Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 05:12 pm BST

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)

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

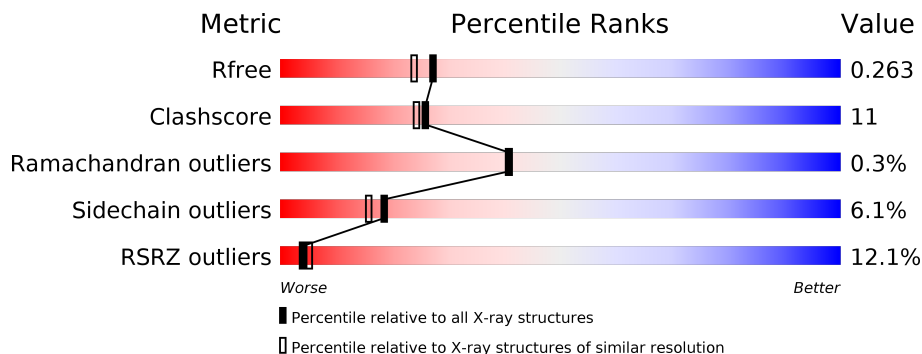|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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	Percentile Ranks	Value
Rfree		0.263
Clashscore		11
Ramachandran outliers		0.3%
Sidechain outliers		6.1%
RSRZ outliers		12.1%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 >=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 <=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	3% / 78% / 19% ··
1	B	392	21% / 69% / 23% ···
1	C	392	3% / 81% / 17% ··
1	D	392	20% / 86% / 11% ··

2 Entry composition (i)

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: $C_4H_{10}O_3$).

PEG

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: $C_{14}H_{30}O_7S$).

PE7
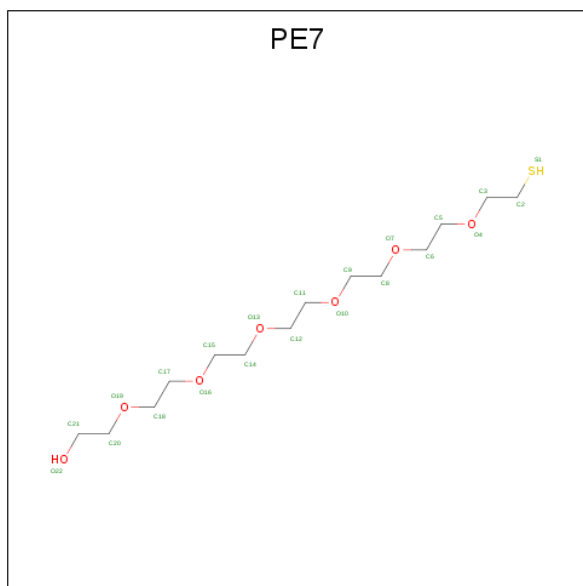
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	O	S	0	0
			22	14	7	1		
4	B	1	Total	C	O	S	0	0
			22	14	7	1		

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

- Molecule 5 is water.

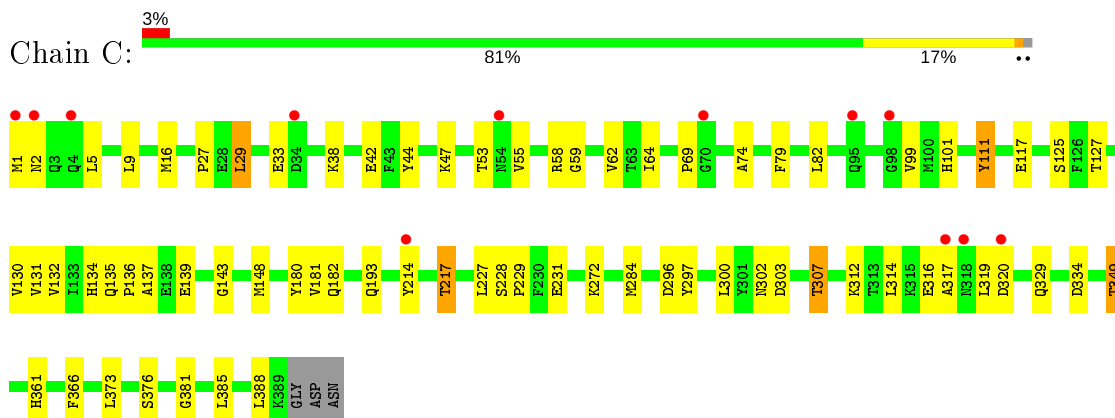| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	125	Total 125	O 125	0	0
5	C	127	Total 127	O 127	0	0
5	D	110	Total 110	O 110	0	0
5	B	113	Total 113	O 113	0	0

