WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 04:42 pm BST

PDB ID	:	8OFU
Title	:	Human adenovirus type 53 fiber-knob protein
Authors	:	Rizkallah, P.J.; Parker, A.L.; Mundy, R.M.; Baker, A.T.
Deposited on	:	2023-03-16
Resolution	:	1.61 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:

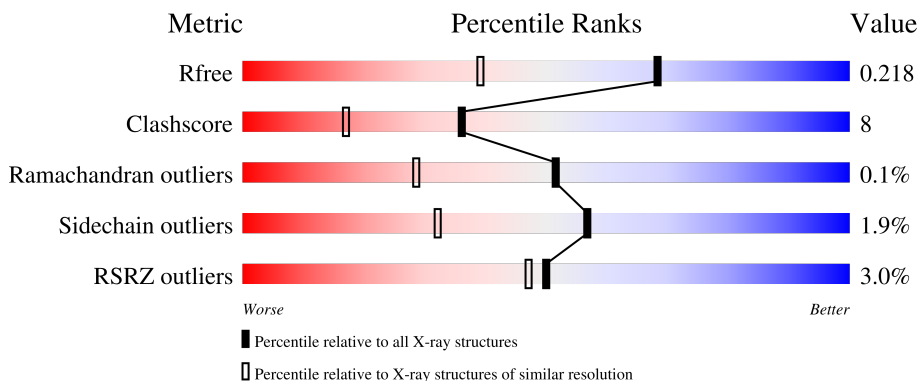|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.61 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	Percentile Ranks	Value
Rfree		0.218
Clashscore		8
Ramachandran outliers		0.1%
Sidechain outliers		1.9%
RSRZ outliers		3.0%

Worse   *Better*

▊ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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 <=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	188	2% / 81% / 15% / ..
1	B	188	2% / 87% / 12% / .
1	C	188	2% / 82% / 15% / ..
1	D	188	4% / 85% / 13% / .
1	E	188	% / 90% / 9% / .

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Length	Quality of chain
1	F	188	

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
2	SO4	A	401	-	-	X	-
2	SO4	F	402	-	-	X	-
3	EDO	A	403	-	-	X	-
3	EDO	A	407	-	-	X	-
3	EDO	C	402	-	-	X	-
3	EDO	D	401	-	-	X	-
3	EDO	D	405	-	-	X	-
3	EDO	F	403	-	-	X	-
4	PEG	C	403	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 10039 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 Fiber protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	2	0
			1475	947	240	280	8			
1	B	188	Total	C	N	O	S	0	2	0
			1509	966	247	289	7			
1	C	184	Total	C	N	O	S	0	0	0
			1461	939	238	278	6			
1	D	184	Total	C	N	O	S	0	1	0
			1467	942	239	279	7			
1	E	188	Total	C	N	O	S	0	4	0
			1526	975	252	292	7			
1	F	184	Total	C	N	O	S	0	0	0
			1461	939	238	278	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	ASN	LYS	conflict	UNP E5RWD1
A	181	ASN	GLU	conflict	UNP E5RWD1
A	184	LEU	ARG	conflict	UNP E5RWD1
B	180	ASN	LYS	conflict	UNP E5RWD1
B	181	ASN	GLU	conflict	UNP E5RWD1
B	184	LEU	ARG	conflict	UNP E5RWD1
C	180	ASN	LYS	conflict	UNP E5RWD1
C	181	ASN	GLU	conflict	UNP E5RWD1
C	184	LEU	ARG	conflict	UNP E5RWD1
D	180	ASN	LYS	conflict	UNP E5RWD1
D	181	ASN	GLU	conflict	UNP E5RWD1
D	184	LEU	ARG	conflict	UNP E5RWD1
E	180	ASN	LYS	conflict	UNP E5RWD1
E	181	ASN	GLU	conflict	UNP E5RWD1
E	184	LEU	ARG	conflict	UNP E5RWD1
F	180	ASN	LYS	conflict	UNP E5RWD1
F	181	ASN	GLU	conflict	UNP E5RWD1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	184	LEU	ARG	conflict	UNP E5RWD1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	E	1	Total 5	O 4	S 1	0	0
2	F	1	Total 5	O 4	S 1	0	0
2	F	1	Total 5	O 4	S 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total 4	C 2	O 2		0	0
3	D	1	Total 4	C 2	O 2		0	0
3	D	1	Total 4	C 2	O 2		0	0
3	D	1	Total 4	C 2	O 2		0	0
3	E	1	Total 4	C 2	O 2		0	0
3	E	1	Total 4	C 2	O 2		0	0
3	E	1	Total 4	C 2	O 2		0	0
3	F	1	Total 4	C 2	O 2		0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

