



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:54 AM UTC

PDB ID : 8GM9 / pdb_00008gm9
Title : Structure of Citrate Synthase(CitA) in Mycobacterium Tuberculosis
Authors : Pathirage, R.; Ronning, D.; Favrot, L.
Deposited on : 2023-03-24
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

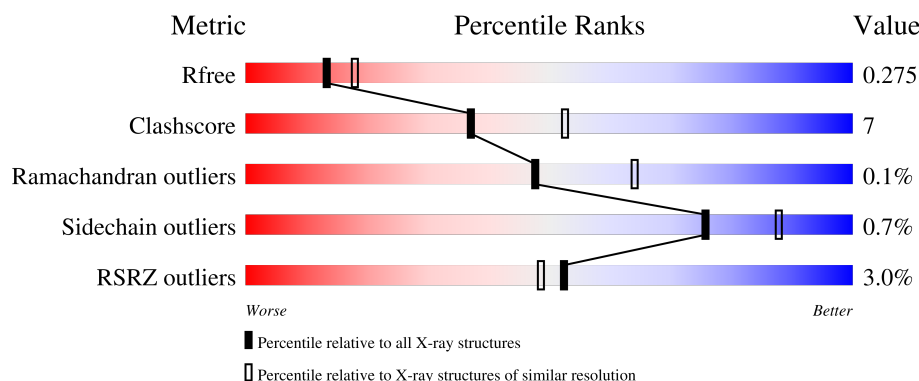
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	379	3% 80% 17% .
1	B	379	4% 75% 19% 6%
1	C	379	2% 78% 15% 7%
1	D	379	2% 81% 16% .

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	AKR	A	406	-	X	-	-
4	AKR	B	404	-	X	-	-
4	AKR	C	404	-	X	-	-
4	AKR	D	404	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11239 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 citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2766	1742	502	509	13			
1	B	356	Total	C	N	O	S	0	0	0
			2697	1697	488	499	13			
1	C	353	Total	C	N	O	S	0	0	0
			2675	1688	483	491	13			
1	D	367	Total	C	N	O	S	0	1	0
			2794	1757	509	515	13			

There are 24 discrepancies between the modelled and reference sequences:

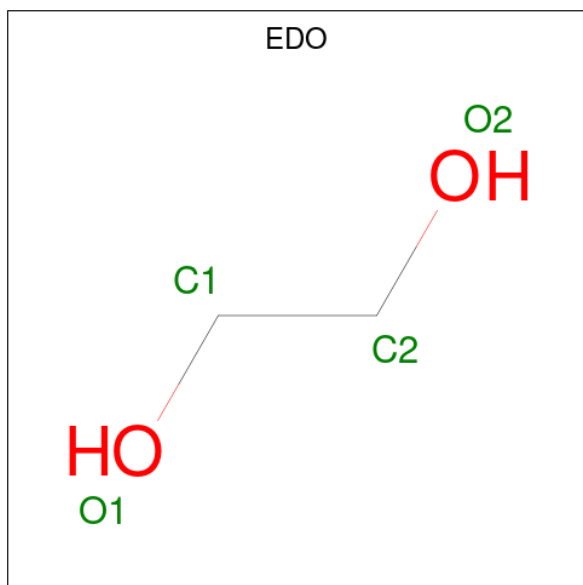
Chain	Residue	Modelled	Actual	Comment	Reference
A	374	HIS	-	expression tag	UNP A0A045JB88
A	375	HIS	-	expression tag	UNP A0A045JB88
A	376	HIS	-	expression tag	UNP A0A045JB88
A	377	HIS	-	expression tag	UNP A0A045JB88
A	378	HIS	-	expression tag	UNP A0A045JB88
A	379	HIS	-	expression tag	UNP A0A045JB88
B	374	HIS	-	expression tag	UNP A0A045JB88
B	375	HIS	-	expression tag	UNP A0A045JB88
B	376	HIS	-	expression tag	UNP A0A045JB88
B	377	HIS	-	expression tag	UNP A0A045JB88
B	378	HIS	-	expression tag	UNP A0A045JB88
B	379	HIS	-	expression tag	UNP A0A045JB88
C	374	HIS	-	expression tag	UNP A0A045JB88
C	375	HIS	-	expression tag	UNP A0A045JB88
C	376	HIS	-	expression tag	UNP A0A045JB88
C	377	HIS	-	expression tag	UNP A0A045JB88
C	378	HIS	-	expression tag	UNP A0A045JB88
C	379	HIS	-	expression tag	UNP A0A045JB88
D	374	HIS	-	expression tag	UNP A0A045JB88
D	375	HIS	-	expression tag	UNP A0A045JB88
D	376	HIS	-	expression tag	UNP A0A045JB88

