



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:03 PM UTC

PDB ID : 4NMJ / pdb_00004nmj
Title : Thermostable aldehyde dehydrogenase from Pyrobaculum sp. complexed with NADP⁺ at 2 Å resolution
Authors : Petrova, T.; Boyko, K.M.; Bezsudnova, E.Y.; Mardanov, A.V.; Gumerov, V.M.; Ravin, N.V.; Popov, V.O.
Deposited on : 2013-11-15
Resolution : 2.00 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:

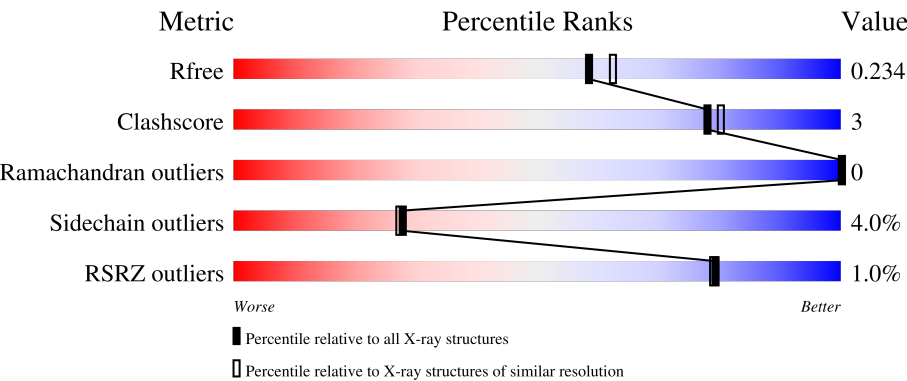
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.00 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.



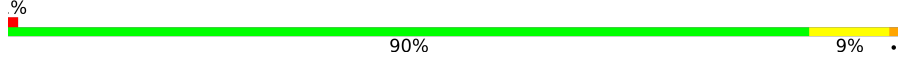
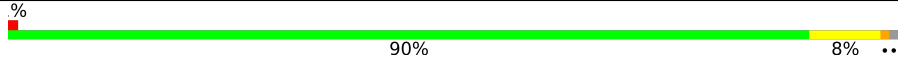
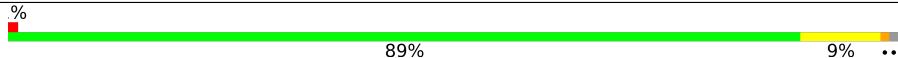
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	491	91%8% ..
1	B	491	% 89%9% ..
1	C	491	% 88%9% ..
1	D	491	% 87%11% ..
1	E	491	2% 90%9% .

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Mol	Chain	Length	Quality of chain
1	F	491	 90%9% .
1	G	491	 90%8% ..
1	H	491	 89%9% ..

2 Entry composition

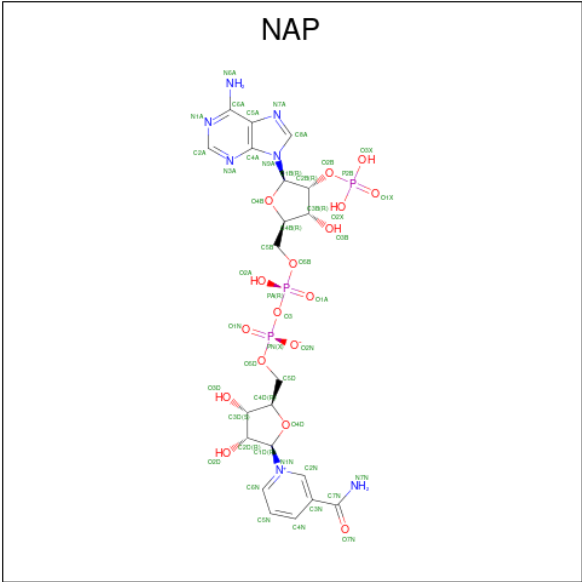
There are 3 unique types of molecules in this entry. The entry contains 33717 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	2	0
			3797	2421	661	703	12			
1	B	485	Total	C	N	O	S	0	2	0
			3784	2408	662	702	12			
1	C	484	Total	C	N	O	S	0	2	0
			3779	2408	659	701	11			
1	D	483	Total	C	N	O	S	0	2	0
			3767	2398	660	698	11			
1	E	485	Total	C	N	O	S	0	2	0
			3779	2408	657	702	12			
1	F	489	Total	C	N	O	S	0	2	0
			3825	2436	668	709	12			
1	G	484	Total	C	N	O	S	0	2	0
			3777	2407	657	701	12			
1	H	484	Total	C	N	O	S	0	2	0
			3771	2402	659	699	11			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	1
			48	21	7	17	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	428	Total	O	0	1
			428	428		
3	B	378	Total	O	0	1
			378	378		
3	C	411	Total	O	0	2
			411	411		
3	D	357	Total	O	0	1
			357	357		

