



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2017 – 08:36 PM EST

PDB ID : 2GX8
Title : The Crystal Structure of Bacillus cereus protein related to NIF3
Authors : Minasov, G.; Brunzelle, J.S.; Shuvalova, L.; Vorontsov, I.I.; Collart, F.R.;
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(MCSG)
Deposited on : 2006-05-08
Resolution : 2.20 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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

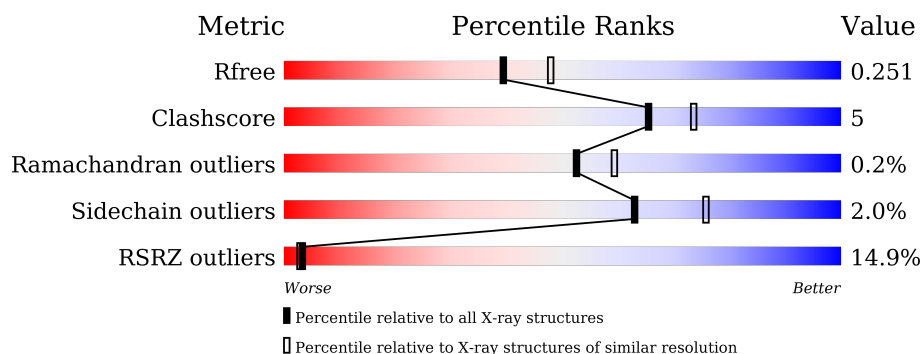
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	397	<div> <div>9%</div> <div>81%</div> <div>8%</div> <div>10%</div> </div>
1	B	397	<div> <div>17%</div> <div>81%</div> <div>10%</div> <div>9%</div> </div>
1	C	397	<div> <div>14%</div> <div>79%</div> <div>12%</div> <div>8%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EPE	A	376	-	-	-	X
3	EPE	B	376	-	-	-	X
3	EPE	C	376	-	-	-	X
3	EPE	C	377	-	-	-	X
4	TRS	A	378	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9083 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 NIF3-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	1	0
			2785	1777	477	520	11			
1	B	361	Total	C	N	O	S	0	0	0
			2788	1777	479	521	11			
1	C	364	Total	C	N	O	S	0	0	0
			2805	1786	482	526	11			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	CLONING ARTIFACT	GB 29897924
A	-22	HIS	-	EXPRESSION TAG	GB 29897924
A	-21	HIS	-	EXPRESSION TAG	GB 29897924
A	-20	HIS	-	EXPRESSION TAG	GB 29897924
A	-19	HIS	-	EXPRESSION TAG	GB 29897924
A	-18	HIS	-	EXPRESSION TAG	GB 29897924
A	-17	HIS	-	EXPRESSION TAG	GB 29897924
A	-16	SER	-	CLONING ARTIFACT	GB 29897924
A	-15	SER	-	CLONING ARTIFACT	GB 29897924
A	-14	GLY	-	CLONING ARTIFACT	GB 29897924
A	-13	VAL	-	CLONING ARTIFACT	GB 29897924
A	-12	ASP	-	CLONING ARTIFACT	GB 29897924
A	-11	LEU	-	CLONING ARTIFACT	GB 29897924
A	-10	GLY	-	CLONING ARTIFACT	GB 29897924
A	-9	THR	-	CLONING ARTIFACT	GB 29897924
A	-8	GLU	-	CLONING ARTIFACT	GB 29897924
A	-7	ASN	-	CLONING ARTIFACT	GB 29897924
A	-6	LEU	-	CLONING ARTIFACT	GB 29897924
A	-5	TYR	-	CLONING ARTIFACT	GB 29897924
A	-4	PHE	-	CLONING ARTIFACT	GB 29897924
A	-3	GLN	-	CLONING ARTIFACT	GB 29897924
A	-2	SER	-	CLONING ARTIFACT	GB 29897924
A	-1	ASN	-	CLONING ARTIFACT	GB 29897924

