



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:20 AM UTC

PDB ID : 7JVH / pdb_00007jvh
Title : Crystal structure of a GH43_12 retrieved from capybara gut metagenome
Authors : Cabral, L.; Domingues, M.N.; Martins, M.P.; Persinoti, G.F.; Morais, M.A.B.;
Murakami, M.T.
Deposited on : 2020-08-21
Resolution : 2.48 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:

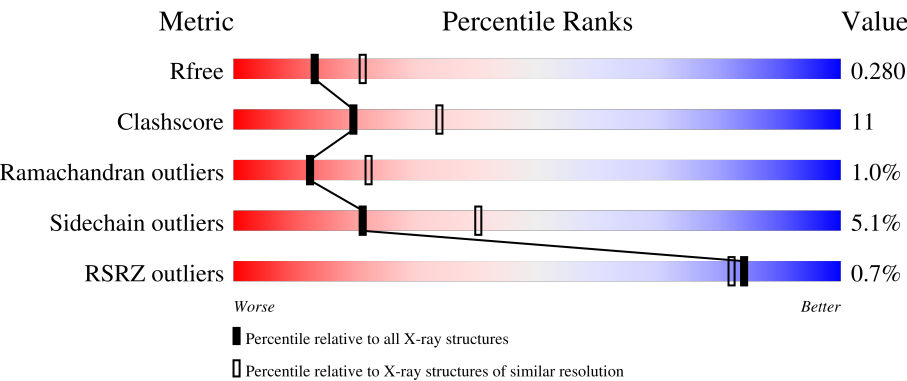
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	567	80%12%• 6%
1	B	567	80%13%• 6%
1	C	567	% 74%17%• 5%
1	D	567	75%15%• 6%
1	E	567	% 62%20%• • 12%

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Mol	Chain	Length	Quality of chain
1	F	567	2% 63% 20% • 12%

2 Entry composition [i](#)

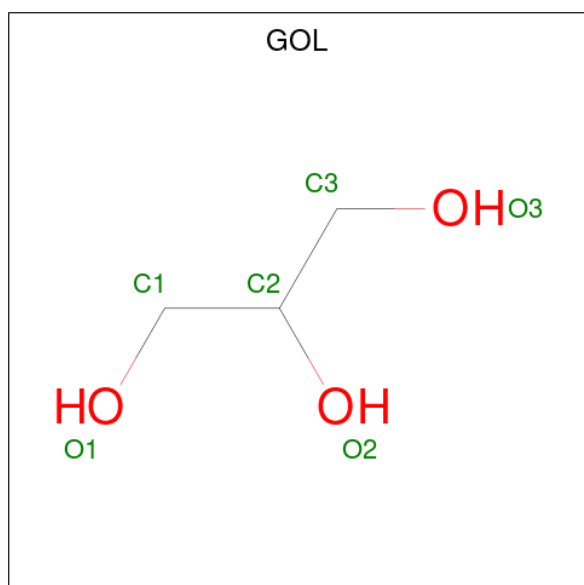
There are 3 unique types of molecules in this entry. The entry contains 25078 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycoside Hydrolase Family 43_12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	Se	0	0	0
			4232	2721	700	793	9	9			
1	B	535	Total	C	N	O	S	Se	0	0	0
			4231	2719	700	794	9	9			
1	C	536	Total	C	N	O	S	Se	0	0	0
			4239	2725	702	794	9	9			
1	D	534	Total	C	N	O	S	Se	0	0	0
			4221	2713	698	792	9	9			
1	E	497	Total	C	N	O	S	Se	0	0	0
			3943	2543	650	733	8	9			
1	F	499	Total	C	N	O	S	Se	0	0	0
			3964	2556	651	740	8	9			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0

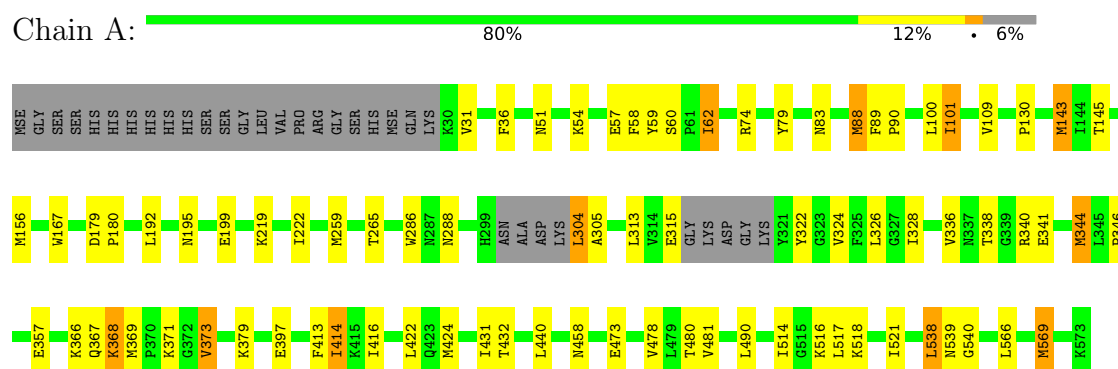
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	64	Total O 64 64	0	0
3	B	52	Total O 52 52	0	0
3	C	32	Total O 32 32	0	0
3	D	31	Total O 31 31	0	0
3	E	4	Total O 4 4	0	0
3	F	5	Total O 5 5	0	0

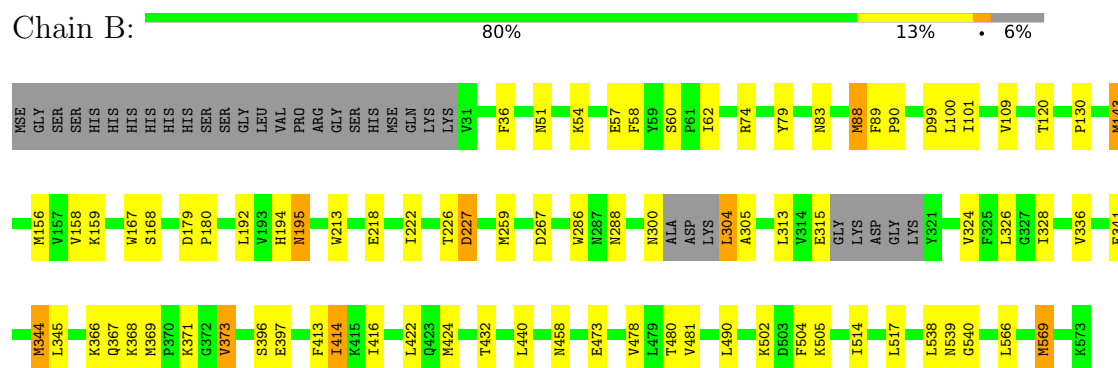
3 Residue-property plots

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.

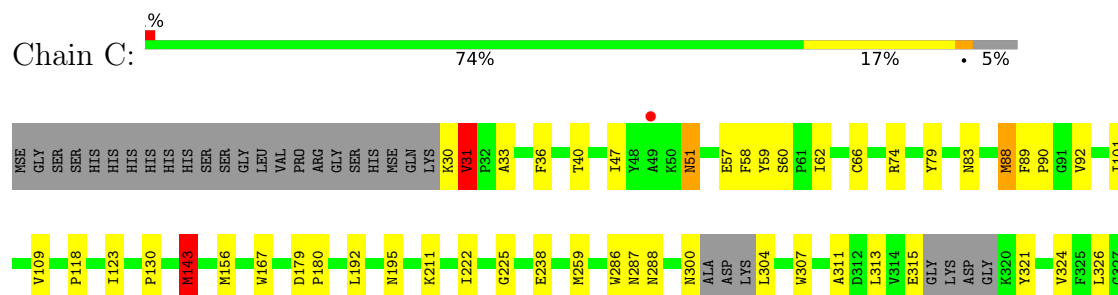
• Molecule 1: Glycoside Hydrolase Family 43_12

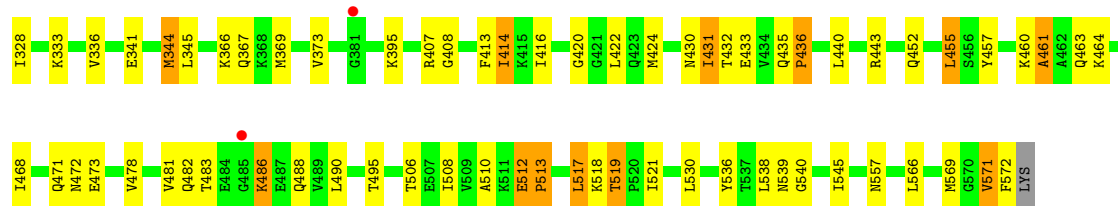


• Molecule 1: Glycoside Hydrolase Family 43_12



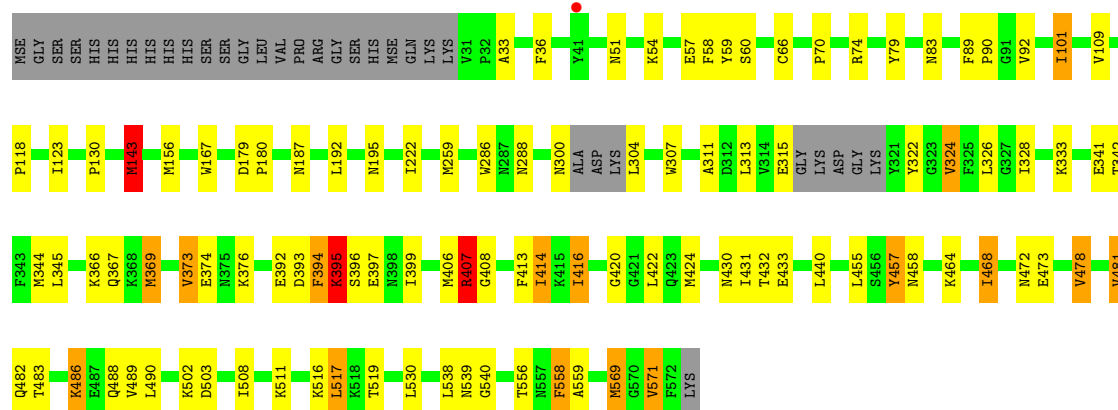
• Molecule 1: Glycoside Hydrolase Family 43_12





