



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:56 AM UTC

PDB ID : 4D1J / pdb_00004d1j
Title : The structure of the GH35 beta-galactosidase Bgl35A from *Cellvibrio japonicas* in complex with 1-Deoxygalactonojirimycin
Authors : Larsbrink, J.; Thompson, A.J.; Lundqvist, M.; Gardner, J.G.; Davies, G.J.; Brumer, H.
Deposited on : 2014-05-02
Resolution : 1.80 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

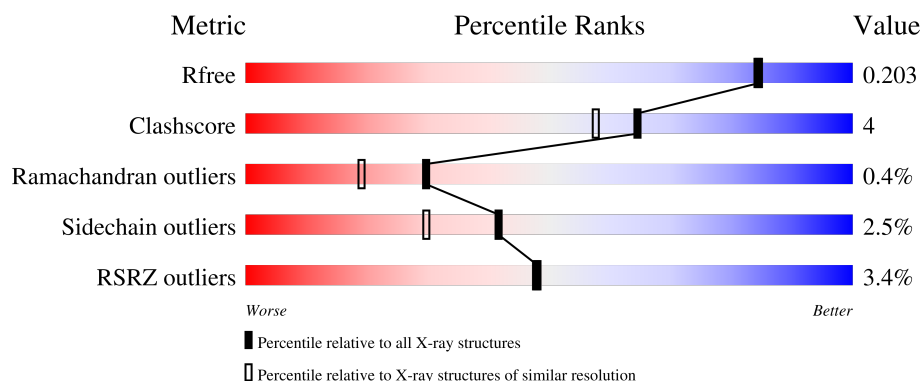
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	540	3% 92% 7% .
1	B	540	3% 91% 8% .
1	C	540	6% 91% 7% .
1	D	540	3% 92% 7% .
1	E	540	2% 91% 6% ..

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Mol	Chain	Length	Quality of chain
1	F	540	2% 91% 6%
1	G	540	3% 92% 6%
1	H	540	6% 92% 6%

2 Entry composition

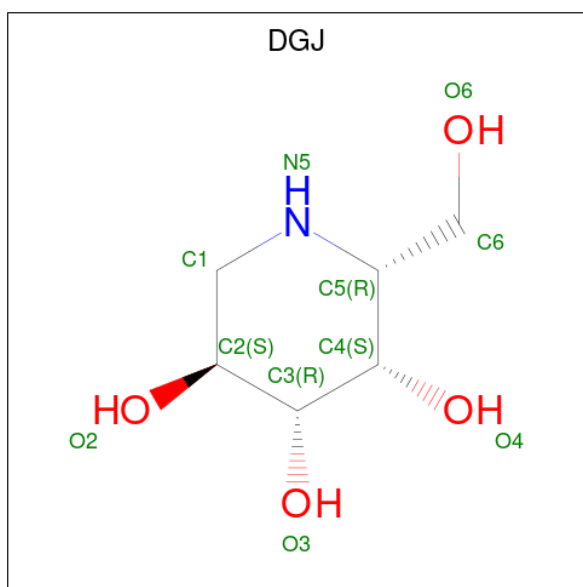
There are 5 unique types of molecules in this entry. The entry contains 37796 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-GALACTOSIDASE, PUTATIVE, BGL35A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	3	0
			4185	2681	711	777	16			
1	B	539	Total	C	N	O	S	0	3	0
			4167	2671	703	777	16			
1	C	539	Total	C	N	O	S	0	6	0
			4190	2689	710	775	16			
1	D	540	Total	C	N	O	S	0	7	0
			4222	2712	715	779	16			
1	E	539	Total	C	N	O	S	0	5	0
			4234	2713	718	787	16			
1	F	539	Total	C	N	O	S	0	12	0
			4244	2725	712	790	17			
1	G	540	Total	C	N	O	S	0	7	0
			4224	2712	712	783	17			
1	H	539	Total	C	N	O	S	0	4	0
			4181	2677	714	775	15			

- Molecule 2 is (2R,3S,4R,5S)-2-(hydroxymethyl)piperidine-3,4,5-triol (CCD ID: DGJ) (formula: C₆H₁₃NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	1	4		
2	B	1	Total	C	N	O	0	0
			11	6	1	4		
2	C	1	Total	C	N	O	0	0
			11	6	1	4		
2	D	1	Total	C	N	O	0	0
			11	6	1	4		
2	E	1	Total	C	N	O	0	0
			11	6	1	4		
2	F	1	Total	C	N	O	0	0
			11	6	1	4		
2	G	1	Total	C	N	O	0	0
			11	6	1	4		
2	H	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

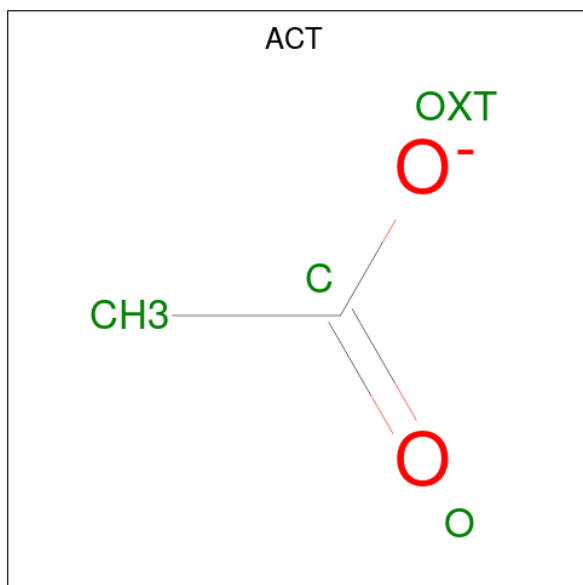
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Na	0	0
			4	4		
3	B	2	Total	Na	0	0
			2	2		
3	D	4	Total	Na	0	0
			4	4		
3	E	4	Total	Na	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	4	Total	Na	0	0
			4	4		
3	G	4	Total	Na	0	0
			4	4		
3	H	1	Total	Na	0	0
			1	1		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	493	Total	O	0	0
			493	493		

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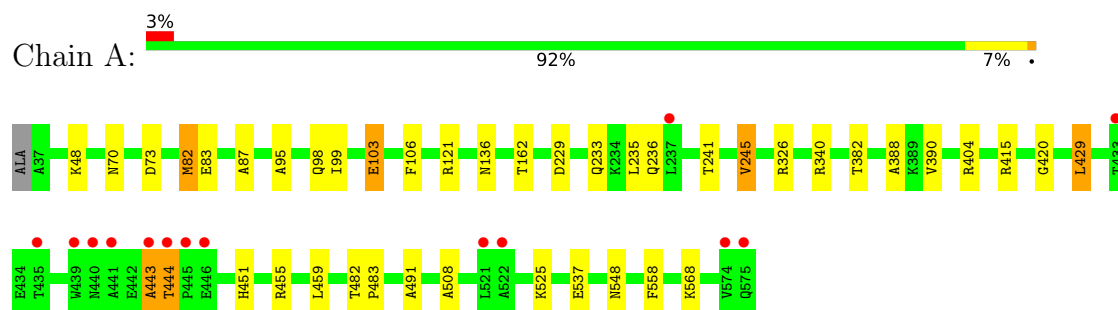
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	491	Total 491	O 491	0	0
5	C	409	Total 409	O 409	0	0
5	D	535	Total 535	O 535	0	0
5	E	567	Total 571	O 571	0	4
5	F	564	Total 564	O 564	0	0
5	G	556	Total 559	O 559	0	3
5	H	396	Total 396	O 396	0	0

