



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 12:32 AM UTC

PDB ID : 5NKM / pdb_00005nkm
Title : SMG8-SMG9 complex
Authors : Li, L.; Basquin, J.; Conti, E.
Deposited on : 2017-03-31
Resolution : 2.49 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

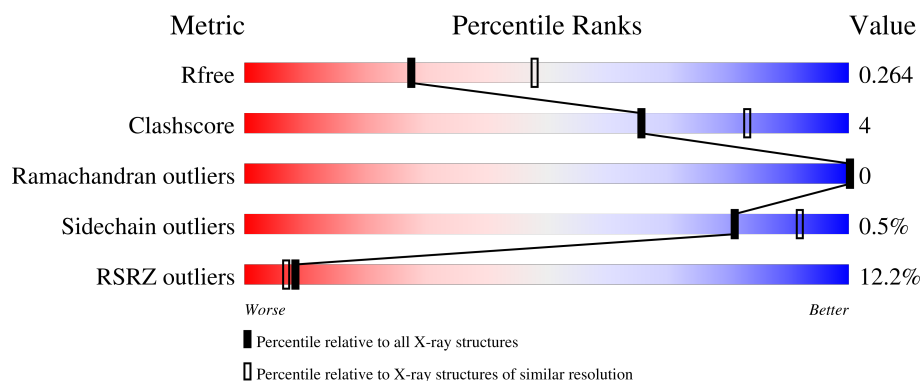
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	429	8% 76% 20%
1	C	429	10% 74% 7% 19%
2	B	317	9% 72% 10% 18%
3	D	305	10% 78% 8% 14%
3	F	305	12% 72% 11% 15%

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Mol	Chain	Length	Quality of chain
4	E	419	11% 76% 7% 16%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27997 atoms, of which 13638 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 Protein smg-8.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	345	Total	C	H	N	O	S	Se	0	0	0
			5217	1671	2550	462	514	11	9			
1	C	347	Total	C	H	N	O	S	Se	0	0	0
			5160	1661	2504	464	511	11	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP O62301
A	424	HIS	-	expression tag	UNP O62301
A	425	HIS	-	expression tag	UNP O62301
A	426	HIS	-	expression tag	UNP O62301
A	427	HIS	-	expression tag	UNP O62301
A	428	HIS	-	expression tag	UNP O62301
A	429	HIS	-	expression tag	UNP O62301
C	1	MSE	-	initiating methionine	UNP O62301
C	424	HIS	-	expression tag	UNP O62301
C	425	HIS	-	expression tag	UNP O62301
C	426	HIS	-	expression tag	UNP O62301
C	427	HIS	-	expression tag	UNP O62301
C	428	HIS	-	expression tag	UNP O62301
C	429	HIS	-	expression tag	UNP O62301

- Molecule 2 is a protein called Protein smg-9.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	B	260	Total	C	H	N	O	S	Se	0	0	0
			4035	1299	1996	345	386	2	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	59	MSE	-	initiating methionine	UNP Q9XWJ1

- Molecule 3 is a protein called Protein smg-9.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
3	D	263	Total	C	H	N	O	S	Se	0	0	0
			3999	1295	1960	341	393	2	8			
3	F	258	Total	C	H	N	O	S	Se	0	0	0
			3931	1276	1928	342	376	2	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	59	MSE	-	initiating methionine	UNP Q9XWJ1
F	59	MSE	-	initiating methionine	UNP Q9XWJ1

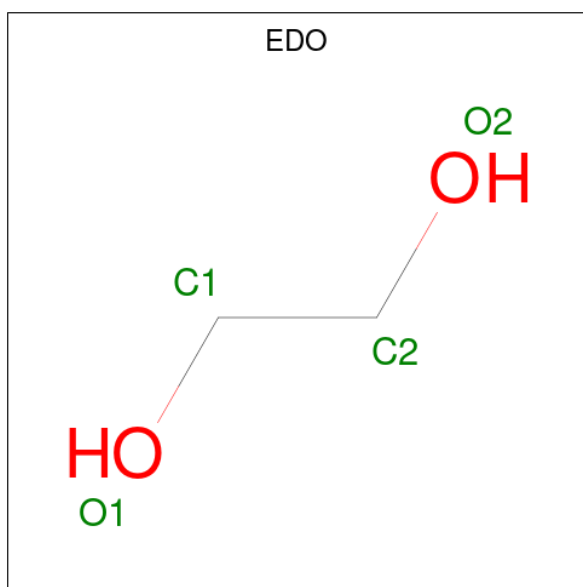
- Molecule 4 is a protein called Protein smg-8.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
4	E	351	Total	C	H	N	O	S	Se	0	0	0
			5301	1704	2590	473	514	11	9			

There is a discrepancy between the modelled and reference sequences:

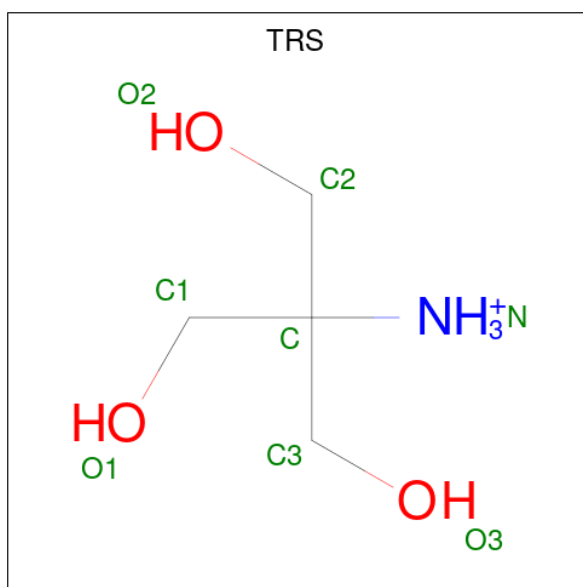
Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MSE	-	initiating methionine	UNP O62301

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



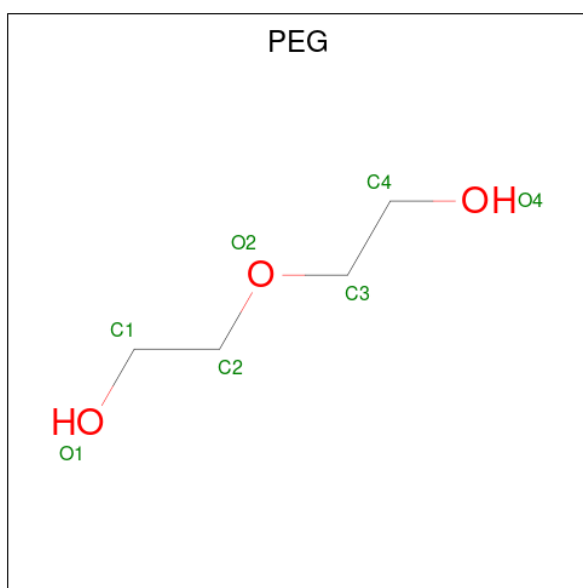
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		
5	D	1	Total	C	H	O	0	0
			10	2	6	2		
5	D	1	Total	C	H	O	0	0
			10	2	6	2		
5	E	1	Total	C	H	O	0	0
			10	2	6	2		
5	E	1	Total	C	H	O	0	0
			10	2	6	2		
5	E	1	Total	C	H	O	0	0
			10	2	6	2		
5	E	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
6	E	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	H	O	0	0
			17	4	10	3		
7	C	1	Total	C	H	O	0	0
			17	4	10	3		

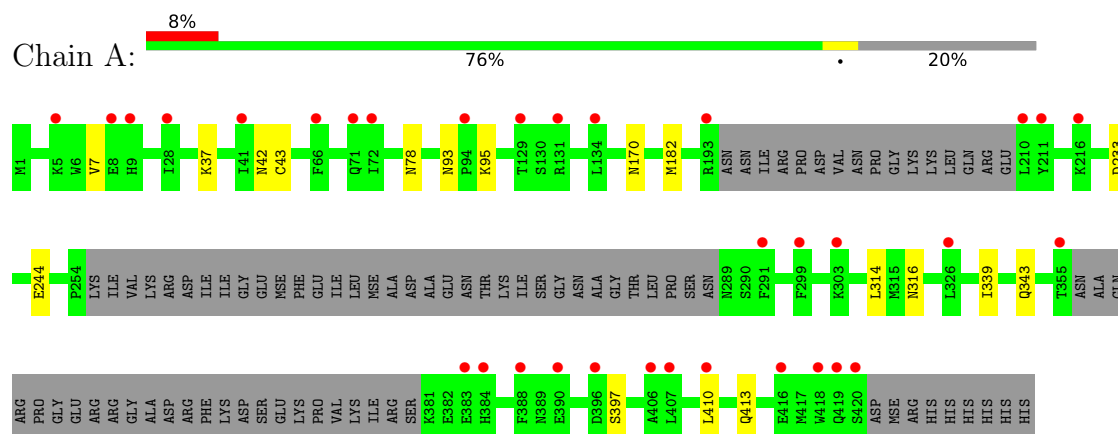
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	38	Total 38	O 38	0	0
8	B	27	Total 27	O 27	0	0
8	C	34	Total 34	O 34	0	0
8	D	22	Total 22	O 22	0	0
8	E	34	Total 34	O 34	0	0
8	F	15	Total 15	O 15	0	0

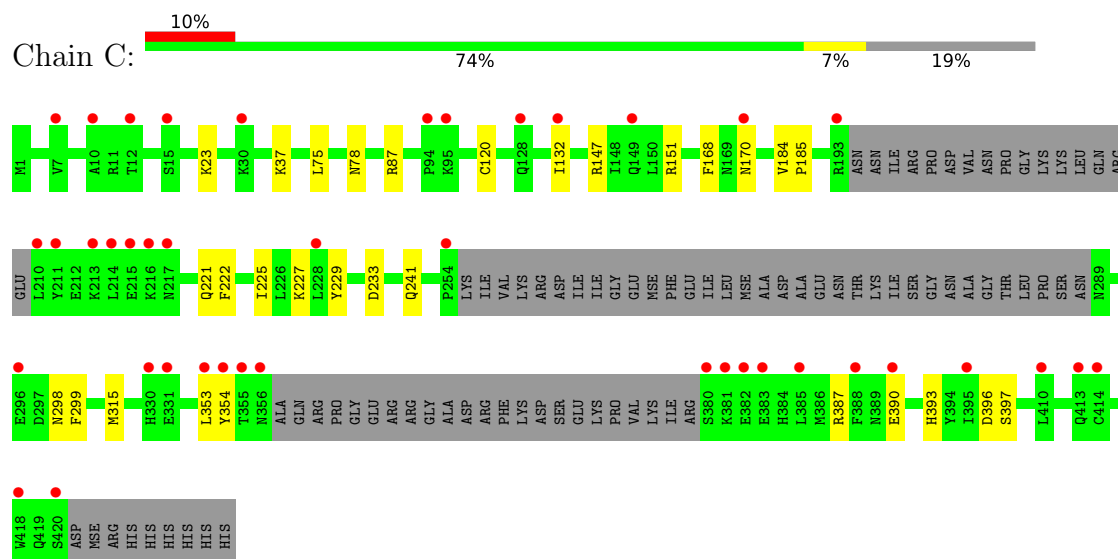
3 Residue-property plots [i](#)