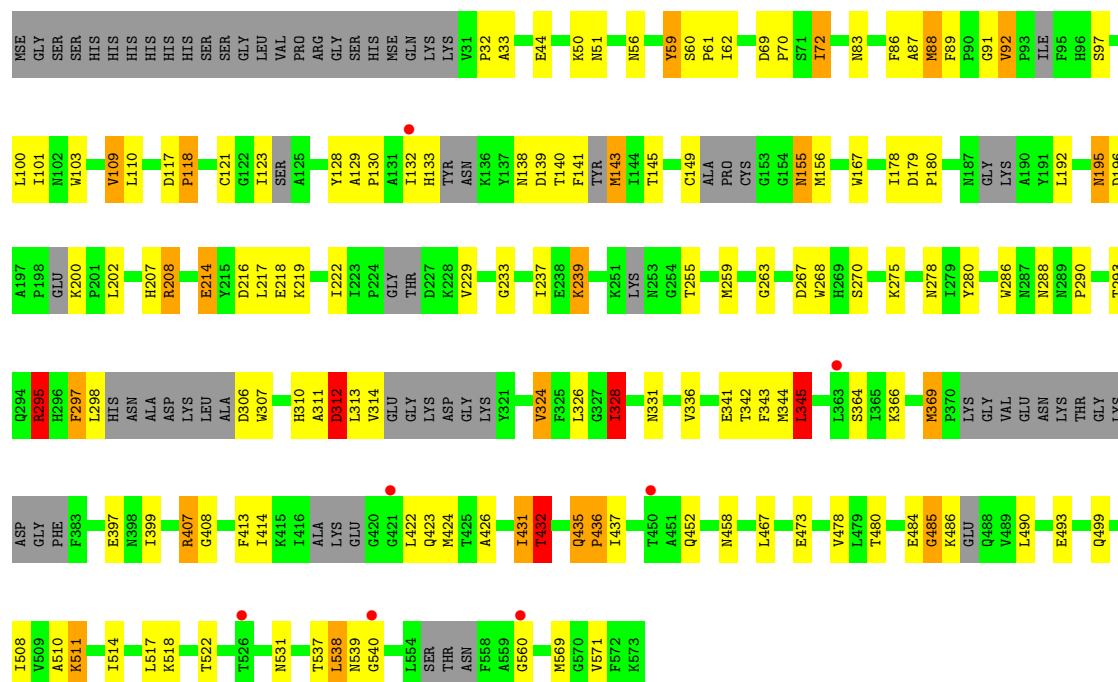
• Molecule 1: Glycoside Hydrolase Family 43_12

Chain D: 75% 15% 6%

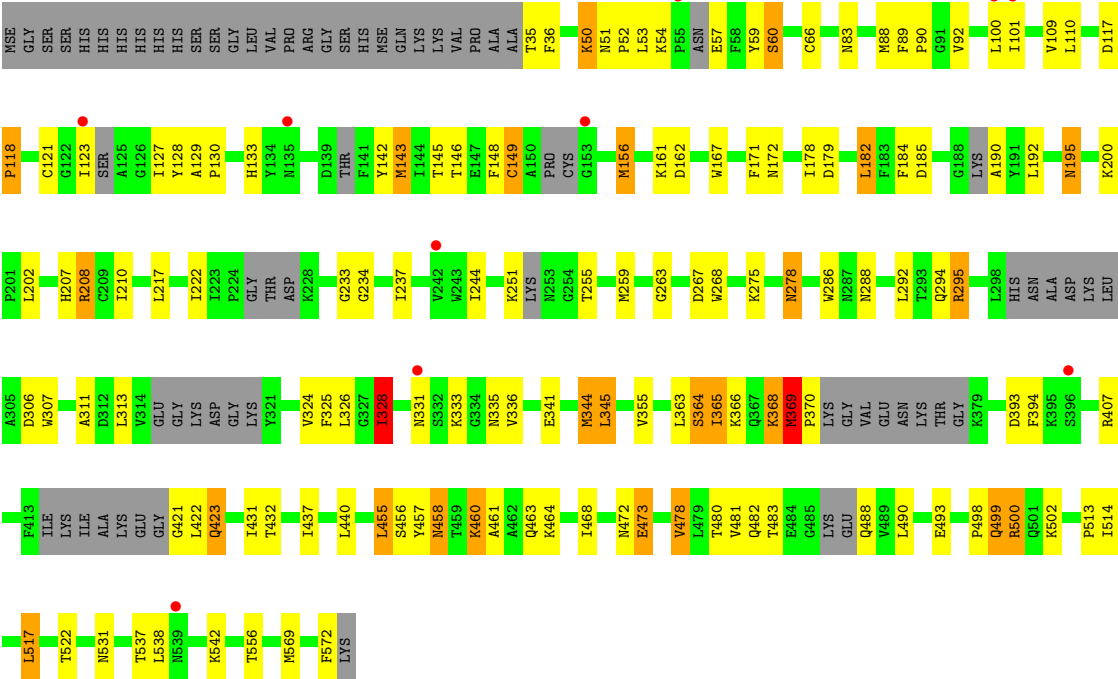


• Molecule 1: Glycoside Hydrolase Family 43_12

Chain E: 62% 20% 12%



• Molecule 1: Glycoside Hydrolase Family 43_12



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	107.22Å 107.38Å 132.53Å 99.03° 113.38° 108.45°	Depositor
Resolution (Å)	49.20 – 2.48 49.20 – 2.48	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.20-2.48) 95.9 (49.20-2.48)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.8	Depositor
R, R_{free}	0.246 , 0.278 0.250 , 0.280	Depositor DCC
R_{free} test set	8303 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.437 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25078	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: GOL

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	0.65	1/4343 (0.0%)	0.87	3/5887 (0.1%)
1	B	0.67	2/4342 (0.0%)	0.91	6/5887 (0.1%)
1	C	0.80	7/4350 (0.2%)	1.10	21/5898 (0.4%)
1	D	0.74	4/4332 (0.1%)	1.07	19/5876 (0.3%)
1	E	0.79	6/4037 (0.1%)	1.12	27/5459 (0.5%)
1	F	0.73	3/4062 (0.1%)	1.10	20/5498 (0.4%)
All	All	0.73	23/25466 (0.1%)	1.03	96/34505 (0.3%)

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	B	0	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	513	PRO	N-CA	18.04	1.69	1.47
1	F	118	PRO	N-CA	17.89	1.70	1.47
1	E	436	PRO	N-CA	17.48	1.69	1.47
1	E	118	PRO	N-CA	15.56	1.67	1.47
1	F	345	LEU	C-N	13.52	1.51	1.33
1	D	408	GLY	C-N	13.51	1.50	1.33
1	C	408	GLY	C-N	13.50	1.50	1.33
1	E	408	GLY	C-N	13.46	1.50	1.33
1	E	345	LEU	C-N	12.68	1.50	1.33
1	C	345	LEU	C-N	12.60	1.50	1.33
1	D	369	MSE	C-N	12.49	1.50	1.33
1	B	345	LEU	C-N	12.36	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	345	LEU	C-N	11.85	1.49	1.33
1	C	512	GLU	C-N	9.79	1.45	1.33
1	E	89	PHE	C-N	8.44	1.50	1.34
1	B	60	SER	C-N	8.14	1.49	1.34
1	E	60	SER	C-N	8.05	1.49	1.34
1	A	60	SER	C-N	7.97	1.49	1.34
1	F	60	SER	C-N	7.92	1.49	1.34
1	C	60	SER	C-N	7.70	1.48	1.34
1	D	60	SER	C-N	7.60	1.48	1.34
1	C	31	VAL	C-N	7.58	1.51	1.33
1	C	51	ASN	N-CA	5.12	1.50	1.46