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	CLONING ARTIFACT	GB 29897924
B	-23	MET	-	CLONING ARTIFACT	GB 29897924
B	-22	HIS	-	EXPRESSION TAG	GB 29897924
B	-21	HIS	-	EXPRESSION TAG	GB 29897924
B	-20	HIS	-	EXPRESSION TAG	GB 29897924
B	-19	HIS	-	EXPRESSION TAG	GB 29897924
B	-18	HIS	-	EXPRESSION TAG	GB 29897924
B	-17	HIS	-	EXPRESSION TAG	GB 29897924
B	-16	SER	-	CLONING ARTIFACT	GB 29897924
B	-15	SER	-	CLONING ARTIFACT	GB 29897924
B	-14	GLY	-	CLONING ARTIFACT	GB 29897924
B	-13	VAL	-	CLONING ARTIFACT	GB 29897924
B	-12	ASP	-	CLONING ARTIFACT	GB 29897924
B	-11	LEU	-	CLONING ARTIFACT	GB 29897924
B	-10	GLY	-	CLONING ARTIFACT	GB 29897924
B	-9	THR	-	CLONING ARTIFACT	GB 29897924
B	-8	GLU	-	CLONING ARTIFACT	GB 29897924
B	-7	ASN	-	CLONING ARTIFACT	GB 29897924
B	-6	LEU	-	CLONING ARTIFACT	GB 29897924
B	-5	TYR	-	CLONING ARTIFACT	GB 29897924
B	-4	PHE	-	CLONING ARTIFACT	GB 29897924
B	-3	GLN	-	CLONING ARTIFACT	GB 29897924
B	-2	SER	-	CLONING ARTIFACT	GB 29897924
B	-1	ASN	-	CLONING ARTIFACT	GB 29897924
B	0	ALA	-	CLONING ARTIFACT	GB 29897924
C	-23	MET	-	CLONING ARTIFACT	GB 29897924
C	-22	HIS	-	EXPRESSION TAG	GB 29897924
C	-21	HIS	-	EXPRESSION TAG	GB 29897924
C	-20	HIS	-	EXPRESSION TAG	GB 29897924
C	-19	HIS	-	EXPRESSION TAG	GB 29897924
C	-18	HIS	-	EXPRESSION TAG	GB 29897924
C	-17	HIS	-	EXPRESSION TAG	GB 29897924
C	-16	SER	-	CLONING ARTIFACT	GB 29897924
C	-15	SER	-	CLONING ARTIFACT	GB 29897924
C	-14	GLY	-	CLONING ARTIFACT	GB 29897924
C	-13	VAL	-	CLONING ARTIFACT	GB 29897924
C	-12	ASP	-	CLONING ARTIFACT	GB 29897924
C	-11	LEU	-	CLONING ARTIFACT	GB 29897924
C	-10	GLY	-	CLONING ARTIFACT	GB 29897924
C	-9	THR	-	CLONING ARTIFACT	GB 29897924
C	-8	GLU	-	CLONING ARTIFACT	GB 29897924
C	-7	ASN	-	CLONING ARTIFACT	GB 29897924

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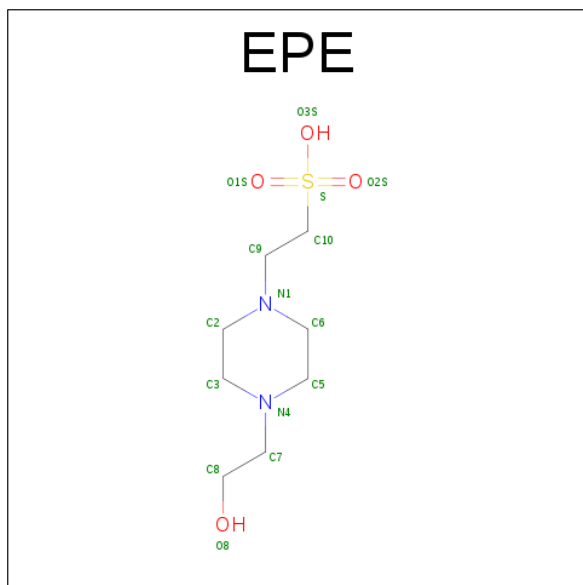
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	LEU	-	CLONING ARTIFACT	GB 29897924
C	-5	TYR	-	CLONING ARTIFACT	GB 29897924
C	-4	PHE	-	CLONING ARTIFACT	GB 29897924
C	-3	GLN	-	CLONING ARTIFACT	GB 29897924
C	-2	SER	-	CLONING ARTIFACT	GB 29897924
C	-1	ASN	-	CLONING ARTIFACT	GB 29897924
C	0	ALA	-	CLONING ARTIFACT	GB 29897924

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



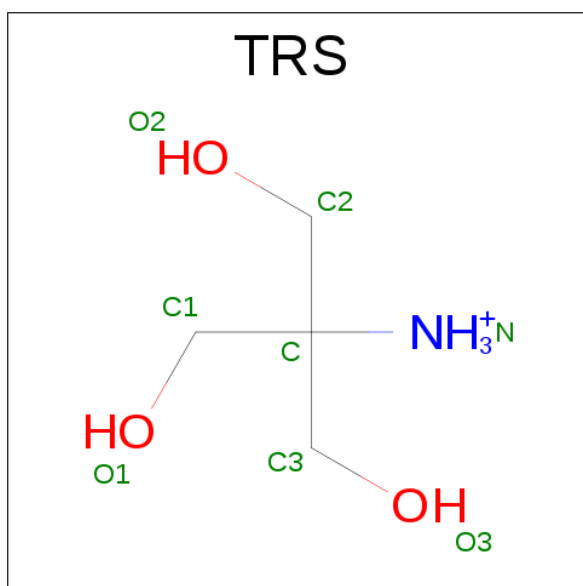
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