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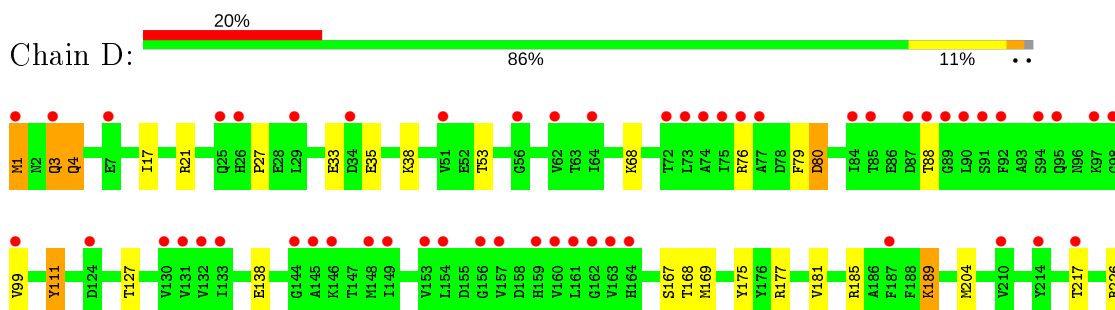
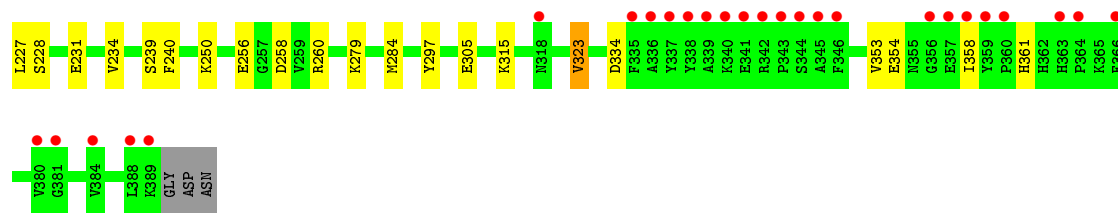- Molecule 1: Peptidase, M20/M25/M40 family
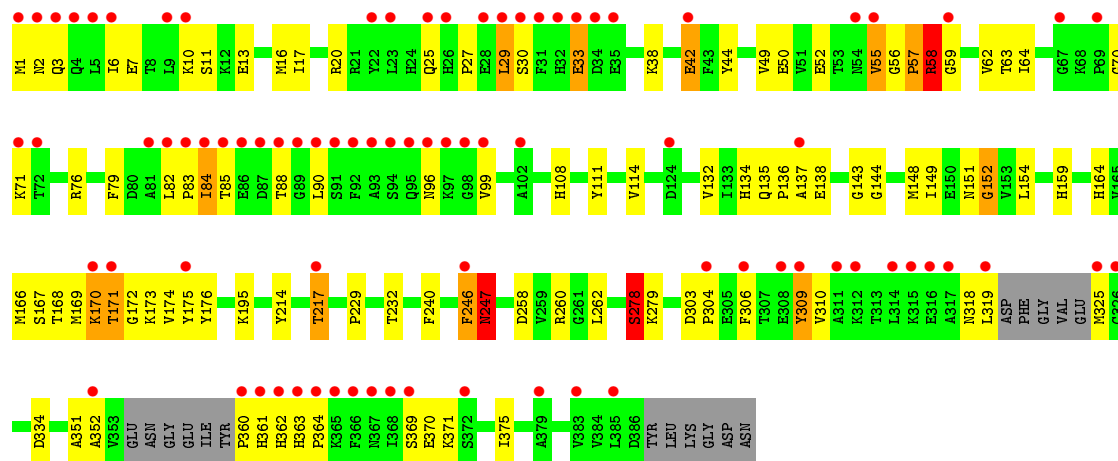

- Molecule 1: Peptidase, M20/M25/M40 family

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

L227 S228 E231 V234 S239 F240 K250 E256 G257 D258 V259 R260 K279 M284 Y297 E305 K315 N318 V323 D334 F335 A336 Y337 Y338 A339 K340 E341 R342 P343 S344 A345 F346 V353 E354 N355 G356 E357 I358 Y359 P360 H361 H362 H363 P364 K365 F366

