Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:37 AM GMT

PDB ID	:	3FDS
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

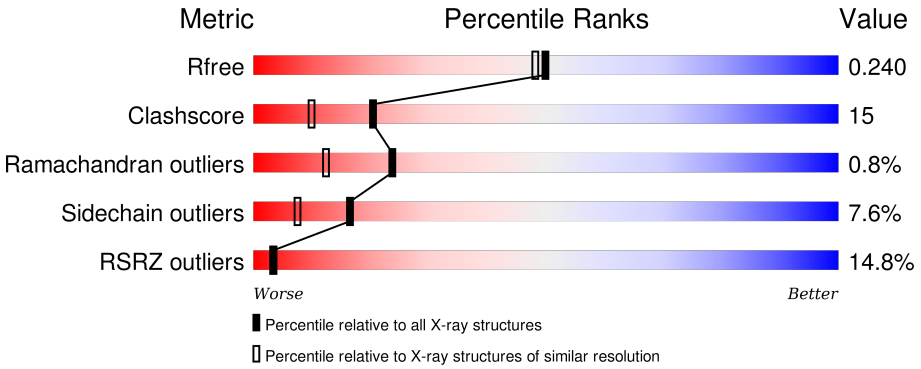
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (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 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 <=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	15%, 75%, 20%
2	C	249	14%, 69%, 26%
3	D	245	15%, 77%, 17%

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	354	-	-	-	X
4	EDO	A	355	-	-	-	X
4	EDO	A	357	-	-	-	X
4	EDO	A	358	-	-	X	-
4	EDO	A	359	-	-	-	X
4	EDO	A	360	-	-	-	X
4	EDO	C	250	-	-	-	X
4	EDO	C	253	-	-	-	X
4	EDO	C	255	-	-	-	X
4	EDO	C	256	-	-	-	X
4	EDO	C	257	-	-	-	X
4	EDO	D	246	-	-	-	X
5	PEG	A	369	-	-	X	X
6	1PE	A	370	-	-	X	-
7	GOL	C	260	-	-	X	X
7	GOL	C	261	-	-	X	X
8	PGE	D	247	-	-	X	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	UNP P57766

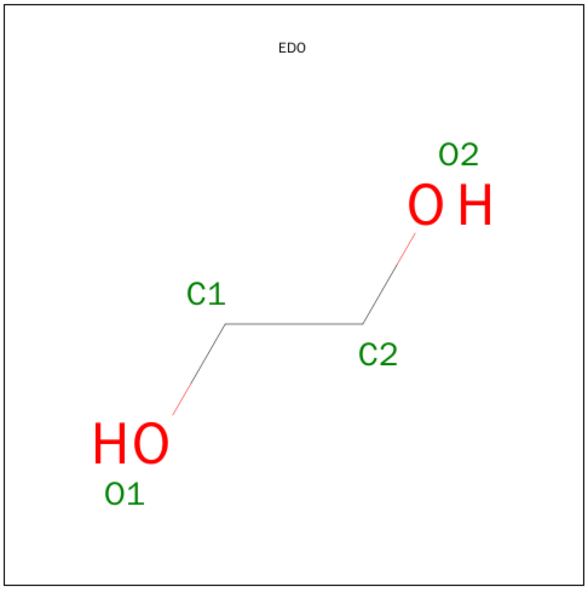
- Molecule 3 is a protein called DNA polymerase sliding clamp C.

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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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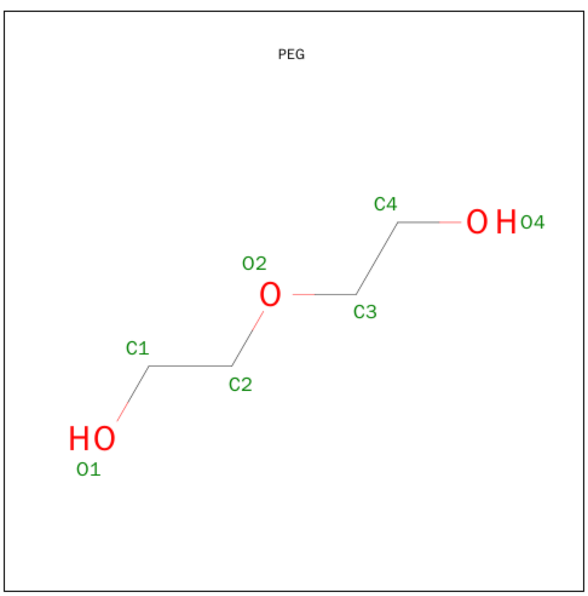
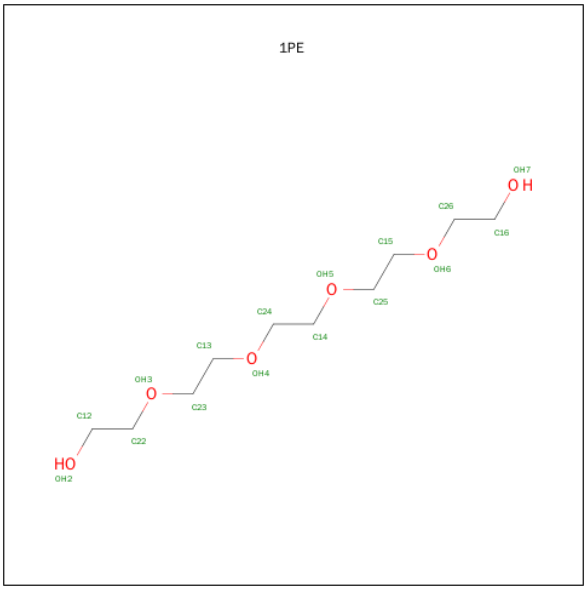
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0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

