



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2016 – 11:10 PM EST

PDB ID : 5GYD
Title : Crystal Structure of Mdm12
Authors : Jeong, H.; Park, J.; Lee, C.
Deposited on : 2016-09-22
Resolution : 3.11 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

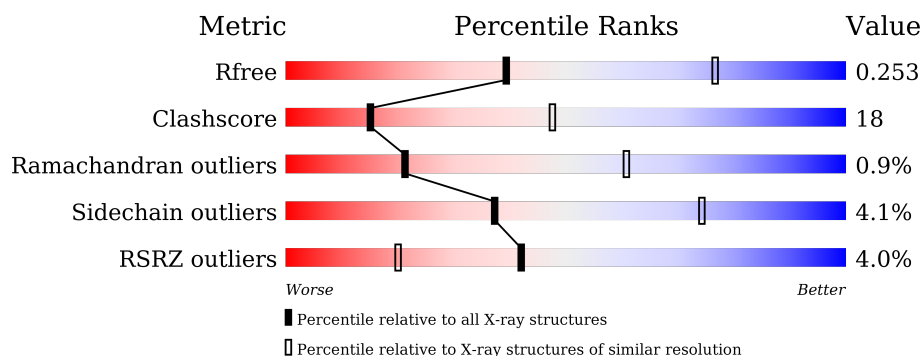
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	272	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>19%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	272	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>25%</div> <div>•</div> <div>18%</div> </div> </div>
1	C	272	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>17%</div> <div>•</div> <div>16%</div> </div> </div>
1	D	272	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>16%</div> <div>•</div> <div>18%</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEE	A	301	-	-	-	X
2	PEE	B	301	-	-	-	X
2	PEE	C	301	-	-	-	X
2	PEE	D	302	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7385 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.

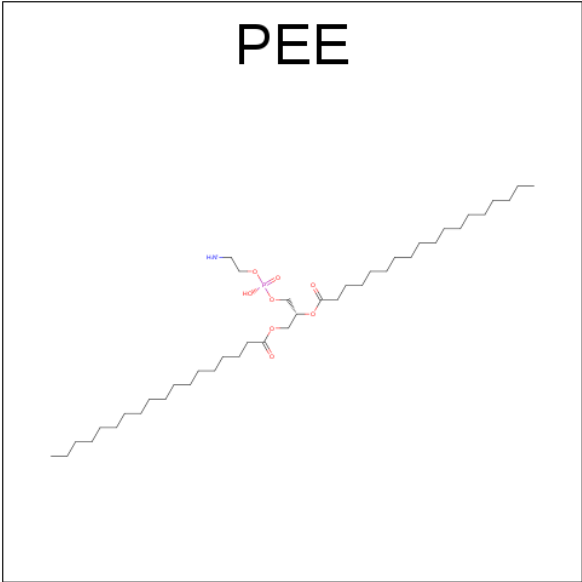
- Molecule 1 is a protein called Mitochondrial distribution and morphology protein 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1814	1168	290	350	6			
1	B	224	Total	C	N	O	S	0	0	0
			1791	1156	286	343	6			
1	C	228	Total	C	N	O	S	0	0	0
			1821	1173	291	351	6			
1	D	222	Total	C	N	O	S	0	0	0
			1774	1143	283	342	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q92328
B	0	GLY	-	expression tag	UNP Q92328
C	0	GLY	-	expression tag	UNP Q92328
D	0	GLY	-	expression tag	UNP Q92328

- Molecule 2 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₈₃NO₈P).

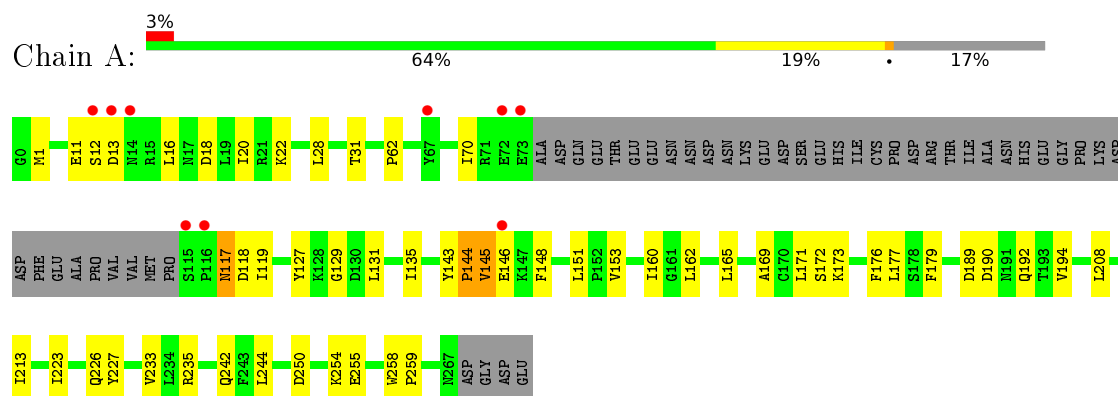


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
2	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
2	D	1	Total	C				0	0
			16	16					
2	D	1	Total	C				0	0
			16	16					