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: Protein smg-8

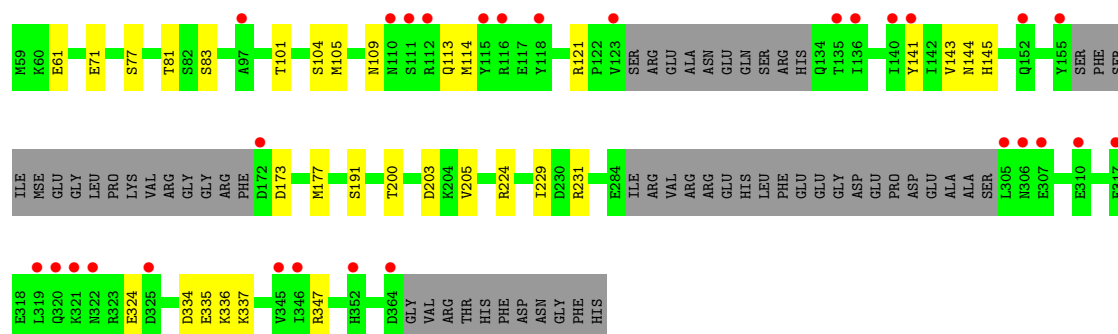


• Molecule 1: Protein smg-8

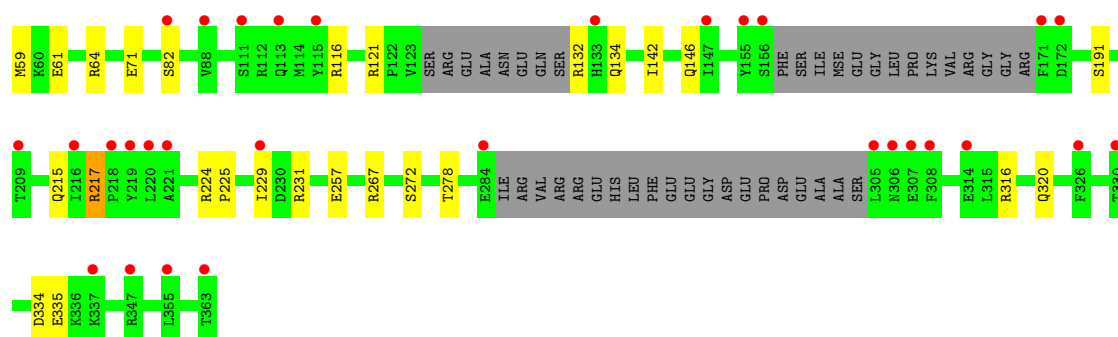
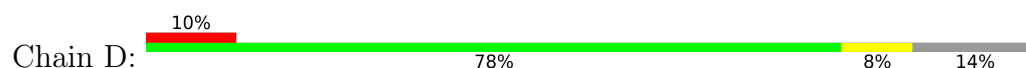


