



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:15 PM GMT

PDB ID : 1JF5
Title : CRYSTAL STRUCTURE OF THERMOACTINOMYCES VULGARIS R-47
ALPHA-AMYLASE 2 MUTANT F286A
Authors : Ohtaki, A.; Kondo, S.; Shimura, Y.; Tonozuka, T.; Sakano, Y.; Kamitori, S.
Deposited on : 2001-06-20
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

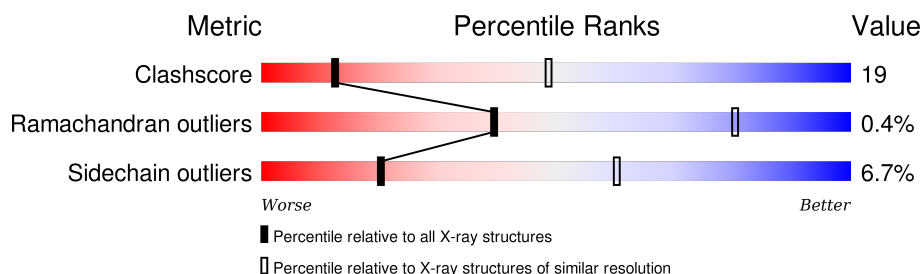
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	585	
1	B	585	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9542 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 ALPHA AMYLASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4770	3050	831	874	15			
1	B	585	Total	C	N	O	S	0	0	0
			4770	3050	831	874	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ALA	PHE	ENGINEERED	UNP Q08751
B	286	ALA	PHE	ENGINEERED	UNP Q08751

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

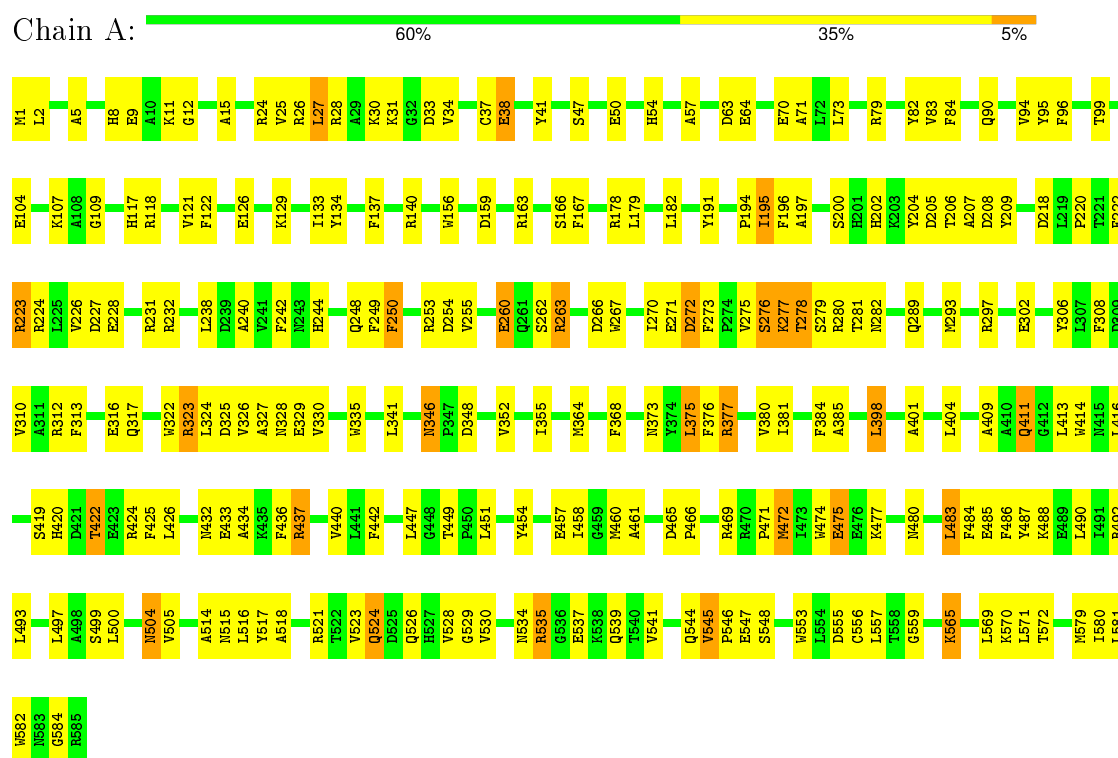
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

3 Residue-property plots [i](#)

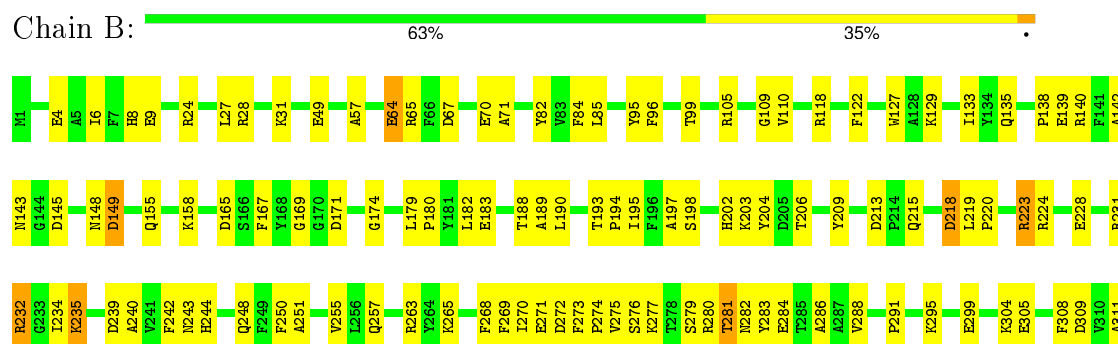
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: ALPHA AMYLASE II



