



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:45 AM GMT

PDB ID : 2IJX
Title : Crystal structure of PCNA3 monomer from *Sulfolobus solfataricus*.
Authors : Hlinkova, V.; Ling, H.
Deposited on : 2006-10-01
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

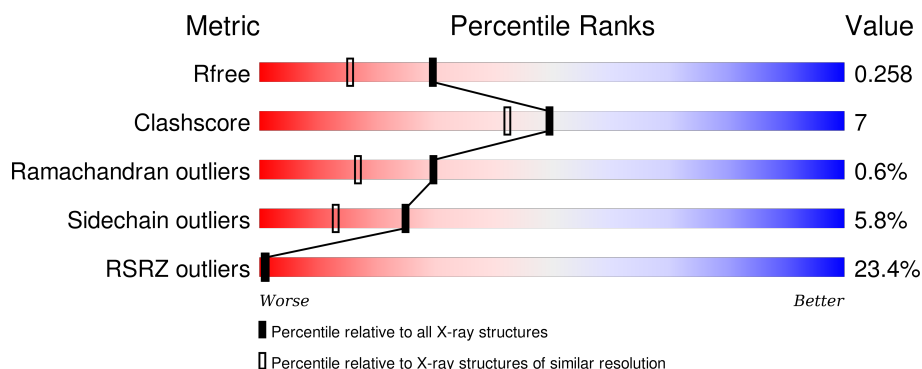
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	244	<div> <div>27%</div> <div>77%</div> <div>21%</div> <div>..</div> </div>
1	B	244	<div> <div>18%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	C	244	<div> <div>23%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>
1	D	244	<div> <div>26%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	D	616	-	-	-	X

2 Entry composition [i](#)

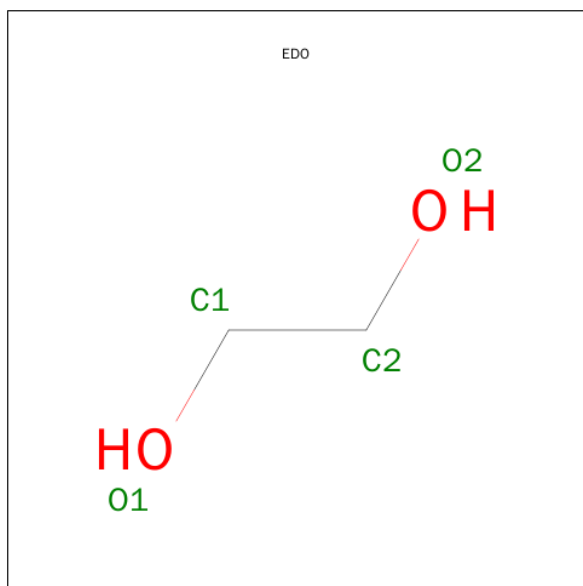
There are 3 unique types of molecules in this entry. The entry contains 8406 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 sliding clamp A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	3	0
			1948	1239	314	391	4			
1	B	244	Total	C	N	O	S	0	6	0
			1954	1243	313	393	5			
1	C	244	Total	C	N	O	S	0	5	0
			1955	1243	312	395	5			
1	D	244	Total	C	N	O	S	0	0	0
			1934	1229	312	389	4			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total 123	O 123	0	0

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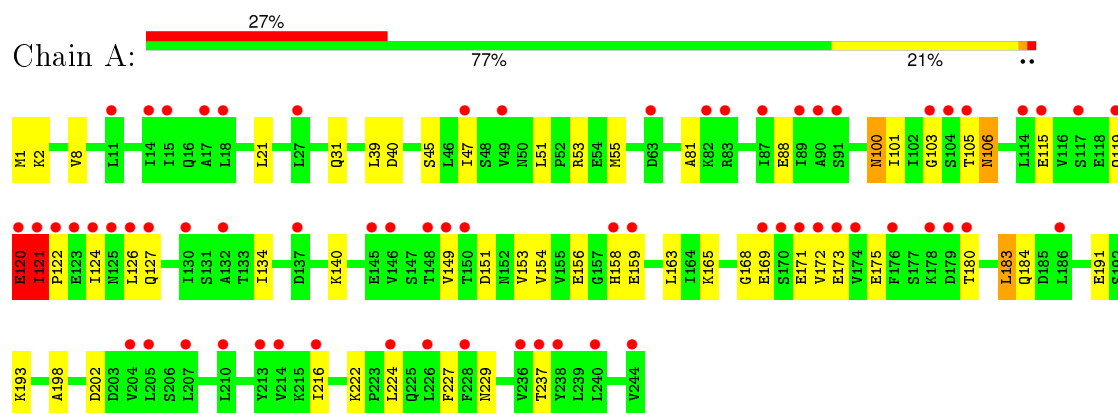
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	150	Total 150	O 150	0	0
3	C	119	Total 119	O 119	0	0
3	D	143	Total 143	O 143	0	0

