



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:26 PM GMT

PDB ID : 4EWT  
Title : The crystal structure of a putative aminohydrolase from methicillin resistant Staphylococcus aureus  
Authors : Girish, T.S.; Vivek, B.; Colaco, M.; Misquith, S.; Gopal, B.  
Deposited on : 2012-04-27  
Resolution : 2.10 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

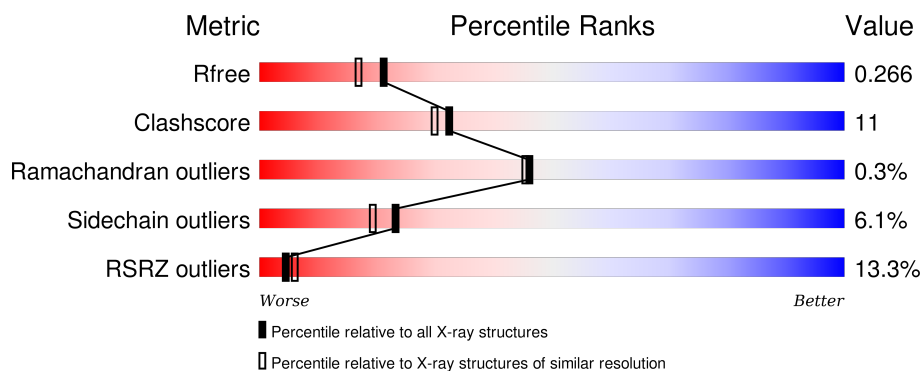
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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  $\geq 3$ , 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	392	<div> <div>3%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>
1	B	392	<div> <div>23%</div> <div>69%</div> <div>23%</div> <div>..</div> </div>
1	C	392	<div> <div>5%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>
1	D	392	<div> <div>21%</div> <div>86%</div> <div>11%</div> <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
3	PEG	A	403	-	-	-	X
4	PE7	B	403	-	-	-	X
4	PE7	B	404	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12344 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.

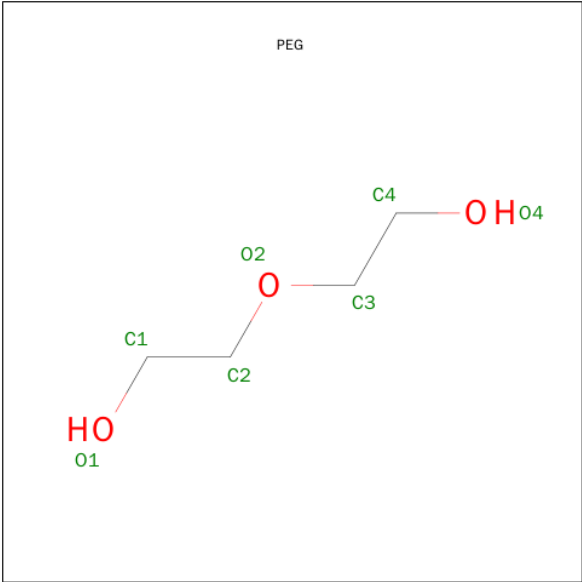
- Molecule 1 is a protein called Peptidase, M20/M25/M40 family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	1	0
			2985	1896	499	577	13			
1	C	389	Total	C	N	O	S	0	1	0
			2996	1907	496	580	13			
1	D	389	Total	C	N	O	S	0	2	0
			2980	1892	496	578	14			
1	B	375	Total	C	N	O	S	0	1	0
			2827	1795	473	546	13			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

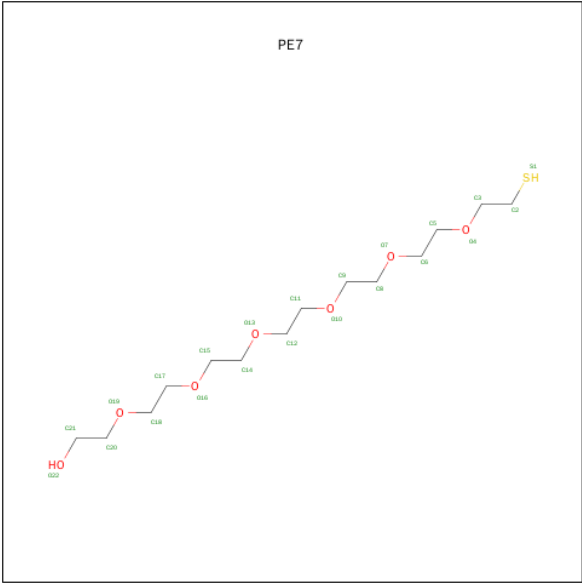
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		
2	D	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 4 is 1-DEOXY-1-THIO-HEPTAETHYLENE GLYCOL (three-letter code: PE7) (formula: C<sub>14</sub>H<sub>30</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	O	S	0	0
			22	14	7	1		
4	B	1	Total	C	O	S	0	0
			22	14	7	1		

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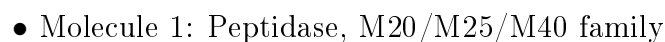
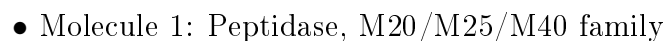
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	S	0	0
			22	14	7	1		

