Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2023 – 06:51 PM JST

PDB ID	:	7WU1
Title	:	Crystal structure of phospholipase D from Moritella sp. JT01
Authors	:	Wang, Y.H.; Mao, X.J.; Wang, J.; Wang, F.H.
Deposited on	:	2022-02-05
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

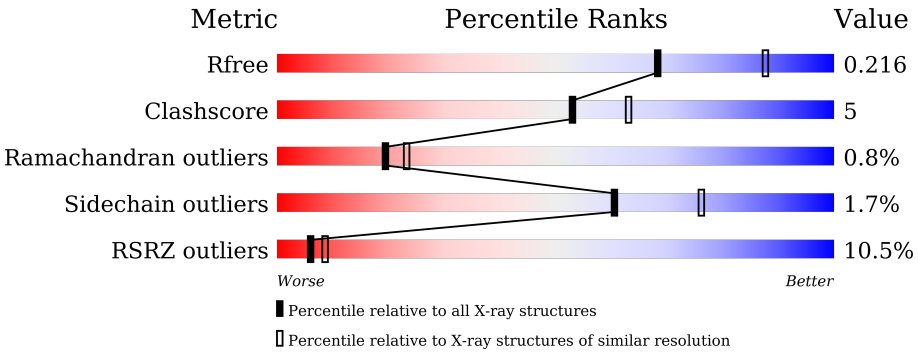
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	557	7% 89% 7%
1	B	557	11% 87% 9%
1	C	557	10% 88% 7%
1	D	557	12% 85% 10%
1	E	557	11% 89% 8%
1	F	557	11% 86% 10%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	C	610	-	-	-	X
3	NA	D	608	-	-	-	X
3	NA	E	601	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 51186 atoms, of which 24695 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 Phospholipase D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	538	Total	C	H	N	O	S	0	0	0
			8294	2661	4085	703	831	14			
1	B	542	Total	C	H	N	O	S	0	0	0
			8351	2679	4113	707	837	15			
1	C	542	Total	C	H	N	O	S	0	0	0
			8354	2682	4111	708	838	15			
1	D	542	Total	C	H	N	O	S	0	0	0
			8346	2677	4108	708	838	15			
1	E	545	Total	C	H	N	O	S	0	0	0
			8395	2694	4133	711	842	15			
1	F	545	Total	C	H	N	O	S	0	0	0
			8395	2694	4133	711	842	15			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP A0A137SLD1
A	2	HIS	-	expression tag	UNP A0A137SLD1
A	3	HIS	-	expression tag	UNP A0A137SLD1
A	4	HIS	-	expression tag	UNP A0A137SLD1
A	5	HIS	-	expression tag	UNP A0A137SLD1
A	6	HIS	-	expression tag	UNP A0A137SLD1
A	7	HIS	-	expression tag	UNP A0A137SLD1
B	1	MET	-	expression tag	UNP A0A137SLD1
B	2	HIS	-	expression tag	UNP A0A137SLD1
B	3	HIS	-	expression tag	UNP A0A137SLD1
B	4	HIS	-	expression tag	UNP A0A137SLD1
B	5	HIS	-	expression tag	UNP A0A137SLD1
B	6	HIS	-	expression tag	UNP A0A137SLD1
B	7	HIS	-	expression tag	UNP A0A137SLD1
C	1	MET	-	expression tag	UNP A0A137SLD1
C	2	HIS	-	expression tag	UNP A0A137SLD1
C	3	HIS	-	expression tag	UNP A0A137SLD1

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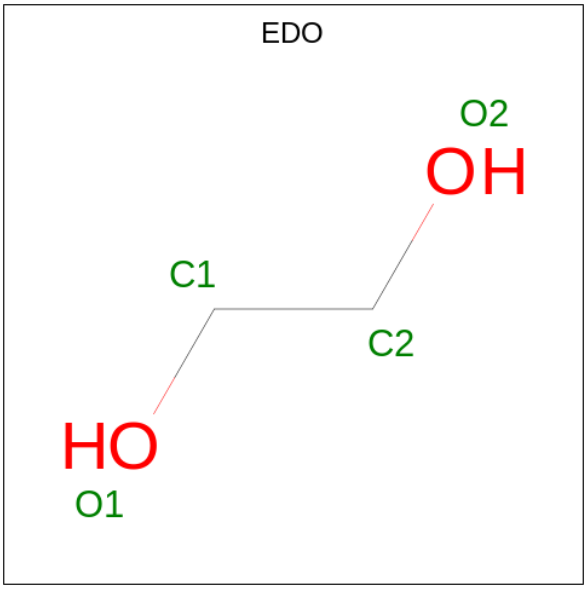
Chain	Residue	Modelled	Actual	Comment	Reference
C	4	HIS	-	expression tag	UNP A0A137SLD1
C	5	HIS	-	expression tag	UNP A0A137SLD1
C	6	HIS	-	expression tag	UNP A0A137SLD1
C	7	HIS	-	expression tag	UNP A0A137SLD1
D	1	MET	-	expression tag	UNP A0A137SLD1
D	2	HIS	-	expression tag	UNP A0A137SLD1
D	3	HIS	-	expression tag	UNP A0A137SLD1
D	4	HIS	-	expression tag	UNP A0A137SLD1
D	5	HIS	-	expression tag	UNP A0A137SLD1
D	6	HIS	-	expression tag	UNP A0A137SLD1
D	7	HIS	-	expression tag	UNP A0A137SLD1
E	1	MET	-	expression tag	UNP A0A137SLD1
E	2	HIS	-	expression tag	UNP A0A137SLD1
E	3	HIS	-	expression tag	UNP A0A137SLD1
E	4	HIS	-	expression tag	UNP A0A137SLD1
E	5	HIS	-	expression tag	UNP A0A137SLD1
E	6	HIS	-	expression tag	UNP A0A137SLD1
E	7	HIS	-	expression tag	UNP A0A137SLD1
F	1	MET	-	expression tag	UNP A0A137SLD1
F	2	HIS	-	expression tag	UNP A0A137SLD1
F	3	HIS	-	expression tag	UNP A0A137SLD1
F	4	HIS	-	expression tag	UNP A0A137SLD1
F	5	HIS	-	expression tag	UNP A0A137SLD1
F	6	HIS	-	expression tag	UNP A0A137SLD1
F	7	HIS	-	expression tag	UNP A0A137SLD1

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total Na 9 9	0	0
3	B	10	Total Na 10 10	0	0
3	C	11	Total Na 11 11	0	0
3	D	8	Total Na 8 8	0	0
3	E	3	Total Na 3 3	0	0
3	F	6	Total Na 6 6	0	0

- Molecule 4 is water.

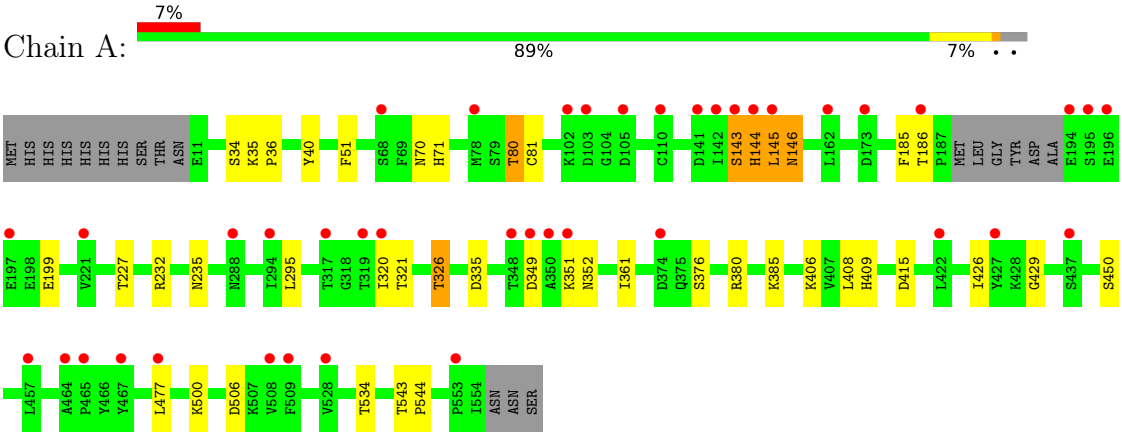
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	256	Total O 256 256	0	0
4	B	146	Total O 146 146	0	0
4	C	198	Total O 198 198	0	0
4	D	144	Total O 144 144	0	0
4	E	146	Total O 146 146	0	0
4	F	94	Total O 94 94	0	0