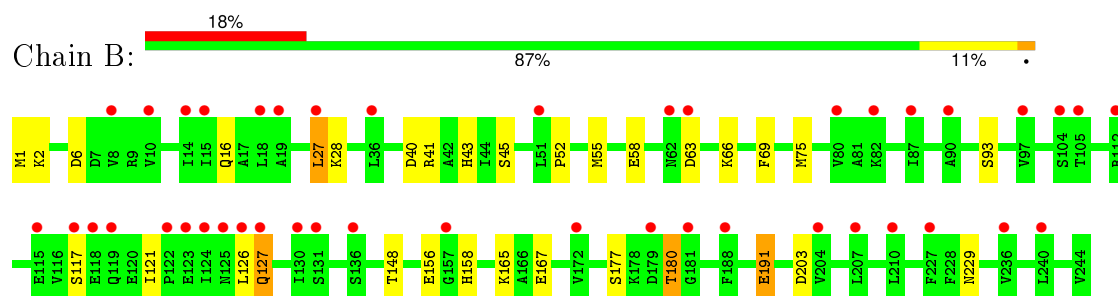
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

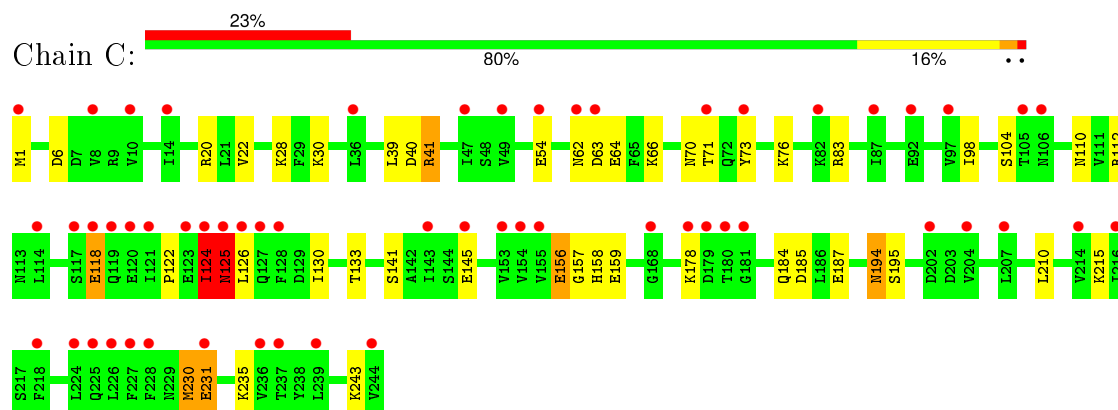
• Molecule 1: DNA polymerase sliding clamp A



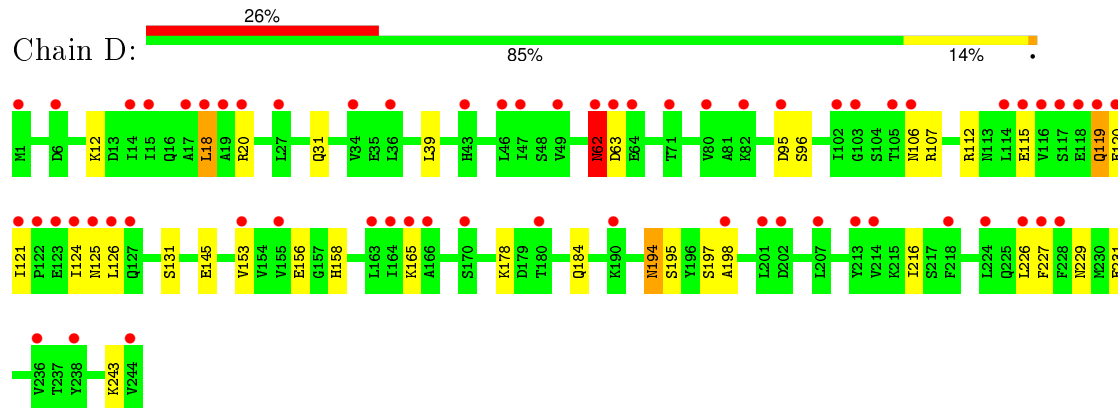
• Molecule 1: DNA polymerase sliding clamp A