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



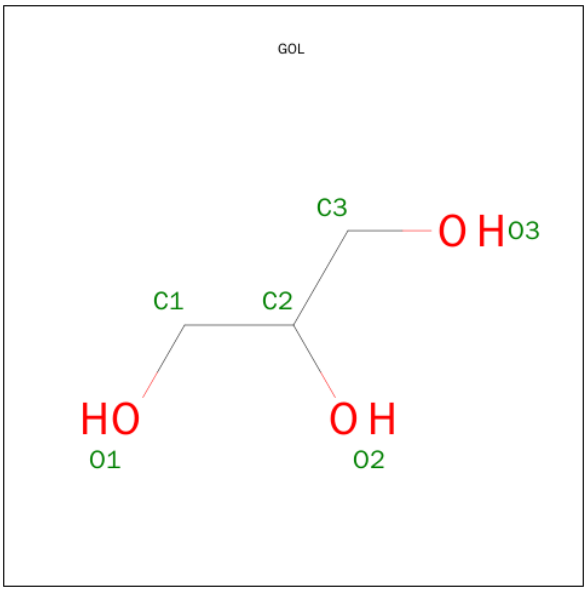
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0

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



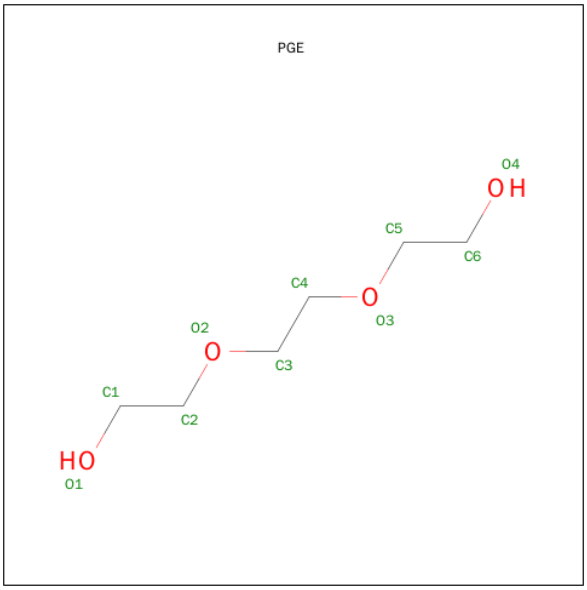
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 16 10 6	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 9 is water.

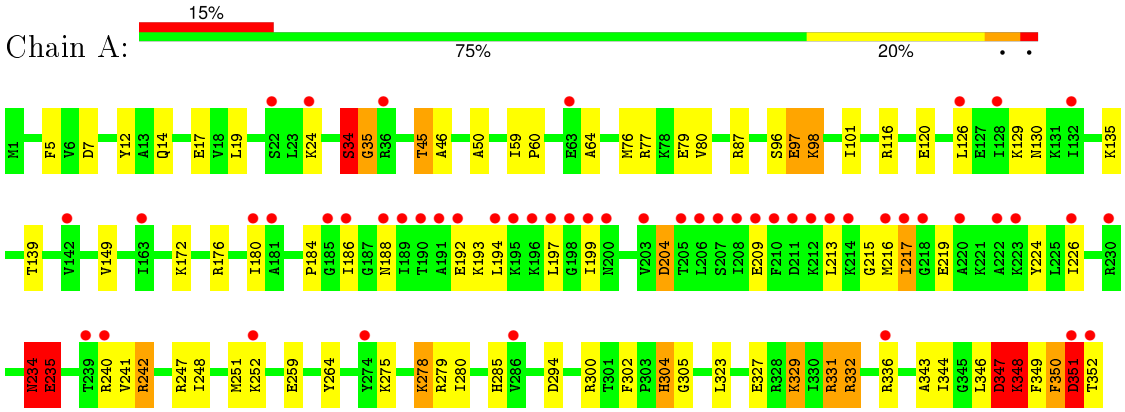
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	160	Total O 160 160	0	0
9	C	99	Total O 99 99	0	0
9	D	58	Total O 58 58	0	0

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 errors 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.