• Molecule 1: ALPHA AMYLASE II





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.60Å 118.05Å 113.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.39 – 3.20	Depositor
% Data completeness (in resolution range)	99.7 (38.39-3.20)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.214 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9542	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.54	0/4899	0.70	0/6632
1	B	0.53	0/4899	0.70	0/6632
All	All	0.54	0/9798	0.70	0/13264

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4770	0	4603	192	0
1	B	4770	0	4603	181	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	9542	0	9206	365	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 19.

All (365) 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:A:275:VAL:HA	1:A:282:ASN:HD21	1.22	1.05
1:B:545:VAL:HG21	1:B:569:LEU:HD13	1.39	1.04
1:A:328:ASN:HB3	1:A:355:ILE:HD12	1.40	1.02
1:B:535:ARG:HD3	1:B:539:GLN:HE22	1.30	0.96
1:A:514:ALA:HB1	1:A:539:GLN:HE22	1.31	0.94
1:A:223:ARG:NH1	1:A:223:ARG:HB3	1.88	0.89
1:B:243:ASN:HD21	1:B:295:LYS:NZ	1.74	0.85
1:A:579:MET:HE2	1:A:581:LEU:HD21	1.58	0.85
1:B:458:ILE:HD11	1:B:460:MET:HG3	1.61	0.82
1:B:535:ARG:HD3	1:B:539:GLN:NE2	1.95	0.81
1:A:433:GLU:HG2	1:A:437:ARG:HD2	1.63	0.80
1:A:255:VAL:HG22	1:A:262:SER:OG	1.81	0.80
1:B:223:ARG:HB3	1:B:223:ARG:NH2	1.98	0.78
1:A:254:ASP:OD2	1:A:262:SER:HB2	1.84	0.78
1:A:416:LEU:HD23	1:A:416:LEU:H	1.49	0.78
1:B:183:GLU:OE2	1:B:232:ARG:HG3	1.84	0.77
1:A:277:LYS:HB2	1:A:277:LYS:NZ	2.02	0.74
1:B:416:LEU:H	1:B:416:LEU:HD23	1.52	0.74
1:A:275:VAL:O	1:A:276:SER:HB2	1.87	0.73
1:B:545:VAL:HG21	1:B:569:LEU:CD1	2.18	0.73
1:B:190:LEU:HD13	1:B:234:ILE:HG21	1.70	0.72
1:A:223:ARG:HB3	1:A:223:ARG:HH11	1.53	0.72
1:B:401:ALA:O	1:B:404:LEU:HB2	1.90	0.72
1:B:135:GLN:HB2	1:B:451:LEU:HD21	1.70	0.71
1:A:197:ALA:HB3	1:A:208:ASP:HB3	1.73	0.70
1:A:582:TRP:CE2	1:A:584:GLY:HA2	2.26	0.70
1:A:485:GLU:HA	1:A:488:LYS:HD3	1.73	0.70
1:A:275:VAL:HA	1:A:282:ASN:ND2	2.03	0.69
1:B:219:LEU:HD11	1:B:317:GLN:OE1	1.92	0.69
1:B:243:ASN:HD21	1:B:295:LYS:HZ1	1.38	0.69
1:B:190:LEU:HD13	1:B:234:ILE:CG2	2.22	0.69
1:B:386:THR:OG1	1:B:388:GLU:HG3	1.93	0.69
1:B:467:ASP:OD2	1:B:470:ARG:NH1	2.26	0.68
1:B:542:LEU:HD21	1:B:568:GLN:NE2	2.08	0.68
1:A:398:LEU:HD21	1:A:442:PHE:CZ	2.29	0.68
1:A:401:ALA:HA	1:A:404:LEU:HD13	1.76	0.68
1:B:133:ILE:CD1	1:B:189:ALA:HB3	2.24	0.67
1:B:309:ASP:OD2	1:B:312:ARG:NH2	2.27	0.67
1:A:515:ASN:ND2	1:A:534:ASN:HB3	2.11	0.66
1:A:514:ALA:HB1	1:A:539:GLN:NE2	2.08	0.66
1:A:514:ALA:CB	1:A:539:GLN:HE22	2.07	0.66
1:B:328:ASN:HB3	1:B:355:ILE:HG12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ASP:O	1:B:349:ALA:HA	1.96	0.66
1:B:198:SER:HB3	1:B:203:LYS:HG3	1.79	0.65
1:A:306:TYR:O	1:A:310:VAL:HG23	1.97	0.65
1:B:219:LEU:HB3	1:B:220:PRO:HD3	1.78	0.64