3 Residue-property plots (i)

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

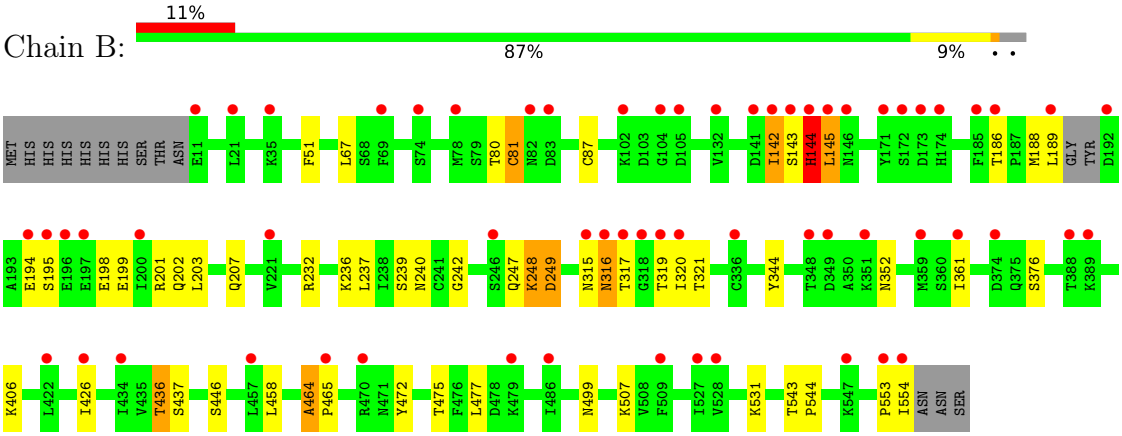
• Molecule 1: Phospholipase D

Chain A:



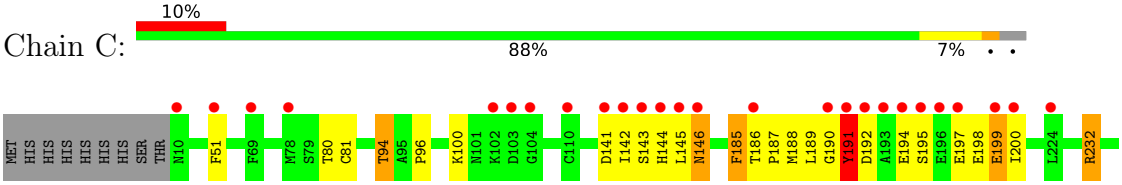
• Molecule 1: Phospholipase D

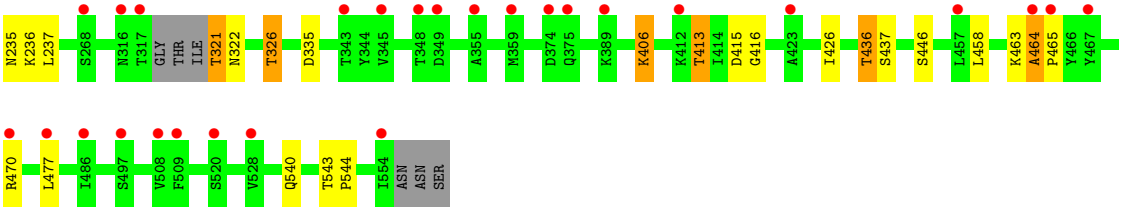
Chain B:



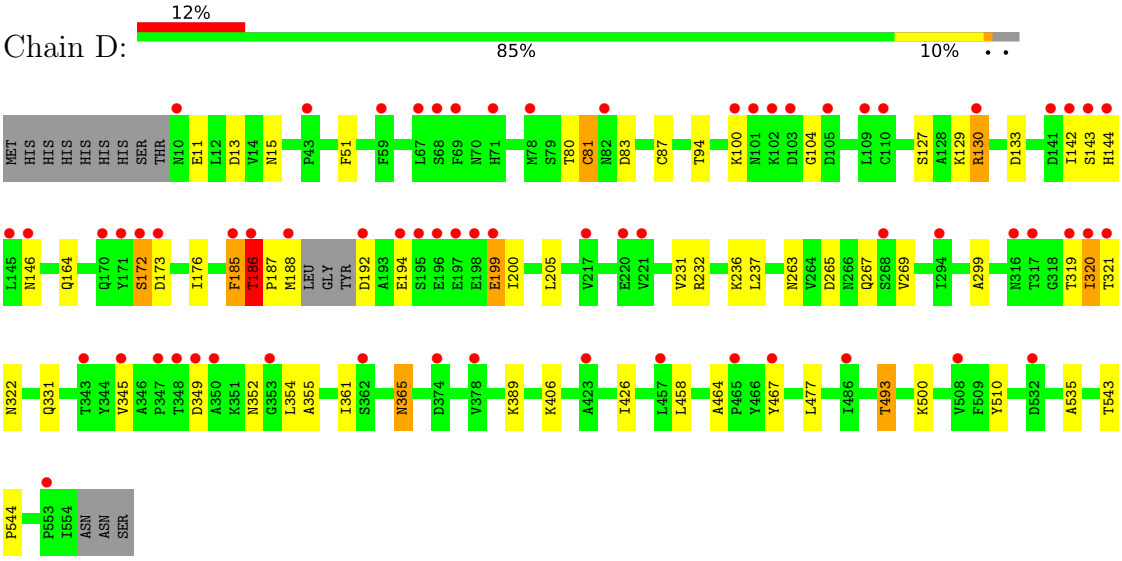
• Molecule 1: Phospholipase D

Chain C:

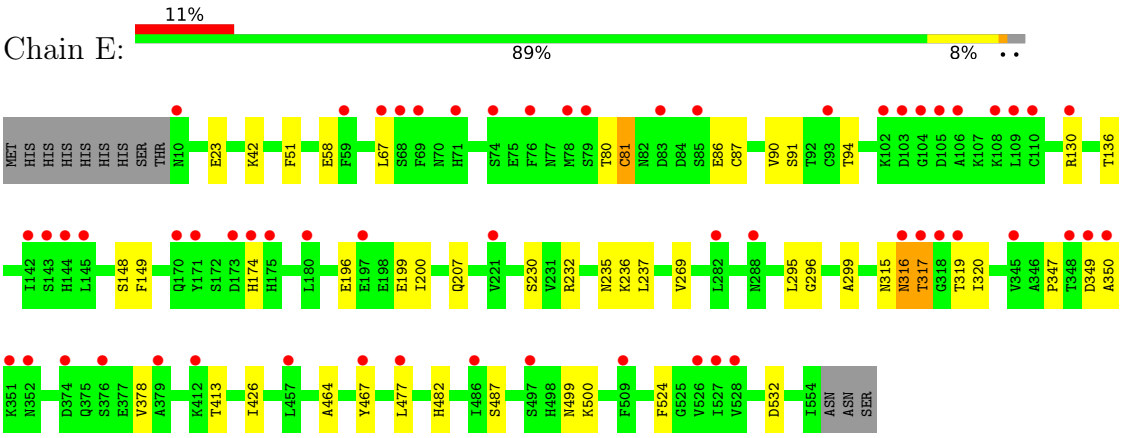




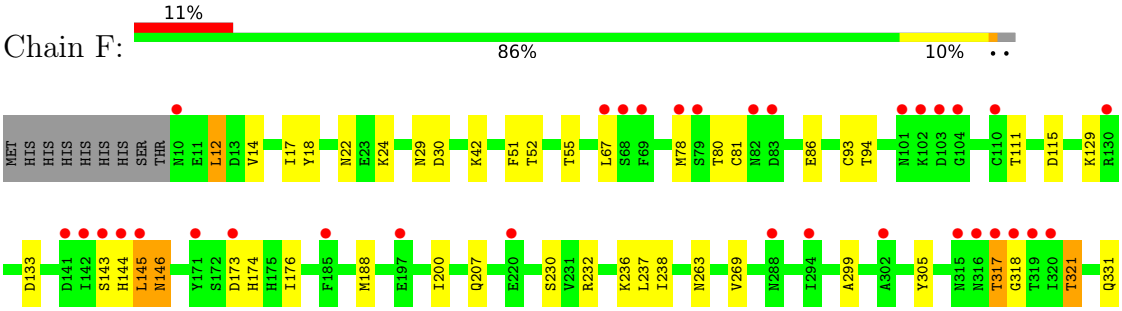
• Molecule 1: Phospholipase D

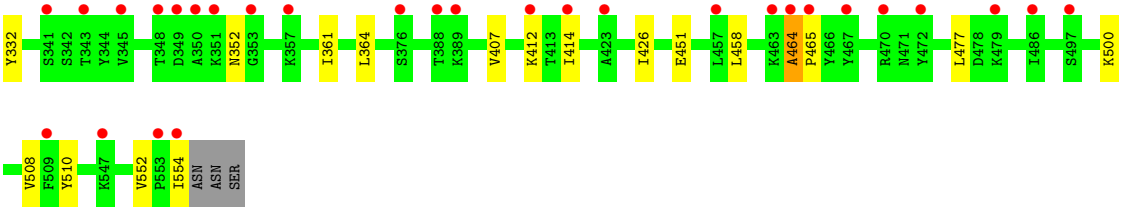


• Molecule 1: Phospholipase D



• Molecule 1: Phospholipase D




Y332
S341
S342
T343
Y344
V345
T348
D349
A350
K351
N352
G353
K357
I361
L364
S376
T388
K389
V407
K412
T413
I414
A423
I426
E451
L457
L458
K463
A464
P465
Y466
Y467
R470
N471
Y472
L477
D478
K479
I486
S497
K500

V508
F509
Y510
K547
V552
P553
I554
ASN
ASN
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.90Å 216.64Å 277.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 2.30 19.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.81-2.30) 99.9 (19.81-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.30Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.212 , 0.216 0.212 , 0.216	Depositor DCC
R_{free} test set	2000 reflections (0.80%)	wwPDB-VP
Wilson B-factor (Å^2)	66.3	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	51186	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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

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	0.59	2/4299 (0.0%)	0.62	0/5850
1	B	0.51	1/4328 (0.0%)	0.59	1/5889 (0.0%)
1	C	0.54	1/4334 (0.0%)	0.61	0/5897
1	D	0.48	1/4328 (0.0%)	0.59	2/5889 (0.0%)
1	E	0.47	1/4354 (0.0%)	0.56	0/5926
1	F	0.44	1/4354 (0.0%)	0.55	0/5926
All	All	0.51	7/25997 (0.0%)	0.59	3/35377 (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	A	0	2
1	B	0	3
1	C	0	4
1	D	0	2
1	E	0	1
1	F	0	1
All	All	0	13