• Molecule 1: DNA polymerase sliding clamp A



● Molecule 1: DNA polymerase sliding clamp A



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.77Å 85.77Å 264.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.62 – 1.90 29.56 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.62-1.90) 96.3 (29.56-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.204 , 0.251 0.210 , 0.258	Depositor DCC
R_{free} test set	1530 reflections (2.06%)	DCC
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 75802 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8406	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.37% 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, 0.375 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: 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	0.70	0/1983	0.84	1/2671 (0.0%)
1	B	0.76	0/2002	0.80	2/2696 (0.1%)
1	C	0.78	2/1999 (0.1%)	0.86	5/2694 (0.2%)
1	D	0.72	0/1960	0.81	1/2641 (0.0%)
All	All	0.74	2/7944 (0.0%)	0.83	9/10702 (0.1%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	159	GLU	CD-OE1	5.25	1.31	1.25
1	C	156	GLU	CD-OE2	5.13	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	GLU	OE1-CD-OE2	9.17	134.30	123.30
1	C	41	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	C	41	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	D	18	LEU	CA-CB-CG	6.49	130.23	115.30
1	C	124	ILE	CG1-CB-CG2	5.94	124.48	111.40
1	A	121	ILE	N-CA-C	5.57	126.03	111.00
1	C	83	ARG	NE-CZ-NH1	5.43	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	203	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	GLY	Peptide
1	A	120	GLU	Peptide