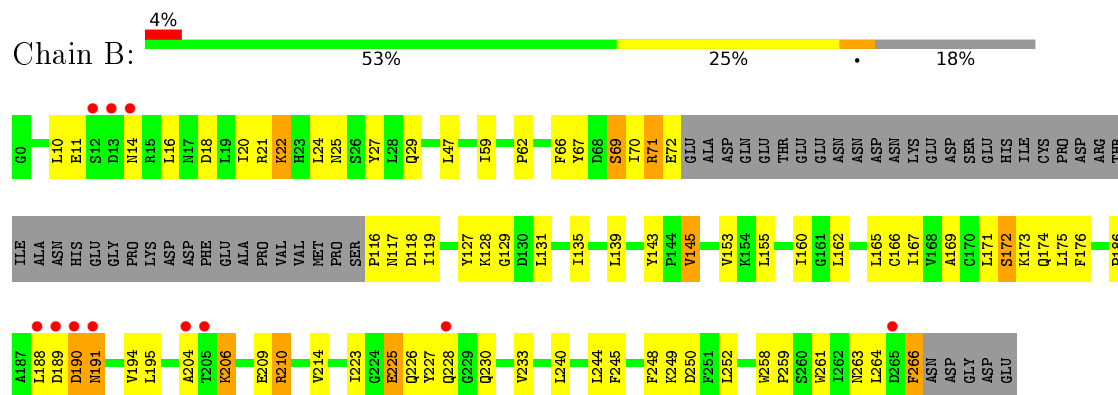
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

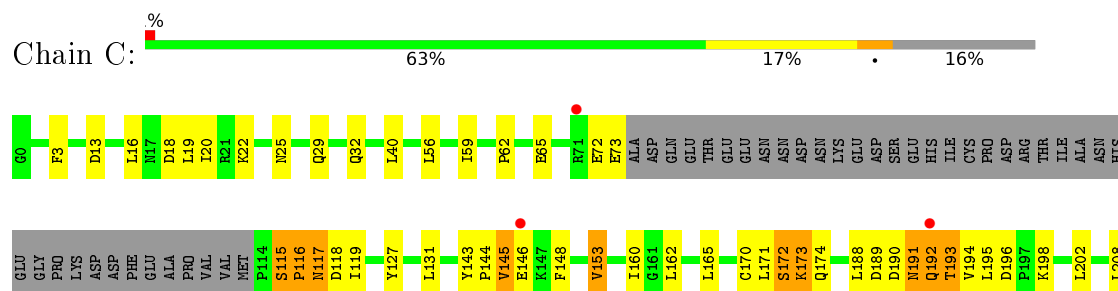
• Molecule 1: Mitochondrial distribution and morphology protein 12

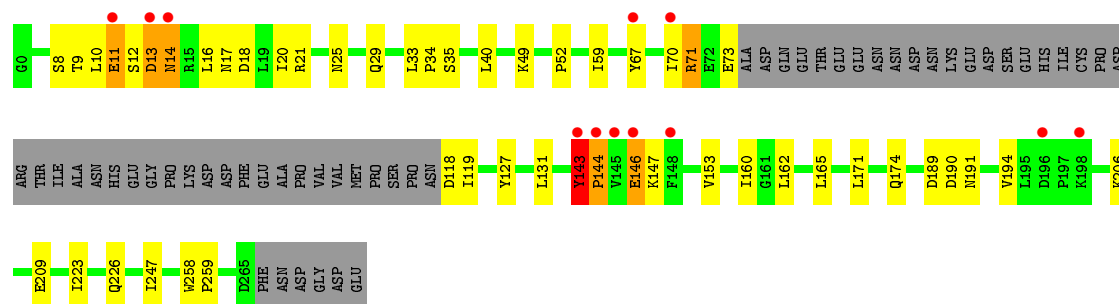


• Molecule 1: Mitochondrial distribution and morphology protein 12



• Molecule 1: Mitochondrial distribution and morphology protein 12





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	142.59 Å 219.07 Å 73.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.68 – 3.11 32.68 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.4 (32.68-3.11) 94.1 (32.68-3.11)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 3.12 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.214 , 0.254 0.215 , 0.253	Depositor DCC
R_{free} test set	1892 reflections (4.77%)	DCC
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.1	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	0.92	EDS
Total number of atoms	7385	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: PEE