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	512	GLU	CA-C-N	17.45	138.22	119.90
1	C	512	GLU	C-N-CA	17.45	138.22	119.90
1	F	161	LYS	N-CA-C	-14.87	84.49	108.73
1	F	117	ASP	CA-C-N	14.59	138.07	119.84
1	F	117	ASP	C-N-CA	14.59	138.07	119.84
1	E	431	ILE	N-CA-C	-14.45	87.78	108.58
1	E	435	GLN	CA-C-N	14.25	137.65	119.84
1	E	435	GLN	C-N-CA	14.25	137.65	119.84
1	E	117	ASP	CA-C-N	14.15	137.52	119.84
1	E	117	ASP	C-N-CA	14.15	137.52	119.84
1	F	345	LEU	CA-C-N	14.01	134.00	119.85
1	F	345	LEU	C-N-CA	14.01	134.00	119.85
1	E	408	GLY	CA-C-N	13.92	135.03	119.99
1	E	408	GLY	C-N-CA	13.92	135.03	119.99
1	D	457	TYR	N-CA-C	13.29	129.28	113.20
1	C	408	GLY	CA-C-N	13.27	134.32	119.99
1	C	408	GLY	C-N-CA	13.27	134.32	119.99
1	D	408	GLY	CA-C-N	13.10	134.14	119.99
1	D	408	GLY	C-N-CA	13.10	134.14	119.99
1	F	355	VAL	N-CA-C	12.91	122.49	110.74
1	E	345	LEU	CA-C-N	12.73	132.89	119.78
1	E	345	LEU	C-N-CA	12.73	132.89	119.78
1	C	345	LEU	CA-C-N	12.01	131.77	119.76
1	C	345	LEU	C-N-CA	12.01	131.77	119.76
1	D	345	LEU	CA-C-N	11.87	132.00	119.78
1	D	345	LEU	C-N-CA	11.87	132.00	119.78
1	D	369	MSE	CA-C-N	11.54	131.66	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	MSE	C-N-CA	11.54	131.66	119.78
1	B	345	LEU	CA-C-N	11.43	131.55	119.78
1	B	345	LEU	C-N-CA	11.43	131.55	119.78
1	C	31	VAL	CA-C-N	11.29	133.95	119.84
1	C	31	VAL	C-N-CA	11.29	133.95	119.84
1	F	364	SER	N-CA-C	11.01	128.46	112.94
1	E	328	ILE	N-CA-C	9.46	120.07	112.12
1	F	171	PHE	N-CA-C	9.41	124.76	113.28
1	C	345	LEU	O-C-N	-9.09	115.42	121.88
1	F	328	ILE	N-CA-C	8.64	119.38	112.12
1	C	143	MSE	CG-SE-CE	8.17	116.89	98.92
1	E	510	ALA	N-CA-C	8.12	128.10	110.80
1	B	345	LEU	O-C-N	-8.08	116.19	121.85
1	D	345	LEU	O-C-N	-8.02	116.23	121.85
1	D	143	MSE	CG-SE-CE	8.01	116.53	98.92
1	A	344	MSE	CG-SE-CE	7.88	116.27	98.92
1	E	436	PRO	CA-N-CD	-7.87	100.98	112.00
1	E	118	PRO	CA-N-CD	-7.81	101.07	112.00
1	E	432	THR	N-CA-CB	7.71	123.53	110.49
1	C	513	PRO	CA-N-CD	-7.49	101.51	112.00
1	E	118	PRO	CA-C-O	-7.22	107.47	120.60
1	F	118	PRO	CA-N-CD	-7.18	101.94	112.00
1	C	513	PRO	N-CA-C	-7.18	99.96	110.80
1	B	344	MSE	CG-SE-CE	7.11	114.57	98.92
1	F	369	MSE	CG-SE-CE	7.09	114.51	98.92
1	E	88	MSE	CG-SE-CE	7.00	114.32	98.92
1	B	88	MSE	CG-SE-CE	6.74	113.76	98.92
1	D	558	PHE	CA-C-N	6.55	134.05	121.54
1	D	558	PHE	C-N-CA	6.55	134.05	121.54
1	D	392	GLU	N-CA-C	6.49	123.15	110.56
1	E	208	ARG	CB-CG-CD	-6.41	96.55	111.30
1	D	394	PHE	CB-CA-C	6.16	121.01	110.79
1	E	263	GLY	N-CA-C	-6.08	103.23	112.84
1	F	278	ASN	CB-CA-C	6.05	122.83	109.94
1	F	263	GLY	N-CA-C	-5.99	103.38	112.84
1	A	88	MSE	CG-SE-CE	5.98	112.09	98.92
1	C	344	MSE	CG-SE-CE	5.93	111.97	98.92
1	F	208	ARG	CG-CD-NE	5.85	124.88	112.00
1	E	312	ASP	CB-CA-C	5.85	121.27	109.68
1	C	51	ASN	CA-CB-CG	5.82	118.42	112.60
1	C	30	LYS	CA-C-N	5.73	132.73	122.13
1	C	30	LYS	C-N-CA	5.73	132.73	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	471	GLN	N-CA-C	-5.66	103.98	111.96
1	F	59	TYR	CA-C-N	5.63	132.00	122.65
1	F	59	TYR	C-N-CA	5.63	132.00	122.65
1	D	406	MSE	CG-SE-CE	5.63	111.31	98.92
1	E	297	PHE	N-CA-C	5.62	122.76	110.80
1	E	435	GLN	O-C-N	-5.61	118.12	121.71
1	D	187	ASN	N-CA-C	-5.60	101.11	109.96
1	C	59	TYR	CA-C-N	5.53	129.97	122.56
1	C	59	TYR	C-N-CA	5.53	129.97	122.56
1	F	59	TYR	O-C-N	5.47	129.51	123.16
1	F	88	MSE	CG-SE-CE	5.45	110.91	98.92
1	F	295	ARG	CG-CD-NE	5.38	123.83	112.00
1	C	88	MSE	CG-SE-CE	5.37	110.74	98.92
1	E	431	ILE	N-CA-CB	5.34	116.54	110.72
1	E	59	TYR	CA-C-N	5.33	131.50	122.65
1	E	59	TYR	C-N-CA	5.33	131.50	122.65
1	A	59	TYR	O-C-N	5.30	129.31	123.16
1	E	59	TYR	O-C-N	5.29	129.29	123.16
1	D	369	MSE	CG-SE-CE	5.24	110.45	98.92
1	C	436	PRO	CB-CA-C	-5.24	104.25	111.21
1	D	59	TYR	CA-C-N	5.21	129.55	122.56
1	D	59	TYR	C-N-CA	5.21	129.55	122.56
1	E	295	ARG	CB-CG-CD	5.14	123.13	111.30
1	B	267	ASP	N-CA-C	5.11	118.28	111.75
1	D	558	PHE	CA-C-O	-5.08	114.17	120.57
1	F	267	ASP	N-CA-C	5.04	118.21	111.75
1	E	267	ASP	N-CA-C	5.02	118.18	111.75

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	226	THR	Mainchain
1	B	227	ASP	Mainchain

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	4232	0	4103	54	0
1	B	4231	0	4096	57	0
1	C	4239	0	4109	97	0
1	D	4221	0	4083	87	0
1	E	3943	0	3807	135	0
1	F	3964	0	3804	140	0
2	A	18	0	24	1	0
2	B	12	0	16	0	0
2	C	12	0	16	3	0
2	D	12	0	16	0	0
2	F	6	0	8	0	0
3	A	64	0	0	0	0
3	B	52	0	0	0	0
3	C	32	0	0	0	0
3	D	31	0	0	0	0
3	E	4	0	0	0	0
3	F	5	0	0	0	0
All	All	25078	0	24082	562	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 11.