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	1948	0	1969	38	0
1	B	1954	0	1977	19	1
1	C	1955	0	1970	39	1
1	D	1934	0	1945	25	0
2	A	12	0	18	0	0
2	B	20	0	30	0	0
2	C	32	0	48	1	0
2	D	16	0	24	1	0
3	A	123	0	0	1	0
3	B	150	0	0	4	0
3	C	119	0	0	5	0
3	D	143	0	0	7	0
All	All	8406	0	7981	112	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ARG:HB2	3:C:643:HOH:O	1.60	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:GLU:OE2	1:C:158:HIS:HE1	1.46	0.97
1:A:100:ASN:HD21	1:A:106:ASN:ND2	1.62	0.97
1:A:100:ASN:HD21	1:A:106:ASN:HD21	1.10	0.95
1:C:124:ILE:HG23	1:D:124:ILE:CG1	2.03	0.88
1:A:100:ASN:ND2	1:A:106:ASN:HD21	1.72	0.88
1:B:127:GLN:HE22	1:D:125:ASN:HA	1.45	0.82
1:C:124:ILE:HG23	1:D:124:ILE:HG13	1.63	0.79
1:C:156:GLU:OE2	1:C:158:HIS:CE1	2.36	0.78
1:C:28:LYS:HE3	1:C:64:GLU:OE2	1.83	0.77
1:C:133[B]:THR:HG23	1:C:184:GLN:HB3	1.66	0.76
1:D:227:PHE:CZ	1:D:229:ASN:OD1	2.39	0.75
1:C:133[A]:THR:HG21	1:C:184:GLN:HE21	1.50	0.75
1:B:177:SER:OG	1:B:180:THR:HG23	1.86	0.74
1:A:100:ASN:ND2	1:A:106:ASN:ND2	2.32	0.74
1:C:28:LYS:CE	1:C:64:GLU:OE2	2.35	0.73
1:C:54:GLU:HG2	3:C:690:HOH:O	1.89	0.72
1:D:20:ARG:HB2	3:D:640:HOH:O	1.90	0.72
1:C:187:GLU:OE2	1:C:215:LYS:NZ	2.24	0.71
1:C:130:ILE:HD13	1:C:157:GLY:HA3	1.73	0.71
1:C:28:LYS:HE2	1:C:30:LYS:NZ	2.07	0.70
1:C:133[A]:THR:CG2	1:C:184:GLN:HE21	2.07	0.68
1:C:133[B]:THR:HG22	1:C:185:ASP:HB3	1.75	0.68
1:C:70:ASN:HD22	1:C:73:TYR:H	1.43	0.67
1:C:124:ILE:HG23	1:D:124:ILE:HG12	1.76	0.66
1:C:133[A]:THR:HG21	1:C:184:GLN:NE2	2.14	0.63
1:D:107:ARG:HD2	3:D:620:HOH:O	2.02	0.60
1:D:227:PHE:CE2	1:D:229:ASN:OD1	2.55	0.60
1:A:119:GLN:HE22	1:B:167:GLU:CG	2.16	0.59
1:A:165:LYS:HB3	1:A:173:GLU:HG2	1.83	0.59
1:C:141:SER:O	1:C:145:GLU:HG3	2.02	0.59
1:A:127:GLN:HE22	1:C:125:ASN:HA	1.68	0.58
1:C:235:LYS:NZ	3:C:709:HOH:O	2.37	0.58
1:C:28:LYS:HE2	1:C:30:LYS:HZ2	1.69	0.57
1:A:39:LEU:HD11	1:A:121:ILE:HD13	1.87	0.57
1:B:127:GLN:NE2	1:D:125:ASN:HA	2.19	0.56
1:C:130:ILE:CD1	1:C:157:GLY:HA3	2.36	0.56
1:A:149:VAL:HG21	1:A:172:VAL:HG21	1.88	0.55
1:C:22:VAL:O	1:C:71[B]:THR:HG21	2.07	0.54
1:A:159:GLU:CD	1:A:159:GLU:H	2.11	0.54
1:B:158:HIS:ND1	1:B:191:GLU:OE2	2.36	0.54
1:A:51:LEU:HD22	1:A:55:MET:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PHE:CE2	1:A:229:ASN:ND2	2.77	0.53
1:A:216:ILE:CG1	1:A:224:LEU:HD11	2.39	0.53
1:A:149:VAL:HG21	1:A:169:GLU:OE2	2.09	0.52
1:D:39:LEU:HD12	1:D:119:GLN:NE2	2.24	0.52
1:D:115:GLU:HG3	3:D:694:HOH:O	2.08	0.52
1:C:210:LEU:HB3	1:C:230:MET:HG3	1.91	0.52
1:A:40:ASP:OD1	1:A:45:SER:N	2.42	0.52
1:D:31:GLN:NE2	3:D:670:HOH:O	2.43	0.51
1:B:127:GLN:NE2	1:D:126:LEU:H	2.08	0.51