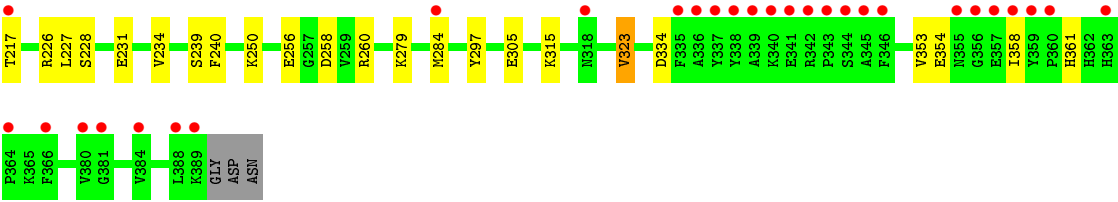
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	125	Total	O	0	0
			125	125		
5	C	127	Total	O	0	0
			127	127		
5	D	110	Total	O	0	0
			110	110		
5	B	113	Total	O	0	0
			113	113		

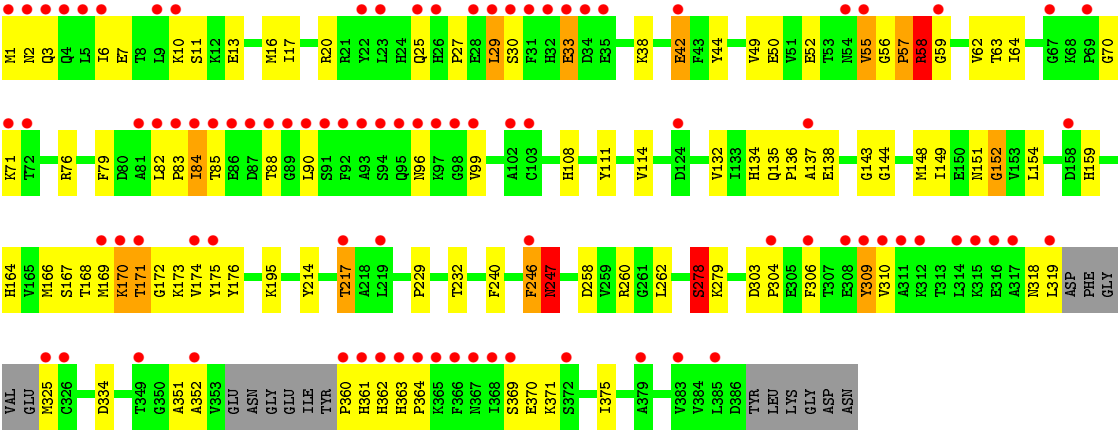


- Molecule 1: Peptidase, M20/M25/M40 family





● Molecule 1: Peptidase, M20/M25/M40 family





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.62Å 120.11Å 132.41Å 115.40° 94.64° 96.55°	Depositor
Resolution (Å)	39.32 – 2.10 39.32 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.8 (39.32-2.10) 80.1 (39.32-2.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.199 , 0.229 0.241 , 0.266	Depositor DCC
$R_{free}$ test set	7153 reflections (5.63%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.0	EDS
Estimated twinning fraction	0.016 for -h,-k,h+k+l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 133737 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12344	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, PE7, MN

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	0.61	0/3052	0.67	1/4134 (0.0%)
1	B	0.77	1/2890 (0.0%)	0.78	8/3917 (0.2%)
1	C	0.62	2/3065 (0.1%)	0.62	0/4152
1	D	0.64	0/3048	0.64	1/4130 (0.0%)
All	All	0.66	3/12055 (0.0%)	0.68	10/16333 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	278	SER	CB-OG	-7.51	1.32	1.42
1	C	272	LYS	CD-CE	-5.77	1.36	1.51
1	C	180	TYR	CD1-CE1	-5.26	1.31	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	PRO	N-CA-C	-7.69	92.10	112.10
1	B	152	GLY	N-CA-C	7.21	131.12	113.10
1	B	151	ASN	O-C-N	-7.11	111.12	123.20
1	B	151	ASN	N-CA-C	-6.56	93.28	111.00
1	A	88	THR	N-CA-C	-6.03	94.73	111.00
1	B	246	PHE	CB-CA-C	-5.73	98.93	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	ARG	C-N-CA	-5.71	110.30	122.30
1	B	55	VAL	CB-CA-C	-5.66	100.66	111.40
1	D	80	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	247	ASN	CB-CA-C	-5.13	100.13	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	152	GLY	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	2985	0	2920	68	0
1	B	2827	0	2709	92	0
1	C	2996	0	2932	53	0
1	D	2980	0	2895	47	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	7	0	10	0	0
4	B	44	0	60	1	0
4	D	22	0	30	0	0
5	A	125	0	0	7	0
5	B	113	0	0	2	0
5	C	127	0	0	1	0
5	D	110	0	0	3	0
All	All	12344	0	11556	247	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 11.