All (562) 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:436:PRO:N	1:E:436:PRO:CA	1.69	1.42
1:C:513:PRO:N	1:C:513:PRO:CA	1.69	1.38
1:F:118:PRO:N	1:F:118:PRO:CA	1.70	1.34
1:F:36:PHE:CE1	1:F:455:LEU:HD13	1.69	1.25
1:E:118:PRO:HB2	1:E:407:ARG:HA	1.15	1.11
1:F:423:GLN:O	1:F:423:GLN:HG2	1.57	1.03
1:B:397:GLU:HA	1:B:416:ILE:HD12	1.42	1.00
1:A:100:LEU:HB3	1:A:344:MSE:HE1	1.44	0.99
1:D:118:PRO:O	1:D:407:ARG:HB3	1.63	0.98
1:F:36:PHE:CE1	1:F:455:LEU:CD1	2.48	0.97
1:C:130:PRO:HB3	1:C:143:MSE:HE2	1.48	0.96
1:C:490:LEU:HD23	1:C:512:GLU:O	1.64	0.96
1:E:128:TYR:CE2	1:E:178:ILE:HD12	2.00	0.96
1:F:128:TYR:CE2	1:F:178:ILE:HD12	2.00	0.96
1:F:36:PHE:HE1	1:F:455:LEU:HD13	1.27	0.96
1:D:130:PRO:HB3	1:D:143:MSE:HE2	1.48	0.95
1:E:306:ASP:O	1:E:328:ILE:HG22	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:ILE:HG13	1:E:369:MSE:HE3	1.52	0.90
1:E:214:GLU:HG3	1:E:280:TYR:OH	1.72	0.89
1:B:100:LEU:HB3	1:B:344:MSE:HE1	1.53	0.89
1:F:182:LEU:HD13	1:F:184:PHE:CE2	2.07	0.89
1:D:92:VAL:HG21	1:D:143:MSE:HE3	1.56	0.88
1:D:424:MSE:HG3	1:D:571:VAL:HG21	1.54	0.88
1:D:424:MSE:HG3	1:D:571:VAL:CG2	2.03	0.88
1:C:490:LEU:HD21	1:C:512:GLU:HB2	1.55	0.87
1:A:265:THR:HG21	1:A:340:ARG:HH11	1.36	0.87
1:E:118:PRO:O	1:E:407:ARG:HB3	1.75	0.87
1:F:92:VAL:HB	1:F:109:VAL:HG12	1.55	0.87
1:C:92:VAL:HG21	1:C:143:MSE:HE3	1.57	0.87
1:E:426:ALA:HB2	1:E:571:VAL:HG22	1.57	0.85
1:E:431:ILE:O	1:E:432:THR:HG23	1.75	0.85
1:F:100:LEU:HB3	1:F:344:MSE:HE1	1.57	0.83
1:F:331:ASN:HD21	1:F:335:ASN:HB2	1.42	0.82
1:F:182:LEU:HD13	1:F:184:PHE:CZ	2.14	0.82
1:F:364:SER:O	1:F:365:ILE:HG22	1.80	0.82
1:B:88:MSE:HE2	1:B:566:LEU:HD21	1.62	0.81
1:C:464:LYS:HG2	1:C:482:GLN:HG2	1.62	0.81
1:A:88:MSE:HE2	1:A:566:LEU:HD21	1.64	0.80
1:E:306:ASP:O	1:E:328:ILE:CG2	2.29	0.80
1:E:92:VAL:HG22	1:E:109:VAL:CG1	2.13	0.79
1:E:100:LEU:HB3	1:E:344:MSE:HE1	1.64	0.79
1:D:457:TYR:OH	1:D:483:THR:HG23	1.83	0.79
1:D:464:LYS:HE2	1:D:482:GLN:CD	2.08	0.79
1:E:195:ASN:HD21	1:E:208:ARG:HD2	1.47	0.78
1:C:483:THR:HG22	1:C:488:GLN:HE21	1.46	0.78
1:F:101:ILE:HG13	1:F:369:MSE:HG2	1.66	0.78
1:F:498:PRO:HB2	1:F:500:ARG:HE	1.48	0.77
1:E:33:ALA:HB3	1:E:571:VAL:HG21	1.67	0.77
1:E:259:MSE:HE1	1:E:313:LEU:HD11	1.66	0.77
1:F:259:MSE:HE1	1:F:313:LEU:HD11	1.66	0.77
1:E:306:ASP:C	1:E:328:ILE:CG2	2.57	0.77
1:F:307:TRP:H	1:F:328:ILE:CG2	1.98	0.77
1:E:87:ALA:HB2	1:E:121:CYS:SG	2.25	0.76
1:B:259:MSE:HE1	1:B:313:LEU:HD11	1.67	0.76
1:D:130:PRO:CB	1:D:143:MSE:HE2	2.15	0.76
1:C:130:PRO:CB	1:C:143:MSE:HE2	2.16	0.76
1:E:92:VAL:CG1	1:E:109:VAL:HG13	2.16	0.75
1:D:430:ASN:OD1	1:D:433:GLU:HG3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:MSE:HE1	1:D:313:LEU:HD11	1.70	0.74
1:C:413:PHE:CD1	1:C:414:ILE:HD12	2.23	0.73
1:D:413:PHE:CD1	1:D:414:ILE:HD12	2.23	0.73
1:E:311:ALA:HA	1:E:324:VAL:O	1.88	0.73
1:F:146:THR:HG21	1:F:148:PHE:CE2	2.23	0.73
1:E:484:GLU:OE2	1:E:511:LYS:NZ	2.21	0.73
1:E:293:THR:OG1	1:E:295:ARG:HD2	1.88	0.73
1:A:259:MSE:HE1	1:A:313:LEU:HD11	1.70	0.72
1:E:51:ASN:O	1:E:366:LYS:NZ	2.22	0.72
1:C:259:MSE:HE1	1:C:313:LEU:HD11	1.70	0.72
1:D:457:TYR:CG	1:D:457:TYR:O	2.43	0.72
1:C:513:PRO:N	1:C:513:PRO:C	2.47	0.71
1:E:92:VAL:HG22	1:E:109:VAL:HG12	1.70	0.71
1:C:424:MSE:HG3	1:C:571:VAL:CG2	2.21	0.71
1:F:51:ASN:O	1:F:366:LYS:CE	2.39	0.70
1:E:92:VAL:CG2	1:E:109:VAL:CG1	2.69	0.70
1:F:423:GLN:O	1:F:423:GLN:CG	2.39	0.70
1:E:155:ASN:OD1	1:E:155:ASN:N	2.24	0.70
1:F:483:THR:HG23	1:F:488:GLN:HE21	1.56	0.70
1:D:538:LEU:O	1:D:540:GLY:N	2.25	0.70
1:C:486:LYS:HG2	1:C:486:LYS:O	1.90	0.70
1:E:522:THR:OG1	1:E:537:THR:HB	1.91	0.69
1:F:407:ARG:HH12	1:F:473:GLU:HG3	1.57	0.69
1:E:69:ASP:HA	1:E:310:HIS:ND1	2.07	0.69
1:C:538:LEU:O	1:C:540:GLY:N	2.25	0.69
1:E:538:LEU:O	1:E:540:GLY:N	2.25	0.69
1:B:538:LEU:O	1:B:540:GLY:N	2.26	0.69
1:E:128:TYR:CE2	1:E:179:ASP:OD1	2.45	0.69
1:E:133:HIS:NE2	1:E:312:ASP:OD2	2.26	0.69
1:F:128:TYR:CE2	1:F:179:ASP:OD1	2.45	0.69
1:E:33:ALA:CB	1:E:571:VAL:HG21	2.22	0.69
1:F:92:VAL:HB	1:F:109:VAL:CG1	2.22	0.69
1:D:369:MSE:HE2	1:D:373:VAL:HB	1.75	0.68
1:A:538:LEU:O	1:A:540:GLY:N	2.26	0.68
1:C:455:LEU:HD23	1:C:455:LEU:O	1.94	0.67
1:E:118:PRO:HB2	1:E:407:ARG:CA	2.09	0.67
1:F:118:PRO:HB2	1:F:407:ARG:HA	1.77	0.67
1:C:130:PRO:HB3	1:C:143:MSE:CE	2.24	0.67
1:E:436:PRO:N	1:E:436:PRO:C	2.52	0.67
1:C:92:VAL:HG11	1:C:143:MSE:HE3	1.77	0.67
1:E:72:ILE:HD13	1:E:314:VAL:HG11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:PRO:O	1:F:366:LYS:NZ	2.27	0.67
1:B:369:MSE:HE2	1:B:373:VAL:HB	1.77	0.66
1:F:109:VAL:HG23	1:F:167:TRP:CD1	2.30	0.66
1:A:101:ILE:HG21	1:A:369:MSE:HE3	1.77	0.66
1:F:51:ASN:O	1:F:366:LYS:HE2	1.95	0.66
1:E:490:LEU:CD2	1:E:514:ILE:HD13	2.26	0.66
1:E:200:LYS:O	1:E:202:LEU:HD12	1.96	0.65
1:F:200:LYS:O	1:F:202:LEU:HD12	1.96	0.65
1:E:130:PRO:HB2	1:E:143:MSE:HE3	1.79	0.65
1:F:331:ASN:ND2	1:F:335:ASN:HB2	2.10	0.65
1:D:92:VAL:HG11	1:D:143:MSE:HE3	1.79	0.65
1:F:101:ILE:HG13	1:F:369:MSE:CG	2.26	0.65
1:F:311:ALA:HA	1:F:324:VAL:O	1.97	0.65
1:B:130:PRO:HB2	1:B:143:MSE:HE3	1.79	0.65
1:C:468:ILE:HD12	1:C:478:VAL:HG22	1.78	0.65
1:F:130:PRO:HB2	1:F:143:MSE:HE3	1.79	0.65
1:F:513:PRO:O	1:F:514:ILE:HD13	1.97	0.65
1:E:118:PRO:CB	1:E:407:ARG:HA	2.09	0.64
1:F:294:GLN:HB2	1:F:306:ASP:O	1.97	0.64
1:D:130:PRO:HB3	1:D:143:MSE:CE	2.25	0.64
1:D:424:MSE:HG3	1:D:571:VAL:HG22	1.80	0.64
1:D:517:LEU:HD13	1:D:519:THR:O	1.97	0.64
1:E:56:ASN:O	1:E:369:MSE:HG3	1.98	0.64
1:C:435:GLN:HB3	1:C:436:PRO:HD2	1.79	0.64
1:F:464:LYS:HG2	1:F:482:GLN:HG2	1.80	0.63
1:E:33:ALA:HB3	1:E:571:VAL:CG2	2.28	0.63
1:E:202:LEU:HD13	1:E:207:HIS:CE1	2.34	0.63
1:F:123:ILE:HG12	1:F:472:ASN:HB3	1.80	0.63
1:F:202:LEU:HD13	1:F:207:HIS:CE1	2.34	0.63
1:F:522:THR:HB	1:F:537:THR:OG1	1.98	0.63
1:E:33:ALA:CB	1:E:571:VAL:CG2	2.76	0.63
1:E:216:ASP:OD1	1:E:218:GLU:CG	2.47	0.63
1:F:234:GLY:HA2	1:F:244:ILE:HG21	1.79	0.63
1:F:490:LEU:HD23	1:F:514:ILE:HG13	1.81	0.63
1:C:430:ASN:OD1	1:C:433:GLU:HG3	1.99	0.63
1:A:130:PRO:HB2	1:A:143:MSE:HE3	1.79	0.62
1:F:35:THR:CG2	1:F:456:SER:HB2	2.29	0.62
1:F:51:ASN:HB3	1:F:366:LYS:HE3	1.80	0.62
1:C:490:LEU:HD11	1:C:536:TYR:CD1	2.34	0.62
1:B:396:SER:O	1:B:416:ILE:CD1	2.47	0.62
1:F:483:THR:HG23	1:F:488:GLN:NE2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:MSE:HG3	1:C:571:VAL:HG21	1.81	0.62