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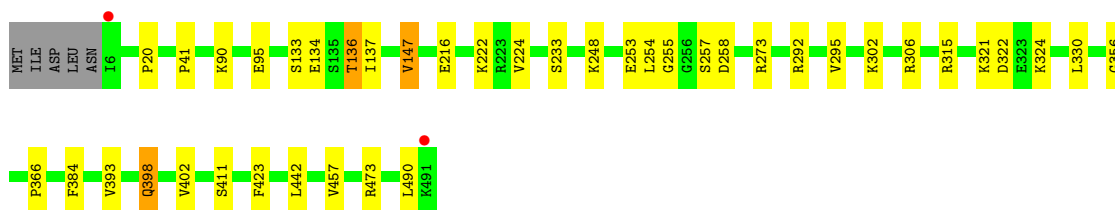
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	323	Total 323	O 323	0	1
3	F	375	Total 375	O 375	0	1
3	G	360	Total 360	O 360	0	1
3	H	422	Total 422	O 422	0	1

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.

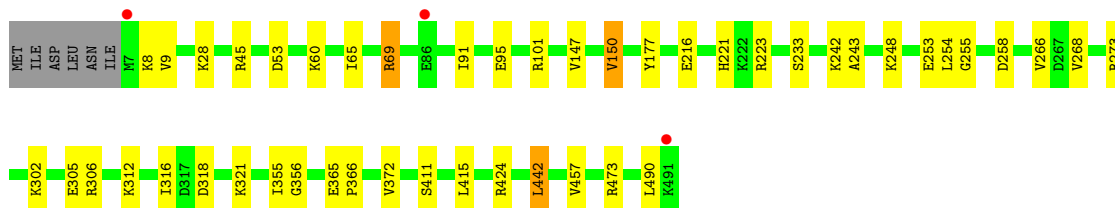
- Molecule 1: Aldehyde dehydrogenase

Chain A:  91% 8% ..



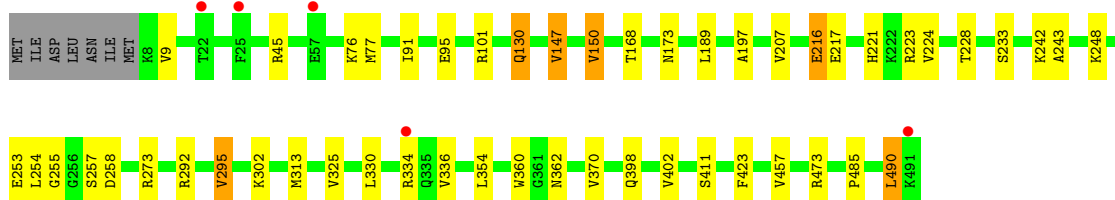
- Molecule 1: Aldehyde dehydrogenase

Chain B:  89% 9% ..



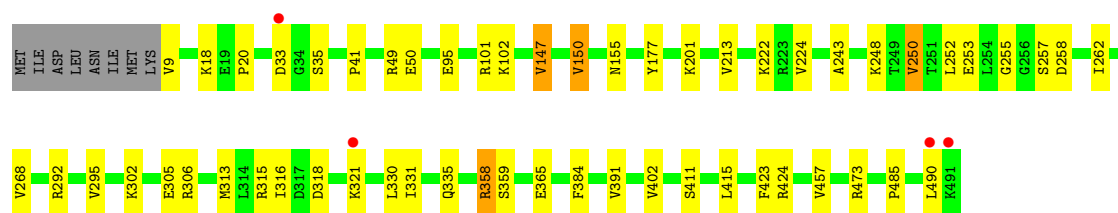
- Molecule 1: Aldehyde dehydrogenase

Chain C:  88% 9% ..

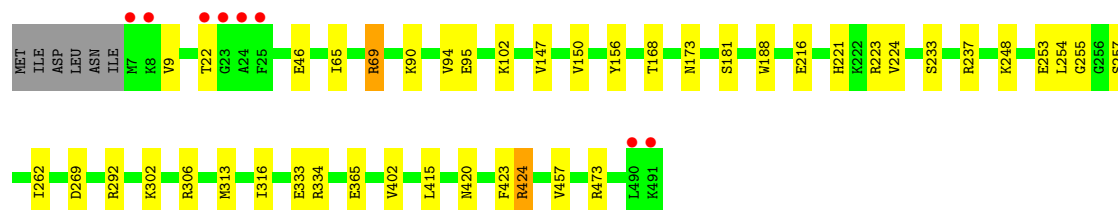
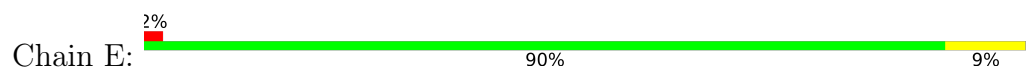