1:B:240:ALA:HB1	1:B:242:PHE:CE1	2.32	0.64
1:A:47:SER:HB3	1:A:50:GLU:HG3	1.79	0.64
1:B:27:LEU:HD23	1:B:28:ARG:N	2.13	0.64
1:A:523:VAL:HG22	1:A:524:GLN:HG2	1.80	0.64
1:A:133:ILE:HD12	1:A:449:THR:HG21	1.79	0.64
1:B:328:ASN:HD22	1:B:328:ASN:N	1.95	0.63
1:A:398:LEU:HD21	1:A:442:PHE:HZ	1.64	0.63
1:B:27:LEU:HD12	1:B:84:PHE:CD2	2.33	0.62
1:B:331:ASP:OD2	1:B:333:ALA:HB3	1.99	0.62
1:A:84:PHE:HB2	1:A:96:PHE:HB3	1.81	0.62
1:B:255:VAL:O	1:B:275:VAL:HG21	1.99	0.62
1:A:224:ARG:HA	1:A:224:ARG:HE	1.63	0.62
1:B:271:GLU:HB2	1:B:282:ASN:O	2.00	0.61
1:A:475:GLU:OE1	1:A:477:LYS:HB2	2.01	0.61
1:A:544:GLN:O	1:A:545:VAL:HG13	2.01	0.60
1:A:218:ASP:OD1	1:A:220:PRO:HD2	2.02	0.60
1:A:118:ARG:O	1:A:121:VAL:HG23	2.01	0.60
1:B:84:PHE:HB2	1:B:96:PHE:HB3	1.83	0.60
1:B:228:GLU:OE2	1:B:231:ARG:NH1	2.35	0.60
1:A:224:ARG:NE	1:A:224:ARG:HA	2.17	0.60
1:A:133:ILE:HD12	1:A:449:THR:CG2	2.32	0.60
1:A:409:ALA:O	1:A:413:LEU:HD13	2.02	0.60
1:B:243:ASN:HD21	1:B:295:LYS:HZ2	1.47	0.59
1:A:38:GLU:OE1	1:A:54:HIS:HB3	2.02	0.59
1:B:269:PHE:HB2	1:B:284:GLU:HB3	1.84	0.59
1:B:129:LYS:HA	1:B:411:GLN:OE1	2.02	0.59
1:A:535:ARG:NH2	1:A:537:GLU:HB2	2.17	0.59
1:B:582:TRP:CE2	1:B:584:GLY:HA2	2.38	0.59
1:B:545:VAL:HG23	1:B:545:VAL:O	2.02	0.59
1:A:297:ARG:HH12	1:B:118:ARG:HH22	1.49	0.58
1:B:547:GLU:HG2	1:B:551:LYS:NZ	2.18	0.58
1:B:401:ALA:HA	1:B:404:LEU:HD13	1.84	0.58
1:B:582:TRP:CZ2	1:B:584:GLY:HA2	2.39	0.58
1:B:545:VAL:CG2	1:B:569:LEU:HD13	2.25	0.58
1:A:2:LEU:H	1:A:2:LEU:HD12	1.68	0.58
1:B:330:VAL:HB	1:B:335:TRP:NE1	2.19	0.58
1:B:547:GLU:HG2	1:B:551:LYS:HZ2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ARG:HD2	1:B:70:GLU:HG2	1.86	0.58
1:A:263:ARG:O	1:A:263:ARG:HD2	2.04	0.57
1:B:133:ILE:HD12	1:B:189:ALA:HB3	1.86	0.57
1:A:346:ASN:ND2	1:A:348:ASP:H	2.02	0.57
1:B:458:ILE:C	1:B:458:ILE:HD12	2.24	0.57
1:B:145:ASP:HB3	1:B:148:ASN:ND2	2.18	0.57
1:A:516:LEU:HD13	1:A:541:VAL:HG11	1.86	0.57
1:A:324:LEU:HD13	1:A:335:TRP:CZ3	2.40	0.57
1:A:277:LYS:HB2	1:A:277:LYS:HZ2	1.69	0.56
1:A:79:ARG:HH22	1:B:288:VAL:HG22	1.69	0.56
1:A:324:LEU:HD13	1:A:335:TRP:CH2	2.40	0.56
1:B:273:PHE:HA	1:B:274:PRO:C	2.25	0.56
1:A:381:ILE:O	1:A:385:ALA:HB3	2.06	0.56
1:B:223:ARG:HB3	1:B:223:ARG:CZ	2.35	0.56
1:B:516:LEU:C	1:B:516:LEU:HD23	2.27	0.56
1:A:195:ILE:O	1:A:196:PHE:HD2	1.89	0.56
1:A:31:LYS:HE3	1:A:63:ASP:O	2.05	0.55
1:A:223:ARG:CZ	1:A:223:ARG:HB3	2.36	0.55
1:B:139:GLU:OE2	1:B:140:ARG:NH1	2.39	0.55
1:A:202:HIS:CE1	1:A:205:ASP:OD1	2.59	0.55
1:A:228:GLU:OE1	1:A:231:ARG:NH1	2.37	0.55
1:A:276:SER:O	1:A:277:LYS:HB2	2.05	0.55
1:B:143:ASN:ND2	1:B:169:GLY:O	2.39	0.55
1:B:276:SER:OG	1:B:277:LYS:N	2.40	0.55
1:A:419:SER:OG	1:A:422:THR:HG23	2.07	0.55
1:A:270:ILE:HD13	1:A:275:VAL:HG21	1.88	0.55
1:B:425:PHE:HB3	1:B:436:PHE:HE1	1.70	0.54
1:B:197:ALA:HA	1:B:213:ASP:HB2	1.89	0.54
1:A:289:GLN:HE21	1:A:289:GLN:HA	1.71	0.54
