



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:34 AM UTC

PDB ID : 2G56 / pdb_00002g56
Title : crystal structure of human insulin-degrading enzyme in complex with insulin B chain
Authors : Shen, Y.; Tang, W.-J.
Deposited on : 2006-02-22
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

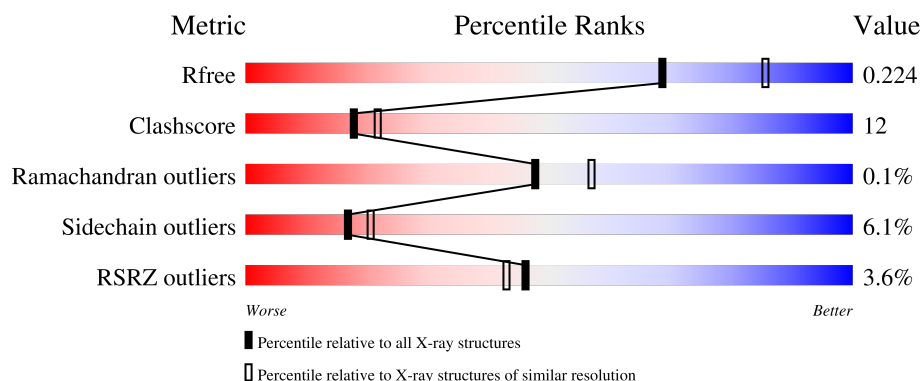
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	990	3% 69% 24% • •
1	B	990	2% 71% 23% • •
2	C	30	33% 37% 13% 10% 40%
2	D	30	37% 37% 20% 7% 37%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16964 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	964	Total	C	N	O	S	0	0	0
			7853	5053	1319	1447	34			
1	B	964	Total	C	N	O	S	0	0	0
			7850	5052	1318	1446	34			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	initiating methionine	UNP Q5T5N2
A	31	HIS	-	expression tag	UNP Q5T5N2
A	32	HIS	-	expression tag	UNP Q5T5N2
A	33	HIS	-	expression tag	UNP Q5T5N2
A	34	HIS	-	expression tag	UNP Q5T5N2
A	35	HIS	-	expression tag	UNP Q5T5N2
A	36	HIS	-	expression tag	UNP Q5T5N2
A	37	ALA	-	cloning artifact	UNP Q5T5N2
A	38	ALA	-	cloning artifact	UNP Q5T5N2
A	39	GLY	-	cloning artifact	UNP Q5T5N2
A	40	ILE	-	cloning artifact	UNP Q5T5N2
A	41	PRO	-	cloning artifact	UNP Q5T5N2
A	111	GLN	GLU	engineered mutation	UNP Q5T5N2
B	30	MET	-	initiating methionine	UNP Q5T5N2
B	31	HIS	-	expression tag	UNP Q5T5N2
B	32	HIS	-	expression tag	UNP Q5T5N2
B	33	HIS	-	expression tag	UNP Q5T5N2
B	34	HIS	-	expression tag	UNP Q5T5N2
B	35	HIS	-	expression tag	UNP Q5T5N2
B	36	HIS	-	expression tag	UNP Q5T5N2
B	37	ALA	-	cloning artifact	UNP Q5T5N2
B	38	ALA	-	cloning artifact	UNP Q5T5N2
B	39	GLY	-	cloning artifact	UNP Q5T5N2
B	40	ILE	-	cloning artifact	UNP Q5T5N2
B	41	PRO	-	cloning artifact	UNP Q5T5N2

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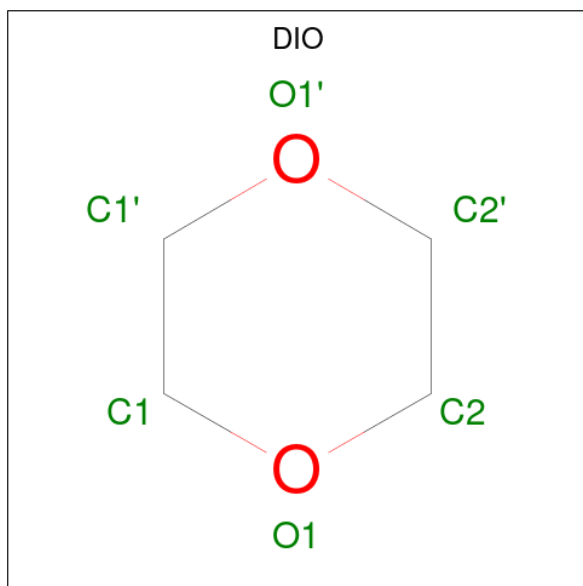
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Chain	Residue	Modelled	Actual	Comment	Reference
B	111	GLN	GLU	engineered mutation	UNP Q5T5N2

- Molecule 2 is a protein called Insulin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	0	0	0
			103	63	20	20			
2	D	19	Total	C	N	O	0	0	0
			108	66	21	21			

- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: C₄H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	541	Total	O	0	0
			541	541		
4	B	500	Total	O	0	0
			500	500		
4	C	2	Total	O	0	0
			2	2		

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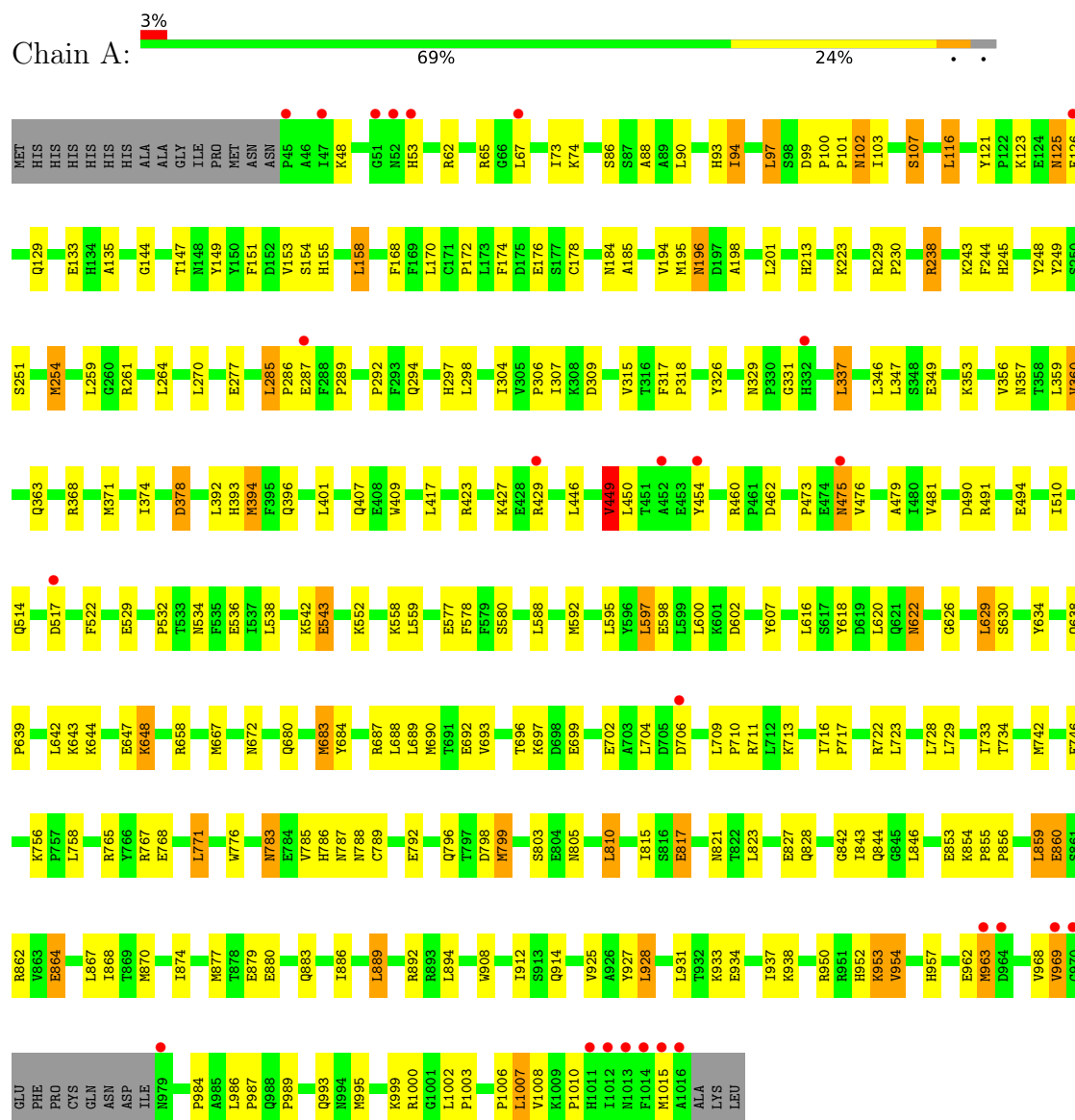
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	O	0	0
			1	1		