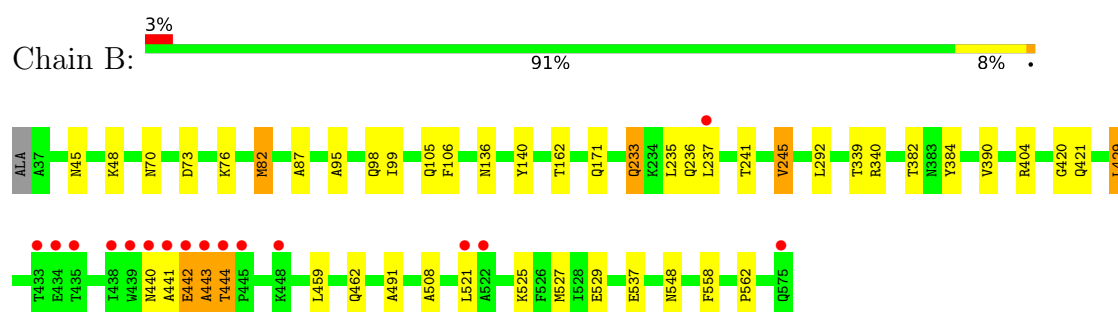
3 Residue-property plots [i](#)

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.

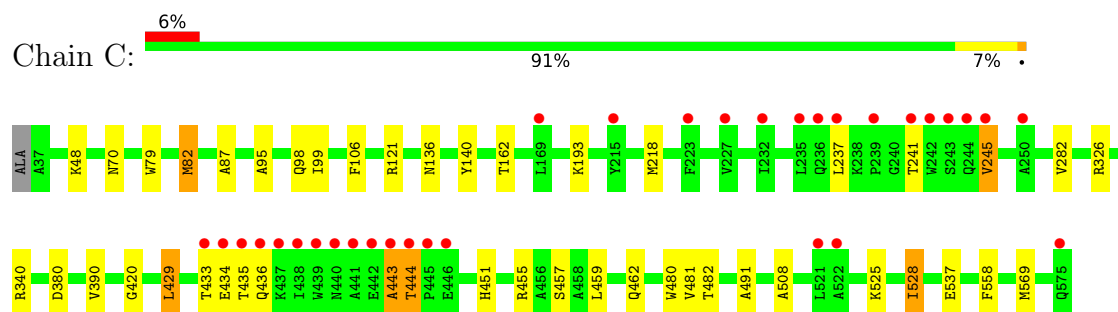
- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A



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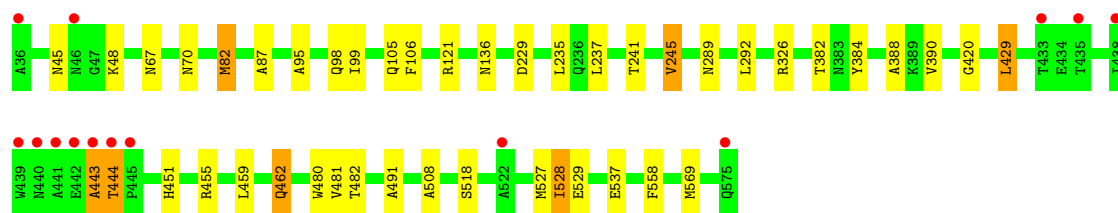


- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A

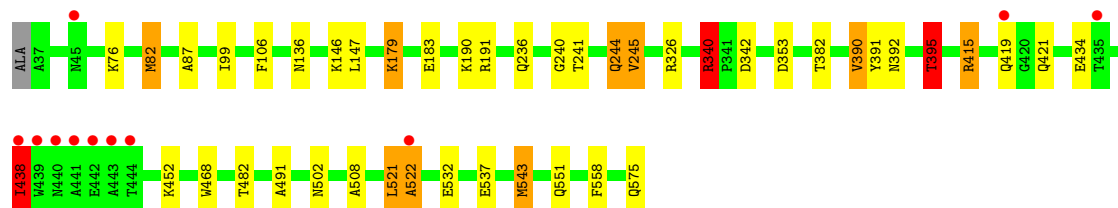
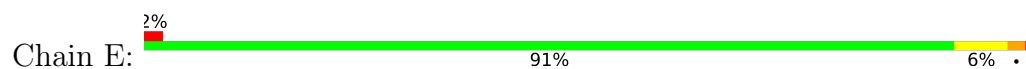


- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A

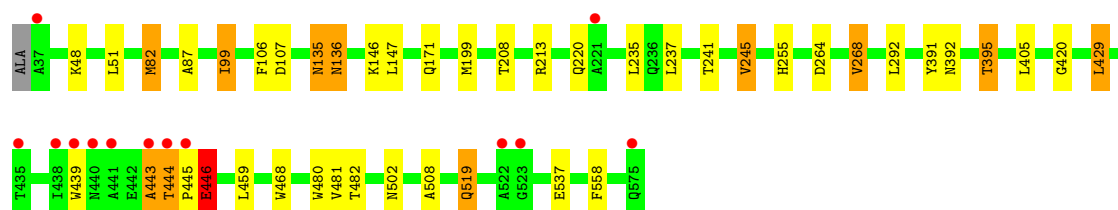




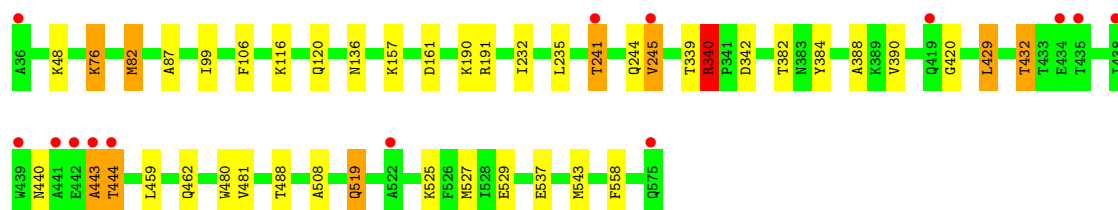
- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A



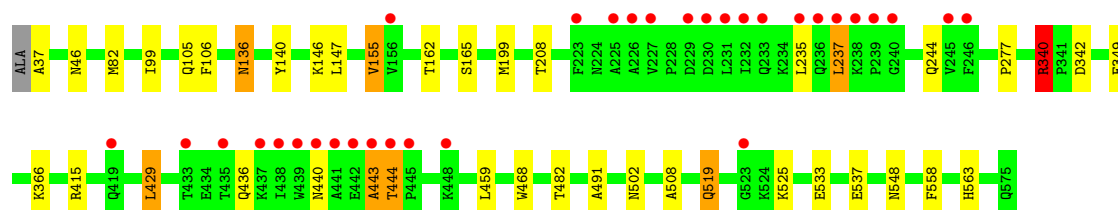
- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A



- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A



- Molecule 1: BETA-GALACTOSIDASE, PUTATIVE, BGL35A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.26Å 116.09Å 116.11Å 90.00° 90.05° 90.04°	Depositor
Resolution (Å)	116.11 – 1.80 116.11 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.1 (116.11-1.80) 97.1 (116.11-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.172 , 0.195 0.181 , 0.203	Depositor DCC
R_{free} test set	23426 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.077 for h,l,-k 0.077 for h,-l,k 0.057 for h,-k,-l 0.027 for -h,k,-l 0.028 for -h,-k,l 0.028 for -h,l,k 0.035 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	37796	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.60% 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: NA, ACT, DGJ