1:B:142:ALA:O	1:B:174:GLY:HA3	2.08	0.54
1:B:232:ARG:HG3	1:B:232:ARG:HH11	1.73	0.54
1:B:193:THR:HB	1:B:194:PRO:HD2	1.90	0.54
1:B:145:ASP:HB3	1:B:148:ASN:HD21	1.73	0.54
1:A:518:ALA:HA	1:A:530:VAL:O	2.08	0.54
1:B:281:THR:HG23	1:B:291:PRO:HB3	1.91	0.53
1:A:376:PHE:O	1:A:380:VAL:HG23	2.07	0.53
1:A:281:THR:OG1	1:A:289:GLN:NE2	2.41	0.53
1:A:416:LEU:H	1:A:416:LEU:CD2	2.21	0.53
1:A:195:ILE:O	1:A:195:ILE:HG13	2.09	0.53
1:A:41:TYR:HB3	1:A:82:TYR:HB3	1.91	0.53
1:B:355:ILE:HG22	1:B:357:HIS:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PHE:O	1:A:95:TYR:HA	2.08	0.53
1:A:126:GLU:OE1	1:A:129:LYS:HE3	2.09	0.53
1:A:267:TRP:CZ2	1:A:302:GLU:HB3	2.44	0.53
1:B:383:PHE:CE1	1:B:391:ALA:HA	2.44	0.52
1:A:289:GLN:HE21	1:A:289:GLN:CA	2.23	0.52
1:B:441:LEU:HD13	1:B:578:GLY:HA3	1.89	0.52
1:A:24:ARG:HD2	1:A:70:GLU:CD	2.30	0.52
1:A:202:HIS:HE1	1:A:205:ASP:OD1	1.92	0.52
1:A:134:TYR:CZ	1:A:454:TYR:HA	2.45	0.52
1:A:117:HIS:HB3	1:B:299:GLU:CD	2.30	0.52
1:A:579:MET:CE	1:A:581:LEU:HD21	2.34	0.52
1:B:357:HIS:O	1:B:358:ASP:C	2.48	0.52
1:A:99:THR:OG1	1:A:109:GLY:HA3	2.09	0.52
1:B:180:PRO:HG3	1:B:232:ARG:HH22	1.75	0.52
1:A:504:ASN:N	1:A:504:ASN:HD22	2.07	0.52
1:B:6:ILE:HG23	1:B:27:LEU:HD21	1.91	0.51
1:B:138:PRO:HG3	1:B:195:ILE:CG2	2.40	0.51
1:A:486:PHE:CZ	1:A:490:LEU:HD11	2.44	0.51
1:A:289:GLN:HA	1:A:289:GLN:NE2	2.25	0.51
1:B:133:ILE:HD13	1:B:189:ALA:HB3	1.92	0.51
1:B:8:HIS:CG	1:B:9:GLU:N	2.79	0.51
1:B:149:ASP:N	1:B:149:ASP:OD2	2.43	0.50
1:B:193:THR:HB	1:B:194:PRO:CD	2.42	0.50
1:A:223:ARG:HH22	1:A:227:ASP:CG	2.15	0.50
1:A:297:ARG:NH1	1:B:118:ARG:HH12	2.10	0.50
1:A:535:ARG:HG3	1:A:539:GLN:OE1	2.11	0.50
1:A:117:HIS:HB3	1:B:299:GLU:OE2	2.11	0.50
1:B:554:LEU:O	1:B:581:LEU:HA	2.12	0.50
1:A:57:ALA:HB2	1:A:71:ALA:HB2	1.94	0.50
1:B:143:ASN:ND2	1:B:169:GLY:HA3	2.26	0.49
1:B:138:PRO:HG3	1:B:195:ILE:HG22	1.93	0.49
1:A:178:ARG:HG3	1:A:474:TRP:CZ2	2.48	0.49
1:A:457:GLU:HA	1:A:487:TYR:CE1	2.47	0.49
1:B:308:PHE:O	1:B:311:ALA:HB3	2.12	0.49
1:B:444:MET:HG3	1:B:490:LEU:HB3	1.92	0.49
1:A:326:VAL:O	1:A:326:VAL:HG12	2.13	0.49
1:A:163:ARG:NH1	1:A:163:ARG:HB2	2.28	0.49
1:B:99:THR:OG1	1:B:109:GLY:HA3	2.13	0.49
1:A:2:LEU:N	1:A:2:LEU:HD12	2.28	0.49
1:A:324:LEU:HB2	1:A:327:ALA:HB2	1.94	0.48
1:B:179:LEU:N	1:B:180:PRO:CD	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:ASP:OD1	1:B:469:ARG:NH2	2.46	0.48
1:B:323:ARG:C	1:B:323:ARG:HD2	2.33	0.48
1:A:352:VAL:HG21	1:A:414:TRP:CZ2	2.48	0.48
1:A:432:ASN:OD1	1:A:434:ALA:N	2.46	0.48
1:A:197:ALA:O	1:A:207:ALA:HB3	2.14	0.48
1:B:206:THR:HG21	1:B:209:TYR:CG	2.49	0.48
1:B:255:VAL:HG12	1:B:275:VAL:CG1	2.44	0.48
1:A:380:VAL:HG12	1:A:425:PHE:CZ	2.49	0.48
1:B:533:ASN:ND2	1:B:574:ARG:O	2.47	0.48
1:B:324:LEU:HD13	1:B:335:TRP:CH2	2.49	0.48
1:B:244:HIS:CD2	1:B:286:ALA:HB2	2.48	0.48
1:A:411:GLN:HA	1:A:447:LEU:HD11	1.96	0.48
1:B:328:ASN:ND2	1:B:328:ASN:N	2.62	0.47