3 Residue-property plots

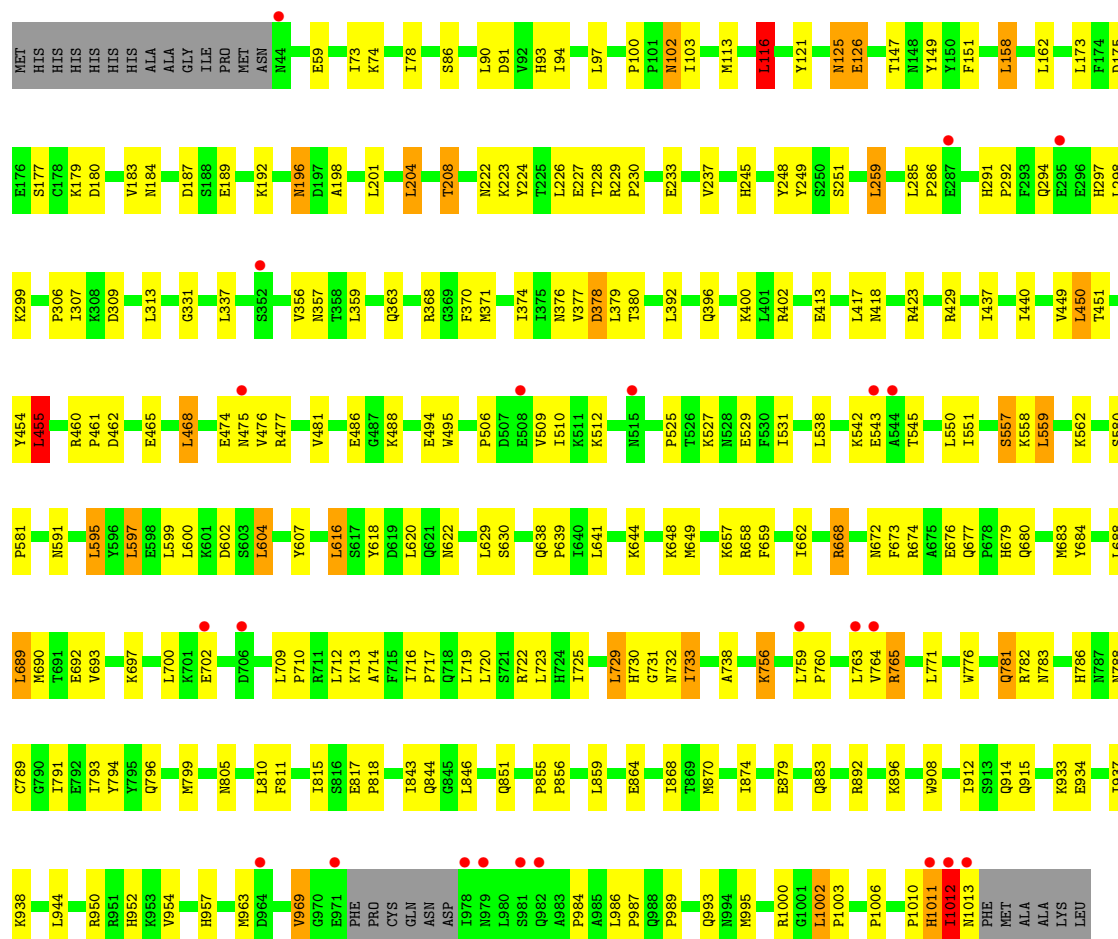
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Insulin-degrading enzyme

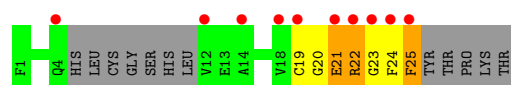
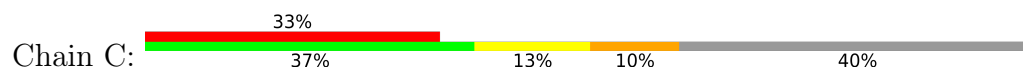


• Molecule 1: Insulin-degrading enzyme





- Molecule 2: Insulin



- Molecule 2: Insulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	262.25Å 262.25Å 90.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.75 – 2.20 29.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.1 (29.75-2.20) 95.0 (29.75-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.225 0.203 , 0.224	Depositor DCC
R_{free} test set	17390 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16964	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.43	4/8049 (0.0%)	0.86	13/10887 (0.1%)
1	B	0.46	5/8046 (0.1%)	0.89	18/10884 (0.2%)
2	C	1.81	3/102 (2.9%)	3.53	17/137 (12.4%)
2	D	1.32	1/107 (0.9%)	2.02	5/144 (3.5%)
All	All	0.48	13/16304 (0.1%)	0.93	53/22052 (0.2%)

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
2	C	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	23	GLY	N-CA	-9.31	1.35	1.45
1	A	254	MET	SD-CE	-7.74	1.60	1.79
1	A	394	MET	SD-CE	-7.71	1.60	1.79
2	C	23	GLY	CA-C	-7.67	1.45	1.51
1	A	683	MET	SD-CE	-7.55	1.60	1.79
1	B	371	MET	SD-CE	-7.33	1.61	1.79
1	B	1010	PRO	CA-C	-6.25	1.45	1.52
1	B	1011	HIS	CA-C	6.19	1.61	1.53
1	B	1010	PRO	C-O	6.09	1.31	1.23
2	D	10	HIS	CA-CB	-5.90	1.41	1.53
1	B	690	MET	SD-CE	-5.88	1.64	1.79
1	A	690	MET	SD-CE	-5.87	1.64	1.79
2	C	25	PHE	CA-CB	-5.41	1.42	1.53