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	0.77	2/4305 (0.0%)	0.84	6/5873 (0.1%)
1	B	0.73	0/4287	0.81	3/5854 (0.1%)
1	C	0.75	0/4321	0.82	4/5899 (0.1%)
1	D	0.78	0/4356	0.82	2/5944 (0.0%)
1	E	0.79	0/4361	0.91	11/5945 (0.2%)
1	F	0.79	1/4393 (0.0%)	0.83	1/5997 (0.0%)
1	G	0.81	0/4358	0.88	6/5945 (0.1%)
1	H	0.72	0/4304	0.86	5/5875 (0.1%)
All	All	0.77	3/34685 (0.0%)	0.85	38/47332 (0.1%)

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	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	GLU	CA-C	5.78	1.60	1.52
1	F	446	GLU	N-CA	5.23	1.52	1.46
1	A	483	PRO	CA-C	5.18	1.54	1.51

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	340	ARG	NE-CZ-NH2	-15.65	105.12	119.20
1	G	340	ARG	NE-CZ-NH2	-15.23	105.49	119.20
1	H	340	ARG	NE-CZ-NH2	-14.22	106.40	119.20
1	E	340	ARG	NE-CZ-NH1	14.09	135.59	121.50
1	G	340	ARG	NE-CZ-NH1	13.95	135.45	121.50
1	H	340	ARG	NE-CZ-NH1	13.12	134.62	121.50
1	G	76	LYS	CD-CE-NZ	10.24	144.66	111.90
1	E	521	LEU	N-CA-C	9.66	124.41	112.23
1	E	340	ARG	CD-NE-CZ	9.07	137.10	124.40
1	G	340	ARG	CD-NE-CZ	8.53	136.34	124.40
1	H	340	ARG	CD-NE-CZ	8.40	136.16	124.40
1	A	103	GLU	O-C-N	-8.21	112.77	122.87
1	E	244	GLN	CB-CA-C	7.74	124.01	110.85
1	E	340	ARG	CB-CG-CD	-6.63	96.05	111.30
1	G	340	ARG	CB-CG-CD	-6.60	96.12	111.30
1	A	103	GLU	CA-C-N	6.44	134.04	121.41
1	A	103	GLU	C-N-CA	6.44	134.04	121.41
1	H	340	ARG	CB-CG-CD	-6.44	96.50	111.30
1	F	443	ALA	N-CA-C	5.85	120.80	113.43
1	E	183	GLU	CG-CD-OE2	-5.73	105.23	118.40
1	E	179	LYS	N-CA-CB	5.67	118.45	110.12
1	C	443	ALA	N-CA-C	5.63	120.52	113.43
1	A	443	ALA	N-CA-C	5.54	120.41	113.43
1	E	183	GLU	CG-CD-OE1	5.54	131.13	118.40
1	G	443	ALA	N-CA-C	5.54	120.41	113.43
1	D	443	ALA	N-CA-C	5.50	120.36	113.43
1	H	443	ALA	N-CA-C	5.44	120.28	113.43
1	A	340	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	B	340	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	B	233	GLN	CB-CA-C	-5.38	102.68	110.96
1	E	438	ILE	N-CA-CB	5.34	118.20	110.52
1	E	395	THR	CB-CA-C	5.33	119.63	110.79
1	A	340	ARG	NE-CZ-NH2	-5.29	114.43	119.20
1	D	537	GLU	CA-CB-CG	5.29	124.67	114.10
1	C	326	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	B	443	ALA	N-CA-C	-5.18	96.49	111.00
1	C	282	VAL	N-CA-C	5.12	115.34	108.17
1	C	340	ARG	NE-CZ-NH1	5.01	126.51	121.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	GLU	Peptide
1	B	442	GLU	Peptide

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	4185	0	3989	30	0
1	B	4167	0	3951	38	0
1	C	4190	0	3985	29	0
1	D	4222	0	4051	40	0
1	E	4234	0	4084	42	0
1	F	4244	0	4071	37	0
1	G	4224	0	4050	38	0
1	H	4181	0	3974	35	0
2	A	11	0	13	0	0
2	B	11	0	13	0	0
2	C	11	0	13	0	0
2	D	11	0	13	0	0
2	E	11	0	13	0	0
2	F	11	0	13	1	0
2	G	11	0	13	0	0
2	H	11	0	13	1	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	1	0	0	0	0
4	C	8	0	6	0	0
4	D	8	0	6	0	0
4	F	4	0	3	0	0
5	A	493	0	0	11	0
5	B	491	0	0	10	0
5	C	409	0	0	4	0
5	D	535	0	0	10	0
5	E	571	0	0	12	0
5	F	564	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	559	0	0	10	0
5	H	396	0	0	10	0
All	All	37796	0	32274	257	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 4.

