



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:23 PM UTC

PDB ID : 5TD8 / pdb_00005td8
Title : Crystal structure of an Extended Dwarf Ndc80 Complex
Authors : Valverde, R.; Ingram, J.; Harrison, S.C.
Deposited on : 2016-09-17
Resolution : 7.53 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

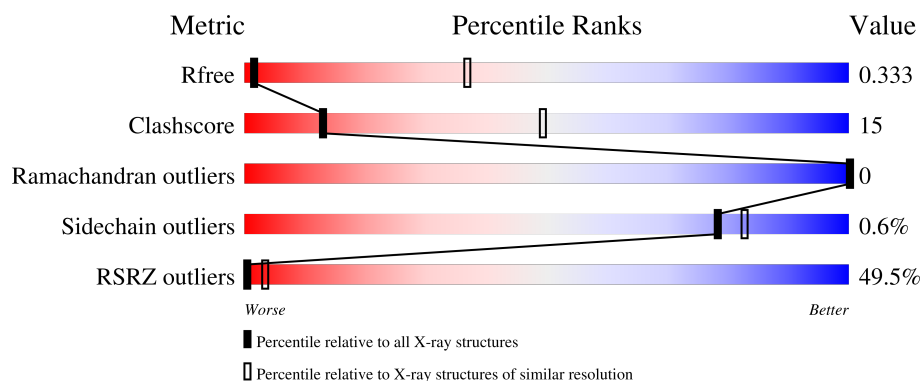
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.53 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}	180053	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	279	42% 70% 22% 8%
2	B	198	45% 60% 34% 6%
3	C	114	56% 61% 36% .
4	D	129	47% 84% 15% ..
5	E	145	39% 62% 10% 28%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12626 atoms, of which 6191 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 Kinetochore protein NDC80.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	256	Total	C	H	N	O	S	0	0	0
			4302	1385	2144	363	404	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	SER	-	expression tag	UNP P40460
A	112	ASN	-	expression tag	UNP P40460
A	113	ALA	-	expression tag	UNP P40460

- Molecule 2 is a protein called Kinetochore protein NUF2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	186	Total	C	H	N	O	S	0	0	0
			2902	964	1376	247	303	12			

- Molecule 3 is a protein called Kinetochore protein SPC24.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	111	Total	C	H	N	O	S	0	0	0
			1839	578	917	162	181	1			

- Molecule 4 is a protein called Kinetochore protein SPC25.

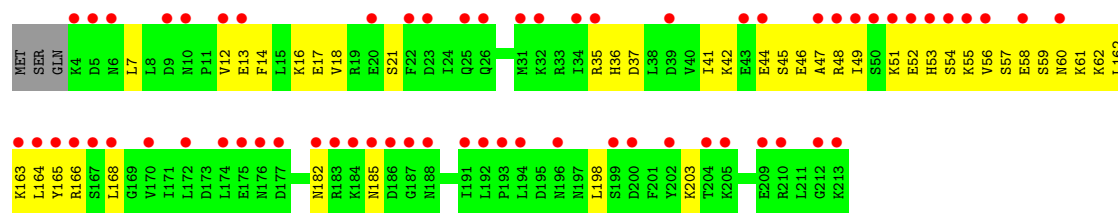
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	128	Total	C	H	N	O	S	0	0	0
			2011	632	998	190	186	5			

- Molecule 5 is a protein called nanobody.

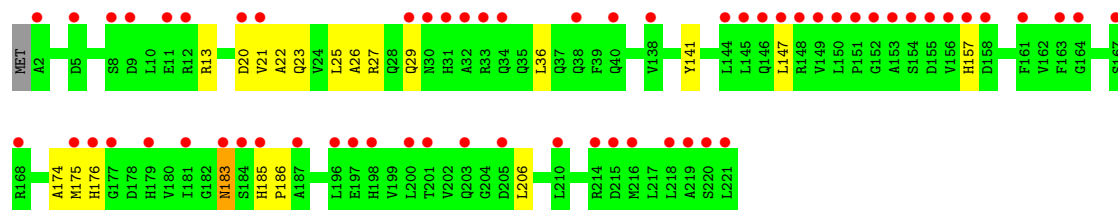
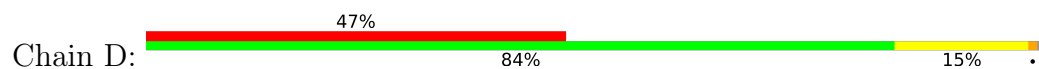
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	105	Total	C	H	N	O	S	0	0	0
			1566	512	756	143	152	3			