V380 G381 V384 L388 K389 GLY ASP ASN

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

Chain B:

21%

69% 23%

M1 N2 Q3 Q4 L5 I6 E7 T8 L9 K10 S11 K12 E13 M16 I17 R20 R21 Y22 L23 H24 Q25 H26 P27 E28 L29 S30 F31 H32 E33 D34 E35 K38 E42 F43 Y44 V49 E50 V51 E52 T53 N54 V55 G56 P57 R58 G59 V62 T63 I64 G67 K68 P69 G70

K71 T72 R76 F79 D80 A81 L82 P83 I84 T85 E86 D87 T88 G89 L90 S91 F92 A93 S94 Q95 N96 K97 G98 V99 A102 H108 Y111 V114 D124 V132 I133 H134 Q135 P136 A137 E138 G143 G144 M148 I149 E150 N151 G152 V153 L154 H159 H164 V165

M166 S167 T168 M169 K170 T171 G172 K173 V174 Y175 Y176 K195 Y214 T217 P229 T232 F240 F246 N247 D258 V259 R260 G261 L262 S278 K279 D303 P304 E305 F306 T307 E308 Y309 V310 A311 K312 T313 L314 K315 E316 A317 N318 L319 ASP PHE GLY VAL GLU M325 C326

D334 A351 A352 V353 GLU ASN GLY GLU ILE TYR P360 H361 H362 H363 P364 K365 F366 N367 I368 S369 E370 K371 S372 I375 A379 V383 V384 L385 D386 TYR LEU LYS GLY ASP ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	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) 93.9 (39.32-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.199 , 0.229 0.240 , 0.263	Depositor DCC
R_{free} test set	6731 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.2	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12344	wwPDB-VP
Average B, all atoms (Å^2)	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.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, 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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:A:39:TYR:O	1:A:42:GLU:HG3	1.78	0.82
1:B:159:HIS:HD2	1:B:306:PHE:CD2	1.96	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:A:136:PRO:CD	1:A:148:MET:CE	2.68	0.71
1:B:1:MET:C	1:B:2:ASN:OD1	2.29	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:A:234:VAL:HG22	1:C:229:PRO:HG3	1.77	0.66
1:C:317:ALA:CB	1:C:319:LEU:CD1	2.74	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:A:363:HIS:CD2	1:A:365:LYS:HG2	2.34	0.62
1:B:52:GLU:OE2	1:B:55:VAL:HG21	1.99	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:A:39:TYR:HA	1:A:42:GLU:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214[A]:TYR:HE2	1:B:217:THR:HG23	1.65	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:CD2	1:B:176:TYR:N	2.70	0.57
1:B:176:TYR:CZ	1:B:325:MET:HG2	2.39	0.57
1:C:135:GLN:HA	1:C:148:MET:HE3	1.86	0.57
1:A:137:ALA:O	1:A:143:GLY:HA2	2.05	0.57
1:A:363:HIS:CD2	1:A:365:LYS:H	2.22	0.57
1:B:159:HIS:CD2	1:B:306:PHE:CG	2.92	0.57
1:A:195:LYS:HE3	5:A:613:HOH:O	2.04	0.57
1:D:297:TYR:CE2	1:D:334:ASP:HB3	2.39	0.57
1:C:214[A]:TYR:HE2	1:B:217:THR:CG2	2.18	0.56
1:A:134:HIS:HD2	5:A:549:HOH:O	1.87	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: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: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:D:1:MET:CE	1:D:4:GLN:H	2.19	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:C:33:GLU:HG3	1:C:79:PHE:CE1	2.42	0.54
1:A:214:TYR:CE1	1:D:217:THR:HG22	2.38	0.54
1:B:176:TYR:HD2	1:B:176:TYR:N	2.05	0.54
1:C:317:ALA:HB1	1:C:319:LEU:HD11	1.90	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:A:55:VAL:O	1:A:151:ASN:CG	2.48	0.53
1:C:303:ASP:O	1:C:307:THR:CG2	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:MET:HE1	1:D:175:TYR:CD2	2.40	0.53
1:D:1:MET:HE1	1:D:4:GLN:H	1.72	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:A:44:TYR:OH	1:A:134:HIS:HE1	1.92	0.51
1:C:312:LYS:HE2	1:C:316:GLU:OE2	2.10	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:B:16:MET:HG2	1:B:114:VAL:HG21	1.93	0.50
1:D:1:MET:HE3	1:D:1:MET:C	2.32	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:B:3:GLN:O	1:B:7:GLU:N	2.30	0.49
1:C:319:LEU:N	1:C:319:LEU:HD12	2.27	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:163:VAL:HG22	1:A:347:ILE:HG13	1.94	0.48
1:A:71:LYS:HB2	1:A:388:LEU:HD23	1.95	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:167:SER:H	1:A:361:HIS:HE1	1.61	0.48
1:A:387:TYR:HD2	1:A:388:LEU:HG	1.77	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:B:149:ILE:HG12	1:B:154:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:GLY:HA2	1:C:148:MET:HE1	1.95	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: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:C:59:GLY:HA2	1:C:148:MET:CE	2.45	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: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: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: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:33:GLU:HG3	1:A:79:PHE:CE1	2.52	0.44
1:A:71:LYS:NZ	5:A:510:HOH:O	2.47	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: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:C:47:LYS:HD3	1:C:117:GLU:HG3	2.02	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: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: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:C:62:VAL:HB	1:C:132:VAL:HB	2.02	0.41
1:D:1:MET:CE	1:D:4:GLN:HG3	2.51	0.41
1:B:108:HIS:NE2	1:B:164:HIS:HA	2.35	0.40
1:B:171:THR:HG21	1:B:369:SER:CB	2.51	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:B:166:MET:C	1:B:168:THR:H	2.24	0.40
1:D:17:ILE:O	1:D:21:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	388/392 (99%)	377 (97%)	11 (3%)	0	100	100
1	B	370/392 (94%)	343 (93%)	22 (6%)	5 (1%)	11	6
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%)	41	41