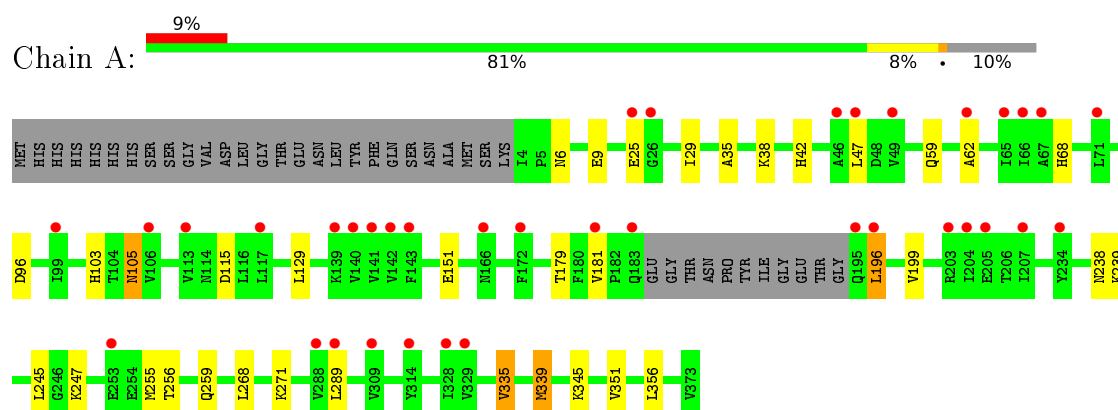
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	233	Total	O	0	0
			233	233		
5	B	220	Total	O	0	0
			220	220		
5	C	163	Total	O	0	0
			163	163		