• Molecule 2: Protein smg-9

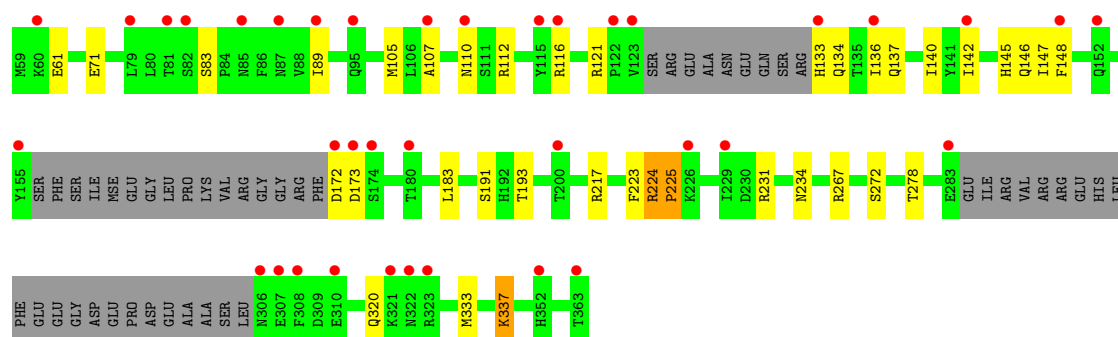




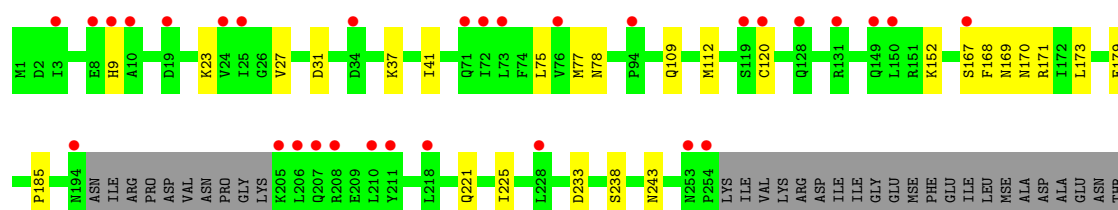
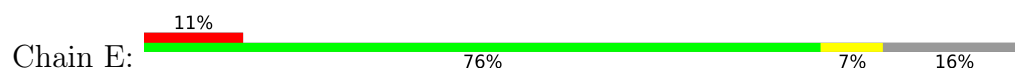
● Molecule 3: Protein smg-9

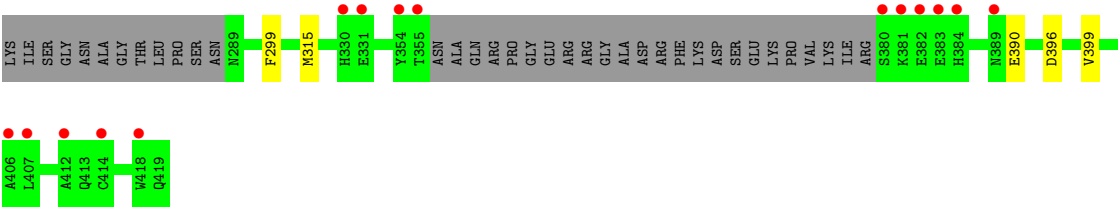


● Molecule 3: Protein smg-9



● Molecule 4: Protein smg-8





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.08Å 111.08Å 374.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.41 – 2.49 62.41 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.8 (62.41-2.49) 99.8 (62.41-2.49)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.225 , 0.260 0.228 , 0.264	Depositor DCC
R_{free} test set	4712 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 86.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27997	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, EDO, TRS

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	0.13	0/2694	0.30	0/3628
1	C	0.14	0/2682	0.32	0/3614
2	B	0.15	0/2063	0.38	0/2784
3	D	0.14	0/2062	0.35	0/2788
3	F	0.14	0/2026	0.49	3/2738 (0.1%)
4	E	0.14	0/2739	0.31	0/3687
All	All	0.14	0/14266	0.36	3/19239 (0.0%)

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
3	F	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	224	ARG	CA-C-N	-11.20	108.17	120.94
3	F	224	ARG	C-N-CA	-11.20	108.17	120.94
3	F	225	PRO	N-CA-C	-5.24	107.97	114.68

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	224	ARG	Peptide

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	2667	2550	2550	11	0
1	C	2656	2504	2509	24	0
2	B	2039	1996	2001	20	0
3	D	2039	1960	1965	19	0
3	F	2003	1928	1947	23	0
4	E	2711	2590	2591	19	0
5	A	8	12	12	1	0
5	C	8	12	12	0	0
5	D	8	12	12	2	0
5	E	20	30	30	2	0
6	C	8	12	12	0	0
6	E	8	12	12	1	0
7	C	14	20	20	0	0
8	A	38	0	0	0	0
8	B	27	0	0	1	0
8	C	34	0	0	6	0
8	D	22	0	0	1	0
8	E	34	0	0	0	0
8	F	15	0	0	0	0
All	All	14359	13638	13673	105	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 4.