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1011	HIS	N-CA-C	-18.89	86.17	110.53
2	C	24	PHE	CA-C-O	13.72	134.80	120.40
2	C	25	PHE	N-CA-C	12.32	145.49	111.00
2	C	23	GLY	CA-C-N	-11.06	106.93	123.07
2	C	23	GLY	C-N-CA	-11.06	106.93	123.07
1	A	449	VAL	CB-CA-C	-10.89	97.77	112.04
2	D	22	ARG	N-CA-C	10.86	133.93	110.80
2	C	20	GLY	CA-C-N	-10.86	105.14	122.73
2	C	20	GLY	C-N-CA	-10.86	105.14	122.73
2	C	24	PHE	CA-C-N	9.74	139.24	121.70
2	C	24	PHE	C-N-CA	9.74	139.24	121.70
2	C	25	PHE	CA-C-O	-8.97	105.56	120.80
1	B	494	GLU	N-CA-C	8.10	119.80	110.97
2	C	24	PHE	N-CA-C	7.87	121.80	108.02
2	C	19	CYS	N-CA-C	-7.86	96.43	109.24
2	D	21	GLU	CA-C-N	7.86	136.55	121.54
2	D	21	GLU	C-N-CA	7.86	136.55	121.54
2	D	21	GLU	N-CA-C	7.58	126.94	110.80
2	C	22	ARG	CA-C-O	7.55	128.66	120.43
1	A	121	TYR	CA-C-N	7.53	127.07	119.24
1	A	121	TYR	C-N-CA	7.53	127.07	119.24
1	B	1012	ILE	N-CA-C	7.47	124.87	109.34
1	A	494	GLU	N-CA-C	7.19	119.11	111.28
1	A	953	LYS	N-CA-C	6.97	120.26	108.90
2	D	20	GLY	N-CA-C	-6.71	97.28	113.18
1	B	455	LEU	N-CA-C	6.70	119.06	108.67
1	A	307	ILE	N-CA-C	-6.65	104.69	110.74
1	A	116	LEU	N-CA-C	6.61	120.34	112.93
2	C	23	GLY	CA-C-O	-6.55	115.87	121.57
1	A	449	VAL	N-CA-C	6.44	117.96	110.62
1	A	449	VAL	N-CA-CB	6.42	118.50	110.47
1	B	116	LEU	N-CA-C	6.32	120.01	112.93
1	A	853	GLU	N-CA-C	-6.22	105.69	113.28
2	C	21	GLU	N-CA-C	5.96	119.20	109.24
1	B	944	LEU	N-CA-C	5.86	120.44	113.12
1	A	378	ASP	N-CA-C	-5.85	101.86	110.52
1	B	677	GLN	CA-C-N	5.77	125.90	119.32
1	B	677	GLN	C-N-CA	5.77	125.90	119.32
1	B	495	TRP	N-CA-C	5.75	118.49	111.82
2	C	22	ARG	O-C-N	5.39	129.36	123.27
1	B	378	ASP	N-CA-C	-5.39	102.78	110.59
2	C	24	PHE	O-C-N	5.26	130.07	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	476	VAL	N-CA-C	5.19	117.02	108.97
1	B	380	THR	N-CA-C	-5.15	103.24	110.35
2	C	23	GLY	N-CA-C	5.12	119.73	111.38
1	B	121	TYR	CA-C-N	5.11	124.90	119.28
1	B	121	TYR	C-N-CA	5.11	124.90	119.28
1	A	304	ILE	N-CA-C	5.10	115.83	108.48
1	A	374	ILE	N-CA-C	5.04	116.85	108.99
1	B	557	SER	N-CA-C	5.04	117.04	109.23
1	B	545	THR	CA-C-N	5.03	124.52	119.19
1	B	545	THR	C-N-CA	5.03	124.52	119.19
1	B	307	ILE	N-CA-C	-5.00	105.97	110.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	21	GLU	Mainchain
2	C	22	ARG	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	7853	0	7773	211	0
1	B	7850	0	7765	181	0
2	C	103	0	66	1	0
2	D	108	0	68	5	0
3	A	6	0	8	1	0
4	A	541	0	0	20	0
4	B	500	0	0	17	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
All	All	16964	0	15680	387	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 12.