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

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

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	171	Total 171	O 171	0	0
5	B	188	Total 188	O 188	0	0
5	C	152	Total 152	O 152	0	0
5	D	149	Total 149	O 149	0	0
5	E	204	Total 204	O 204	0	0
5	F	118	Total 118	O 118	0	0

3 Residue-property plots ⓘ

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.
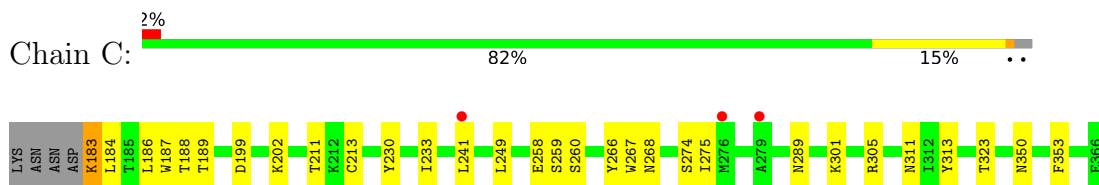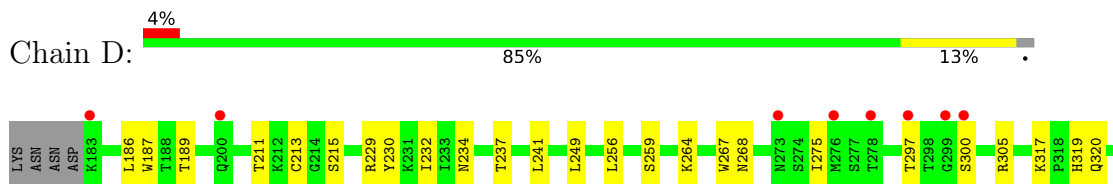
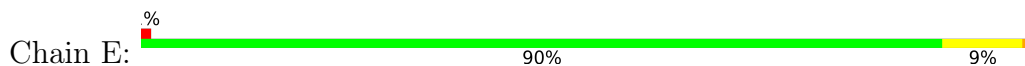- Molecule 1: Fiber protein
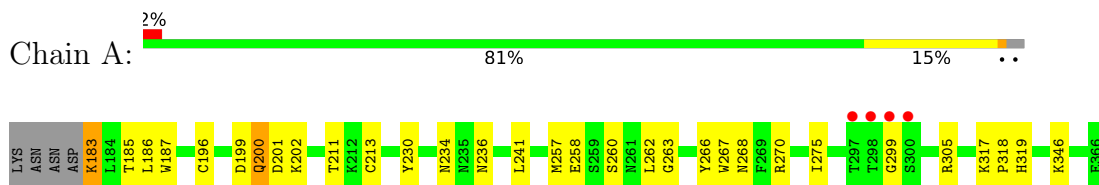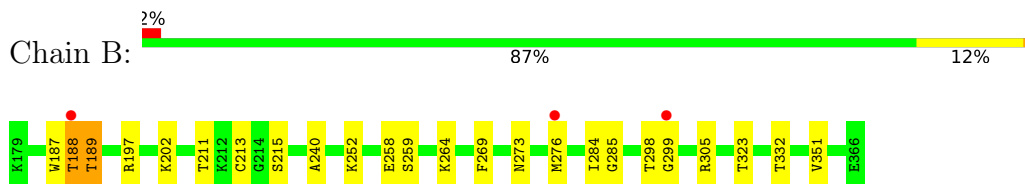
Chain A:

- Molecule 1: Fiber protein

Chain B:

- Molecule 1: Fiber protein

Chain C:

- Molecule 1: Fiber protein

Chain D:

- Molecule 1: Fiber protein

Chain E:

K179 W187 T188 T189 P194 R197 T211 K212 C213 V226 R229 Y230 T237 L241 K242 S259 N268 N273 S274 I275 K295 T298 G299 S300 E366

• Molecule 1: Fiber protein

Chain F:

7%

88%

9%

LYS ASN ASN ASP K183 L186 W187 D201 T207 C213 L249 S259 W267 N268 F269 R270 N271 Q272 N273 S274 I275 M276 S277 T278 A279 Y280 E281 K282 A283 F286 N289 R305 Y313 E366
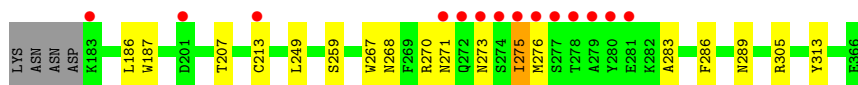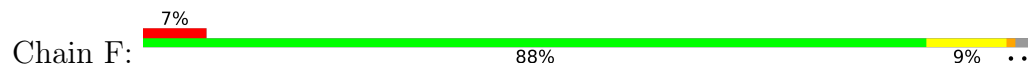
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	206.31Å 60.53Å 93.84Å 90.00° 91.80° 90.00°	Depositor
Resolution (Å)	68.42 – 1.61 68.32 – 1.61	Depositor EDS
% Data completeness (in resolution range)	99.3 (68.42-1.61) 99.3 (68.32-1.61)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 1.61Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.191 , 0.213 0.197 , 0.218	Depositor DCC
R_{free} test set	7463 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10039	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, EDO, PEG