1:B:232:ARG:CG	1:B:232:ARG:HH11	2.27	0.47
1:B:281:THR:HG22	1:B:283:TYR:CE2	2.49	0.47
1:A:297:ARG:HH11	1:B:118:ARG:HH12	1.62	0.47
1:B:65:ARG:HG2	1:B:65:ARG:HH11	1.78	0.47
1:A:297:ARG:HH12	1:B:118:ARG:NH2	2.11	0.47
1:A:436:PHE:O	1:A:440:VAL:HG23	2.14	0.47
1:B:422:THR:OG1	1:B:423:GLU:N	2.46	0.47
1:B:447:LEU:HB2	1:B:505:VAL:CG2	2.45	0.47
1:B:143:ASN:HA	1:B:171:ASP:OD2	2.15	0.47
1:A:24:ARG:HD2	1:A:70:GLU:CG	2.44	0.47
1:A:565:LYS:O	1:A:565:LYS:HG2	2.14	0.47
1:B:223:ARG:HB3	1:B:223:ARG:HH21	1.77	0.47
1:B:475:GLU:OE2	1:B:475:GLU:HA	2.14	0.47
1:A:493:LEU:HD11	1:A:556:CYS:HB3	1.97	0.47
1:A:133:ILE:CD1	1:A:449:THR:HG21	2.45	0.47
1:B:324:LEU:HD13	1:B:335:TRP:CZ3	2.49	0.47
1:A:499:SER:HG	1:A:526:GLN:HG2	1.80	0.47
1:B:504:ASN:HD22	1:B:504:ASN:N	2.13	0.46
1:B:480:ASN:ND2	1:B:483:LEU:HB2	2.30	0.46
1:A:324:LEU:HD12	1:A:368:PHE:CE2	2.50	0.46
1:A:377:ARG:HH11	1:A:377:ARG:HG2	1.80	0.46
1:A:194:PRO:HG2	1:A:204:TYR:CE1	2.51	0.46
1:B:377:ARG:CZ	1:B:381:ILE:HD11	2.46	0.46
1:B:206:THR:HG21	1:B:209:TYR:CD1	2.51	0.46
1:B:453:TYR:HB3	1:B:456:ASP:OD2	2.15	0.46
1:B:504:ASN:HD22	1:B:504:ASN:C	2.19	0.46
1:B:582:TRP:CH2	1:B:584:GLY:HA2	2.51	0.46
1:A:330:VAL:HG22	1:A:335:TRP:NE1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:THR:OG1	1:B:462:GLY:O	2.29	0.46
1:B:582:TRP:CE2	1:B:584:GLY:CA	3.00	0.45
1:B:65:ARG:NH1	1:B:65:ARG:HG2	2.31	0.45
1:B:31:LYS:HG3	1:B:67:ASP:OD1	2.17	0.45
1:A:8:HIS:HD2	1:A:26:ARG:O	1.98	0.45
1:B:564:GLY:HA3	1:B:569:LEU:HD12	1.99	0.45
1:A:83:VAL:HG22	1:A:84:PHE:N	2.31	0.45
1:A:27:LEU:HD13	1:A:84:PHE:CD2	2.52	0.45
1:A:545:VAL:HG21	1:A:569:LEU:HB2	1.97	0.45
1:A:569:LEU:HG	1:A:571:LEU:HD13	1.99	0.45
1:A:497:LEU:HD12	1:A:500:LEU:CD1	2.47	0.45
1:B:357:HIS:HA	1:B:374:TYR:OH	2.16	0.45
1:A:420:HIS:N	1:A:420:HIS:ND1	2.65	0.45
1:A:313:PHE:O	1:A:317:GLN:HG2	2.17	0.45
1:A:424:ARG:HD2	1:A:461:ALA:C	2.37	0.45
1:A:140:ARG:HG2	1:A:469:ARG:O	2.17	0.45
1:A:312:ARG:O	1:A:316:GLU:HG3	2.17	0.45
1:A:271:GLU:HG2	1:A:282:ASN:O	2.17	0.45
1:B:218:ASP:HB2	1:B:220:PRO:HD2	1.99	0.45
1:A:27:LEU:HD22	1:A:37:CYS:SG	2.57	0.45
1:A:30:LYS:HB3	1:A:33:ASP:HB2	1.97	0.45
1:A:523:VAL:HG13	1:A:523:VAL:O	2.17	0.44
1:B:271:GLU:OE2	1:B:283:TYR:HA	2.17	0.44
1:A:454:TYR:CG	1:A:454:TYR:O	2.70	0.44
1:B:82:TYR:C	1:B:110:VAL:HG23	2.37	0.44
1:B:416:LEU:CD2	1:B:416:LEU:H	2.25	0.44
1:A:484:PHE:CE1	1:A:488:LYS:HD2	2.52	0.44
1:A:380:VAL:HG13	1:A:384:PHE:HD1	1.82	0.44
1:B:64:GLU:HG3	1:B:393:ARG:NH2	2.33	0.44
1:A:1:MET:HE3	1:A:94:VAL:HG12	1.99	0.44
1:A:260:GLU:HG2	1:A:260:GLU:H	1.40	0.44
1:B:499:SER:HA	1:B:523:VAL:HG12	1.99	0.44
1:A:278:THR:C	1:A:280:ARG:H	2.21	0.44
1:B:27:LEU:HD23	1:B:28:ARG:O	2.18	0.44
1:A:483:LEU:O	1:A:486:PHE:HB3	2.17	0.44
1:A:206:THR:HG21	1:A:209:TYR:CZ	2.53	0.44
1:B:263:ARG:HG3	1:B:263:ARG:O	2.18	0.44
1:A:341:LEU:HD23	1:A:341:LEU:C	2.38	0.44