- Molecule 1: Aldehyde dehydrogenase

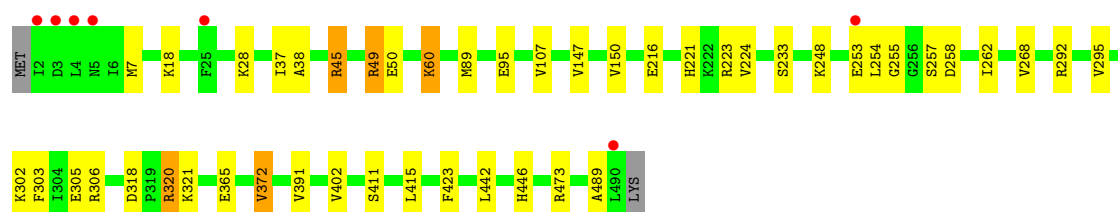
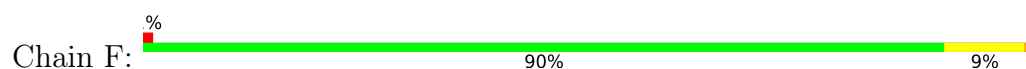
Chain D:  87% 11% ..



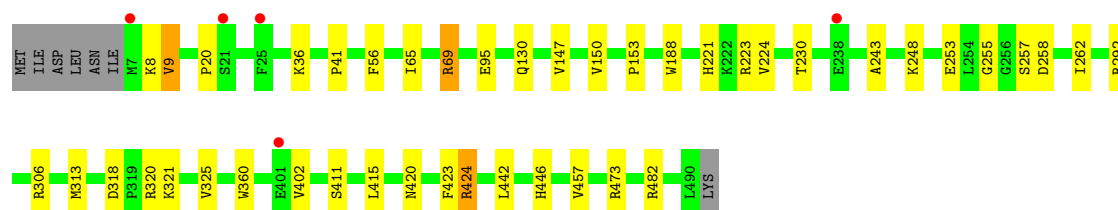
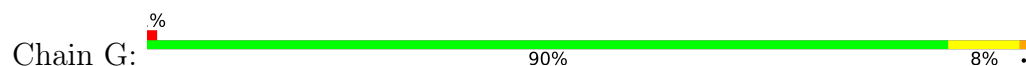
• Molecule 1: Aldehyde dehydrogenase



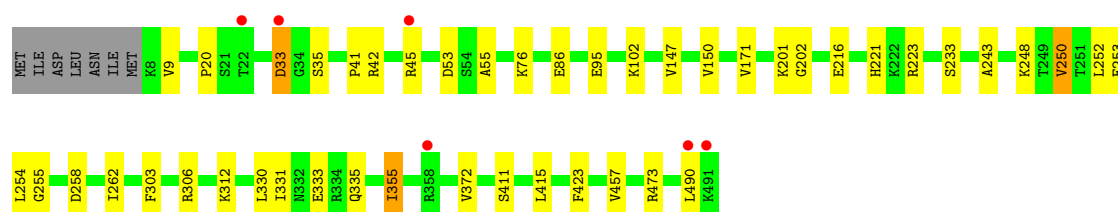
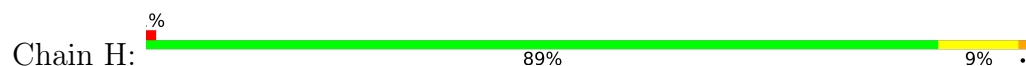
• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	164.48Å 184.39Å 207.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.09 – 2.00 28.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (28.09-2.00) 99.4 (28.09-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 1.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.201 , 0.233 0.201 , 0.234	Depositor DCC
R_{free} test set	21029 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33717	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3933e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	0/3876	0.75	0/5253
1	B	0.46	0/3862	0.77	1/5235 (0.0%)
1	C	0.46	0/3858	0.80	1/5230 (0.0%)
1	D	0.44	0/3845	0.78	0/5213
1	E	0.44	0/3858	0.75	0/5232
1	F	0.45	0/3904	0.76	0/5291
1	G	0.44	0/3856	0.76	0/5228
1	H	0.46	0/3849	0.76	0/5218
All	All	0.45	0/30908	0.77	2/41900 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	295	VAL	CB-CA-C	-7.05	100.12	110.62
1	B	266	VAL	CB-CA-C	-5.40	105.40	111.45

There are no chirality outliers.

There are no planarity outliers.

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	3797	0	3801	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3784	0	3781	23	0
1	C	3779	0	3777	27	0
1	D	3767	0	3766	29	0
1	E	3779	0	3761	19	0
1	F	3825	0	3829	25	0
1	G	3777	0	3768	20	0
1	H	3771	0	3770	22	0
2	A	48	0	13	2	0
2	B	48	0	13	1	0
2	C	48	0	13	1	0
2	D	48	0	13	3	0
2	E	48	0	13	2	0
2	F	48	0	13	1	0
2	G	48	0	13	1	0
2	H	48	0	13	1	0
3	A	428	0	0	0	0
3	B	378	0	0	3	0
3	C	411	0	0	2	0
3	D	357	0	0	3	0
3	E	323	0	0	1	0
3	F	375	0	0	2	0
3	G	360	0	0	2	0
3	H	422	0	0	2	0
All	All	33717	0	30357	173	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 3.