All (247) 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:D:1:MET:SD	1:D:3:GLN:HG3	1.71	1.31
1:B:371:LYS:O	1:B:375:ILE:HD12	1.34	1.22
1:B:2:ASN:O	1:B:6:ILE:HG12	1.37	1.21
1:C:82:LEU:HD21	1:C:139:GLU:HG2	1.18	1.14
1:A:88:THR:CG2	1:A:90:LEU:HG	1.78	1.14
1:A:88:THR:HG22	1:A:90:LEU:HG	1.28	1.12
1:A:136:PRO:HD2	1:A:148:MET:HE3	1.31	1.10
1:B:17:ILE:HG23	1:B:370:GLU:OE2	1.51	1.08
1:C:136:PRO:HD2	1:C:148:MET:HE3	1.35	1.07
1:B:173:LYS:HG2	1:B:174:VAL:H	1.19	1.05
1:D:169:MET:HE3	1:D:175:TYR:CD2	1.92	1.03
1:D:169:MET:CE	1:D:175:TYR:CD2	2.41	1.02
1:B:136:PRO:HD2	1:B:148:MET:HE3	1.41	1.02
1:C:82:LEU:CD2	1:C:139:GLU:HG2	1.90	1.01
1:B:55:VAL:HG12	1:B:55:VAL:O	1.60	0.98
1:C:136:PRO:HD2	1:C:148:MET:CE	1.94	0.98
1:A:136:PRO:HD2	1:A:148:MET:CE	1.97	0.95
1:B:135:GLN:HA	1:B:148:MET:HE3	1.49	0.94
1:B:136:PRO:HD2	1:B:148:MET:CE	1.99	0.91
1:C:82:LEU:HD21	1:C:139:GLU:CG	2.01	0.90
5:A:595:HOH:O	1:B:217:THR:HG21	1.72	0.88
1:B:136:PRO:CD	1:B:148:MET:HE3	2.04	0.86
1:A:387:TYR:O	1:A:388:LEU:HB2	1.78	0.83
1:D:167:SER:H	1:D:361:HIS:CE1	1.97	0.83
1:B:159:HIS:HD2	1:B:306:PHE:CD2	1.96	0.82
1:A:39:TYR:O	1:A:42:GLU:HG3	1.78	0.82
1:B:246:PHE:O	1:B:247:ASN:HB2	1.78	0.82
1:B:56:GLY:O	1:B:57:PRO:C	2.17	0.82
1:C:302:ASN:HB3	1:C:307:THR:HG21	1.61	0.82
1:A:88:THR:HG21	1:A:90:LEU:CD1	2.12	0.80
1:A:136:PRO:CD	1:A:148:MET:HE3	2.11	0.80
1:B:171:THR:OG1	1:B:352:ALA:N	2.14	0.80
1:B:246:PHE:O	1:B:247:ASN:CB	2.27	0.79
1:A:168:THR:HB	5:A:581:HOH:O	1.81	0.79
1:B:170:LYS:O	1:B:171:THR:CB	2.30	0.79
1:B:17:ILE:CG2	1:B:370:GLU:OE2	2.31	0.79
1:A:135:GLN:HA	1:A:148:MET:HE3	1.64	0.79
1:A:88:THR:HG21	1:A:90:LEU:HG	1.65	0.78
1:C:317:ALA:HB3	1:C:319:LEU:CD1	2.13	0.78
1:B:173:LYS:HG2	1:B:174:VAL:N	1.98	0.78
1:B:361:HIS:O	1:B:362:HIS:HB2	1.83	0.77
1:B:169:MET:HB3	1:B:175:TYR:CE2	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:PRO:HB2	1:B:363:HIS:CB	2.15	0.75
1:A:145:ALA:O	1:A:149:ILE:HG12	1.86	0.75
1:A:214:TYR:HE1	1:D:217:THR:HG22	1.52	0.74
1:B:195:LYS:HD2	4:B:403:PE7:H172	1.69	0.73
1:A:88:THR:CG2	1:A:90:LEU:CG	2.62	0.73
1:B:136:PRO:CD	1:B:148:MET:CE	2.66	0.73
1:C:134:HIS:HD2	5:C:587:HOH:O	1.71	0.72
1:D:169:MET:HE3	1:D:175:TYR:CG	2.24	0.72
1:A:159:HIS:HD2	1:A:387:TYR:OH	1.71	0.72
1:D:167:SER:H	1:D:361:HIS:HE1	1.36	0.72
1:D:234:VAL:HG22	1:B:229:PRO:HG3	1.70	0.72
1:B:1:MET:C	1:B:2:ASN:OD1	2.29	0.71
1:A:136:PRO:CD	1:A:148:MET:CE	2.68	0.71
1:A:88:THR:HG21	1:A:90:LEU:CG	2.20	0.71
1:B:171:THR:HG1	1:B:352:ALA:N	1.86	0.71
1:A:363:HIS:HD2	1:A:365:LYS:H	1.38	0.70
1:C:137:ALA:O	1:C:143:GLY:HA2	1.91	0.70
1:D:169:MET:HE3	1:D:175:TYR:CE2	2.26	0.70
1:B:159:HIS:HD2	1:B:306:PHE:CE2	2.09	0.70
1:C:1:MET:CB	1:C:2:ASN:HA	2.21	0.69
1:B:258:ASP:OD2	1:B:260:ARG:NH1	2.26	0.69
1:B:159:HIS:CD2	1:B:306:PHE:CD2	2.81	0.68
1:B:88:THR:OG1	1:B:90:LEU:HD12	1.93	0.68
1:B:279:LYS:HE2	5:B:508:HOH:O	1.93	0.67
1:D:33:GLU:HG3	1:D:79:PHE:CE1	2.30	0.66
1:B:318:ASN:O	1:B:319:LEU:C	2.30	0.66
1:C:317:ALA:CB	1:C:319:LEU:CD1	2.74	0.66
1:A:234:VAL:HG22	1:C:229:PRO:HG3	1.77	0.66
1:B:56:GLY:O	1:B:59:GLY:N	2.23	0.65
1:C:136:PRO:CD	1:C:148:MET:CE	2.73	0.64
1:D:1:MET:SD	1:D:3:GLN:CG	2.67	0.63
1:A:247:ASN:OD1	1:A:247:ASN:N	2.28	0.63
1:B:170:LYS:O	1:B:171:THR:OG1	2.17	0.62
1:A:135:GLN:HA	1:A:148:MET:CE	2.29	0.62
1:B:306:PHE:O	1:B:310:VAL:HG13	1.99	0.62
1:C:317:ALA:CB	1:C:319:LEU:HD11	2.29	0.62
1:B:52:GLU:OE2	1:B:55:VAL:HG21	1.99	0.62
1:A:363:HIS:CD2	1:A:365:LYS:HG2	2.34	0.62
1:B:56:GLY:O	1:B:58:ARG:N	2.33	0.62
1:B:170:LYS:O	1:B:171:THR:HB	2.00	0.62
1:C:214[A]:TYR:HE2	1:B:217:THR:HG23	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:TYR:HA	1:A:42:GLU:HG2	1.82	0.61