All (105) 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:23:LYS:NZ	1:C:299:PHE:O	2.03	0.92
4:E:233:ASP:O	4:E:238:SER:OG	1.88	0.90
4:E:23:LYS:NZ	4:E:299:PHE:O	2.05	0.89
1:C:185:PRO:O	8:C:601:HOH:O	1.92	0.85
3:F:61:GLU:OE1	3:F:121:ARG:NH2	2.09	0.84
1:C:393:HIS:O	1:C:397:SER:OG	1.96	0.84
3:D:191:SER:O	3:D:231:ARG:NH2	2.11	0.83
3:F:191:SER:O	3:F:231:ARG:NH2	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:SER:O	2:B:231:ARG:NH2	2.15	0.79
1:C:298:ASN:OD1	8:C:602:HOH:O	2.02	0.78
1:C:170:ASN:ND2	8:C:604:HOH:O	2.20	0.75
2:B:77:SER:O	2:B:336:LYS:NZ	2.20	0.73
1:C:227:LYS:NZ	1:C:233:ASP:OD2	2.22	0.72
3:F:172:ASP:OD1	3:F:173:ASP:N	2.23	0.71
1:C:241:GLN:N	8:C:601:HOH:O	2.25	0.69
3:F:110:ASN:O	3:F:112:ARG:N	2.26	0.67
1:C:87:ARG:NH2	3:D:257:GLU:OE1	2.28	0.66
2:B:81:THR:N	2:B:335:GLU:OE2	2.29	0.66
3:D:71:GLU:OE2	4:E:170:ASN:ND2	2.30	0.65
2:B:113:GLN:OE1	2:B:114:MSE:N	2.30	0.64
3:F:333:MSE:HG3	3:F:337:LYS:HB3	1.80	0.64
3:F:116:ARG:O	3:F:121:ARG:NH1	2.32	0.63
2:B:224:ARG:O	2:B:337:LYS:NZ	2.33	0.62
1:C:229:TYR:O	8:C:603:HOH:O	2.16	0.61
3:D:215:GLN:O	5:D:401:EDO:O2	2.07	0.61
1:C:184:VAL:O	1:C:184:VAL:HG23	2.02	0.60
4:E:167:SER:OG	4:E:169:ASN:O	2.22	0.58
3:D:61:GLU:OE1	3:D:121:ARG:NH2	2.34	0.57
2:B:71:GLU:OE1	1:C:170:ASN:ND2	2.37	0.56
1:C:390:GLU:N	1:C:390:GLU:OE1	2.39	0.56
3:D:142:ILE:O	8:D:501:HOH:O	2.18	0.56
3:D:64:ARG:NH2	3:D:134:GLN:OE1	2.36	0.55
4:E:77:MSE:HE1	4:E:109:GLN:HG3	1.87	0.55
4:E:171:ARG:NE	5:E:503:EDO:O2	2.36	0.55
3:D:217:ARG:NE	5:D:402:EDO:O1	2.34	0.54
2:B:200:THR:O	2:B:203:ASP:HB2	2.08	0.54
3:D:272:SER:O	3:D:278:THR:OG1	2.26	0.54
2:B:347:ARG:NH2	8:B:401:HOH:O	2.40	0.53
4:E:31:ASP:O	6:E:506:TRS:O2	2.15	0.53
3:D:334:ASP:OD1	3:D:335:GLU:N	2.42	0.53
4:E:75:LEU:HD11	4:E:315:MSE:HE1	1.90	0.52
4:E:390:GLU:N	4:E:390:GLU:OE1	2.42	0.51
1:C:396:ASP:O	3:D:267:ARG:NH2	2.43	0.51
1:A:244:GLU:HB3	3:F:133:HIS:O	2.12	0.50
3:F:272:SER:O	3:F:278:THR:OG1	2.29	0.49
3:F:83:SER:CB	3:F:145:HIS:CE1	2.96	0.48
4:E:27:VAL:HG21	4:E:41:ILE:CD1	2.43	0.48
1:A:37:LYS:HE2	1:A:78:ASN:HA	1.95	0.48
2:B:173:ASP:O	2:B:177:MSE:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:LYS:HE2	1:C:78:ASN:HA	1.95	0.47
3:F:107:ALA:HA	3:F:148:PHE:CE2	2.50	0.47
3:D:316:ARG:O	3:D:320:GLN:OE1	2.33	0.46
3:F:134:GLN:OE1	3:F:137:GLN:NE2	2.46	0.46
2:B:104:SER:HB3	2:B:109:ASN:OD1	2.15	0.46
4:E:77:MSE:HE3	4:E:112:MSE:HB2	1.97	0.46
3:D:116:ARG:O	3:D:121:ARG:NH1	2.49	0.46
4:E:399:VAL:O	3:F:267:ARG:NH1	2.49	0.46
1:A:93:ASN:OD1	1:A:95:LYS:N	2.49	0.46
1:C:353:LEU:O	1:C:354:TYR:CB	2.64	0.45
2:B:141:TYR:CE2	2:B:143:VAL:HG13	2.52	0.45
3:F:89:ILE:HG12	3:F:148:PHE:CD1	2.51	0.45
4:E:37:LYS:HE2	4:E:78:ASN:HA	1.98	0.44
3:D:59:MSE:HE3	3:D:142:ILE:HB	2.00	0.44
3:F:110:ASN:C	3:F:112:ARG:H	2.22	0.44
1:C:75:LEU:HD11	1:C:315:MSE:HE1	1.99	0.44
1:C:241:GLN:HG2	8:C:601:HOH:O	2.17	0.44
1:C:147:ARG:O	1:C:151:ARG:HG3	2.16	0.43
1:C:397:SER:CB	3:D:229:ILE:HD11	2.48	0.43
1:C:184:VAL:O	1:C:184:VAL:CG2	2.65	0.43
3:F:320:GLN:N	3:F:320:GLN:OE1	2.51	0.43
3:F:142:ILE:HA	3:F:146:GLN:O	2.19	0.43
3:F:136:ILE:HB	3:F:183:LEU:HD21	2.01	0.43
1:A:7:VAL:HG11	1:A:316:ASN:HB2	2.01	0.43
2:B:334:ASP:OD1	2:B:335:GLU:N	2.51	0.43
3:D:142:ILE:HA	3:D:146:GLN:O	2.19	0.43
2:B:83:SER:OG	2:B:145:HIS:ND1	2.49	0.43
1:A:170:ASN:HD21	3:F:71:GLU:HB2	1.83	0.43
2:B:83:SER:HB3	2:B:145:HIS:CE1	2.54	0.42
1:A:397:SER:CB	2:B:229:ILE:HD11	2.48	0.42
3:D:132:ARG:NH1	4:E:243:ASN:O	2.52	0.42
3:F:110:ASN:O	3:F:110:ASN:ND2	2.48	0.42
3:D:224:ARG:HA	3:D:225:PRO:C	2.44	0.42
3:F:193:THR:HA	3:F:234:ASN:O	2.20	0.42
3:D:82:SER:HA	3:D:334:ASP:OD1	2.19	0.42
2:B:231:ARG:NH1	2:B:324:GLU:O	2.52	0.42
2:B:203:ASP:OD1	2:B:205:VAL:HG12	2.20	0.42
1:A:182:MSE:HE2	1:A:314:LEU:HD13	2.02	0.41
4:E:152:LYS:HG2	4:E:179:GLU:OE2	2.21	0.41
3:F:140:ILE:HD11	3:F:147:ILE:HG23	2.02	0.41
4:E:221:GLN:O	4:E:225:ILE:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ILE:O	1:A:343:GLN:HG3	2.21	0.41
4:E:173:LEU:HD21	5:E:503:EDO:C2	2.50	0.41
1:A:233:ASP:N	5:A:501:EDO:O1	2.42	0.41
2:B:61:GLU:OE2	2:B:121:ARG:NH2	2.53	0.41
1:C:120:CYS:O	1:C:185:PRO:HB3	2.21	0.41
2:B:101:THR:O	2:B:105:MSE:HG2	2.21	0.40
1:A:42:ASN:OD1	1:A:43:CYS:N	2.54	0.40
1:A:410:LEU:O	1:A:413:GLN:N	2.54	0.40
2:B:83:SER:HG	2:B:145:HIS:CE1	2.38	0.40
1:C:221:GLN:O	1:C:225:ILE:HD12	2.21	0.40
1:C:354:TYR:CB	1:C:387:ARG:O	2.69	0.40
4:E:396:ASP:OD1	3:F:267:ARG:NH2	2.54	0.40
1:C:132:ILE:HD13	1:C:222:PHE:HD1	1.87	0.40
3:F:223:PHE:CE2	3:F:225:PRO:HD2	2.56	0.40
4:E:120:CYS:O	4:E:185:PRO:HB3	2.21	0.40