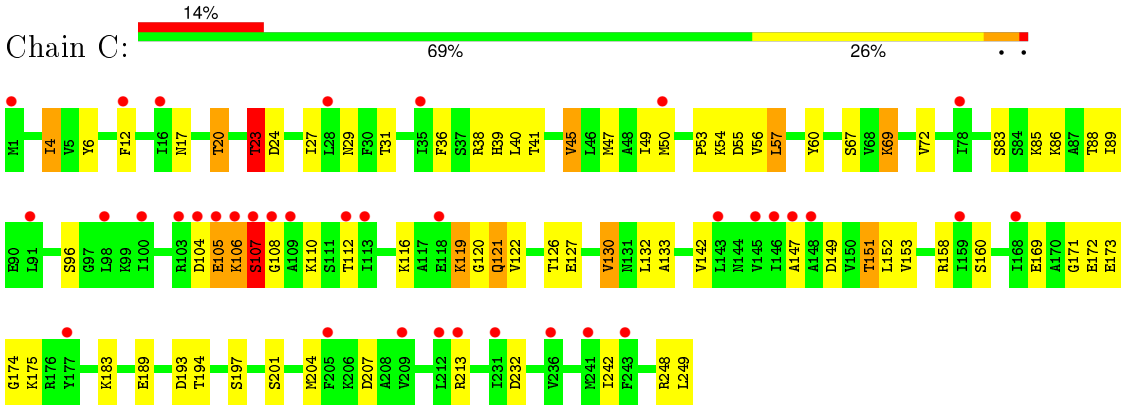
- Molecule 1: DNA polymerase IV

Chain A:



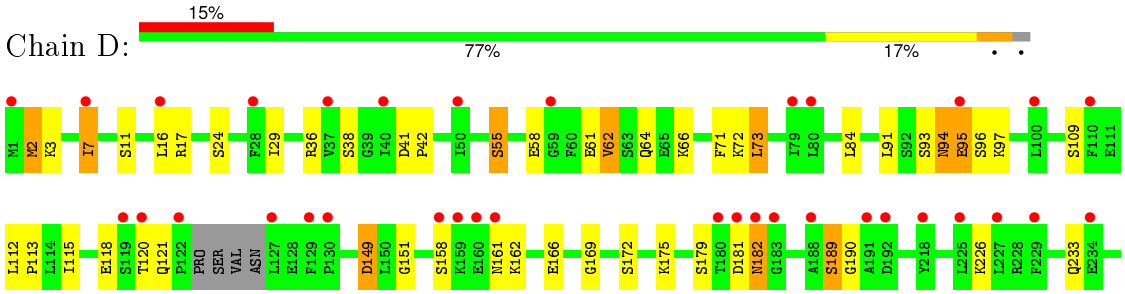
- Molecule 2: DNA polymerase sliding clamp B

Chain C:



- Molecule 3: DNA polymerase sliding clamp C

Chain D:




G237
Y240
A245

4 Data and refinement statistics (i)

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 29.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.88-2.05) 97.1 (29.90-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.4.0062	Depositor
R, R_{free}	0.190 , 0.240 0.192 , 0.240	Depositor DCC
R_{free} test set	1301 reflections (2.05%)	DCC
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 66.2	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 68498 reflections	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PEG, GOL, PGE, EDO, 1PE