All (257) 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:E:146:LYS:HE3	1:G:527[A]:MET:HE1	1.35	1.08
1:D:527[A]:MET:HE1	1:F:146:LYS:HE3	1.33	1.04
1:D:527[A]:MET:HE2	1:F:147:LEU:HD21	1.39	1.00
1:F:468:TRP:HE1	1:F:502:ASN:HD22	1.09	1.00
1:B:527[A]:MET:HE1	1:H:146:LYS:HE3	1.44	0.99
1:E:147:LEU:HD21	1:G:527[A]:MET:HE2	1.43	0.97
1:C:218:MET:HE1	5:C:2141:HOH:O	1.64	0.96
1:B:527[A]:MET:HE2	1:H:147:LEU:HD21	1.48	0.94
1:H:468:TRP:HE1	1:H:502:ASN:HD22	1.12	0.93
1:E:468:TRP:HE1	1:E:502:ASN:HD22	1.07	0.92
1:H:105:GLN:HG3	5:H:2084:HOH:O	1.68	0.91
1:D:326[B]:ARG:NH1	5:D:2322:HOH:O	2.09	0.86
1:B:45:ASN:CB	5:B:2014:HOH:O	2.24	0.85
1:E:146:LYS:HE3	1:G:527[A]:MET:CE	2.07	0.84
1:D:105:GLN:HG3	5:D:2105:HOH:O	1.78	0.83
1:D:527[A]:MET:CE	1:F:146:LYS:HE3	2.08	0.83
1:E:146:LYS:CE	1:G:527[A]:MET:HE1	2.12	0.80
1:F:392:ASN:H	1:F:395:THR:HG23	1.45	0.80
1:G:382[B]:THR:CG2	1:G:388:ALA:O	2.30	0.80
1:A:95:ALA:H	1:A:98:GLN:HE21	1.31	0.79
1:C:193:LYS:H	1:D:289:ASN:HD21	1.29	0.79
1:C:380:ASP:OD2	1:H:563:HIS:HE1	1.64	0.79
1:E:392:ASN:H	1:E:395:THR:HG23	1.46	0.79
1:B:95:ALA:H	1:B:98:GLN:HE21	1.30	0.78
1:F:48:LYS:NZ	1:F:420:GLY:O	2.15	0.77
1:D:527[A]:MET:HE1	1:F:146:LYS:CE	2.12	0.77
1:D:95:ALA:H	1:D:98:GLN:HE21	1.32	0.76
1:B:48:LYS:NZ	1:B:420:GLY:O	2.16	0.76
1:C:48:LYS:NZ	1:C:420:GLY:O	2.16	0.76
1:B:339:THR:O	5:B:2307:HOH:O	2.04	0.76
1:A:326:ARG:NH1	5:A:2292:HOH:O	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:440:ASN:CB	5:G:2416:HOH:O	2.34	0.75
1:F:392:ASN:H	1:F:395:THR:CG2	2.00	0.75
1:C:95:ALA:H	1:C:98:GLN:HE21	1.32	0.74
1:B:105:GLN:HG3	5:B:2095:HOH:O	1.89	0.73
1:D:382[B]:THR:CG2	1:D:388:ALA:O	2.36	0.72
1:D:527[A]:MET:HE2	1:F:147:LEU:CD2	2.17	0.72
1:B:521:LEU:CB	5:B:2422:HOH:O	2.38	0.72
1:A:48:LYS:NZ	1:A:420:GLY:O	2.15	0.72
1:A:229:ASP:CB	5:A:2110:HOH:O	2.37	0.71
1:B:527[A]:MET:CE	1:H:146:LYS:HE3	2.18	0.71
1:D:48:LYS:NZ	1:D:420:GLY:O	2.17	0.71
1:C:528[A]:ILE:CD1	1:C:569:MET:SD	2.79	0.70
1:D:528[A]:ILE:CD1	1:D:569:MET:SD	2.80	0.70
1:E:392:ASN:H	1:E:395:THR:CG2	2.04	0.70
1:E:236:GLN:CB	5:E:2121:HOH:O	2.39	0.70
1:A:236:GLN:CB	5:A:2235:HOH:O	2.39	0.70
1:B:527[A]:MET:HE1	1:H:146:LYS:CE	2.21	0.69
1:G:432:THR:HG21	5:G:2426:HOH:O	1.93	0.69
1:D:518:SER:O	5:D:2466:HOH:O	2.10	0.69
1:E:147:LEU:CD2	1:G:527[A]:MET:HE2	2.18	0.69
1:B:527[A]:MET:HE2	1:H:147:LEU:CD2	2.22	0.69
1:B:421:GLN:CB	5:B:2203:HOH:O	2.40	0.69
1:G:382[B]:THR:HG21	1:G:388:ALA:O	1.93	0.68
1:F:264:ASP:O	1:F:268:VAL:HG13	1.94	0.67
1:B:236:GLN:CB	5:B:2240:HOH:O	2.41	0.66
1:E:532:GLU:CD	1:E:543[B]:MET:HE3	2.21	0.66
1:C:433:THR:O	1:C:435:THR:N	2.29	0.65
1:H:340:ARG:HD3	1:H:342:ASP:OD1	1.97	0.65
1:E:340:ARG:HD3	1:E:342:ASP:OD1	1.98	0.64
1:G:339:THR:O	5:G:2331:HOH:O	2.14	0.64
1:F:213:ARG:HH22	1:F:220:GLN:HE22	1.46	0.63
1:G:340:ARG:HD3	1:G:342:ASP:OD1	1.99	0.63
1:H:440:ASN:CB	5:H:2299:HOH:O	2.45	0.63
1:G:232:ILE:CB	5:G:2256:HOH:O	2.46	0.63
1:D:528[A]:ILE:HD12	1:D:569:MET:SD	2.39	0.62
1:D:382[B]:THR:HG22	1:D:384:TYR:H	1.65	0.61
1:C:528[A]:ILE:HD12	1:C:569:MET:SD	2.39	0.61
1:E:452:LYS:HE2	5:E:2448:HOH:O	1.98	0.61
1:C:457:SER:O	5:C:2324:HOH:O	2.17	0.60
1:F:99[A]:ILE:CD1	1:F:107:ASP:O	2.50	0.60
1:F:443:ALA:O	1:F:444:THR:CB	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:76:LYS:HE2	5:G:2052:HOH:O	2.02	0.59
1:F:445:PRO:O	1:F:446:GLU:CB	2.50	0.59
1:F:99[A]:ILE:HD13	1:F:107:ASP:O	2.03	0.58
1:B:171:GLN:HG2	5:B:2081:HOH:O	2.02	0.58
1:B:440:ASN:C	1:B:442:GLU:H	2.11	0.58
1:A:326:ARG:HG3	1:A:326:ARG:HH11	1.69	0.57
1:E:240:GLY:HA2	1:E:244:GLN:HE21	1.68	0.57
1:E:382[A]:THR:HG23	5:E:2380:HOH:O	2.03	0.57
1:C:443:ALA:O	1:C:444:THR:CB	2.53	0.57
1:D:67:ASN:HB2	1:E:551:GLN:HE22	1.70	0.57
1:E:390:VAL:O	1:E:395:THR:HG21	2.05	0.56
1:D:382[B]:THR:HG21	1:D:388:ALA:O	2.05	0.56
1:F:439:TRP:CB	5:F:2416:HOH:O	2.54	0.56
1:H:155:VAL:HG13	1:H:165:SER:O	2.05	0.56
1:H:349:GLU:OE1	2:H:600:DGJ:H1	2.05	0.56
1:F:171:GLN:HG2	5:F:2092:HOH:O	2.07	0.55
1:H:199:MET:HG2	1:H:277:PRO:HB2	1.90	0.54
1:G:443:ALA:O	1:G:444:THR:CB	2.56	0.54
1:E:468:TRP:HE1	1:E:502:ASN:ND2	1.91	0.54
1:G:382[B]:THR:HG22	1:G:384:TYR:H	1.74	0.53
1:D:443:ALA:O	1:D:444:THR:CB	2.56	0.53
1:F:391:TYR:HA	1:F:395:THR:HG21	1.90	0.53
1:F:136:ASN:HD22	1:F:208:THR:HA	1.73	0.53
1:G:527[A]:MET:HE3	1:G:529:GLU:HA	1.90	0.53
1:E:391:TYR:HA	1:E:395:THR:HG21	1.90	0.53
1:E:326[B]:ARG:NH2	1:E:353:ASP:OD2	2.29	0.53
1:D:229:ASP:CB	5:D:2263:HOH:O	2.56	0.53
1:E:575:GLN:HA	5:E:2564:HOH:O	2.08	0.53
1:H:443:ALA:O	1:H:444:THR:CB	2.57	0.53
1:E:452:LYS:CE	5:E:2448:HOH:O	2.56	0.52
1:B:382[B]:THR:HG23	1:B:384:TYR:H	1.75	0.52
1:H:436:GLN:CB	5:H:2298:HOH:O	2.57	0.52
1:E:532:GLU:OE2	1:E:543[B]:MET:HE3	2.10	0.52
1:D:382[B]:THR:HG23	5:D:2346:HOH:O	2.09	0.52
1:A:443:ALA:O	1:A:444:THR:CB	2.57	0.51
1:F:208:THR:OG1	1:F:255:HIS:HE1	1.93	0.51
1:H:46:ASN:ND2	5:H:2016:HOH:O	2.37	0.51
1:H:366:LYS:NZ	5:H:2254:HOH:O	2.41	0.51
1:A:326:ARG:HD3	5:A:2294:HOH:O	2.10	0.51
1:B:76:LYS:HE2	5:B:2045:HOH:O	2.11	0.51
1:B:440:ASN:O	1:B:442:GLU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:LYS:CD	1:G:527[A]:MET:HE1	2.41	0.50
1:E:532:GLU:HG2	1:E:543[B]:MET:CE	2.41	0.50
1:B:443:ALA:O	1:B:444:THR:CB	2.59	0.50
1:D:480:TRP:CG	1:D:481[B]:VAL:H	2.29	0.50
1:D:528[A]:ILE:HD13	1:D:569:MET:HE1	1.94	0.50
1:D:480:TRP:CG	1:D:481[A]:VAL:H	2.29	0.50
1:G:488[A]:THR:HG23	5:G:2470:HOH:O	2.11	0.50
1:B:382[B]:THR:CG2	1:B:384:TYR:H	2.25	0.49
1:E:521:LEU:O	1:E:522:ALA:HB3	2.11	0.49
1:G:519:GLN:HG2	5:G:2444:HOH:O	2.11	0.49
1:D:527[A]:MET:HE1	1:F:146:LYS:CD	2.42	0.49
1:G:508:ALA:HB3	1:G:558:PHE:CD1	2.47	0.49
1:H:415[A]:ARG:NH2	5:H:2280:HOH:O	2.46	0.49
1:A:568:LYS:HE2	5:A:2442:HOH:O	2.10	0.49
1:C:480:TRP:CG	1:C:481:VAL:H	2.30	0.49
1:C:380:ASP:OD2	1:H:563:HIS:CE1	2.54	0.49
1:G:480:TRP:CG	1:G:481:VAL:H	2.30	0.49
1:H:136:ASN:HD22	1:H:208:THR:HA	1.77	0.49
1:C:528[A]:ILE:HD13	1:C:569:MET:HE1	1.94	0.48