1:A:401:ALA:O	1:A:404:LEU:HB2	2.17	0.44
1:A:516:LEU:HD23	1:A:517:TYR:N	2.32	0.43
1:A:504:ASN:ND2	1:A:504:ASN:C	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ASP:HA	1:A:466:PRO:HA	1.78	0.43
1:A:12:GLY:HA2	1:A:364:MET:CE	2.48	0.43
1:B:255:VAL:HG11	1:B:270:ILE:HD11	2.01	0.43
1:A:179:LEU:HB3	1:A:232:ARG:HD2	2.00	0.43
1:B:27:LEU:HD23	1:B:27:LEU:C	2.39	0.43
1:B:197:ALA:HA	1:B:213:ASP:CB	2.47	0.43
1:B:499:SER:OG	1:B:523:VAL:HG12	2.19	0.43
1:B:426:LEU:HD23	1:B:461:ALA:HB2	2.00	0.43
1:B:424:ARG:HD2	1:B:461:ALA:C	2.39	0.43
1:B:305:GLU:OE2	1:B:305:GLU:HA	2.19	0.43
1:A:375:LEU:HD12	1:A:375:LEU:HA	1.83	0.43
1:B:57:ALA:HB2	1:B:71:ALA:HB2	1.99	0.43
1:B:158:LYS:CD	1:B:478:GLU:HB3	2.49	0.43
1:B:376:PHE:CE1	1:B:415:ASN:HB3	2.54	0.43
1:A:191:TYR:CE1	1:A:323:ARG:HG3	2.53	0.43
1:B:425:PHE:HB3	1:B:436:PHE:CE1	2.51	0.43
1:A:352:VAL:HG21	1:A:414:TRP:CE2	2.54	0.43
1:A:137:PHE:CE1	1:A:469:ARG:HD3	2.54	0.43
1:B:158:LYS:HD2	1:B:478:GLU:HB3	2.00	0.43
1:A:222:PHE:O	1:A:226:VAL:HG23	2.19	0.43
1:B:95:TYR:CE2	1:B:105:ARG:HB2	2.54	0.43
1:A:240:ALA:HB2	1:A:322:TRP:CE3	2.54	0.43
1:B:250:PHE:CG	1:B:251:ALA:N	2.87	0.43
1:B:277:LYS:HG3	1:B:280:ARG:HB3	2.01	0.43
1:A:497:LEU:HD12	1:A:500:LEU:HD11	2.00	0.43
1:B:268:PHE:CD1	1:B:268:PHE:N	2.86	0.43
1:A:244:HIS:ND1	1:A:293:MET:HB3	2.33	0.43
1:A:528:VAL:HA	1:A:581:LEU:O	2.19	0.43
1:B:182:LEU:HD13	1:B:190:LEU:HD11	2.01	0.42
1:B:240:ALA:HB1	1:B:242:PHE:CZ	2.54	0.42
1:A:200:SER:OG	1:A:202:HIS:CE1	2.72	0.42
1:A:275:VAL:O	1:A:276:SER:CB	2.58	0.42
1:A:41:TYR:CB	1:A:82:TYR:HB3	2.49	0.42
1:A:222:PHE:CZ	1:A:238:LEU:HD11	2.54	0.42
1:A:156:TRP:CE2	1:A:471:PRO:HB2	2.54	0.42
1:B:202:HIS:O	1:B:203:LYS:HB2	2.19	0.42
1:B:255:VAL:HG12	1:B:275:VAL:HG11	2.00	0.42
1:A:73:LEU:CD1	1:A:73:LEU:N	2.83	0.42
1:A:134:TYR:OH	1:A:454:TYR:HA	2.18	0.42
1:A:232:ARG:HH21	1:A:232:ARG:HG3	1.84	0.42
1:A:557:LEU:HG	1:A:580:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ILE:CG2	1:B:27:LEU:HD21	2.49	0.42
1:A:447:LEU:HB2	1:A:505:VAL:CG2	2.48	0.42
1:B:515:ASN:HD21	1:B:534:ASN:ND2	2.18	0.42
1:B:257:GLN:HB2	1:B:257:GLN:HE21	1.65	0.42
1:B:573:LEU:HA	1:B:577:GLN:OE1	2.20	0.42
1:A:553:TRP:CD1	1:A:581:LEU:HB3	2.55	0.42
1:A:206:THR:HG21	1:A:209:TYR:CE2	2.54	0.42
1:A:57:ALA:CB	1:A:71:ALA:HB2	2.48	0.42
1:B:82:TYR:N	1:B:110:VAL:HG22	2.35	0.42
1:B:263:ARG:HG3	1:B:263:ARG:HH21	1.85	0.42
1:A:277:LYS:HB2	1:A:277:LYS:HZ3	1.83	0.42
1:A:570:LYS:O	1:A:571:LEU:HD12	2.20	0.42
1:A:373:ASN:ND2	1:A:413:LEU:HD23	2.35	0.42
1:B:533:ASN:O	1:B:576:TYR:HA	2.19	0.42
1:B:519:PHE:CE1	1:B:530:VAL:HB	2.55	0.42
1:A:324:LEU:CB	1:A:327:ALA:HB2	2.50	0.41
1:A:324:LEU:CD1	1:A:368:PHE:CE2	3.03	0.41
1:B:377:ARG:HE	1:B:418:ASP:HA	1.85	0.41
1:A:5:ALA:HB1	1:B:4:GLU:HB3	2.01	0.41
1:A:11:LYS:N	1:A:15:ALA:HB3	2.35	0.41
1:A:555:ASP:O	1:A:559:GLY:N	2.41	0.41
1:B:460:MET:HG2	1:B:473:ILE:HD12	2.02	0.41