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	0.95	7/2975 (0.2%)	0.94	18/3989 (0.5%)
2	C	0.79	0/2036	0.88	5/2741 (0.2%)
3	D	0.89	1/1969 (0.1%)	0.89	1/2657 (0.0%)
All	All	0.89	8/6980 (0.1%)	0.91	24/9387 (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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	ARG	CZ-NH2	8.79	1.44	1.33
1	A	259[A]	GLU	CD-OE1	-8.55	1.16	1.25
1	A	259[B]	GLU	CD-OE1	-8.55	1.16	1.25
1	A	209	GLU	CD-OE2	8.09	1.34	1.25
3	D	189	SER	C-N	6.77	1.45	1.33
1	A	176	ARG	CD-NE	6.62	1.57	1.46
1	A	176	ARG	CZ-NH1	5.81	1.40	1.33
1	A	219	GLU	C-O	5.11	1.33	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	35	GLY	N-CA-C	-9.82	88.55	113.10
1	A	176	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	A	348	LYS	N-CA-C	-8.49	88.07	111.00
3	D	73	LEU	CA-CB-CG	-8.37	96.05	115.30
1	A	235	GLU	N-CA-C	-7.90	89.67	111.00
1	A	259[A]	GLU	OE1-CD-OE2	-7.87	113.86	123.30
1	A	259[B]	GLU	OE1-CD-OE2	-7.87	113.86	123.30
1	A	176	ARG	NH1-CZ-NH2	6.45	126.49	119.40
2	C	173	GLU	C-N-CA	-6.36	108.95	122.30
2	C	23	THR	CB-CA-C	-6.31	94.57	111.60
1	A	259[A]	GLU	CG-CD-OE1	6.21	130.72	118.30
1	A	259[B]	GLU	CG-CD-OE1	6.21	130.72	118.30
1	A	97	GLU	N-CA-C	6.16	127.64	111.00
1	A	176	ARG	NE-CZ-NH1	-6.09	117.25	120.30
1	A	304	HIS	C-N-CA	-6.08	109.52	122.30
1	A	332	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	34[A]	SER	C-N-CA	5.82	134.52	122.30
1	A	34[B]	SER	C-N-CA	5.82	134.52	122.30
2	C	112	THR	O-C-N	5.72	131.85	122.70
2	C	232	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	347	ASP	CB-CG-OD1	-5.66	113.21	118.30
1	A	97	GLU	C-N-CA	5.24	134.79	121.70
1	A	204	ASP	CB-CG-OD2	5.11	122.90	118.30
2	C	149	ASP	CB-CG-OD2	-5.06	113.75	118.30

