Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 04:55 pm BST

PDB ID	:	8BB7
Title	:	Crystal structure of Mouse Plexin-B1 (20-535) in complex with VHH15
Authors	:	Cowan, R.; Hall, G.; Carr, M.
Deposited on	:	2022-10-12
Resolution	:	2.95 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:

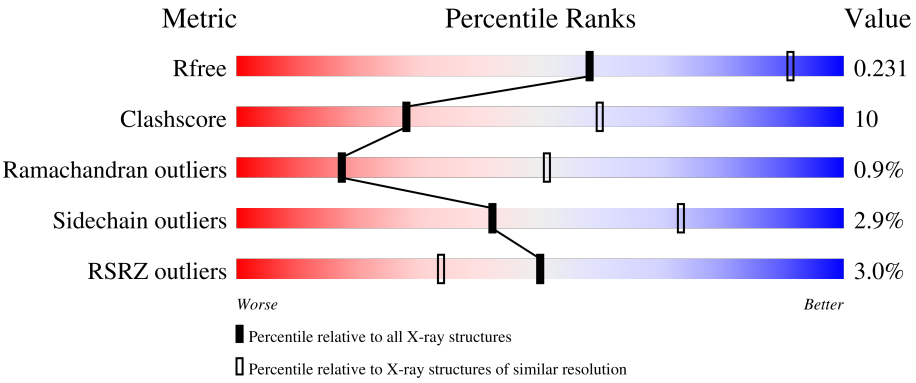
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	523	2% 70% 20% • 8%
1	B	523	% 72% 19% • 7%
2	C	130	12% 66% 25% • 7%
2	D	130	2% 74% 19% • 5%

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	NAG	B	603	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9504 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 Plexin-B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	485	Total	C	N	O	S	0	0	0
			3678	2318	642	697	21			
1	A	479	Total	C	N	O	S	0	0	0
			3630	2288	631	690	21			

There are 14 discrepancies between the modelled and reference sequences:

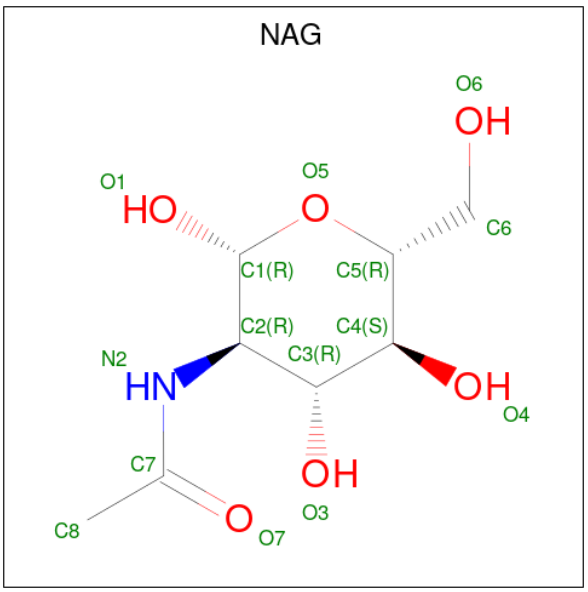
Chain	Residue	Modelled	Actual	Comment	Reference
B	536	LYS	-	expression tag	UNP Q8CJH3
B	537	HIS	-	expression tag	UNP Q8CJH3
B	538	HIS	-	expression tag	UNP Q8CJH3
B	539	HIS	-	expression tag	UNP Q8CJH3
B	540	HIS	-	expression tag	UNP Q8CJH3
B	541	HIS	-	expression tag	UNP Q8CJH3
B	542	HIS	-	expression tag	UNP Q8CJH3
A	536	LYS	-	expression tag	UNP Q8CJH3
A	537	HIS	-	expression tag	UNP Q8CJH3
A	538	HIS	-	expression tag	UNP Q8CJH3
A	539	HIS	-	expression tag	UNP Q8CJH3
A	540	HIS	-	expression tag	UNP Q8CJH3
A	541	HIS	-	expression tag	UNP Q8CJH3
A	542	HIS	-	expression tag	UNP Q8CJH3

- Molecule 2 is a protein called VHH15 Nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	124	Total	C	N	O	S	0	0	0
			941	584	165	186	6			
2	C	121	Total	C	N	O	S	0	0	0
			921	573	161	181	6			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	112	Total O 112 112	0	0
4	D	23	Total O 23 23	0	0
4	A	79	Total O 79 79	0	0