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Chain	Residue	Modelled	Actual	Comment	Reference
D	377	HIS	-	expression tag	UNP A0A045JB88
D	378	HIS	-	expression tag	UNP A0A045JB88
D	379	HIS	-	expression tag	UNP A0A045JB88

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



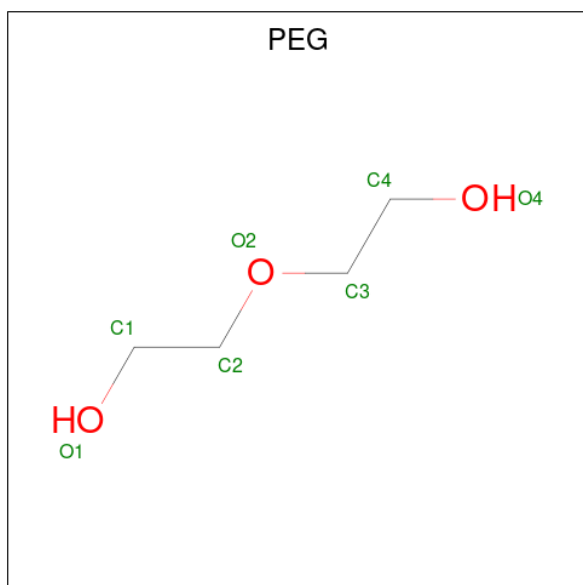
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total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

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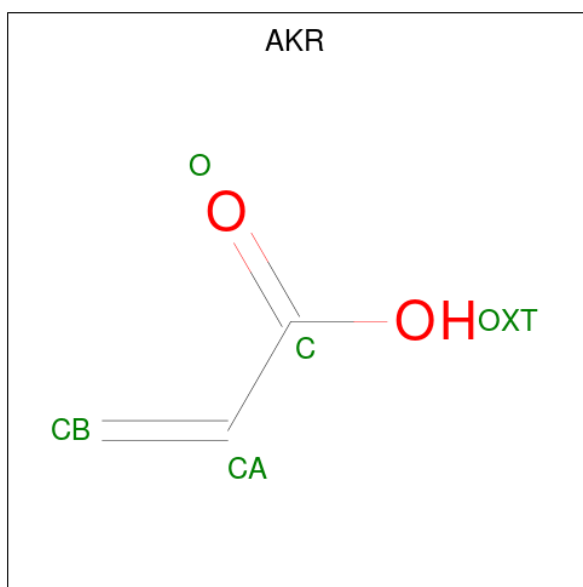
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is ACRYLIC ACID (CCD ID: AKR) (formula: $C_3H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	3	2		
4	B	1	Total	C	O	0	0
			5	3	2		
4	C	1	Total	C	O	0	0
			5	3	2		
4	D	1	Total	C	O	0	0
			5	3	2		

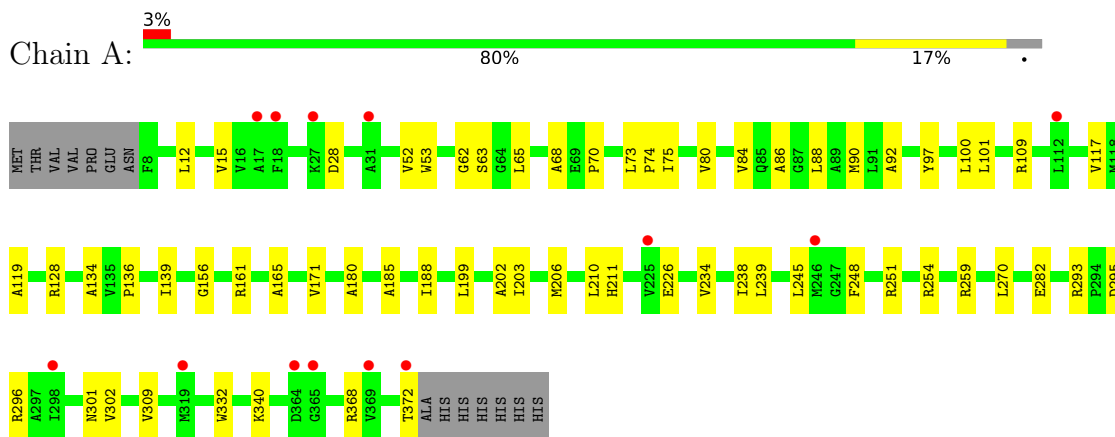
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	27	Total	O	0	0
			27	27		
5	C	58	Total	O	0	0
			58	58		
5	D	63	Total	O	0	0
			63	63		