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 (i)

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%)	16	14
1	B	290/326 (89%)	272 (94%)	18 (6%)	18	15
1	C	318/326 (98%)	299 (94%)	19 (6%)	19	16
1	D	314/326 (96%)	297 (95%)	17 (5%)	22	20
All	All	1238/1304 (95%)	1163 (94%)	75 (6%)	18	16

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
4	PE7	B	404	-	21,21,21	0.52	0	20,20,20	0.53	0
4	PE7	D	403	-	21,21,21	0.48	0	20,20,20	0.77	0
4	PE7	B	403	-	21,21,21	0.52	0	20,20,20	0.67	0
3	PEG	A	403	-	6,6,6	0.42	0	5,5,5	0.31	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
4	PE7	B	404	-	-	7/19/19/19	-
4	PE7	D	403	-	-	6/19/19/19	-
4	PE7	B	403	-	-	12/19/19/19	-
3	PEG	A	403	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	PE7	S1-C2-C3-O4
4	B	403	PE7	O16-C17-C18-O19
4	D	403	PE7	O10-C11-C12-O13
3	A	403	PEG	O2-C3-C4-O4
4	B	403	PE7	O4-C5-C6-O7
4	B	403	PE7	O7-C8-C9-O10
4	B	404	PE7	O16-C17-C18-O19
4	B	403	PE7	O10-C11-C12-O13
4	B	404	PE7	O7-C8-C9-O10
4	B	404	PE7	O19-C20-C21-O22
4	B	404	PE7	C15-C14-O13-C12
4	B	404	PE7	C17-C18-O19-C20
4	B	403	PE7	C9-C8-O7-C6
4	D	403	PE7	O7-C8-C9-O10
4	D	403	PE7	C12-C11-O10-C9
4	D	403	PE7	C6-C5-O4-C3
4	B	403	PE7	C17-C18-O19-C20
4	B	403	PE7	C15-C14-O13-C12

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Mol	Chain	Res	Type	Atoms
4	B	403	PE7	C14-C15-O16-C17
4	D	403	PE7	O19-C20-C21-O22
4	B	403	PE7	C12-C11-O10-C9
4	B	404	PE7	S1-C2-C3-O4
4	D	403	PE7	C21-C20-O19-C18
4	B	403	PE7	C18-C17-O16-C15
4	B	403	PE7	C11-C12-O13-C14
4	B	404	PE7	C21-C20-O19-C18