1:D:118:PRO:HG2	1:D:407:ARG:HA	1.82	0.62
1:E:32:PRO:CD	1:F:460:LYS:HD3	2.30	0.62
1:B:120:THR:HB	2:C:602:GOL:O2	1.99	0.61
1:E:202:LEU:HD13	1:E:207:HIS:HE1	1.65	0.61
1:E:522:THR:HG1	1:E:537:THR:HB	1.64	0.61
1:F:202:LEU:HD13	1:F:207:HIS:HE1	1.65	0.61
1:E:297:PHE:O	1:E:298:LEU:HB3	2.01	0.61
1:C:461:ALA:HB1	1:C:463:GLN:HG3	1.83	0.60
1:F:57:GLU:HA	1:F:368:LYS:HA	1.83	0.60
1:C:455:LEU:CD2	1:C:521:ILE:CG2	2.78	0.60
1:C:92:VAL:CG2	1:C:143:MSE:HE3	2.31	0.60
1:D:92:VAL:CG2	1:D:143:MSE:HE3	2.30	0.60
1:D:517:LEU:CD1	1:D:519:THR:O	2.48	0.60
1:C:490:LEU:CD2	1:C:512:GLU:HB2	2.31	0.60
1:E:69:ASP:HB3	1:E:310:HIS:CE1	2.37	0.60
1:F:35:THR:HG22	1:F:456:SER:HB2	1.82	0.60
1:C:315:GLU:HB2	1:C:321:TYR:CE2	2.37	0.60
1:B:62:ILE:HD13	1:B:344:MSE:HB2	1.84	0.60
1:C:518:LYS:HG2	1:C:518:LYS:O	2.02	0.60
1:D:413:PHE:CE1	1:D:414:ILE:HD12	2.36	0.60
1:F:36:PHE:CD1	1:F:455:LEU:CB	2.84	0.60
1:F:130:PRO:CB	1:F:143:MSE:HE3	2.32	0.59
1:E:216:ASP:OD1	1:E:218:GLU:HG3	2.01	0.59
1:A:369:MSE:HE2	1:A:373:VAL:HB	1.84	0.59
1:E:490:LEU:HD23	1:E:514:ILE:HG21	1.83	0.59
1:B:158:VAL:CG1	1:B:168:SER:O	2.51	0.59
1:E:239:LYS:O	1:E:239:LYS:HG2	2.01	0.59
1:A:109:VAL:HG13	1:A:167:TRP:CD1	2.38	0.59
1:A:357:GLU:HG2	1:C:288:ASN:HB2	1.85	0.59
1:E:270:SER:OG	1:E:290:PRO:CB	2.51	0.59
1:E:92:VAL:HG11	1:E:110:LEU:HG	1.84	0.59
1:B:130:PRO:CB	1:B:143:MSE:HE3	2.33	0.58
1:F:133:HIS:CG	1:F:182:LEU:HD11	2.37	0.58
1:C:413:PHE:CE1	1:C:414:ILE:HD12	2.37	0.58
1:E:92:VAL:HG13	1:E:109:VAL:HG13	1.84	0.58
1:C:495:THR:HG22	1:C:506:THR:HA	1.86	0.58
1:F:133:HIS:HB2	1:F:182:LEU:HD11	1.86	0.58
1:F:146:THR:CG2	1:F:148:PHE:CE2	2.86	0.58
1:E:138:ASN:O	1:E:139:ASP:OD1	2.21	0.58
1:B:101:ILE:HG21	1:B:369:MSE:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:VAL:O	1:C:31:VAL:HG13	2.04	0.58
1:D:109:VAL:HG13	1:D:167:TRP:CD1	2.39	0.57
1:F:133:HIS:CG	1:F:182:LEU:CD1	2.86	0.57
1:C:455:LEU:CD2	1:C:521:ILE:HG22	2.34	0.57
1:E:59:TYR:CE1	1:E:366:LYS:NZ	2.72	0.57
1:C:109:VAL:HG13	1:C:167:TRP:CD1	2.39	0.57
1:B:304:LEU:HD13	1:B:305:ALA:HB2	1.85	0.57
1:E:130:PRO:CB	1:E:143:MSE:HE3	2.34	0.57
1:A:130:PRO:CB	1:A:143:MSE:HE3	2.33	0.57
1:D:457:TYR:O	1:D:457:TYR:CD1	2.57	0.57
1:F:195:ASN:OD1	1:F:208:ARG:NH1	2.37	0.57
1:F:328:ILE:HG13	1:F:336:VAL:HG21	1.86	0.57
1:A:54:LYS:NZ	1:C:238:GLU:OE2	2.34	0.57
1:F:328:ILE:CD1	1:F:336:VAL:HG21	2.34	0.57
1:A:88:MSE:CE	1:A:566:LEU:HD21	2.35	0.56
1:D:468:ILE:HG12	1:D:478:VAL:HG13	1.87	0.56
1:B:158:VAL:HG12	1:B:167:TRP:HB3	1.87	0.56
1:B:109:VAL:HG13	1:B:167:TRP:CD1	2.39	0.56
1:D:70:PRO:HB3	1:D:342:THR:HG23	1.87	0.56
1:F:514:ILE:O	1:F:514:ILE:HG22	2.04	0.56
1:F:133:HIS:CB	1:F:182:LEU:HD11	2.35	0.56
1:B:158:VAL:HG13	1:B:168:SER:O	2.05	0.56
1:D:101:ILE:HD12	1:D:369:MSE:HG2	1.88	0.56
1:E:432:THR:HA	1:E:473:GLU:O	2.06	0.56
1:C:36:PHE:CE1	1:C:455:LEU:HD12	2.41	0.56
1:C:424:MSE:HG3	1:C:571:VAL:HG22	1.88	0.56
1:F:36:PHE:CD1	1:F:455:LEU:HB3	2.41	0.56
1:F:109:VAL:HG23	1:F:167:TRP:CG	2.39	0.55
1:F:92:VAL:CB	1:F:109:VAL:HG12	2.31	0.55
1:C:62:ILE:HD13	1:C:344:MSE:HE3	1.88	0.55
1:C:483:THR:HG22	1:C:488:GLN:NE2	2.20	0.55
1:E:328:ILE:CD1	1:E:336:VAL:HG21	2.37	0.55
1:F:365:ILE:HG23	1:F:366:LYS:HG2	1.89	0.55
1:E:91:GLY:C	1:E:92:VAL:HG12	2.31	0.55
1:E:32:PRO:HD3	1:F:460:LYS:HD3	1.88	0.54
1:A:54:LYS:HB2	1:A:57:GLU:OE1	2.07	0.54
1:E:214:GLU:N	1:E:214:GLU:OE1	2.39	0.54
1:A:304:LEU:HD13	1:A:305:ALA:HB2	1.88	0.54
1:E:397:GLU:O	1:E:399:ILE:HD12	2.07	0.54
1:C:333:LYS:HE2	1:C:530:LEU:HD12	1.89	0.54
1:C:490:LEU:HD11	1:C:536:TYR:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:PHE:CE1	1:A:367:GLN:HB2	2.42	0.54
1:E:423:GLN:CD	1:F:460:LYS:HB3	2.33	0.54
1:F:307:TRP:H	1:F:328:ILE:HG22	1.72	0.54
1:B:88:MSE:CE	1:B:566:LEU:HD21	2.35	0.54
1:D:464:LYS:HE2	1:D:482:GLN:OE1	2.08	0.54
1:F:268:TRP:CD2	1:F:295:ARG:HD3	2.42	0.54
1:A:432:THR:HA	1:A:473:GLU:O	2.08	0.54
1:B:54:LYS:HB2	1:B:57:GLU:OE1	2.08	0.54
1:D:101:ILE:HG21	1:D:369:MSE:HE3	1.89	0.54
1:A:62:ILE:HD13	1:A:344:MSE:HB2	1.90	0.54
1:D:54:LYS:HB2	1:D:57:GLU:OE1	2.08	0.54
1:C:517:LEU:HD12	1:C:519:THR:HG23	1.90	0.53
1:F:457:TYR:OH	1:F:483:THR:OG1	2.25	0.53
1:D:311:ALA:HA	1:D:324:VAL:O	2.09	0.53
1:E:32:PRO:HD2	1:F:460:LYS:HD3	1.90	0.53
1:B:432:THR:HA	1:B:473:GLU:O	2.09	0.53
1:C:455:LEU:HD22	1:C:521:ILE:HG23	1.90	0.53
1:E:478:VAL:HG22	1:E:480:THR:HG23	1.89	0.53
1:D:558:PHE:O	1:D:558:PHE:HD1	1.92	0.53
1:F:407:ARG:HH12	1:F:473:GLU:CG	2.20	0.53
1:A:259:MSE:CE	1:A:313:LEU:HD11	2.39	0.53
1:C:457:TYR:C	1:C:457:TYR:CD1	2.85	0.53
1:D:92:VAL:HG21	1:D:143:MSE:CE	2.36	0.53
1:D:414:ILE:HG12	1:D:422:LEU:HD22	1.90	0.53
1:C:414:ILE:HG12	1:C:422:LEU:HD22	1.91	0.53
1:E:91:GLY:O	1:E:92:VAL:CG1	2.57	0.52
1:F:432:THR:HA	1:F:473:GLU:O	2.09	0.52
1:E:216:ASP:OD1	1:E:218:GLU:HG2	2.09	0.52
1:E:485:GLY:O	1:E:486:LYS:C	2.53	0.52
1:F:182:LEU:CD1	1:F:184:PHE:CE2	2.88	0.52
1:F:307:TRP:H	1:F:328:ILE:HG21	1.73	0.52
1:F:458:ASN:C	1:F:460:LYS:H	2.17	0.52
1:C:40:THR:OG1	1:C:452:GLN:HG3	2.09	0.52
1:C:300:ASN:HD21	1:C:304:LEU:N	2.08	0.52
1:C:432:THR:HA	1:C:473:GLU:O	2.09	0.52
1:F:500:ARG:CD	1:F:500:ARG:H	2.23	0.52
1:D:259:MSE:CE	1:D:313:LEU:HD11	2.40	0.52
1:B:130:PRO:HA	1:B:143:MSE:HE1	1.92	0.52
1:E:109:VAL:HG23	1:E:167:TRP:CD2	2.45	0.52
1:F:36:PHE:CD1	1:F:455:LEU:HB2	2.44	0.52
1:F:53:LEU:HD23	1:F:366:LYS:CD	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:ALA:HB2	1:F:217:LEU:HD21	1.91	0.52
1:D:432:THR:HA	1:D:473:GLU:O	2.09	0.52
1:F:461:ALA:HB1	1:F:463:GLN:HG3	1.91	0.52
1:A:397:GLU:HA	1:A:416:ILE:HG13	1.92	0.51
1:E:91:GLY:C	1:E:92:VAL:CG1	2.83	0.51
1:E:92:VAL:CG1	1:E:110:LEU:HG	2.41	0.51
1:B:109:VAL:HG13	1:B:167:TRP:CG	2.45	0.51
1:A:130:PRO:HA	1:A:143:MSE:HE1	1.91	0.51
1:C:109:VAL:HG13	1:C:167:TRP:CG	2.45	0.51
1:D:36:PHE:CE2	1:D:569:MSE:HB2	2.46	0.51
1:D:109:VAL:HG13	1:D:167:TRP:CG	2.45	0.51
1:E:297:PHE:O	1:E:298:LEU:CB	2.58	0.51
1:E:490:LEU:HD21	1:E:514:ILE:HD13	1.91	0.51
1:A:109:VAL:HG13	1:A:167:TRP:CG	2.45	0.51
1:C:468:ILE:HG23	1:C:478:VAL:HG22	1.92	0.51
1:D:413:PHE:CE1	1:D:414:ILE:CD1	2.94	0.51
1:C:369:MSE:HE2	1:C:373:VAL:HB	1.91	0.51
1:D:464:LYS:HG2	1:D:482:GLN:HG2	1.93	0.51
1:F:51:ASN:O	1:F:366:LYS:HE3	2.10	0.51
1:F:130:PRO:HA	1:F:143:MSE:HE1	1.93	0.51
1:B:36:PHE:CE2	1:B:569:MSE:HB2	2.46	0.51
1:D:300:ASN:HD21	1:D:304:LEU:N	2.08	0.51