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	0.29	0/1849	0.55	0/2509
1	B	0.34	0/1826	0.61	0/2477
1	C	0.31	0/1857	0.55	0/2520
1	D	0.33	0/1807	0.57	1/2451 (0.0%)
All	All	0.32	0/7339	0.57	1/9957 (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
1	B	0	1
1	C	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	143	TYR	C-N-CD	-6.19	106.97	120.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	225	GLU	Peptide
1	C	116	PRO	Peptide
1	C	117	ASN	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	1814	0	1821	60	0
1	B	1791	0	1805	81	0
1	C	1821	0	1829	55	0
1	D	1774	0	1788	49	0
2	A	51	0	82	8	0
2	B	51	0	82	18	0
2	C	51	0	82	15	0
2	D	32	0	62	0	0
All	All	7385	0	7551	262	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 18.

All (262) 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:116:PRO:CB	1:B:117:ASN:HA	1.40	1.46
2:A:301:PEE:H7	2:A:301:PEE:C11	1.56	1.31
1:D:143:TYR:CD2	1:D:144:PRO:HD2	1.69	1.25
1:C:195:LEU:O	1:C:202:LEU:CD1	1.85	1.22
2:A:301:PEE:C3	2:A:301:PEE:H14	1.71	1.18
1:B:116:PRO:HB2	1:B:117:ASN:HA	1.19	1.18
1:C:195:LEU:O	1:C:202:LEU:HD12	1.01	1.18
1:A:190:ASP:O	1:A:192:GLN:OE1	1.63	1.16
1:D:8:SER:O	1:D:12:SER:HB2	1.44	1.14
1:C:144:PRO:O	1:C:145:VAL:HG12	1.47	1.14
1:B:116:PRO:HB3	1:B:117:ASN:HA	1.22	1.12
1:D:143:TYR:HD2	1:D:144:PRO:CD	1.63	1.11
1:B:116:PRO:CB	1:B:117:ASN:CA	2.30	1.09
1:C:192:GLN:O	1:C:193:THR:HG22	1.56	1.05
1:B:176:PHE:CE2	1:B:263:ASN:ND2	2.22	1.05
1:A:145:VAL:HG12	1:A:146:GLU:H	1.20	1.03
2:B:301:PEE:H2	2:B:301:PEE:H11	1.38	1.00
1:B:71:ARG:HG2	1:B:72:GLU:N	1.78	0.97
1:B:172:SER:N	1:B:173:LYS:HA	1.80	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:HG12	1:A:146:GLU:N	1.80	0.93
1:B:71:ARG:HG2	1:B:72:GLU:H	1.30	0.92
1:B:116:PRO:HB2	1:B:117:ASN:CA	1.96	0.91
1:D:143:TYR:HD2	1:D:144:PRO:HD2	1.10	0.91
1:A:119:ILE:CD1	1:B:173:LYS:NZ	2.35	0.90
2:B:301:PEE:H29	2:B:301:PEE:C43	2.01	0.89
2:C:301:PEE:O5	2:C:301:PEE:H14	1.73	0.88
1:B:176:PHE:CD2	1:B:263:ASN:ND2	2.42	0.88
2:C:301:PEE:H30	2:C:301:PEE:H76	1.56	0.87
1:A:119:ILE:HD12	1:B:173:LYS:NZ	1.90	0.86
1:D:14:ASN:O	1:D:17:ASN:HB3	1.75	0.86
2:B:301:PEE:H73	2:B:301:PEE:H29	1.55	0.85
1:A:145:VAL:CG1	1:A:146:GLU:H	1.89	0.84
2:C:301:PEE:C3	2:C:301:PEE:H12	2.08	0.83
1:D:10:LEU:C	1:D:11:GLU:HG3	1.97	0.81
1:A:255:GLU:OE1	2:A:301:PEE:H11	1.81	0.81
1:A:119:ILE:CD1	1:B:173:LYS:HZ1	1.95	0.80
1:D:143:TYR:CD2	1:D:144:PRO:CD	2.46	0.80
1:B:59:ILE:HD11	1:B:119:ILE:HD11	1.63	0.80
1:B:69:SER:HG	1:B:261:TRP:HZ2	1.26	0.80
1:C:192:GLN:O	1:C:193:THR:CG2	2.30	0.80
1:C:144:PRO:O	1:C:145:VAL:CG1	2.30	0.78
2:C:301:PEE:O5	2:C:301:PEE:H1	1.82	0.78
1:A:119:ILE:HD12	1:B:173:LYS:HZ2	1.49	0.77
1:C:165:LEU:HD13	1:C:194:VAL:HG21	1.66	0.77
2:C:301:PEE:H7	2:C:301:PEE:H12	1.67	0.77
2:C:301:PEE:O5	2:C:301:PEE:C11	2.32	0.77
1:C:19:LEU:HD23	2:C:301:PEE:H3	1.67	0.77
1:B:71:ARG:CG	1:B:72:GLU:N	2.48	0.76
2:B:301:PEE:H11	2:B:301:PEE:C1	2.14	0.76
1:A:119:ILE:HD11	1:B:173:LYS:HZ1	1.52	0.75
1:B:226:GLN:OE1	1:B:226:GLN:N	2.20	0.75
1:B:69:SER:OG	1:B:261:TRP:HZ2	1.68	0.75
1:A:119:ILE:HD11	1:B:173:LYS:NZ	2.02	0.74
1:A:119:ILE:CD1	1:B:173:LYS:HZ2	2.01	0.74
