0
4	EDO	A	356	-	3,3,3	0.44	0	2,2,2	0.62	0
4	EDO	A	367	-	3,3,3	0.56	0	2,2,2	0.49	0
4	EDO	A	360	-	3,3,3	0.40	0	2,2,2	0.36	0
7	GOL	C	260	-	5,5,5	0.65	0	5,5,5	1.21	0
4	EDO	A	354	-	3,3,3	0.59	0	2,2,2	0.26	0
4	EDO	A	368	-	3,3,3	0.79	0	2,2,2	0.79	0
4	EDO	C	252	-	3,3,3	0.47	0	2,2,2	0.43	0
4	EDO	C	257	-	3,3,3	0.52	0	2,2,2	0.21	0
5	PEG	C	259	-	6,6,6	0.91	0	5,5,5	0.92	0
8	PGE	D	247	-	9,9,9	0.92	0	8,8,8	1.45	2 (25%)
4	EDO	C	253	-	3,3,3	0.47	0	2,2,2	0.55	0
4	EDO	A	362	-	3,3,3	0.50	0	2,2,2	0.51	0
7	GOL	C	261	-	5,5,5	1.06	1 (20%)	5,5,5	1.61	2 (40%)
4	EDO	C	251	-	3,3,3	0.57	0	2,2,2	0.10	0
4	EDO	C	258	-	3,3,3	0.51	0	2,2,2	0.48	0
4	EDO	A	365	-	3,3,3	0.54	0	2,2,2	0.33	0
4	EDO	C	256	-	3,3,3	0.45	0	2,2,2	0.52	0
4	EDO	A	363	-	3,3,3	0.51	0	2,2,2	0.37	0
4	EDO	C	255	-	3,3,3	0.52	0	2,2,2	0.25	0
4	EDO	A	366	-	3,3,3	0.77	0	2,2,2	0.33	0
4	EDO	A	359	-	3,3,3	0.58	0	2,2,2	0.26	0
4	EDO	A	353	-	3,3,3	0.42	0	2,2,2	0.49	0
6	1PE	A	370	-	15,15,15	0.60	0	14,14,14	0.81	0
4	EDO	D	246	-	3,3,3	0.63	0	2,2,2	0.21	0
4	EDO	A	364	-	3,3,3	0.55	0	2,2,2	0.15	0
4	EDO	A	355	-	3,3,3	0.55	0	2,2,2	0.37	0
4	EDO	A	357	-	3,3,3	0.48	0	2,2,2	0.03	0
4	EDO	A	358	-	3,3,3	0.37	0	2,2,2	0.17	0
4	EDO	A	361	-	3,3,3	0.39	0	2,2,2	0.59	0
4	EDO	C	254	-	3,3,3	0.78	0	2,2,2	0.16	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
5	PEG	A	369	-	-	4/4/4/4	-
7	GOL	A	371	-	-	1/4/4/4	-
4	EDO	C	250	-	-	1/1/1/1	-
4	EDO	A	356	-	-	1/1/1/1	-
4	EDO	A	367	-	-	0/1/1/1	-
4	EDO	A	360	-	-	1/1/1/1	-
7	GOL	C	260	-	-	2/4/4/4	-
4	EDO	A	354	-	-	1/1/1/1	-
4	EDO	A	368	-	-	1/1/1/1	-
4	EDO	C	252	-	-	1/1/1/1	-
4	EDO	C	257	-	-	1/1/1/1	-
5	PEG	C	259	-	-	2/4/4/4	-
8	PGE	D	247	-	-	5/7/7/7	-
4	EDO	C	253	-	-	1/1/1/1	-
4	EDO	A	362	-	-	1/1/1/1	-
7	GOL	C	261	-	-	2/4/4/4	-
4	EDO	C	251	-	-	1/1/1/1	-
4	EDO	C	258	-	-	0/1/1/1	-
4	EDO	A	365	-	-	0/1/1/1	-
4	EDO	C	256	-	-	1/1/1/1	-