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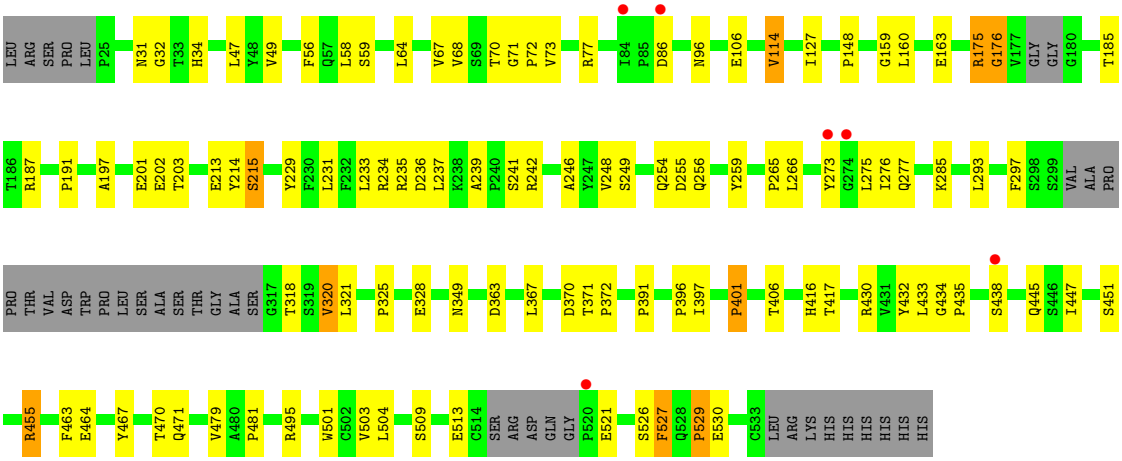
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	8	Total O 8 8	0	0

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.

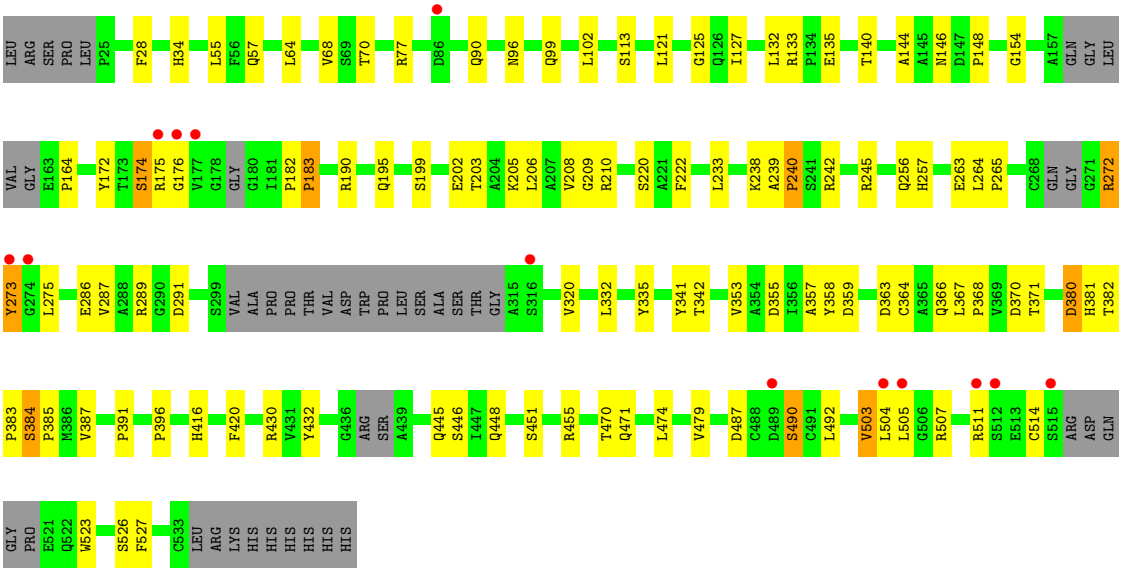
• Molecule 1: Plexin-B1

Chain B:



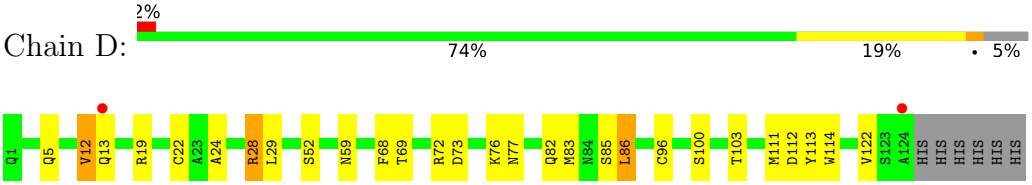
• Molecule 1: Plexin-B1

Chain A:



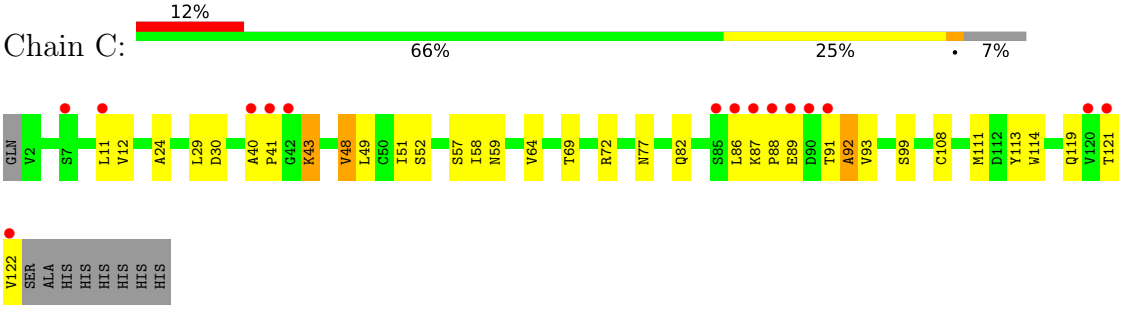
• Molecule 2: VHH15 Nanobody

Chain D:



• Molecule 2: VHH15 Nanobody

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.54Å 108.99Å 94.04Å 90.00° 90.37° 90.00°	Depositor
Resolution (Å)	47.15 – 2.95 47.15 – 2.95	Depositor EDS
% Data completeness (in resolution range)	84.8 (47.15-2.95) 78.0 (47.15-2.95)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.203 , 0.229 0.205 , 0.231	Depositor DCC
R_{free} test set	1703 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.017 for l,k,-h 0.039 for h,-k,-l 0.027 for l,-k,h	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	9504	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: NAG

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	0.40	1/3717 (0.0%)	0.65	2/5077 (0.0%)
1	B	0.37	0/3768	0.62	1/5148 (0.0%)
2	C	0.40	1/939 (0.1%)	0.65	0/1267
2	D	0.50	2/959 (0.2%)	0.63	2/1294 (0.2%)
All	All	0.40	4/9383 (0.0%)	0.63	5/12786 (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	4
1	B	0	4
2	D	0	1
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	12	VAL	C-N	8.34	1.53	1.34
2	D	13	GLN	C-N	7.83	1.49	1.34
1	A	470	THR	C-N	-6.95	1.18	1.34
2	C	48	VAL	C-N	-5.13	1.22	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	12	VAL	O-C-N	6.70	133.41	122.70
1	A	470	THR	O-C-N	-6.60	112.13	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	72	PRO	N-CA-C	-6.04	96.41	112.10
2	D	12	VAL	CA-C-N	-5.77	104.50	117.20
1	A	503	VAL	O-C-N	5.18	130.99	122.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	ARG	Sidechain
1	A	272	ARG	Sidechain
1	A	455	ARG	Sidechain
1	A	507	ARG	Sidechain
1	B	175	ARG	Sidechain
1	B	234	ARG	Sidechain
1	B	235	ARG	Sidechain
1	B	455	ARG	Sidechain
2	D	19	ARG	Sidechain

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	3630	0	3514	74	1
1	B	3678	0	3571	70	1
2	C	921	0	877	24	0
2	D	941	0	899	16	0
3	A	70	0	65	4	0
3	B	42	0	39	0	0
4	A	79	0	0	3	0
4	B	112	0	0	0	0
4	C	8	0	0	0	0
4	D	23	0	0	1	0
All	All	9504	0	8965	180	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 10.