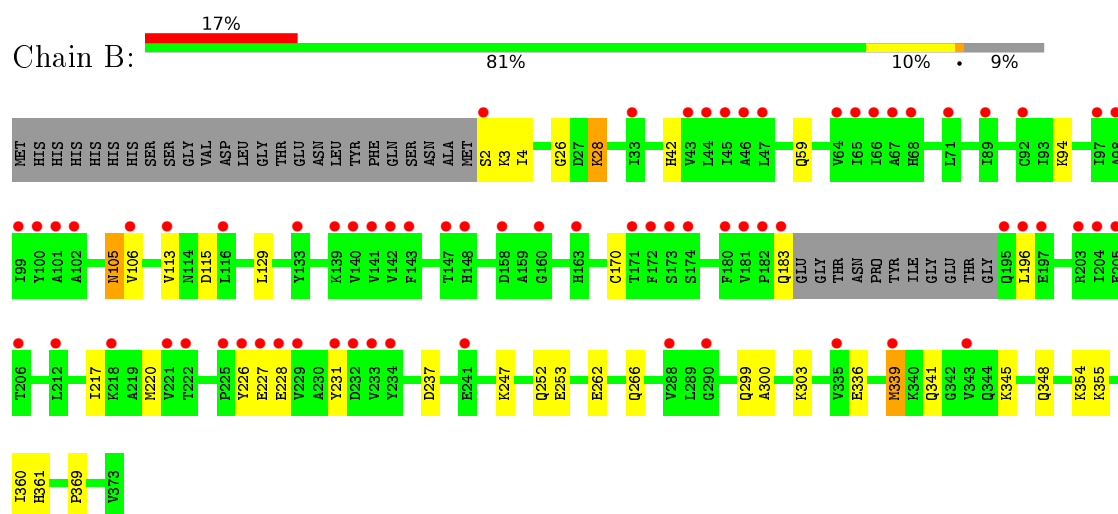
3 Residue-property plots

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

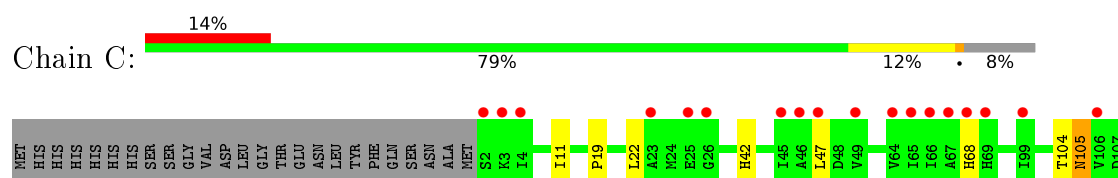
• Molecule 1: NIF3-related protein

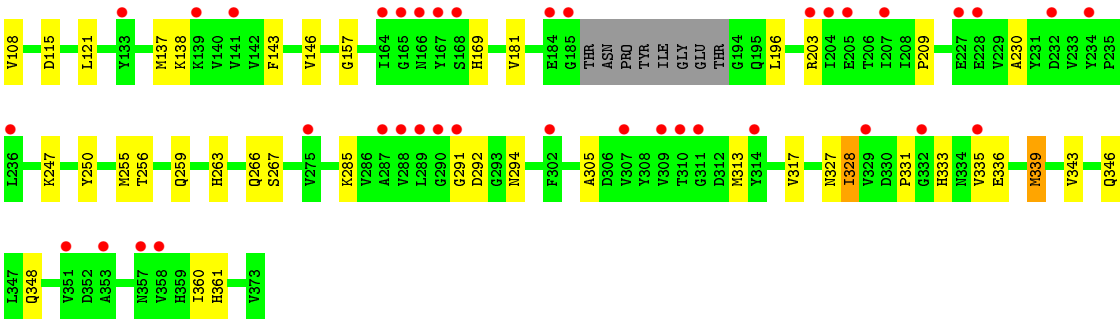


• Molecule 1: NIF3-related protein



• Molecule 1: NIF3-related protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.04Å 95.04Å 260.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.96 – 2.20 28.07 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (28.96-2.20) 97.8 (28.07-2.20)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.261 0.191 , 0.251	Depositor DCC
R_{free} test set	3421 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9083	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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: ZN, EPE, 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	0.66	0/2837	0.83	0/3838
1	B	0.75	1/2839 (0.0%)	0.84	1/3839 (0.0%)
1	C	0.65	0/2856	0.79	0/3861
All	All	0.68	1/8532 (0.0%)	0.82	1/11538 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	183	GLN	C-O	17.40	1.56	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	ASP	CB-CG-OD1	6.07	123.77	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2785	0	2815	24	0
1	B	2788	0	2825	27	0
1	C	2805	0	2837	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	30	0	34	0	0
3	B	15	0	17	1	0
3	C	30	0	36	1	0
4	A	8	0	11	2	0
5	A	233	0	0	3	0
5	B	220	0	0	3	0
5	C	163	0	0	2	0
All	All	9083	0	8575	85	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 5.