1:E:382[A]:THR:HG22	5:E:2357:HOH:O	2.13	0.48
1:E:415:ARG:O	1:E:419:GLN:HG2	2.13	0.48
1:A:326:ARG:HH11	1:A:326:ARG:CG	2.24	0.48
1:A:70:ASN:HD22	1:A:98:GLN:NE2	2.11	0.48
1:E:532:GLU:CD	1:E:543[B]:MET:CE	2.86	0.48
1:G:241:THR:HG22	1:G:244:GLN:CG	2.44	0.48
1:A:415:ARG:NH1	5:A:2371:HOH:O	2.41	0.48
1:B:527[A]:MET:HE3	1:B:529:GLU:HA	1.95	0.48
1:F:429:LEU:HD22	1:F:459:LEU:HG	1.96	0.48
1:A:229:ASP:CB	5:A:2228:HOH:O	2.61	0.47
1:C:162:THR:O	1:H:525:LYS:HE3	2.14	0.47
1:A:382:THR:OG1	1:A:388:ALA:O	2.33	0.47
1:A:429:LEU:HD22	1:A:459:LEU:HG	1.97	0.47
1:G:157:LYS:HE3	1:G:161:ASP:HB2	1.95	0.47
1:B:527[A]:MET:HE1	1:H:146:LYS:CD	2.45	0.47
1:G:241:THR:HG22	1:G:244:GLN:HG3	1.97	0.47
1:G:429:LEU:HD22	1:G:459:LEU:HG	1.97	0.47
1:A:525:LYS:HE3	1:B:162:THR:O	2.15	0.46
1:G:48:LYS:NZ	1:G:420:GLY:O	2.48	0.46
1:A:525:LYS:HE2	5:A:2438:HOH:O	2.15	0.46
1:D:482:THR:HG21	5:D:2236:HOH:O	2.14	0.46
1:H:429:LEU:HD22	1:H:459:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:480:TRP:CG	1:F:481:VAL:H	2.33	0.46
1:B:429:LEU:HD22	1:B:459:LEU:HG	1.97	0.46
1:B:525:LYS:HE3	1:H:162:THR:O	2.16	0.46
1:C:528[A]:ILE:HD13	1:C:569:MET:SD	2.56	0.46
1:C:140:TYR:CZ	1:H:548:ASN:HB3	2.51	0.46
1:C:429:LEU:HD22	1:C:459:LEU:HG	1.98	0.46
1:E:146:LYS:HG3	1:G:527[A]:MET:HE1	1.98	0.45
1:A:229:ASP:O	1:A:233:GLN:HG2	2.16	0.45
1:D:241:THR:O	1:D:245:VAL:HG13	2.17	0.45
1:E:241:THR:O	1:E:245:VAL:HG13	2.16	0.45
1:A:241:THR:O	1:A:245:VAL:HG13	2.16	0.45
1:D:528[A]:ILE:HD13	1:D:569:MET:SD	2.56	0.45
1:D:527[A]:MET:HE3	1:D:529:GLU:HA	1.98	0.45
1:A:482:THR:HG23	5:A:2413:HOH:O	2.16	0.45
1:A:83:GLU:OE1	1:A:121[B]:ARG:NH2	2.50	0.45
1:F:508:ALA:HB3	1:F:558:PHE:CD1	2.52	0.45
1:A:508:ALA:HB3	1:A:558:PHE:CD1	2.52	0.44
1:B:70:ASN:HD22	1:B:98:GLN:NE2	2.15	0.44
1:E:482:THR:HG23	5:E:2482:HOH:O	2.16	0.44
1:G:241:THR:O	1:G:245:VAL:HG13	2.18	0.44
1:A:82:MET:HG2	1:A:87:ALA:HB3	2.00	0.44
1:B:241:THR:O	1:B:245:VAL:HG13	2.17	0.44
1:F:135:ASN:N	1:F:135:ASN:HD22	2.16	0.44
1:C:70:ASN:HD22	1:C:98:GLN:NE2	2.16	0.44
1:F:395:THR:HB	5:F:2365:HOH:O	2.17	0.44
1:A:99:ILE:O	1:A:106:PHE:HA	2.18	0.44
1:C:241:THR:O	1:C:245:VAL:HG13	2.17	0.44
1:D:382[B]:THR:HG23	1:D:388:ALA:O	2.17	0.44
1:D:508:ALA:HB3	1:D:558:PHE:CD1	2.52	0.44
1:E:421:GLN:NE2	5:E:2425:HOH:O	2.51	0.44
1:B:70:ASN:HD22	1:B:98:GLN:HE22	1.66	0.44
1:D:99:ILE:O	1:D:106:PHE:HA	2.17	0.44
1:D:382[B]:THR:CG2	5:D:2346:HOH:O	2.64	0.44
1:D:527[A]:MET:HE1	1:F:146:LYS:HG3	2.00	0.44
1:G:116:LYS:O	1:G:120:GLN:HG2	2.17	0.44
1:B:527[A]:MET:HE1	1:H:146:LYS:HG3	2.00	0.43
1:D:121[B]:ARG:NH2	5:D:2065:HOH:O	2.48	0.43
1:G:99:ILE:O	1:G:106:PHE:HA	2.18	0.43
1:G:190:LYS:HG3	1:G:191[B]:ARG:HG2	2.01	0.43
1:B:76:LYS:CE	5:B:2045:HOH:O	2.66	0.43
1:B:440:ASN:C	1:B:442:GLU:N	2.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:LYS:HG3	1:E:191:ARG:HG2	2.01	0.43
1:E:99:ILE:O	1:E:106:PHE:HA	2.17	0.43
1:E:508:ALA:HB3	1:E:558:PHE:CD1	2.54	0.43
1:F:241:THR:O	1:F:245:VAL:HG13	2.17	0.43
1:H:508:ALA:HB3	1:H:558:PHE:CD1	2.54	0.43
1:B:404[B]:ARG:NH1	1:B:562:PRO:HD3	2.32	0.43
1:E:421:GLN:HG3	5:E:2424:HOH:O	2.19	0.43
1:B:508:ALA:HB3	1:B:558:PHE:CD1	2.54	0.43
1:D:429:LEU:HD22	1:D:459:LEU:HG	2.00	0.43
1:G:157:LYS:NZ	5:G:2169:HOH:O	2.51	0.43
1:A:162:THR:O	1:C:525:LYS:HE3	2.18	0.43
1:C:99:ILE:O	1:C:106:PHE:HA	2.19	0.43
1:H:99:ILE:O	1:H:106:PHE:HA	2.19	0.43
1:H:244:GLN:CB	5:H:2176:HOH:O	2.67	0.42
1:D:482:THR:HG23	5:D:2447:HOH:O	2.19	0.42
1:B:99:ILE:O	1:B:106:PHE:HA	2.19	0.42
1:F:519[B]:GLN:H	1:F:519[B]:GLN:NE2	2.17	0.42
1:G:76:LYS:HE3	5:G:2054:HOH:O	2.18	0.42
1:E:236:GLN:CB	5:E:2260:HOH:O	2.67	0.42
1:E:240:GLY:CA	1:E:244:GLN:HE21	2.29	0.42
1:G:82:MET:HG2	1:G:87:ALA:HB3	2.01	0.42
1:A:326:ARG:NH1	1:A:326:ARG:CG	2.82	0.42
1:F:135:ASN:HD21	2:F:600:DGJ:H2	1.84	0.42
1:H:519:GLN:HG2	5:H:2313:HOH:O	2.19	0.42
1:B:82:MET:HG2	1:B:87:ALA:HB3	2.02	0.42
1:C:433:THR:O	1:C:436:GLN:N	2.40	0.42
1:E:76:LYS:HE2	5:E:2051:HOH:O	2.20	0.42
1:G:190:LYS:HG3	1:G:191[A]:ARG:HG2	2.02	0.42
1:C:508:ALA:HB3	1:C:558:PHE:CD1	2.55	0.41
1:D:82:MET:HG2	1:D:87:ALA:HB3	2.01	0.41
1:D:451:HIS:CE1	1:D:455:ARG:HD2	2.55	0.41
1:D:462:GLN:HB3	5:D:2425:HOH:O	2.20	0.41
1:G:462:GLN:HB3	5:G:2435:HOH:O	2.20	0.41
1:A:451:HIS:CE1	1:A:455:ARG:HD2	2.55	0.41
1:H:482:THR:HG23	5:H:2322:HOH:O	2.19	0.41
1:G:241:THR:H	1:G:244:GLN:NE2	2.19	0.41
1:C:482[A]:THR:HG23	5:C:2345:HOH:O	2.21	0.41
1:C:482[B]:THR:HG23	5:C:2345:HOH:O	2.21	0.41
1:C:82:MET:HG2	1:C:87:ALA:HB3	2.02	0.41
1:D:70:ASN:HD22	1:D:98:GLN:NE2	2.18	0.41
1:B:73:ASP:HB2	5:B:2044:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:HIS:CE1	1:C:455:ARG:HD2	2.56	0.41
1:B:548:ASN:HB3	1:H:140:TYR:CZ	2.56	0.41
1:E:482:THR:HG21	5:E:2228:HOH:O	2.20	0.41
1:H:533:GLU:OE2	1:H:563:HIS:HD2	2.04	0.41
1:F:51:LEU:HD22	1:F:199[A]:MET:HE1	2.02	0.41
1:F:482[A]:THR:HG21	5:F:2457:HOH:O	2.20	0.41
1:C:121[B]:ARG:HG2	1:C:121[B]:ARG:HH11	1.86	0.41
1:H:235:LEU:HB2	1:H:237:LEU:HD22	2.02	0.41
1:F:264:ASP:O	1:F:268:VAL:CG1	2.67	0.40
1:G:190:LYS:CG	1:G:191[B]:ARG:HG2	2.51	0.40
1:A:548:ASN:HB3	1:B:140:TYR:CZ	2.56	0.40
1:C:79:TRP:HB3	1:C:121[B]:ARG:CZ	2.51	0.40
1:F:82:MET:HG2	1:F:87:ALA:HB3	2.03	0.40
1:E:434:GLU:O	1:E:438:ILE:HG23	2.20	0.40
1:H:37:ALA:N	5:H:2004:HOH:O	2.53	0.40
1:A:73:ASP:HB2	5:A:2045:HOH:O	2.21	0.40
1:A:404:ARG:HD2	5:A:2361:HOH:O	2.22	0.40
1:E:82:MET:HG2	1:E:87:ALA:HB3	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	540/540 (100%)	519 (96%)	19 (4%)	2 (0%)	30	19
1	B	540/540 (100%)	519 (96%)	18 (3%)	3 (1%)	21	11
1	C	543/540 (101%)	524 (96%)	16 (3%)	3 (1%)	21	11
1	D	545/540 (101%)	525 (96%)	18 (3%)	2 (0%)	30	19
1	E	542/540 (100%)	524 (97%)	16 (3%)	2 (0%)	30	19
1	F	549/540 (102%)	528 (96%)	19 (4%)	2 (0%)	30	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	545/540 (101%)	525 (96%)	19 (4%)	1 (0%)	43	31
1	H	541/540 (100%)	522 (96%)	17 (3%)	2 (0%)	30	19
All	All	4345/4320 (101%)	4186 (96%)	142 (3%)	17 (0%)	30	19