2:A:301:PEE:H7	2:A:301:PEE:H14	0.79	0.74
1:A:177:LEU:HD11	2:A:301:PEE:H31	1.70	0.73
1:B:225:GLU:HG3	1:B:228:GLN:N	2.04	0.73
2:B:301:PEE:H30	2:B:301:PEE:H79	1.70	0.72
2:B:301:PEE:H72	2:B:301:PEE:H29	1.72	0.72
1:C:143:TYR:HB3	1:C:144:PRO:CD	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:LEU:HD11	2:C:301:PEE:H56	1.72	0.71
1:D:143:TYR:CG	1:D:144:PRO:HD2	2.24	0.71
1:D:14:ASN:HD22	1:D:14:ASN:N	1.86	0.71
1:B:116:PRO:HB3	1:B:117:ASN:CA	2.09	0.71
2:C:301:PEE:H8	2:C:301:PEE:H12	1.73	0.70
1:A:117:ASN:C	1:A:117:ASN:OD1	2.30	0.70
1:C:59:ILE:HD11	1:C:119:ILE:HD11	1.75	0.69
1:A:255:GLU:OE1	2:A:301:PEE:C5	2.42	0.68
1:D:8:SER:O	1:D:12:SER:CB	2.34	0.67
1:B:225:GLU:HG3	1:B:228:GLN:H	1.57	0.67
2:B:301:PEE:C1	2:B:301:PEE:O4	2.42	0.67
1:D:59:ILE:HD11	1:D:119:ILE:HD11	1.76	0.67
1:B:172:SER:N	1:B:173:LYS:CA	2.56	0.66
1:C:118:ASP:HB3	1:C:170:CYS:O	1.94	0.66
1:D:147:LYS:HG2	1:D:147:LYS:O	1.95	0.66
1:C:145:VAL:HG22	1:C:146:GLU:H	1.61	0.66
2:A:301:PEE:C3	2:A:301:PEE:C11	2.41	0.66
1:D:143:TYR:HD2	1:D:144:PRO:HD3	1.60	0.65
1:B:264:LEU:HB3	1:B:266:PHE:CZ	2.31	0.65
1:C:62:PRO:HB3	1:C:171:LEU:HD11	1.77	0.65
1:B:188:LEU:CD2	1:B:194:VAL:HG12	2.27	0.65
1:B:155:LEU:HD13	1:B:244:LEU:HD22	1.79	0.64
1:C:145:VAL:HG12	1:C:148:PHE:HB2	1.80	0.64
1:C:191:ASN:OD1	1:C:191:ASN:N	2.30	0.64
1:A:143:TYR:HB3	1:A:144:PRO:HD3	1.80	0.63
1:B:16:LEU:HD11	2:B:301:PEE:H17	1.79	0.63
1:A:143:TYR:CD2	1:A:144:PRO:HD3	2.34	0.63
1:C:171:LEU:O	1:C:174:GLN:N	2.29	0.63
1:B:204:ALA:HA	1:B:210:ARG:NH2	2.13	0.62
1:C:143:TYR:HB3	1:C:144:PRO:HD2	1.80	0.62
2:B:301:PEE:H3	2:B:301:PEE:O4	1.98	0.62
1:B:206:LYS:HD2	1:B:209:GLU:OE1	2.00	0.62
1:A:189:ASP:O	1:A:190:ASP:CG	2.39	0.61
1:B:11:GLU:HB3	1:B:14:ASN:O	2.00	0.61
1:B:71:ARG:O	1:B:72:GLU:C	2.38	0.61
1:A:172:SER:N	1:A:173:LYS:HA	2.15	0.61
1:A:153:VAL:HG22	1:A:223:ILE:HG22	1.82	0.60
1:B:66:PHE:HA	1:B:69:SER:HB2	1.82	0.60
1:B:20:ILE:HG23	2:B:301:PEE:H48	1.82	0.60
1:B:24:LEU:HD11	1:B:248:PHE:HE1	1.66	0.60
1:A:143:TYR:HB3	1:A:144:PRO:CD	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:LEU:O	1:C:196:ASP:C	2.38	0.60
1:D:171:LEU:O	1:D:174:GLN:N	2.35	0.60
1:B:188:LEU:HD21	1:B:194:VAL:HG12	1.83	0.60
1:A:144:PRO:HG2	1:A:148:PHE:CD2	2.38	0.59
1:C:165:LEU:CD1	1:C:194:VAL:HG21	2.33	0.59
1:A:18:ASP:O	1:A:22:LYS:HG3	2.03	0.58
1:A:143:TYR:HD2	1:A:144:PRO:HD3	1.67	0.58
1:A:16:LEU:O	1:A:20:ILE:HG12	2.03	0.58
1:B:225:GLU:HA	1:B:227:TYR:H	1.67	0.58
1:B:204:ALA:HA	1:B:210:ARG:HH21	1.69	0.58
1:D:165:LEU:HD23	1:D:194:VAL:HG21	1.86	0.58
1:B:27:TYR:OH	1:B:250:ASP:OD2	2.21	0.58
1:A:189:ASP:O	1:A:190:ASP:CB	2.52	0.58
1:A:144:PRO:O	1:A:145:VAL:HB	2.05	0.57
1:D:14:ASN:O	1:D:17:ASN:N	2.37	0.57
1:B:165:LEU:HD23	1:B:194:VAL:HG11	1.87	0.57
1:C:192:GLN:O	1:C:193:THR:CB	2.53	0.56
1:A:1:MET:SD	2:B:301:PEE:H74	2.46	0.56
1:C:143:TYR:CB	1:C:144:PRO:CD	2.83	0.56
1:A:28:LEU:O	1:A:31:THR:OG1	2.22	0.56
1:A:135:ILE:HD12	1:A:244:LEU:HD21	1.87	0.56
1:C:29:GLN:NE2	1:C:40:LEU:O	2.38	0.56
1:C:56:LEU:HD13	1:D:10:LEU:HD22	1.87	0.55
1:D:14:ASN:O	1:D:17:ASN:CB	2.50	0.55
1:B:131:LEU:HD23	1:B:160:ILE:HD12	1.88	0.55