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	0.66	0/1509	0.83	1/2046 (0.0%)
1	B	0.68	0/1543	0.86	1/2092 (0.0%)
1	C	0.67	0/1495	0.78	1/2028 (0.0%)
1	D	0.69	0/1501	0.82	1/2036 (0.0%)
1	E	0.68	0/1560	0.90	3/2115 (0.1%)
1	F	0.67	0/1495	0.80	1/2028 (0.0%)
All	All	0.68	0/9103	0.83	8/12345 (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	B	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	189	THR	CA-CB-OG1	-9.97	88.06	109.00
1	E	188	THR	C-N-CA	-9.79	97.23	121.70
1	E	188	THR	O-C-N	-7.36	110.93	122.70
1	D	305	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	B	305	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	C	305	ARG	CG-CD-NE	-5.27	100.74	111.80
1	F	305	ARG	CG-CD-NE	-5.17	100.93	111.80
1	A	305	ARG	CG-CD-NE	-5.16	100.97	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	188	THR	Mainchain

5.2 Too-close contacts ⓘ

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	1475	0	1468	32	1
1	B	1509	0	1500	25	0
1	C	1461	0	1456	28	0
1	D	1467	0	1460	23	0
1	E	1526	0	1517	17	0
1	F	1461	0	1456	25	1
2	A	10	0	0	6	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	E	5	0	0	0	0
2	F	10	0	0	2	0
3	A	20	0	30	17	0
3	B	24	0	36	7	0
3	C	4	0	6	5	0
3	D	24	0	36	11	0
3	E	12	0	18	0	0
3	F	4	0	6	4	0
4	C	14	0	20	5	0
4	D	7	0	10	3	0
4	F	14	0	20	1	0
5	A	171	0	0	8	1
5	B	188	0	0	5	0
5	C	152	0	0	2	0
5	D	149	0	0	2	1
5	E	204	0	0	2	0
5	F	118	0	0	1	0
All	All	10039	0	9039	145	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 8.