All (85) 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:105:ASN:H	1:B:105:ASN:HD22	1.08	0.99
1:A:105:ASN:HD22	1:A:105:ASN:H	1.06	0.98
1:A:105:ASN:HD22	1:A:105:ASN:N	1.81	0.77
1:C:105:ASN:HD22	1:C:105:ASN:H	1.30	0.76
1:B:348:GLN:HE22	1:B:360:ILE:H	1.33	0.74
1:C:348:GLN:HE22	1:C:360:ILE:H	1.34	0.72
1:A:105:ASN:ND2	1:A:105:ASN:H	1.86	0.71
1:C:137:MET:HE2	1:C:209:PRO:HA	1.74	0.69
1:C:115:ASP:OD1	1:C:247:LYS:HE3	1.92	0.69
1:C:143:PHE:CE2	1:C:203:ARG:HG3	2.27	0.69
1:B:59:GLN:HG3	5:B:460:HOH:O	1.95	0.67
1:B:26:GLY:O	1:B:28:LYS:HE3	1.96	0.66
1:B:105:ASN:ND2	1:B:105:ASN:H	1.87	0.66
1:B:299:GLN:HE21	1:B:303:LYS:HE2	1.59	0.66
5:A:553:HOH:O	1:B:170:CYS:SG	2.54	0.65
1:B:105:ASN:N	1:B:105:ASN:HD22	1.88	0.63
1:B:217:ILE:HD11	1:B:231:TYR:CE1	2.33	0.62
1:C:263:HIS:O	1:C:267:SER:HB2	2.00	0.61
1:A:115:ASP:OD1	1:A:247:LYS:HE3	2.01	0.61
1:C:138:LYS:HE2	5:C:498:HOH:O	2.01	0.59
1:A:6:ASN:HB2	1:A:9:GLU:HG2	1.84	0.59
1:B:262:GLU:O	1:B:266:GLN:HG2	2.03	0.59
1:B:348:GLN:NE2	1:B:360:ILE:H	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:MET:HB3	1:C:259:GLN:HG3	1.85	0.57
1:A:255:MET:HB2	1:A:259:GLN:HG3	1.86	0.57
1:A:151:GLU:HG3	5:A:420:HOH:O	2.06	0.55
1:A:351:VAL:HG22	1:A:356:LEU:HB2	1.88	0.55
1:C:291:GLY:HA2	1:C:333:HIS:CD2	2.43	0.54
1:B:94:LYS:HE3	5:B:482:HOH:O	2.06	0.54
1:B:106:VAL:HG12	1:B:113:VAL:HG23	1.88	0.53
1:C:105:ASN:N	1:C:105:ASN:HD22	2.04	0.53
1:C:42:HIS:HD2	1:C:361:HIS:NE2	2.06	0.53
1:A:42:HIS:HB2	1:A:62:ALA:HA	1.91	0.53
1:A:38:LYS:NZ	1:A:96:ASP:O	2.42	0.52
1:C:181:VAL:HG22	1:C:196:LEU:HA	1.92	0.52
1:B:217:ILE:HA	1:B:220:MET:HE3	1.93	0.51
1:B:226:TYR:C	1:B:228:GLU:H	2.13	0.51
1:B:115:ASP:OD1	1:B:247:LYS:HE2	2.10	0.51
1:B:217:ILE:HD11	1:B:231:TYR:CZ	2.46	0.50
1:B:129:LEU:HD11	1:B:300:ALA:HA	1.93	0.50
1:B:26:GLY:O	1:B:28:LYS:CE	2.59	0.50
1:C:263:HIS:O	1:C:267:SER:CB	2.59	0.50
1:C:285:LYS:HG3	1:C:305:ALA:HA	1.93	0.50
1:A:47:LEU:HD12	1:A:68:HIS:HB3	1.95	0.48
1:A:35:ALA:O	1:A:38:LYS:HD2	2.13	0.48
1:C:256:THR:OG1	1:C:259:GLN:HG2	2.13	0.48
1:B:105:ASN:ND2	1:B:105:ASN:N	2.56	0.48
1:C:146:VAL:HG23	5:C:499:HOH:O	2.13	0.48
1:A:29:ILE:HG22	1:A:103:HIS:H	1.79	0.48
1:C:348:GLN:NE2	1:C:360:ILE:H	2.08	0.48
1:B:2:SER:HA	1:B:355:LYS:O	2.13	0.47
1:B:341:GLN:O	1:B:345:LYS:HG3	2.15	0.47
3:B:376:EPE:O3S	5:B:394:HOH:O	2.20	0.47
1:C:250:TYR:CE2	1:C:285:LYS:HB3	2.49	0.47
1:A:181:VAL:HG22	1:A:196:LEU:HA	1.96	0.47
1:A:68:HIS:HB2	1:A:339:MET:CE	2.45	0.46
1:C:292:ASP:OD2	1:C:294:ASN:ND2	2.48	0.46
1:A:179:THR:O	1:B:170:CYS:HA	2.16	0.45
1:A:239:LYS:H	4:A:378:TRS:H31	1.81	0.45
1:C:121:LEU:O	1:C:263:HIS:HE1	2.00	0.45
1:C:104:THR:O	1:C:108:VAL:HG23	2.17	0.45
1:A:238:ASN:HA	4:A:378:TRS:H31	1.98	0.45
1:B:252:GLN:HG3	1:B:253:GLU:HG2	1.97	0.44
1:C:343:VAL:HA	1:C:346:GLN:HE21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:MET:HE1	1:C:317:VAL:HG12	1.99	0.44
1:C:230:ALA:HB3	3:C:377:EPE:H22	1.99	0.43
1:B:3:LYS:HG3	1:B:4:ILE:H	1.84	0.43
1:C:11:ILE:HA	1:C:11:ILE:HD13	1.83	0.43
1:C:313:MET:CE	1:C:317:VAL:HG12	2.49	0.43
1:C:336:GLU:O	1:C:339:MET:HB3	2.19	0.43
1:A:268:LEU:HB3	1:A:335:VAL:CG2	2.49	0.42
1:A:268:LEU:HD13	1:A:335:VAL:HG21	2.01	0.42
1:A:129:LEU:HB3	1:A:245:LEU:O	2.19	0.42
1:B:336:GLU:O	1:B:339:MET:HB3	2.18	0.42
1:C:105:ASN:H	1:C:105:ASN:ND2	2.08	0.42
1:C:157:GLY:HA3	1:C:169:HIS:CD2	2.55	0.42
1:C:327:ASN:C	1:C:328:ILE:HG12	2.40	0.42
1:A:105:ASN:N	1:A:105:ASN:ND2	2.55	0.41
1:A:256:THR:HG23	1:A:259:GLN:HE21	1.84	0.41
1:C:19:PRO:HG2	1:C:22:LEU:HG	2.03	0.41
1:C:331:PRO:HB2	1:C:335:VAL:HG11	2.02	0.41
1:C:138:LYS:HA	1:C:138:LYS:HD3	1.95	0.41
1:C:47:LEU:HD12	1:C:68:HIS:HB3	2.03	0.41
1:B:42:HIS:HD2	1:B:361:HIS:NE2	2.19	0.40
1:A:59:GLN:HB3	5:A:499:HOH:O	2.20	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	356/397 (90%)	347 (98%)	8 (2%)	1 (0%)	46	50
1	B	357/397 (90%)	347 (97%)	9 (2%)	1 (0%)	46	50
1	C	360/397 (91%)	349 (97%)	11 (3%)	0	100	100
All	All	1073/1191 (90%)	1043 (97%)	28 (3%)	2 (0%)	52	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	B	227	GLU