1:D:353:VAL:HG23	1:D:353:VAL:O	2.01	0.59
1:D:204:MET:CE	1:D:204:MET:HA	2.33	0.59
1:B:171:THR:HG22	1:B:171:THR:O	2.03	0.59
1:A:279:LYS:HD2	5:D:601:HOH:O	2.03	0.58
1:D:169:MET:CE	1:D:175:TYR:CG	2.82	0.58
1:D:315:LYS:HG3	1:D:323:VAL:HG13	1.86	0.58
1:A:2:ASN:HB3	5:A:592:HOH:O	2.04	0.57
1:C:135:GLN:HA	1:C:148:MET:CE	2.35	0.57
1:B:176:TYR:N	1:B:176:TYR:CD2	2.70	0.57
1:C:135:GLN:HA	1:C:148:MET:HE3	1.86	0.57
1:B:176:TYR:CZ	1:B:325:MET:HG2	2.39	0.57
1:A:363:HIS:CD2	1:A:365:LYS:H	2.22	0.57
1:A:137:ALA:O	1:A:143:GLY:HA2	2.05	0.57
1:B:159:HIS:CD2	1:B:306:PHE:CG	2.92	0.57
1:D:297:TYR:CE2	1:D:334:ASP:HB3	2.39	0.57
1:A:195:LYS:HE3	5:A:613:HOH:O	2.04	0.57
1:C:214[A]:TYR:HE2	1:B:217:THR:CG2	2.18	0.56
1:C:44:TYR:OH	1:C:134:HIS:HE1	1.88	0.56
1:D:204:MET:HA	1:D:204:MET:HE2	1.86	0.56
1:A:134:HIS:HD2	5:A:549:HOH:O	1.87	0.56
1:B:149:ILE:HG23	1:B:154:LEU:HD12	1.88	0.56
1:C:217:THR:HG23	1:B:214:TYR:HE1	1.70	0.56
1:D:1:MET:CE	1:D:4:GLN:H	2.19	0.56
1:B:136:PRO:HD2	1:B:148:MET:HE2	1.88	0.56
1:C:349:THR:HG21	1:C:376:SER:OG	2.05	0.56
1:C:303:ASP:O	1:C:307:THR:HG23	2.06	0.55
1:B:52:GLU:OE2	1:B:55:VAL:CG2	2.55	0.55
1:C:296:ASP:CG	1:C:297:TYR:H	2.10	0.55
1:D:168:THR:HA	1:D:358:ILE:HD12	1.89	0.54
1:A:214:TYR:CE1	1:D:217:THR:HG22	2.38	0.54
1:C:33:GLU:HG3	1:C:79:PHE:CE1	2.42	0.54
1:C:317:ALA:HB1	1:C:319:LEU:HD11	1.90	0.54
1:B:176:TYR:N	1:B:176:TYR:HD2	2.05	0.54
1:B:44:TYR:OH	1:B:134:HIS:HE1	1.90	0.53
1:D:297:TYR:CZ	1:D:334:ASP:HB3	2.43	0.53
1:D:177:ARG:HB3	1:D:181:VAL:HG12	1.90	0.53
1:C:38:LYS:O	1:C:42:GLU:HG2	2.09	0.53
1:C:214[A]:TYR:CE2	1:D:217:THR:HG23	2.43	0.53
1:D:1:MET:HE1	1:D:4:GLN:H	1.72	0.53
1:D:169:MET:HE1	1:D:175:TYR:CD2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ASP:O	1:C:307:THR:CG2	2.57	0.53
1:A:55:VAL:O	1:A:151:ASN:CG	2.48	0.53
1:A:6:ILE:HG22	1:A:10:LYS:HD2	1.91	0.52
1:B:44:TYR:CE2	1:B:62:VAL:HG11	2.45	0.52
1:A:206:ASN:ND2	1:D:226:ARG:HH12	2.07	0.52
1:B:176:TYR:H	1:B:176:TYR:HD2	1.58	0.52
5:A:595:HOH:O	1:C:217:THR:HG21	2.09	0.52
1:B:173:LYS:CG	1:B:174:VAL:H	2.05	0.52
1:B:50:GLU:HB3	1:B:63:THR:HG23	1.92	0.52
1:D:185:ARG:HG2	1:D:260:ARG:HD3	1.92	0.52
1:B:13:GLU:O	1:B:16:MET:N	2.41	0.51
1:C:312:LYS:HE2	1:C:316:GLU:OE2	2.10	0.51
1:A:44:TYR:OH	1:A:134:HIS:HE1	1.92	0.51
1:A:87:ASP:C	1:A:88:THR:O	2.44	0.51
1:B:55:VAL:CG1	1:B:55:VAL:O	2.29	0.51
1:B:50:GLU:HB3	1:B:63:THR:CG2	2.41	0.51
1:C:136:PRO:CD	1:C:148:MET:HE3	2.24	0.50
1:B:62:VAL:HG22	1:B:132:VAL:HB	1.93	0.50
1:D:1:MET:HE3	1:D:1:MET:C	2.32	0.50
1:B:16:MET:HG2	1:B:114:VAL:HG21	1.93	0.50
1:A:118:THR:O	1:A:121:GLU:HG2	2.12	0.50
1:B:138:GLU:HG2	1:B:334:ASP:OD2	2.12	0.50
1:B:232:THR:HB	1:B:262:LEU:HB2	1.94	0.50
1:A:384:VAL:O	1:A:387:TYR:O	2.29	0.49
1:C:319:LEU:N	1:C:319:LEU:HD12	2.27	0.49
1:B:3:GLN:O	1:B:7:GLU:N	2.30	0.49
1:A:189:LYS:HG2	1:A:256:GLU:HG2	1.94	0.49
1:C:214[A]:TYR:CE2	1:B:217:THR:HG23	2.47	0.49
1:C:316:GLU:C	1:C:317:ALA:O	2.50	0.49
1:D:185:ARG:HD3	1:D:260:ARG:CZ	2.42	0.49
1:D:239:SER:HB3	1:D:256:GLU:HB2	1.94	0.49
1:A:71:LYS:HB2	1:A:388:LEU:HD23	1.95	0.48
1:A:163:VAL:HG22	1:A:347:ILE:HG13	1.94	0.48
1:A:3:GLN:H	1:A:3:GLN:CD	2.12	0.48
1:B:52:GLU:HB3	1:B:55:VAL:HG23	1.96	0.48
1:A:387:TYR:HD2	1:A:388:LEU:HG	1.77	0.48
1:A:167:SER:H	1:A:361:HIS:HE1	1.61	0.48
1:A:62:VAL:HG22	1:A:132:VAL:HB	1.95	0.48
1:D:138:GLU:HG2	1:D:334:ASP:OD2	2.13	0.48
1:D:167:SER:N	1:D:361:HIS:HE1	2.08	0.48
1:C:59:GLY:HA2	1:C:148:MET:HE1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ILE:HG12	1:B:154:LEU:CD1	2.44	0.47
1:A:108:HIS:NE2	1:A:165:VAL:HG22	2.29	0.47