All (387) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:THR:HG23	1:B:477:ARG:HH22	1.11	1.08
1:A:315:VAL:HG21	1:A:394:MET:HE1	1.37	1.04
1:B:892:ARG:HD2	4:B:1459:HOH:O	1.57	1.02
1:B:208:THR:CG2	1:B:477:ARG:HH22	1.77	0.97
1:B:817:GLU:HG3	1:B:818:PRO:HD3	1.47	0.97
1:B:765:ARG:NH1	1:B:914:GLN:OE1	2.02	0.93
1:B:864:GLU:HG2	1:B:986:LEU:HD21	1.49	0.92
1:A:94:ILE:HD11	1:A:244:PHE:CZ	2.05	0.91
1:A:309:ASP:H	1:A:672:ASN:HD21	1.17	0.89
1:A:680:GLN:OE1	2:C:25:PHE:CB	2.20	0.88
1:A:102:ASN:H	1:A:102:ASN:HD22	1.22	0.88
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.23	0.87
1:A:879:GLU:HG2	4:A:1330:HOH:O	1.74	0.86
1:B:102:ASN:HD22	1:B:102:ASN:H	1.22	0.85
1:A:765:ARG:NH1	1:A:914:GLN:OE1	2.10	0.85
1:A:815:ILE:HA	1:A:870:MET:HE2	1.58	0.84
1:B:309:ASP:H	1:B:672:ASN:HD21	1.24	0.83
1:A:864:GLU:HG2	1:A:986:LEU:HD21	1.58	0.83
1:A:886:ILE:HG23	1:A:928:LEU:HD22	1.58	0.83
1:A:534:ASN:OD1	1:A:536:GLU:HG2	1.79	0.83
1:A:689:LEU:HG	1:A:995:MET:HE2	1.62	0.82
1:B:294:GLN:H	1:B:297:HIS:HD2	1.25	0.82
1:B:429:ARG:HD2	4:B:1352:HOH:O	1.80	0.81
1:A:287:GLU:HG2	1:A:289:PRO:HD3	1.63	0.80
1:B:950:ARG:HD2	4:B:1252:HOH:O	1.83	0.79
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.64	0.79
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.31	0.78
1:B:208:THR:HG23	1:B:477:ARG:NH2	1.96	0.77
1:A:309:ASP:H	1:A:672:ASN:ND2	1.83	0.77
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.33	0.76
1:A:294:GLN:H	1:A:297:HIS:HD2	1.31	0.76
1:B:604:LEU:HD13	1:B:648:LYS:HG2	1.65	0.76
1:A:1000:ARG:HD2	4:B:1297:HOH:O	1.85	0.76
1:B:783:ASN:ND2	1:B:786:HIS:H	1.83	0.76
1:B:59:GLU:OE2	4:B:1464:HOH:O	2.02	0.76
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.85	0.75
1:B:791:ILE:HD11	1:B:793:ILE:HD11	1.69	0.75
1:A:538:LEU:HD23	1:A:734:THR:HG23	1.69	0.74
1:A:184:ASN:HD21	1:A:223:LYS:NZ	1.85	0.74
1:B:674:ARG:HD3	4:B:1239:HOH:O	1.88	0.73
1:A:783:ASN:HD22	1:A:785:VAL:H	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:ASN:ND2	1:A:785:VAL:H	1.88	0.72
1:B:309:ASP:H	1:B:672:ASN:ND2	1.86	0.72
1:A:711:ARG:O	1:A:711:ARG:NH2	2.24	0.71
1:B:817:GLU:HG3	1:B:818:PRO:CD	2.19	0.71
1:B:451:THR:HB	1:B:455:LEU:HD22	1.72	0.70
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.39	0.70
1:A:135:ALA:HA	1:A:892:ARG:NH2	2.08	0.69
1:A:102:ASN:HD22	1:A:102:ASN:N	1.90	0.69
1:B:538:LEU:H	1:B:732:ASN:HD21	1.38	0.69
1:A:491:ARG:HD2	4:A:1220:HOH:O	1.93	0.68
1:B:689:LEU:HD13	1:B:995:MET:HE2	1.73	0.68
1:B:709:LEU:HG	1:B:713:LYS:HE3	1.75	0.68
1:A:174:PHE:O	1:A:238:ARG:HD3	1.94	0.68
1:B:683:MET:HE1	2:D:23:GLY:HA2	1.76	0.67
1:A:88:ALA:HB3	1:A:151:PHE:CE2	2.29	0.67
1:A:716:ILE:HB	1:A:717:PRO:HD3	1.76	0.67
1:A:517:ASP:HB2	4:A:1230:HOH:O	1.93	0.67
1:B:102:ASN:HD22	1:B:102:ASN:N	1.88	0.67
1:B:527:LYS:HD2	1:B:529:GLU:OE2	1.95	0.67
1:A:298:LEU:HD21	1:A:318:PRO:HG2	1.77	0.67
1:A:100:PRO:HG2	1:A:103:ILE:HB	1.76	0.66
1:B:868:ILE:HD12	1:B:984:PRO:HD3	1.76	0.66
1:A:315:VAL:CG2	1:A:394:MET:HE1	2.21	0.66
1:A:368:ARG:HD2	4:A:1195:HOH:O	1.96	0.66
1:B:1012:ILE:O	1:B:1013:ASN:CB	2.43	0.66
1:A:294:GLN:H	1:A:297:HIS:CD2	2.13	0.65
1:A:722:ARG:HB3	1:A:758:LEU:HD13	1.78	0.65
1:B:543:GLU:N	1:B:543:GLU:OE2	2.30	0.64
1:B:658:ARG:NH2	4:B:1480:HOH:O	2.30	0.64
1:B:102:ASN:H	1:B:102:ASN:ND2	1.95	0.64
1:B:294:GLN:H	1:B:297:HIS:CD2	2.12	0.64
1:A:883:GLN:NE2	4:A:1094:HOH:O	2.30	0.64
1:B:883:GLN:NE2	4:B:1458:HOH:O	2.30	0.64
1:B:125:ASN:HD22	1:B:125:ASN:H	1.46	0.64
1:B:229:ARG:HB3	1:B:230:PRO:HD3	1.80	0.63
1:A:194:VAL:HG12	1:A:195:MET:HE2	1.81	0.63
1:A:771:LEU:HD21	1:A:954:VAL:HG12	1.80	0.63
1:B:781:GLN:HE21	1:B:782:ARG:H	1.45	0.63
1:A:309:ASP:N	1:A:672:ASN:HD21	1.95	0.63
1:A:317:PHE:HD2	1:A:475:ASN:HD21	1.47	0.63
1:A:934:GLU:HG2	1:A:938:LYS:HE3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:969:VAL:HG21	1:A:989:PRO:HD2	1.81	0.62
1:A:709:LEU:HG	1:A:713:LYS:HE3	1.81	0.62
1:A:363:GLN:NE2	1:A:371:MET:HE1	2.14	0.62
1:B:815:ILE:HG22	1:B:870:MET:HE2	1.81	0.62
1:A:889:LEU:HB3	1:A:928:LEU:HD11	1.82	0.62
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.16	0.62
1:B:716:ILE:HB	1:B:717:PRO:HD3	1.81	0.62
1:A:908:TRP:CZ2	1:A:912:ILE:HD11	2.34	0.61
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.13	0.61
1:B:100:PRO:HG2	1:B:103:ILE:HB	1.82	0.61
1:A:125:ASN:H	1:A:125:ASN:HD22	1.47	0.61
1:A:767:ARG:NH1	1:A:1006:PRO:HA	2.16	0.61
1:B:357:ASN:HB2	1:B:378:ASP:OD1	2.01	0.61
1:B:874:ILE:O	1:B:933:LYS:HD2	2.02	0.60
1:A:643:LYS:HE3	1:A:647:GLU:OE2	2.00	0.60
1:A:950:ARG:HD2	4:A:1303:HOH:O	2.01	0.60
1:A:168:PHE:O	1:A:172:PRO:HG3	2.01	0.60
1:B:423:ARG:NH2	4:B:1464:HOH:O	2.28	0.59
1:B:474:GLU:C	1:B:475:ASN:HD22	2.11	0.59
1:B:331:GLY:HA3	1:B:363:GLN:HE21	1.67	0.59
1:A:99:ASP:OD2	1:A:107:SER:HB3	2.02	0.59
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.84	0.58
1:A:803:SER:HA	1:A:927:TYR:CE2	2.37	0.58
1:B:423:ARG:NE	4:B:1464:HOH:O	2.27	0.58
1:A:102:ASN:H	1:A:102:ASN:ND2	1.96	0.58
1:B:94:ILE:HG13	1:B:248:TYR:HB3	1.85	0.58
1:B:285:LEU:HD13	1:B:286:PRO:O	2.03	0.58
1:A:129:GLN:O	1:A:133:GLU:HG3	2.04	0.58
1:A:957:HIS:HD2	4:A:1306:HOH:O	1.86	0.58
1:B:285:LEU:HD22	1:B:286:PRO:HD2	1.86	0.58
1:B:679:HIS:HD2	1:B:851:GLN:OE1	1.86	0.57
1:A:196:ASN:C	1:A:196:ASN:HD22	2.11	0.57
1:A:580:SER:HB2	1:A:723:LEU:HD23	1.85	0.57
1:B:208:THR:CG2	1:B:477:ARG:NH2	2.60	0.57
1:A:317:PHE:HD2	1:A:475:ASN:ND2	2.02	0.57
1:A:97:LEU:HB2	1:A:144:GLY:O	2.04	0.57
1:A:475:ASN:ND2	1:A:475:ASN:C	2.63	0.57
1:A:1002:LEU:C	1:B:1006:PRO:HB3	2.29	0.57
1:B:597:LEU:HG	1:B:620:LEU:HG	1.87	0.57
1:B:760:PRO:HA	1:B:763:LEU:HD23	1.85	0.57
1:B:402:ARG:HG2	1:B:468:LEU:HD13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:GLY:HA3	1:B:363:GLN:NE2	2.20	0.57
1:A:490:ASP:OD1	1:A:491:ARG:HG3	2.04	0.57
1:A:597:LEU:HG	1:A:620:LEU:HG	1.87	0.57
1:A:407:GLN:HG3	1:A:409:TRP:CD1	2.39	0.56
1:A:185:ALA:HB2	1:A:828:GLN:HE22	1.70	0.56