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	297/328 (90%)	289 (97%)	8 (3%)	52	64
1	B	298/328 (91%)	292 (98%)	6 (2%)	63	76
1	C	299/328 (91%)	295 (99%)	4 (1%)	76	87
All	All	894/984 (91%)	876 (98%)	18 (2%)	63	76

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	196	LEU
1	A	199	VAL
1	A	271	LYS
1	A	289	LEU
1	A	335	VAL
1	A	339	MET
1	A	345	LYS
1	B	28	LYS
1	B	105	ASN
1	B	196	LEU
1	B	339	MET
1	B	354	LYS
1	B	369	PRO
1	C	105	ASN
1	C	266	GLN
1	C	328	ILE
1	C	339	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	21	HIS
1	A	74	ASN
1	A	105	ASN
1	A	259	GLN
1	A	263	HIS
1	A	341	GLN
1	B	42	HIS
1	B	95	ASN
1	B	105	ASN
1	B	169	HIS
1	B	195	GLN
1	B	213	GLN
1	B	252	GLN
1	B	299	GLN
1	B	327	ASN
1	B	341	GLN
1	B	344	GLN
1	B	346	GLN
1	B	348	GLN
1	C	42	HIS
1	C	59	GLN
1	C	105	ASN
1	C	125	ASN
1	C	148	HIS
1	C	163	HIS
1	C	183	GLN
1	C	195	GLN
1	C	263	HIS
1	C	266	GLN
1	C	341	GLN
1	C	346	GLN
1	C	348	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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	EPE	A	376	-	15,15,15	0.89	1 (6%)	19,20,20	2.01	7 (36%)
3	EPE	A	377	-	15,15,15	0.94	1 (6%)	19,20,20	2.46	5 (26%)
4	TRS	A	378	-	7,7,7	1.64	2 (28%)	9,9,9	1.77	1 (11%)
3	EPE	B	376	-	15,15,15	0.94	1 (6%)	19,20,20	1.97	5 (26%)
3	EPE	C	376	-	15,15,15	1.11	1 (6%)	19,20,20	2.32	8 (42%)
3	EPE	C	377	-	15,15,15	0.69	1 (6%)	19,20,20	2.15	7 (36%)

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	EPE	A	376	-	-	0/9/19/19	0/1/1/1
3	EPE	A	377	-	-	0/9/19/19	0/1/1/1
4	TRS	A	378	-	-	0/9/9/9	0/0/0/0
3	EPE	B	376	-	-	0/9/19/19	0/1/1/1
3	EPE	C	376	-	-	0/9/19/19	0/1/1/1
3	EPE	C	377	-	-	0/9/19/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	378	TRS	C-N	-3.28	1.46	1.50
4	A	378	TRS	O2-C2	-2.54	1.34	1.42
3	C	377	EPE	C10-S	2.04	1.80	1.77
3	A	376	EPE	C10-S	3.01	1.82	1.77
3	A	377	EPE	C10-S	3.27	1.82	1.77
3	B	376	EPE	C10-S	3.28	1.82	1.77
3	C	376	EPE	C10-S	3.88	1.83	1.77