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	CYS	CB-SG	-13.21	1.59	1.82
1	C	81	CYS	CB-SG	-10.54	1.64	1.82
1	E	81	CYS	CB-SG	-8.30	1.68	1.82
1	B	81	CYS	CB-SG	-7.86	1.68	1.82
1	D	81	CYS	CB-SG	-6.22	1.71	1.82
1	F	81	CYS	CB-SG	-5.61	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	PHE	C-N	5.34	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	186	THR	C-N-CD	-8.19	102.58	120.60
1	B	249	ASP	CB-CG-OD1	6.12	123.81	118.30
1	D	186	THR	C-N-CA	5.82	146.43	122.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	LEU	Peptide
1	A	80	THR	Peptide
1	B	145	LEU	Peptide
1	B	248	LYS	Peptide
1	B	80	THR	Peptide
1	C	185	PHE	Peptide
1	C	191	TYR	Peptide
1	C	463	LYS	Peptide
1	C	80	THR	Peptide
1	D	185	PHE	Peptide
1	D	80	THR	Peptide
1	E	80	THR	Peptide
1	F	80	THR	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	4209	4085	4084	33	0
1	B	4238	4113	4113	54	0
1	C	4243	4111	4109	52	0
1	D	4238	4108	4108	61	0
1	E	4262	4133	4132	31	0
1	F	4262	4133	4132	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	8	12	12	2	0
3	A	9	0	0	0	0
3	B	10	0	0	0	0
3	C	11	0	0	0	0
3	D	8	0	0	0	0
3	E	3	0	0	0	0
3	F	6	0	0	0	0
4	A	256	0	0	6	0
4	B	146	0	0	7	0
4	C	198	0	0	2	1
4	D	144	0	0	6	0
4	E	146	0	0	7	1
4	F	94	0	0	1	0
All	All	26491	24695	24690	269	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (269) 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:100:LYS:NZ	1:D:164:GLN:OE1	1.83	1.11
1:D:186:THR:HG23	1:D:187:PRO:HA	1.35	1.08
1:D:127:SER:OG	4:D:701:HOH:O	1.85	0.93
1:D:186:THR:HG23	1:D:187:PRO:CA	2.00	0.91
1:D:186:THR:HG21	1:D:188:MET:HG2	1.56	0.88
1:C:413:THR:HG22	1:C:415:ASP:H	1.39	0.86
1:B:472:TYR:O	1:B:475:THR:HG22	1.74	0.85
1:E:482:HIS:ND1	4:E:704:HOH:O	2.10	0.84
1:A:227:THR:HG23	1:A:326:THR:HG22	1.61	0.82
1:F:200:ILE:HD11	1:F:321:THR:HG23	1.63	0.81
1:E:315:ASN:O	1:E:317:THR:N	2.14	0.81
1:F:207:GLN:OE1	1:F:230:SER:OG	1.97	0.81
1:F:464:ALA:HB1	1:F:465:PRO:HD2	1.61	0.81
1:F:464:ALA:HB1	1:F:465:PRO:CD	2.13	0.79
1:B:464:ALA:HB1	1:B:465:PRO:CD	2.13	0.78
1:E:317:THR:O	4:E:702:HOH:O	2.02	0.78
1:E:207:GLN:OE1	1:E:230:SER:OG	1.99	0.77
1:A:450:SER:OG	4:A:701:HOH:O	2.03	0.77
1:C:321:THR:N	4:C:702:HOH:O	2.19	0.75
1:D:142:ILE:HD12	1:D:143:SER:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:ALA:HB1	1:C:465:PRO:HD2	1.69	0.73
1:B:458:LEU:HD13	1:B:477:LEU:HD12	1.70	0.73
1:A:349:ASP:OD1	1:A:352:ASN:HB2	1.89	0.73
1:C:142:ILE:O	1:C:142:ILE:HG22	1.88	0.73
1:F:14:VAL:HA	1:F:17:ILE:HD12	1.71	0.73
1:D:263:ASN:O	4:D:702:HOH:O	2.07	0.72
1:D:361:ILE:HD11	1:D:510:TYR:HE2	1.53	0.72
1:B:464:ALA:HB1	1:B:465:PRO:HD2	1.70	0.72
1:E:58:GLU:O	4:E:703:HOH:O	2.06	0.72
1:C:232:ARG:NH1	1:C:321:THR:O	2.22	0.72
1:A:409:HIS:ND1	4:A:704:HOH:O	2.22	0.72
1:D:406:LYS:NZ	4:D:705:HOH:O	2.23	0.72
1:F:361:ILE:HD11	1:F:510:TYR:HE1	1.55	0.72
1:C:326:THR:HG21	1:C:335:ASP:O	1.91	0.71
1:C:464:ALA:HB1	1:C:465:PRO:CD	2.20	0.71
1:D:361:ILE:HD12	1:D:361:ILE:O	1.90	0.70
1:F:407:VAL:O	4:F:701:HOH:O	2.10	0.69
1:B:142:ILE:HD13	1:B:142:ILE:H	1.57	0.69
1:A:145:LEU:HG	1:A:146:ASN:N	2.08	0.68
1:D:192:ASP:OD1	4:D:703:HOH:O	2.11	0.68
1:A:429:GLY:O	4:A:703:HOH:O	2.11	0.68
1:F:52:THR:O	1:F:55:THR:HG22	1.94	0.67
1:E:524:PHE:O	4:E:705:HOH:O	2.13	0.67
1:D:185:PHE:O	1:D:186:THR:HG22	1.94	0.66
1:C:187:PRO:HB3	1:C:199:GLU:HG3	1.77	0.66
1:F:361:ILE:HD12	1:F:361:ILE:O	1.95	0.66
1:A:199:GLU:OE1	1:A:232:ARG:NH2	2.27	0.66
1:D:11:GLU:OE2	1:D:389:LYS:NZ	2.27	0.66
1:F:317:THR:O	1:F:317:THR:HG23	1.97	0.65
1:D:186:THR:OG1	1:D:187:PRO:C	2.35	0.65
1:F:458:LEU:HD13	1:F:477:LEU:HD12	1.78	0.65
1:C:413:THR:HG22	1:C:415:ASP:N	2.12	0.65
1:A:71:HIS:H	1:A:80:THR:HG22	1.62	0.65
1:F:24:LYS:HE3	1:F:414:ILE:HD12	1.78	0.64
1:C:232:ARG:NH2	1:C:321:THR:O	2.29	0.64
1:B:315:ASN:O	1:B:317:THR:N	2.30	0.64
1:F:552:VAL:HG12	1:F:554:ILE:HG12	1.79	0.64
1:E:295:LEU:HD23	1:E:296:GLY:N	2.12	0.64
1:F:78:MET:CE	1:F:111:THR:HG22	2.27	0.64
1:F:361:ILE:HD11	1:F:510:TYR:CE1	2.33	0.63
1:C:142:ILE:O	1:C:144:HIS:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:THR:CG2	1:C:415:ASP:H	2.12	0.62
1:A:70:ASN:HB3	1:A:80:THR:HG22	1.81	0.62
1:F:12:LEU:HD12	1:F:508:VAL:HG21	1.81	0.62
1:B:240:ASN:OD1	1:B:242:GLY:N	2.32	0.61
1:B:188:MET:HG3	1:B:199:GLU:HG2	1.82	0.61
1:D:361:ILE:HD11	1:D:510:TYR:CE2	2.35	0.60
1:B:236:LYS:O	1:B:237:LEU:HB2	2.02	0.59
1:B:464:ALA:CB	1:B:465:PRO:CD	2.80	0.59