- Molecule 6 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

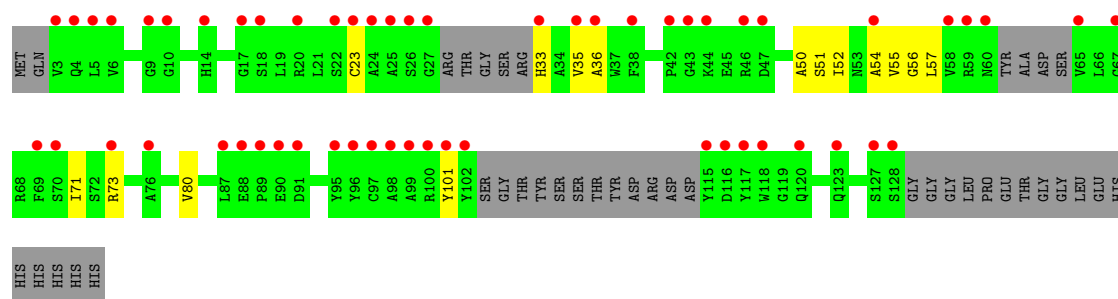
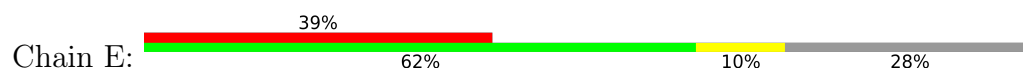
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Hg	0	0
			2	2		
6	B	2	Total	Hg	0	0
			2	2		
6	D	2	Total	Hg	0	0
			2	2		



● Molecule 4: Kinetochore protein SPC25



● Molecule 5: nanobody



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	226.82Å 226.82Å 237.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.41 – 7.53 113.41 – 7.53	Depositor EDS
% Data completeness (in resolution range)	99.7 (113.41-7.53) 99.7 (113.41-7.53)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 7.45Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.312 , 0.328 0.314 , 0.333	Depositor DCC
R_{free} test set	204 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.016 for -l,-k,-h 0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	12626	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: HG

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	0.24	0/2199	0.44	0/2958
2	B	0.20	0/1547	0.45	0/2083
3	C	0.29	0/933	0.62	0/1251
4	D	0.16	0/1030	0.40	0/1392
5	E	0.14	0/826	0.36	0/1116
All	All	0.22	0/6535	0.46	0/8800

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	2158	2144	2171	54	2
2	B	1526	1376	1493	66	0
3	C	922	917	932	72	2
4	D	1013	998	999	16	0
5	E	810	756	771	17	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	D	2	0	0	0	0
All	All	6435	6191	6366	192	2

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 15.