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	89	1
2	C	1991	0	2071	76	0
3	D	1930	0	1943	44	1
4	A	64	0	96	11	0
4	C	36	0	54	6	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	4	1
9	D	58	0	0	0	0
All	All	7313	0	7312	209	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 (209) 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
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:304:HIS:N	4:A:358:EDO:H12	1.84	0.91
1:A:188:ASN:H	1:A:352:THR:C	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:351:ASP:HB3	1:A:352:THR:CB	2.07	0.83
1:A:96:SER:OG	1:A:98:LYS:HB3	1.77	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:153:VAL:HG22	5:C:259:PEG:H11	1.63	0.79
2:C:45:VAL:HG21	7:C:261:GOL:H31	1.62	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
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
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
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
3:D:169:GLY:HA2	4:D:246:EDO:H22	1.74	0.69
2:C:248:ARG:HE	7:C:261:GOL:C2	2.05	0.69
1:A:87:ARG:HH22	4:A:360:EDO:H21	1.57	0.69
3:D:95:GLU:CD	3:D:95:GLU:H	1.96	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:304:HIS:H	4:A:358:EDO:C1	1.99	0.67
1:A:101:ILE:H	1:A:240:ARG:HH22	1.42	0.67
1:A:216:MET:N	1:A:217:ILE:CA	2.58	0.67
1:A:130:ASN:HD21	6:A:370:1PE:H132	1.59	0.67
3:D:179:SER:H	3:D:182:ASN:HD21	1.43	0.66
1:A:278:LYS:CD	1:A:278:LYS:H	2.08	0.66
1:A:34[B]:SER:HB3	1:A:35:GLY:CA	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:45:VAL:HG11	7:C:261:GOL:H32	1.77	0.66
2:C:248:ARG:NE	7:C:261:GOL:H2	2.11	0.65
2:C:171:GLY:O	7:C:260:GOL:C3	2.37	0.65
2:C:160:SER:HB3	2:C:197:SER:HB3	1.78	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
2:C:45:VAL:CG2	7:C:261:GOL:H12	2.28	0.62
1:A:278:LYS:H	1:A:278:LYS:HD3	1.63	0.62
3:D:118:GLU:HA	3:D:118:GLU:OE2	1.99	0.62
1:A:331:ARG:O	1:A:331:ARG:HD3	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
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
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:2:MET:HE2	3:D:93:SER:HB3	1.85	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:HH11	3:D:36:ARG:HB2	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:188:ASN:O	1:A:192:GLU:HB2	2.06	0.56
1:A:129:LYS:HB3	4:A:366:EDO:H11	1.88	0.56
1:A:87:ARG:NH2	4:A:360:EDO:H21	2.21	0.55
2:C:106:LYS:O	2:C:107:SER:C	2.44	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
2:C:40:LEU:HD11	2:C:47[A]:MET:HE2	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34[A]:SER:CB	1:A:35:GLY:CA	2.85	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
3:D:94:ASN:HD22	3:D:94:ASN:C	2.13	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: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:327:GLU:H	1:A:327:GLU:CD	2.13	0.51
1:A:344:ILE:HD13	2:C:249:LEU:CD1	2.40	0.51
1:A:327:GLU:CD	1:A:327:GLU:N	2.64	0.51
2:C:45:VAL:CG2	7:C:261:GOL:C1	2.88	0.51
2:C:31:THR:HG22	2:C:122[A]:VAL:HG21	1.93	0.51
1:A:351:ASP:CB	1:A:352:THR:CB	2.87	0.51
1:A:275:LYS:O	1:A:279[A]:ARG:NH2	2.43	0.51
3:D:94:ASN:ND2	3:D:97:LYS:H	2.09	0.50
2:C:17:ASN:O	2:C:20:THR:HB	2.11	0.50
2:C:133:ALA:CB	2:C:194:THR:HG22	2.40	0.50
1:A:280:ILE:CG2	1:A:305:GLY:HA3	2.41	0.50
1:A:116:ARG:HD2	1:A:120:GLU:OE1	2.11	0.50
2:C:207:ASP:OD2	4:C:253:EDO:H11	2.11	0.50
2:C:158:ARG:HB3	2:C:169[B]:GLU:CG	2.43	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:C	1:A:349:PHE:H	2.00	0.48
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
3:D:115[A]:ILE:HG12	8:D:247:PGE:H12	1.94	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
1:A:60:PRO:HB3	4:A:354:EDO:H21	1.95	0.48
1:A:46:ALA:HB1	1:A:50:ALA:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:213:LEU:C	1:A:215:GLY:HA3	2.35	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:188:ASN:N	1:A:352:THR:C	2.56	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
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
2:C:45:VAL:HG21	7:C:261:GOL:H11	1.93	0.46
2:C:23:THR:HG23	9:C:616:HOH:O	2.16	0.46
3:D:55:SER:HB2	3:D:233:GLN:HG3	1.97	0.46
1:A:347:ASP:C	1:A:349:PHE:N	2.59	0.45
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:172:LYS:NZ	9:A:652:HOH:O	2.45	0.45
1:A:348:LYS:HA	1:A:348:LYS:HD2	1.86	0.45
2:C:174:GLY:CA	3:D:113:PRO:HG3	2.36	0.45
2:C:106:LYS:O	2:C:107:SER:O	2.35	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
1:A:126:LEU:HB2	6:A:370:1PE: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
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:201:SER:HB3	7:C:261:GOL:H11	2.01	0.42
3:D:182:ASN:HD22	3:D:182:ASN:C	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:71:PHE:HA	8:D:247:PGE:H2	2.02	0.42
2:C:45:VAL:HG22	2:C:204:MET:HG3	2.01	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
3:D:71:PHE:HA	8:D:247:PGE:H12	2.01	0.41
1:A:149:VAL:HG13	1:A:184:PRO:HD2	2.02	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
6:A:370:1PE:C24	9:A:559:HOH:O	2.63	0.41
2:C:107:SER:HA	2:C:108:GLY:HA3	1.67	0.41
2:C:45:VAL:HG21	7:C:261:GOL:C3	2.43	0.41
1:A:5:PHE:CE2	1:A:7:ASP:HB2	2.56	0.41
1:A:59:ILE:HD11	1:A:64:ALA:HB2	2.03	0.40
3:D:71:PHE:CA	8:D:247:PGE:H2	2.51	0.40
3:D:2:MET:HG3	3:D:93:SER:OG	2.21	0.40
2:C:49:ILE:CD1	2:C:127:GLU:HG2	2.51	0.40
3:D:62[A]:VAL:HG13	3:D:64:GLN:O	2.21	0.40
2:C:160:SER:HB3	2:C:197:SER:CB	2.50	0.40
1:A:346:LEU:O	1:A:347:ASP:C	2.59	0.40
2:C:183:LYS:HZ2	2:C:189:GLU:HA	1.85	0.40
2:C:152:LEU:O	9:C:382:HOH:O	2.22	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%)	11 3
2	C	257/249 (103%)	247 (96%)	8 (3%)	2 (1%)	24 12
3	D	240/245 (98%)	234 (98%)	6 (2%)	0	100 100
All	All	860/846 (102%)	826 (96%)	26 (3%)	8 (1%)	24 10

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	318/309 (103%)	300 (94%)	18 (6%)	25 15
2	C	230/220 (104%)	210 (91%)	20 (9%)	13 5
3	D	219/219 (100%)	198 (90%)	21 (10%)	10 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	767/748 (102%)	708 (92%)	59 (8%)	16 7

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	45	THR
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	242	ARG
1	A	252	LYS
1	A	278	LYS
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	104	ASP
2	C	105	GLU
2	C	106	LYS
2	C	107	SER
2	C	110	LYS
2	C	119	LYS
2	C	126	THR
2	C	130	VAL
2	C	151[A]	THR
2	C	151[B]	THR
2	C	213[A]	ARG

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Mol	Chain	Res	Type
2	C	213[B]	ARG
3	D	2	MET
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
3	D	109	SER
3	D	120	THR
3	D	121	GLN
3	D	149	ASP
3	D	172	SER
3	D	181	ASP
3	D	182	ASN