All (173) 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:F:255:GLY:H	2:F:500[C]:NAP:H71N	1.22	0.83
1:B:255:GLY:H	2:B:500[C]:NAP:H71N	1.26	0.80
1:B:316:ILE:HD12	1:B:365:GLU:HG2	1.64	0.79
1:A:255:GLY:H	2:A:500[C]:NAP:H71N	1.31	0.78
1:E:255:GLY:H	2:E:500[C]:NAP:H71N	1.30	0.77
1:G:255:GLY:H	2:G:500[C]:NAP:H71N	1.31	0.76
1:H:45:ARG:HH22	1:H:216:GLU:HG2	1.52	0.75
1:F:268:VAL:HG21	1:F:302:LYS:HE3	1.70	0.73
1:B:28:LYS:HE2	1:B:95:GLU:HG3	1.68	0.73
1:G:20:PRO:HG3	1:G:41:PRO:HB3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:VAL:HG21	1:B:302:LYS:HE3	1.74	0.70
1:H:255:GLY:H	2:H:500[C]:NAP:H71N	1.39	0.70
1:D:315:ARG:NH1	3:D:848:HOH:O	2.26	0.69
1:C:490:LEU:HD13	1:D:313:MET:HE1	1.73	0.68
1:D:316:ILE:HD12	1:D:365:GLU:HG2	1.78	0.66
1:G:420:ASN:O	1:G:424:ARG:HD3	1.96	0.65
1:D:20:PRO:HG3	1:D:41:PRO:HB3	1.78	0.65
1:B:65:ILE:HD12	1:B:69:ARG:HB3	1.79	0.65
1:E:292:ARG:NH2	1:E:402:VAL:O	2.30	0.64
1:B:305:GLU:OE1	1:B:306:ARG:NH1	2.30	0.64
1:A:315:ARG:NH2	1:A:322:ASP:OD2	2.23	0.63
1:C:313:MET:HE1	1:D:490:LEU:HB2	1.80	0.63
1:G:292:ARG:NH2	1:G:402:VAL:O	2.31	0.63
1:D:292:ARG:NH2	1:D:402:VAL:O	2.33	0.61
1:B:221:HIS:HE1	1:B:223:ARG:HG3	1.66	0.61
1:E:420:ASN:O	1:E:424:ARG:HD3	2.01	0.60
1:C:45:ARG:NH1	1:C:217:GLU:OE1	2.30	0.60
1:D:321:LYS:NZ	3:D:751:HOH:O	2.34	0.60
1:D:318:ASP:HB3	1:D:321:LYS:HG2	1.82	0.60
1:C:216:GLU:OE1	1:C:242:LYS:NZ	2.28	0.59
1:H:76:LYS:NZ	3:H:1006:HOH:O	2.27	0.59
1:A:147:VAL:HG22	1:A:224:VAL:HA	1.84	0.59
1:D:201:LYS:NZ	3:D:829:HOH:O	2.34	0.59
1:G:318:ASP:OD1	1:G:320:ARG:HD3	2.02	0.58
1:H:33:ASP:HB3	1:H:35:SER:H	1.66	0.58
1:E:237:ARG:NH1	3:E:920:HOH:O	2.24	0.58
1:D:18:LYS:NZ	1:D:50:GLU:OE2	2.34	0.56
1:C:292:ARG:NH2	1:C:402:VAL:O	2.38	0.56
1:C:257:SER:OG	1:C:292:ARG:HD2	2.06	0.56
1:D:243:ALA:HB1	1:D:248:LYS:HG3	1.87	0.55
1:C:255:GLY:H	2:C:500[C]:NAP:H71N	1.53	0.55
1:C:147:VAL:HG22	1:C:224:VAL:HA	1.88	0.55
1:F:224:VAL:HB	1:F:248:LYS:HE3	1.89	0.54
1:F:257:SER:OG	1:F:292:ARG:HD2	2.07	0.54
1:A:273:ARG:NH1	1:B:490:LEU:HD13	2.22	0.54
1:A:490:LEU:HD13	1:B:273:ARG:NH1	2.23	0.54
1:C:302:LYS:NZ	3:C:987:HOH:O	2.40	0.54
1:E:65:ILE:HD12	1:E:69:ARG:HB3	1.90	0.53
1:H:243:ALA:HB1	1:H:248:LYS:HG3	1.91	0.53
1:D:255:GLY:H	2:D:500[C]:NAP:H71N	1.57	0.53
1:H:45:ARG:NH2	1:H:216:GLU:HG2	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:318:ASP:OD1	1:F:320:ARG:HD3	2.09	0.52
1:F:45:ARG:NH2	1:F:49:ARG:HH22	2.07	0.52
1:F:221:HIS:HE1	1:F:223:ARG:HG3	1.75	0.52
1:E:224:VAL:O	1:E:248:LYS:HE3	2.11	0.51
1:A:134:GLU:O	1:A:136:THR:HG22	2.11	0.51
1:H:221:HIS:HE1	1:H:223:ARG:HG3	1.75	0.51
1:H:250:VAL:HG13	1:H:252:LEU:HG	1.92	0.51
1:F:223:ARG:HD3	3:F:911:HOH:O	2.11	0.51
1:B:318:ASP:HB3	1:B:321:LYS:HG3	1.91	0.51
1:E:168:THR:HG22	1:E:173:ASN:HB2	1.93	0.50
1:B:243:ALA:HB1	1:B:248:LYS:HG3	1.94	0.50
1:F:262:ILE:HG12	1:F:415:LEU:HD12	1.92	0.50
1:G:223:ARG:HD3	3:G:786:HOH:O	2.11	0.50
1:C:243:ALA:HB1	1:C:248:LYS:HG3	1.95	0.49
1:F:372:VAL:HG22	1:F:391:VAL:HG12	1.94	0.49
1:B:45:ARG:HH12	1:B:216:GLU:HG2	1.77	0.49
1:H:331:ILE:HG22	1:H:335:GLN:HG3	1.95	0.49
1:B:221:HIS:CE1	1:B:223:ARG:HG3	2.47	0.49
1:G:262:ILE:HG12	1:G:415:LEU:HD12	1.95	0.49
1:F:292:ARG:NH2	1:F:402:VAL:O	2.45	0.49
1:D:384:PHE:CE1	2:D:500[C]:NAP:H2D	2.48	0.49
1:B:233:SER:HA	1:B:254:LEU:HB3	1.95	0.48
1:B:306:ARG:HH11	1:B:306:ARG:HA	1.78	0.48
1:B:424:ARG:HD3	3:B:902:HOH:O	2.13	0.48
1:C:336:VAL:HG21	1:C:362:ASN:HA	1.95	0.48
1:C:485:PRO:O	1:D:101:ARG:NH1	2.46	0.47
1:G:130:GLN:HG3	3:G:663:HOH:O	2.14	0.47
1:A:292:ARG:NH2	1:A:402:VAL:O	2.47	0.47
1:A:136:THR:HG21	3:B:901:HOH:O	2.14	0.47
1:B:312:LYS:HG3	1:B:355:ILE:CD1	2.44	0.47
1:E:423:PHE:HZ	1:H:423:PHE:HZ	1.61	0.47
1:C:91:ILE:HG13	1:C:189:LEU:HD11	1.97	0.46
1:E:313:MET:HE2	1:F:489:ALA:HB3	1.97	0.46
1:D:313:MET:HE2	1:D:313:MET:HB3	1.71	0.46