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PE7 B 404

Bond lengths — Bond angles

Torsions — Rings

Ligand PE7 D 403

Bond lengths — Bond angles

Torsions — Rings

Ligand PE7 B 403

Bond lengths

Bond angles

Torsions

Rings
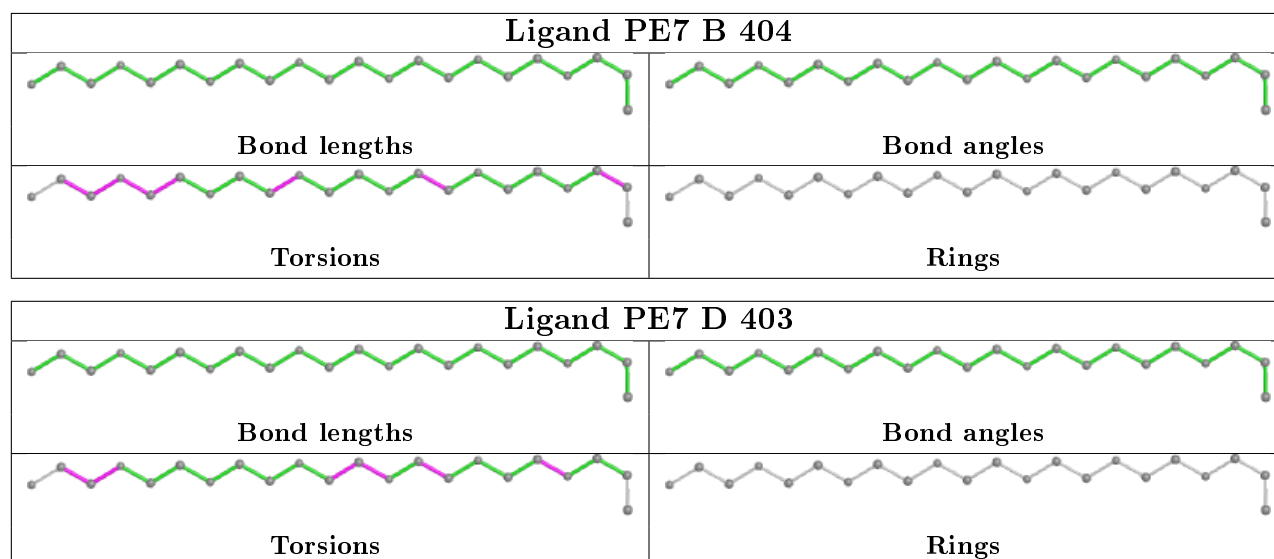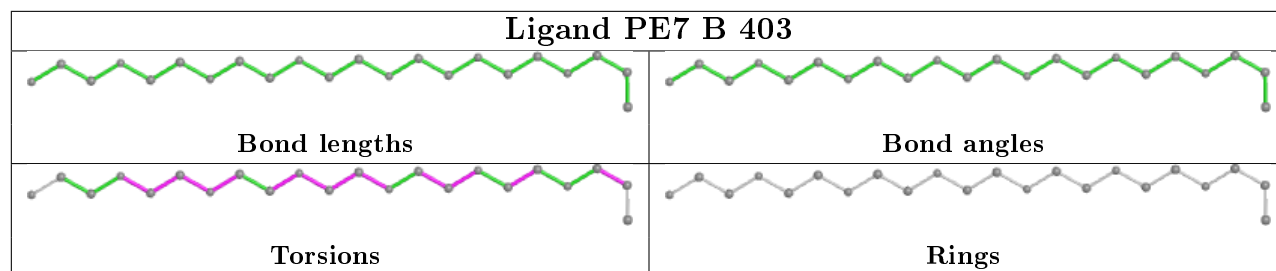
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	389/392 (99%)	0.24	11 (2%)	53	59	10, 38, 67, 92	0
1	B	375/392 (95%)	1.08	83 (22%)	0	0	10, 37, 64, 76	0
1	C	389/392 (99%)	0.29	12 (3%)	49	55	11, 36, 57, 70	0
1	D	389/392 (99%)	1.04	80 (20%)	1	1	10, 44, 91, 130	0
All	All	1542/1568 (98%)	0.65	186 (12%)	4	5	10, 38, 71, 130	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	98	GLY	7.9
1	D	214[A]	TYR	6.3
1	B	89	GLY	6.1
1	B	29	LEU	6.0
1	B	1	MET	6.0
1	B	93	ALA	5.8
1	D	160	VAL	5.6
1	B	137	ALA	5.6
1	B	87	ASP	5.4
1	C	214[A]	TYR	5.4
1	B	314	LEU	5.3
1	B	85	THR	5.3
1	D	343	PRO	5.3
1	D	339	ALA	5.2
1	B	90	LEU	5.2
1	B	88	THR	4.7
1	D	87	ASP	4.7
1	D	360	PRO	4.6
1	B	95	GLN	4.6
1	B	96	ASN	4.6
1	D	337	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	344	SER	4.5
1	B	34	ASP	4.4
1	B	94	SER	4.4
1	B	326	CYS	4.4
1	B	25	GLN	4.4
1	D	338	TYR	4.3
1	B	81	ALA	4.2
1	B	366	PHE	4.2
1	D	153	VAL	4.2
1	D	133	ILE	4.2
1	D	161	LEU	4.1
1	D	89	GLY	4.1
1	D	359	TYR	4.1