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

Mol	Chain	Res	Type
1	A	14	GLN
1	A	130	ASN
1	A	188	ASN
1	A	234	ASN
1	A	285	HIS
2	C	135	ASN
3	D	27	ASN
3	D	64	GLN
3	D	94	ASN
3	D	161	ASN
3	D	182	ASN
3	D	233	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
4	EDO	A	353	-	3,3,3	0.46	0	2,2,2	0.54	0
4	EDO	A	354	-	3,3,3	0.63	0	2,2,2	0.30	0
4	EDO	A	355	-	3,3,3	0.57	0	2,2,2	0.41	0
4	EDO	A	356	-	3,3,3	0.47	0	2,2,2	0.68	0
4	EDO	A	357	-	3,3,3	0.52	0	2,2,2	0.04	0
4	EDO	A	358	-	3,3,3	0.42	0	2,2,2	0.21	0
4	EDO	A	359	-	3,3,3	0.62	0	2,2,2	0.29	0
4	EDO	A	360	-	3,3,3	0.45	0	2,2,2	0.40	0
4	EDO	A	361	-	3,3,3	0.43	0	2,2,2	0.65	0
4	EDO	A	362	-	3,3,3	0.54	0	2,2,2	0.56	0
4	EDO	A	363	-	3,3,3	0.54	0	2,2,2	0.41	0
4	EDO	A	364	-	3,3,3	0.59	0	2,2,2	0.17	0
4	EDO	A	365	-	3,3,3	0.58	0	2,2,2	0.37	0
4	EDO	A	366	-	3,3,3	0.79	0	2,2,2	0.33	0
4	EDO	A	367	-	3,3,3	0.61	0	2,2,2	0.53	0
4	EDO	A	368	-	3,3,3	0.81	0	2,2,2	0.86	0
5	PEG	A	369	-	6,6,6	0.59	0	5,5,5	0.43	0
6	1PE	A	370	-	15,15,15	0.60	0	14,14,14	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	GOL	A	371	-	5,5,5	0.51	0	5,5,5	0.76	0
4	EDO	C	250	-	3,3,3	0.64	0	2,2,2	0.49	0
4	EDO	C	251	-	3,3,3	0.60	0	2,2,2	0.11	0
4	EDO	C	252	-	3,3,3	0.51	0	2,2,2	0.48	0
4	EDO	C	253	-	3,3,3	0.53	0	2,2,2	0.61	0
4	EDO	C	254	-	3,3,3	0.81	0	2,2,2	0.18	0
4	EDO	C	255	-	3,3,3	0.56	0	2,2,2	0.29	0
4	EDO	C	256	-	3,3,3	0.48	0	2,2,2	0.56	0
4	EDO	C	257	-	3,3,3	0.57	0	2,2,2	0.24	0
4	EDO	C	258	-	3,3,3	0.54	0	2,2,2	0.53	0
5	PEG	C	259	-	6,6,6	0.88	0	5,5,5	0.91	0
7	GOL	C	260	-	5,5,5	0.57	0	5,5,5	1.14	0
7	GOL	C	261	-	5,5,5	1.02	1 (20%)	5,5,5	1.49	1 (20%)
4	EDO	D	246	-	3,3,3	0.66	0	2,2,2	0.22	0
8	PGE	D	247	-	9,9,9	0.92	0	8,8,8	1.45	2 (25%)