1:B:149:ILE:HG12	1:B:154:LEU:HD12	1.97	0.47
1:B:84:ILE:HD12	1:B:364:PRO:HA	1.96	0.47
1:C:59:GLY:HA2	1:C:148:MET:CE	2.45	0.47
1:C:29:LEU:HD13	1:C:99:VAL:HG13	1.96	0.47
1:C:16:MET:HB3	1:C:373:LEU:HD23	1.97	0.47
1:A:284:MET:HE3	1:D:284:MET:SD	2.54	0.47
1:D:35:GLU:O	1:D:38:LYS:HG2	2.16	0.46
1:B:30:SER:HB3	1:B:137:ALA:HA	1.98	0.46
1:B:169:MET:O	1:B:170:LYS:C	2.54	0.46
1:B:176:TYR:HE2	1:B:325:MET:N	2.14	0.46
1:B:136:PRO:O	1:B:144:GLY:HA2	2.16	0.46
1:C:69:PRO:O	1:C:127:THR:HB	2.16	0.45
1:D:228:SER:HB3	1:D:231:GLU:HG3	1.97	0.45
1:A:44:TYR:CE2	1:A:62:VAL:HG11	2.52	0.45
1:B:2:ASN:N	1:B:2:ASN:OD1	2.48	0.45
1:D:234:VAL:HG22	1:B:229:PRO:CG	2.44	0.45
1:A:203:HIS:H	1:A:203:HIS:CD2	2.35	0.45
1:A:164:HIS:HB2	1:A:346:PHE:CZ	2.51	0.45
1:A:88:THR:HG21	1:A:90:LEU:HD12	1.94	0.45
1:B:303:ASP:HA	1:B:304:PRO:HD3	1.80	0.45
1:A:239:SER:HB3	1:A:256:GLU:HB2	1.99	0.44
1:A:284:MET:CE	1:D:284:MET:SD	3.05	0.44
1:B:33:GLU:HG3	1:B:79:PHE:CE1	2.52	0.44
1:B:1:MET:O	1:B:2:ASN:OD1	2.34	0.44
1:A:71:LYS:NZ	5:A:510:HOH:O	2.47	0.44
1:A:33:GLU:HG3	1:A:79:PHE:CE1	2.52	0.44
1:B:38:LYS:O	1:B:42:GLU:HG2	2.18	0.44
1:B:171:THR:OG1	1:B:351:ALA:C	2.56	0.44
1:D:189:LYS:HE3	1:D:189:LYS:HB3	1.89	0.44
1:A:167:SER:H	1:A:361:HIS:CE1	2.36	0.44
1:A:361:HIS:O	1:A:362:HIS:HB2	2.18	0.44
1:A:369:SER:OG	1:A:371:LYS:HG2	2.18	0.44
1:C:182:GLN:HG2	1:C:329:GLN:HB2	2.00	0.43
1:D:80:ASP:OD2	1:D:138:GLU:N	2.51	0.43
1:A:39:TYR:HA	1:A:42:GLU:CG	2.47	0.43
1:C:127:THR:O	1:C:388:LEU:HB3	2.17	0.43
1:C:74:ALA:HA	1:C:131:VAL:O	2.18	0.43
1:B:176:TYR:CE2	1:B:325:MET:N	2.86	0.43
1:B:306:PHE:O	1:B:309:TYR:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:TYR:CD1	1:C:111:TYR:C	2.93	0.43
1:C:228:SER:HB3	1:C:231:GLU:HG3	2.00	0.43
1:A:59:GLY:HA2	1:A:148:MET:CE	2.49	0.42
1:A:61:LYS:HE2	1:A:153:VAL:HA	2.01	0.42
1:C:1:MET:CB	1:C:2:ASN:CA	2.92	0.42
1:C:5:LEU:HD21	1:C:381:GLY:HA3	2.01	0.42
1:D:169:MET:CE	1:D:175:TYR:CE2	2.94	0.42
1:A:2:ASN:O	1:A:6:ILE:HG12	2.20	0.42
1:A:351:ALA:HB1	1:A:368:ILE:HB	2.02	0.42
1:A:219:LEU:HD11	1:A:274:ILE:HG12	2.02	0.42
1:D:250:LYS:HE2	5:D:531:HOH:O	2.18	0.42
1:B:57:PRO:O	1:B:58:ARG:C	2.57	0.42
1:B:49:VAL:HG12	1:B:64:ILE:HG12	2.02	0.42
1:B:25:GLN:C	1:B:27:PRO:HD3	2.41	0.41
1:C:47:LYS:HD3	1:C:117:GLU:HG3	2.02	0.41
1:A:20:ARG:CG	1:A:21:ARG:N	2.80	0.41
1:B:278:SER:HB3	5:B:534:HOH:O	2.20	0.41
1:B:137:ALA:O	1:B:143:GLY:HA2	2.20	0.41
1:B:159:HIS:HD2	1:B:306:PHE:CG	2.32	0.41
1:B:29:LEU:HD13	1:B:99:VAL:HG13	2.01	0.41
1:C:361:HIS:HA	1:C:366:PHE:CD1	2.55	0.41
1:A:55:VAL:O	1:A:151:ASN:CB	2.69	0.41
1:A:359:TYR:CB	1:A:365:LYS:HG3	2.50	0.41
1:B:82:LEU:HA	1:B:83:PRO:HD3	1.95	0.41
1:D:127:THR:HG23	5:D:576:HOH:O	2.21	0.41
1:D:177:ARG:HB3	1:D:181:VAL:CG1	2.49	0.41
1:D:258:ASP:OD1	1:D:260:ARG:NH1	2.52	0.41
1:A:27:PRO:HG2	1:A:99:VAL:HG22	2.02	0.41
1:C:27:PRO:HB3	1:C:101:HIS:CD2	2.56	0.41
1:D:1:MET:CE	1:D:4:GLN:HG3	2.51	0.41
1:C:62:VAL:HB	1:C:132:VAL:HB	2.02	0.41
1:B:171:THR:HG21	1:B:369:SER:CB	2.51	0.40
1:B:108:HIS:NE2	1:B:164:HIS:HA	2.35	0.40
1:C:296:ASP:O	1:C:297:TYR:C	2.60	0.40
1:D:111:TYR:C	1:D:111:TYR:CD1	2.95	0.40
1:C:64:ILE:HB	1:C:130:VAL:HB	2.03	0.40
1:B:371:LYS:O	1:B:375:ILE:CD1	2.30	0.40
1:A:25:GLN:HE21	1:A:92:PHE:HA	1.86	0.40
1:D:17:ILE:O	1:D:21:ARG:HG3	2.22	0.40
1:B:166:MET:C	1:B:168:THR:H	2.24	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	388/392 (99%)	377 (97%)	11 (3%)	0	100	100
1	B	370/392 (94%)	343 (93%)	22 (6%)	5 (1%)	14	7
1	C	388/392 (99%)	379 (98%)	9 (2%)	0	100	100
1	D	389/392 (99%)	379 (97%)	10 (3%)	0	100	100
All	All	1535/1568 (98%)	1478 (96%)	52 (3%)	5 (0%)	46	45