1	B	309	TYR	4.1
1	B	92	PHE	4.1
1	B	325	MET	4.0
1	B	2	ASN	4.0
1	B	82	LEU	4.0
1	B	99	VAL	4.0
1	B	69	PRO	4.0
1	D	75	ILE	4.0
1	B	22	TYR	3.9
1	D	74	ALA	3.9
1	B	312	LYS	3.9
1	B	170	LYS	3.8
1	B	97	LYS	3.8
1	D	145	ALA	3.8
1	D	363	HIS	3.8
1	B	363	HIS	3.8
1	D	163	VAL	3.7
1	B	26	HIS	3.7
1	B	83	PRO	3.7
1	B	91	SER	3.7
1	D	154	LEU	3.7
1	D	335	PHE	3.7
1	B	30	SER	3.6
1	B	98	GLY	3.6
1	B	317	ALA	3.6
1	B	32	HIS	3.6
1	D	162	GLY	3.6
1	B	364	PRO	3.6
1	B	352	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	159	HIS	3.5
1	D	91	SER	3.5
1	D	357	GLU	3.5
1	D	384	VAL	3.5
1	D	90	LEU	3.5
1	D	345	ALA	3.5
1	D	389	LYS	3.5
1	D	157	VAL	3.5
1	B	86	GLU	3.4
1	B	319	LEU	3.4
1	B	84	ILE	3.4
1	A	95	GLN	3.3
1	B	368	ILE	3.3
1	A	355	ASN	3.3
1	D	336	ALA	3.1
1	D	3	GLN	3.1
1	D	99	VAL	3.1
1	D	62	VAL	3.1
1	D	131	VAL	3.1
1	D	132	VAL	3.1
1	D	1	MET	3.0
1	D	26	HIS	3.0
1	D	148	MET	3.0
1	B	171	THR	2.9
1	C	1	MET	2.9
1	B	59	GLY	2.9
1	B	306	PHE	2.9
1	A	318	ASN	2.9
1	B	385	LEU	2.8
1	D	72	THR	2.8
1	D	85	THR	2.8
1	C	4	GLN	2.8
1	D	388	LEU	2.8
1	D	84	ILE	2.8
1	D	364	PRO	2.8
1	B	308	GLU	2.8
1	B	304	PRO	2.7
1	D	95	GLN	2.7
1	D	34	ASP	2.7
1	B	3	GLN	2.7
1	B	31	PHE	2.7
1	B	360	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	311	ALA	2.7
1	D	342	ARG	2.7
1	B	383	VAL	2.6
1	B	124	ASP	2.6
1	B	379	ALA	2.6