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
4	EDO	A	353	-	-	0/1/1/1	0/0/0/0
4	EDO	A	354	-	-	0/1/1/1	0/0/0/0
4	EDO	A	355	-	-	0/1/1/1	0/0/0/0
4	EDO	A	356	-	-	0/1/1/1	0/0/0/0
4	EDO	A	357	-	-	0/1/1/1	0/0/0/0
4	EDO	A	358	-	-	0/1/1/1	0/0/0/0
4	EDO	A	359	-	-	0/1/1/1	0/0/0/0
4	EDO	A	360	-	-	0/1/1/1	0/0/0/0
4	EDO	A	361	-	-	0/1/1/1	0/0/0/0
4	EDO	A	362	-	-	0/1/1/1	0/0/0/0
4	EDO	A	363	-	-	0/1/1/1	0/0/0/0
4	EDO	A	364	-	-	0/1/1/1	0/0/0/0
4	EDO	A	365	-	-	0/1/1/1	0/0/0/0
4	EDO	A	366	-	-	0/1/1/1	0/0/0/0
4	EDO	A	367	-	-	0/1/1/1	0/0/0/0
4	EDO	A	368	-	-	0/1/1/1	0/0/0/0
5	PEG	A	369	-	-	0/4/4/4	0/0/0/0
6	1PE	A	370	-	-	0/13/13/13	0/0/0/0
7	GOL	A	371	-	-	0/4/4/4	0/0/0/0
4	EDO	C	250	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	251	-	-	0/1/1/1	0/0/0/0
4	EDO	C	252	-	-	0/1/1/1	0/0/0/0
4	EDO	C	253	-	-	0/1/1/1	0/0/0/0
4	EDO	C	254	-	-	0/1/1/1	0/0/0/0
4	EDO	C	255	-	-	0/1/1/1	0/0/0/0
4	EDO	C	256	-	-	0/1/1/1	0/0/0/0
4	EDO	C	257	-	-	0/1/1/1	0/0/0/0
4	EDO	C	258	-	-	0/1/1/1	0/0/0/0
5	PEG	C	259	-	-	0/4/4/4	0/0/0/0
7	GOL	C	260	-	-	0/4/4/4	0/0/0/0
7	GOL	C	261	-	-	0/4/4/4	0/0/0/0
4	EDO	D	246	-	-	0/1/1/1	0/0/0/0
8	PGE	D	247	-	-	0/7/7/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	261	GOL	O2-C2	-2.02	1.37	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	261	GOL	O1-C1-C2	2.04	120.10	110.18
8	D	247	PGE	O3-C4-C3	2.29	120.55	110.36
8	D	247	PGE	C3-O2-C2	2.74	125.10	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	354	EDO	1	0
4	A	358	EDO	7	0
4	A	360	EDO	2	0
4	A	366	EDO	1	0
5	A	369	PEG	4	0
6	A	370	1PE	7	0
7	A	371	GOL	1	0
4	C	250	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	251	EDO	1	0
4	C	253	EDO	2	0
4	C	255	EDO	1	0
4	C	256	EDO	1	0
5	C	259	PEG	2	0
7	C	260	GOL	4	0
7	C	261	GOL	15	0
4	D	246	EDO	3	0
8	D	247	PGE	17	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, 95^{th} 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%)	0.84	52 (14%)	3	3	31, 45, 53, 58	0
2	C	249/249 (100%)	0.85	36 (14%)	3	3	39, 46, 60, 66	0
3	D	241/245 (98%)	0.79	37 (15%)	3	3	37, 45, 55, 81	0
All	All	842/846 (99%)	0.83	125 (14%)	3	3	31, 45, 56, 81	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	LYS	8.7
1	A	213	LEU	8.1
1	A	352	THR	7.5
1	A	210	PHE	7.2
2	C	107	SER	7.1
1	A	208	ILE	6.6
1	A	214	LYS	5.9
1	A	216	MET	5.8
1	A	206	LEU	5.7
3	D	245	ALA	5.7
1	A	220	ALA	5.5
1	A	195	LYS	5.4
1	A	209	GLU	5.4
1	A	198	GLY	5.3
3	D	160	GLU	5.2
1	A	207	SER	5.2
1	A	197	LEU	5.1
1	A	199	ILE	5.1
1	A	190	THR	5.0
2	C	213[A]	ARG	4.8
2	C	109	ALA	4.8
3	D	122	PRO	4.6
1	A	191	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	200	ASN	4.4
1	A	211	ASP	4.4
1	A	351	ASP	4.4
2	C	212	LEU	4.4
2	C	106	LYS	4.3
1	A	192	GLU	4.3
1	A	189	ILE	4.2
2	C	146[A]	ILE	4.1
3	D	183	GLY	4.0
1	A	217	ILE	4.0
2	C	105	GLU	3.9
3	D	161	ASN	3.7
1	A	226	ILE	3.7
2	C	143	LEU	3.7
2	C	205	PHE	3.6
1	A	188	ASN	3.6
1	A	205	THR	3.6
1	A	194	LEU	3.5
2	C	16	ILE	3.5
3	D	180	THR	3.4
2	C	28	LEU	3.4
3	D	127	LEU	3.4
3	D	192	ASP	3.4
1	A	286	VAL	3.3
1	A	203	VAL	3.3
3	D	159	LYS	3.3
3	D	50	ILE	3.2
3	D	218	TYR	3.1
3	D	182	ASN	3.1