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	LYS
1	B	171	THR
1	B	167	SER
1	B	70	GLY
1	B	172	GLY

### 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	316/326 (97%)	295 (93%)	21 (7%)	21	17
1	B	290/326 (89%)	272 (94%)	18 (6%)	23	19
1	C	318/326 (98%)	299 (94%)	19 (6%)	24	20
1	D	314/326 (96%)	297 (95%)	17 (5%)	27	24
All	All	1238/1304 (95%)	1163 (94%)	75 (6%)	23	19

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	5	LEU
1	A	7	GLU
1	A	20	ARG
1	A	29	LEU
1	A	42	GLU
1	A	50	GLU
1	A	51	VAL
1	A	53	THR
1	A	87	ASP
1	A	99	VAL
1	A	111	TYR
1	A	204	MET
1	A	206	ASN
1	A	240	PHE
1	A	258	ASP
1	A	279	LYS
1	A	319	LEU
1	A	320	ASP
1	A	325	MET
1	A	334	ASP
1	C	9	LEU
1	C	29	LEU
1	C	53	THR
1	C	55	VAL
1	C	58	ARG
1	C	111	TYR
1	C	125	SER
1	C	181	VAL
1	C	193	GLN
1	C	217	THR
1	C	227	LEU
1	C	284	MET
1	C	300	LEU
1	C	307	THR
1	C	314	LEU
1	C	320	ASP
1	C	334	ASP
1	C	349	THR
1	C	385	LEU
1	D	1	MET
1	D	3	GLN