All (145) 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)
3:A:403:EDO:H21	5:A:576:HOH:O	1.79	0.81
3:A:403:EDO:C2	5:A:576:HOH:O	2.30	0.80
1:E:273:ASN:HD21	1:F:289:ASN:HD21	1.30	0.80
1:E:237[A]:THR:HG21	5:E:556:HOH:O	1.83	0.79
1:C:258:GLU:O	3:C:402:EDO:H12	1.83	0.78
1:E:230:TYR:HE1	1:E:241:LEU:HD11	1.52	0.75
1:B:259:SER:HA	3:B:402:EDO:H21	1.68	0.75
1:F:273:ASN:ND2	5:F:501:HOH:O	2.19	0.74
1:A:183:LYS:HD3	1:A:185:THR:H	1.53	0.74
1:A:213[A]:CYS:O	1:C:211:THR:HG21	1.87	0.74
1:A:213[B]:CYS:O	1:C:211:THR:HG21	1.87	0.73
1:C:260:SER:O	3:C:402:EDO:H11	1.86	0.73
1:C:260:SER:O	3:C:402:EDO:C1	2.36	0.73
1:E:211:THR:HG21	1:F:213:CYS:O	1.90	0.71
3:A:407:EDO:H12	5:A:535:HOH:O	1.90	0.71
1:F:268:ASN:HB3	1:F:275:ILE:HG23	1.70	0.71
1:B:273:ASN:HD21	1:C:289:ASN:HD21	1.40	0.70
1:F:270:ARG:O	1:F:271:ASN:ND2	2.24	0.70
1:D:319:HIS:CD2	4:D:407:PEG:H41	2.27	0.69
1:C:233:ILE:HD11	1:C:353:PHE:HB2	1.77	0.67
1:B:202:LYS:N	2:B:401:SO4:O2	2.20	0.67
1:F:207:THR:CG2	3:F:403:EDO:H21	2.24	0.67
1:B:197:ARG:NH2	1:B:258:GLU:O	2.28	0.67
1:A:319:HIS:HB2	3:A:407:EDO:C1	2.26	0.66
1:A:262:LEU:O	3:A:403:EDO:H11	1.96	0.65
1:B:188:THR:O	1:B:189:THR:O	2.15	0.65
5:D:527:HOH:O	3:F:403:EDO:H22	1.98	0.64
1:E:230:TYR:CE1	1:E:241:LEU:HD11	2.31	0.64
1:F:283:ALA:HA	2:F:402:SO4:O2	1.98	0.63
1:E:273:ASN:ND2	1:F:289:ASN:HD21	1.95	0.63
1:B:264:LYS:HE3	3:B:404:EDO:H22	1.80	0.62
1:B:299:GLY:O	5:B:501:HOH:O	2.16	0.62
1:C:313:TYR:OH	4:C:403:PEG:H31	1.99	0.61
1:F:207:THR:HG21	3:F:403:EDO:H21	1.82	0.61
1:C:233:ILE:HD11	1:C:353:PHE:HD2	1.66	0.60
3:C:402:EDO:H22	5:C:504:HOH:O	2.01	0.60
1:C:274:SER:HB2	5:C:621:HOH:O	2.02	0.59
1:D:319:HIS:HB2	3:D:401:EDO:H12	1.84	0.59
1:F:268:ASN:HB3	1:F:275:ILE:CG2	2.34	0.58
5:B:578:HOH:O	3:D:401:EDO:H12	2.04	0.58
1:B:252:LYS:O	1:B:284:ILE:HD11	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:THR:C	1:B:189:THR:O	2.43	0.56
3:A:403:EDO:H22	5:A:576:HOH:O	2.00	0.56
1:D:297:THR:OG1	1:D:300:SER:HB2	2.06	0.56
1:B:258:GLU:HG3	1:B:264:LYS:HD3	1.87	0.56
1:F:270:ARG:HE	1:F:273:ASN:H	1.53	0.55
1:B:188:THR:O	1:B:189:THR:C	2.44	0.55
1:F:207:THR:O	3:F:403:EDO:H12	2.07	0.55
1:A:319:HIS:HB3	2:A:401:SO4:O4	2.06	0.54
1:D:213[A]:CYS:HB3	1:F:213:CYS:SG	2.47	0.54
1:A:260:SER:HB2	3:A:403:EDO:H11	1.88	0.54
1:C:260:SER:O	3:C:402:EDO:H12	2.07	0.54
1:F:268:ASN:HB3	1:F:275:ILE:HG12	1.89	0.54
1:D:232:ILE:O	3:D:404:EDO:H22	2.08	0.53
1:F:313:TYR:OH	4:F:404:PEG:H31	2.07	0.53
1:A:196:CYS:C	2:A:402:SO4:O3	2.46	0.53
1:A:230:TYR:CE1	1:A:241:LEU:HD11	2.44	0.53
1:D:319:HIS:O	3:D:405:EDO:C2	2.56	0.53
1:A:263:GLY:HA2	3:A:403:EDO:H22	1.92	0.52
1:C:230:TYR:CE1	1:C:241:LEU:HD11	2.45	0.52
1:C:233:ILE:HD11	1:C:353:PHE:CD2	2.43	0.52
1:C:313:TYR:OH	4:C:403:PEG:C3	2.58	0.52
1:F:275:ILE:HG22	1:F:276:MET:O	2.11	0.51
1:B:211:THR:HG21	1:C:213:CYS:O	2.10	0.51
1:A:211:THR:HG21	1:B:213:CYS:O	2.10	0.51
1:A:319:HIS:HB2	3:A:407:EDO:H12	1.92	0.51
1:C:323:THR:HG23	4:C:404:PEG:H22	1.93	0.50
1:D:268:ASN:HB3	1:D:275:ILE:HB	1.94	0.50
1:D:211:THR:HG21	1:E:213:CYS:O	2.12	0.50
1:D:319:HIS:O	3:D:405:EDO:H22	2.12	0.49
1:A:270:ARG:HD3	1:B:215:SER:OG	2.12	0.49
1:A:319:HIS:HB2	3:A:407:EDO:H11	1.94	0.49
5:A:601:HOH:O	4:C:403:PEG:H21	2.13	0.49
1:B:269:PHE:HB2	1:B:276[B]:MET:HE3	1.95	0.49
1:E:295:LYS:O	1:E:298:THR:HB	2.13	0.48
1:F:286:PHE:HD1	2:F:402:SO4:O2	1.97	0.48
1:A:317:LYS:HB3	3:A:407:EDO:H22	1.96	0.48
1:F:268:ASN:CB	1:F:275:ILE:HG23	2.42	0.48
1:A:236:ASN:OD1	1:E:197:ARG:NH2	2.35	0.48