1:D:186:THR:HG22	1:D:232:ARG:NH2	2.16	0.59
1:B:198:GLU:OE1	1:B:201:ARG:NH1	2.36	0.59
1:B:239:SER:HA	1:C:191:TYR:HE2	1.67	0.59
1:B:189:LEU:HD11	1:C:406:LYS:HD3	1.83	0.59
1:F:464:ALA:CB	1:F:465:PRO:CD	2.81	0.58
1:C:436:THR:CG2	1:C:437:SER:O	2.51	0.58
1:E:487:SER:O	4:E:707:HOH:O	2.17	0.58
1:D:172:SER:O	1:D:173:ASP:HB2	2.04	0.58
1:B:142:ILE:O	1:B:143:SER:OG	2.13	0.58
1:A:227:THR:CG2	1:A:326:THR:HG22	2.33	0.58
1:B:344:TYR:CE2	4:B:701:HOH:O	2.56	0.57
1:D:426:ILE:HG21	1:D:477:LEU:HD23	1.87	0.57
1:E:235:ASN:CG	1:E:320:ILE:HD11	2.24	0.57
1:C:190:GLY:N	4:C:701:HOH:O	2.17	0.56
1:F:78:MET:HE2	1:F:111:THR:HG22	1.87	0.56
1:C:191:TYR:HA	1:C:192:ASP:CG	2.25	0.56
1:C:232:ARG:NH2	1:C:321:THR:HG22	2.19	0.56
1:C:464:ALA:CB	1:C:465:PRO:HD2	2.35	0.56
1:C:464:ALA:CB	1:C:465:PRO:CD	2.83	0.56
1:F:42:LYS:HE3	1:F:352:ASN:ND2	2.20	0.56
1:C:200:ILE:HD11	1:C:321:THR:O	2.07	0.55
1:B:436:THR:HG21	4:B:773:HOH:O	2.06	0.55
1:B:248:LYS:HB3	1:C:191:TYR:HB2	1.88	0.55
1:C:232:ARG:CZ	1:C:321:THR:O	2.55	0.55
1:C:188:MET:HE3	1:C:188:MET:HA	1.89	0.54
1:F:464:ALA:CB	1:F:465:PRO:HD2	2.33	0.54
1:A:326:THR:HG21	1:A:335:ASP:O	2.07	0.54
1:C:436:THR:HG22	1:C:437:SER:O	2.08	0.54
1:B:507:LYS:HD2	1:B:531:LYS:HD3	1.88	0.54
1:D:200:ILE:HD11	1:D:321:THR:HA	1.90	0.54
1:D:172:SER:OG	1:D:173:ASP:N	2.38	0.54
1:D:319:THR:HB	1:D:320:ILE:HD12	1.88	0.54
1:C:190:GLY:O	1:C:191:TYR:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:LEU:HD12	1:D:355:ALA:N	2.22	0.54
1:F:426:ILE:HG21	1:F:477:LEU:HD23	1.89	0.54
1:A:143:SER:O	1:A:144:HIS:O	2.26	0.53
1:F:78:MET:HE2	1:F:111:THR:HA	1.90	0.53
1:A:35:LYS:HD3	1:A:36:PRO:HD2	1.90	0.53
1:F:12:LEU:CD1	1:F:508:VAL:HG21	2.39	0.53
1:C:413:THR:HB	1:C:416:GLY:O	2.08	0.53
1:B:144:HIS:CE1	1:B:145:LEU:HD13	2.44	0.53
1:B:436:THR:CG2	1:B:437:SER:O	2.56	0.53
1:C:436:THR:HG23	1:C:446:SER:HB3	1.89	0.53
1:D:265:ASP:O	1:D:267:GLN:HG3	2.08	0.53
1:B:67:LEU:HD22	1:B:67:LEU:H	1.72	0.53
1:B:144:HIS:CG	1:B:145:LEU:H	2.27	0.53
1:D:185:PHE:O	1:D:188:MET:HE2	2.09	0.52
1:E:236:LYS:O	1:E:237:LEU:HB2	2.09	0.52
1:F:78:MET:HE1	1:F:111:THR:HG22	1.91	0.52
1:B:142:ILE:O	1:B:142:ILE:HG12	2.10	0.52
1:C:426:ILE:HG21	1:C:477:LEU:HD23	1.91	0.52
1:D:320:ILE:HG22	1:D:321:THR:H	1.75	0.51
1:B:436:THR:HG22	1:B:437:SER:O	2.10	0.51
1:D:320:ILE:HD12	1:D:320:ILE:N	2.25	0.51
1:B:189:LEU:CD1	1:C:406:LYS:HD3	2.39	0.51
1:B:458:LEU:HD13	1:B:477:LEU:CD1	2.40	0.51
1:D:192:ASP:N	4:D:703:HOH:O	2.43	0.51
1:D:100:LYS:HE3	1:D:104:GLY:HA2	1.91	0.51
1:D:186:THR:OG1	1:D:187:PRO:O	2.27	0.51
1:A:426:ILE:HG21	1:A:477:LEU:HD23	1.93	0.51
1:B:247:GLN:OE1	4:B:702:HOH:O	2.19	0.51
1:C:142:ILE:O	1:C:142:ILE:CG2	2.58	0.51
1:D:81:CYS:SG	1:D:87:CYS:SG	3.09	0.51
1:D:186:THR:CG2	1:D:199:GLU:OE2	2.59	0.50
1:C:470:ARG:HG3	1:C:470:ARG:HH11	1.77	0.50
1:A:199:GLU:OE1	1:A:232:ARG:NH1	2.41	0.50
1:B:315:ASN:O	1:B:316:ASN:C	2.50	0.50
1:D:236:LYS:O	1:D:237:LEU:HB2	2.10	0.50
1:B:142:ILE:C	1:B:143:SER:HG	2.10	0.49
1:D:232:ARG:NH1	1:D:321:THR:HG21	2.28	0.49
1:E:90:VAL:O	1:E:90:VAL:HG22	2.12	0.49
1:F:451:GLU:OE1	1:F:554:ILE:HG21	2.13	0.49
1:D:205:LEU:HD11	1:F:332:TYR:O	2.13	0.49
1:E:349:ASP:OD1	1:E:349:ASP:O	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:TYR:OH	1:C:194:GLU:HG2	2.12	0.49
1:F:18:TYR:CZ	1:F:22:ASN:ND2	2.81	0.49
1:F:176:ILE:N	1:F:176:ILE:HD12	2.28	0.49
1:C:188:MET:SD	1:C:235:ASN:OD1	2.71	0.48
1:B:319:THR:HG23	1:B:320:ILE:H	1.78	0.48
1:E:199:GLU:OE2	1:E:232:ARG:NH1	2.46	0.48
1:E:269:VAL:HG21	1:E:299:ALA:HA	1.96	0.48
1:A:543:THR:HB	1:A:544:PRO:HD3	1.94	0.48
1:B:464:ALA:CB	1:B:465:PRO:HD2	2.41	0.48
1:B:344:TYR:OH	4:B:701:HOH:O	1.85	0.47
1:C:185:PHE:CD1	1:C:186:THR:HA	2.50	0.47
1:B:361:ILE:HG13	1:B:376:SER:HA	1.95	0.47
1:B:188:MET:HG3	1:B:199:GLU:OE2	2.15	0.47
1:C:543:THR:HB	1:C:544:PRO:HD3	1.97	0.47
1:F:22:ASN:HD21	1:F:29:ASN:ND2	2.13	0.47
1:C:191:TYR:CD1	1:C:192:ASP:N	2.83	0.47
1:C:195:SER:O	1:C:199:GLU:HG2	2.15	0.47
1:E:464:ALA:HB2	1:E:467:TYR:CZ	2.50	0.47
1:B:426:ILE:HG21	1:B:477:LEU:HD23	1.96	0.47
1:E:347:PRO:HD2	1:E:350:ALA:HB2	1.96	0.47
1:E:42:LYS:HB3	1:E:42:LYS:HE2	1.78	0.46
1:B:143:SER:O	1:B:144:HIS:O	2.33	0.46
1:B:319:THR:HG23	1:B:320:ILE:N	2.31	0.46
1:E:148:SER:HB3	1:E:149:PHE:CD2	2.50	0.46
1:E:237:LEU:HD12	1:F:238:ILE:HG22	1.98	0.46
1:F:317:THR:O	1:F:317:THR:CG2	2.63	0.46
1:D:458:LEU:HD13	1:D:477:LEU:HD12	1.98	0.46