1	C	95	GLN	2.6
1	D	149	ILE	2.6
1	B	102	ALA	2.6
1	B	367	ASN	2.6
1	D	210	VAL	2.6
1	D	94	SER	2.6
1	B	372	SER	2.6
1	C	320	ASP	2.6
1	D	356	GLY	2.6
1	D	318	ASN	2.6
1	A	320	ASP	2.6
1	B	316	GLU	2.6
1	D	358	ILE	2.6
1	D	380	VAL	2.5
1	B	67	GLY	2.5
1	A	67	GLY	2.5
1	D	64	ILE	2.5
1	D	29	LEU	2.5
1	D	73	LEU	2.5
1	B	28	GLU	2.5
1	B	175	TYR	2.5
1	A	96	ASN	2.5
1	B	9	LEU	2.5
1	D	97	LYS	2.5
1	D	130	VAL	2.5
1	C	54	ASN	2.5
1	D	92	PHE	2.5
1	D	366	PHE	2.5
1	B	246	PHE	2.5
1	B	33	GLU	2.4
1	B	362	HIS	2.4
1	A	246	PHE	2.4
1	B	23	LEU	2.4
1	B	35	GLU	2.4
1	D	146	LYS	2.4
1	D	340	LYS	2.4
1	D	164	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	346	PHE	2.4
1	D	144	GLY	2.4
1	C	2	ASN	2.4
1	B	54	ASN	2.4
1	B	42	GLU	2.4
1	B	369	SER	2.4
1	C	98	GLY	2.4
1	D	76	ARG	2.3
1	D	187	PHE	2.3
1	B	217	THR	2.3
1	A	7	GLU	2.3
1	D	77	ALA	2.3
1	A	88	THR	2.2
1	D	51	VAL	2.2
1	D	25	GLN	2.2
1	C	34	ASP	2.2
1	B	5	LEU	2.2
1	B	10	LYS	2.2
1	B	365	LYS	2.2
1	C	317	ALA	2.2
1	D	56	GLY	2.2
1	D	124	ASP	2.2
1	A	93	ALA	2.2
1	B	6	ILE	2.1
1	B	71	LYS	2.1
1	D	341	GLU	2.1
1	C	70	GLY	2.1
1	C	318	ASN	2.1
1	B	4	GLN	2.1
1	D	156	GLY	2.1
1	D	88	THR	2.1
1	B	72	THR	2.1
1	D	7	GLU	2.1
1	D	381	GLY	2.1
1	B	361	HIS	2.1
1	D	217	THR	2.1
1	A	34	ASP	2.0
1	B	55	VAL	2.0
1	B	315	LYS	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. 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