1:B:259:SER:HB2	1:D:234:ASN:ND2	2.28	0.48
1:C:202:LYS:N	2:C:401:SO4:O4	2.42	0.48
1:A:200:GLN:HG3	1:A:201:ASP:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ALA:HB1	4:D:407:PEG:H21	1.95	0.47
1:D:319:HIS:HB2	3:D:401:EDO:C1	2.44	0.47
1:A:319:HIS:ND1	2:A:401:SO4:O3	2.47	0.47
1:C:233:ILE:CD1	1:C:353:PHE:HB2	2.43	0.47
1:A:258:GLU:HG2	3:A:405:EDO:C1	2.44	0.47
3:A:406:EDO:C1	5:A:558:HOH:O	2.63	0.47
1:C:268:ASN:HB3	1:C:275:ILE:HB	1.96	0.47
1:F:275:ILE:CG2	1:F:276:MET:O	2.63	0.47
1:B:273:ASN:ND2	1:C:289:ASN:HD21	2.10	0.47
1:C:202:LYS:HE2	1:C:266:TYR:OH	2.15	0.46
1:B:351:VAL:HG13	3:B:403:EDO:H12	1.96	0.46
5:B:637:HOH:O	3:D:405:EDO:C1	2.63	0.46
3:B:407:EDO:H22	5:E:549:HOH:O	2.16	0.46
1:D:256:LEU:O	1:D:264:LYS:HE3	2.16	0.46
1:C:350:ASN:CG	1:C:350:ASN:O	2.53	0.46
2:A:401:SO4:O2	1:E:241:LEU:HD12	2.16	0.46
1:A:262:LEU:O	3:A:403:EDO:C1	2.63	0.45
5:B:503:HOH:O	1:D:317:LYS:NZ	2.50	0.45
1:A:318:PRO:HB3	3:B:405:EDO:H11	1.99	0.45
1:C:188:THR:O	1:C:189:THR:C	2.53	0.45
1:E:273:ASN:HD22	1:E:273:ASN:HA	1.62	0.45
1:A:258:GLU:HG2	3:A:405:EDO:H12	1.99	0.45
1:D:319:HIS:CG	4:D:407:PEG:H41	2.51	0.45
1:B:285:GLY:H	3:B:406:EDO:H11	1.82	0.44
1:C:183:LYS:HG3	1:C:184:LEU:N	2.33	0.44
1:C:313:TYR:CZ	4:C:403:PEG:H31	2.53	0.44
1:C:249:LEU:HD12	1:C:259:SER:OG	2.18	0.43
1:D:249:LEU:HD12	1:D:259:SER:OG	2.17	0.43
2:A:401:SO4:O2	1:E:242:LYS:N	2.48	0.43
1:A:258:GLU:OE2	5:A:501:HOH:O	2.21	0.43
1:D:230:TYR:CE1	1:D:241:LEU:HD11	2.53	0.43
1:F:271:ASN:OD1	1:F:276:MET:HA	2.19	0.43
1:C:186:LEU:HG	1:C:267:TRP:CZ2	2.54	0.43
1:F:271:ASN:ND2	1:F:276:MET:HG2	2.34	0.43
1:A:270:ARG:HH11	1:B:215:SER:HB3	1.83	0.43
1:A:346:LYS:HD3	3:A:406:EDO:H21	2.00	0.43
1:B:273:ASN:HD22	1:B:273:ASN:HA	1.63	0.43
1:C:233:ILE:CD1	1:C:353:PHE:HD2	2.32	0.43
1:A:268:ASN:HB3	1:A:275:ILE:HB	2.01	0.42
1:A:202:LYS:HE2	1:A:266:TYR:OH	2.19	0.42
1:D:320:GLN:HG3	3:D:401:EDO:H11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:THR:HG21	3:B:405:EDO:H12	2.01	0.42
1:D:237:THR:O	3:D:402:EDO:H22	2.20	0.42
1:A:183:LYS:HD3	1:A:185:THR:N	2.30	0.42
1:D:229:ARG:HD2	1:D:230:TYR:CE2	2.54	0.42
5:B:637:HOH:O	3:D:405:EDO:H12	2.20	0.42
1:D:186:LEU:HG	1:D:267:TRP:CZ2	2.55	0.42
1:D:189:THR:HG23	5:D:524:HOH:O	2.19	0.42
1:F:186:LEU:HG	1:F:267:TRP:CZ2	2.55	0.42
1:A:257:MET:O	3:A:403:EDO:H12	2.20	0.41
1:D:215:SER:OG	1:F:270:ARG:HD3	2.20	0.41
1:F:271:ASN:OD1	1:F:276:MET:HG2	2.20	0.41
1:A:234:ASN:ND2	1:E:259:SER:HB2	2.36	0.41
1:A:186:LEU:HG	1:A:267:TRP:CZ2	2.55	0.41
1:B:276[B]:MET:HE3	1:B:276[B]:MET:HB2	1.91	0.41
1:A:319:HIS:HE1	5:A:654:HOH:O	2.04	0.41
1:D:232:ILE:O	3:D:404:EDO:C2	2.70	0.40
1:F:249:LEU:HD12	1:F:259:SER:OG	2.21	0.40
1:E:268:ASN:HB3	1:E:275:ILE:HB	2.03	0.40
1:E:194:PRO:HG3	1:E:226:VAL:HG21	2.03	0.40
2:A:401:SO4:O2	1:E:241:LEU:HA	2.21	0.40
1:E:229[A]:ARG:HH11	1:E:241:LEU:HD13	1.86	0.40
1:B:188:THR:O	1:B:188:THR:OG1	2.35	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)
1:A:299:GLY:O	1:F:271:ASN:CB[1_554]	2.00	0.20
5:A:652:HOH:O	5:D:570:HOH:O[1_554]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/188 (98%)	176 (96%)	8 (4%)	0	100	100
1	B	188/188 (100%)	180 (96%)	7 (4%)	1 (0%)	29	11
1	C	182/188 (97%)	176 (97%)	6 (3%)	0	100	100
1	D	183/188 (97%)	176 (96%)	7 (4%)	0	100	100
1	E	190/188 (101%)	183 (96%)	7 (4%)	0	100	100
1	F	182/188 (97%)	175 (96%)	7 (4%)	0	100	100
All	All	1109/1128 (98%)	1066 (96%)	42 (4%)	1 (0%)	51	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	189	THR