1:A:165:LEU:HD23	1:A:194:VAL:HG21	1.89	0.55
1:A:190:ASP:OD1	1:A:190:ASP:C	2.45	0.54
1:B:47:LEU:HD12	1:B:131:LEU:HD13	1.89	0.54
1:A:144:PRO:O	1:A:148:PHE:HB2	2.06	0.54
1:B:139:LEU:HD13	1:B:240:LEU:HD22	1.89	0.54
2:A:301:PEE:H79	2:A:301:PEE:H30	1.90	0.53
1:B:67:TYR:HA	1:B:70:ILE:HD12	1.90	0.53
1:A:143:TYR:CB	1:A:144:PRO:HD3	2.38	0.53
2:B:301:PEE:H30	2:B:301:PEE:C46	2.38	0.53
1:A:70:ILE:HD11	1:A:176:PHE:HZ	1.74	0.53
1:A:145:VAL:CG1	1:A:146:GLU:N	2.50	0.53
1:A:11:GLU:O	1:A:11:GLU:HG3	2.10	0.52
1:B:135:ILE:HD12	1:B:244:LEU:HD21	1.90	0.52
1:B:72:GLU:OE1	1:B:72:GLU:HA	2.10	0.52
1:D:143:TYR:CB	1:D:144:PRO:HD2	2.39	0.52
1:C:250:ASP:OD1	1:C:254:LYS:NZ	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:ASN:ND2	1:D:14:ASN:N	2.57	0.52
1:A:250:ASP:O	1:A:254:LYS:HG3	2.10	0.52
1:B:166:CYS:SG	1:B:167:ILE:N	2.83	0.52
1:A:62:PRO:HB3	1:A:171:LEU:HD11	1.93	0.51
1:C:20:ILE:HD12	2:C:301:PEE:C34	2.40	0.51
1:C:20:ILE:HD12	2:C:301:PEE:H55	1.91	0.51
1:C:13:ASP:OD1	1:C:13:ASP:N	2.43	0.51
1:B:214:VAL:HG21	1:B:252:LEU:HD21	1.92	0.51
1:B:25:ASN:O	1:B:29:GLN:HG2	2.12	0.50
2:B:301:PEE:H31	2:B:301:PEE:C25	2.41	0.50
1:B:66:PHE:O	1:B:69:SER:N	2.45	0.50
1:A:143:TYR:CB	1:A:144:PRO:CD	2.89	0.50
1:C:16:LEU:O	1:C:20:ILE:HG12	2.10	0.50
2:B:301:PEE:C19	2:B:301:PEE:H79	2.40	0.50
1:A:117:ASN:O	1:A:117:ASN:OD1	2.30	0.49
1:B:173:LYS:O	1:B:174:GLN:C	2.50	0.49
1:C:25:ASN:O	1:C:29:GLN:HG2	2.11	0.49
1:D:14:ASN:CB	1:D:17:ASN:HB3	2.42	0.49
1:B:230:GLN:HB2	1:B:233:VAL:HG12	1.95	0.49
1:C:189:ASP:O	1:C:191:ASN:OD1	2.31	0.49
1:A:151:LEU:HD22	1:A:227:TYR:CZ	2.47	0.49
1:B:230:GLN:N	1:B:230:GLN:OE1	2.45	0.49
2:C:301:PEE:C2	2:C:301:PEE:O5	2.53	0.49
1:C:115:SER:HB2	1:C:173:LYS:HZ1	1.78	0.48
1:B:171:LEU:O	1:B:174:GLN:N	2.47	0.48
1:A:171:LEU:C	1:A:173:LYS:HA	2.33	0.48
1:B:169:ALA:O	1:B:175:LEU:HA	2.14	0.48
1:D:71:ARG:HD2	1:D:71:ARG:C	2.33	0.48
1:A:235:ARG:NH2	1:C:65:GLU:OE2	2.47	0.48
1:A:227:TYR:HB3	1:A:233:VAL:HG11	1.95	0.47
1:A:179:PHE:HB3	1:A:213:ILE:HD13	1.96	0.47
1:B:143:TYR:OH	1:B:230:GLN:NE2	2.42	0.47
1:B:223:ILE:HB	1:B:228:GLN:HG2	1.97	0.47
1:C:172:SER:OG	1:C:173:LYS:NZ	2.35	0.47
1:C:174:GLN:OE1	1:C:174:GLN:HA	2.15	0.47
1:D:14:ASN:HB3	1:D:17:ASN:CB	2.44	0.47
1:B:223:ILE:HB	1:B:228:GLN:CG	2.45	0.47
1:D:127:TYR:HB3	1:D:162:LEU:HB3	1.97	0.47
2:B:301:PEE:H72	2:B:301:PEE:C19	2.44	0.47
1:D:25:ASN:O	1:D:29:GLN:HG2	2.15	0.46
1:C:253:ARG:HG2	1:C:257:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:PRO:HB3	1:B:118:ASP:H	1.79	0.46
1:D:206:LYS:NZ	1:D:209:GLU:OE2	2.32	0.46
1:A:144:PRO:HG2	1:A:148:PHE:CG	2.50	0.46
1:A:190:ASP:C	1:A:192:GLN:OE1	2.47	0.46
1:B:66:PHE:O	1:B:69:SER:HB2	2.15	0.46
1:D:153:VAL:HG22	1:D:223:ILE:HG22	1.98	0.46
1:B:22:LYS:HA	1:B:25:ASN:HB2	1.97	0.46
1:B:10:LEU:HD12	1:B:10:LEU:O	2.16	0.46
1:D:131:LEU:HD23	1:D:160:ILE:HD12	1.97	0.46
2:B:301:PEE:H31	2:B:301:PEE:H37	1.27	0.45
1:B:145:VAL:O	1:B:145:VAL:HG12	2.15	0.45
1:C:3:PHE:CE1	1:D:52:PRO:HD2	2.51	0.45
1:A:208:LEU:HD21	1:C:245:PHE:CD2	2.50	0.45
2:C:301:PEE:H13	2:C:301:PEE:O5	2.14	0.45
1:C:20:ILE:HG23	2:C:301:PEE:H54	1.99	0.45
1:A:189:ASP:O	1:A:190:ASP:OD1	2.35	0.45