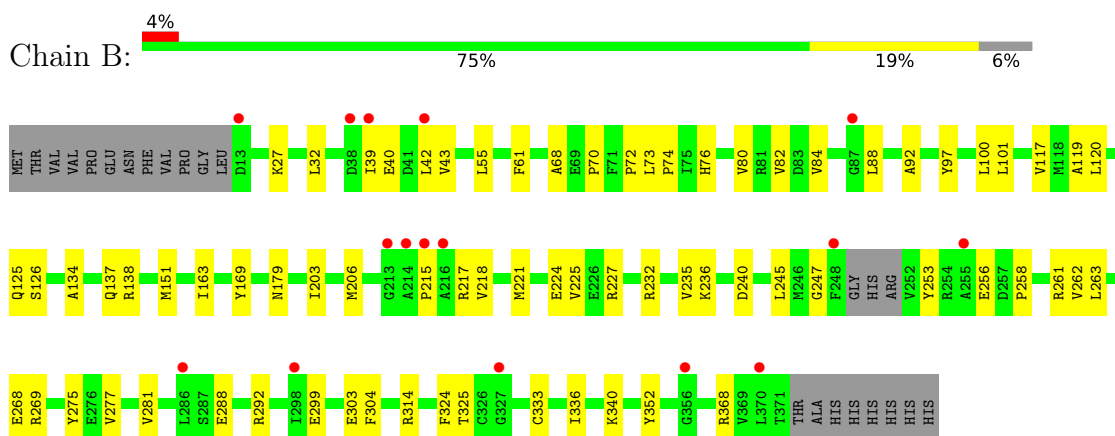
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

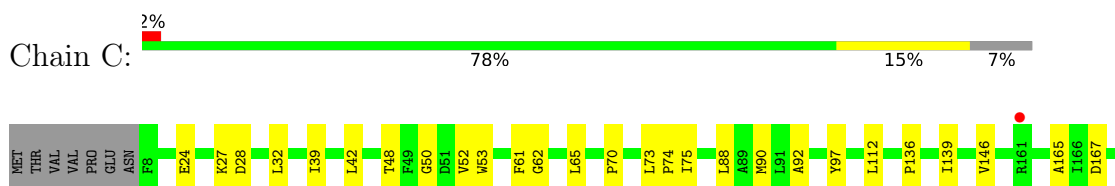
• Molecule 1: citrate synthase

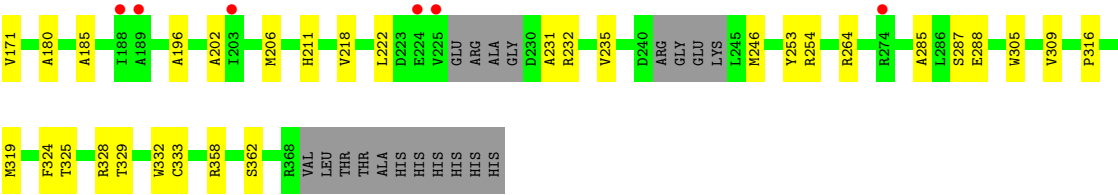


• Molecule 1: citrate synthase

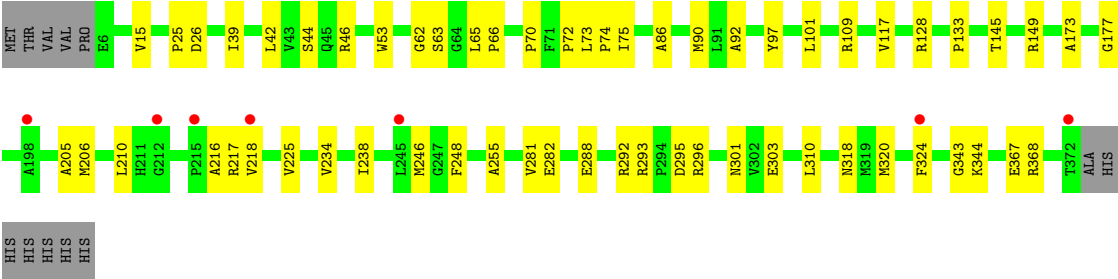
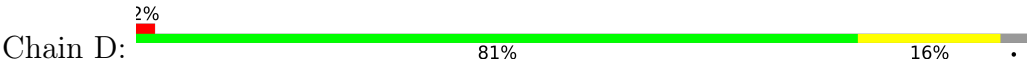


• Molecule 1: citrate synthase





● Molecule 1: citrate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.33Å 121.03Å 99.58Å 90.00° 94.73° 90.00°	Depositor
Resolution (Å)	43.06 – 2.40 43.06 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.3 (43.06-2.40) 84.5 (43.06-2.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.44 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158:000	Depositor
R, R_{free}	0.220 , 0.275 0.220 , 0.275	Depositor DCC
R_{free} test set	1998 reflections (2.31%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.805	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11239	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, AKR, 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	0.08	0/2829	0.22	0/3853
1	B	0.08	0/2756	0.23	0/3752
1	C	0.09	0/2736	0.23	0/3726
1	D	0.10	0/2857	0.26	1/3890 (0.0%)
All	All	0.09	0/11178	0.24	1/15221 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	255	ALA	CB-CA-C	-5.04	109.18	116.54

There are no chirality outliers.