There are no symmetry-related clashes.

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	337/429 (79%)	324 (96%)	13 (4%)	0	100	100
1	C	339/429 (79%)	324 (96%)	15 (4%)	0	100	100
2	B	252/317 (80%)	245 (97%)	7 (3%)	0	100	100
3	D	255/305 (84%)	246 (96%)	9 (4%)	0	100	100
3	F	250/305 (82%)	241 (96%)	9 (4%)	0	100	100
4	E	343/419 (82%)	332 (97%)	11 (3%)	0	100	100
All	All	1776/2204 (81%)	1712 (96%)	64 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	288/378 (76%)	288 (100%)	0	100	100
1	C	281/378 (74%)	280 (100%)	1 (0%)	84	93
2	B	219/279 (78%)	218 (100%)	1 (0%)	81	92
3	D	216/269 (80%)	215 (100%)	1 (0%)	81	92
3	F	211/269 (78%)	208 (99%)	3 (1%)	59	81
4	E	287/369 (78%)	285 (99%)	2 (1%)	76	89
All	All	1502/1942 (77%)	1494 (100%)	8 (0%)	81	92

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

Mol	Chain	Res	Type
2	B	144	ASN
1	C	168	PHE
3	D	217	ARG
4	E	9	HIS
4	E	168	PHE
3	F	105	MSE
3	F	217	ARG
3	F	337	LYS

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	17	GLN
1	A	250	HIS
1	C	114	HIS
1	C	241	GLN
3	D	145	HIS
4	E	93	ASN
4	E	192	GLN
4	E	250	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	EDO	A	501	-	3,3,3	0.41	0	2,2,2	0.28	0
6	TRS	C	503	-	7,7,7	0.34	0	9,9,9	0.26	0
5	EDO	E	502	-	3,3,3	0.43	0	2,2,2	0.35	0
5	EDO	A	502	-	3,3,3	0.44	0	2,2,2	0.31	0
5	EDO	E	501	-	3,3,3	0.44	0	2,2,2	0.34	0
5	EDO	C	501	-	3,3,3	0.42	0	2,2,2	0.33	0
5	EDO	E	505	-	3,3,3	0.42	0	2,2,2	0.33	0
5	EDO	C	502	-	3,3,3	0.40	0	2,2,2	0.41	0
6	TRS	E	506	-	7,7,7	0.32	0	9,9,9	0.36	0
7	PEG	C	505	-	6,6,6	0.50	0	5,5,5	0.30	0
7	PEG	C	504	-	6,6,6	0.49	0	5,5,5	0.47	0
5	EDO	E	504	-	3,3,3	0.43	0	2,2,2	0.35	0
5	EDO	D	401	-	3,3,3	0.40	0	2,2,2	0.20	0
5	EDO	D	402	-	3,3,3	0.36	0	2,2,2	0.47	0
5	EDO	E	503	-	3,3,3	0.42	0	2,2,2	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	501	-	-	0/1/1/1	-
6	TRS	C	503	-	-	2/9/9/9	-
5	EDO	E	502	-	-	0/1/1/1	-
5	EDO	A	502	-	-	1/1/1/1	-
5	EDO	E	501	-	-	0/1/1/1	-
5	EDO	C	501	-	-	1/1/1/1	-
5	EDO	E	505	-	-	0/1/1/1	-
5	EDO	C	502	-	-	1/1/1/1	-
6	TRS	E	506	-	-	8/9/9/9	-
7	PEG	C	505	-	-	2/4/4/4	-
7	PEG	C	504	-	-	1/4/4/4	-
5	EDO	E	504	-	-	0/1/1/1	-
5	EDO	D	401	-	-	0/1/1/1	-
5	EDO	D	402	-	-	1/1/1/1	-
5	EDO	E	503	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	506	TRS	C1-C-C3-O3
6	E	506	TRS	C2-C-C3-O3
6	E	506	TRS	N-C-C3-O3
7	C	505	PEG	O1-C1-C2-O2
5	C	502	EDO	O1-C1-C2-O2
6	E	506	TRS	C1-C-C2-O2
6	E	506	TRS	C3-C-C2-O2
5	A	502	EDO	O1-C1-C2-O2
7	C	504	PEG	O1-C1-C2-O2
6	E	506	TRS	C3-C-C1-O1
6	E	506	TRS	N-C-C2-O2
7	C	505	PEG	O2-C3-C4-O4
5	C	501	EDO	O1-C1-C2-O2
5	D	402	EDO	O1-C1-C2-O2
6	C	503	TRS	C3-C-C2-O2
6	C	503	TRS	C1-C-C2-O2