All (180) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ASN:HD21	3:A:601:NAG:C1	1.84	0.88
1:B:416:HIS:HB3	1:B:432:TYR:HE1	1.42	0.83
1:A:286:GLU:HG3	1:A:287:VAL:H	1.46	0.80
1:A:335:TYR:HE1	1:A:353:VAL:HG21	1.47	0.78
1:B:231:LEU:HD11	1:B:293:LEU:HD21	1.67	0.75
1:A:384:SER:HB3	1:A:385:PRO:HD3	1.69	0.74
1:A:183:PRO:HG2	1:A:206:LEU:HD23	1.69	0.72
1:A:206:LEU:HG	1:A:208:VAL:HG23	1.72	0.72
1:A:263:GLU:HB2	1:A:387:VAL:HG23	1.72	0.71
1:B:367:LEU:HB3	1:B:371:THR:HG21	1.73	0.69
1:A:335:TYR:CE1	1:A:353:VAL:HG21	2.27	0.68
2:D:85:SER:O	2:D:86:LEU:HB2	1.92	0.68
1:B:417:THR:H	1:B:434:GLY:HA2	1.60	0.67
1:B:213:GLU:O	1:B:237:LEU:HD21	1.98	0.64
2:C:52:SER:O	2:C:72:ARG:NH1	2.31	0.63
1:A:140:THR:HG23	1:A:199:SER:HB2	1.81	0.62
1:A:102:LEU:HD11	1:A:154:GLY:HA3	1.81	0.62
1:B:34:HIS:HA	1:B:471:GLN:O	2.00	0.62
1:A:320:VAL:CG1	1:A:396:PRO:HB3	2.30	0.61
1:A:238:LYS:HD2	1:A:238:LYS:O	2.01	0.61
1:B:297:PHE:HB2	1:B:320:VAL:HG12	1.82	0.60
1:B:64:LEU:HD11	1:B:67:VAL:HG22	1.85	0.59
1:B:31:ASN:HD21	3:A:601:NAG:C2	2.15	0.58
1:A:286:GLU:HG3	1:A:287:VAL:N	2.16	0.58
1:B:32:GLY:O	2:D:103:THR:OG1	2.16	0.58
1:B:406:THR:O	1:B:455:ARG:HG2	2.03	0.57
1:B:432:TYR:OH	1:B:435:PRO:HD2	2.05	0.57
1:A:256:GLN:HG2	4:A:723:HOH:O	2.05	0.57
1:A:182:PRO:CG	1:A:205:LYS:HD2	2.35	0.56
1:A:341:TYR:CE1	1:A:382:THR:HB	2.40	0.56
1:B:430:ARG:HH21	1:B:445:GLN:HE22	1.54	0.56
1:A:182:PRO:HG3	1:A:205:LYS:HD2	1.88	0.56
1:A:342:THR:O	1:A:366:GLN:HA	2.06	0.55
1:A:34:HIS:HA	1:A:471:GLN:O	2.07	0.55
1:A:77:ARG:HD3	1:A:175:ARG:HD3	1.88	0.55
1:A:487:ASP:OD1	1:A:490:SER:HB2	2.07	0.54
1:A:77:ARG:O	1:A:176:GLY:HA3	2.07	0.54
1:A:511:ARG:HB2	1:A:523:TRP:CE3	2.43	0.54
1:A:242:ARG:NH1	4:A:701:HOH:O	2.25	0.54
1:B:233:LEU:CD1	1:B:276:ILE:HG22	2.38	0.53
2:C:91:THR:HG23	2:C:121:THR:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:99:SER:HB2	2:C:111:MET:SD	2.48	0.53
1:B:416:HIS:HB3	1:B:432:TYR:CE1	2.32	0.53
1:A:148:PRO:HG2	2:C:113:TYR:OH	2.09	0.53
2:C:91:THR:O	2:C:92:ALA:HB2	2.10	0.52
1:B:529:PRO:O	1:B:530:GLU:HB2	2.10	0.52
1:A:256:GLN:CG	4:A:723:HOH:O	2.58	0.52
1:A:164:PRO:HD3	1:A:190:ARG:NH2	2.24	0.51
2:D:12:VAL:HG23	2:D:122:VAL:HG22	1.93	0.50
1:A:335:TYR:HE1	1:A:353:VAL:CG2	2.21	0.50
1:A:68:VAL:HG23	1:A:127:ILE:HG13	1.93	0.50
1:A:272:ARG:HH11	1:A:272:ARG:HB3	1.76	0.50
1:B:233:LEU:HD21	1:B:275:LEU:HD22	1.94	0.50
1:B:451:SER:OG	1:B:471:GLN:HB2	2.12	0.50
2:D:5:GLN:O	2:D:22:CYS:HA	2.12	0.50
1:B:318:THR:HA	1:B:401:PRO:O	2.12	0.49
1:A:380:ASP:HB2	1:A:381:HIS:CD2	2.47	0.49
2:C:51:ILE:HG13	2:C:58:ILE:HG12	1.94	0.49
1:A:233:LEU:HD22	1:A:275:LEU:HD22	1.94	0.49
1:A:99:GLN:HG2	1:A:144:ALA:HB1	1.94	0.49