1:D:153:VAL:HG23	1:D:198:ALA:HB2	1.92	0.51
1:A:127:GLN:NE2	1:C:125:ASN:HA	2.26	0.51
1:C:194:ASN:HD22	1:C:195:SER:H	1.59	0.51
1:D:12:LYS:NZ	3:D:715:HOH:O	2.43	0.51
1:C:28:LYS:HE2	1:C:30:LYS:HZ1	1.75	0.50
1:A:216:ILE:HG13	1:A:224:LEU:HD11	1.93	0.50
1:A:39:LEU:HD11	1:A:121:ILE:CD1	2.41	0.50
1:D:121:ILE:H	1:D:121:ILE:HD12	1.77	0.49
1:D:156:GLU:OE1	1:D:158:HIS:HE1	1.94	0.49
1:A:163:LEU:HD12	1:A:163:LEU:N	2.28	0.49
1:A:124:ILE:HG22	1:A:126:LEU:HG	1.94	0.49
1:C:124:ILE:HG22	1:C:125:ASN:H	1.77	0.49
1:B:2:LYS:HE2	1:B:58:GLU:OE1	2.12	0.49
1:A:8:VAL:HG11	1:A:81:ALA:HB1	1.95	0.48
1:C:231:GLU:OE2	3:C:724:HOH:O	2.20	0.48
1:A:2:LYS:HE3	1:A:88:GLU:OE2	2.13	0.48
1:D:96:SER:HB2	3:D:749:HOH:O	2.14	0.48
1:B:16:GLN:NE2	3:B:659:HOH:O	2.46	0.47
1:A:153:VAL:HG23	1:A:198:ALA:HB2	1.96	0.47
1:C:126:LEU:HD23	1:C:126:LEU:N	2.29	0.47
1:C:98:ILE:HD12	1:C:110:ASN:OD1	2.15	0.47
1:C:178:LYS:HG2	3:C:653:HOH:O	2.15	0.47
1:B:52:PRO:O	1:B:55:MET:HG2	2.15	0.46
1:A:175:GLU:O	1:A:180:THR:HG21	2.15	0.46
1:A:149:VAL:CG2	1:A:169:GLU:OE2	2.64	0.46
1:D:145:GLU:HG3	3:D:699:HOH:O	2.16	0.46
1:B:66:LYS:NZ	3:B:720:HOH:O	2.46	0.46
1:D:194:ASN:HD22	1:D:195:SER:H	1.64	0.46
1:C:243:LYS:HA	2:C:618:EDO:H21	1.97	0.46
1:D:227:PHE:O	2:D:610:EDO:H22	2.16	0.45
1:D:216:ILE:HG22	1:D:226:LEU:CD2	2.47	0.45
1:A:127:GLN:O	1:A:222:LYS:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ILE:HA	1:A:122:PRO:HD3	1.94	0.45
1:C:28:LYS:HZ2	1:C:66:LYS:HE2	1.82	0.44
1:A:21:LEU:HD12	1:A:47:ILE:CD1	2.46	0.44
1:A:156:GLU:HG3	1:A:163:LEU:HB2	1.99	0.44
1:A:158:HIS:CD2	3:A:685:HOH:O	2.70	0.43
1:A:39:LEU:HD12	1:A:39:LEU:N	2.33	0.43
1:A:227:PHE:HE2	1:A:229:ASN:ND2	2.15	0.43
1:A:8:VAL:HG21	1:A:101:ILE:HD12	2.00	0.43
1:A:171:GLU:O	1:A:171:GLU:HG2	2.18	0.43
1:A:134:ILE:HG22	1:A:183:LEU:HD23	2.00	0.43
1:B:229:ASN:ND2	3:B:652:HOH:O	2.35	0.43
1:B:40:ASP:OD1	1:B:45:SER:N	2.45	0.43
1:C:118:GLU:CD	1:C:118:GLU:H	2.22	0.43
1:B:16:GLN:N	1:B:75[A]:MET:HE1	2.34	0.43
1:B:27:LEU:HD22	1:B:69:PHE:CE2	2.53	0.43
1:C:22:VAL:HG23	1:C:71[A]:THR:HG21	2.01	0.42
1:B:40:ASP:O	1:B:43:HIS:HD2	2.01	0.42
1:A:154:VAL:HG11	1:A:193:LYS:HZ2	1.85	0.42
1:D:62:ASN:HA	1:D:63:ASP:HA	1.79	0.41
1:A:227:PHE:HD1	1:A:237:THR:HG22	1.85	0.41
1:B:28:LYS:HE2	3:B:734:HOH:O	2.20	0.41
1:C:28:LYS:NZ	1:C:66:LYS:HE2	2.35	0.41
1:B:156:GLU:OE2	1:B:158:HIS:NE2	2.53	0.41
1:D:197:SER:HA	1:D:243:LYS:HD2	2.03	0.41
1:A:21:LEU:HD12	1:A:47:ILE:HD12	2.02	0.41
1:C:39:LEU:HD11	1:C:122:PRO:HD3	2.02	0.40
1:D:156:GLU:OE2	1:D:165:LYS:NZ	2.48	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ASP:OD2	1:C:6:ASP:OD2[3_545]	2.15	0.05