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Mol	Chain	Res	Type	Atoms
6	E	506	TRS	N-C-C1-O1

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	EDO	1	0
6	E	506	TRS	1	0
5	D	401	EDO	1	0
5	D	402	EDO	1	0
5	E	503	EDO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	335/429 (78%)	0.80	33 (9%) 13 11	62, 92, 145, 171	0
1	C	337/429 (78%)	0.85	41 (12%) 8 7	63, 90, 163, 208	0
2	B	252/317 (79%)	0.89	29 (11%) 9 8	59, 91, 142, 175	0
3	D	255/305 (83%)	1.03	30 (11%) 9 7	61, 99, 153, 206	0
3	F	250/305 (81%)	1.06	37 (14%) 5 4	66, 97, 143, 163	0
4	E	341/419 (81%)	0.88	46 (13%) 7 5	60, 86, 150, 187	0
All	All	1770/2204 (80%)	0.91	216 (12%) 8 7	59, 92, 151, 208	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	194	ASN	6.9
3	D	156	SER	6.7
2	B	306	ASN	5.6
4	E	418	TRP	5.5
3	F	322	ASN	5.3
2	B	111	SER	4.9
1	C	128	GLN	4.8
4	E	380	SER	4.7
4	E	384	HIS	4.7
3	F	155	TYR	4.7
1	C	356	ASN	4.6
1	C	254	PRO	4.5
3	D	305	LEU	4.5
1	A	193	ARG	4.4
3	F	307	GLU	4.3
1	C	210	LEU	4.3
3	F	85	ASN	4.3
4	E	253	ASN	4.3
3	F	173	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
3	F	133	HIS	4.2
2	B	155	TYR	4.2
3	D	155	TYR	4.1
4	E	8	GLU	4.1
4	E	72	ILE	4.1
1	A	72	ILE	4.1
1	A	41	ILE	4.0
4	E	128	GLN	3.9
4	E	76	VAL	3.8
2	B	110	ASN	3.8
3	D	172	ASP	3.8
1	C	414	CYS	3.7
1	A	134	LEU	3.7
2	B	136	ILE	3.7
3	F	115	TYR	3.7
3	D	220	LEU	3.7
4	E	19	ASP	3.7
4	E	207	GLN	3.6
3	F	81	THR	3.6
3	F	123	VAL	3.6
1	C	132	ILE	3.5
1	A	383	GLU	3.5
3	D	219	TYR	3.5
1	A	211	TYR	3.5
2	B	305	LEU	3.5
1	C	149	GLN	3.5
1	C	410	LEU	3.5
2	B	322	ASN	3.4
1	C	193	ARG	3.4
1	C	211	TYR	3.4
4	E	206	LEU	3.4
3	F	122	PRO	3.4
3	F	107	ALA	3.4
1	A	94	PRO	3.3
1	A	390	GLU	3.3
2	B	320	GLN	3.3
1	C	228	LEU	3.3
1	C	7	VAL	3.2
4	E	389	ASN	3.2
4	E	25	ILE	3.2
4	E	208	ARG	3.1
2	B	140	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	385	LEU	3.1
3	F	172	ASP	3.1
1	C	418	TRP	3.1
1	A	299	PHE	3.0
3	D	171	PHE	3.0
3	D	111	SER	3.0
1	A	303	LYS	3.0
1	C	216	LYS	3.0
2	B	97	ALA	3.0
3	F	152	GLN	3.0
1	C	214	LEU	2.9
1	C	10	ALA	2.9
3	F	226	LYS	2.9
2	B	118	TYR	2.9
4	E	210	LEU	2.9
1	A	418	TRP	2.9
3	D	326	PHE	2.9
3	D	306	ASN	2.9
1	A	407	LEU	2.9
3	F	136	ILE	2.8
3	F	180	THR	2.8
2	B	152	GLN	2.8
1	C	217	ASN	2.8
3	D	133	HIS	2.8
1	C	94	PRO	2.8
1	A	410	LEU	2.8
3	F	79	LEU	2.8
1	C	215	GLU	2.8
4	E	9	HIS	2.8
4	E	94	PRO	2.7
2	B	135	THR	2.7
1	A	419	GLN	2.7
1	C	330	HIS	2.7
1	C	354	TYR	2.7
1	A	129	THR	2.7
1	C	420	SER	2.7
3	F	60	LYS	2.7
4	E	149	GLN	2.7
1	A	291	PHE	2.7
3	D	115	TYR	2.7
2	B	325	ASP	2.6
4	E	414	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	229	ILE	2.6
3	F	323	ARG	2.6
4	E	331	GLU	2.6
1	A	406	ALA	2.6
3	F	321	LYS	2.6
4	E	412	ALA	2.6