1:A:137:ILE:HD12	1:C:423:PHE:CD2	2.50	0.46
1:F:423:PHE:HZ	1:G:423:PHE:HZ	1.62	0.46
1:D:250:VAL:HG13	1:D:252:LEU:HG	1.98	0.45
1:F:28:LYS:HE3	1:F:37:ILE:HD12	1.98	0.45
1:F:233:SER:HA	1:F:254:LEU:HB3	1.96	0.45
1:H:312:LYS:HG3	1:H:355:ILE:HD12	1.99	0.45
1:G:243:ALA:HB1	1:G:248:LYS:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ARG:NH2	3:C:944:HOH:O	2.45	0.45
1:G:224:VAL:O	1:G:248:LYS:HE3	2.16	0.45
1:B:258:ASP:OD2	1:B:411:SER:HB3	2.17	0.45
1:F:89:MET:HG3	1:F:107:VAL:HG21	1.99	0.45
1:C:490:LEU:HD12	1:C:490:LEU:HA	1.78	0.45
1:D:155:ASN:HD21	2:D:500[C]:NAP:H5N	1.82	0.45
1:E:233:SER:HA	1:E:254:LEU:HB3	1.99	0.45
1:H:233:SER:HA	1:H:254:LEU:HB3	1.99	0.45
1:D:147:VAL:HG22	1:D:224:VAL:HA	1.98	0.45
1:F:258:ASP:OD2	1:F:411:SER:HB3	2.17	0.45
1:H:20:PRO:HD3	1:H:41:PRO:HB3	1.99	0.44
1:G:153:PRO:HD3	1:G:230:THR:HB	1.98	0.44
1:H:201:LYS:NZ	3:H:986:HOH:O	2.50	0.44
1:H:76:LYS:HB3	1:H:76:LYS:HE3	1.73	0.44
1:D:33:ASP:HB3	1:D:35:SER:H	1.83	0.44
1:D:257:SER:OG	1:D:292:ARG:HD2	2.16	0.44
1:D:331:ILE:HG22	1:D:335:GLN:HG3	2.00	0.44
1:A:133:SER:HB2	1:A:136:THR:HG21	2.00	0.44
1:C:233:SER:HA	1:C:254:LEU:HB3	2.00	0.44
1:G:258:ASP:OD2	1:G:411:SER:HB3	2.18	0.44
1:C:354:LEU:HD11	1:C:370:VAL:HG13	1.98	0.43
1:E:257:SER:OG	1:E:292:ARG:HD2	2.18	0.43
1:F:365:GLU:HG2	3:F:680:HOH:O	2.18	0.43
1:F:305:GLU:OE1	1:F:306:ARG:NH1	2.52	0.43
1:E:9:VAL:HG13	1:E:188:TRP:CD1	2.53	0.43
1:G:306:ARG:HA	1:G:306:ARG:HD3	1.81	0.43
1:G:313:MET:HE1	1:H:490:LEU:HD13	2.01	0.43
1:A:258:ASP:OD2	1:A:411:SER:HB3	2.19	0.43
1:A:356:GLY:HA3	1:A:366:PRO:O	2.19	0.43
1:D:150:VAL:HG22	1:D:177:TYR:HD1	1.84	0.43
1:F:302:LYS:HB3	1:F:302:LYS:HE2	1.53	0.43
1:G:65:ILE:HD12	1:G:69:ARG:HB3	1.99	0.43
1:A:224:VAL:O	1:A:248:LYS:HE3	2.17	0.43
1:A:257:SER:OG	1:A:292:ARG:HD2	2.18	0.43
1:E:181:SER:OG	2:E:500[C]:NAP:O3X	2.32	0.43
1:F:18:LYS:NZ	1:F:50:GLU:OE2	2.29	0.43
1:E:269:ASP:HA	1:E:306:ARG:HG2	2.00	0.43
1:G:257:SER:OG	1:G:292:ARG:HD2	2.19	0.43
1:C:168:THR:HG22	1:C:173:ASN:HB2	2.01	0.43
1:H:258:ASP:OD2	1:H:411:SER:HB3	2.19	0.43
1:A:423:PHE:HZ	1:D:423:PHE:HZ	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:VAL:HB	1:G:188:TRP:CG	2.54	0.43
1:E:221:HIS:HE1	1:E:223:ARG:HG3	1.84	0.42
1:E:90:LYS:O	1:E:94:VAL:HG23	2.19	0.42
1:B:91:ILE:O	1:B:95:GLU:HB3	2.19	0.42
1:C:76:LYS:HG2	1:C:197:ALA:HA	2.01	0.42
1:C:150:VAL:HB	1:C:228:THR:HG23	2.02	0.42
1:C:221:HIS:HE1	1:C:223:ARG:HG3	1.83	0.42
1:D:358:ARG:HG3	1:D:359:SER:N	2.33	0.42
1:H:306:ARG:HD3	1:H:306:ARG:HA	1.69	0.42
1:C:101:ARG:HG2	1:D:485:PRO:HB2	2.01	0.42
1:D:262:ILE:HG12	1:D:415:LEU:HD12	2.02	0.42
1:C:258:ASP:OD2	1:C:411:SER:HB3	2.19	0.42
3:B:887:HOH:O	1:C:130:GLN:HG3	2.19	0.42
1:G:221:HIS:HE1	1:G:223:ARG:HG3	1.85	0.42
1:H:55:ALA:HA	1:H:202:GLY:O	2.20	0.41
1:F:60:LYS:HB3	1:F:60:LYS:HE2	1.55	0.41
1:A:306:ARG:HD3	1:A:306:ARG:HA	1.75	0.41
1:A:393:VAL:HB	1:A:398:GLN:HB3	2.03	0.41
1:B:53:ASP:OD1	1:B:223:ARG:NH2	2.52	0.41
1:B:442:LEU:HD23	1:B:442:LEU:HA	1.93	0.41
1:D:268:VAL:HG21	1:D:302:LYS:HE2	2.02	0.41
1:G:56:PHE:CD1	1:G:223:ARG:HD2	2.55	0.41
1:F:295:VAL:HG21	1:F:303:PHE:CD2	2.55	0.41
1:H:53:ASP:OD1	1:H:223:ARG:NH2	2.49	0.41
1:A:384:PHE:CZ	2:A:500[C]:NAP:H3D	2.56	0.41
1:H:262:ILE:HD13	1:H:303:PHE:CE1	2.56	0.41
1:A:20:PRO:HD3	1:A:41:PRO:HB3	2.03	0.41
1:C:77:MET:HE3	1:C:77:MET:HB2	1.84	0.41
1:D:321:LYS:HA	1:D:321:LYS:HD3	1.76	0.41
1:F:318:ASP:HB3	1:F:321:LYS:HG3	2.02	0.41
1:D:258:ASP:OD2	1:D:411:SER:HB3	2.20	0.40
1:H:262:ILE:HG12	1:H:415:LEU:HD12	2.03	0.40
1:A:233:SER:HA	1:A:254:LEU:HB3	2.03	0.40
1:E:316:ILE:HD12	1:E:365:GLU:HG2	2.03	0.40
1:B:150:VAL:HG22	1:B:177:TYR:HD1	1.87	0.40
1:C:224:VAL:O	1:C:248:LYS:HE3	2.22	0.40
1:E:102:LYS:HE2	1:E:156:TYR:CZ	2.56	0.40
1:F:7:MET:HE3	1:F:38:ALA:HB2	2.04	0.40
1:B:356:GLY:HA3	1:B:366:PRO:O	2.21	0.40
1:E:262:ILE:HG12	1:E:415:LEU:HD12	2.02	0.40