There are no planarity outliers.

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	2766	0	2742	42	0
1	B	2697	0	2672	49	0
1	C	2675	0	2644	36	0
1	D	2794	0	2766	44	0
2	A	16	0	24	6	0
2	B	8	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	12	0	18	5	0
2	D	12	0	18	1	0
3	A	7	0	10	3	0
3	B	14	0	20	2	0
4	A	5	0	3	0	0
4	B	5	0	3	1	0
4	C	5	0	3	0	0
4	D	5	0	3	0	0
5	A	70	0	0	1	0
5	B	27	0	0	0	0
5	C	58	0	0	0	0
5	D	63	0	0	1	0
All	All	11239	0	10938	155	0

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

All (155) 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:B:256:GLU:HB3	1:B:261:ARG:HD3	1.61	0.81
1:A:100:LEU:HD22	1:A:340:LYS:HD2	1.69	0.74
1:B:215:PRO:HA	1:B:303:GLU:HB3	1.70	0.73
1:B:368:ARG:HG3	1:C:62:GLY:HA2	1.69	0.73
1:D:39:ILE:HA	1:D:42:LEU:HD12	1.70	0.72
1:C:232:ARG:HH12	1:C:287:SER:HB2	1.55	0.71
1:B:55:LEU:HB2	1:B:61:PHE:HE1	1.56	0.71
1:A:128:ARG:HH22	2:A:401:EDO:H22	1.56	0.70
1:D:75:ILE:HD11	1:D:90:MET:HE1	1.74	0.68
1:B:39:ILE:HA	1:B:42:LEU:HD12	1.77	0.67
1:A:368:ARG:HD2	1:D:62:GLY:HA2	1.77	0.66
1:B:70:PRO:HB2	1:D:70:PRO:HB2	1.76	0.66
1:D:367:GLU:HG2	1:D:368:ARG:HD3	1.78	0.64
1:A:101:LEU:HD13	1:D:210:LEU:HD21	1.80	0.63
1:D:92:ALA:HA	1:D:97:TYR:HB2	1.80	0.62
1:D:218:VAL:HG12	1:D:246:MET:HB3	1.81	0.62
1:A:12:LEU:HD22	1:A:15:VAL:HG21	1.81	0.61
1:D:128[B]:ARG:NH1	1:D:133:PRO:O	2.34	0.60
1:A:92:ALA:HA	1:A:97:TYR:HB2	1.84	0.60
1:A:301:ASN:HA	2:A:403:EDO:H21	1.84	0.59
1:B:92:ALA:HA	1:B:97:TYR:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PRO:HB2	1:C:70:PRO:HB2	1.85	0.58
1:B:333:CYS:HA	1:B:336:ILE:HD12	1.85	0.58
1:B:138:ARG:HG2	1:B:138:ARG:HH11	1.68	0.57
1:A:340:LYS:NZ	5:A:502:HOH:O	2.38	0.56
1:D:73:LEU:HD12	1:D:74:PRO:HD2	1.88	0.56
1:A:75:ILE:HG23	1:D:90:MET:HE2	1.88	0.55
1:C:231:ALA:O	1:C:235:VAL:HG12	2.06	0.55
1:C:73:LEU:HD12	1:C:74:PRO:HD2	1.87	0.55
1:C:328:ARG:HH12	2:C:401:EDO:H12	1.72	0.55
1:B:72:PRO:HD2	1:D:72:PRO:HD2	1.89	0.55
1:B:240:ASP:OD1	1:B:292:ARG:NH2	2.39	0.54
1:B:88:LEU:HD21	1:B:119:ALA:HB2	1.88	0.54
1:D:234:VAL:O	1:D:238:ILE:HG13	2.08	0.54
1:C:146:VAL:HB	2:C:402:EDO:H22	1.89	0.53
1:A:128:ARG:HD3	3:A:404:PEG:H21	1.91	0.53
1:D:293:ARG:HB3	1:D:296:ARG:HG2	1.90	0.53
1:D:301:ASN:HB3	1:D:303:GLU:OE1	2.08	0.53
1:D:343:GLY:HA2	2:D:402:EDO:H12	1.91	0.52
1:B:40:GLU:OE2	1:B:261:ARG:NH2	2.40	0.52
1:A:293:ARG:HD3	1:A:296:ARG:HG3	1.91	0.52
1:C:50:GLY:HA3	2:C:402:EDO:H21	1.91	0.51
1:A:134:ALA:HB1	3:A:404:PEG:H11	1.93	0.51