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	166/168 (99%)	162 (98%)	4 (2%)	49	22
1	B	170/168 (101%)	166 (98%)	4 (2%)	49	22
1	C	164/168 (98%)	159 (97%)	5 (3%)	41	15
1	D	165/168 (98%)	164 (99%)	1 (1%)	86	76
1	E	172/168 (102%)	167 (97%)	5 (3%)	42	16
1	F	164/168 (98%)	162 (99%)	2 (1%)	71	52
All	All	1001/1008 (99%)	980 (98%)	21 (2%)	57	27

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	LYS
1	A	187	TRP
1	A	199	ASP
1	A	200	GLN

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Mol	Chain	Res	Type
1	B	187	TRP
1	B	298	THR
1	B	332[A]	THR
1	B	332[B]	THR
1	C	183	LYS
1	C	187	TRP
1	C	199	ASP
1	C	301	LYS
1	C	311	ASN
1	D	187	TRP
1	E	187	TRP
1	E	197	ARG
1	E	229[A]	ARG
1	E	229[B]	ARG
1	E	298	THR
1	F	187	TRP
1	F	275	ILE

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

Mol	Chain	Res	Type
1	A	319	HIS
1	B	200	GLN
1	B	273	ASN
1	C	311	ASN
1	D	311	ASN
1	E	200	GLN
1	E	273	ASN
1	F	236	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