1:B:233:LEU:HD11	1:B:276:ILE:HG22	1.94	0.49
1:A:70:THR:HB	1:A:96:ASN:ND2	2.28	0.49
1:B:275:LEU:O	1:B:277:GLN:HG2	2.13	0.48
2:C:11:LEU:H	2:C:11:LEU:HD23	1.79	0.48
1:B:504:LEU:HB2	1:B:521:GLU:HG2	1.96	0.48
1:A:367:LEU:HD23	1:A:371:THR:HG21	1.94	0.48
1:B:430:ARG:HH12	1:B:481:PRO:HD3	1.79	0.48
1:B:495:ARG:HG3	1:B:526:SER:O	2.14	0.47
1:B:47:LEU:HD21	1:B:467:TYR:CE1	2.49	0.47
1:B:495:ARG:HG2	1:B:527:PHE:CD1	2.49	0.47
1:B:501:TRP:CD1	1:B:503:VAL:HG22	2.49	0.47
1:B:325:PRO:HG2	1:B:328:GLU:HB2	1.96	0.47
1:B:371:THR:OG1	1:B:372:PRO:HD3	2.14	0.47
1:A:264:LEU:HD13	1:A:332:LEU:HD23	1.97	0.47
1:B:185:THR:OG1	1:B:187:ARG:NH1	2.48	0.47
2:D:68:PHE:CE1	2:D:83:MET:HB3	2.50	0.47
1:B:233:LEU:HD12	1:B:246:ALA:HA	1.96	0.47
2:C:48:VAL:HG13	2:C:64:VAL:HG11	1.97	0.47
2:D:69:THR:HB	2:D:82:GLN:HB3	1.96	0.46
1:A:70:THR:HB	1:A:96:ASN:HD22	1.79	0.46
1:A:272:ARG:HG2	1:A:273:TYR:N	2.30	0.46
1:B:160:LEU:HD21	1:B:254:GLN:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:VAL:HG21	2:D:86:LEU:HD13	1.97	0.46
1:A:222:PHE:HB2	1:A:289:ARG:HH22	1.80	0.46
1:B:175:ARG:O	1:B:176:GLY:C	2.54	0.46
1:B:464:GLU:O	1:B:479:VAL:HG22	2.15	0.46
1:A:355:ASP:HA	1:A:364:CYS:SG	2.55	0.46
1:B:255:ASP:OD2	1:B:259:TYR:N	2.49	0.46
1:A:368:PRO:C	1:A:370:ASP:H	2.17	0.46
1:B:73:VAL:CG2	1:B:114:VAL:HG21	2.46	0.45
1:B:160:LEU:HD21	1:B:254:GLN:HB2	1.98	0.45
1:A:195:GLN:O	1:A:195:GLN:HG3	2.16	0.45
1:B:49:VAL:HB	1:B:56:PHE:HB2	1.98	0.45
1:A:504:LEU:HG	1:A:505:LEU:HD12	1.98	0.45
1:B:233:LEU:CD2	1:B:275:LEU:HD22	2.47	0.45
1:A:55:LEU:HG	1:A:127:ILE:HD12	1.99	0.45
1:A:64:LEU:HB2	3:A:601:NAG:H3	1.99	0.45
1:B:509:SER:HB2	1:B:513:GLU:OE1	2.17	0.45
1:A:265:PRO:HD2	1:A:391:PRO:HA	1.99	0.45
1:B:56:PHE:HB3	1:B:58:LEU:HD13	1.99	0.45
2:D:52:SER:O	2:D:72:ARG:NH1	2.50	0.44
1:B:201:GLU:H	1:B:201:GLU:HG3	1.58	0.44
1:B:447:ILE:HB	1:B:470:THR:HG21	1.98	0.44
1:B:495:ARG:CG	1:B:527:PHE:HA	2.47	0.44
2:D:86:LEU:HD23	2:D:86:LEU:HA	1.64	0.44
1:B:349:ASN:N	1:B:349:ASN:OD1	2.50	0.44
1:A:28:PHE:HB3	1:A:474:LEU:HB3	2.00	0.44
1:B:241:SER:O	1:B:242:ARG:C	2.55	0.44
1:B:159:GLY:HA3	1:B:163:GLU:CD	2.38	0.44
1:A:121:LEU:HB2	1:A:132:LEU:HB3	1.99	0.44
1:A:382:THR:O	1:A:383:PRO:C	2.56	0.44
2:C:87:LYS:O	2:C:122:VAL:HG21	2.16	0.44
1:A:113:SER:O	1:A:146:ASN:HA	2.18	0.44
1:A:357:ALA:HB2	1:A:387:VAL:HB	2.00	0.44
1:B:34:HIS:CG	2:D:100:SER:HB2	2.52	0.43
1:B:214:TYR:O	1:B:215:SER:C	2.55	0.43
1:A:416:HIS:HB3	1:A:432:TYR:CE2	2.52	0.43
1:A:320:VAL:HG13	1:A:396:PRO:HB3	2.00	0.43
1:B:73:VAL:HG21	1:B:114:VAL:HG11	1.99	0.43
1:B:229:TYR:HA	1:B:249:SER:O	2.18	0.43
1:A:203:THR:O	1:A:257:HIS:HA	2.18	0.43