1:B:76:HIS:ND1	2:B:401:EDO:O1	2.44	0.51
1:C:92:ALA:HA	1:C:97:TYR:HB2	1.92	0.51
1:D:75:ILE:CD1	1:D:90:MET:HE1	2.40	0.51
1:B:340:LYS:HZ1	3:B:402:PEG:H42	1.76	0.51
1:A:28:ASP:HA	1:A:254:ARG:HB2	1.93	0.50
1:D:288:GLU:HG3	1:D:292:ARG:HE	1.77	0.50
1:B:235:VAL:HG13	1:B:245:LEU:HD21	1.92	0.49
1:B:55:LEU:HB2	1:B:61:PHE:CE1	2.43	0.49
1:C:165:ALA:HB1	1:C:309:VAL:HG13	1.94	0.49
1:D:310:LEU:HB2	1:D:320:MET:HE2	1.95	0.49
1:D:217:ARG:NH1	5:D:509:HOH:O	2.44	0.49
1:C:185:ALA:HB2	1:C:202:ALA:HB2	1.94	0.49
1:B:68:ALA:HB2	1:B:117:VAL:HG22	1.95	0.48
1:A:52:VAL:HG11	1:A:171:VAL:HG23	1.96	0.48
1:A:239:LEU:HD21	1:A:245:LEU:HB2	1.96	0.48
1:B:236:LYS:HZ2	1:B:292:ARG:HE	1.60	0.48
1:B:73:LEU:HD12	1:B:74:PRO:HD2	1.96	0.48
1:A:62:GLY:HA2	1:D:368:ARG:HB2	1.95	0.48
2:A:405:EDO:H11	1:D:25:PRO:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ALA:HB1	1:D:324:PHE:CE1	2.49	0.48
1:B:134:ALA:HB1	3:B:403:PEG:H11	1.94	0.48
1:B:169:TYR:HA	1:B:263:LEU:HD21	1.96	0.48
1:A:248:PHE:CZ	1:A:282:GLU:HA	2.49	0.48
1:C:235:VAL:HG21	1:C:285:ALA:HA	1.95	0.48
1:A:63:SER:O	1:A:109:ARG:NH2	2.37	0.47
1:A:68:ALA:HB2	1:A:117:VAL:HG22	1.96	0.47
1:C:28:ASP:OD1	1:C:254:ARG:NH1	2.47	0.47
1:C:136:PRO:HD2	1:C:139:ILE:HD12	1.97	0.47
1:B:236:LYS:HD3	1:B:288:GLU:CD	2.40	0.47
1:A:73:LEU:HD12	1:A:74:PRO:HD2	1.96	0.47
1:A:86:ALA:HB1	1:D:90:MET:HE3	1.97	0.47
1:B:80:VAL:HG13	1:B:126:SER:HB3	1.96	0.46
1:B:27:LYS:HA	1:B:253:TYR:CD1	2.50	0.46
1:A:185:ALA:HB2	1:A:202:ALA:HB2	1.98	0.46
1:B:84:VAL:HG13	1:B:203:ILE:HD13	1.97	0.46
1:D:216:ALA:HB1	1:D:246:MET:HG3	1.97	0.46
1:A:210:LEU:HG	1:D:101:LEU:HD11	1.98	0.46
1:B:247:GLY:HA3	1:B:304:PHE:HB2	1.97	0.46
1:C:112:LEU:HD12	1:C:333:CYS:SG	2.56	0.46
1:A:53:TRP:CD2	1:A:65:LEU:HD13	2.51	0.46
1:B:32:LEU:HD23	1:B:39:ILE:HD13	1.98	0.46
1:A:156:GLY:HA3	2:A:401:EDO:H21	1.97	0.46
1:C:167:ASP:O	1:C:171:VAL:HG12	2.16	0.46
1:D:66:PRO:O	1:D:117:VAL:HG11	2.16	0.45
1:C:206:MET:HE2	1:C:332:TRP:CZ2	2.51	0.45
1:B:277:VAL:O	1:B:281:VAL:HG13	2.15	0.45
1:D:65:LEU:HG	1:D:117:VAL:HG12	1.97	0.45
1:A:90:MET:SD	1:D:75:ILE:HD12	2.56	0.45
1:A:88:LEU:HD11	1:A:119:ALA:HB2	1.96	0.45
1:A:128:ARG:HD3	3:A:404:PEG:H31	1.98	0.45
1:A:234:VAL:O	1:A:238:ILE:HG13	2.16	0.45
1:B:206:MET:HE2	1:B:325:THR:HA	1.99	0.45
1:C:264:ARG:HG3	1:C:305:TRP:CZ2	2.52	0.45
1:C:88:LEU:O	1:C:196:ALA:HB1	2.17	0.45
1:C:218:VAL:HG12	1:C:246:MET:HB2	1.99	0.45
1:A:161:ARG:NH1	1:A:270:LEU:O	2.44	0.45
1:A:251:ARG:HA	2:A:403:EDO:H11	1.98	0.45