1:D:333:LYS:HE2	1:D:530:LEU:HD12	1.92	0.50
1:A:265:THR:O	1:A:265:THR:HG22	2.10	0.50
1:E:91:GLY:O	1:E:92:VAL:HG13	2.11	0.50
1:E:233:GLY:HA3	1:E:237:ILE:CD1	2.41	0.50
1:F:50:LYS:HD3	1:F:50:LYS:N	2.27	0.50
1:F:233:GLY:HA3	1:F:237:ILE:CD1	2.42	0.50
1:E:326:LEU:C	1:E:326:LEU:HD12	2.36	0.50
1:C:326:LEU:C	1:C:326:LEU:HD12	2.37	0.50
1:C:413:PHE:CE1	1:C:414:ILE:CD1	2.94	0.50
1:E:92:VAL:HG11	1:E:109:VAL:HG13	1.92	0.50
1:F:328:ILE:HG13	1:F:336:VAL:CG2	2.41	0.50
1:E:130:PRO:HA	1:E:143:MSE:HE1	1.94	0.50
1:A:326:LEU:HD12	1:A:326:LEU:C	2.37	0.50
1:A:478:VAL:HG12	1:A:480:THR:HG23	1.93	0.50
1:C:510:ALA:HB1	1:C:545:ILE:HD11	1.92	0.50
1:E:59:TYR:HE1	1:E:366:LYS:NZ	2.10	0.50
1:E:195:ASN:OD1	1:E:208:ARG:NH1	2.44	0.50
1:F:259:MSE:CE	1:F:313:LEU:HD11	2.39	0.50
1:F:537:THR:HG22	1:F:542:LYS:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:SER:O	1:B:416:ILE:HD13	2.12	0.49
1:E:328:ILE:HG13	1:E:336:VAL:CG2	2.42	0.49
1:D:431:ILE:HD11	1:D:468:ILE:HG21	1.94	0.49
1:E:431:ILE:O	1:E:431:ILE:HG22	2.10	0.49
1:A:36:PHE:CE2	1:A:569:MSE:HB2	2.47	0.49
1:D:326:LEU:HA	1:D:341:GLU:O	2.12	0.49
1:E:61:PRO:HB3	1:E:343:PHE:CD1	2.47	0.49
1:A:431:ILE:HG22	2:A:602:GOL:H32	1.94	0.49
1:D:326:LEU:HD12	1:D:326:LEU:C	2.37	0.49
1:B:504:PHE:CE2	1:C:225:GLY:HA3	2.47	0.49
1:C:118:PRO:O	1:C:407:ARG:HB3	2.12	0.49
1:F:326:LEU:HD12	1:F:326:LEU:C	2.36	0.49
1:B:326:LEU:C	1:B:326:LEU:HD12	2.38	0.49
1:C:326:LEU:HA	1:C:341:GLU:O	2.12	0.49
1:D:517:LEU:C	1:D:517:LEU:HD12	2.37	0.49
1:F:54:LYS:O	1:F:57:GLU:HB2	2.13	0.49
1:C:286:TRP:CD2	1:C:288:ASN:HB3	2.48	0.49
1:D:92:VAL:HG11	1:D:143:MSE:CE	2.42	0.49
1:E:128:TYR:CG	1:E:129:ALA:N	2.79	0.49
1:B:158:VAL:CG1	1:B:167:TRP:HB3	2.42	0.49
1:C:495:THR:CG2	1:C:506:THR:OG1	2.60	0.49
1:F:478:VAL:HG13	1:F:493:GLU:HB2	1.95	0.49
1:B:286:TRP:CD2	1:B:288:ASN:HB3	2.48	0.49
1:B:478:VAL:HG12	1:B:480:THR:HG23	1.93	0.49
1:E:328:ILE:HG13	1:E:336:VAL:HG21	1.94	0.49
1:F:123:ILE:HG12	1:F:472:ASN:CB	2.42	0.49
1:B:83:ASN:C	1:B:130:PRO:HG3	2.38	0.49
1:D:397:GLU:HB3	1:D:416:ILE:HD13	1.94	0.49
1:A:83:ASN:C	1:A:130:PRO:HG3	2.38	0.48
1:A:286:TRP:CD2	1:A:288:ASN:HB3	2.48	0.48
1:D:83:ASN:C	1:D:130:PRO:HG3	2.38	0.48
1:D:481:VAL:HG13	1:D:490:LEU:HD21	1.94	0.48
1:E:268:TRP:CD1	1:E:295:ARG:HH21	2.32	0.48
1:F:326:LEU:HA	1:F:341:GLU:O	2.13	0.48
1:B:300:ASN:HD21	1:B:304:LEU:N	2.11	0.48
1:E:478:VAL:CG1	1:E:493:GLU:HB2	2.43	0.48
1:F:36:PHE:HD1	1:F:455:LEU:HB3	1.78	0.48
1:C:92:VAL:HG11	1:C:143:MSE:CE	2.41	0.48
1:D:51:ASN:HB3	1:D:366:LYS:HD2	1.94	0.48
1:D:395:LYS:HG2	1:D:420:GLY:HA3	1.95	0.48
1:E:286:TRP:CD2	1:E:288:ASN:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:LYS:NZ	2:C:602:GOL:H2	2.29	0.48
1:D:394:PHE:HZ	1:D:569:MSE:HE1	1.79	0.48
1:D:489:VAL:HG11	1:D:511:LYS:HE2	1.95	0.48
1:E:140:THR:O	1:E:141:PHE:HB2	2.13	0.48
1:E:233:GLY:HA3	1:E:237:ILE:HD13	1.95	0.48
1:A:328:ILE:HD12	1:A:336:VAL:HG21	1.94	0.48
1:C:47:ILE:HG13	1:C:47:ILE:O	2.13	0.48
1:E:214:GLU:CD	1:E:214:GLU:H	2.19	0.48
1:E:508:ILE:N	1:E:508:ILE:HD12	2.28	0.48
1:F:83:ASN:C	1:F:130:PRO:HG3	2.39	0.48
1:F:537:THR:HG22	1:F:542:LYS:HB2	1.96	0.48
1:C:92:VAL:CG1	1:C:143:MSE:HE3	2.44	0.48
1:D:286:TRP:CD2	1:D:288:ASN:HB3	2.48	0.48
1:E:83:ASN:C	1:E:130:PRO:HG3	2.39	0.48
1:E:128:TYR:HE2	1:E:179:ASP:OD1	1.93	0.48
1:E:290:PRO:HG3	1:E:295:ARG:HH11	1.79	0.48
1:E:326:LEU:HA	1:E:341:GLU:O	2.13	0.48
1:F:128:TYR:HE2	1:F:179:ASP:OD1	1.93	0.48
1:C:83:ASN:C	1:C:130:PRO:HG3	2.38	0.48
1:D:508:ILE:HD12	1:D:508:ILE:N	2.29	0.48
1:A:51:ASN:HB3	1:A:366:LYS:HD2	1.96	0.48
1:F:490:LEU:HD23	1:F:514:ILE:CG1	2.42	0.48
1:D:538:LEU:HD23	1:D:538:LEU:H	1.79	0.47
1:D:483:THR:HG22	1:D:488:GLN:HE21	1.78	0.47
1:D:558:PHE:O	1:D:558:PHE:CD1	2.67	0.47
1:E:306:ASP:C	1:E:328:ILE:HG22	2.31	0.47
1:F:368:LYS:HB3	1:F:368:LYS:HE2	1.53	0.47
1:C:508:ILE:N	1:C:508:ILE:HD12	2.29	0.47
1:E:306:ASP:HB3	1:E:328:ILE:HG21	1.95	0.47
1:F:286:TRP:CD2	1:F:288:ASN:HB3	2.48	0.47
1:C:211:LYS:HZ2	2:C:602:GOL:H2	1.78	0.47
1:E:259:MSE:CE	1:E:313:LEU:HD11	2.38	0.47
1:F:210:ILE:HG12	1:F:244:ILE:HD12	1.96	0.47
1:F:233:GLY:HA3	1:F:237:ILE:HD13	1.96	0.47
1:A:326:LEU:HA	1:A:341:GLU:O	2.13	0.47
1:D:481:VAL:HG13	1:D:490:LEU:CD2	2.44	0.47
1:F:468:ILE:HD11	1:F:572:PHE:CE2	2.50	0.47
1:B:326:LEU:HA	1:B:341:GLU:O	2.13	0.47
1:C:259:MSE:CE	1:C:313:LEU:HD11	2.40	0.47
1:C:395:LYS:HD3	1:C:420:GLY:HA3	1.97	0.47
1:D:70:PRO:CB	1:D:342:THR:HG23	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ASN:HB3	1:B:366:LYS:HD2	1.96	0.47
1:D:558:PHE:CD1	1:D:558:PHE:C	2.93	0.47
1:C:311:ALA:HA	1:C:324:VAL:O	2.15	0.46
1:C:443:ARG:HA	1:C:566:LEU:HD23	1.97	0.46
1:D:424:MSE:SE	1:D:571:VAL:HG22	2.64	0.46
1:B:99:ASP:HB2	1:B:373:VAL:HG11	1.97	0.46
1:C:40:THR:OG1	1:C:452:GLN:CG	2.64	0.46
1:E:311:ALA:CA	1:E:324:VAL:O	2.62	0.46
1:B:259:MSE:CE	1:B:313:LEU:HD11	2.39	0.46
1:E:70:PRO:HB3	1:E:342:THR:HG23	1.96	0.46
1:F:192:LEU:C	1:F:192:LEU:HD23	2.41	0.46
1:E:431:ILE:O	1:E:431:ILE:CG2	2.59	0.46
1:D:58:PHE:CD1	1:D:369:MSE:HG2	2.51	0.46
1:C:490:LEU:CD2	1:C:512:GLU:O	2.49	0.46
1:D:413:PHE:O	1:D:424:MSE:HA	2.16	0.46
1:B:328:ILE:HD12	1:B:336:VAL:HG21	1.97	0.46
1:C:62:ILE:CD1	1:C:344:MSE:HE3	2.45	0.46
1:D:33:ALA:HB3	1:D:571:VAL:HG11	1.98	0.46
1:F:36:PHE:CZ	1:F:455:LEU:HD13	2.42	0.46
1:C:192:LEU:C	1:C:192:LEU:HD23	2.41	0.46
1:C:455:LEU:HD23	1:C:455:LEU:C	2.41	0.46
1:F:522:THR:HB	1:F:537:THR:HG1	1.81	0.46
1:B:158:VAL:HG11	1:B:168:SER:O	2.16	0.45
1:E:192:LEU:C	1:E:192:LEU:HD23	2.41	0.45
1:A:74:ARG:HD2	1:A:79:TYR:CE1	2.52	0.45
1:D:192:LEU:HD23	1:D:192:LEU:C	2.41	0.45
1:F:307:TRP:CE2	1:F:328:ILE:HD12	2.51	0.45
1:D:464:LYS:HE2	1:D:482:GLN:NE2	2.31	0.45
1:B:74:ARG:HD2	1:B:79:TYR:CE1	2.51	0.45
1:F:328:ILE:CG1	1:F:336:VAL:HG21	2.47	0.45
1:B:158:VAL:HG12	1:B:159:LYS:N	2.32	0.45
1:A:514:ILE:HD12	1:A:517:LEU:HD13	1.98	0.45
1:C:413:PHE:O	1:C:424:MSE:HA	2.16	0.45
1:D:322:TYR:CD1	1:D:344:MSE:HE3	2.51	0.45
1:D:424:MSE:CG	1:D:571:VAL:HG22	2.45	0.45
1:E:128:TYR:HE2	1:E:178:ILE:HD12	1.70	0.45
1:F:110:LEU:HD11	1:F:156:MSE:HE1	1.99	0.45
1:A:192:LEU:C	1:A:192:LEU:HD23	2.41	0.45
1:F:307:TRP:CD2	1:F:328:ILE:HD12	2.52	0.45
1:F:369:MSE:HB3	1:F:370:PRO:CD	2.47	0.45
1:A:324:VAL:HG12	1:A:344:MSE:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LEU:C	1:B:192:LEU:HD23	2.41	0.45