1:A:783:ASN:HD22	1:A:783:ASN:C	2.14	0.56
1:B:449:VAL:HG13	1:B:450:LEU:HD13	1.86	0.56
1:A:74:LYS:HE2	4:A:1462:HOH:O	2.04	0.56
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.86	0.56
1:A:789:CYS:SG	1:A:963:MET:HE1	2.46	0.56
1:B:147:THR:HG22	1:B:149:TYR:CE1	2.41	0.56
1:A:125:ASN:HB3	1:A:821:ASN:ND2	2.20	0.55
1:A:184:ASN:HD21	1:A:223:LYS:HZ1	1.53	0.55
1:A:783:ASN:ND2	1:A:786:HIS:H	2.04	0.55
1:A:196:ASN:ND2	1:A:198:ALA:H	2.03	0.55
1:B:461:PRO:O	1:B:465:GLU:HG3	2.07	0.55
1:B:184:ASN:HD21	1:B:223:LYS:NZ	2.04	0.55
1:A:349:GLU:O	1:A:353:LYS:HG3	2.06	0.55
1:A:684:TYR:OH	1:A:697:LYS:HG2	2.06	0.55
1:B:356:VAL:CG1	1:B:377:VAL:HB	2.36	0.55
1:A:1006:PRO:HB3	1:B:1002:LEU:C	2.31	0.54
1:A:874:ILE:HG22	1:A:937:ILE:HD11	1.90	0.54
1:B:474:GLU:HG2	1:B:475:ASN:ND2	2.23	0.54
1:B:259:LEU:HD12	1:B:259:LEU:C	2.33	0.54
1:B:733:ILE:HD13	1:B:733:ILE:N	2.23	0.54
1:B:673:PHE:CD1	1:B:697:LYS:HE3	2.42	0.54
1:A:460:ARG:NH1	1:A:462:ASP:OD2	2.41	0.54
1:B:392:LEU:O	1:B:396:GLN:HG3	2.08	0.54
1:A:823:LEU:N	1:A:823:LEU:HD12	2.21	0.54
1:A:229:ARG:HB3	1:A:230:PRO:HD3	1.90	0.53
1:A:73:ILE:HG13	1:A:251:SER:HB2	1.90	0.53
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.89	0.53
1:B:709:LEU:N	1:B:710:PRO:HD2	2.23	0.53
1:A:94:ILE:HD11	1:A:244:PHE:HZ	1.71	0.53
1:A:598:GLU:OE2	4:A:1455:HOH:O	2.18	0.53
1:A:622:ASN:HD22	1:A:622:ASN:H	1.54	0.53
1:B:591:ASN:O	1:B:595:LEU:HD22	2.07	0.53
1:A:658:ARG:NH2	4:A:1192:HOH:O	2.41	0.53
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.42	0.52
1:B:180:ASP:O	1:B:183:VAL:HG12	2.10	0.52
1:B:374:ILE:HD12	1:B:376:ASN:ND2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:879:GLU:HB2	4:B:1510:HOH:O	2.08	0.52
1:A:696:THR:OG1	1:A:699:GLU:HG3	2.08	0.52
1:A:331:GLY:HA3	1:A:363:GLN:OE1	2.09	0.52
1:B:602:ASP:OD1	1:B:658:ARG:HD3	2.09	0.52
1:A:821:ASN:HB2	4:A:1063:HOH:O	2.10	0.52
1:A:53:HIS:HB3	4:A:1384:HOH:O	2.09	0.52
1:A:155:HIS:ND1	1:A:261:ARG:HD2	2.25	0.51
1:A:742:MET:O	1:A:746:GLU:HG3	2.09	0.51
1:B:580:SER:HB2	1:B:723:LEU:HD23	1.91	0.51
1:A:1015:MET:CB	4:A:1250:HOH:O	2.58	0.51
1:B:418:ASN:HB3	1:B:454:TYR:O	2.10	0.51
1:B:599:LEU:HD21	1:B:659:PHE:HA	1.92	0.51
1:B:413:GLU:HG2	1:B:531:ILE:HD11	1.93	0.51
1:A:532:PRO:HG3	1:A:634:TYR:CD2	2.46	0.51
1:A:600:LEU:HD11	1:A:648:LYS:HB3	1.91	0.51
1:A:259:LEU:C	1:A:259:LEU:HD23	2.37	0.50
1:A:688:LEU:O	1:A:999:LYS:HE2	2.11	0.50
1:A:810:LEU:HA	1:A:889:LEU:HD12	1.92	0.50
1:A:170:LEU:HD21	1:A:277:GLU:HG3	1.93	0.50
1:B:551:ILE:HD11	1:B:559:LEU:HD13	1.93	0.50
1:A:969:VAL:HG21	1:A:989:PRO:CD	2.42	0.50
1:A:184:ASN:ND2	1:A:223:LYS:NZ	2.58	0.50
1:A:393:HIS:HE1	4:A:1189:HOH:O	1.95	0.50
1:A:815:ILE:CA	1:A:870:MET:HE2	2.34	0.50
1:A:479:ALA:HB2	3:A:1020:DIO:H12	1.93	0.50
1:B:298:LEU:HD13	1:B:475:ASN:HA	1.93	0.50
1:A:285:LEU:HD23	1:A:286:PRO:HD2	1.93	0.49
1:A:799:MET:HE1	1:A:1006:PRO:HG2	1.94	0.49
1:A:908:TRP:CE2	1:A:912:ILE:HD11	2.47	0.49
1:B:600:LEU:CD2	1:B:649:MET:HG2	2.41	0.49
1:B:789:CYS:SG	1:B:963:MET:SD	3.10	0.49
1:A:392:LEU:O	1:A:396:GLN:HG3	2.12	0.49
1:A:692:GLU:HG2	1:A:693:VAL:HG23	1.95	0.49
1:A:67:LEU:HD12	1:A:67:LEU:C	2.37	0.49
1:A:815:ILE:HG22	1:A:870:MET:HE2	1.95	0.49
1:B:229:ARG:O	1:B:233:GLU:HG3	2.13	0.49
1:B:359:LEU:C	1:B:359:LEU:HD23	2.38	0.49
1:B:680:GLN:HE22	2:D:24:PHE:HA	1.76	0.49
1:B:776:TRP:CE3	1:B:989:PRO:HB3	2.47	0.49
1:B:229:ARG:HG3	1:B:229:ARG:HH11	1.77	0.49
1:B:559:LEU:HD21	1:B:729:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:ASN:ND2	1:B:844:GLN:HE22	2.05	0.49
1:A:1006:PRO:HD3	1:B:1003:PRO:HB3	1.95	0.48
1:B:506:PRO:HG2	1:B:509:VAL:CG2	2.43	0.48
1:A:359:LEU:C	1:A:359:LEU:HD23	2.38	0.48
1:A:877:MET:O	1:A:933:LYS:NZ	2.41	0.48
1:A:65:ARG:HB3	1:A:264:LEU:HD22	1.94	0.48
1:A:473:PRO:O	1:A:476:VAL:HG12	2.14	0.48
1:B:969:VAL:HG21	1:B:989:PRO:CD	2.43	0.48
1:A:618:TYR:HA	1:A:630:SER:O	2.13	0.48
1:A:602:ASP:OD1	1:A:658:ARG:HD3	2.13	0.48
1:A:184:ASN:HD21	1:A:223:LYS:HZ2	1.60	0.48
1:A:776:TRP:HA	1:A:953:LYS:O	2.14	0.48
1:B:356:VAL:HG13	1:B:377:VAL:HB	1.96	0.48
1:B:843:ILE:HG22	1:B:844:GLN:N	2.28	0.48
1:A:196:ASN:HD22	1:A:198:ALA:N	2.12	0.47
1:A:689:LEU:CG	1:A:995:MET:HE2	2.39	0.47
1:B:224:TYR:CE2	1:B:229:ARG:HD2	2.48	0.47
1:B:313:LEU:HB2	1:B:379:LEU:HD11	1.96	0.47
1:A:429:ARG:CZ	4:A:1086:HOH:O	2.62	0.47
1:A:933:LYS:O	1:A:937:ILE:HG12	2.15	0.47
1:A:346:LEU:HA	1:A:522:PHE:CE2	2.49	0.47
1:A:607:TYR:CE2	1:A:644:LYS:HG2	2.50	0.47
1:B:638:GLN:HB2	1:B:639:PRO:HD3	1.96	0.47
1:B:196:ASN:ND2	1:B:198:ALA:H	2.13	0.47
1:B:915:GLN:O	1:B:1011:HIS:HB3	2.14	0.47
1:A:798:ASP:CG	1:A:799:MET:H	2.23	0.47
1:A:702:GLU:OE2	1:B:759:LEU:HD11	2.14	0.47
1:B:113:MET:HA	1:B:116:LEU:HD22	1.96	0.47
1:B:616:LEU:HD22	1:B:641:LEU:HD23	1.97	0.47
1:A:475:ASN:C	1:A:475:ASN:HD22	2.22	0.47
1:A:600:LEU:HD23	1:A:620:LEU:HD21	1.96	0.46
1:A:86:SER:HB3	1:A:158:LEU:HG	1.97	0.46
1:B:622:ASN:HD22	1:B:622:ASN:H	1.62	0.46
1:A:538:LEU:HD23	1:A:734:THR:CG2	2.43	0.46
1:A:796:GLN:HB3	1:A:952:HIS:HB2	1.98	0.46
1:A:842:GLY:HA3	1:A:1008:VAL:HG23	1.97	0.46
1:A:1010:PRO:HG2	4:A:1525:HOH:O	2.15	0.46
1:B:684:TYR:CZ	1:B:688:LEU:HD11	2.50	0.46
1:A:196:ASN:HD22	1:A:198:ALA:H	1.62	0.46
1:B:562:LYS:HD3	1:B:730:HIS:CE1	2.50	0.46
1:A:357:ASN:HB2	1:A:378:ASP:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:MET:HA	1:A:792:GLU:OE2	2.16	0.46
1:B:600:LEU:HD21	1:B:649:MET:HG2	1.97	0.46
1:A:934:GLU:CG	1:A:938:LYS:HE3	2.46	0.46
1:A:968:VAL:HG23	1:A:969:VAL:HG23	1.97	0.46
1:B:90:LEU:C	1:B:90:LEU:HD23	2.41	0.46
1:A:1003:PRO:HB3	1:B:1006:PRO:HD3	1.98	0.46
1:B:618:TYR:HA	1:B:630:SER:O	2.16	0.46
1:B:683:MET:HE1	2:D:23:GLY:CA	2.44	0.46
1:B:783:ASN:HD22	1:B:786:HIS:H	1.58	0.46
1:B:874:ILE:HG22	1:B:937:ILE:HD11	1.97	0.46
1:B:934:GLU:HG2	1:B:938:LYS:HE3	1.97	0.46
1:A:245:HIS:O	1:A:249:TYR:HB2	2.16	0.46
1:B:245:HIS:O	1:B:249:TYR:HB2	2.15	0.46
1:A:93:HIS:HE1	1:A:368:ARG:NH2	2.02	0.46
1:A:446:LEU:O	1:A:449:VAL:HG22	2.15	0.46