1:B:352:TYR:CG	1:C:24:GLU:HB2	2.52	0.45
1:C:48:THR:OG1	2:C:402:EDO:O2	2.27	0.44
1:A:188:ILE:HG12	1:D:205:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:GLU:HA	1:B:299:GLU:OE1	2.18	0.44
1:D:206:MET:O	1:D:206:MET:HE3	2.18	0.44
1:B:100:LEU:HD22	1:B:340:LYS:HG3	2.00	0.44
1:B:224:GLU:HA	1:B:227:ARG:HG2	1.98	0.44
1:B:258:PRO:O	1:B:262:VAL:HG12	2.17	0.44
1:D:63:SER:HB2	1:D:109:ARG:NH2	2.32	0.44
1:D:145:THR:O	1:D:149:ARG:HG3	2.17	0.44
1:C:32:LEU:HB3	1:C:39:ILE:HD13	2.00	0.44
1:C:180:ALA:HB3	1:C:211:HIS:CD2	2.53	0.44
2:A:405:EDO:H12	1:D:177:GLY:HA3	1.99	0.44
1:C:39:ILE:HA	1:C:42:LEU:HD12	2.00	0.43
1:A:259:ARG:HB2	1:A:302:VAL:HG21	2.01	0.43
1:A:180:ALA:HB3	1:A:211:HIS:CD2	2.53	0.43
1:D:248:PHE:CZ	1:D:282:GLU:HA	2.54	0.43
1:B:82:VAL:HG11	1:C:90:MET:HA	2.01	0.43
1:C:232:ARG:NH2	1:C:288:GLU:OE1	2.51	0.43
1:B:43:VAL:HG21	1:B:262:VAL:HG21	1.99	0.43
1:B:70:PRO:HG3	1:B:137:GLN:HG3	2.00	0.43
1:B:268:GLU:HB3	1:B:275:TYR:CZ	2.53	0.43
1:B:303:GLU:H	1:B:303:GLU:CD	2.27	0.43
1:D:65:LEU:HG	1:D:117:VAL:CG1	2.48	0.43
1:B:206:MET:HE3	1:B:324:PHE:CG	2.53	0.43
1:D:295:ASP:C	1:D:296:ARG:HD3	2.43	0.43
1:B:236:LYS:HA	1:B:236:LYS:HD2	1.60	0.43
1:B:120:LEU:HB3	4:B:404:AKR:HB3	2.01	0.43
1:C:358:ARG:HH21	1:C:362:SER:C	2.26	0.43
1:D:225:VAL:HG21	1:D:281:VAL:HG22	2.01	0.42
1:C:75:ILE:HD11	1:C:90:MET:SD	2.59	0.42
1:A:165:ALA:HB1	1:A:309:VAL:HG13	2.02	0.42
1:A:206:MET:HE2	1:A:332:TRP:CZ2	2.55	0.42
1:D:53:TRP:CD2	1:D:65:LEU:HD13	2.54	0.42
1:A:199:LEU:O	1:A:203:ILE:HG12	2.19	0.42
1:C:53:TRP:CD2	1:C:65:LEU:HD13	2.54	0.42
1:A:80:VAL:O	1:A:84:VAL:HG12	2.20	0.42
1:A:136:PRO:HD2	1:A:139:ILE:HD12	2.02	0.42
1:C:52:VAL:HG11	1:C:171:VAL:HG23	2.02	0.42
1:B:125:GLN:O	2:B:401:EDO:H11	2.20	0.42
1:C:27:LYS:HA	1:C:253:TYR:CD2	2.55	0.42
1:B:268:GLU:HG2	1:B:269:ARG:N	2.34	0.41
1:B:314:ARG:HA	1:B:314:ARG:HD3	1.81	0.41
1:B:151:MET:HG3	1:B:163:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:ASN:H	1:D:318:ASN:ND2	2.18	0.41
1:C:316:PRO:HD2	1:C:319:MET:SD	2.60	0.41
1:C:324:PHE:HZ	2:C:401:EDO:H21	1.85	0.41
1:D:344:LYS:HA	1:D:344:LYS:HD2	1.87	0.41
1:C:325:THR:O	1:C:329:THR:HG23	2.21	0.41
1:D:248:PHE:HZ	1:D:282:GLU:HA	1.86	0.40
1:C:222:LEU:HD23	1:C:222:LEU:HA	1.94	0.40
1:A:372:THR:HB	1:D:46:ARG:NH2	2.36	0.40
1:B:221:MET:O	1:B:225:VAL:HG22	2.21	0.40
1:B:232:ARG:NE	1:B:288:GLU:OE2	2.54	0.40
1:A:86:ALA:HB1	1:D:86:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