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	434	GLU
1	F	446	GLU
1	B	441	ALA
1	B	444	THR
1	E	522	ALA
1	F	444	THR
1	A	444	THR
1	C	444	THR
1	D	444	THR
1	G	444	THR
1	H	444	THR
1	A	491	ALA
1	C	491	ALA
1	E	491	ALA
1	B	491	ALA
1	D	491	ALA
1	H	491	ALA

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	423/452 (94%)	416 (98%)	7 (2%)	53	45
1	B	419/452 (93%)	408 (97%)	11 (3%)	40	28
1	C	421/452 (93%)	411 (98%)	10 (2%)	43	31
1	D	429/452 (95%)	417 (97%)	12 (3%)	38	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	436/452 (96%)	424 (97%)	12 (3%)	38	26
1	F	436/452 (96%)	420 (96%)	16 (4%)	30	18
1	G	430/452 (95%)	415 (96%)	15 (4%)	32	19
1	H	420/452 (93%)	412 (98%)	8 (2%)	50	41
All	All	3414/3616 (94%)	3323 (97%)	91 (3%)	42	27

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	MET
1	A	136	ASN
1	A	235	LEU
1	A	245	VAL
1	A	390	VAL
1	A	429	LEU
1	A	537	GLU
1	B	82	MET
1	B	136	ASN
1	B	233	GLN
1	B	235	LEU
1	B	237	LEU
1	B	245	VAL
1	B	292	LEU
1	B	390	VAL
1	B	429	LEU
1	B	462	GLN
1	B	537	GLU
1	C	82	MET
1	C	136	ASN
1	C	237	LEU
1	C	245	VAL
1	C	390	VAL
1	C	429	LEU
1	C	462	GLN
1	C	528[A]	ILE
1	C	528[B]	ILE
1	C	537	GLU
1	D	45	ASN
1	D	82	MET
1	D	136	ASN
1	D	235	LEU