1:B:70:THR:HB	1:B:96:ASN:ND2	2.34	0.43
2:C:12:VAL:HG21	2:C:86:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ARG:HB2	1:B:175:ARG:HD2	2.00	0.43
1:B:191:PRO:HG3	1:B:197:ALA:HA	1.99	0.43
1:B:470:THR:O	1:B:471:GLN:HB2	2.18	0.43
2:D:73:ASP:OD2	2:D:76:LYS:HE3	2.19	0.43
1:A:183:PRO:CG	1:A:206:LEU:HD23	2.46	0.43
1:A:202:GLU:HG3	1:A:203:THR:HG23	1.99	0.43
2:D:111:MET:HB2	2:D:114:TRP:CZ2	2.54	0.43
2:C:108:CYS:HB2	2:C:111:MET:CE	2.49	0.43
1:B:265:PRO:HG2	1:B:391:PRO:HA	2.01	0.43
2:C:49:LEU:HD12	2:C:59:ASN:O	2.19	0.43
2:D:28:ARG:NH2	4:D:201:HOH:O	2.47	0.42
1:A:172:TYR:CZ	1:A:174:SER:HB2	2.54	0.42
1:A:384:SER:HB3	1:A:385:PRO:CD	2.45	0.42
2:C:24:ALA:HB2	2:C:29:LEU:HD23	2.01	0.42
3:A:602:NAG:H82	3:A:602:NAG:H2	1.92	0.42
2:C:11:LEU:HA	2:C:121:THR:O	2.19	0.42
1:A:286:GLU:HG3	1:A:287:VAL:HG23	2.01	0.42
2:C:88:PRO:HA	2:C:122:VAL:HB	2.01	0.42
1:B:320:VAL:HG22	1:B:396:PRO:HB3	2.01	0.42
2:C:108:CYS:HB2	2:C:111:MET:HE2	2.01	0.42
2:D:83:MET:HB2	2:D:83:MET:HE3	1.76	0.42
1:A:55:LEU:HB3	1:A:68:VAL:HB	2.00	0.42
1:B:236:ASP:O	1:B:239:ALA:HB3	2.20	0.42
1:B:321:LEU:O	1:B:397:ILE:HG12	2.20	0.42
1:A:492:LEU:HD22	1:A:526:SER:HA	2.02	0.42
2:C:86:LEU:HD23	2:C:86:LEU:HA	1.94	0.41
1:A:291:ASP:OD1	1:A:291:ASP:N	2.48	0.41
1:B:47:LEU:HD21	1:B:467:TYR:CZ	2.55	0.41
1:B:285:LYS:HG3	1:B:463:PHE:HD2	1.85	0.41
1:A:90:GLN:H	1:A:90:GLN:HG2	1.56	0.41
1:A:209:GLY:O	1:A:210:ARG:HB2	2.20	0.41
2:C:40:ALA:HB3	2:C:43:LYS:HD3	2.01	0.41
2:C:49:LEU:HD11	2:C:58:ILE:CG2	2.51	0.41
1:B:70:THR:HB	1:B:96:ASN:HD22	1.85	0.41
1:A:358:TYR:O	1:A:359:ASP:C	2.59	0.41
1:A:273:TYR:CD1	1:A:320:VAL:HG21	2.55	0.41
2:C:69:THR:HG22	2:C:82:GLN:HB3	2.02	0.41
1:B:202:GLU:O	1:B:202:GLU:HG2	2.20	0.41
1:B:430:ARG:NH2	1:B:445:GLN:HE22	2.16	0.41
1:A:57:GLN:HE22	1:A:125:GLY:HA2	1.86	0.41
1:A:430:ARG:HE	1:A:445:GLN:NE2	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLU:N	1:A:195:GLN:OE1	2.49	0.41
1:A:448:GLN:HE21	1:A:451:SER:HB2	1.84	0.41
2:C:93:VAL:HA	2:C:119:GLN:HA	2.03	0.41
2:D:24:ALA:HB2	2:D:29:LEU:HD23	2.02	0.41
1:A:380:ASP:OD1	1:A:380:ASP:N	2.54	0.41
1:B:68:VAL:HG23	1:B:127:ILE:HG13	2.02	0.40
1:A:148:PRO:HG2	2:C:113:TYR:CZ	2.56	0.40
2:C:87:LYS:HB3	2:C:88:PRO:HD2	2.03	0.40
1:B:417:THR:HG22	1:B:433:LEU:HD12	2.03	0.40
1:A:239:ALA:HB1	1:A:240:PRO:HD2	2.03	0.40
1:B:148:PRO:HG2	2:D:113:TYR:CE1	2.56	0.40
1:B:248:VAL:HB	1:B:266:LEU:HD11	2.03	0.40
2:C:40:ALA:O	2:C:41:PRO:C	2.60	0.40
1:B:203:THR:HG23	1:B:256:GLN:O	2.22	0.40
1:A:64:LEU:HD12	1:A:64:LEU:HA	1.90	0.40
1:A:420:PHE:CZ	1:A:479:VAL:HG12	2.57	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)
1:B:370:ASP:OD1	1:A:446:SER:OG[2_555]	2.19	0.01