4	EDO	A	363	-	-	1/1/1/1	-
4	EDO	C	255	-	-	1/1/1/1	-
4	EDO	A	366	-	-	1/1/1/1	-
4	EDO	A	359	-	-	0/1/1/1	-
4	EDO	A	353	-	-	1/1/1/1	-
6	1PE	A	370	-	-	8/13/13/13	-
4	EDO	D	246	-	-	0/1/1/1	-
4	EDO	A	364	-	-	0/1/1/1	-
4	EDO	A	355	-	-	1/1/1/1	-
4	EDO	A	357	-	-	1/1/1/1	-
4	EDO	A	358	-	-	0/1/1/1	-
4	EDO	A	361	-	-	1/1/1/1	-
4	EDO	C	254	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	261	GOL	O2-C2	-2.03	1.37	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	247	PGE	C3-O2-C2	2.70	125.10	113.26
8	D	247	PGE	O3-C4-C3	2.24	120.55	110.35
7	C	261	GOL	O1-C1-C2	2.16	120.10	110.38
7	C	261	GOL	O3-C3-C2	2.03	119.50	110.38

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	261	GOL	C1-C2-C3-O3
5	C	259	PEG	C4-C3-O2-C2
8	D	247	PGE	C1-C2-O2-C3
6	A	370	1PE	OH4-C13-C23-OH3
5	A	369	PEG	O1-C1-C2-O2
8	D	247	PGE	O3-C5-C6-O4
6	A	370	1PE	OH5-C14-C24-OH4
7	C	261	GOL	O2-C2-C3-O3
4	A	353	EDO	O1-C1-C2-O2
4	A	366	EDO	O1-C1-C2-O2
4	C	250	EDO	O1-C1-C2-O2
4	C	253	EDO	O1-C1-C2-O2
4	C	255	EDO	O1-C1-C2-O2
5	A	369	PEG	O2-C3-C4-O4
8	D	247	PGE	O1-C1-C2-O2
5	A	369	PEG	C1-C2-O2-C3
4	A	356	EDO	O1-C1-C2-O2
4	A	362	EDO	O1-C1-C2-O2
4	A	363	EDO	O1-C1-C2-O2
4	A	368	EDO	O1-C1-C2-O2
4	C	256	EDO	O1-C1-C2-O2
7	A	371	GOL	O2-C2-C3-O3
6	A	370	1PE	C23-C13-OH4-C24
6	A	370	1PE	C12-C22-OH3-C23
8	D	247	PGE	C6-C5-O3-C4
6	A	370	1PE	C24-C14-OH5-C25
8	D	247	PGE	C4-C3-O2-C2
6	A	370	1PE	C13-C23-OH3-C22
4	C	254	EDO	O1-C1-C2-O2
6	A	370	1PE	OH2-C12-C22-OH3
6	A	370	1PE	C16-C26-OH6-C15
4	A	355	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	C	260	GOL	O1-C1-C2-O2
4	A	360	EDO	O1-C1-C2-O2
4	A	361	EDO	O1-C1-C2-O2
4	C	251	EDO	O1-C1-C2-O2
4	C	252	EDO	O1-C1-C2-O2
4	C	257	EDO	O1-C1-C2-O2
5	C	259	PEG	O1-C1-C2-O2
4	A	357	EDO	O1-C1-C2-O2
7	C	260	GOL	O1-C1-C2-C3
5	A	369	PEG	C4-C3-O2-C2
4	A	354	EDO	O1-C1-C2-O2

There are no ring outliers.