1:C:58:PHE:CD1	1:C:369:MSE:HG2	2.52	0.45
1:C:490:LEU:CD1	1:C:536:TYR:CD1	3.00	0.45
1:D:222:ILE:O	1:D:222:ILE:HD12	2.17	0.45
1:E:413:PHE:O	1:E:424:MSE:HA	2.17	0.45
1:F:53:LEU:HD23	1:F:366:LYS:HD3	1.98	0.45
1:F:468:ILE:HD11	1:F:572:PHE:HE2	1.82	0.44
1:B:396:SER:C	1:B:416:ILE:HD13	2.41	0.44
1:A:538:LEU:HD12	1:A:538:LEU:HA	1.82	0.44
1:F:345:LEU:HD11	1:F:363:LEU:HD21	1.99	0.44
1:D:92:VAL:CG1	1:D:143:MSE:HE3	2.46	0.44
1:E:33:ALA:CB	1:E:571:VAL:HG23	2.47	0.44
1:E:97:SER:HB3	1:E:103:TRP:CZ3	2.52	0.44
1:E:132:ILE:O	1:E:133:HIS:C	2.61	0.44
1:F:92:VAL:CG1	1:F:109:VAL:HG12	2.48	0.44
1:A:222:ILE:HD12	1:A:222:ILE:O	2.17	0.44
1:E:478:VAL:HG13	1:E:493:GLU:HB2	1.99	0.44
1:F:422:LEU:HD11	1:F:440:LEU:HD23	1.99	0.44
1:A:413:PHE:O	1:A:424:MSE:HA	2.17	0.44
1:E:222:ILE:HD12	1:E:222:ILE:O	2.18	0.44
1:F:142:TYR:HB3	1:F:182:LEU:HD21	2.00	0.44
1:D:58:PHE:CE1	1:D:367:GLN:HB2	2.52	0.44
1:F:222:ILE:O	1:F:222:ILE:HD12	2.18	0.44
1:F:233:GLY:O	1:F:244:ILE:HG12	2.18	0.44
1:A:481:VAL:HG22	1:A:490:LEU:HD21	2.00	0.44
1:B:514:ILE:HD12	1:B:517:LEU:HD13	1.98	0.44
1:F:292:LEU:HD21	1:F:325:PHE:CG	2.53	0.44
1:F:488:GLN:N	1:F:488:GLN:CD	2.76	0.44
1:C:495:THR:HG22	1:C:506:THR:CA	2.48	0.44
1:B:481:VAL:HG22	1:B:490:LEU:HD21	2.00	0.43
1:C:431:ILE:HG13	1:C:572:PHE:CZ	2.53	0.43
1:E:97:SER:CB	1:E:103:TRP:CE3	3.01	0.43
1:A:199:GLU:HA	1:A:199:GLU:OE1	2.18	0.43
1:C:431:ILE:HG13	1:C:572:PHE:HZ	1.83	0.43
1:D:33:ALA:HB3	1:D:571:VAL:CG1	2.48	0.43
1:D:397:GLU:CB	1:D:416:ILE:HD13	2.49	0.43
1:E:431:ILE:O	1:E:432:THR:CG2	2.58	0.43
1:E:514:ILE:HD12	1:E:517:LEU:HD13	2.00	0.43
1:E:195:ASN:ND2	1:E:208:ARG:HD2	2.23	0.43
1:E:255:THR:HG21	1:E:275:LYS:HE2	2.01	0.43
1:F:255:THR:HG21	1:F:275:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:345:LEU:HD11	1:F:363:LEU:CD2	2.48	0.43
1:D:394:PHE:CZ	1:D:569:MSE:HE1	2.53	0.43
1:B:413:PHE:O	1:B:424:MSE:HA	2.18	0.43
1:C:222:ILE:HD12	1:C:222:ILE:O	2.18	0.43
1:A:322:TYR:CD2	1:A:346:PRO:HA	2.53	0.43
1:B:58:PHE:CE1	1:B:367:GLN:HB2	2.53	0.43
1:B:222:ILE:HD12	1:B:222:ILE:O	2.18	0.43
1:C:74:ARG:HD2	1:C:79:TYR:CE1	2.54	0.43
1:C:455:LEU:CD2	1:C:521:ILE:HG23	2.48	0.43
1:E:109:VAL:HG23	1:E:167:TRP:CG	2.53	0.43
1:A:101:ILE:CG2	1:A:369:MSE:HE3	2.48	0.42
1:A:521:ILE:HG13	1:A:538:LEU:HD13	2.01	0.42
1:E:109:VAL:HA	1:E:167:TRP:CE3	2.54	0.42
1:F:458:ASN:HB2	1:F:460:LYS:HD2	2.01	0.42
1:F:461:ALA:CB	1:F:463:GLN:HG3	2.49	0.42
1:A:328:ILE:HD12	1:A:336:VAL:CG2	2.49	0.42
1:D:503:ASP:OD1	1:D:503:ASP:N	2.39	0.42
1:E:426:ALA:HB2	1:E:571:VAL:CG2	2.40	0.42
1:F:35:THR:HG23	1:F:35:THR:O	2.20	0.42
1:F:394:PHE:HB2	1:F:421:GLY:N	2.34	0.42
1:B:414:ILE:HG12	1:B:422:LEU:HD22	2.01	0.42
1:E:307:TRP:CD2	1:E:328:ILE:HD12	2.55	0.42
1:A:143:MSE:HE1	1:A:145:THR:HB	2.02	0.42
1:A:179:ASP:N	1:A:180:PRO:CD	2.83	0.42
1:B:179:ASP:N	1:B:180:PRO:CD	2.83	0.42
1:E:490:LEU:HD23	1:E:514:ILE:CG2	2.49	0.42
1:F:292:LEU:HD21	1:F:325:PHE:CD2	2.54	0.42
1:F:499:GLN:HG3	1:F:500:ARG:NE	2.34	0.42
1:C:58:PHE:CE1	1:C:367:GLN:HB2	2.55	0.42
1:D:123:ILE:HG12	1:D:472:ASN:HB3	2.00	0.42
1:D:502:LYS:HD3	1:D:502:LYS:C	2.44	0.42
1:E:290:PRO:HG3	1:E:295:ARG:NH1	2.35	0.42
1:F:490:LEU:HD13	1:F:490:LEU:HA	1.92	0.42
1:E:307:TRP:CE2	1:E:328:ILE:HD12	2.54	0.42
1:A:414:ILE:HG12	1:A:422:LEU:HD22	2.02	0.41
1:B:481:VAL:HG22	1:B:490:LEU:CD2	2.50	0.41
1:C:57:GLU:OE1	1:C:366:LYS:HE3	2.20	0.41
1:C:422:LEU:HD11	1:C:440:LEU:HD23	2.02	0.41
1:E:286:TRP:CE2	1:E:288:ASN:HB3	2.55	0.41
1:D:286:TRP:CE2	1:D:288:ASN:HB3	2.56	0.41
1:F:60:SER:O	1:F:365:ILE:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:TRP:CZ3	1:B:227:ASP:HB3	2.55	0.41
1:B:538:LEU:HA	1:B:538:LEU:HD23	1.74	0.41
1:F:185:ASP:OD1	1:F:251:LYS:NZ	2.51	0.41
1:C:33:ALA:HB3	1:C:571:VAL:HG11	2.01	0.41
1:C:179:ASP:N	1:C:180:PRO:CD	2.84	0.41
1:C:286:TRP:CE2	1:C:288:ASN:HB3	2.56	0.41
1:D:486:LYS:HD2	1:D:486:LYS:O	2.20	0.41
1:E:196:ASP:O	1:E:208:ARG:HD3	2.20	0.41
1:F:143:MSE:HE1	1:F:145:THR:HB	2.03	0.41
1:A:89:PHE:HA	1:A:90:PRO:C	2.46	0.41
1:F:393:ASP:O	1:F:421:GLY:N	2.53	0.41
1:A:368:LYS:CE	1:C:287:ASN:OD1	2.69	0.41
1:A:481:VAL:HG22	1:A:490:LEU:CD2	2.50	0.41
1:D:74:ARG:HD2	1:D:79:TYR:CE1	2.56	0.41
1:D:307:TRP:CD2	1:D:328:ILE:HD13	2.56	0.41
1:D:422:LEU:HD11	1:D:440:LEU:HD23	2.01	0.41
1:E:345:LEU:HD23	1:E:345:LEU:HA	1.86	0.41
1:F:128:TYR:CG	1:F:129:ALA:N	2.79	0.41
1:B:422:LEU:HD11	1:B:440:LEU:HD23	2.02	0.41
1:C:89:PHE:HA	1:C:90:PRO:C	2.46	0.41
1:D:179:ASP:N	1:D:180:PRO:CD	2.84	0.41
1:E:128:TYR:CD2	1:E:179:ASP:OD1	2.74	0.41
1:E:435:GLN:HB3	1:E:436:PRO:HD2	2.02	0.41
1:F:286:TRP:CE2	1:F:288:ASN:HB3	2.55	0.41
1:A:286:TRP:CE2	1:A:288:ASN:HB3	2.56	0.41
1:B:286:TRP:CE2	1:B:288:ASN:HB3	2.56	0.41
1:B:324:VAL:HG12	1:B:344:MSE:HG3	2.02	0.41
1:C:92:VAL:HG21	1:C:143:MSE:CE	2.38	0.41
1:E:92:VAL:CG2	1:E:109:VAL:HG13	2.46	0.41
1:E:97:SER:HB2	1:E:103:TRP:CD2	2.56	0.41
1:C:307:TRP:CD2	1:C:328:ILE:HD13	2.56	0.41
1:D:89:PHE:HA	1:D:90:PRO:C	2.46	0.41
1:E:143:MSE:HE1	1:E:145:THR:HB	2.03	0.41
1:F:128:TYR:HE2	1:F:178:ILE:HD12	1.71	0.41
1:A:516:LYS:O	1:A:518:LYS:HG3	2.21	0.41
1:E:100:LEU:HD22	1:E:344:MSE:HE1	2.02	0.41
1:E:499:GLN:HG2	1:E:560:GLY:CA	2.51	0.40
1:F:92:VAL:CG2	1:F:127:ILE:HG21	2.51	0.40
1:B:89:PHE:HA	1:B:90:PRO:C	2.45	0.40
1:C:118:PRO:HG2	1:C:407:ARG:HA	2.04	0.40
1:D:468:ILE:HG23	1:D:478:VAL:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:SER:HB2	1:E:103:TRP:CE3	2.57	0.40
1:F:118:PRO:CB	1:F:407:ARG:HA	2.49	0.40
1:B:194:HIS:ND1	1:B:195:ASN:O	2.54	0.40
1:C:123:ILE:HG12	1:C:472:ASN:HB3	2.03	0.40
1:C:336:VAL:HG12	1:C:557:ASN:OD1	2.22	0.40
1:F:92:VAL:CG1	1:F:109:VAL:CG1	3.00	0.40
1:F:133:HIS:CG	1:F:182:LEU:HD12	2.57	0.40
1:F:478:VAL:HG22	1:F:480:THR:HG23	2.02	0.40
1:A:422:LEU:HD11	1:A:440:LEU:HD23	2.02	0.40
1:B:328:ILE:HD12	1:B:336:VAL:CG2	2.51	0.40
1:E:179:ASP:N	1:E:180:PRO:CD	2.84	0.40
1:F:89:PHE:HA	1:F:90:PRO:C	2.45	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	529/567 (93%)	498 (94%)	28 (5%)	3 (1%)	21	35
1	B	529/567 (93%)	497 (94%)	30 (6%)	2 (0%)	30	46
1	C	530/567 (94%)	500 (94%)	26 (5%)	4 (1%)	16	28
1	D	528/567 (93%)	489 (93%)	31 (6%)	8 (2%)	8	14
1	E	465/567 (82%)	425 (91%)	34 (7%)	6 (1%)	9	16
1	F	473/567 (83%)	438 (93%)	28 (6%)	7 (2%)	8	14
All	All	3054/3402 (90%)	2847 (93%)	177 (6%)	30 (1%)	12	22