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	363/379 (96%)	354 (98%)	9 (2%)	0	100	100
1	B	352/379 (93%)	339 (96%)	13 (4%)	0	100	100
1	C	347/379 (92%)	337 (97%)	9 (3%)	1 (0%)	36	50
1	D	366/379 (97%)	359 (98%)	6 (2%)	1 (0%)	36	50
All	All	1428/1516 (94%)	1389 (97%)	37 (3%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	26	ASP
1	C	61	PHE

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	278/291 (96%)	276 (99%)	2 (1%)	76	88
1	B	271/291 (93%)	267 (98%)	4 (2%)	57	77
1	C	269/291 (92%)	269 (100%)	0	100	100
1	D	281/291 (97%)	279 (99%)	2 (1%)	76	88
All	All	1099/1164 (94%)	1091 (99%)	8 (1%)	76	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	GLU
1	A	295	ASP
1	B	101	LEU
1	B	179	ASN
1	B	217	ARG
1	B	218	VAL
1	D	15	VAL
1	D	44	SER

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	76	HIS
1	A	283	GLN
1	B	45	GLN
1	B	132	GLN
1	B	301	ASN
1	C	110	GLN
1	D	76	HIS
1	D	318	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

19 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	C	403	-	3,3,3	0.43	0	2,2,2	0.38	0
3	PEG	B	403	-	6,6,6	0.51	0	5,5,5	0.24	0
4	AKR	D	404	-	4,4,4	1.59	1 (25%)	4,4,4	1.38	1 (25%)
2	EDO	C	402	-	3,3,3	0.41	0	2,2,2	0.35	0
3	PEG	A	404	-	6,6,6	0.51	0	5,5,5	0.26	0
4	AKR	B	404	-	4,4,4	1.58	1 (25%)	4,4,4	1.37	1 (25%)
2	EDO	A	403	-	3,3,3	0.41	0	2,2,2	0.35	0
2	EDO	B	401	-	3,3,3	0.43	0	2,2,2	0.30	0
2	EDO	A	405	-	3,3,3	0.43	0	2,2,2	0.39	0
2	EDO	C	401	-	3,3,3	0.42	0	2,2,2	0.37	0
3	PEG	B	402	-	6,6,6	0.50	0	5,5,5	0.27	0
4	AKR	A	406	-	4,4,4	1.60	1 (25%)	4,4,4	1.36	1 (25%)
4	AKR	C	404	-	4,4,4	1.61	1 (25%)	4,4,4	1.35	1 (25%)
2	EDO	D	402	-	3,3,3	0.42	0	2,2,2	0.34	0
2	EDO	D	401	-	3,3,3	0.43	0	2,2,2	0.36	0
2	EDO	D	403	-	3,3,3	0.42	0	2,2,2	0.38	0
2	EDO	A	401	-	3,3,3	0.43	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	402	-	3,3,3	0.42	0	2,2,2	0.38	0
2	EDO	B	405	-	3,3,3	0.43	0	2,2,2	0.37	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	C	403	-	-	0/1/1/1	-
3	PEG	B	403	-	-	0/4/4/4	-
4	AKR	D	404	-	-	2/2/2/2	-
2	EDO	C	402	-	-	0/1/1/1	-
3	PEG	A	404	-	-	2/4/4/4	-
4	AKR	B	404	-	-	2/2/2/2	-
2	EDO	A	403	-	-	0/1/1/1	-
2	EDO	B	401	-	-	0/1/1/1	-
2	EDO	A	405	-	-	0/1/1/1	-
2	EDO	C	401	-	-	0/1/1/1	-
3	PEG	B	402	-	-	1/4/4/4	-
4	AKR	A	406	-	-	2/2/2/2	-
4	AKR	C	404	-	-	2/2/2/2	-
2	EDO	D	402	-	-	0/1/1/1	-
2	EDO	D	401	-	-	0/1/1/1	-
2	EDO	D	403	-	-	0/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	A	402	-	-	0/1/1/1	-
2	EDO	B	405	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	404	AKR	CA-C	2.40	1.53	1.46
4	A	406	AKR	CA-C	2.37	1.53	1.46
4	D	404	AKR	CA-C	2.37	1.53	1.46
4	B	404	AKR	CA-C	2.36	1.53	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	404	AKR	OXT-C-CA	2.13	119.99	114.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	AKR	OXT-C-CA	2.13	119.98	114.19
4	C	404	AKR	OXT-C-CA	2.10	119.92	114.19
4	A	406	AKR	OXT-C-CA	2.10	119.91	114.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	406	AKR	O-C-CA-CB
4	A	406	AKR	OXT-C-CA-CB
4	B	404	AKR	O-C-CA-CB
4	B	404	AKR	OXT-C-CA-CB
4	C	404	AKR	O-C-CA-CB
4	C	404	AKR	OXT-C-CA-CB
4	D	404	AKR	O-C-CA-CB
4	D	404	AKR	OXT-C-CA-CB
3	A	404	PEG	O2-C3-C4-O4
3	B	402	PEG	C1-C2-O2-C3
3	A	404	PEG	C4-C3-O2-C2