2	C	209	VAL	3.1
1	A	186	ILE	3.0
3	D	191	ALA	3.0
2	C	145	VAL	2.9
3	D	120	THR	2.9
1	A	22	SER	2.8
2	C	12	PHE	2.8
3	D	229	PHE	2.8
1	A	185	GLY	2.8
1	A	230	ARG	2.8
3	D	130	PRO	2.8
3	D	110	PHE	2.7
3	D	129	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	108	GLY	2.7
1	A	212	LYS	2.7
3	D	80	LEU	2.7
3	D	95	GLU	2.6
1	A	274	TYR	2.6
2	C	112	THR	2.6
1	A	336[A]	ARG	2.6
2	C	100	ILE	2.6
1	A	181	ALA	2.6
2	C	35	ILE	2.6
3	D	37	VAL	2.6
1	A	180	ILE	2.5
2	C	177	TYR	2.5
3	D	188	ALA	2.5
3	D	237	GLY	2.5
3	D	16	LEU	2.5
1	A	142	VAL	2.5
1	A	240	ARG	2.5
2	C	148	ALA	2.4
2	C	231	ILE	2.4
1	A	24	LYS	2.4
3	D	227	LEU	2.4
2	C	147	ALA	2.3
1	A	163	ILE	2.3
1	A	218	GLY	2.3
3	D	100	LEU	2.3
2	C	104	ASP	2.3
3	D	1[A]	MET	2.3
1	A	223	LYS	2.3
1	A	128	ILE	2.3
2	C	103	ARG	2.3
3	D	28	PHE	2.2
2	C	1	MET	2.2
2	C	50	MET	2.2
2	C	241[A]	MET	2.2
2	C	113	ILE	2.2
1	A	239	THR	2.2
2	C	236	VAL	2.2
2	C	168	ILE	2.2
3	D	225	LEU	2.2
3	D	234	GLU	2.2
3	D	7	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	126	LEU	2.1
2	C	91	LEU	2.1
1	A	63[A]	GLU	2.1
3	D	158	SER	2.1
3	D	181	ASP	2.1
3	D	59	GLY	2.1
3	D	119	SER	2.1
2	C	98	LEU	2.1
1	A	222	ALA	2.1
2	C	243	PHE	2.1
3	D	40	ILE	2.1
1	A	36	ARG	2.1
1	A	252	LYS	2.1
2	C	78	ILE	2.0
3	D	79	ILE	2.0
2	C	118	GLU	2.0
1	A	132	ILE	2.0
2	C	159	ILE	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 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, 95^{th} 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
4	EDO	C	253	4/4	0.85	0.44	15.79	46,55,56,61	0
4	EDO	A	359	4/4	0.90	0.25	11.06	46,57,58,64	0
4	EDO	C	250	4/4	0.93	0.45	9.18	40,49,49,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	GOL	C	261	6/6	0.94	0.34	7.62	39,47,48,49	0
8	PGE	D	247	10/10	0.86	0.33	6.44	15,39,49,53	2
4	EDO	A	360	4/4	0.81	0.19	6.33	61,63,63,66	0
4	EDO	D	246	4/4	0.66	0.32	4.87	51,53,55,55	0
4	EDO	C	255	4/4	0.64	0.28	4.47	50,51,51,52	4
4	EDO	A	357	4/4	0.85	0.41	4.41	46,47,48,49	4
4	EDO	A	354	4/4	0.83	0.19	4.21	47,49,50,51	4
4	EDO	C	256	4/4	0.87	0.33	3.53	53,56,58,62	0
5	PEG	A	369	7/7	0.86	0.22	3.31	59,61,64,64	0
4	EDO	A	355	4/4	0.69	0.25	3.16	48,48,49,50	4
7	GOL	C	260	6/6	0.82	0.26	2.72	41,44,50,50	0
4	EDO	C	257	4/4	0.74	0.20	2.00	44,46,48,48	4
5	PEG	C	259	7/7	0.88	0.21	0.92	31,47,54,55	0
4	EDO	C	254	4/4	0.78	0.19	0.84	55,57,58,59	0
7	GOL	A	371	6/6	0.96	0.12	-0.12	34,46,49,51	0
4	EDO	A	366	4/4	0.85	0.21	-0.37	53,60,61,61	0
6	1PE	A	370	16/16	0.88	0.18	-0.44	50,58,70,73	0
4	EDO	A	367	4/4	0.79	0.19	-0.56	51,61,62,63	0
4	EDO	A	356	4/4	0.87	0.11	-1.52	54,56,56,59	0
4	EDO	C	258	4/4	0.80	0.29	-	48,49,49,50	4
4	EDO	C	251	4/4	0.84	0.16	-	56,63,65,69	0
4	EDO	A	363	4/4	0.87	0.16	-	64,65,65,67	0
4	EDO	C	252	4/4	0.65	0.21	-	53,54,54,54	4
4	EDO	A	358	4/4	0.95	0.27	-	43,45,46,46	0
4	EDO	A	365	4/4	0.87	0.18	-	51,51,51,51	4
4	EDO	A	361	4/4	0.83	0.18	-	50,51,51,51	4
4	EDO	A	353	4/4	0.77	0.45	-	52,52,53,53	4
4	EDO	A	362	4/4	0.90	0.15	-	56,56,56,57	4
4	EDO	A	368	4/4	0.72	0.45	-	52,54,54,55	0
4	EDO	A	364	4/4	0.88	0.24	-	44,45,45,48	4

6.5 Other polymers

There are no such residues in this entry.