All (192) 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:249:GLN:OE1	1:A:270:ARG:NH1	2.07	0.88
3:C:21:SER:HB3	5:E:57:LEU:HG	1.57	0.86
2:B:148:GLU:O	2:B:152:GLY:N	2.13	0.81
3:C:61:LYS:O	3:C:164:LEU:HB2	1.81	0.80
3:C:61:LYS:O	3:C:164:LEU:CB	2.32	0.78
3:C:21:SER:CB	5:E:57:LEU:HG	2.15	0.76
2:B:143:PHE:O	2:B:147:MET:N	2.19	0.76
1:A:298:GLU:OE1	1:A:302:GLN:NE2	2.22	0.73
3:C:56:VAL:O	3:C:60:ASN:HB2	1.88	0.73
3:C:46:GLU:O	3:C:49:ILE:N	2.18	0.72
3:C:165:TYR:OH	4:D:147:LEU:O	2.09	0.71
2:B:431:GLU:CD	3:C:16:LYS:HG2	2.16	0.70
1:A:235:CYS:SG	2:B:64:SER:OG	2.51	0.67
3:C:45:SER:O	3:C:49:ILE:HG23	1.93	0.67
1:A:262:ASP:OD1	1:A:263:GLU:N	2.29	0.66
3:C:55:LYS:O	3:C:59:SER:OG	2.13	0.65
2:B:34:SER:O	2:B:37:THR:OG1	2.13	0.64
3:C:59:SER:O	3:C:162:LEU:CB	2.45	0.64
3:C:18:VAL:HA	5:E:55:VAL:HG13	1.80	0.64
3:C:55:LYS:O	3:C:59:SER:CB	2.46	0.63
1:A:230:ILE:O	1:A:234:MET:HG2	1.98	0.63
1:A:147:HIS:HB2	1:A:148:PRO:HD3	1.81	0.63
1:A:148:PRO:HB2	1:A:151:ILE:HB	1.80	0.63
3:C:59:SER:O	3:C:162:LEU:HG	2.00	0.62
3:C:54:SER:O	3:C:58:GLU:HB2	2.01	0.61
3:C:62:LYS:O	3:C:165:TYR:CG	2.54	0.61
3:C:62:LYS:O	3:C:165:TYR:CD2	2.54	0.60
1:A:224:TRP:HE1	2:B:80:ILE:HG22	1.66	0.60
3:C:59:SER:O	3:C:162:LEU:HB2	2.01	0.60
1:A:203:ASN:OD1	1:A:205:SER:OG	2.20	0.59
2:B:88:LEU:O	2:B:92:LYS:HG2	2.01	0.59
3:C:164:LEU:HG	4:D:206:LEU:CD2	2.33	0.59
3:C:46:GLU:O	3:C:49:ILE:HG12	2.03	0.59
2:B:440:ASN:OD1	4:D:13:ARG:NH2	2.35	0.58
1:A:287:TYR:CZ	2:B:129:TYR:HB2	2.37	0.58
4:D:23:GLN:O	4:D:27:ARG:N	2.31	0.58
1:A:173:LEU:O	2:B:92:LYS:NZ	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:CYS:O	2:B:143:PHE:HB3	2.04	0.57
1:A:128:ILE:HB	1:A:223:HIS:CG	2.40	0.57
2:B:147:MET:O	2:B:151:LEU:N	2.25	0.57
2:B:450:MET:O	2:B:451:GLN:HB2	2.05	0.57
1:A:289:SER:O	1:A:292:LYS:N	2.37	0.56
1:A:311:PHE:CE2	2:B:150:LEU:HD12	2.40	0.56
2:B:97:PHE:HZ	2:B:126:VAL:HG11	1.69	0.56
1:A:299:PRO:O	1:A:303:GLU:HB2	2.06	0.56
3:C:61:LYS:O	3:C:164:LEU:HB3	2.04	0.56
1:A:271:TYR:OH	1:A:318:ASP:OD2	2.20	0.56
3:C:18:VAL:HA	5:E:55:VAL:CG1	2.36	0.55
1:A:157:PRO:HG3	1:A:215:TRP:CE2	2.41	0.55
3:C:62:LYS:HA	3:C:164:LEU:HB3	1.89	0.55
3:C:164:LEU:O	3:C:168:LEU:HG	2.07	0.54
2:B:42:VAL:HG13	2:B:90:LEU:HD21	1.89	0.54
1:A:629:GLU:O	1:A:632:LYS:HB2	2.08	0.54
3:C:21:SER:HB2	5:E:55:VAL:CG1	2.38	0.54
2:B:85:LEU:O	2:B:89:VAL:HG23	2.07	0.54
5:E:50:ALA:HB3	5:E:71:ILE:HD12	1.88	0.53
2:B:145:LEU:O	2:B:149:SER:N	2.28	0.53
3:C:12:VAL:O	3:C:16:LYS:HG3	2.09	0.53
3:C:57:SER:O	3:C:61:LYS:HB2	2.09	0.53
3:C:13:GLU:OE1	5:E:33:HIS:NE2	2.39	0.53
1:A:287:TYR:HB2	2:B:129:TYR:CZ	2.44	0.52
2:B:91:ASN:HA	2:B:111:LEU:HD11	1.91	0.52
2:B:41:MET:HG3	2:B:114:PRO:CG	2.40	0.52