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	245/244 (100%)	239 (98%)	3 (1%)	3 (1%)	16	5
1	B	248/244 (102%)	244 (98%)	4 (2%)	0	100	100
1	C	247/244 (101%)	242 (98%)	4 (2%)	1 (0%)	39	27
1	D	242/244 (99%)	239 (99%)	1 (0%)	2 (1%)	24	11
All	All	982/976 (101%)	964 (98%)	12 (1%)	6 (1%)	30	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	THR
1	A	168	GLY
1	C	125	ASN
1	D	62	ASN
1	A	120	GLU
1	D	106	ASN

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	223/220 (101%)	209 (94%)	14 (6%)	22	10
1	B	226/220 (103%)	214 (95%)	12 (5%)	28	16
1	C	225/220 (102%)	211 (94%)	14 (6%)	23	11
1	D	220/220 (100%)	209 (95%)	11 (5%)	30	18
All	All	894/880 (102%)	843 (94%)	51 (6%)	25	13

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	31	GLN
1	A	53	ARG
1	A	100	ASN
1	A	106	ASN
1	A	115	GLU
1	A	120	GLU
1	A	121	ILE
1	A	140	LYS
1	A	151	ASP
1	A	183	LEU
1	A	184	GLN
1	A	191	GLU
1	A	202	ASP
1	B	1	MET
1	B	27	LEU
1	B	41	ARG
1	B	63	ASP
1	B	93	SER
1	B	117	SER
1	B	121	ILE
1	B	126	LEU
1	B	127	GLN
1	B	165	LYS
1	B	180	THR
1	B	191	GLU
1	C	1	MET
1	C	40	ASP
1	C	41	ARG
1	C	62	ASN
1	C	63	ASP
1	C	76	LYS
1	C	104	SER
1	C	112	ARG
1	C	118	GLU
1	C	124	ILE
1	C	125	ASN
1	C	194	ASN
1	C	230	MET
1	C	231	GLU
1	D	18	LEU
1	D	62	ASN
1	D	95	ASP

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Mol	Chain	Res	Type
1	D	112	ARG
1	D	119	GLN
1	D	120	GLU
1	D	131	SER
1	D	178	LYS
1	D	184	GLN
1	D	194	ASN
1	D	231	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	100	ASN
1	A	106	ASN
1	A	119	GLN
1	A	127	GLN
1	A	158	HIS
1	A	229	ASN
1	B	43	HIS
1	B	119	GLN
1	B	127	GLN
1	C	16	GLN
1	C	62	ASN
1	C	70	ASN
1	C	158	HIS
1	C	184	GLN
1	C	194	ASN
1	D	31	GLN
1	D	43	HIS
1	D	62	ASN
1	D	119	GLN
1	D	125	ASN
1	D	158	HIS
1	D	194	ASN