1:C:458:LEU:HD23	1:C:470:ARG:CZ	2.46	0.46
1:C:436:THR:HG23	1:C:437:SER:O	2.17	0.45
1:B:543:THR:HB	1:B:544:PRO:HD3	1.98	0.45
1:D:320:ILE:HG22	1:D:321:THR:N	2.31	0.45
1:B:232:ARG:NH2	1:B:321:THR:O	2.50	0.45
1:F:305:TYR:CE1	1:F:364:LEU:HD21	2.51	0.45
1:B:317:THR:O	1:B:317:THR:HG22	2.17	0.45
1:B:499:ASN:HA	4:B:719:HOH:O	2.16	0.45
1:E:81:CYS:SG	1:E:87:CYS:SG	3.15	0.45
1:E:378:VAL:HG22	1:E:413:THR:HB	1.97	0.45
1:F:317:THR:HA	1:F:318:GLY:HA2	1.59	0.45
1:D:13:ASP:OD2	1:D:15:ASN:HB2	2.17	0.45
1:A:385:LYS:NZ	1:A:415:ASP:O	2.49	0.45
1:D:186:THR:HG23	1:D:187:PRO:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:426:ILE:HG21	1:E:477:LEU:HD23	2.00	0.44
1:B:248:LYS:O	1:B:249:ASP:HB3	2.17	0.44
1:B:436:THR:HG23	1:B:446:SER:HB3	1.99	0.44
1:D:535:ALA:O	4:D:704:HOH:O	2.21	0.44
1:B:344:TYR:CZ	4:B:701:HOH:O	2.52	0.44
1:D:543:THR:HB	1:D:544:PRO:HD3	2.00	0.44
2:A:602:EDO:C2	4:A:923:HOH:O	2.64	0.44
1:B:249:ASP:HB3	1:B:406:LYS:NZ	2.33	0.44
1:C:197:GLU:HG2	1:C:198:GLU:H	1.81	0.44
1:A:385:LYS:HE2	1:A:385:LYS:HB2	1.78	0.44
1:D:133:ASP:HB3	1:D:263:ASN:HB3	1.99	0.44
1:D:186:THR:CG2	1:D:187:PRO:CA	2.84	0.44
1:D:464:ALA:HB2	1:D:467:TYR:CZ	2.52	0.44
1:F:145:LEU:O	1:F:146:ASN:C	2.56	0.44
1:C:232:ARG:NH1	1:C:322:ASN:HA	2.33	0.44
1:F:67:LEU:HD12	1:F:86:GLU:O	2.17	0.44
1:E:136:THR:OG1	4:E:706:HOH:O	2.16	0.43
1:E:315:ASN:O	1:E:316:ASN:C	2.57	0.43
1:C:470:ARG:HG3	1:C:470:ARG:NH1	2.31	0.43
1:A:144:HIS:CG	1:A:145:LEU:H	2.36	0.43
1:B:248:LYS:CB	1:C:191:TYR:HB2	2.46	0.43
1:D:269:VAL:HG21	1:D:299:ALA:HA	1.99	0.43
1:A:186:THR:O	1:A:186:THR:HG23	2.17	0.43
1:A:232:ARG:HH11	1:A:235:ASN:ND2	2.17	0.43
1:A:361:ILE:CG1	1:A:376:SER:HA	2.48	0.43
1:D:142:ILE:HD12	1:D:143:SER:HB3	2.00	0.43
1:C:185:PHE:CE1	1:C:189:LEU:HD22	2.54	0.43
1:D:185:PHE:HD2	1:D:186:THR:HB	1.83	0.43
1:B:203:LEU:O	1:B:207:GLN:HG3	2.18	0.43
1:B:361:ILE:CG1	1:B:376:SER:HA	2.49	0.43
1:F:133:ASP:HB3	1:F:263:ASN:HB3	2.00	0.43
1:A:232:ARG:NH1	1:A:321:THR:HG21	2.34	0.43
1:D:231:VAL:HA	1:D:322:ASN:OD1	2.19	0.43
1:B:553:PRO:O	1:B:554:ILE:HB	2.19	0.42
1:D:142:ILE:HD12	1:D:143:SER:CA	2.49	0.42
1:F:236:LYS:O	1:F:237:LEU:HB2	2.19	0.42
2:A:602:EDO:H21	4:A:923:HOH:O	2.18	0.42
1:F:269:VAL:HG21	1:F:299:ALA:HA	2.00	0.42
1:F:129:LYS:O	1:F:174:HIS:HE1	2.03	0.42
1:B:202:GLN:NE2	4:B:705:HOH:O	2.36	0.42
1:E:196:GLU:O	1:E:200:ILE:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LYS:HZ1	1:A:415:ASP:HB3	1.85	0.42
1:C:236:LYS:O	1:C:237:LEU:HB2	2.20	0.42
1:E:87:CYS:HB3	1:E:91:SER:OG	2.19	0.42
1:A:34:SER:OG	4:A:702:HOH:O	2.07	0.42
1:C:458:LEU:HD13	1:C:477:LEU:HD12	2.02	0.42
1:D:185:PHE:O	1:D:232:ARG:NH2	2.53	0.42
1:B:186:THR:HB	1:B:232:ARG:HD2	2.01	0.42
1:D:130:ARG:HE	1:D:130:ARG:HB3	1.56	0.42
1:D:345:VAL:HG23	1:D:345:VAL:O	2.18	0.42
1:D:493:THR:HG23	1:D:493:THR:O	2.19	0.42
1:A:506:ASP:C	1:A:534:THR:HG21	2.40	0.42
1:E:67:LEU:HD11	1:E:86:GLU:HA	2.02	0.42
1:D:176:ILE:N	1:D:176:ILE:HD12	2.35	0.41
1:A:145:LEU:CG	1:A:146:ASN:N	2.80	0.41
1:D:319:THR:CB	1:D:320:ILE:HD12	2.50	0.41
1:B:67:LEU:HD22	1:B:67:LEU:N	2.34	0.41
1:A:385:LYS:NZ	1:A:415:ASP:HB3	2.35	0.41
1:C:188:MET:HA	1:C:188:MET:CE	2.50	0.41
1:C:232:ARG:HH12	1:C:322:ASN:HA	1.85	0.41
1:D:83:ASP:C	1:D:83:ASP:OD1	2.59	0.41
1:F:188:MET:HB2	1:F:188:MET:HE2	1.69	0.41
1:A:145:LEU:HG	1:A:146:ASN:H	1.85	0.41
1:F:67:LEU:HD12	1:F:86:GLU:C	2.41	0.41
1:C:199:GLU:N	1:C:199:GLU:OE1	2.54	0.41
1:D:349:ASP:OD2	1:D:352:ASN:ND2	2.48	0.41
1:E:316:ASN:O	1:E:317:THR:C	2.58	0.41
1:B:81:CYS:SG	1:B:87:CYS:SG	3.19	0.41
1:D:192:ASP:HB3	1:D:194:GLU:OE1	2.21	0.41
1:E:130:ARG:HG3	1:E:130:ARG:HH11	1.85	0.41
1:D:127:SER:O	1:D:129:LYS:HE2	2.20	0.40
1:A:295:LEU:HD23	1:A:295:LEU:C	2.42	0.40
1:E:235:ASN:ND2	1:E:320:ILE:HD11	2.36	0.40
1:A:326:THR:CG2	1:A:335:ASP:O	2.70	0.40
1:A:406:LYS:HE3	1:A:408:LEU:HD21	2.03	0.40
1:B:194:GLU:OE2	1:B:195:SER:HB2	2.22	0.40
1:D:185:PHE:O	1:D:186:THR:CG2	2.65	0.40
1:D:200:ILE:CD1	1:D:321:THR:HA	2.49	0.40
1:C:94:THR:HG22	1:C:96:PRO:HD3	2.03	0.40
1:C:187:PRO:O	1:C:192:ASP:HA	2.22	0.40
1:E:499:ASN:HA	4:E:749:HOH:O	2.21	0.40
1:F:78:MET:CE	1:F:115:ASP:OD2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:LEU:O	1:F:145:LEU:HG	2.20	0.40
1:A:40:TYR:CE1	1:A:351:LYS:HA	2.56	0.40
1:D:186:THR:HG21	1:D:188:MET:CG	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:894:HOH:O	4:E:843:HOH:O[3_656]	1.99	0.21