1:A:132:ILE:HA	1:A:226:VAL:HG11	1.92	0.52
2:B:87:VAL:HG13	2:B:112:TYR:OH	2.08	0.52
1:A:632:LYS:O	1:A:636:ASN:CG	2.53	0.52
1:A:312:VAL:HG12	2:B:150:LEU:HD11	1.91	0.51
1:A:315:ILE:HG21	2:B:150:LEU:HD13	1.91	0.51
3:C:41:ILE:O	3:C:44:GLU:N	2.43	0.51
3:C:52:GLU:O	3:C:56:VAL:HB	2.10	0.51
1:A:632:LYS:O	1:A:636:ASN:HB2	2.11	0.50
3:C:59:SER:O	3:C:162:LEU:CG	2.59	0.50
3:C:45:SER:C	3:C:49:ILE:HG23	2.37	0.50
3:C:60:ASN:HA	3:C:162:LEU:HB2	1.92	0.49
3:C:162:LEU:O	3:C:166:ARG:HB2	2.11	0.49
3:C:21:SER:OG	5:E:57:LEU:HG	2.12	0.49
5:E:33:HIS:ND1	5:E:101:TYR:O	2.45	0.49
1:A:315:ILE:HG21	2:B:150:LEU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:HIS:HD1	3:C:36:HIS:C	2.21	0.49
3:C:55:LYS:O	3:C:59:SER:HB3	2.11	0.49
1:A:311:PHE:CD2	2:B:143:PHE:CE1	3.00	0.48
3:C:54:SER:O	3:C:58:GLU:CB	2.61	0.48
3:C:62:LYS:O	3:C:165:TYR:HB2	2.14	0.48
3:C:54:SER:HA	3:C:57:SER:OG	2.13	0.48
3:C:48:ARG:HA	3:C:51:LYS:HB2	1.95	0.48
1:A:148:PRO:HB2	1:A:151:ILE:CB	2.44	0.48
1:A:288:LYS:O	1:A:292:LYS:HB2	2.14	0.48
1:A:632:LYS:O	1:A:636:ASN:CB	2.62	0.48
1:A:141:PHE:CE2	1:A:148:PRO:HG3	2.50	0.47
2:B:149:SER:O	2:B:153:GLN:N	2.36	0.47
1:A:236:LEU:HD11	2:B:92:LYS:HG3	1.97	0.47
1:A:295:ASP:O	1:A:299:PRO:HD2	2.15	0.47
2:B:101:ILE:HD11	2:B:122:LEU:HB3	1.95	0.47
2:B:415:LYS:O	2:B:416:GLN:C	2.56	0.47
1:A:315:ILE:HD13	2:B:150:LEU:HB3	1.95	0.47
1:A:642:LEU:O	1:A:645:GLN:HG2	2.14	0.47
1:A:147:HIS:CB	1:A:148:PRO:HD3	2.45	0.46
1:A:115:ASP:HB3	1:A:116:PRO:HD3	1.97	0.46
4:D:23:GLN:HA	4:D:26:ALA:HB3	1.97	0.46
2:B:57:VAL:HG11	2:B:90:LEU:HD13	1.96	0.46
2:B:79:ASN:O	2:B:79:ASN:OD1	2.32	0.46
3:C:44:GLU:O	3:C:48:ARG:HB2	2.16	0.46
3:C:14:PHE:O	3:C:18:VAL:HG23	2.15	0.46
3:C:17:GLU:C	5:E:55:VAL:HG21	2.41	0.46
3:C:162:LEU:O	3:C:166:ARG:CB	2.64	0.46
4:D:175:MET:HG3	4:D:176:HIS:CE1	2.50	0.46
3:C:21:SER:HB2	5:E:55:VAL:HB	1.97	0.46
3:C:53:HIS:O	3:C:57:SER:CB	2.65	0.45
1:A:246:GLN:OE1	1:A:277:LYS:NZ	2.30	0.45
2:B:81:TYR:O	2:B:85:LEU:HG	2.16	0.45
3:C:62:LYS:O	3:C:165:TYR:CB	2.64	0.45
3:C:46:GLU:C	3:C:49:ILE:H	2.17	0.45
1:A:158:THR:HG23	1:A:161:GLY:H	1.81	0.45
3:C:165:TYR:CE2	4:D:141:TYR:HB3	2.51	0.45
4:D:21:VAL:O	4:D:22:ALA:C	2.60	0.45
2:B:126:VAL:O	2:B:129:TYR:HB3	2.16	0.45
3:C:162:LEU:O	3:C:166:ARG:CG	2.65	0.45
2:B:427:GLU:HB3	3:C:12:VAL:HG11	1.99	0.44
4:D:157:HIS:HA	4:D:174:ALA:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:PHE:CZ	2:B:126:VAL:HG11	2.52	0.44
2:B:107:ASN:OD1	2:B:109:THR:CB	2.65	0.44
3:C:52:GLU:O	3:C:56:VAL:HG23	2.17	0.44
2:B:33:ILE:O	2:B:33:ILE:HG22	2.18	0.44
3:C:45:SER:O	3:C:49:ILE:N	2.51	0.44
1:A:157:PRO:HG3	1:A:215:TRP:CZ2	2.53	0.44
3:C:182:ASN:OD1	3:C:185:ASN:HA	2.17	0.44
1:A:678:LEU:HD21	4:D:36:LEU:HD12	2.00	0.43