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 ⓘ

20 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	$\# Z > 2$
2	EDO	A	604	-	3,3,3	0.41	0	2,2,2	0.31	0
2	EDO	A	609	-	3,3,3	0.60	0	2,2,2	0.32	0
2	EDO	A	614	-	3,3,3	0.62	0	2,2,2	0.69	0
2	EDO	B	601	-	3,3,3	0.56	0	2,2,2	0.55	0
2	EDO	B	605	-	3,3,3	0.35	0	2,2,2	0.53	0
2	EDO	B	612	-	3,3,3	0.54	0	2,2,2	0.30	0
2	EDO	B	613	-	3,3,3	0.50	0	2,2,2	0.13	0
2	EDO	B	617	-	3,3,3	0.65	0	2,2,2	0.43	0
2	EDO	C	602	-	3,3,3	0.63	0	2,2,2	0.61	0
2	EDO	C	603	-	3,3,3	0.45	0	2,2,2	0.67	0
2	EDO	C	606	-	3,3,3	0.37	0	2,2,2	0.26	0
2	EDO	C	607	-	3,3,3	0.55	0	2,2,2	0.04	0
2	EDO	C	611	-	3,3,3	0.50	0	2,2,2	0.70	0
2	EDO	C	615	-	3,3,3	0.51	0	2,2,2	0.29	0
2	EDO	C	618	-	3,3,3	0.83	0	2,2,2	0.55	0
2	EDO	C	620	-	3,3,3	0.66	0	2,2,2	0.09	0
2	EDO	D	608	-	3,3,3	0.48	0	2,2,2	0.38	0
2	EDO	D	610	-	3,3,3	0.44	0	2,2,2	0.31	0
2	EDO	D	616	-	3,3,3	0.39	0	2,2,2	0.64	0
2	EDO	D	619	-	3,3,3	0.43	0	2,2,2	0.50	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	EDO	A	604	-	-	0/1/1/1	0/0/0/0
2	EDO	A	609	-	-	0/1/1/1	0/0/0/0
2	EDO	A	614	-	-	0/1/1/1	0/0/0/0
2	EDO	B	601	-	-	0/1/1/1	0/0/0/0
2	EDO	B	605	-	-	0/1/1/1	0/0/0/0
2	EDO	B	612	-	-	0/1/1/1	0/0/0/0
2	EDO	B	613	-	-	0/1/1/1	0/0/0/0
2	EDO	B	617	-	-	0/1/1/1	0/0/0/0
2	EDO	C	602	-	-	0/1/1/1	0/0/0/0
2	EDO	C	603	-	-	0/1/1/1	0/0/0/0
2	EDO	C	606	-	-	0/1/1/1	0/0/0/0
2	EDO	C	607	-	-	0/1/1/1	0/0/0/0
2	EDO	C	611	-	-	0/1/1/1	0/0/0/0
2	EDO	C	615	-	-	0/1/1/1	0/0/0/0
2	EDO	C	618	-	-	0/1/1/1	0/0/0/0
2	EDO	C	620	-	-	0/1/1/1	0/0/0/0
2	EDO	D	608	-	-	0/1/1/1	0/0/0/0
2	EDO	D	610	-	-	0/1/1/1	0/0/0/0
2	EDO	D	616	-	-	0/1/1/1	0/0/0/0
2	EDO	D	619	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	618	EDO	1	0
2	D	610	EDO	1	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	244/244 (100%)	1.54	66 (27%) 1 1	32, 42, 54, 67	0
1	B	244/244 (100%)	1.16	43 (17%) 2 2	33, 42, 50, 63	0
1	C	244/244 (100%)	1.32	56 (22%) 1 1	29, 41, 48, 55	1 (0%)
1	D	244/244 (100%)	1.49	63 (25%) 1 1	29, 42, 49, 57	0
All	All	976/976 (100%)	1.38	228 (23%) 1 1	29, 42, 50, 67	1 (0%)