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	PEG	1	0
2	C	402	EDO	3	0
3	A	404	PEG	3	0
4	B	404	AKR	1	0
2	A	403	EDO	2	0
2	B	401	EDO	2	0
2	A	405	EDO	2	0
2	C	401	EDO	2	0
3	B	402	PEG	1	0
2	D	402	EDO	1	0
2	A	401	EDO	2	0

5.7 Other polymers [i](#)

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	365/379 (96%)	0.31	13 (3%) 46 42	39, 50, 87, 108	0
1	B	356/379 (93%)	0.52	16 (4%) 38 34	45, 64, 90, 98	0
1	C	353/379 (93%)	0.44	7 (1%) 65 60	42, 56, 87, 99	0
1	D	367/379 (96%)	0.31	7 (1%) 66 62	25, 54, 76, 111	1 (0%)
All	All	1441/1516 (95%)	0.39	43 (2%) 52 48	25, 55, 87, 111	1 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	PRO	7.3
1	B	214	ALA	4.5
1	C	225	VAL	4.3
1	B	216	ALA	4.3
1	D	245	LEU	4.2
1	A	18	PHE	4.0
1	B	286	LEU	3.8
1	A	27	LYS	3.6
1	B	87	GLY	3.5
1	D	324	PHE	3.1
1	D	198	ALA	3.1
1	B	298	ILE	3.1
1	B	13	ASP	3.1
1	B	327	GLY	3.0
1	C	188	ILE	2.8
1	D	372	THR	2.8
1	B	248	PHE	2.7
1	C	274	ARG	2.6
1	C	203	ILE	2.6
1	D	212	GLY	2.6
1	A	225	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	38	ASP	2.5
1	A	17	ALA	2.5
1	B	213	GLY	2.4
1	B	370	LEU	2.4
1	A	31	ALA	2.4
1	A	319	MET	2.4
1	D	218	VAL	2.4
1	A	246	MET	2.4
1	A	372	THR	2.3
1	B	356	GLY	2.3
1	A	364	ASP	2.3
1	C	189	ALA	2.3
1	A	112	LEU	2.2
1	D	215	PRO	2.2
1	B	255	ALA	2.2
1	B	39	ILE	2.2
1	C	161	ARG	2.2
1	A	369	VAL	2.1
1	B	42	LEU	2.1
1	A	365	GLY	2.0
1	C	224	GLU	2.0
1	A	298	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	C	403	4/4	0.63	0.21	70,71,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	403	4/4	0.73	0.28	51,53,56,59	0
3	PEG	B	402	7/7	0.75	0.12	79,82,94,99	0
2	EDO	D	401	4/4	0.77	0.15	62,66,71,71	0
2	EDO	A	402	4/4	0.77	0.22	53,56,56,61	0
2	EDO	B	401	4/4	0.83	0.26	57,59,61,68	0
2	EDO	A	401	4/4	0.83	0.12	63,69,74,82	0
3	PEG	B	403	7/7	0.84	0.23	46,51,55,59	0
2	EDO	C	402	4/4	0.85	0.15	52,61,62,68	0
2	EDO	D	403	4/4	0.86	0.20	58,61,63,66	0
3	PEG	A	404	7/7	0.86	0.19	45,48,52,64	0
2	EDO	B	405	4/4	0.88	0.13	57,57,62,65	0
4	AKR	D	404	5/5	0.88	0.12	57,59,67,74	0
4	AKR	A	406	5/5	0.89	0.09	50,51,53,59	0
2	EDO	D	402	4/4	0.89	0.18	47,53,59,65	0
4	AKR	B	404	5/5	0.91	0.19	58,61,62,66	0
2	EDO	C	401	4/4	0.91	0.11	54,59,59,61	0
2	EDO	A	405	4/4	0.92	0.12	53,54,67,73	0
4	AKR	C	404	5/5	0.93	0.12	45,53,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.