There are no symmetry-related clashes.

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	486/491 (99%)	476 (98%)	10 (2%)	0	100	100
1	B	485/491 (99%)	474 (98%)	11 (2%)	0	100	100
1	C	484/491 (99%)	468 (97%)	16 (3%)	0	100	100
1	D	483/491 (98%)	474 (98%)	9 (2%)	0	100	100
1	E	485/491 (99%)	473 (98%)	12 (2%)	0	100	100
1	F	489/491 (100%)	479 (98%)	10 (2%)	0	100	100
1	G	484/491 (99%)	471 (97%)	13 (3%)	0	100	100
1	H	484/491 (99%)	471 (97%)	13 (3%)	0	100	100
All	All	3880/3928 (99%)	3786 (98%)	94 (2%)	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	402/408 (98%)	385 (96%)	17 (4%)	26	25
1	B	400/408 (98%)	385 (96%)	15 (4%)	29	29
1	C	400/408 (98%)	382 (96%)	18 (4%)	24	23
1	D	398/408 (98%)	378 (95%)	20 (5%)	22	20
1	E	398/408 (98%)	383 (96%)	15 (4%)	29	29
1	F	406/408 (100%)	392 (97%)	14 (3%)	32	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	399/408 (98%)	381 (96%)	18 (4%)	24	23
1	H	398/408 (98%)	380 (96%)	18 (4%)	24	23
All	All	3201/3264 (98%)	3066 (96%)	135 (4%)	28	25