1:B:259:LEU:C	1:B:259:LEU:CD1	2.89	0.46
1:B:796:GLN:HB3	1:B:952:HIS:HB2	1.97	0.46
1:B:908:TRP:CZ2	1:B:912:ILE:HD11	2.51	0.46
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.51	0.45
1:A:868:ILE:HD12	1:A:984:PRO:HD3	1.99	0.45
1:B:356:VAL:HG11	1:B:377:VAL:HB	1.98	0.45
1:B:957:HIS:HD2	4:B:1503:HOH:O	1.98	0.45
1:B:799:MET:SD	1:B:1006:PRO:HG2	2.56	0.45
1:A:243:LYS:HB2	1:A:243:LYS:NZ	2.31	0.45
1:A:337:LEU:HD23	1:A:401:LEU:HD22	1.99	0.45
1:A:558:LYS:HZ3	1:A:558:LYS:HB2	1.81	0.45
1:A:927:TYR:CE2	1:A:931:LEU:HD11	2.52	0.45
1:B:908:TRP:CE2	1:B:912:ILE:HD11	2.52	0.45
1:A:151:PHE:CD1	1:A:151:PHE:C	2.94	0.45
1:B:187:ASP:OD1	1:B:222:ASN:HB2	2.17	0.45
1:B:805:ASN:HD22	1:B:844:GLN:NE2	2.07	0.45
1:B:815:ILE:C	1:B:818:PRO:HD2	2.42	0.45
1:A:771:LEU:HD21	1:A:954:VAL:CG1	2.46	0.45
1:A:588:LEU:O	1:A:592:MET:HG3	2.17	0.45
1:B:74:LYS:HE2	4:B:1309:HOH:O	2.16	0.45
1:B:126:GLU:HG3	4:B:1370:HOH:O	2.17	0.45
1:B:460:ARG:HD2	1:B:462:ASP:OD2	2.17	0.45
1:B:969:VAL:HG21	1:B:989:PRO:HD3	1.98	0.45
1:A:407:GLN:HG3	1:A:409:TRP:NE1	2.31	0.45
1:A:517:ASP:OD2	1:A:517:ASP:C	2.60	0.45
1:A:823:LEU:N	1:A:823:LEU:CD1	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:GLU:C	1:B:230:PRO:HD2	2.42	0.45
1:A:90:LEU:HD21	1:A:254:MET:HE3	1.98	0.44
1:A:135:ALA:HA	1:A:892:ARG:CZ	2.47	0.44
1:A:429:ARG:NH2	4:A:1086:HOH:O	2.49	0.44
1:A:706:ASP:CG	1:B:722:ARG:HH12	2.25	0.44
2:D:19:CYS:O	2:D:21:GLU:N	2.50	0.44
1:B:437:ILE:HA	1:B:440:ILE:HG12	1.99	0.44
1:A:968:VAL:HG23	1:A:969:VAL:CG2	2.48	0.44
1:B:676:GLU:OE2	1:B:676:GLU:HA	2.17	0.44
1:B:811:PHE:CE1	1:B:815:ILE:HD13	2.52	0.44
1:B:151:PHE:CD1	1:B:151:PHE:C	2.95	0.44
1:B:299:LYS:HD2	1:B:510:ILE:HD12	1.99	0.44
1:A:787:ASN:OD1	1:A:962:GLU:HG2	2.17	0.44
1:A:817:GLU:HB3	4:A:1319:HOH:O	2.16	0.44
1:B:175:ASP:OD2	1:B:177:SER:HB3	2.17	0.44
1:A:559:LEU:HD11	1:A:729:LEU:HG	2.00	0.44
1:B:600:LEU:HD23	1:B:620:LEU:CD2	2.48	0.44
1:B:731:GLY:C	1:B:733:ILE:HD13	2.43	0.44
1:A:306:PRO:HB3	1:A:481:VAL:CG1	2.48	0.43
1:B:692:GLU:HG2	1:B:693:VAL:HG23	2.00	0.43
1:A:170:LEU:CD2	1:A:277:GLU:HG3	2.49	0.43
1:B:189:GLU:O	1:B:192:LYS:HG2	2.17	0.43
1:B:402:ARG:CG	1:B:468:LEU:HD13	2.48	0.43
1:B:506:PRO:HG2	1:B:509:VAL:HG23	2.00	0.43
1:B:100:PRO:HB2	1:B:102:ASN:ND2	2.34	0.43
1:A:90:LEU:HD11	1:A:254:MET:CE	2.48	0.43
1:A:543:GLU:CD	1:A:543:GLU:H	2.27	0.43
1:A:776:TRP:CD2	1:A:989:PRO:HB3	2.53	0.43
1:A:815:ILE:HG22	1:A:870:MET:CE	2.48	0.43
1:A:176:GLU:OE2	1:A:238:ARG:HG3	2.19	0.43
1:A:684:TYR:CZ	1:A:688:LEU:HD11	2.53	0.43
1:A:213:HIS:CE1	1:A:292:PRO:HG3	2.54	0.43
1:A:805:ASN:ND2	1:A:844:GLN:HE22	2.11	0.43
1:A:843:ILE:HG22	1:A:844:GLN:N	2.33	0.43
1:B:309:ASP:O	1:B:668:ARG:HG2	2.19	0.43
1:B:622:ASN:H	1:B:622:ASN:ND2	2.17	0.43
1:B:794:TYR:HB3	1:B:954:VAL:HG13	1.99	0.43
1:A:638:GLN:N	1:A:639:PRO:CD	2.82	0.43
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.53	0.43
1:B:986:LEU:HA	1:B:987:PRO:HD3	1.89	0.43
1:A:359:LEU:HD23	1:A:360:VAL:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ILE:O	1:B:259:LEU:HA	2.18	0.42
1:A:326:TYR:HA	1:A:329:ASN:OD1	2.19	0.42
1:A:629:LEU:HD22	1:A:630:SER:N	2.33	0.42
1:B:722:ARG:HD2	1:B:756:LYS:HB2	2.01	0.42
1:B:843:ILE:HG22	1:B:844:GLN:H	1.84	0.42
1:B:600:LEU:HD23	1:B:620:LEU:HD21	2.01	0.42
1:B:933:LYS:O	1:B:937:ILE:HG12	2.19	0.42
1:A:768:GLU:HB3	1:A:843:ILE:HG13	2.01	0.42
1:B:299:LYS:HD2	1:B:510:ILE:CD1	2.49	0.42
1:A:510:ILE:O	1:A:514:GLN:HG3	2.19	0.42
1:A:53:HIS:ND1	1:A:53:HIS:N	2.62	0.42
1:B:557:SER:HA	1:B:725:ILE:O	2.19	0.42
1:B:729:LEU:HD23	1:B:738:ALA:HA	2.02	0.42
1:A:423:ARG:NE	4:A:1542:HOH:O	2.53	0.42
1:A:860:GLU:OE2	1:A:957:HIS:HE1	2.03	0.42
1:A:968:VAL:C	1:A:969:VAL:CG2	2.93	0.42
1:A:100:PRO:HA	1:A:101:PRO:HD3	1.95	0.42
1:A:733:ILE:HG12	1:A:734:THR:N	2.34	0.42
1:B:306:PRO:HB3	1:B:481:VAL:CG1	2.49	0.42
1:B:810:LEU:HD23	1:B:810:LEU:O	2.20	0.42
1:B:714:ALA:O	1:B:717:PRO:HD2	2.20	0.42
1:A:116:LEU:CD1	1:A:178:CYS:HB3	2.49	0.42
1:B:179:LYS:HD2	1:B:237:VAL:HB	2.02	0.42
1:B:400:LYS:HD3	4:B:1189:HOH:O	2.19	0.42
4:B:1433:HOH:O	2:D:2:VAL:HG13	2.20	0.42
1:A:767:ARG:HH12	1:A:1006:PRO:HA	1.82	0.41
1:A:62:ARG:HD3	1:A:427:LYS:HE3	2.02	0.41
1:A:125:ASN:HD22	1:A:125:ASN:N	2.10	0.41
1:A:153:VAL:HG22	1:A:154:SER:N	2.34	0.41
1:A:94:ILE:HD13	1:A:248:TYR:CG	2.55	0.41
1:B:73:ILE:HG13	1:B:251:SER:HB2	2.03	0.41
1:B:184:ASN:HD21	1:B:223:LYS:HZ1	1.66	0.41
1:A:48:LYS:NZ	4:A:1113:HOH:O	2.52	0.41
1:A:94:ILE:CD1	1:A:244:PHE:CZ	2.91	0.41
1:B:378:ASP:OD2	1:B:378:ASP:C	2.64	0.41
1:A:667:MET:HE2	1:A:704:LEU:HD23	2.02	0.41
1:A:855:PRO:HA	1:A:856:PRO:HD3	1.89	0.41
1:B:204:LEU:O	1:B:208:THR:HB	2.21	0.41
1:B:525:PRO:HG3	4:B:1296:HOH:O	2.20	0.41
1:B:580:SER:HA	1:B:581:PRO:HD3	1.88	0.41
1:A:622:ASN:H	1:A:622:ASN:ND2	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:LEU:HD23	1:B:1000:ARG:HG2	2.03	0.41
1:B:90:LEU:HD23	1:B:91:ASP:N	2.35	0.41
1:B:817:GLU:N	1:B:818:PRO:CD	2.84	0.41
1:A:196:ASN:C	1:A:196:ASN:ND2	2.76	0.41
1:A:578:PHE:O	1:A:626:GLY:HA3	2.21	0.41
1:A:986:LEU:HA	1:A:987:PRO:HD3	1.92	0.41
1:B:291:HIS:ND1	1:B:292:PRO:HD2	2.36	0.41
1:B:607:TYR:CE2	1:B:644:LYS:HG2	2.55	0.41
1:B:196:ASN:HD21	1:B:198:ALA:HB3	1.86	0.41
1:B:855:PRO:HA	1:B:856:PRO:HD3	1.94	0.41
1:A:894:LEU:HG	1:A:925:VAL:HG21	2.03	0.40
1:B:224:TYR:OH	1:B:229:ARG:NH1	2.53	0.40
1:A:460:ARG:NH1	1:A:462:ASP:CG	2.80	0.40
1:B:550:LEU:HD11	1:B:558:LYS:HG2	2.03	0.40
1:A:854:LYS:HB2	1:A:859:LEU:CD1	2.51	0.40
1:A:577:GLU:OE2	1:A:577:GLU:HA	2.22	0.40
1:B:86:SER:HB3	1:B:158:LEU:HG	2.04	0.40
1:B:102:ASN:N	1:B:102:ASN:ND2	2.59	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	960/990 (97%)	928 (97%)	32 (3%)	0	100	100
1	B	960/990 (97%)	931 (97%)	27 (3%)	2 (0%)	43	51
2	C	14/30 (47%)	14 (100%)	0	0	100	100
2	D	15/30 (50%)	12 (80%)	3 (20%)	0	100	100
All	All	1949/2040 (96%)	1885 (97%)	62 (3%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	228	THR
1	B	1012	ILE