34 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	#$|Z| > 2$
3	EDO	E	403	-	3,3,3	0.10	0	2,2,2	0.25	0
3	EDO	B	405	-	3,3,3	0.09	0	2,2,2	0.44	0
3	EDO	D	401	-	3,3,3	0.57	0	2,2,2	0.23	0
2	SO4	C	401	-	4,4,4	0.44	0	6,6,6	0.07	0
2	SO4	F	401	-	4,4,4	0.45	0	6,6,6	0.06	0
4	PEG	C	403	-	6,6,6	0.13	0	5,5,5	0.16	0
2	SO4	A	402	-	4,4,4	0.51	0	6,6,6	0.10	0
3	EDO	E	404	-	3,3,3	0.03	0	2,2,2	0.32	0
4	PEG	F	405	-	6,6,6	0.25	0	5,5,5	0.14	0
3	EDO	E	402	-	3,3,3	0.12	0	2,2,2	0.42	0
4	PEG	D	407	-	6,6,6	0.30	0	5,5,5	0.19	0
3	EDO	D	406	-	3,3,3	0.18	0	2,2,2	0.23	0
3	EDO	F	403	-	3,3,3	0.48	0	2,2,2	0.08	0
2	SO4	F	402	-	4,4,4	0.44	0	6,6,6	0.09	0
3	EDO	B	402	-	3,3,3	0.07	0	2,2,2	0.39	0
3	EDO	D	403	-	3,3,3	0.23	0	2,2,2	0.10	0
3	EDO	D	404	-	3,3,3	0.49	0	2,2,2	0.16	0
3	EDO	D	402	-	3,3,3	0.25	0	2,2,2	0.39	0
3	EDO	B	407	-	3,3,3	0.07	0	2,2,2	0.21	0
3	EDO	B	406	-	3,3,3	0.20	0	2,2,2	0.38	0
4	PEG	F	404	-	6,6,6	0.17	0	5,5,5	0.12	0
3	EDO	B	403	-	3,3,3	0.45	0	2,2,2	0.12	0
2	SO4	A	401	-	4,4,4	0.50	0	6,6,6	0.11	0
3	EDO	B	404	-	3,3,3	0.36	0	2,2,2	0.25	0
3	EDO	A	407	-	3,3,3	0.37	0	2,2,2	0.19	0
3	EDO	A	406	-	3,3,3	0.24	0	2,2,2	0.09	0
3	EDO	A	403	-	3,3,3	0.50	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	EDO	A	405	-	3,3,3	0.13	0	2,2,2	0.40	0
3	EDO	D	405	-	3,3,3	0.44	0	2,2,2	0.08	0
2	SO4	B	401	-	4,4,4	0.49	0	6,6,6	0.14	0
3	EDO	C	402	-	3,3,3	0.28	0	2,2,2	0.66	0
4	PEG	C	404	-	6,6,6	0.15	0	5,5,5	0.11	0
3	EDO	A	404	-	3,3,3	0.34	0	2,2,2	0.02	0
2	SO4	E	401	-	4,4,4	0.38	0	6,6,6	0.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	E	403	-	-	1/1/1/1	-
3	EDO	B	405	-	-	1/1/1/1	-
3	EDO	D	401	-	-	1/1/1/1	-
4	PEG	C	403	-	-	3/4/4/4	-
3	EDO	E	404	-	-	1/1/1/1	-
4	PEG	F	405	-	-	3/4/4/4	-
3	EDO	E	402	-	-	0/1/1/1	-
4	PEG	D	407	-	-	2/4/4/4	-
3	EDO	D	406	-	-	0/1/1/1	-
3	EDO	F	403	-	-	0/1/1/1	-
3	EDO	B	402	-	-	1/1/1/1	-
3	EDO	D	403	-	-	1/1/1/1	-
3	EDO	D	404	-	-	0/1/1/1	-
3	EDO	D	402	-	-	0/1/1/1	-
3	EDO	B	407	-	-	0/1/1/1	-
3	EDO	B	406	-	-	1/1/1/1	-
4	PEG	F	404	-	-	2/4/4/4	-
3	EDO	B	403	-	-	0/1/1/1	-
3	EDO	B	404	-	-	1/1/1/1	-
3	EDO	A	407	-	-	1/1/1/1	-
3	EDO	A	406	-	-	0/1/1/1	-
3	EDO	A	403	-	-	0/1/1/1	-
3	EDO	A	405	-	-	1/1/1/1	-
3	EDO	D	405	-	-	0/1/1/1	-
3	EDO	C	402	-	-	1/1/1/1	-
4	PEG	C	404	-	-	2/4/4/4	-
3	EDO	A	404	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	403	PEG	O2-C3-C4-O4
4	C	404	PEG	O1-C1-C2-O2
4	F	404	PEG	O2-C3-C4-O4
4	D	407	PEG	O1-C1-C2-O2
3	A	405	EDO	O1-C1-C2-O2
3	A	407	EDO	O1-C1-C2-O2
3	B	402	EDO	O1-C1-C2-O2
3	B	405	EDO	O1-C1-C2-O2
3	E	403	EDO	O1-C1-C2-O2
4	C	403	PEG	O1-C1-C2-O2
3	C	402	EDO	O1-C1-C2-O2
3	D	403	EDO	O1-C1-C2-O2
3	B	406	EDO	O1-C1-C2-O2
4	D	407	PEG	C4-C3-O2-C2
4	F	405	PEG	C1-C2-O2-C3
4	C	404	PEG	O2-C3-C4-O4
4	F	404	PEG	O1-C1-C2-O2
4	F	405	PEG	O1-C1-C2-O2
3	D	401	EDO	O1-C1-C2-O2
4	C	403	PEG	C4-C3-O2-C2
3	B	404	EDO	O1-C1-C2-O2
3	E	404	EDO	O1-C1-C2-O2
4	F	405	PEG	O2-C3-C4-O4

There are no ring outliers.