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Mol	Chain	Res	Type
1	D	4	GLN
1	D	27	PRO
1	D	53	THR
1	D	68	LYS
1	D	76	ARG
1	D	88	THR
1	D	99	VAL
1	D	111	TYR
1	D	189	LYS
1	D	227	LEU
1	D	240	PHE
1	D	279	LYS
1	D	305	GLU
1	D	323	VAL
1	D	354	GLU
1	B	10	LYS
1	B	11	SER
1	B	20	ARG
1	B	29	LEU
1	B	33	GLU
1	B	42	GLU
1	B	58	ARG
1	B	71	LYS
1	B	76	ARG
1	B	84	ILE
1	B	85	THR
1	B	96	ASN
1	B	111	TYR
1	B	217	THR
1	B	240	PHE
1	B	247	ASN
1	B	278	SER
1	B	309	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	54	ASN
1	A	95	GLN
1	A	96	ASN
1	A	134	HIS

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Mol	Chain	Res	Type
1	A	159	HIS
1	A	203	HIS
1	A	206	ASN
1	A	220	GLN
1	A	361	HIS
1	A	363	HIS
1	C	134	HIS
1	D	25	GLN
1	D	95	GLN
1	D	193	GLN
1	D	245	GLN
1	D	361	HIS
1	D	362	HIS
1	B	96	ASN
1	B	134	HIS
1	B	159	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	PEG	A	403	-	6,6,6	0.42	0	5,5,5	0.33	0
4	PE7	B	403	-	21,21,21	0.52	0	20,20,20	0.67	0
4	PE7	B	404	-	21,21,21	0.53	0	20,20,20	0.54	0
4	PE7	D	403	-	21,21,21	0.49	0	20,20,20	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	403	-	-	0/4/4/4	0/0/0/0
4	PE7	B	403	-	-	0/19/19/19	0/0/0/0
4	PE7	B	404	-	-	0/19/19/19	0/0/0/0
4	PE7	D	403	-	-	0/19/19/19	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	PE7	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	389/392 (99%)	0.30	13 (3%) 50 59	10, 38, 67, 92	0
1	B	375/392 (95%)	1.17	90 (24%) 1 1	10, 37, 64, 76	0
1	C	389/392 (99%)	0.36	18 (4%) 36 45	11, 36, 57, 70	0
1	D	389/392 (99%)	1.11	84 (21%) 1 1	10, 44, 91, 130	0
All	All	1542/1568 (98%)	0.73	205 (13%) 4 6	10, 38, 71, 130	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	98	GLY	8.0
1	B	29	LEU	6.5
1	D	214[A]	TYR	6.4
1	B	89	GLY	6.4
1	B	93	ALA	6.1
1	B	1	MET	6.0
1	D	160	VAL	5.9
1	B	137	ALA	5.8
1	B	87	ASP	5.6
1	C	214[A]	TYR	5.6
1	B	314	LEU	5.6
1	B	85	THR	5.5
1	B	90	LEU	5.4
1	D	339	ALA	5.3
1	D	343	PRO	5.3
1	B	88	THR	5.1
1	D	360	PRO	4.9
1	B	95	GLN	4.8
1	D	87	ASP	4.8
1	B	34	ASP	4.7
1	D	344	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	96	ASN	4.6
1	B	94	SER	4.6
1	B	81	ALA	4.6
1	D	153	VAL	4.5
1	B	25	GLN	4.5
1	B	92	PHE	4.5
1	B	326	CYS	4.5
1	B	366	PHE	4.5
1	D	337	TYR	4.4
1	B	82	LEU	4.4
1	D	133	ILE	4.3
1	B	99	VAL	4.3
1	D	89	GLY	4.2
1	B	69	PRO	4.2
1	B	309	TYR	4.2
1	B	2	ASN	4.2
1	D	161	LEU	4.2
1	D	75	ILE	4.1
1	D	338	TYR	4.1
1	B	22	TYR	4.1
1	D	359	TYR	4.0
1	B	325	MET	4.0
1	D	74	ALA	4.0
1	B	97	LYS	3.9
1	B	170	LYS	3.9
1	B	312	LYS	3.9
1	B	317	ALA	3.9
1	B	98	GLY	3.9
1	D	335	PHE	3.9
1	B	363	HIS	3.9
1	D	384	VAL	3.9
1	B	83	PRO	3.8
1	D	145	ALA	3.8
1	B	91	SER	3.8
1	B	26	HIS	3.8
1	D	163	VAL	3.8
1	D	345	ALA	3.8
1	B	30	SER	3.8
1	D	154	LEU	3.8
1	D	363	HIS	3.8
1	B	364	PRO	3.7
1	D	389	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	352	ALA	3.7
1	B	32	HIS	3.7
1	B	368	ILE	3.7
1	D	91	SER	3.6
1	D	159	HIS	3.6
1	D	162	GLY	3.6
1	B	84	ILE	3.6
1	D	357	GLU	3.6
1	B	86	GLU	3.6
1	B	319	LEU	3.5