1	A	416	GLU	2.6
3	D	216	ILE	2.5
4	E	407	LEU	2.5
1	A	5	LYS	2.5
2	B	112	ARG	2.5
3	F	89	ILE	2.5
2	B	310	GLU	2.5
3	D	337	LYS	2.5
4	E	381	LYS	2.5
4	E	355	THR	2.5
4	E	354	TYR	2.5
3	F	306	ASN	2.5
2	B	115	TYR	2.5
1	A	384	HIS	2.5
4	E	120	CYS	2.4
2	B	172	ASP	2.4
3	F	352	HIS	2.4
4	E	10	ALA	2.4
3	D	209	THR	2.4
3	F	283	GLU	2.4
1	A	28	ILE	2.4
2	B	346	ILE	2.4
4	E	218	LEU	2.4
1	A	388	PHE	2.4
1	C	30	LYS	2.4
2	B	307	GLU	2.4
2	B	364	ASP	2.4
1	A	9	HIS	2.4
1	A	131	ARG	2.4
3	F	148	PHE	2.4
3	D	314	GLU	2.4
3	D	330	THR	2.4
3	F	310	GLU	2.4
1	A	420	SER	2.4
3	D	308	PHE	2.4
3	D	147	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	308	PHE	2.3
4	E	24	VAL	2.3
3	F	82	SER	2.3
3	D	355	LEU	2.3
4	E	211	TYR	2.3
2	B	317	GLU	2.3
3	D	284	GLU	2.3
4	E	383	GLU	2.3
4	E	406	ALA	2.3
4	E	167	SER	2.3
4	E	3	ILE	2.3
4	E	150	LEU	2.3
1	A	216	LYS	2.3
4	E	205	LYS	2.3
1	C	296	GLU	2.3
4	E	254	PRO	2.3
3	F	95	GLN	2.3
4	E	330	HIS	2.3
4	E	73	LEU	2.3
4	E	34	ASP	2.3
1	C	388	PHE	2.3
3	F	110	ASN	2.2
1	C	12	THR	2.2
3	F	200	THR	2.2
3	D	113	GLN	2.2
3	F	142	ILE	2.2
3	D	347	ARG	2.2
2	B	141	TYR	2.2
1	C	382	GLU	2.2
1	A	71	GLN	2.2
1	C	413	GLN	2.2
3	F	229	ILE	2.2
1	C	390	GLU	2.2
2	B	345	VAL	2.2
2	B	321	LYS	2.2
3	F	363	THR	2.2
3	D	82	SER	2.2
3	D	218	PRO	2.2
1	C	353	LEU	2.1
4	E	228	LEU	2.1
4	E	382	GLU	2.1
3	D	221	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	170	ASN	2.1
1	A	326	LEU	2.1
1	A	8	GLU	2.1
1	C	331	GLU	2.1
1	C	383	GLU	2.1
3	D	307	GLU	2.1
4	E	131	ARG	2.1
3	F	87	ASN	2.1
1	A	210	LEU	2.1
1	A	355	THR	2.1
1	C	355	THR	2.1
3	F	116	ARG	2.1
1	C	381	LYS	2.1
1	C	15	SER	2.1
4	E	71	GLN	2.1
2	B	116	ARG	2.1
1	A	396	ASP	2.1
2	B	352	HIS	2.1
1	A	66	PHE	2.0
2	B	123	VAL	2.0
2	B	319	LEU	2.0
1	C	95	LYS	2.0
1	C	395	ILE	2.0
1	C	380	SER	2.0
3	F	174	SER	2.0
3	D	88	VAL	2.0
1	C	213	LYS	2.0
3	D	363	THR	2.0
4	E	119	SER	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 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
7	PEG	C	504	7/7	0.64	0.17	110,132,133,133	0
5	EDO	A	502	4/4	0.76	0.18	121,145,146,146	0
5	EDO	C	502	4/4	0.77	0.20	92,111,111,111	0
5	EDO	E	503	4/4	0.78	0.28	112,134,135,135	0
5	EDO	E	501	4/4	0.79	0.26	83,99,101,102	0
5	EDO	E	502	4/4	0.79	0.12	99,119,120,120	0
5	EDO	E	504	4/4	0.82	0.24	78,94,96,97	0
5	EDO	A	501	4/4	0.82	0.20	124,148,149,150	0
6	TRS	E	506	8/8	0.83	0.18	98,119,121,121	0
5	EDO	D	401	4/4	0.83	0.28	107,129,136,136	0
7	PEG	C	505	7/7	0.83	0.21	133,160,160,160	0
5	EDO	C	501	4/4	0.85	0.18	85,103,105,105	0
5	EDO	D	402	4/4	0.87	0.27	98,118,118,119	0
5	EDO	E	505	4/4	0.91	0.28	89,107,108,108	0
6	TRS	C	503	8/8	0.92	0.14	88,108,111,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.