1:B:194:PRO:HD3	1:B:239:ASP:OD1	2.19	0.41
1:B:555:ASP:OD1	1:B:579:MET:HG2	2.20	0.41
1:A:555:ASP:OD1	1:A:579:MET:HG2	2.20	0.41
1:B:127:TRP:CE3	1:B:235:LYS:HD3	2.56	0.41
1:A:529:GLY:N	1:A:581:LEU:O	2.46	0.41
1:B:228:GLU:O	1:B:232:ARG:HD3	2.20	0.41
1:A:504:ASN:O	1:A:521:ARG:HA	2.20	0.41
1:B:464:THR:OG1	1:B:465:ASP:N	2.53	0.41
1:A:240:ALA:HB1	1:A:242:PHE:CE1	2.55	0.41
1:A:458:ILE:HD11	1:A:472:MET:SD	2.60	0.41
1:B:24:ARG:HD2	1:B:70:GLU:CG	2.50	0.41
1:A:346:ASN:HD22	1:A:346:ASN:C	2.23	0.41
1:B:574:ARG:HB3	1:B:575:PRO:CD	2.51	0.41
1:B:442:PHE:O	1:B:443:GLN:C	2.58	0.41
1:A:104:GLU:OE1	1:A:107:LYS:HD3	2.21	0.41
1:B:165:ASP:N	1:B:165:ASP:OD2	2.50	0.41
1:B:232:ARG:CG	1:B:232:ARG:NH1	2.83	0.41
1:B:542:LEU:HD21	1:B:568:GLN:CD	2.40	0.41
1:A:454:TYR:CD1	1:A:454:TYR:O	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:SER:HG	1:A:526:GLN:CD	2.22	0.41
1:A:8:HIS:CG	1:A:9:GLU:N	2.88	0.41
1:B:352:VAL:HG21	1:B:414:TRP:CZ2	2.55	0.41
1:A:250:PHE:CD1	1:A:250:PHE:C	2.94	0.41
1:B:582:TRP:CD2	1:B:584:GLY:HA2	2.56	0.41
1:A:1:MET:SD	1:A:34:VAL:HG22	2.60	0.41
1:A:273:PHE:CD1	1:A:275:VAL:HG23	2.55	0.41
1:A:515:ASN:HD22	1:A:534:ASN:HB3	1.83	0.41
1:B:202:HIS:ND1	1:B:204:TYR:HB2	2.36	0.41
1:A:326:VAL:HG12	1:A:329:GLU:HB2	2.02	0.41
1:A:488:LYS:O	1:A:492:ARG:HG3	2.20	0.41
1:A:195:ILE:CG1	1:A:195:ILE:O	2.66	0.41
1:B:193:THR:O	1:B:194:PRO:C	2.60	0.41
1:A:57:ALA:HA	1:A:71:ALA:HB2	2.03	0.41
1:A:325:ASP:OD1	1:A:326:VAL:HG23	2.20	0.41
1:B:377:ARG:NE	1:B:417:LEU:O	2.53	0.41
1:A:278:THR:O	1:A:279:SER:HB2	2.21	0.41
1:A:12:GLY:HA2	1:A:364:MET:SD	2.61	0.41
1:B:555:ASP:OD2	1:B:555:ASP:C	2.60	0.41
1:B:304:LYS:HB2	1:B:304:LYS:HE3	1.92	0.41
1:A:546:PRO:O	1:A:548:SER:N	2.54	0.41
1:A:271:GLU:HG3	1:A:272:ASP:CG	2.41	0.41
1:A:416:LEU:HB3	1:A:451:LEU:HD23	2.03	0.41
1:B:475:GLU:O	1:B:476:GLU:C	2.59	0.41
1:B:499:SER:HA	1:B:523:VAL:CG1	2.51	0.41
1:B:564:GLY:CA	1:B:569:LEU:HD12	2.52	0.40
1:A:308:PHE:HB3	1:A:341:LEU:CD1	2.51	0.40
1:B:49:GLU:H	1:B:49:GLU:HG3	1.61	0.40
1:A:426:LEU:HA	1:A:436:PHE:HD1	1.85	0.40
1:A:249:PHE:O	1:A:250:PHE:C	2.59	0.40
1:B:335:TRP:HA	1:B:335:TRP:CE3	2.57	0.40
1:A:480:ASN:OD1	1:A:483:LEU:HB2	2.21	0.40
1:B:483:LEU:O	1:B:486:PHE:HB3	2.21	0.40
1:B:158:LYS:NZ	1:B:478:GLU:O	2.52	0.40
1:B:550:GLY:HA2	1:B:585:ARG:NH2	2.36	0.40
1:A:248:GLN:HA	1:A:253:ARG:HD3	2.03	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	583/585 (100%)	556 (95%)	23 (4%)	4 (1%)	26	72
1	B	583/585 (100%)	548 (94%)	34 (6%)	1 (0%)	52	88
All	All	1166/1170 (100%)	1104 (95%)	57 (5%)	5 (0%)	39	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	547	GLU
1	A	276	SER
1	A	277	LYS
1	B	328	ASN
1	A	195	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	492/492 (100%)	456 (93%)	36 (7%)	17	57
1	B	492/492 (100%)	462 (94%)	30 (6%)	23	64
All	All	984/984 (100%)	918 (93%)	66 (7%)	20	60