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LYS
1	A	95	GLU
1	A	136	THR
1	A	147	VAL
1	A	216	GLU
1	A	222	LYS
1	A	253[A]	GLU
1	A	253[B]	GLU
1	A	295	VAL
1	A	302	LYS
1	A	321	LYS
1	A	324	LYS
1	A	330	LEU
1	A	398	GLN
1	A	442	LEU
1	A	457	VAL
1	A	473	ARG
1	B	8	LYS
1	B	9	VAL
1	B	60	LYS
1	B	69	ARG
1	B	101	ARG
1	B	147	VAL
1	B	150	VAL
1	B	242	LYS
1	B	253[A]	GLU
1	B	253[B]	GLU
1	B	372	VAL
1	B	415	LEU
1	B	442	LEU
1	B	457	VAL
1	B	473	ARG
1	C	9	VAL
1	C	95	GLU

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Mol	Chain	Res	Type
1	C	130	GLN
1	C	147	VAL
1	C	150	VAL
1	C	207	VAL
1	C	216	GLU
1	C	253[A]	GLU
1	C	253[B]	GLU
1	C	295	VAL
1	C	325	VAL
1	C	330	LEU
1	C	334	ARG
1	C	360	TRP
1	C	398	GLN
1	C	457	VAL
1	C	473	ARG
1	C	490	LEU
1	D	9	VAL
1	D	49	ARG
1	D	95	GLU
1	D	102	LYS
1	D	147	VAL
1	D	150	VAL
1	D	213	VAL
1	D	222	LYS
1	D	250	VAL
1	D	253[A]	GLU
1	D	253[B]	GLU
1	D	295	VAL
1	D	305	GLU
1	D	306	ARG
1	D	330	LEU
1	D	358	ARG
1	D	391	VAL
1	D	424	ARG
1	D	457	VAL
1	D	473	ARG
1	E	22	THR
1	E	46	GLU
1	E	69	ARG
1	E	95	GLU
1	E	147	VAL
1	E	150	VAL