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	534/557 (96%)	501 (94%)	29 (5%)	4 (1%)	22	26
1	B	538/557 (97%)	501 (93%)	34 (6%)	3 (1%)	25	31
1	C	538/557 (97%)	499 (93%)	34 (6%)	5 (1%)	17	20
1	D	538/557 (97%)	506 (94%)	27 (5%)	5 (1%)	17	20
1	E	543/557 (98%)	515 (95%)	26 (5%)	2 (0%)	34	42
1	F	543/557 (98%)	509 (94%)	28 (5%)	6 (1%)	14	15
All	All	3234/3342 (97%)	3031 (94%)	178 (6%)	25 (1%)	19	23

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	146	ASN
1	B	144	HIS
1	B	316	ASN
1	B	464	ALA

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Mol	Chain	Res	Type
1	C	146	ASN
1	C	191	TYR
1	C	464	ALA
1	D	186	THR
1	E	316	ASN
1	E	317	THR
1	F	12	LEU
1	F	144	HIS
1	F	317	THR
1	F	464	ALA
1	C	141	ASP
1	D	365	ASN
1	F	143	SER
1	F	146	ASN
1	C	143	SER
1	D	144	HIS
1	D	146	ASN
1	A	143	SER
1	A	320	ILE
1	D	320	ILE

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	475/492 (96%)	471 (99%)	4 (1%)	81	91
1	B	478/492 (97%)	473 (99%)	5 (1%)	76	87
1	C	478/492 (97%)	465 (97%)	13 (3%)	44	61
1	D	478/492 (97%)	469 (98%)	9 (2%)	57	73
1	E	480/492 (98%)	473 (98%)	7 (2%)	65	79
1	F	480/492 (98%)	469 (98%)	11 (2%)	50	67
All	All	2869/2952 (97%)	2820 (98%)	49 (2%)	60	76

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	PHE
1	A	326	THR
1	A	380	ARG
1	A	500	LYS
1	B	51	PHE
1	B	142	ILE
1	B	144	HIS
1	B	352	ASN
1	B	436	THR
1	C	51	PHE
1	C	94	THR
1	C	100	LYS
1	C	145	LEU
1	C	146	ASN
1	C	199	GLU
1	C	232	ARG
1	C	321	THR
1	C	326	THR
1	C	406	LYS
1	C	413	THR
1	C	436	THR
1	C	540	GLN
1	D	51	PHE
1	D	94	THR
1	D	130	ARG
1	D	172	SER
1	D	199	GLU
1	D	331	GLN
1	D	365	ASN
1	D	493	THR
1	D	500	LYS
1	E	23	GLU
1	E	51	PHE
1	E	94	THR
1	E	174	HIS
1	E	319	THR
1	E	500	LYS
1	E	532	ASP
1	F	30	ASP
1	F	51	PHE
1	F	93	CYS
1	F	94	THR
1	F	145	LEU

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Mol	Chain	Res	Type
1	F	173	ASP
1	F	232	ARG
1	F	321	THR
1	F	331	GLN
1	F	412	LYS
1	F	500	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	352	ASN
1	C	462	HIS
1	C	482	HIS
1	C	551	HIS
1	D	311	ASN
1	D	315	ASN
1	E	70	ASN
1	F	10	ASN
1	F	22	ASN
1	F	174	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 49 ligands modelled in this entry, 47 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	EDO	A	601	-	3,3,3	0.61	0	2,2,2	0.20	0
2	EDO	A	602	-	3,3,3	0.70	0	2,2,2	0.69	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	EDO	A	601	-	-	0/1/1/1	-
2	EDO	A	602	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	EDO	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	538/557 (96%)	0.54	41 (7%) 13 18	49, 64, 98, 155	0
1	B	542/557 (97%)	0.70	62 (11%) 5 7	54, 75, 119, 172	0
1	C	542/557 (97%)	0.68	53 (9%) 7 10	54, 70, 107, 207	0
1	D	542/557 (97%)	0.68	65 (11%) 4 6	54, 78, 121, 169	0
1	E	545/557 (97%)	0.64	59 (10%) 5 8	58, 80, 111, 153	0
1	F	545/557 (97%)	0.67	62 (11%) 5 7	61, 84, 116, 176	0
All	All	3254/3342 (97%)	0.65	342 (10%) 6 8	49, 76, 113, 207	0