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	377	EPE	C5-C6-N1	-2.88	105.03	110.65
3	C	377	EPE	C3-C2-N1	-2.66	105.46	110.65
3	C	377	EPE	O2S-S-O1S	-2.27	107.56	113.96
3	B	376	EPE	O3S-S-O1S	-2.17	106.45	111.26
3	A	376	EPE	C9-N1-C6	-2.17	106.52	111.25
3	C	376	EPE	C9-N1-C6	-2.10	106.69	111.25
3	C	376	EPE	C9-N1-C2	-2.07	106.75	111.25
3	A	376	EPE	C6-N1-C2	2.04	113.44	108.87
3	C	376	EPE	C2-C3-N4	2.17	114.89	110.65
3	A	376	EPE	O3S-S-C10	2.33	109.83	104.99
3	A	377	EPE	O3S-S-C10	2.41	110.00	104.99
3	C	376	EPE	O3S-S-C10	2.46	110.10	104.99
3	A	376	EPE	C7-N4-C3	2.52	116.74	111.25
3	B	376	EPE	C7-N4-C3	2.62	116.95	111.25
3	C	377	EPE	C7-N4-C3	2.72	117.18	111.25
3	C	377	EPE	O1S-S-C10	2.97	108.97	106.87
3	B	376	EPE	C5-N4-C3	3.13	115.88	108.87
3	C	376	EPE	C7-N4-C3	3.19	118.19	111.25
3	A	376	EPE	O2S-S-C10	3.42	109.28	106.87
3	C	376	EPE	C7-N4-C5	3.44	118.74	111.25
3	C	377	EPE	C7-N4-C5	3.61	119.11	111.25
3	A	376	EPE	O1S-S-C10	3.66	109.46	106.87
3	A	376	EPE	C5-N4-C3	3.90	117.61	108.87
3	B	376	EPE	O3S-S-C10	3.97	113.23	104.99
3	A	377	EPE	O2S-S-C10	4.05	109.73	106.87
3	C	376	EPE	C5-N4-C3	4.09	118.03	108.87
3	A	377	EPE	C5-N4-C3	4.44	118.80	108.87
4	A	378	TRS	O2-C2-C	4.65	121.97	110.92
3	A	377	EPE	C7-N4-C5	4.68	121.44	111.25
3	B	376	EPE	C7-N4-C5	4.93	121.98	111.25
3	A	377	EPE	O1S-S-C10	5.57	110.80	106.87
3	C	377	EPE	C5-N4-C3	5.57	121.35	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	376	EPE	O1S-S-C10	6.25	111.28	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	378	TRS	2	0
3	B	376	EPE	1	0
3	C	377	EPE	1	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	359/397 (90%)	0.44	37 (10%) 9 8	44, 57, 66, 72	0
1	B	361/397 (90%)	0.94	69 (19%) 2 1	44, 57, 68, 79	0
1	C	364/397 (91%)	0.69	56 (15%) 3 2	41, 56, 68, 88	0
All	All	1084/1191 (91%)	0.69	162 (14%) 3 3	41, 57, 68, 88	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	141	VAL	9.1
1	B	196	LEU	8.2
1	B	183	GLN	7.2
1	B	181	VAL	7.2
1	C	2	SER	7.2
1	B	180	PHE	6.8
1	B	182	PRO	6.7
1	C	25	GLU	6.2
1	B	195	GLN	5.9
1	B	2	SER	5.8
1	B	204	ILE	5.8
1	B	66	ILE	5.5
1	C	234	TYR	5.4
1	B	203	ARG	5.4
1	A	141	VAL	5.3
1	C	184	GLU	5.2
1	B	67	ALA	5.2
1	C	185	GLY	5.0
1	C	47	LEU	5.0
1	C	167	TYR	4.8
1	C	141	VAL	4.7
1	A	49	VAL	4.7
1	B	205	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	232	ASP	4.5
1	B	197	GLU	4.5
1	B	65	ILE	4.4
1	A	196	LEU	4.4
1	A	253	GLU	4.3
1	B	234	TYR	4.3
1	B	142	VAL	4.2
1	B	45	ILE	4.2
1	B	172	PHE	4.2
1	A	203	ARG	4.1
1	B	140	VAL	4.1
1	C	26	GLY	4.1
1	A	309	VAL	4.0
1	B	106	VAL	4.0
1	C	164	ILE	4.0
1	C	46	ALA	4.0
1	B	226	TYR	3.9
1	C	203	ARG	3.9
1	B	143	PHE	3.8
1	C	165	GLY	3.8
1	A	143	PHE	3.8
1	C	309	VAL	3.8
1	A	25	GLU	3.7
1	C	289	LEU	3.7