25 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	405	EDO	2	0
3	D	401	EDO	4	0
2	C	401	SO4	1	0
4	C	403	PEG	4	0
2	A	402	SO4	1	0
4	D	407	PEG	3	0
3	F	403	EDO	4	0
2	F	402	SO4	2	0
3	B	402	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	404	EDO	2	0
3	D	402	EDO	1	0
3	B	407	EDO	1	0
3	B	406	EDO	1	0
4	F	404	PEG	1	0
3	B	403	EDO	1	0
2	A	401	SO4	5	0
3	B	404	EDO	1	0
3	A	407	EDO	5	0
3	A	406	EDO	2	0
3	A	403	EDO	8	0
3	A	405	EDO	2	0
3	D	405	EDO	4	0
2	B	401	SO4	1	0
3	C	402	EDO	5	0
4	C	404	PEG	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	184/188 (97%)	-0.20	4 (2%)	62	60	14, 21, 37, 71	0
1	B	188/188 (100%)	-0.21	3 (1%)	72	71	14, 21, 33, 58	0
1	C	184/188 (97%)	-0.11	3 (1%)	72	71	17, 29, 52, 59	0
1	D	184/188 (97%)	-0.18	8 (4%)	35	31	14, 24, 49, 67	0
1	E	188/188 (100%)	-0.36	1 (0%)	91	90	14, 21, 30, 54	0
1	F	184/188 (97%)	0.21	14 (7%)	13	11	17, 30, 56, 91	0
All	All	1112/1128 (98%)	-0.14	33 (2%)	50	47	14, 24, 48, 91	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	275	ILE	13.8
1	F	272	GLN	10.5
1	F	271	ASN	7.1
1	F	277	SER	5.7
1	F	273	ASN	5.7
1	F	274	SER	5.6
1	A	300	SER	5.2
1	A	298	THR	4.9
1	F	276	MET	4.0
1	A	297	THR	4.0
1	A	299	GLY	3.7
1	F	280	TYR	3.2
1	D	276	MET	3.1
1	F	278	THR	3.1
1	F	281	GLU	3.1
1	F	279	ALA	3.0
1	E	300	SER	2.7
1	C	241	LEU	2.6
1	D	299	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	183	LYS	2.5
1	B	299	GLY	2.5
1	B	276[A]	MET	2.5
1	B	188	THR	2.4
1	F	213	CYS	2.4
1	D	297	THR	2.4
1	D	300	SER	2.3
1	C	276	MET	2.3
1	F	183	LYS	2.2
1	D	273	ASN	2.2
1	D	278	THR	2.2
1	C	279	ALA	2.1
1	F	201	ASP	2.0
1	D	200	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	C	402	4/4	0.65	0.20	39,39,40,40	0
4	PEG	F	405	7/7	0.66	0.20	47,50,53,53	0
3	EDO	E	403	4/4	0.68	0.24	42,43,43,44	0
3	EDO	B	402	4/4	0.77	0.32	42,43,44,47	0
3	EDO	D	406	4/4	0.78	0.22	36,40,41,41	0
3	EDO	B	406	4/4	0.79	0.20	28,32,34,35	0
3	EDO	B	405	4/4	0.80	0.20	40,40,41,41	0
3	EDO	E	404	4/4	0.81	0.22	43,44,45,46	0
3	EDO	B	407	4/4	0.81	0.14	41,41,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
3	EDO	A	405	4/4	0.82	0.32	34,41,43,44	0
3	EDO	D	403	4/4	0.82	0.24	26,32,37,41	0
4	PEG	D	407	7/7	0.83	0.28	24,32,46,46	0
3	EDO	E	402	4/4	0.83	0.24	35,35,36,39	0
3	EDO	D	402	4/4	0.87	0.25	31,34,36,41	0
2	SO4	E	401	5/5	0.87	0.35	69,72,77,81	0
2	SO4	F	402	5/5	0.88	0.24	33,33,34,34	5
4	PEG	F	404	7/7	0.89	0.17	38,40,44,44	0
4	PEG	C	403	7/7	0.89	0.11	37,40,42,42	0
3	EDO	D	401	4/4	0.90	0.15	23,26,27,28	0
3	EDO	D	404	4/4	0.90	0.30	29,32,34,38	0
3	EDO	A	407	4/4	0.91	0.16	28,30,31,31	0
4	PEG	C	404	7/7	0.92	0.10	36,37,39,40	0
3	EDO	A	403	4/4	0.92	0.22	26,29,30,35	0
3	EDO	A	404	4/4	0.92	0.25	33,41,42,45	0
2	SO4	B	401	5/5	0.92	0.22	31,32,33,35	5
2	SO4	C	401	5/5	0.93	0.25	33,35,36,37	5
2	SO4	F	401	5/5	0.93	0.25	33,34,35,37	5
3	EDO	D	405	4/4	0.93	0.20	28,32,33,33	0
3	EDO	B	403	4/4	0.94	0.14	29,30,30,30	0
3	EDO	F	403	4/4	0.95	0.28	25,27,27,27	0
2	SO4	A	402	5/5	0.96	0.26	23,29,30,31	5
3	EDO	B	404	4/4	0.96	0.19	27,32,33,37	0
3	EDO	A	406	4/4	0.96	0.16	35,35,35,37	0
2	SO4	A	401	5/5	0.97	0.23	23,26,27,28	5

6.5 Other polymers ⓘ

There are no such residues in this entry.