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	467/523 (89%)	432 (92%)	32 (7%)	3 (1%)	25	60
1	B	477/523 (91%)	435 (91%)	36 (8%)	6 (1%)	12	41
2	C	119/130 (92%)	114 (96%)	4 (3%)	1 (1%)	19	53
2	D	122/130 (94%)	114 (93%)	7 (6%)	1 (1%)	19	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1185/1306 (91%)	1095 (92%)	79 (7%)	11 (1%)	17 51

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	86	LEU
1	B	71	GLY
1	B	176	GLY
1	B	215	SER
1	B	401	PRO
1	B	438	SER
2	C	92	ALA
1	B	529	PRO
1	A	384	SER
1	A	183	PRO
1	A	240	PRO

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	394/430 (92%)	384 (98%)	10 (2%)	47 76
1	B	399/430 (93%)	391 (98%)	8 (2%)	55 80
2	C	96/104 (92%)	90 (94%)	6 (6%)	18 48
2	D	98/104 (94%)	93 (95%)	5 (5%)	24 56
All	All	987/1068 (92%)	958 (97%)	29 (3%)	42 73

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	59	SER
1	B	86	ASP
1	B	106	GLU
1	B	114	VAL

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Mol	Chain	Res	Type
1	B	273	TYR
1	B	320	VAL
1	B	363	ASP
1	B	527	PHE
2	D	28	ARG
2	D	59	ASN
2	D	77	ASN
2	D	96	CYS
2	D	112	ASP
1	A	174	SER
1	A	220	SER
1	A	245	ARG
1	A	273	TYR
1	A	363	ASP
1	A	380	ASP
1	A	490	SER
1	A	503	VAL
1	A	514	CYS
1	A	527	PHE
2	C	30	ASP
2	C	43	LYS
2	C	57	SER
2	C	77	ASN
2	C	89	GLU
2	C	114	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	31	ASN
1	B	445	GLN
1	B	494	HIS
2	D	5	GLN
1	A	445	GLN
1	A	485	HIS
2	C	3	GLN