18 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	369	PEG	4	0
7	A	371	GOL	1	0
4	C	250	EDO	1	0
4	A	360	EDO	2	0
7	C	260	GOL	4	0
4	A	354	EDO	1	0
4	C	257	EDO	1	0
5	C	259	PEG	2	0
8	D	247	PGE	17	0
4	C	253	EDO	2	0
7	C	261	GOL	15	0
4	C	251	EDO	1	0
4	C	256	EDO	1	0
4	C	255	EDO	1	0
4	A	366	EDO	1	0
6	A	370	1PE	7	0
4	D	246	EDO	3	0
4	A	358	EDO	7	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	352/352 (100%)	1.17	58 (16%) 4 4	14, 44, 53, 58	12 (3%)
2	C	249/249 (100%)	1.20	35 (14%) 6 5	21, 46, 59, 66	10 (4%)
3	D	241/245 (98%)	1.07	33 (13%) 6 6	21, 45, 55, 81	4 (1%)
All	All	842/846 (99%)	1.15	126 (14%) 5 5	14, 45, 56, 81	26 (3%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	352	THR	7.1
1	A	174	LEU	4.7
1	A	239	THR	4.2
1	A	345	GLY	4.1
1	A	211	ASP	4.1
1	A	210	PHE	4.1
3	D	203	ALA	3.9
2	C	151[A]	THR	3.9
1	A	180	ILE	3.9
1	A	237	ILE	3.9
2	C	120	GLY	3.8
1	A	178	LEU	3.8
1	A	176	ARG	3.7
3	D	191	ALA	3.6
3	D	243	PRO	3.6
1	A	197	LEU	3.6
2	C	109	ALA	3.6
2	C	116	LYS	3.5
3	D	245	ALA	3.5
3	D	210	ARG	3.5
2	C	107	SER	3.4
3	D	218	TYR	3.4
1	A	188	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	236	PRO	3.4
2	C	184	ASP	3.3
1	A	198	GLY	3.3
1	A	233	TYR	3.3
1	A	187	GLY	3.2
1	A	183	VAL	3.2
2	C	203[A]	GLU	3.2
2	C	152	LEU	3.2
2	C	193	ASP	3.2
3	D	183	GLY	3.2
3	D	144	ILE	3.2
3	D	149	ASP	3.1
2	C	164	ASP	3.1
2	C	45	VAL	3.1
2	C	148	ALA	3.1
1	A	69	PRO	3.0
2	C	213[A]	ARG	3.0
1	A	179	ASP	3.0
1	A	173	ARG	2.9
3	D	178	LEU	2.9
1	A	343	ALA	2.9
2	C	122[A]	VAL	2.9
2	C	174	GLY	2.9
1	A	213	LEU	2.8
2	C	210	LYS	2.8
3	D	127	LEU	2.8
2	C	23	THR	2.8
3	D	120	THR	2.8
1	A	344	ILE	2.8
1	A	214	LYS	2.8
2	C	236	VAL	2.8
1	A	220	ALA	2.7
1	A	186	ILE	2.7
2	C	62	ILE	2.7
1	A	217	ILE	2.6
2	C	135	ASN	2.6
1	A	184	PRO	2.6
1	A	200	ASN	2.6
1	A	190	THR	2.6
3	D	176	VAL	2.6
2	C	113	ILE	2.5
1	A	71	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	189	ILE	2.5
3	D	223	ILE	2.5
1	A	195	LYS	2.5
2	C	106	LYS	2.5
2	C	6	TYR	2.5
1	A	168	ASP	2.5
3	D	104	GLY	2.5
3	D	220	GLY	2.5
1	A	45	THR	2.4
2	C	88	THR	2.4
1	A	349	PHE	2.4
2	C	108	GLY	2.4
1	A	175	ILE	2.4
1	A	182	ASP	2.4
1	A	199	ILE	2.4
3	D	242	ALA	2.4
1	A	347	ASP	2.4
2	C	1	MET	2.4
2	C	191	SER	2.4
2	C	131	ASN	2.3