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Mol	Chain	Res	Type
1	E	216	GLU
1	E	253[A]	GLU
1	E	253[B]	GLU
1	E	302	LYS
1	E	333	GLU
1	E	334	ARG
1	E	424	ARG
1	E	457	VAL
1	E	473	ARG
1	F	45	ARG
1	F	49	ARG
1	F	60	LYS
1	F	95	GLU
1	F	147	VAL
1	F	150	VAL
1	F	216	GLU
1	F	253[A]	GLU
1	F	253[B]	GLU
1	F	320	ARG
1	F	372	VAL
1	F	442	LEU
1	F	446	HIS
1	F	473	ARG
1	G	8	LYS
1	G	9	VAL
1	G	36	LYS
1	G	69	ARG
1	G	95	GLU
1	G	147	VAL
1	G	150	VAL
1	G	253[A]	GLU
1	G	253[B]	GLU
1	G	321	LYS
1	G	325	VAL
1	G	360	TRP
1	G	424	ARG
1	G	442	LEU
1	G	446	HIS
1	G	457	VAL
1	G	473	ARG
1	G	482	ARG
1	H	9	VAL

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Mol	Chain	Res	Type
1	H	33	ASP
1	H	42	ARG
1	H	86	GLU
1	H	95	GLU
1	H	102	LYS
1	H	147	VAL
1	H	150	VAL
1	H	171	VAL
1	H	250	VAL
1	H	253[A]	GLU
1	H	253[B]	GLU
1	H	330	LEU
1	H	333	GLU
1	H	355	ILE
1	H	372	VAL
1	H	457	VAL
1	H	473	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	375	ASN
1	B	192	GLN
1	B	285	GLN
1	B	375	ASN
1	C	285	GLN
1	C	362	ASN
1	C	375	ASN
1	D	26	GLN
1	D	115	GLN
1	E	362	ASN
1	F	64	ASN
1	G	285	GLN
1	G	362	ASN
1	H	285	GLN
1	H	362	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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 [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, 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	486/491 (98%)	-0.36	2 (0%) 88 88	6, 16, 32, 59	2 (0%)
1	B	485/491 (98%)	-0.26	3 (0%) 85 85	7, 16, 36, 57	2 (0%)
1	C	484/491 (98%)	-0.17	5 (1%) 79 79	7, 18, 33, 68	2 (0%)
1	D	483/491 (98%)	-0.16	4 (0%) 82 82	8, 19, 39, 68	2 (0%)
1	E	485/491 (98%)	-0.21	8 (1%) 70 70	7, 19, 37, 59	2 (0%)
1	F	489/491 (99%)	-0.30	7 (1%) 73 73	7, 17, 34, 54	2 (0%)
1	G	484/491 (98%)	-0.30	5 (1%) 79 79	7, 18, 33, 46	2 (0%)
1	H	484/491 (98%)	-0.22	6 (1%) 76 76	6, 16, 36, 71	2 (0%)
All	All	3880/3928 (98%)	-0.25	40 (1%) 79 79	6, 17, 36, 71	16 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	491	LYS	6.5
1	D	491	LYS	5.5
1	F	2	ILE	4.9
1	A	491	LYS	4.9
1	C	491	LYS	4.4
1	E	491	LYS	4.1
1	B	491	LYS	3.8
1	E	25	PHE	3.5
1	F	4	LEU	3.4
1	H	490	LEU	3.4
1	E	22	THR	3.4
1	E	7	MET	3.3
1	C	25	PHE	3.3
1	H	33	ASP	3.2
1	D	321	LYS	2.9
1	F	5	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	7	MET	2.8
1	D	33	ASP	2.7
1	G	25	PHE	2.7
1	D	490	LEU	2.6
1	F	25	PHE	2.6
1	F	3	ASP	2.5
1	C	334	ARG	2.5
1	G	238	GLU	2.3
1	A	6	ILE	2.3
1	C	22	THR	2.3
1	B	86	GLU	2.2
1	E	8	LYS	2.2
1	G	7	MET	2.2
1	F	253[A]	GLU	2.2
1	E	24	ALA	2.1
1	E	23	GLY	2.1
1	H	22	THR	2.1
1	H	45	ARG	2.1
1	H	358	ARG	2.1
1	G	401	GLU	2.0
1	E	490	LEU	2.0
1	F	490	LEU	2.0
1	C	57	GLU	2.0
1	G	21	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 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($\text{\AA}^2$)	Q<0.9
2	NAP	D	500[C]	48/48	0.86	0.14	16,27,33,38	21
2	NAP	E	500[C]	48/48	0.88	0.12	18,29,37,40	21
2	NAP	B	500[C]	48/48	0.89	0.12	15,23,28,33	21
2	NAP	C	500[C]	48/48	0.91	0.11	16,23,32,36	17
2	NAP	F	500[C]	48/48	0.91	0.11	16,24,30,32	17
2	NAP	G	500[C]	48/48	0.91	0.11	16,23,30,34	17
2	NAP	H	500[C]	48/48	0.91	0.11	13,23,31,37	17
2	NAP	A	500[C]	48/48	0.93	0.10	14,22,28,34	17

6.5 Other polymers [i](#)

There are no such residues in this entry.