1:B:47:LEU:HA	1:B:131:LEU:HD13	1.98	0.45
1:B:18:ASP:OD1	1:B:21:ARG:NH1	2.50	0.44
1:C:253:ARG:HG2	1:C:257:ALA:CB	2.46	0.44
2:C:301:PEE:C5	2:C:301:PEE:H8	2.45	0.44
1:A:127:TYR:HB3	1:A:162:LEU:HB3	1.98	0.44
1:B:127:TYR:HB3	1:B:162:LEU:HB3	1.99	0.44
1:B:62:PRO:HG2	1:B:67:TYR:CE2	2.53	0.44
1:D:171:LEU:O	1:D:174:GLN:O	2.35	0.44
1:C:115:SER:HB2	1:D:118:ASP:N	2.33	0.44
1:C:226:GLN:HG3	1:C:226:GLN:H	1.42	0.44
1:A:131:LEU:HD22	1:A:160:ILE:HD12	2.00	0.44
2:B:301:PEE:H65	2:B:301:PEE:H58	1.22	0.44
1:D:171:LEU:N	1:D:171:LEU:HD12	2.33	0.44
1:D:10:LEU:HG	1:D:11:GLU:CD	2.39	0.43
1:B:116:PRO:HB3	1:B:118:ASP:N	2.34	0.43
1:D:10:LEU:HG	1:D:11:GLU:HG3	2.00	0.43
1:C:144:PRO:O	1:C:148:PHE:HB2	2.17	0.43
1:C:188:LEU:HD22	1:C:194:VAL:HG22	1.99	0.43
1:B:249:LYS:O	1:B:252:LEU:HG	2.19	0.43
2:B:301:PEE:H31	2:B:301:PEE:H42	2.01	0.43
1:C:62:PRO:CB	1:C:171:LEU:HD11	2.47	0.43
1:B:266:PHE:CD2	1:B:266:PHE:N	2.86	0.43
1:B:69:SER:OG	1:B:261:TRP:CZ2	2.47	0.43
1:A:153:VAL:CG2	1:A:223:ILE:HG22	2.47	0.43
1:D:29:GLN:NE2	1:D:40:LEU:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:LEU:HG	1:D:11:GLU:CG	2.48	0.42
1:D:258:TRP:CD2	1:D:259:PRO:HA	2.54	0.42
1:C:144:PRO:O	1:C:145:VAL:CB	2.66	0.42
1:D:258:TRP:CG	1:D:259:PRO:HA	2.53	0.42
1:B:225:GLU:OE1	1:B:228:GLN:HB2	2.19	0.42
1:C:127:TYR:HB3	1:C:162:LEU:HB3	2.02	0.42
1:B:186:PRO:O	1:B:189:ASP:HB2	2.19	0.42
1:C:131:LEU:HD22	1:C:160:ILE:HD12	2.00	0.42
1:D:13:ASP:O	1:D:14:ASN:HB2	2.19	0.42
1:A:258:TRP:CG	1:A:259:PRO:HA	2.54	0.42
1:C:145:VAL:HG22	1:C:146:GLU:N	2.32	0.42
1:C:72:GLU:HB3	1:C:73:GLU:OE2	2.19	0.42
1:C:18:ASP:O	1:C:22:LYS:HG3	2.20	0.42
1:D:247:ILE:HD13	1:D:247:ILE:HA	1.92	0.42
1:B:258:TRP:CG	1:B:259:PRO:HA	2.55	0.41
1:D:33:LEU:HA	1:D:34:PRO:HD3	1.92	0.41
1:C:153:VAL:CG2	1:C:223:ILE:HG22	2.50	0.41
1:D:49:LYS:HB2	1:D:49:LYS:HE2	1.57	0.41
1:A:192:GLN:N	1:A:192:GLN:OE1	2.53	0.41
1:C:143:TYR:HB3	1:C:144:PRO:HD3	1.99	0.41
1:A:144:PRO:CG	1:A:148:PHE:CD2	3.02	0.41
1:B:127:TYR:CZ	1:B:129:GLY:HA3	2.55	0.41
1:B:128:LYS:HG3	1:B:128:LYS:O	2.20	0.41
1:D:14:ASN:HB2	1:D:17:ASN:HB3	2.03	0.41
1:B:190:ASP:HB3	1:B:191:ASN:H	1.58	0.41
1:B:194:VAL:HG23	1:B:195:LEU:HD22	2.00	0.41
1:D:190:ASP:OD1	1:D:191:ASN:N	2.54	0.41
1:A:242:GLN:HA	1:C:208:LEU:HG	2.03	0.41
1:A:127:TYR:CZ	1:A:129:GLY:HA3	2.55	0.41
1:D:146:GLU:H	1:D:146:GLU:HG3	1.50	0.41
1:D:16:LEU:O	1:D:20:ILE:HG12	2.21	0.41
1:A:226:GLN:H	1:A:226:GLN:HG2	1.63	0.41
1:B:245:PHE:CZ	1:B:249:LYS:HD2	2.56	0.41
1:C:196:ASP:OD1	1:C:198:LYS:HG2	2.21	0.41
1:D:67:TYR:O	1:D:70:ILE:HG22	2.21	0.40
1:A:169:ALA:HB3	1:A:176:PHE:HB2	2.03	0.40
1:D:14:ASN:HB3	1:D:17:ASN:HB2	2.02	0.40
1:D:18:ASP:HA	1:D:21:ARG:HB3	2.03	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	223/272 (82%)	208 (93%)	12 (5%)	3 (1%)	15	50
1	B	220/272 (81%)	209 (95%)	10 (4%)	1 (0%)	34	72
1	C	224/272 (82%)	211 (94%)	10 (4%)	3 (1%)	15	50
1	D	218/272 (80%)	208 (95%)	9 (4%)	1 (0%)	34	72
All	All	885/1088 (81%)	836 (94%)	41 (5%)	8 (1%)	21	61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	VAL
1	C	116	PRO
1	C	145	VAL
1	D	144	PRO
1	C	193	THR
1	A	144	PRO
1	A	118	ASP
1	B	145	VAL