3	D	192	ASP	2.3
2	C	175	LYS	2.3
3	D	8	ASP	2.3
3	D	171	LEU	2.3
2	C	64	SER	2.3
2	C	126	THR	2.3
1	A	218	GLY	2.3
1	A	11	PHE	2.2
1	A	181	ALA	2.2
3	D	196	SER	2.2
3	D	47	PHE	2.2
3	D	129	PHE	2.2
2	C	27	ILE	2.2
1	A	203	VAL	2.2
3	D	1[A]	MET	2.2
2	C	111	SER	2.2
1	A	50	ALA	2.2
3	D	221	SER	2.2
1	A	10	TYR	2.2
1	A	278	LYS	2.2
3	D	146	GLU	2.1
2	C	17	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	231	ASP	2.1
3	D	122	PRO	2.1
1	A	53	PHE	2.1
1	A	32	VAL	2.1
1	A	238	ARG	2.1
2	C	46	LEU	2.1
1	A	206	LEU	2.1
1	A	216	MET	2.1
3	D	182	ASN	2.1
3	D	142	ASP	2.1
3	D	184	THR	2.1
1	A	138	ILE	2.1
1	A	62	VAL	2.1
1	A	34[A]	SER	2.1
3	D	161	ASN	2.0
1	A	207	SER	2.0
3	D	136	LEU	2.0
1	A	25	GLY	2.0
3	D	190	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	C	252	4/4	0.54	0.33	53,54,54,54	4
4	EDO	C	255	4/4	0.54	0.23	50,51,51,52	4
4	EDO	C	258	4/4	0.61	0.25	48,49,49,50	4
4	EDO	A	361	4/4	0.66	0.23	50,51,51,51	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	367	4/4	0.67	0.20	51,61,62,63	0
4	EDO	A	353	4/4	0.67	0.26	52,52,53,53	4
4	EDO	A	362	4/4	0.73	0.23	56,56,56,57	4
4	EDO	A	355	4/4	0.74	0.30	48,48,49,50	4
4	EDO	A	365	4/4	0.75	0.22	51,51,51,51	4
4	EDO	C	257	4/4	0.76	0.21	44,46,48,48	4
4	EDO	A	368	4/4	0.77	0.18	52,54,54,55	0
4	EDO	A	354	4/4	0.78	0.14	47,49,50,51	4
4	EDO	A	357	4/4	0.79	0.21	46,47,48,49	4
5	PEG	A	369	7/7	0.79	0.16	59,61,64,64	0
6	1PE	A	370	16/16	0.79	0.17	50,58,70,73	0
4	EDO	A	356	4/4	0.81	0.19	54,56,56,59	0
5	PEG	C	259	7/7	0.82	0.16	31,47,54,55	0
4	EDO	A	364	4/4	0.82	0.23	44,45,45,48	4
4	EDO	A	366	4/4	0.83	0.19	53,60,61,61	0
4	EDO	A	363	4/4	0.83	0.13	64,65,65,67	0
4	EDO	C	254	4/4	0.83	0.17	55,57,58,59	0
4	EDO	C	256	4/4	0.85	0.19	53,56,58,62	0
4	EDO	A	359	4/4	0.85	0.14	46,57,58,64	0
8	PGE	D	247	10/10	0.85	0.14	15,39,49,53	2
4	EDO	D	246	4/4	0.86	0.14	51,53,55,55	0
4	EDO	C	251	4/4	0.87	0.15	56,63,65,69	0
4	EDO	A	360	4/4	0.87	0.12	61,63,63,66	0
4	EDO	C	250	4/4	0.87	0.27	40,49,49,57	0
7	GOL	C	261	6/6	0.89	0.23	39,47,48,49	0
4	EDO	C	253	4/4	0.89	0.18	46,55,56,61	0
7	GOL	C	260	6/6	0.90	0.20	41,44,50,50	0
7	GOL	A	371	6/6	0.92	0.14	34,46,49,51	0
4	EDO	A	358	4/4	0.92	0.18	43,45,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.