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Mol	Chain	Res	Type
1	D	237	LEU
1	D	245	VAL
1	D	292	LEU
1	D	390	VAL
1	D	429	LEU
1	D	462	GLN
1	D	528[A]	ILE
1	D	528[B]	ILE
1	E	82	MET
1	E	136	ASN
1	E	179	LYS
1	E	245	VAL
1	E	340	ARG
1	E	390	VAL
1	E	395	THR
1	E	415	ARG
1	E	438	ILE
1	E	537	GLU
1	E	543[A]	MET
1	E	543[B]	MET
1	F	82	MET
1	F	99[A]	ILE
1	F	99[B]	ILE
1	F	135	ASN
1	F	136	ASN
1	F	235	LEU
1	F	237	LEU
1	F	245	VAL
1	F	268	VAL
1	F	292	LEU
1	F	395	THR
1	F	405	LEU
1	F	429	LEU
1	F	519[A]	GLN
1	F	519[B]	GLN
1	F	537	GLU
1	G	82	MET
1	G	136	ASN
1	G	235	LEU
1	G	241	THR
1	G	245	VAL
1	G	340	ARG

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Mol	Chain	Res	Type
1	G	390	VAL
1	G	429	LEU
1	G	432	THR
1	G	519	GLN
1	G	525[A]	LYS
1	G	525[B]	LYS
1	G	537	GLU
1	G	543[A]	MET
1	G	543[B]	MET
1	H	82	MET
1	H	136	ASN
1	H	155	VAL
1	H	237	LEU
1	H	340	ARG
1	H	429	LEU
1	H	519	GLN
1	H	537	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	172	ASN
1	A	275	ASN
1	A	398	GLN
1	A	421	GLN
1	A	451	HIS
1	A	462	GLN
1	B	98	GLN
1	B	172	ASN
1	B	233	GLN
1	B	275	ASN
1	B	451	HIS
1	B	462	GLN
1	B	487	ASN
1	C	46	ASN
1	C	98	GLN
1	C	172	ASN
1	C	275	ASN
1	C	451	HIS
1	C	462	GLN
1	D	98	GLN

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Mol	Chain	Res	Type
1	D	172	ASN
1	D	275	ASN
1	D	289	ASN
1	D	451	HIS
1	D	462	GLN
1	E	49	HIS
1	E	172	ASN
1	E	244	GLN
1	E	275	ASN
1	E	421	GLN
1	E	451	HIS
1	E	502	ASN
1	E	551	GLN
1	F	46	ASN
1	F	49	HIS
1	F	135	ASN
1	F	136	ASN
1	F	201	GLN
1	F	220	GLN
1	F	224	ASN
1	F	255	HIS
1	F	275	ASN
1	F	502	ASN
1	G	49	HIS
1	G	224	ASN
1	G	244	GLN
1	G	275	ASN
1	G	401	GLN
1	G	462	GLN
1	G	487	ASN
1	H	45	ASN
1	H	46	ASN
1	H	49	HIS
1	H	136	ASN
1	H	172	ASN
1	H	275	ASN
1	H	451	HIS
1	H	502	ASN
1	H	563	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 23 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DGJ	D	600	-	11,11,11	1.13	1 (9%)	13,15,15	1.32	2 (15%)
2	DGJ	G	600	-	11,11,11	0.99	1 (9%)	13,15,15	1.10	0
2	DGJ	A	600	-	11,11,11	0.89	1 (9%)	13,15,15	1.04	0
4	ACT	F	605	-	3,3,3	0.81	0	3,3,3	1.07	0
2	DGJ	F	600	-	11,11,11	0.97	1 (9%)	13,15,15	1.11	0
2	DGJ	H	600	-	11,11,11	0.57	0	13,15,15	0.84	0
4	ACT	C	601	-	3,3,3	0.76	0	3,3,3	0.64	0
4	ACT	C	602	-	3,3,3	0.97	0	3,3,3	0.62	0
4	ACT	D	605	-	3,3,3	0.92	0	3,3,3	0.19	0
4	ACT	D	606	-	3,3,3	1.09	0	3,3,3	0.49	0
2	DGJ	C	600	-	11,11,11	0.85	0	13,15,15	0.95	1 (7%)
2	DGJ	E	600	-	11,11,11	1.22	1 (9%)	13,15,15	0.71	0
2	DGJ	B	600	-	11,11,11	0.73	0	13,15,15	0.86	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DGJ	D	600	-	-	0/2/19/19	0/1/1/1
2	DGJ	G	600	-	-	0/2/19/19	0/1/1/1
2	DGJ	A	600	-	-	0/2/19/19	0/1/1/1
2	DGJ	F	600	-	-	0/2/19/19	0/1/1/1
2	DGJ	H	600	-	-	0/2/19/19	0/1/1/1
2	DGJ	C	600	-	-	0/2/19/19	0/1/1/1
2	DGJ	E	600	-	-	0/2/19/19	0/1/1/1
2	DGJ	B	600	-	-	0/2/19/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	600	DGJ	C1-C2	3.43	1.55	1.52
2	D	600	DGJ	C1-N5	2.92	1.51	1.47
2	A	600	DGJ	O2-C2	2.10	1.47	1.43
2	G	600	DGJ	C1-N5	-2.06	1.44	1.47
2	F	600	DGJ	C1-C2	-2.02	1.50	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	DGJ	C1-C2-C3	2.53	113.34	110.25
2	D	600	DGJ	O2-C2-C1	2.27	114.04	109.65
2	C	600	DGJ	C2-C3-C4	-2.01	107.33	110.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	600	DGJ	1	0
2	H	600	DGJ	1	0