5:E:36:ALA:HB2	5:E:51:SER:CB	2.48	0.43
2:B:420:ASP:O	2:B:423:VAL:HB	2.18	0.43
2:B:147:MET:HG3	2:B:148:GLU:N	2.32	0.43
3:C:57:SER:O	3:C:61:LYS:CB	2.66	0.43
2:B:143:PHE:CE2	2:B:147:MET:HE2	2.54	0.43
3:C:52:GLU:O	3:C:56:VAL:CB	2.67	0.43
3:C:59:SER:O	3:C:162:LEU:N	2.50	0.43
2:B:109:THR:HG23	2:B:113:LYS:HG3	1.99	0.43
1:A:135:TYR:CD1	1:A:230:ILE:CD1	3.01	0.43
2:B:414:ILE:O	2:B:415:LYS:C	2.62	0.43
2:B:416:GLN:O	2:B:417:LEU:C	2.61	0.43
3:C:54:SER:HA	3:C:57:SER:HG	1.84	0.43
2:B:443:MET:HE1	4:D:13:ARG:HB3	2.01	0.43
2:B:444:ASN:O	2:B:447:LEU:HB2	2.18	0.43
1:A:226:VAL:O	1:A:230:ILE:HG12	2.18	0.42
3:C:41:ILE:O	3:C:42:LYS:C	2.62	0.42
3:C:46:GLU:O	3:C:47:ALA:C	2.61	0.42
2:B:143:PHE:CD2	2:B:147:MET:HE2	2.54	0.42
2:B:146:GLN:O	2:B:150:LEU:HG	2.18	0.42
4:D:25:LEU:O	4:D:29:GLN:HG3	2.19	0.42
4:D:185:HIS:HB3	4:D:186:PRO:HD3	2.00	0.42
5:E:35:VAL:HG12	5:E:80:VAL:HG11	2.02	0.42
1:A:249:GLN:CD	1:A:270:ARG:HH11	2.25	0.42
2:B:120:GLN:HG3	2:B:121:ARG:N	2.33	0.42
2:B:147:MET:CG	2:B:148:GLU:N	2.83	0.42
2:B:449:TYR:HD2	3:C:35:ARG:HD2	1.85	0.42
2:B:41:MET:HG3	2:B:114:PRO:HG3	2.01	0.42
2:B:153:GLN:O	2:B:407:ILE:C	2.62	0.42
2:B:441:LYS:O	2:B:442:TYR:C	2.62	0.42
3:C:57:SER:O	3:C:61:LYS:CG	2.67	0.42
1:A:157:PRO:HD3	1:A:215:TRP:CH2	2.55	0.42
1:A:624:THR:HB	2:B:410:LEU:HD23	2.02	0.41
4:D:22:ALA:O	4:D:25:LEU:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:183:ASN:N	4:D:183:ASN:OD1	2.52	0.41
3:C:54:SER:O	3:C:58:GLU:CG	2.68	0.41
1:A:261:LEU:HD21	2:B:411:ASN:O	2.19	0.41
5:E:23:CYS:HB3	5:E:80:VAL:HG12	2.01	0.41
2:B:146:GLN:O	2:B:147:MET:C	2.62	0.41
5:E:52:ILE:HD11	5:E:56:GLY:HA2	2.02	0.41
2:B:106:PHE:CZ	2:B:111:LEU:HG	2.56	0.41
4:D:20:ASP:O	4:D:21:VAL:C	2.63	0.41
5:E:55:VAL:O	5:E:55:VAL:HG12	2.21	0.41
2:B:143:PHE:HA	2:B:146:GLN:HB2	2.02	0.41
3:C:53:HIS:O	3:C:57:SER:HB3	2.20	0.41
3:C:36:HIS:C	3:C:36:HIS:ND1	2.78	0.41
1:A:270:ARG:O	1:A:274:MET:HG3	2.21	0.41
1:A:643:HIS:CG	3:C:7:LEU:HD12	2.56	0.41
2:B:34:SER:O	2:B:35:ARG:C	2.63	0.41
2:B:429:GLU:O	2:B:430:ILE:C	2.64	0.41
2:B:443:MET:O	2:B:447:LEU:HD13	2.20	0.41
3:C:56:VAL:O	3:C:56:VAL:HG12	2.20	0.41
3:C:198:LEU:HB2	3:C:203:LYS:HE3	2.03	0.41
5:E:54:ALA:HA	5:E:73:ARG:CZ	2.51	0.41
3:C:60:ASN:O	3:C:163:LYS:HB2	2.21	0.40
1:A:221:MET:HE2	1:A:221:MET:HB3	1.90	0.40
1:A:246:GLN:HA	1:A:249:GLN:HB2	2.03	0.40
1:A:298:GLU:N	1:A:299:PRO:HD2	2.37	0.40
1:A:314:ILE:O	1:A:317:THR:HB	2.22	0.40
2:B:55:ILE:HG22	2:B:56:SER:N	2.37	0.40
3:C:52:GLU:O	3:C:56:VAL:CG2	2.69	0.40
3:C:44:GLU:O	3:C:45:SER:C	2.64	0.40
1:A:675:ILE:CG2	1:A:679:ARG:CZ	3.00	0.40
2:B:35:ARG:O	2:B:37:THR:N	2.48	0.40
1:A:229:ASN:O	1:A:230:ILE:C	2.64	0.40
2:B:106:PHE:O	2:B:107:ASN:CG	2.64	0.40