1	D	90	LEU	3.5
1	D	62	VAL	3.5
1	A	95	GLN	3.5
1	D	157	VAL	3.5
1	A	355	ASN	3.5
1	D	99	VAL	3.4
1	D	1	MET	3.4
1	D	3	GLN	3.3
1	D	131	VAL	3.2
1	D	132	VAL	3.2
1	D	84	ILE	3.2
1	C	4	GLN	3.1
1	B	383	VAL	3.1
1	B	59	GLY	3.1
1	D	85	THR	3.1
1	D	26	HIS	3.1
1	B	306	PHE	3.1
1	A	318	ASN	3.0
1	D	148	MET	3.0
1	B	171	THR	3.0
1	D	72	THR	3.0
1	D	380	VAL	3.0
1	D	336	ALA	3.0
1	D	210	VAL	3.0
1	D	388	LEU	3.0
1	D	34	ASP	2.9
1	B	308	GLU	2.9
1	C	1	MET	2.9
1	B	31	PHE	2.9
1	D	364	PRO	2.9
1	B	385	LEU	2.9
1	B	102	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	372	SER	2.8
1	B	311	ALA	2.8
1	B	304	PRO	2.8
1	B	3	GLN	2.8
1	B	124	ASP	2.8
1	B	360	PRO	2.8
1	D	358	ILE	2.8
1	B	379	ALA	2.8
1	A	67	GLY	2.8
1	C	95	GLN	2.8
1	D	95	GLN	2.8
1	B	316	GLU	2.8
1	D	149	ILE	2.8
1	C	320	ASP	2.7
1	A	320	ASP	2.7
1	D	342	ARG	2.7
1	B	67	GLY	2.7
1	C	98	GLY	2.7
1	D	64	ILE	2.7
1	D	92	PHE	2.7
1	D	366	PHE	2.7
1	C	54	ASN	2.6
1	D	318	ASN	2.6
1	D	73	LEU	2.6
1	B	9	LEU	2.6
1	B	33	GLU	2.6
1	D	94	SER	2.6
1	B	369	SER	2.6
1	D	29	LEU	2.6
1	D	356	GLY	2.6
1	D	340	LYS	2.6
1	D	51	VAL	2.6
1	D	130	VAL	2.6
1	B	175	TYR	2.5
1	D	97	LYS	2.5
1	D	346	PHE	2.5
1	B	246	PHE	2.5
1	A	88	THR	2.5
1	B	28	GLU	2.5
1	B	35	GLU	2.5
1	A	96	ASN	2.5
1	B	217	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	144	GLY	2.5
1	B	362	HIS	2.5
1	A	246	PHE	2.5
1	B	367	ASN	2.5
1	D	76	ARG	2.5
1	C	2	ASN	2.5
1	B	23	LEU	2.5
1	D	164	HIS	2.4
1	B	5	LEU	2.4
1	B	42	GLU	2.4
1	D	187	PHE	2.4
1	A	7	GLU	2.4
1	A	93	ALA	2.4
1	B	6	ILE	2.4
1	B	54	ASN	2.4
1	D	77	ALA	2.4
1	D	124	ASP	2.3
1	D	146	LYS	2.3
1	D	25	GLN	2.3
1	B	10	LYS	2.3
1	B	71	LYS	2.3
1	C	317	ALA	2.3
1	D	156	GLY	2.3
1	C	34	ASP	2.3
1	B	4	GLN	2.3
1	D	381	GLY	2.3
1	B	365	LYS	2.2
1	D	217	THR	2.2
1	D	56	GLY	2.2
1	D	341	GLU	2.2
1	D	88	THR	2.2
1	D	7	GLU	2.2
1	C	318	ASN	2.2
1	B	315	LYS	2.2
1	D	104	GLY	2.2
1	B	55	VAL	2.2
1	B	219	LEU	2.2
1	A	34	ASP	2.2
1	C	55	VAL	2.2
1	C	354	GLU	2.1
1	B	174	VAL	2.1
1	B	349	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	96	ASN	2.1
1	B	103	CYS	2.1
1	B	72	THR	2.1
1	B	158	ASP	2.1
1	C	97	LYS	2.1
1	C	355	ASN	2.1
1	D	152	GLY	2.1
1	B	310	VAL	2.0
1	A	2	ASN	2.0
1	D	355	ASN	2.0
1	C	32	HIS	2.0
1	B	361	HIS	2.0
1	C	70	GLY	2.0
1	A	133	ILE	2.0
1	D	284	MET	2.0
1	B	169	MET	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	PE7	B	403	22/22	0.75	0.24	5.31	54,62,67,67	0
4	PE7	B	404	22/22	0.86	0.17	2.87	40,48,56,61	0
3	PEG	A	403	7/7	0.91	0.21	2.07	36,36,39,41	0
2	MN	A	402	1/1	0.97	0.14	0.77	35,35,35,35	0
4	PE7	D	403	22/22	0.87	0.17	0.73	35,38,52,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	C	402	1/1	0.99	0.11	0.47	35,35,35,35	0
2	MN	D	402	1/1	0.99	0.14	-1.26	35,35,35,35	0
2	MN	B	402	1/1	0.92	0.09	-1.38	48,48,48,48	0
2	MN	A	401	1/1	0.95	0.10	-1.40	55,55,55,55	0
2	MN	B	401	1/1	0.90	0.11	-1.40	69,69,69,69	0
2	MN	C	401	1/1	0.95	0.03	-2.69	49,49,49,49	0
2	MN	D	401	1/1	0.94	0.07	-2.80	57,57,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.