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	209/249 (84%)	206 (99%)	3 (1%)	74	90
1	B	206/249 (83%)	196 (95%)	10 (5%)	31	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	210/249 (84%)	200 (95%)	10 (5%)	31	69
1	D	204/249 (82%)	193 (95%)	11 (5%)	27	64
All	All	829/996 (83%)	795 (96%)	34 (4%)	37	74

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	13	ASP
1	A	117	ASN
1	B	22	LYS
1	B	69	SER
1	B	71	ARG
1	B	153	VAL
1	B	172	SER
1	B	190	ASP
1	B	191	ASN
1	B	206	LYS
1	B	210	ARG
1	B	266	PHE
1	C	32	GLN
1	C	115	SER
1	C	117	ASN
1	C	153	VAL
1	C	172	SER
1	C	173	LYS
1	C	190	ASP
1	C	191	ASN
1	C	192	GLN
1	C	253	ARG
1	D	9	THR
1	D	11	GLU
1	D	13	ASP
1	D	14	ASN
1	D	35	SER
1	D	71	ARG
1	D	73	GLU
1	D	143	TYR
1	D	146	GLU
1	D	189	ASP
1	D	226	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	D	14	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

5 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	PEE	A	301	-	50,50,50	0.58	0	52,55,55	0.85	0
2	PEE	B	301	-	50,50,50	0.59	0	52,55,55	0.85	0
2	PEE	C	301	-	50,50,50	0.58	0	52,55,55	0.85	0
2	PEE	D	301	-	15,15,50	0.29	0	14,14,55	0.89	0
2	PEE	D	302	-	15,15,50	0.29	0	14,14,55	0.88	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	PEE	A	301	-	-	1/54/54/54	0/0/0/0
2	PEE	B	301	-	-	0/54/54/54	0/0/0/0
2	PEE	C	301	-	-	1/54/54/54	0/0/0/0
2	PEE	D	301	-	-	0/13/13/54	0/0/0/0
2	PEE	D	302	-	-	0/13/13/54	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	PEE	C2-O2-C10-C11
2	A	301	PEE	C2-O2-C10-C11