All (2) 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:A:213:SER:N	3:C:37:ASP:OD1[3_745]	2.04	0.16
1:A:213:SER:H	3:C:37:ASP:OD1[3_745]	1.54	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	252/279 (90%)	232 (92%)	20 (8%)	0	100	100
2	B	184/198 (93%)	163 (89%)	21 (11%)	0	100	100
3	C	109/114 (96%)	104 (95%)	5 (5%)	0	100	100
4	D	126/129 (98%)	112 (89%)	14 (11%)	0	100	100
5	E	97/145 (67%)	94 (97%)	3 (3%)	0	100	100
All	All	768/865 (89%)	705 (92%)	63 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/268 (92%)	244 (99%)	2 (1%)	73	80
2	B	175/187 (94%)	174 (99%)	1 (1%)	78	83
3	C	106/109 (97%)	106 (100%)	0	100	100
4	D	107/108 (99%)	106 (99%)	1 (1%)	70	79
5	E	83/115 (72%)	83 (100%)	0	100	100
All	All	717/787 (91%)	713 (99%)	4 (1%)	78	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	681	LEU
2	B	103	VAL
4	D	183	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	189	GLN
1	A	302	GLN
2	B	438	HIS
3	C	188	ASN
4	D	28	GLN
4	D	157	HIS
4	D	176	HIS
4	D	203	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	256/279 (91%)	2.16	118 (46%) 0 4	16, 46, 102, 144	0
2	B	186/198 (93%)	2.30	90 (48%) 0 3	26, 59, 110, 129	0
3	C	111/114 (97%)	2.74	64 (57%) 0 3	20, 42, 54, 65	0
4	D	128/129 (99%)	2.21	61 (47%) 0 4	20, 40, 70, 82	1 (0%)
5	E	105/145 (72%)	2.21	56 (53%) 0 3	23, 38, 53, 69	0
All	All	786/865 (90%)	2.29	389 (49%) 0 3	16, 44, 89, 144	1 (0%)