1	B	102	ALA	3.7
1	B	99	ILE	3.7
1	B	113	VAL	3.7
1	C	66	ILE	3.7
1	A	113	VAL	3.7
1	C	49	VAL	3.7
1	B	46	ALA	3.6
1	A	65	ILE	3.6
1	B	158	ASP	3.6
1	B	221	VAL	3.6
1	C	99	ILE	3.5
1	B	231	TYR	3.5
1	B	47	LEU	3.5
1	B	228	GLU	3.5
1	B	101	ALA	3.5
1	B	68	HIS	3.5
1	A	142	VAL	3.4
1	B	227	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	183	GLN	3.4
1	B	174	SER	3.3
1	B	100	TYR	3.3
1	B	343	VAL	3.3
1	C	67	ALA	3.3
1	C	227	GLU	3.2
1	A	204	ILE	3.2
1	C	205	GLU	3.2
1	B	33	ILE	3.1
1	B	171	THR	3.1
1	C	4	ILE	3.1
1	B	222	THR	3.1
1	B	44	LEU	3.1
1	B	148	HIS	3.0
1	B	206	THR	3.0
1	A	205	GLU	3.0
1	A	234	TYR	3.0
1	B	339	MET	3.0
1	A	140	VAL	3.0
1	A	195	GLN	3.0
1	A	47	LEU	2.9
1	B	212	LEU	2.9
1	C	168	SER	2.9
1	B	173	SER	2.9
1	C	45	ILE	2.8
1	C	275	VAL	2.8
1	C	139	LYS	2.8
1	C	65	ILE	2.8
1	C	166	ASN	2.7
1	C	207	ILE	2.7
1	C	357	ASN	2.7
1	C	302	PHE	2.7
1	B	160	GLY	2.7
1	C	133	TYR	2.6
1	C	291	GLY	2.6
1	A	172	PHE	2.6
1	C	232	ASP	2.6
1	A	289	LEU	2.6
1	B	288	VAL	2.6
1	A	288	VAL	2.6
1	B	233	VAL	2.6
1	A	314[A]	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	68	HIS	2.6
1	C	307	VAL	2.5
1	C	329	VAL	2.5
1	C	290	GLY	2.5
1	B	225	PRO	2.5
1	C	228	GLU	2.5
1	C	314	TYR	2.5
1	B	98	ALA	2.5
1	A	62	ALA	2.5
1	B	139	LYS	2.5
1	A	329	VAL	2.5
1	C	3	LYS	2.4
1	A	71	LEU	2.4
1	B	218	LYS	2.4
1	C	236	LEU	2.4
1	B	97	ILE	2.4
1	A	117	LEU	2.4
1	C	69	HIS	2.4
1	B	43	VAL	2.4
1	B	163	HIS	2.4
1	C	353	ALA	2.3
1	A	328	ILE	2.3
1	B	71	LEU	2.3
1	B	133	TYR	2.3
1	C	204	ILE	2.3
1	C	311	GLY	2.3
1	B	64	VAL	2.3
1	C	64	VAL	2.3
1	C	332	GLY	2.3
1	A	46	ALA	2.2
1	A	207	ILE	2.2
1	B	89	ILE	2.2
1	C	358	VAL	2.2
1	C	23	ALA	2.2
1	A	181	VAL	2.2
1	C	287	ALA	2.2
1	B	229	VAL	2.1
1	A	67	ALA	2.1
1	A	166	ASN	2.1
1	C	288	VAL	2.1
1	B	92	CYS	2.1
1	C	106	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	351	VAL	2.1
1	A	26	GLY	2.1
1	A	139	LYS	2.1
1	A	66	ILE	2.1
1	A	106	VAL	2.1
1	B	335	VAL	2.1
1	B	116	LEU	2.0
1	B	241	GLU	2.0
1	C	335	VAL	2.0
1	A	99	ILE	2.0
1	B	147	THR	2.0
1	B	290	GLY	2.0
1	C	310	THR	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
3	EPE	B	376	15/15	0.97	0.23	11.98	58,61,74,75	0
3	EPE	C	376	15/15	0.93	0.23	4.97	65,66,74,75	0
3	EPE	A	376	15/15	0.90	0.23	4.10	70,72,92,94	0
3	EPE	C	377	15/15	0.78	0.49	3.63	49,64,71,73	15
4	TRS	A	378	8/8	0.68	0.24	2.26	57,58,59,59	8
3	EPE	A	377	15/15	0.95	0.15	-0.89	71,73,76,77	0
2	ZN	A	375	1/1	0.97	0.15	-1.21	67,67,67,67	0
2	ZN	A	374	1/1	0.98	0.11	-1.69	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	B	374	1/1	0.99	0.09	-2.04	53,53,53,53	0
2	ZN	C	374	1/1	0.99	0.09	-2.83	55,55,55,55	0
2	ZN	C	375	1/1	0.99	0.10	-2.91	60,60,60,60	0
2	ZN	B	375	1/1	0.99	0.12	-3.68	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.