5.3.3 RNA

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)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	B	603	1	14,14,15	0.40	0	17,19,21	1.33	3 (17%)
3	NAG	A	601	-	14,14,15	0.45	0	17,19,21	2.98	3 (17%)
3	NAG	B	602	1	14,14,15	0.56	0	17,19,21	0.61	0
3	NAG	A	602	1	14,14,15	0.44	0	17,19,21	0.65	0
3	NAG	A	605	1	14,14,15	0.40	0	17,19,21	0.86	0
3	NAG	B	601	1	14,14,15	0.20	0	17,19,21	0.50	0
3	NAG	A	603	1	14,14,15	0.33	0	17,19,21	0.38	0
3	NAG	A	604	1	14,14,15	0.43	0	17,19,21	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	601	-	-	3/6/23/26	0/1/1/1
3	NAG	B	603	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	B	602	1	-	2/6/23/26	0/1/1/1
3	NAG	A	602	1	-	2/6/23/26	0/1/1/1
3	NAG	A	605	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	601	1	-	2/6/23/26	0/1/1/1
3	NAG	A	603	1	-	4/6/23/26	0/1/1/1
3	NAG	A	604	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	NAG	O5-C1-C2	-9.16	96.83	111.29
3	A	601	NAG	C2-N2-C7	5.14	130.23	122.90
3	A	601	NAG	C1-C2-N2	5.12	119.24	110.49
3	B	603	NAG	C1-C2-N2	3.53	116.52	110.49
3	B	603	NAG	C2-N2-C7	3.04	127.23	122.90
3	B	603	NAG	O5-C1-C2	2.50	115.23	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	603	NAG	C1

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	603	NAG	C3-C2-N2-C7
3	A	601	NAG	C1-C2-N2-C7
3	A	602	NAG	C8-C7-N2-C2
3	A	602	NAG	O7-C7-N2-C2
3	B	601	NAG	O5-C5-C6-O6
3	B	602	NAG	O5-C5-C6-O6
3	A	605	NAG	O5-C5-C6-O6
3	B	601	NAG	C4-C5-C6-O6
3	A	604	NAG	C4-C5-C6-O6
3	A	603	NAG	C8-C7-N2-C2
3	A	603	NAG	O7-C7-N2-C2
3	A	605	NAG	C8-C7-N2-C2
3	A	605	NAG	O7-C7-N2-C2
3	A	604	NAG	O5-C5-C6-O6
3	B	602	NAG	C4-C5-C6-O6
3	A	605	NAG	C4-C5-C6-O6
3	B	603	NAG	O5-C5-C6-O6
3	A	601	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	A	601	NAG	C8-C7-N2-C2
3	A	603	NAG	C4-C5-C6-O6
3	A	603	NAG	O5-C5-C6-O6
3	B	603	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NAG	3	0
3	A	602	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	470:THR	C	471:GLN	N	1.18

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	479/523 (91%)	-0.14	13 (2%) 54 38	22, 41, 73, 108	0
1	B	485/523 (92%)	-0.26	6 (1%) 79 63	18, 35, 71, 103	0
2	C	121/130 (93%)	0.48	15 (12%) 4 2	33, 57, 84, 103	0
2	D	124/130 (95%)	-0.19	2 (1%) 72 55	22, 35, 59, 93	0
All	All	1209/1306 (92%)	-0.13	36 (2%) 50 34	18, 39, 74, 108	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	122	VAL	6.0
2	C	40	ALA	4.4
2	D	124	ALA	4.3
1	A	175	ARG	3.8
1	A	177	VAL	3.8
2	C	41	PRO	3.5
1	A	515	SER	3.4
2	C	88	PRO	3.2
2	C	42	GLY	3.1
1	A	504	LEU	3.0
2	C	121	THR	2.9
2	C	120	VAL	2.9
1	A	505	LEU	2.9
2	C	11	LEU	2.9
1	A	489	ASP	2.8
1	A	273	TYR	2.8
1	B	86	ASP	2.8
1	A	512	SER	2.7
1	B	274	GLY	2.6
1	A	511	ARG	2.6
1	B	273	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	316	SER	2.6
1	B	520	PRO	2.6
2	C	87	LYS	2.5
2	C	86	LEU	2.5
2	C	90	ASP	2.5
1	B	84	ILE	2.3
2	C	89	GLU	2.2
2	C	85	SER	2.2
1	B	438	SER	2.2
1	A	274	GLY	2.2
1	A	176	GLY	2.2
2	D	13	GLN	2.2
2	C	91	THR	2.1
1	A	86	ASP	2.0
2	C	7	SER	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	NAG	B	603	14/15	0.70	0.35	52,85,89,91	0
3	NAG	A	605	14/15	0.81	0.26	72,85,96,99	0
3	NAG	A	603	14/15	0.82	0.37	74,77,86,87	0
3	NAG	B	602	14/15	0.89	0.30	64,73,82,82	0
3	NAG	A	601	14/15	0.89	0.23	29,38,51,72	0
3	NAG	A	604	14/15	0.95	0.22	38,50,56,58	0
3	NAG	A	602	14/15	0.95	0.16	29,33,38,45	0
3	NAG	B	601	14/15	0.96	0.23	37,44,51,55	0

6.5 Other polymers (i)

There are no such residues in this entry.