All (389) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	70	ASP	11.9
1	A	208	SER	9.2
5	E	27	GLY	9.1
4	D	156	VAL	9.0
3	C	9	ASP	8.5
3	C	213	LYS	8.1
2	B	72	HIS	7.5
5	E	128	SER	7.4
1	A	150	SER	7.4
2	B	71	GLY	7.3
4	D	158	ASP	7.3
4	D	155	ASP	7.1
1	A	248	THR	7.1
4	D	8	SER	6.9
3	C	212	GLY	6.9
1	A	676	GLU	6.8
4	D	153	ALA	6.7
3	C	209	GLU	6.7
2	B	24	ASP	6.6
2	B	65	ASN	6.6

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Mol	Chain	Res	Type	RSRZ
2	B	75	GLU	6.5
4	D	2	ALA	6.5
3	C	53	HIS	6.4
2	B	69	GLY	6.2
4	D	185	HIS	6.2
2	B	63	SER	6.2
2	B	74	GLN	6.0
3	C	4	LYS	6.0
3	C	20	GLU	5.8
3	C	205	LYS	5.8
5	E	102	TYR	5.8
1	A	677	GLU	5.8
2	B	111	LEU	5.6
5	E	5	LEU	5.6
1	A	147	HIS	5.6
1	A	249	GLN	5.5
4	D	151	PRO	5.5
3	C	185	ASN	5.4
5	E	69	PHE	5.4
3	C	177	ASP	5.4
2	B	66	GLN	5.3
3	C	44	GLU	5.3
1	A	200	GLU	5.3
1	A	244	ILE	5.3
1	A	682	GLU	5.2
1	A	305	LYS	5.2
2	B	13	LEU	5.1
4	D	144	LEU	5.1
3	C	5	ASP	5.1
1	A	317	THR	5.1
3	C	184	LYS	5.1
5	E	65	VAL	5.1
4	D	183	ASN	5.1
2	B	115	GLU	5.0
1	A	211	GLY	5.0
2	B	77	ASN	5.0
5	E	67	GLY	5.0
2	B	76	GLU	5.0
3	C	187	GLY	5.0
4	D	167	SER	4.9
1	A	188	TYR	4.9
3	C	175	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	73	LEU	4.8
4	D	210	LEU	4.8
2	B	104	GLN	4.8
4	D	168	ARG	4.8
3	C	47	ALA	4.8
1	A	241	ARG	4.7
3	C	26	GLN	4.7
1	A	166	PHE	4.7
2	B	145	LEU	4.7
5	E	9	GLY	4.6
3	C	55	LYS	4.6
1	A	120	ARG	4.6
4	D	176	HIS	4.6
3	C	168	LEU	4.6
2	B	81	TYR	4.6
2	B	34	SER	4.6
1	A	266	GLN	4.6
1	A	115	ASP	4.6
5	E	115	TYR	4.6
4	D	221	LEU	4.6
2	B	26	ALA	4.6
1	A	181	LYS	4.6
2	B	35	ARG	4.5
1	A	152	LYS	4.5
4	D	154	SER	4.5
1	A	276	GLU	4.5
4	D	29	GLN	4.4
5	E	91	ASP	4.4
2	B	51	ASN	4.4
2	B	36	PRO	4.4
1	A	265	ASP	4.3
5	E	120	GLN	4.3
1	A	246	GLN	4.3
3	C	210	ARG	4.3
4	D	220	SER	4.3
1	A	634	ASP	4.3
1	A	285	GLU	4.3
4	D	179	HIS	4.3
3	C	39	ASP	4.3
1	A	242	SER	4.2
1	A	294	GLU	4.2
2	B	15	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	136	LEU	4.2
1	A	138	LYS	4.2
5	E	14	HIS	4.2
1	A	178	GLY	4.2
3	C	163	LYS	4.1
2	B	100	ASN	4.1
3	C	23	ASP	4.1
1	A	681	LEU	4.1
3	C	194	LEU	4.1
1	A	669	ASN	4.1
2	B	448	GLU	4.1
3	C	199	SER	4.1
1	A	175	PRO	4.1
2	B	451	GLN	4.0
2	B	38	SER	4.0
2	B	135	GLU	4.0
4	D	147	LEU	4.0
2	B	113	LYS	4.0
3	C	51	LYS	3.9
3	C	183	ARG	3.9
2	B	80	ILE	3.9
5	E	101	TYR	3.9
3	C	6	ASN	3.9
3	C	202	TYR	3.9
4	D	138	VAL	3.9
2	B	128	ASN	3.9
3	C	167	SER	3.9
2	B	61	LEU	3.9
2	B	413	GLU	3.9
3	C	43	GLU	3.9
1	A	146	ASN	3.9
1	A	293	LEU	3.9
2	B	133	ARG	3.9
4	D	30	ASN	3.8
1	A	264	GLN	3.8
5	E	33	HIS	3.8
5	E	99	ALA	3.8
4	D	218	LEU	3.8
1	A	170	TYR	3.8
1	A	247	ASN	3.8
1	A	159	GLN	3.8
2	B	121	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
5	E	98	ALA	3.8
4	D	9	ASP	3.8
1	A	243	LEU	3.7
3	C	25	GLN	3.7
1	A	137	LYS	3.7
2	B	122	LEU	3.7
1	A	298	GLU	3.7
1	A	184	GLU	3.7
3	C	191	ILE	3.7
5	E	123	GLN	3.7
2	B	422	GLU	3.7
2	B	428	ILE	3.7
1	A	297	TYR	3.7
4	D	203	GLN	3.6
1	A	301	MET	3.6
1	A	132	ILE	3.6
1	A	260	THR	3.6
2	B	16	LEU	3.6
4	D	21	VAL	3.6
1	A	295	ASP	3.5
1	A	201	SER	3.5
5	E	26	SER	3.5
1	A	302	GLN	3.5
2	B	449	TYR	3.5
1	A	245	ASN	3.5
1	A	678	LEU	3.5
5	E	43	GLY	3.5
5	E	23	CYS	3.5
4	D	198	HIS	3.5
5	E	3	VAL	3.5
2	B	37	THR	3.5
5	E	97	CYS	3.5
1	A	192	LYS	3.4
1	A	309	GLU	3.4
3	C	188	ASN	3.4
2	B	58	GLU	3.4
4	D	201	THR	3.4
1	A	179	PHE	3.4
1	A	156	GLN	3.4
4	D	161	PHE	3.3
1	A	222	LEU	3.3
4	D	184	SER	3.3