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	855/883 (97%)	803 (94%)	52 (6%)	17	20
1	B	854/883 (97%)	803 (94%)	51 (6%)	17	21
2	C	4/26 (15%)	4 (100%)	0	100	100
2	D	4/26 (15%)	3 (75%)	1 (25%)	0	0
All	All	1717/1818 (94%)	1613 (94%)	104 (6%)	17	20

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ILE
1	A	97	LEU
1	A	102	ASN
1	A	107	SER
1	A	125	ASN
1	A	158	LEU
1	A	196	ASN
1	A	201	LEU
1	A	238	ARG
1	A	270	LEU
1	A	285	LEU
1	A	337	LEU
1	A	347	LEU
1	A	356	VAL
1	A	360	VAL
1	A	417	LEU
1	A	449	VAL
1	A	450	LEU
1	A	454	TYR
1	A	475	ASN

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Mol	Chain	Res	Type
1	A	529	GLU
1	A	542	LYS
1	A	543	GLU
1	A	595	LEU
1	A	597	LEU
1	A	616	LEU
1	A	622	ASN
1	A	629	LEU
1	A	642	LEU
1	A	648	LYS
1	A	687	ARG
1	A	728	LEU
1	A	756	LYS
1	A	771	LEU
1	A	783	ASN
1	A	788	ASN
1	A	799	MET
1	A	810	LEU
1	A	817	GLU
1	A	846	LEU
1	A	859	LEU
1	A	860	GLU
1	A	864	GLU
1	A	867	LEU
1	A	880	GLU
1	A	889	LEU
1	A	928	LEU
1	A	954	VAL
1	A	963	MET
1	A	969	VAL
1	A	993	GLN
1	A	1007	LEU
1	B	97	LEU
1	B	102	ASN
1	B	116	LEU
1	B	125	ASN
1	B	126	GLU
1	B	158	LEU
1	B	162	LEU
1	B	173	LEU
1	B	196	ASN
1	B	201	LEU