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	244	VAL	12.3
1	A	172	VAL	10.8
1	B	124	ILE	8.9
1	B	122	PRO	7.6
1	D	122	PRO	7.3
1	C	244	VAL	7.2
1	C	124	ILE	6.9
1	A	124	ILE	6.4
1	A	122	PRO	6.2
1	A	173	GLU	6.2
1	A	148	THR	5.9
1	A	123	GLU	5.8
1	A	170	SER	5.6
1	D	47	ILE	5.4
1	C	62	ASN	5.0
1	A	104	SER	4.9
1	A	149	VAL	4.9
1	D	115	GLU	4.9
1	A	171	GLU	4.6
1	A	119	GLN	4.6
1	D	124	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	224	LEU	4.5
1	A	15	ILE	4.5
1	D	236	VAL	4.5
1	B	123	GLU	4.4
1	A	213	TYR	4.4
1	A	236	VAL	4.3
1	B	125	ASN	4.3
1	D	102	ILE	4.2
1	C	226	LEU	4.2
1	A	120	GLU	4.2
1	A	83	ARG	4.2
1	D	63	ASP	4.2
1	A	145	GLU	4.1
1	C	180	THR	4.0
1	B	105	THR	4.0
1	B	181	GLY	4.0
1	C	125	ASN	3.9
1	D	119	GLN	3.9
1	D	95	ASP	3.9
1	D	49	VAL	3.9
1	D	114	LEU	3.9
1	C	179	ASP	3.8
1	D	14	ILE	3.8
1	D	117	SER	3.8
1	D	224	LEU	3.8
1	B	115	GLU	3.7
1	C	71[A]	THR	3.7
1	A	14	ILE	3.7
1	A	238	TYR	3.6
1	A	121	ILE	3.6
1	A	117	SER	3.6
1	D	180	THR	3.6
1	D	123	GLU	3.6
1	D	163	LEU	3.6
1	C	105	THR	3.6
1	D	226	LEU	3.5
1	A	105	THR	3.5
1	A	169	GLU	3.5
1	D	120	GLU	3.5
1	D	105	THR	3.5
1	D	18	LEU	3.5
1	D	106	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	14	ILE	3.5
1	C	63	ASP	3.5
1	A	18	LEU	3.5
1	C	181	GLY	3.4
1	A	63	ASP	3.4
1	B	130	ILE	3.4
1	A	115	GLU	3.4
1	C	227	PHE	3.4
1	A	47	ILE	3.3
1	B	210	LEU	3.3
1	C	120	GLU	3.3
1	A	82	LYS	3.3
1	D	62	ASN	3.3
1	D	155	VAL	3.3
1	D	126	LEU	3.2
1	B	119	GLN	3.2
1	B	10	VAL	3.2
1	B	236	VAL	3.2
1	D	15	ILE	3.2
1	D	103	GLY	3.2
1	A	146	VAL	3.2
1	B	104	SER	3.2
1	A	130	ILE	3.1
1	B	62	ASN	3.1
1	B	117	SER	3.1
1	A	186	LEU	3.1
1	A	91	SER	3.1
1	A	207	LEU	3.1
1	C	49	VAL	3.1
1	B	63	ASP	3.1
1	D	228	PHE	3.0
1	D	125	ASN	3.0
1	D	153	VAL	3.0
1	C	126	LEU	3.0
1	C	128	PHE	3.0
1	B	90	ALA	3.0
1	D	19	ALA	3.0
1	D	27	LEU	3.0
1	D	36	LEU	3.0
1	B	112	ARG	3.0
1	D	6	ASP	3.0
1	A	174	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	127	GLN	2.9
1	D	227	PHE	2.9
1	B	126	LEU	2.9
1	A	150	THR	2.9
1	C	214	VAL	2.9
1	A	126	LEU	2.9
1	A	224	LEU	2.9
1	C	155	VAL	2.9
1	C	236	VAL	2.9
1	D	82	LYS	2.8
1	B	87	ILE	2.8
1	B	172	VAL	2.8
1	B	27	LEU	2.8
1	D	218	PHE	2.8
1	C	117	SER	2.8
1	C	143	ILE	2.8
1	B	18	LEU	2.7
1	C	127	GLN	2.7
1	D	238	TYR	2.7
1	A	103	GLY	2.7
1	C	228	PHE	2.7
1	C	202[A]	ASP	2.7
1	B	240	LEU	2.7
1	D	207	LEU	2.7
1	C	47	ILE	2.6
1	D	34	VAL	2.6
1	D	80	VAL	2.6
1	D	121	ILE	2.6
1	D	17	ALA	2.6
1	D	166	ALA	2.6
1	C	204	VAL	2.6
1	D	164	ILE	2.6
1	C	73	TYR	2.6
1	D	170	SER	2.6
1	C	231	GLU	2.6
1	B	14	ILE	2.5
1	A	210	LEU	2.5
1	B	227	PHE	2.5
1	C	8	VAL	2.5
1	C	237	THR	2.5
1	D	71	THR	2.5
1	D	46	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	2.5
1	C	92	GLU	2.5
1	A	179	ASP	2.5
1	C	216	ILE	2.5
1	C	54	GLU	2.5
1	D	201	LEU	2.5
1	A	180	THR	2.5
1	B	204	VAL	2.5
1	D	202	ASP	2.5
1	B	51	LEU	2.5
1	B	188	PHE	2.4
1	C	97	VAL	2.4
1	A	90	ALA	2.4
1	D	43	HIS	2.4
1	C	207	LEU	2.4
1	A	228	PHE	2.4
1	D	213	TYR	2.4
1	D	190	LYS	2.4
1	A	205	LEU	2.4
1	A	176	PHE	2.4
1	C	87	ILE	2.4
1	C	106	ASN	2.4
1	B	97	VAL	2.4
1	D	1	MET	2.4
1	A	89	ILE	2.3
1	B	131	SER	2.3
1	A	204	VAL	2.3
1	A	226	LEU	2.3
1	D	165	LYS	2.3
1	D	116	VAL	2.3
1	A	11	LEU	2.3
1	B	8	VAL	2.3
1	B	80	VAL	2.3
1	B	179	ASP	2.3
1	B	36	LEU	2.3
1	C	154	VAL	2.3
1	A	240	LEU	2.2
1	C	218	PHE	2.2
1	A	216	ILE	2.2
1	D	118	GLU	2.2
1	A	127	GLN	2.2
1	C	145	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	157	GLY	2.2
1	A	49	VAL	2.2
1	A	158	HIS	2.2
1	A	214	VAL	2.2
1	A	132	ALA	2.2
1	B	19	ALA	2.2
1	B	118	GLU	2.2
1	B	207	LEU	2.2
1	B	136[A]	SER	2.2
1	A	17	ALA	2.1
1	D	64	GLU	2.1
1	C	114	LEU	2.1
1	A	137	ASP	2.1
1	A	87	ILE	2.1
1	A	125[A]	ASN	2.1
1	A	178	LYS	2.1
1	C	82	LYS	2.1
1	C	153	VAL	2.1
1	B	15	ILE	2.1
1	B	82	LYS	2.1
1	C	10	VAL	2.1
1	A	237	THR	2.1
1	C	123	GLU	2.1
1	A	114	LEU	2.1
1	C	36	LEU	2.1
1	A	244	VAL	2.1
1	C	178	LYS	2.0
1	C	225	GLN	2.1
1	C	121	ILE	2.0
1	C	239	LEU	2.0
1	C	168	GLY	2.0
1	D	214	VAL	2.0
1	D	198	ALA	2.0
1	A	27	LEU	2.0
1	C	118	GLU	2.0
1	D	20	ARG	2.0
1	A	159	GLU	2.0
1	B	127	GLN	2.0
1	C	119	GLN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	EDO	D	616	4/4	0.88	0.41	2.51	45,49,49,50	0
2	EDO	D	619	4/4	0.76	0.21	1.46	57,58,58,58	0
2	EDO	C	620	4/4	0.52	0.29	1.35	59,60,60,60	0
2	EDO	B	601	4/4	0.88	0.23	1.22	36,41,41,41	0
2	EDO	A	614	4/4	0.87	0.19	1.11	41,44,44,50	0
2	EDO	C	618	4/4	0.72	0.27	1.01	35,43,44,49	0
2	EDO	B	617	4/4	0.86	0.19	0.03	36,43,44,46	0
2	EDO	C	611	4/4	0.89	0.16	-0.05	34,41,42,42	0
2	EDO	C	607	4/4	0.82	0.16	-0.13	44,46,48,51	0
2	EDO	C	603	4/4	0.78	0.16	-0.25	55,57,57,57	0
2	EDO	A	604	4/4	0.87	0.12	-0.37	49,50,50,51	0
2	EDO	A	609	4/4	0.88	0.21	-0.38	49,52,54,58	0
2	EDO	B	613	4/4	0.71	0.17	-0.44	61,61,62,64	0
2	EDO	C	606	4/4	0.86	0.16	-0.60	35,36,39,42	0
2	EDO	D	610	4/4	0.90	0.16	-0.66	34,36,38,40	0
2	EDO	D	608	4/4	0.94	0.16	-0.88	39,42,44,46	0
2	EDO	C	602	4/4	0.92	0.12	-1.27	35,37,37,38	0
2	EDO	B	605	4/4	0.91	0.11	-1.38	32,33,37,41	0
2	EDO	C	615	4/4	0.88	0.18	-	55,55,56,56	0
2	EDO	B	612	4/4	0.67	0.26	-	61,62,62,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.