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL

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Mol	Chain	Res	Type
1	A	27	LEU
1	A	28	ARG
1	A	38	GLU
1	A	64	GLU
1	A	90	GLN
1	A	122	PHE
1	A	159	ASP
1	A	166	SER
1	A	167	PHE
1	A	182	LEU
1	A	223	ARG
1	A	250	PHE
1	A	260	GLU
1	A	263	ARG
1	A	266	ASP
1	A	272	ASP
1	A	278	THR
1	A	323	ARG
1	A	346	ASN
1	A	375	LEU
1	A	377	ARG
1	A	398	LEU
1	A	411	GLN
1	A	422	THR
1	A	437	ARG
1	A	460	MET
1	A	472	MET
1	A	475	GLU
1	A	483	LEU
1	A	504	ASN
1	A	524	GLN
1	A	535	ARG
1	A	545	VAL
1	A	565	LYS
1	A	572	THR
1	B	64	GLU
1	B	85	LEU
1	B	122	PHE
1	B	149	ASP
1	B	155	GLN
1	B	167	PHE
1	B	188	THR

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Mol	Chain	Res	Type
1	B	215	GLN
1	B	218	ASP
1	B	223	ARG
1	B	224	ARG
1	B	232	ARG
1	B	235	LYS
1	B	248	GLN
1	B	265	LYS
1	B	272	ASP
1	B	279	SER
1	B	281	THR
1	B	323	ARG
1	B	325	ASP
1	B	328	ASN
1	B	364	MET
1	B	382	ARG
1	B	411	GLN
1	B	467	ASP
1	B	504	ASN
1	B	522	THR
1	B	537	GLU
1	B	552	THR
1	B	583	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	22	GLN
1	A	135	GLN
1	A	155	GLN
1	A	289	GLN
1	A	332	HIS
1	A	346	ASN
1	A	367	GLN
1	A	390	HIS
1	A	443	GLN
1	A	504	ASN
1	A	539	GLN
1	A	544	GLN
1	A	563	HIS
1	B	135	GLN

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Mol	Chain	Res	Type
1	B	155	GLN
1	B	243	ASN
1	B	244	HIS
1	B	257	GLN
1	B	328	ASN
1	B	332	HIS
1	B	357	HIS
1	B	367	GLN
1	B	504	ASN
1	B	527	HIS
1	B	534	ASN
1	B	544	GLN
1	B	566	GLN
1	B	568	GLN

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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.