All (342) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	69	PHE	10.4
1	D	142	ILE	10.2
1	A	142	ILE	9.0
1	F	317	THR	8.7
1	D	192	ASP	8.2
1	F	142	ILE	8.0
1	C	191	TYR	7.9
1	C	145	LEU	7.8
1	F	145	LEU	7.5
1	B	317	THR	7.0
1	D	145	LEU	6.9
1	D	186	THR	6.9
1	B	318	GLY	6.8
1	D	144	HIS	6.7
1	C	143	SER	6.7
1	D	143	SER	6.5
1	A	143	SER	6.4
1	D	195	SER	6.4
1	F	143	SER	6.2

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Mol	Chain	Res	Type	RSRZ
1	C	144	HIS	6.1
1	B	142	ILE	6.0
1	B	144	HIS	5.8
1	B	145	LEU	5.8
1	F	318	GLY	5.8
1	B	143	SER	5.8
1	B	319	THR	5.6
1	A	144	HIS	5.5
1	A	195	SER	5.5
1	D	348	THR	5.4
1	D	349	ASP	5.4
1	B	196	GLU	5.4
1	F	554	ILE	5.3
1	C	10	ASN	5.3
1	C	192	ASP	5.2
1	A	196	GLU	5.1
1	E	319	THR	5.0
1	C	142	ILE	4.8
1	D	171	TYR	4.8
1	D	350	ALA	4.8
1	C	186	THR	4.7
1	F	68	SER	4.5
1	E	104	GLY	4.5
1	D	69	PHE	4.5
1	A	194	GLU	4.4
1	F	171	TYR	4.4
1	D	110	CYS	4.4
1	A	197	GLU	4.3
1	C	199	GLU	4.3
1	E	78	MET	4.3
1	B	349	ASP	4.3
1	A	145	LEU	4.2
1	F	67	LEU	4.2
1	B	171	TYR	4.2
1	C	194	GLU	4.2
1	B	104	GLY	4.2
1	E	105	ASP	4.2
1	F	343	THR	4.1
1	E	142	ILE	4.1
1	F	144	HIS	4.1
1	A	349	ASP	4.1
1	C	348	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	319	THR	4.1
1	F	348	THR	4.0
1	C	457	LEU	4.0
1	F	467	TYR	4.0
1	D	141	ASP	4.0
1	D	196	GLU	4.0
1	B	69	PHE	4.0
1	D	374	ASP	3.9
1	E	350	ALA	3.9
1	E	102	LYS	3.9
1	B	189	LEU	3.9
1	C	509	PHE	3.9
1	B	146	ASN	3.9
1	E	349	ASP	3.9
1	D	10	ASN	3.9
1	D	345	VAL	3.8
1	B	348	THR	3.8
1	E	467	TYR	3.8
1	E	318	GLY	3.8
1	C	345	VAL	3.7
1	F	173	ASP	3.7
1	D	59	PHE	3.7
1	E	379	ALA	3.7
1	A	348	THR	3.7
1	D	221	VAL	3.6
1	F	110	CYS	3.6
1	F	197	GLU	3.6
1	B	194	GLU	3.5
1	D	457	LEU	3.5
1	E	10	ASN	3.5
1	B	197	GLU	3.5
1	B	320	ILE	3.5
1	E	144	HIS	3.5
1	D	317	THR	3.5
1	A	509	PHE	3.4
1	E	317	THR	3.4
1	E	68	SER	3.4
1	C	467	TYR	3.4
1	E	69	PHE	3.4
1	D	188	MET	3.4
1	C	465	PRO	3.4
1	F	349	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	103	ASP	3.4
1	E	509	PHE	3.4
1	E	143	SER	3.3
1	E	171	TYR	3.3
1	A	320	ILE	3.3
1	B	11	GLU	3.3
1	F	130	ARG	3.3
1	F	479	LYS	3.3
1	C	349	ASP	3.3
1	B	554	ILE	3.3
1	E	528	VAL	3.3
1	C	141	ASP	3.3
1	F	341	SER	3.3
1	F	388	THR	3.3
1	D	173	ASP	3.3
1	A	508	VAL	3.3
1	F	104	GLY	3.2
1	B	141	ASP	3.2
1	D	320	ILE	3.2
1	C	477	LEU	3.2
1	D	194	GLU	3.2
1	E	345	VAL	3.2
1	E	79	SER	3.2
1	F	553	PRO	3.2
1	B	457	LEU	3.2
1	E	67	LEU	3.2
1	F	78	MET	3.2
1	F	10	ASN	3.1
1	C	110	CYS	3.1
1	D	343	THR	3.1
1	B	82	ASN	3.1
1	F	423	ALA	3.1
1	A	467	TYR	3.1
1	D	78	MET	3.1
1	D	146	ASN	3.1
1	D	347	PRO	3.1
1	E	348	THR	3.1
1	F	141	ASP	3.0
1	B	173	ASP	3.0
1	B	422	LEU	3.0
1	F	320	ILE	3.0
1	E	110	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	467	TYR	3.0
1	D	197	GLU	3.0
1	B	315	ASN	3.0
1	E	106	ALA	3.0
1	F	185	PHE	3.0
1	E	221	VAL	3.0
1	B	195	SER	3.0
1	C	197	GLU	3.0
1	C	146	ASN	3.0
1	F	288	ASN	3.0
1	E	174	HIS	3.0
1	F	353	GLY	2.9
1	F	345	VAL	2.9
1	C	195	SER	2.9
1	A	317	THR	2.9
1	D	67	LEU	2.9
1	E	109	LEU	2.9
1	A	294	ILE	2.9
1	E	477	LEU	2.9
1	C	200	ILE	2.9
1	F	470	ARG	2.9
1	C	190	GLY	2.8
1	E	376	SER	2.8
1	F	79	SER	2.8
1	F	464	ALA	2.8
1	F	457	LEU	2.8
1	D	172	SER	2.8
1	E	173	ASP	2.8
1	A	78	MET	2.8
1	E	457	LEU	2.8
1	B	105	ASP	2.8
1	C	69	PHE	2.8
1	B	528	VAL	2.8
1	B	389	LYS	2.8
1	A	110	CYS	2.8
1	C	196	GLU	2.7
1	B	553	PRO	2.7
1	E	497	SER	2.7
1	E	83	ASP	2.7
1	E	103	ASP	2.7
1	B	470	ARG	2.7
1	A	351	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	141	ASP	2.6
1	F	315	ASN	2.6
1	F	547	LYS	2.6
1	C	343	THR	2.6
1	B	527	ILE	2.6
1	D	486	ILE	2.6
1	F	350	ALA	2.6
1	F	465	PRO	2.6
1	B	102	LYS	2.6
1	C	508	VAL	2.6
1	A	464	ALA	2.6
1	F	316	ASN	2.6
1	D	130	ARG	2.6
1	C	193	ALA	2.6
1	A	374	ASP	2.6
1	B	172	SER	2.6
1	B	132	VAL	2.6
1	E	175	HIS	2.6
1	F	497	SER	2.5
1	B	336	CYS	2.5
1	D	508	VAL	2.5
1	F	463	LYS	2.5
1	B	547	LYS	2.5
1	E	351	LYS	2.5
1	F	103	ASP	2.5
1	A	102	LYS	2.5
1	B	479	LYS	2.5
1	C	102	LYS	2.5
1	C	412	LYS	2.5
1	F	509	PHE	2.5
1	C	470	ARG	2.5
1	D	294	ILE	2.5
1	C	520	SER	2.5
1	D	43	PRO	2.5
1	D	465	PRO	2.5
1	F	389	LYS	2.5
1	A	477	LEU	2.5
1	D	185	PHE	2.4
1	B	186	THR	2.4
1	E	316	ASN	2.4
1	B	361	ILE	2.4
1	B	434	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	170	GLN	2.4
1	B	74	SER	2.4
1	D	268	SER	2.4
1	A	221	VAL	2.4
1	B	185	PHE	2.4
1	A	186	THR	2.4
1	C	317	THR	2.4
1	C	554	ILE	2.4
1	E	527	ILE	2.4
1	F	414	ILE	2.4
1	E	85	SER	2.4
1	D	353	GLY	2.4
1	F	486	ILE	2.4
1	D	198	GLU	2.4
1	F	351	LYS	2.4
1	D	105	ASP	2.4
1	C	528	VAL	2.4
1	C	268	SER	2.3
1	D	362	SER	2.3
1	D	103	ASP	2.3
1	E	170	GLN	2.3
1	B	21	LEU	2.3
1	D	109	LEU	2.3
1	E	145	LEU	2.3
1	C	359	MET	2.3
1	E	130	ARG	2.3
1	E	352	ASN	2.3
1	F	83	ASP	2.3
1	B	509	PHE	2.3
1	D	553	PRO	2.3
1	D	532	ASP	2.3
1	E	180	LEU	2.3
1	B	359	MET	2.3
1	F	102	LYS	2.3
1	A	528	VAL	2.3
1	A	465	PRO	2.3
1	F	82	ASN	2.3
1	D	423	ALA	2.3
1	B	426	ILE	2.3
1	C	464	ALA	2.3
1	A	427	TYR	2.2
1	B	221	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	378	VAL	2.2
1	A	105	ASP	2.2
1	A	553	PRO	2.2
1	D	319	THR	2.2
1	E	288	ASN	2.2
1	F	220	GLU	2.2
1	B	351	LYS	2.2
1	D	102	LYS	2.2
1	E	76	PHE	2.2
1	C	78	MET	2.2
1	A	68	SER	2.2
1	B	388	THR	2.2
1	A	422	LEU	2.2
1	B	192	ASP	2.2
1	E	74	SER	2.2
1	B	316	ASN	2.1
1	E	59	PHE	2.1
1	A	319	THR	2.1
1	A	350	ALA	2.1
1	C	355	ALA	2.1
1	F	302	ALA	2.1
1	E	197	GLU	2.1
1	B	200	ILE	2.1
1	B	246	SER	2.1
1	E	108	LYS	2.1
1	E	71	HIS	2.1
1	D	220	GLU	2.1
1	C	375	GLN	2.1
1	C	104	GLY	2.1
1	F	101	ASN	2.1
1	B	78	MET	2.1
1	C	423	ALA	2.1
1	E	526	VAL	2.1
1	F	376	SER	2.1
1	E	93	CYS	2.1
1	C	316	ASN	2.1
1	D	68	SER	2.1
1	B	486	ILE	2.1
1	F	357	LYS	2.1
1	D	217	VAL	2.1
1	B	35	LYS	2.1
1	C	224	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	486	ILE	2.1
1	A	103	ASP	2.1
1	D	82	ASN	2.1
1	D	321	THR	2.1
1	A	437	SER	2.1
1	C	497	SER	2.1
1	F	472	TYR	2.1
1	D	199	GLU	2.0
1	A	173	ASP	2.0
1	A	457	LEU	2.0
1	B	465	PRO	2.0
1	B	174	HIS	2.0
1	C	51	PHE	2.0
1	E	374	ASP	2.0
1	C	389	LYS	2.0
1	A	162	LEU	2.0
1	C	486	ILE	2.0
1	E	282	LEU	2.0
1	F	294	ILE	2.0
1	A	288	ASN	2.0
1	D	316	ASN	2.0
1	C	374	ASP	2.0
1	E	412	LYS	2.0
1	F	412	LYS	2.0
1	D	71	HIS	2.0
1	D	101	ASN	2.0
1	B	83	ASP	2.0
1	B	374	ASP	2.0
1	D	100	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 monosaccharides 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, 95^{th} 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
3	NA	C	604	1/1	0.61	0.37	73,73,73,73	0
3	NA	C	610	1/1	0.76	0.84	83,83,83,83	0
3	NA	D	608	1/1	0.77	0.43	81,81,81,81	0
3	NA	E	601	1/1	0.77	0.42	76,76,76,76	0
3	NA	B	608	1/1	0.79	0.28	69,69,69,69	0
3	NA	B	609	1/1	0.79	0.38	69,69,69,69	0
3	NA	F	606	1/1	0.80	0.25	86,86,86,86	0
3	NA	F	605	1/1	0.83	0.33	73,73,73,73	0
3	NA	B	606	1/1	0.83	0.28	58,58,58,58	0
3	NA	C	611	1/1	0.84	0.50	71,71,71,71	0
3	NA	B	602	1/1	0.84	0.34	77,77,77,77	0
3	NA	B	603	1/1	0.84	0.32	68,68,68,68	0
2	EDO	A	601	4/4	0.84	0.17	68,79,91,91	0
3	NA	B	607	1/1	0.84	0.42	80,80,80,80	0
3	NA	B	605	1/1	0.85	0.29	75,75,75,75	0
3	NA	C	606	1/1	0.86	0.23	74,74,74,74	0
3	NA	F	601	1/1	0.86	0.39	74,74,74,74	0
3	NA	C	605	1/1	0.87	0.12	88,88,88,88	0
3	NA	C	603	1/1	0.87	0.34	72,72,72,72	0
3	NA	A	606	1/1	0.87	0.75	65,65,65,65	0
3	NA	F	603	1/1	0.88	0.23	84,84,84,84	0
3	NA	C	602	1/1	0.89	0.26	59,59,59,59	0
3	NA	C	609	1/1	0.89	0.37	76,76,76,76	0
3	NA	F	602	1/1	0.90	0.81	79,79,79,79	0
3	NA	D	602	1/1	0.90	0.34	75,75,75,75	0
3	NA	D	605	1/1	0.91	0.42	70,70,70,70	0
3	NA	F	604	1/1	0.91	0.18	79,79,79,79	0
3	NA	D	606	1/1	0.91	0.48	80,80,80,80	0
3	NA	B	601	1/1	0.91	0.45	64,64,64,64	0
3	NA	B	610	1/1	0.92	0.52	95,95,95,95	0
3	NA	A	609	1/1	0.92	0.23	63,63,63,63	0
3	NA	E	602	1/1	0.92	0.88	107,107,107,107	0
3	NA	E	603	1/1	0.92	0.34	69,69,69,69	0
3	NA	D	607	1/1	0.92	1.33	81,81,81,81	0
3	NA	A	610	1/1	0.93	0.54	76,76,76,76	0
3	NA	D	603	1/1	0.93	0.17	80,80,80,80	0
2	EDO	A	602	4/4	0.93	0.13	60,71,81,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	D	601	1/1	0.94	0.39	78,78,78,78	0
3	NA	A	604	1/1	0.94	0.28	63,63,63,63	0
3	NA	A	603	1/1	0.94	0.28	57,57,57,57	0
3	NA	C	608	1/1	0.94	0.48	68,68,68,68	0
3	NA	C	601	1/1	0.95	0.24	56,56,56,56	0
3	NA	B	604	1/1	0.95	0.21	74,74,74,74	0
3	NA	C	607	1/1	0.96	0.27	47,47,47,47	0
3	NA	A	605	1/1	0.96	0.43	63,63,63,63	0
3	NA	A	611	1/1	0.96	0.28	65,65,65,65	0
3	NA	A	607	1/1	0.97	0.30	43,43,43,43	0
3	NA	D	604	1/1	0.98	0.43	61,61,61,61	0
3	NA	A	608	1/1	0.98	0.19	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.