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Mol	Chain	Res	Type
1	B	204	LEU
1	B	208	THR
1	B	226	LEU
1	B	259	LEU
1	B	337	LEU
1	B	417	LEU
1	B	450	LEU
1	B	455	LEU
1	B	468	LEU
1	B	486	GLU
1	B	488	LYS
1	B	512	LYS
1	B	542	LYS
1	B	559	LEU
1	B	595	LEU
1	B	597	LEU
1	B	604	LEU
1	B	616	LEU
1	B	629	LEU
1	B	657	LYS
1	B	668	ARG
1	B	689	LEU
1	B	700	LEU
1	B	702	GLU
1	B	712	LEU
1	B	719	LEU
1	B	720	LEU
1	B	729	LEU
1	B	733	ILE
1	B	756	LYS
1	B	764	VAL
1	B	765	ARG
1	B	771	LEU
1	B	781	GLN
1	B	788	ASN
1	B	846	LEU
1	B	859	LEU
1	B	896	LYS
1	B	969	VAL
1	B	993	GLN
1	B	1002	LEU
2	D	2	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	93	HIS
1	A	102	ASN
1	A	125	ASN
1	A	184	ASN
1	A	196	ASN
1	A	231	ASN
1	A	239	GLN
1	A	297	HIS
1	A	300	GLN
1	A	376	ASN
1	A	393	HIS
1	A	407	GLN
1	A	412	GLN
1	A	475	ASN
1	A	499	GLN
1	A	502	GLN
1	A	575	ASN
1	A	621	GLN
1	A	622	ASN
1	A	672	ASN
1	A	770	GLN
1	A	783	ASN
1	A	805	ASN
1	A	821	ASN
1	A	828	GLN
1	A	922	ASN
1	A	957	HIS
1	A	993	GLN
1	B	52	ASN
1	B	93	HIS
1	B	102	ASN
1	B	125	ASN
1	B	129	GLN
1	B	157	HIS
1	B	184	ASN
1	B	196	ASN
1	B	232	GLN
1	B	252	ASN
1	B	282	ASN
1	B	294	GLN

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Mol	Chain	Res	Type
1	B	297	HIS
1	B	300	GLN
1	B	332	HIS
1	B	363	GLN
1	B	376	ASN
1	B	399	GLN
1	B	475	ASN
1	B	499	GLN
1	B	502	GLN
1	B	515	ASN
1	B	621	GLN
1	B	622	ASN
1	B	672	ASN
1	B	679	HIS
1	B	680	GLN
1	B	732	ASN
1	B	743	GLN
1	B	770	GLN
1	B	781	GLN
1	B	783	ASN
1	B	805	ASN
1	B	828	GLN
1	B	883	GLN
1	B	957	HIS
1	B	993	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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DIO	A	1020	-	6,6,6	0.78	0	6,6,6	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DIO	A	1020	-	-	-	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1020	DIO	1	0

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	964/990 (97%)	0.13	26 (2%) 56 53	21, 31, 46, 62	0
1	B	964/990 (97%)	0.02	23 (2%) 59 56	17, 28, 44, 59	0
2	C	18/30 (60%)	2.31	10 (55%) 0 0	25, 43, 60, 62	0
2	D	19/30 (63%)	2.43	11 (57%) 0 0	28, 41, 56, 56	0
All	All	1965/2040 (96%)	0.12	70 (3%) 46 43	17, 30, 46, 62	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1012	ILE	8.7
1	A	1016	ALA	6.3
2	C	23	GLY	5.6
2	D	24	PHE	5.5
2	D	20	GLY	5.4
2	D	21	GLU	5.4
1	A	964	ASP	5.3
1	B	44	ASN	4.8
1	A	979	ASN	4.6
1	A	1015	MET	4.5
1	B	1011	HIS	4.4
1	A	1012	ILE	4.4
2	C	24	PHE	4.4
2	D	11	LEU	4.3
2	C	19	CYS	4.3
1	B	979	ASN	4.2
1	A	1014	PHE	4.2
1	B	978	ILE	4.0
2	D	19	CYS	4.0
1	A	45	PRO	3.7
2	D	22	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	22	ARG	3.7
1	A	970	GLY	3.6
1	A	1011	HIS	3.6
1	B	964	ASP	3.5
2	C	25	PHE	3.5
1	A	969	VAL	3.5
1	A	475	ASN	3.5
1	B	763	LEU	3.3
2	C	14	ALA	3.2
2	C	12	VAL	3.1
1	A	963	MET	3.0
1	B	543	GLU	2.9
1	B	759	LEU	2.9
2	C	4	GLN	2.8
1	B	971	GLU	2.8
1	B	764	VAL	2.8
2	C	18	VAL	2.8
1	B	475	ASN	2.7
1	A	706	ASP	2.7
2	D	14	ALA	2.6
1	A	287	GLU	2.6
2	D	23	GLY	2.6
1	A	53	HIS	2.6
1	A	1013	ASN	2.6
1	B	981	SER	2.5
1	A	51	GLY	2.4
1	A	454	TYR	2.4
1	B	706	ASP	2.4
1	A	429	ARG	2.4
1	B	982	GLN	2.4
1	B	1013	ASN	2.3
2	D	18	VAL	2.3
1	B	352	SER	2.3
1	B	544	ALA	2.3
2	D	4	GLN	2.3
1	A	47	ILE	2.3
1	A	452	ALA	2.3
1	A	332	HIS	2.2
2	D	12	VAL	2.2
1	A	126	GLU	2.2
2	C	21	GLU	2.2
1	A	52	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	515	ASN	2.2
1	A	517	ASP	2.1
1	B	295	GLU	2.1
1	B	702	GLU	2.1
1	B	287	GLU	2.0
1	A	67	LEU	2.0
1	B	508	GLU	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
3	DIO	A	1020	6/6	0.91	0.12	36,38,39,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.