4	PE7	B	403	22/22	0.76	0.24	54,62,67,67	0
4	PE7	B	404	22/22	0.86	0.18	40,48,56,61	0
4	PE7	D	403	22/22	0.87	0.17	35,38,52,58	0
3	PEG	A	403	7/7	0.93	0.21	36,36,39,41	0
2	MN	B	401	1/1	0.93	0.12	69,69,69,69	0
2	MN	B	402	1/1	0.94	0.09	48,48,48,48	0
2	MN	C	401	1/1	0.95	0.04	49,49,49,49	0
2	MN	A	401	1/1	0.95	0.09	55,55,55,55	0
2	MN	D	401	1/1	0.96	0.07	57,57,57,57	0
2	MN	A	402	1/1	0.98	0.14	35,35,35,35	0
2	MN	D	402	1/1	0.99	0.14	35,35,35,35	0
2	MN	C	402	1/1	0.99	0.11	35,35,35,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
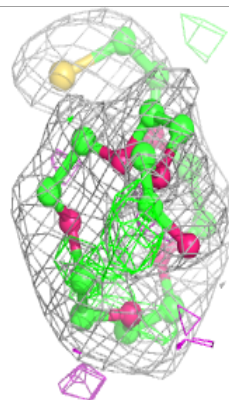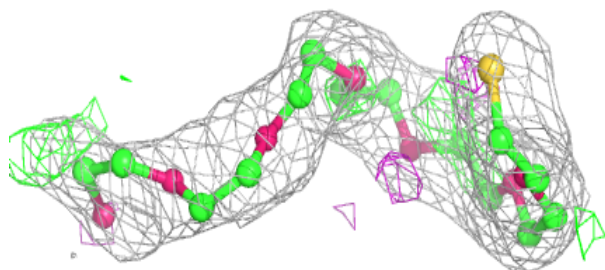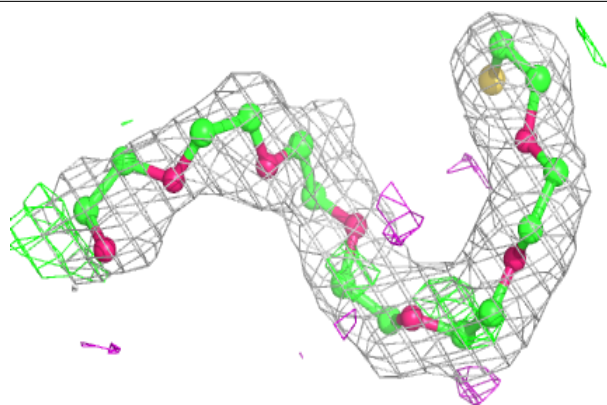
Electron density around PE7 B 403:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
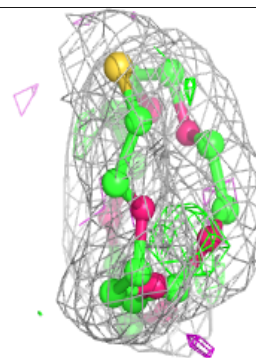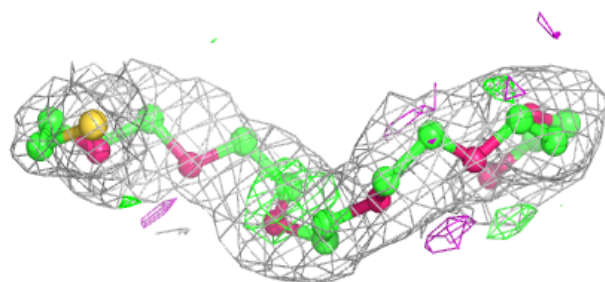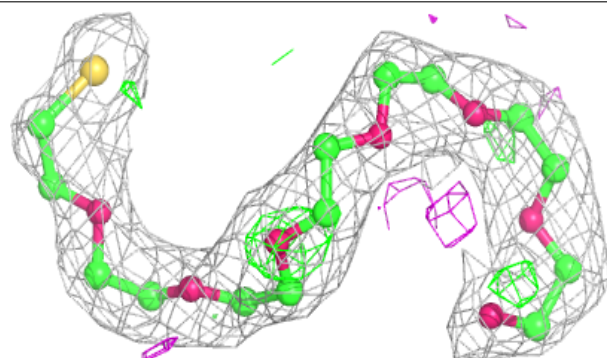and green (positive)
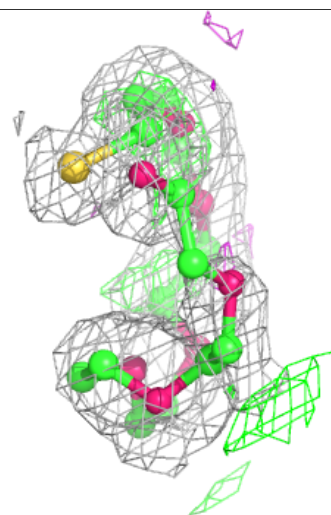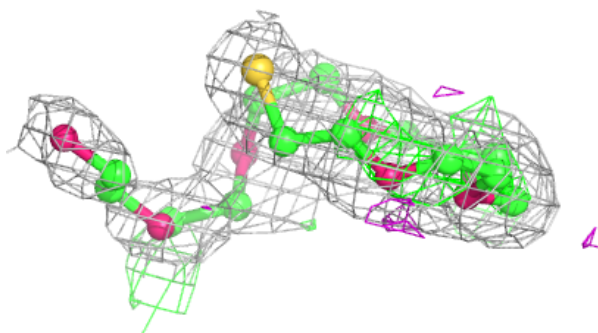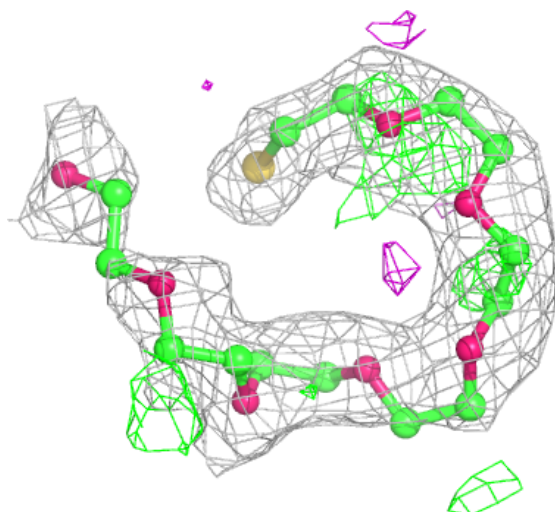
Electron density around PE7 B 404:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around PE7 D 403:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers (i)

There are no such residues in this entry.