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	539/540 (99%)	-0.09	14 (2%)	57	57	17, 26, 49, 93	3 (0%)
1	B	539/540 (99%)	-0.00	16 (2%)	52	52	16, 28, 51, 101	3 (0%)
1	C	539/540 (99%)	0.23	32 (5%)	28	27	16, 29, 56, 108	6 (1%)
1	D	540/540 (100%)	-0.07	14 (2%)	57	57	13, 25, 52, 107	7 (1%)
1	E	539/540 (99%)	-0.20	11 (2%)	65	65	13, 24, 47, 87	5 (0%)
1	F	539/540 (99%)	-0.19	13 (2%)	59	60	13, 23, 47, 97	12 (2%)
1	G	540/540 (100%)	-0.18	14 (2%)	57	57	14, 24, 48, 82	7 (1%)
1	H	539/540 (99%)	0.20	32 (5%)	28	27	17, 29, 62, 102	4 (0%)
All	All	4314/4320 (99%)	-0.04	146 (3%)	48	48	13, 26, 53, 108	47 (1%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	522	ALA	4.9
1	B	443	ALA	4.8
1	D	522	ALA	4.6
1	B	439	TRP	4.6
1	H	439	TRP	4.4
1	C	435	THR	4.2
1	F	440	ASN	4.2
1	H	435	THR	4.1
1	D	443	ALA	4.0
1	A	439	TRP	3.9
1	E	522	ALA	3.9
1	G	522	ALA	3.9
1	D	441	ALA	3.8
1	D	440	ASN	3.8
1	H	245	VAL	3.8
1	C	439	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	439	TRP	3.7
1	C	434	GLU	3.7
1	C	223	PHE	3.7
1	B	438	ILE	3.6
1	H	438	ILE	3.6
1	H	441	ALA	3.6
1	B	444	THR	3.5
1	C	232	ILE	3.5
1	C	433	THR	3.5
1	D	445	PRO	3.5
1	C	522	ALA	3.5
1	B	435	THR	3.4
1	C	445	PRO	3.4
1	D	444	THR	3.4
1	G	444	THR	3.4
1	H	235	LEU	3.4
1	H	443	ALA	3.4
1	E	440	ASN	3.3
1	A	444	THR	3.3
1	H	227	VAL	3.3
1	D	46	ASN	3.3
1	C	441	ALA	3.2
1	G	435	THR	3.2
1	D	438	ILE	3.2
1	D	575	GLN	3.2
1	C	438	ILE	3.2
1	F	435	THR	3.2
1	C	245	VAL	3.2
1	B	521	LEU	3.2
1	H	237	LEU	3.2
1	A	435	THR	3.1
1	D	36	ALA	3.1
1	F	37	ALA	3.1
1	G	438	ILE	3.1
1	E	441	ALA	3.1
1	F	444	THR	3.1
1	B	575	GLN	3.1
1	H	230	ASP	3.0
1	C	215	TYR	3.0
1	C	437	LYS	3.0
1	F	439	TRP	3.0
1	A	440	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	239	PRO	3.0
1	C	436	GLN	3.0
1	B	440	ASN	3.0
1	B	445	PRO	3.0
1	E	438	ILE	3.0
1	G	241	THR	3.0
1	C	446	GLU	3.0
1	H	442	GLU	2.9
1	F	443	ALA	2.9
1	H	232	ILE	2.9
1	A	445	PRO	2.9
1	G	439	TRP	2.9
1	H	445	PRO	2.8
1	C	227	VAL	2.8
1	A	441	ALA	2.8
1	B	237	LEU	2.8
1	F	445	PRO	2.8
1	H	448	LYS	2.7
1	A	433	THR	2.7
1	C	241	THR	2.7
1	A	237	LEU	2.7
1	B	434	GLU	2.7
1	A	443	ALA	2.7
1	H	523	GLY	2.7
1	C	243	SER	2.7
1	F	438	ILE	2.7
1	C	250	ALA	2.6
1	G	36	ALA	2.6
1	C	244	GLN	2.6
1	E	419	GLN	2.6
1	E	435	THR	2.6
1	E	442	GLU	2.6
1	A	522	ALA	2.6
1	D	435	THR	2.6
1	C	237	LEU	2.5
1	E	439	TRP	2.5
1	H	437	LYS	2.5
1	E	443	ALA	2.5
1	G	419	GLN	2.5
1	G	442	GLU	2.5
1	H	419	GLN	2.5
1	B	441	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	443	ALA	2.5
1	H	240	GLY	2.4
1	H	440	ASN	2.4
1	C	521	LEU	2.4
1	C	442	GLU	2.4
1	B	522	ALA	2.4
1	C	444	THR	2.4
1	C	242	TRP	2.4
1	C	235	LEU	2.4
1	B	433	THR	2.4
1	D	442	GLU	2.4
1	G	434	GLU	2.4
1	A	521	LEU	2.3
1	E	444	THR	2.3
1	A	446	GLU	2.3
1	B	442	GLU	2.3
1	H	223	PHE	2.3
1	C	239	PRO	2.3
1	D	433	THR	2.3
1	H	229	ASP	2.3
1	C	443	ALA	2.2
1	B	448	LYS	2.2
1	H	238	LYS	2.2
1	H	226	ALA	2.2
1	F	221	ALA	2.2
1	F	441	ALA	2.2
1	C	440	ASN	2.2
1	C	236	GLN	2.2
1	C	169	LEU	2.2
1	E	45	ASN	2.1
1	C	575	GLN	2.1
1	H	444	THR	2.1
1	H	231	LEU	2.1
1	A	575	GLN	2.1
1	F	575	GLN	2.1
1	H	225	ALA	2.1
1	A	574	VAL	2.1
1	G	245	VAL	2.1
1	G	575	GLN	2.1
1	H	236	GLN	2.1
1	G	441	ALA	2.1
1	H	433	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	156	VAL	2.0
1	H	246	PHE	2.0
1	F	523	GLY	2.0
1	H	233	GLN	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(Å ²)	Q<0.9
3	NA	B	601	1/1	0.87	0.09	47,47,47,47	0
4	ACT	C	601	4/4	0.88	0.16	36,44,45,45	0
4	ACT	D	605	4/4	0.88	0.15	37,37,41,44	0
4	ACT	F	605	4/4	0.91	0.12	37,40,44,45	0
4	ACT	C	602	4/4	0.92	0.14	36,36,36,38	0
4	ACT	D	606	4/4	0.94	0.10	33,34,34,34	0
3	NA	H	601	1/1	0.94	0.06	41,41,41,41	0
3	NA	B	602	1/1	0.95	0.07	42,42,42,42	0
3	NA	D	602	1/1	0.95	0.09	41,41,41,41	0
3	NA	D	604	1/1	0.95	0.11	30,30,30,30	0
3	NA	F	603	1/1	0.96	0.09	30,30,30,30	0
2	DGJ	D	600	11/11	0.97	0.05	17,18,20,20	0
3	NA	G	601	1/1	0.97	0.06	35,35,35,35	0
3	NA	A	604	1/1	0.97	0.09	44,44,44,44	0
3	NA	F	601	1/1	0.97	0.05	26,26,26,26	0
2	DGJ	F	600	11/11	0.98	0.04	15,18,19,19	0
3	NA	E	602	1/1	0.98	0.07	27,27,27,27	0
3	NA	E	603	1/1	0.98	0.07	28,28,28,28	0
3	NA	E	604	1/1	0.98	0.05	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DGJ	G	600	11/11	0.98	0.04	18,18,19,20	0
3	NA	F	602	1/1	0.98	0.05	35,35,35,35	0
2	DGJ	H	600	11/11	0.98	0.04	21,22,23,23	0
3	NA	A	602	1/1	0.98	0.11	35,35,35,35	0
3	NA	G	602	1/1	0.98	0.06	31,31,31,31	0
3	NA	G	603	1/1	0.98	0.06	38,38,38,38	0
2	DGJ	B	600	11/11	0.98	0.05	20,21,24,25	0
2	DGJ	C	600	11/11	0.98	0.04	21,22,22,23	0
2	DGJ	A	600	11/11	0.98	0.04	17,19,21,21	0
3	NA	D	601	1/1	0.98	0.06	33,33,33,33	0
2	DGJ	E	600	11/11	0.98	0.05	17,18,20,21	0
3	NA	D	603	1/1	0.98	0.05	40,40,40,40	0
3	NA	A	603	1/1	0.99	0.04	36,36,36,36	0
3	NA	A	601	1/1	0.99	0.07	29,29,29,29	0
3	NA	E	601	1/1	0.99	0.02	24,24,24,24	0
3	NA	G	604	1/1	0.99	0.07	39,39,39,39	0
3	NA	F	604	1/1	0.99	0.05	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.