There are no ring outliers.

3 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	PEE	8	0
2	B	301	PEE	18	0
2	C	301	PEE	15	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	227/272 (83%)	-0.06	9 (3%)	42	20	51, 86, 162, 225	0
1	B	224/272 (82%)	-0.00	11 (4%)	33	14	42, 94, 182, 216	0
1	C	228/272 (83%)	-0.26	4 (1%)	71	50	38, 73, 154, 216	0
1	D	222/272 (81%)	-0.09	12 (5%)	29	12	37, 77, 179, 238	0
All	All	901/1088 (82%)	-0.10	36 (3%)	42	20	37, 83, 173, 238	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	ASP	6.6
1	B	265	ASP	4.5
1	D	146	GLU	4.4
1	B	14	ASN	4.2
1	B	188	LEU	4.1
1	A	14	ASN	3.9
1	B	191	ASN	3.9
1	D	11	GLU	3.7
1	B	228	GLN	3.6
1	D	144	PRO	3.5
1	C	267	ASN	3.3
1	D	145	VAL	3.3
1	B	190	ASP	3.2
1	D	14	ASN	3.1
1	A	73	GLU	3.0
1	D	198	LYS	3.0
1	A	12	SER	3.0
1	A	115	SER	3.0
1	B	189	ASP	2.9
1	B	12	SER	2.8
1	C	146	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	72	GLU	2.7
1	A	67	TYR	2.6
1	D	143	TYR	2.6
1	B	205	THR	2.6
1	C	192	GLN	2.5
1	B	204	ALA	2.5
1	D	196	ASP	2.4
1	D	70	ILE	2.4
1	D	148	PHE	2.4
1	A	116	PRO	2.3
1	D	13	ASP	2.2
1	D	67	TYR	2.2
1	B	13	ASP	2.2
1	A	146	GLU	2.1
1	C	71	ARG	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PEE	C	301	51/51	0.69	0.42	8.28	91,133,205,232	0
2	PEE	D	302	16/51	0.70	0.57	5.13	84,109,152,155	0
2	PEE	A	301	51/51	0.73	0.38	3.67	88,138,200,222	0
2	PEE	B	301	51/51	0.77	0.37	2.85	89,129,185,207	0
2	PEE	D	301	16/51	0.88	0.32	0.43	86,97,127,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.