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Mol	Chain	Res	Type	RSRZ
5	E	90	GLU	3.3
1	A	670	GLU	3.3
2	B	117	GLN	3.3
3	C	193	PRO	3.3
5	E	118	TRP	3.3
2	B	112	TYR	3.3
5	E	60	ASN	3.2
3	C	52	GLU	3.2
3	C	58	GLU	3.2
3	C	56	VAL	3.2
3	C	200	ASP	3.2
1	A	300	SER	3.2
2	B	99	GLU	3.2
5	E	59	ARG	3.2
1	A	648	HIS	3.2
3	C	165	TYR	3.2
5	E	25	ALA	3.2
1	A	638	LYS	3.2
5	E	117	TYR	3.2
2	B	148	GLU	3.1
5	E	36	ALA	3.1
2	B	39	ASP	3.1
3	C	174	LEU	3.1
3	C	34	ILE	3.1
1	A	240	ASP	3.1
2	B	420	ASP	3.1
1	A	217	LYS	3.1
2	B	139	ASP	3.1
3	C	48	ARG	3.1
5	E	96	TYR	3.1
1	A	176	GLY	3.1
2	B	427	GLU	3.1
5	E	58	VAL	3.1
5	E	70	SER	3.1
1	A	167	LYS	3.1
2	B	68	THR	3.0
1	A	233	ASP	3.0
2	B	96	LYS	3.0
4	D	196	LEU	3.0
1	A	665	GLU	3.0
1	A	189	GLN	3.0
4	D	146	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	134	GLU	3.0
4	D	12	ARG	3.0
5	E	87	LEU	3.0
2	B	79	ASN	3.0
1	A	140	LYS	3.0
1	A	641	LYS	3.0
5	E	38	PHE	3.0
5	E	54	ALA	3.0
5	E	127	SER	2.9
2	B	409	LYS	2.9
3	C	35	ARG	2.9
3	C	54	SER	2.9
3	C	176	ASN	2.9
4	D	214	ARG	2.9
4	D	40	GLN	2.9
1	A	209	ALA	2.9
1	A	263	GLU	2.9
2	B	424	GLU	2.9
2	B	21	GLN	2.9
3	C	182	ASN	2.9
1	A	163	ILE	2.9
5	E	100	ARG	2.9
2	B	78	GLU	2.9
3	C	164	LEU	2.9
4	D	149	VAL	2.8
1	A	224	TRP	2.8
4	D	197	GLU	2.8
1	A	660	ILE	2.8
2	B	131	ARG	2.8
5	E	18	SER	2.8
2	B	146	GLN	2.8
1	A	232	LEU	2.8
4	D	219	ALA	2.8
5	E	95	TYR	2.8
3	C	192	LEU	2.8
1	A	680	ASN	2.7
4	D	157	HIS	2.7
1	A	153	PHE	2.7
2	B	82	LEU	2.7
4	D	187	ALA	2.7
2	B	22	SER	2.7
1	A	160	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
5	E	46	ARG	2.7
3	C	10	ASN	2.7
1	A	636	ASN	2.7
2	B	47	GLN	2.7
5	E	4	GLN	2.7
5	E	20	ARG	2.7
3	C	22	PHE	2.7
5	E	24	ALA	2.7
1	A	226	VAL	2.7
1	A	639	ARG	2.7
2	B	64	SER	2.7
4	D	20	ASP	2.6
1	A	231	LYS	2.6
4	D	177	GLY	2.6
4	D	215	ASP	2.6
2	B	151	LEU	2.6
5	E	17	GLY	2.6
1	A	292	LYS	2.6
3	C	170	VAL	2.6
4	D	33	ARG	2.6
1	A	261	LEU	2.6
2	B	14	GLN	2.6
1	A	308	PHE	2.6
2	B	118	ARG	2.6
3	C	204	THR	2.6
5	E	73	ARG	2.6
2	B	429	GLU	2.6
3	C	196	ASN	2.6
5	E	42	PRO	2.6
2	B	143	PHE	2.6
4	D	152	GLY	2.6
2	B	110	ASP	2.6
2	B	432	TYR	2.6
2	B	435	LEU	2.5
3	C	186	ASP	2.5
3	C	166	ARG	2.5
4	D	164	GLY	2.5
2	B	445	GLU	2.5
4	D	31	HIS	2.5
1	A	144	GLU	2.5
5	E	47	ASP	2.5
1	A	123	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	158	THR	2.5
1	A	149	ILE	2.5
2	B	91	ASN	2.5
5	E	88	GLU	2.5
4	D	150	LEU	2.5
1	A	314	ILE	2.5
5	E	89	PRO	2.5
4	D	163	PHE	2.5
1	A	673	ASN	2.5
2	B	101	ILE	2.4
4	D	5	ASP	2.4
5	E	116	ASP	2.4
2	B	32	ASN	2.4
4	D	200	LEU	2.4
1	A	625	GLU	2.4
2	B	124	SER	2.4
2	B	105	ASP	2.4
4	D	205	ASP	2.4
1	A	204	LYS	2.4
5	E	44	LYS	2.4
2	B	86	ASN	2.4
2	B	93	ILE	2.4
3	C	49	ILE	2.4
5	E	35	VAL	2.4
3	C	12	VAL	2.4
2	B	444	ASN	2.4
1	A	272	GLU	2.3
1	A	311	PHE	2.3
4	D	32	ALA	2.3
3	C	172	LEU	2.3
1	A	141	PHE	2.3
2	B	18	ILE	2.3
1	A	220	GLY	2.3
1	A	223	HIS	2.3
3	C	32	LYS	2.3
4	D	38	GLN	2.3
4	D	148	ARG	2.3
3	C	50	SER	2.3
2	B	92	LYS	2.3
4	D	34	GLN	2.3
1	A	177	TYR	2.2
2	B	152	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	173	LEU	2.2
4	D	145	LEU	2.2
1	A	162	PHE	2.2
1	A	627	LYS	2.2
3	C	60	ASN	2.2
1	A	124	PHE	2.2
2	B	40	TYR	2.2
2	B	136	ARG	2.2
1	A	122	LYS	2.2
3	C	13	GLU	2.2
2	B	450	MET	2.2
3	C	31	MET	2.2
2	B	59	SER	2.1
5	E	10	GLY	2.1
1	A	227	ARG	2.1
4	D	216	MET	2.1
5	E	22	SER	2.1
5	E	76	ALA	2.1
1	A	143	ILE	2.1
1	A	262	ASP	2.1
1	A	196	TYR	2.1
1	A	659	ASN	2.1
1	A	130	GLU	2.1
1	A	165	ILE	2.1
1	A	121	ASP	2.1
5	E	6	VAL	2.1
1	A	278	LEU	2.0
1	A	654	SER	2.0
4	D	181	ILE	2.0
4	D	11	GLU	2.0
4	D	175	MET	2.0
1	A	191	LEU	2.0
1	A	668	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	HG	B	501	1/1	0.71	0.21	208,208,208,208	0
6	HG	D	302	1/1	0.94	0.22	77,77,77,77	1
6	HG	D	301	1/1	0.97	0.08	68,68,68,68	1
6	HG	A	702	1/1	0.97	0.08	144,144,144,144	1
6	HG	A	701	1/1	0.98	0.24	81,81,81,81	1
6	HG	B	502	1/1	0.98	0.06	115,115,115,115	1

6.5 Other polymers [i](#)

There are no such residues in this entry.