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	VAL

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Mol	Chain	Res	Type
1	A	539	ASN
1	B	539	ASN
1	C	539	ASN
1	D	395	LYS
1	D	458	ASN
1	D	539	ASN
1	E	432	THR
1	E	539	ASN
1	F	517	LEU
1	D	393	ASP
1	D	559	ALA
1	E	485	GLY
1	F	172	ASN
1	F	538	LEU
1	A	458	ASN
1	B	458	ASN
1	D	396	SER
1	E	86	PHE
1	C	31	VAL
1	D	407	ARG
1	E	458	ASN
1	F	149	CYS
1	C	66	CYS
1	C	461	ALA
1	D	66	CYS
1	E	511	LYS
1	F	162	ASP
1	F	365	ILE
1	F	66	CYS

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	455/470 (97%)	439 (96%)	16 (4%)	32	55
1	B	455/470 (97%)	442 (97%)	13 (3%)	37	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	456/470 (97%)	439 (96%)	17 (4%)	30	54
1	D	454/470 (97%)	430 (95%)	24 (5%)	20	39
1	E	425/470 (90%)	388 (91%)	37 (9%)	9	18
1	F	426/470 (91%)	397 (93%)	29 (7%)	14	28
All	All	2671/2820 (95%)	2535 (95%)	136 (5%)	21	40

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	A	101	ILE
1	A	143	MSE
1	A	156	MSE
1	A	195	ASN
1	A	219	LYS
1	A	304	LEU
1	A	315	GLU
1	A	338	THR
1	A	368	LYS
1	A	371	LYS
1	A	373	VAL
1	A	379	LYS
1	A	414	ILE
1	A	538	LEU
1	A	569	MSE
1	B	143	MSE
1	B	156	MSE
1	B	195	ASN
1	B	218	GLU
1	B	304	LEU
1	B	315	GLU
1	B	368	LYS
1	B	371	LYS
1	B	373	VAL
1	B	414	ILE
1	B	502	LYS
1	B	505	LYS
1	B	569	MSE
1	C	51	ASN
1	C	88	MSE
1	C	101	ILE

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Mol	Chain	Res	Type
1	C	143	MSE
1	C	156	MSE
1	C	195	ASN
1	C	414	ILE
1	C	416	ILE
1	C	431	ILE
1	C	455	LEU
1	C	460	LYS
1	C	481	VAL
1	C	486	LYS
1	C	517	LEU
1	C	519	THR
1	C	569	MSE
1	C	571	VAL
1	D	101	ILE
1	D	143	MSE
1	D	156	MSE
1	D	195	ASN
1	D	315	GLU
1	D	324	VAL
1	D	373	VAL
1	D	374	GLU
1	D	376	LYS
1	D	395	LYS
1	D	399	ILE
1	D	407	ARG
1	D	414	ILE
1	D	416	ILE
1	D	455	LEU
1	D	468	ILE
1	D	478	VAL
1	D	481	VAL
1	D	486	LYS
1	D	516	LYS
1	D	517	LEU
1	D	556	THR
1	D	569	MSE
1	D	571	VAL
1	E	44	GLU
1	E	50	LYS
1	E	62	ILE
1	E	72	ILE

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Mol	Chain	Res	Type
1	E	88	MSE
1	E	92	VAL
1	E	109	VAL
1	E	123	ILE
1	E	143	MSE
1	E	149	CYS
1	E	155	ASN
1	E	156	MSE
1	E	195	ASN
1	E	214	GLU
1	E	217	LEU
1	E	219	LYS
1	E	229	VAL
1	E	239	LYS
1	E	278	ASN
1	E	295	ARG
1	E	312	ASP
1	E	324	VAL
1	E	328	ILE
1	E	331	ASN
1	E	345	LEU
1	E	364	SER
1	E	369	MSE
1	E	407	ARG
1	E	414	ILE
1	E	422	LEU
1	E	437	ILE
1	E	452	GLN
1	E	467	LEU
1	E	518	LYS
1	E	531	ASN
1	E	538	LEU
1	E	569	MSE
1	F	50	LYS
1	F	121	CYS
1	F	143	MSE
1	F	149	CYS
1	F	156	MSE
1	F	182	LEU
1	F	195	ASN
1	F	278	ASN
1	F	328	ILE

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Mol	Chain	Res	Type
1	F	333	LYS
1	F	344	MSE
1	F	368	LYS
1	F	369	MSE
1	F	423	GLN
1	F	431	ILE
1	F	437	ILE
1	F	455	LEU
1	F	458	ASN
1	F	460	LYS
1	F	473	GLU
1	F	478	VAL
1	F	481	VAL
1	F	499	GLN
1	F	500	ARG
1	F	502	LYS
1	F	517	LEU
1	F	531	ASN
1	F	556	THR
1	F	569	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	HIS
1	A	296	HIS
1	A	539	ASN
1	B	133	HIS
1	B	296	HIS
1	B	435	GLN
1	B	488	GLN
1	B	539	ASN
1	C	423	GLN
1	C	488	GLN
1	C	499	GLN
1	C	539	ASN
1	D	296	HIS
1	D	423	GLN
1	D	488	GLN
1	E	287	ASN
1	E	488	GLN
1	F	248	HIS

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Mol	Chain	Res	Type
1	F	458	ASN
1	F	488	GLN
1	F	539	ASN

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](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	B	601	-	5,5,5	0.12	0	5,5,5	0.40	0
2	GOL	D	602	-	5,5,5	0.11	0	5,5,5	0.37	0
2	GOL	C	601	-	5,5,5	0.11	0	5,5,5	0.34	0
2	GOL	F	601	-	5,5,5	0.10	0	5,5,5	0.26	0
2	GOL	B	602	-	5,5,5	0.12	0	5,5,5	0.36	0
2	GOL	C	602	-	5,5,5	0.16	0	5,5,5	0.37	0
2	GOL	A	601	-	5,5,5	0.10	0	5,5,5	0.27	0
2	GOL	A	602	-	5,5,5	0.09	0	5,5,5	0.29	0
2	GOL	D	601	-	5,5,5	0.10	0	5,5,5	0.33	0
2	GOL	A	603	-	5,5,5	0.09	0	5,5,5	0.24	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	GOL	B	601	-	-	0/4/4/4	-
2	GOL	D	602	-	-	3/4/4/4	-
2	GOL	C	601	-	-	2/4/4/4	-
2	GOL	F	601	-	-	0/4/4/4	-
2	GOL	B	602	-	-	2/4/4/4	-
2	GOL	C	602	-	-	3/4/4/4	-
2	GOL	A	601	-	-	1/4/4/4	-
2	GOL	A	602	-	-	2/4/4/4	-
2	GOL	D	601	-	-	2/4/4/4	-
2	GOL	A	603	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	GOL	C1-C2-C3-O3
2	D	601	GOL	O1-C1-C2-C3
2	D	601	GOL	O1-C1-C2-O2
2	A	602	GOL	C1-C2-C3-O3
2	A	603	GOL	O1-C1-C2-C3
2	B	602	GOL	O1-C1-C2-C3
2	C	602	GOL	C1-C2-C3-O3
2	D	602	GOL	O1-C1-C2-C3
2	C	601	GOL	O2-C2-C3-O3
2	D	602	GOL	O1-C1-C2-O2
2	A	602	GOL	O2-C2-C3-O3
2	B	602	GOL	O1-C1-C2-O2
2	C	602	GOL	O1-C1-C2-O2
2	D	602	GOL	O2-C2-C3-O3
2	C	602	GOL	O2-C2-C3-O3
2	A	603	GOL	O1-C1-C2-O2
2	A	601	GOL	C1-C2-C3-O3
2	A	603	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	GOL	3	0
2	A	602	GOL	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	526/567 (92%)	-0.60	0	100	100	41, 58, 83, 112	0
1	B	526/567 (92%)	-0.64	0	100	100	41, 58, 85, 115	0
1	C	527/567 (92%)	-0.34	3 (0%)	85	83	45, 74, 120, 155	0
1	D	525/567 (92%)	-0.38	1 (0%)	91	90	44, 75, 121, 167	0
1	E	488/567 (86%)	0.18	7 (1%)	73	71	101, 118, 147, 190	0
1	F	490/567 (86%)	0.18	10 (2%)	65	62	102, 118, 151, 178	0
All	All	3082/3402 (90%)	-0.28	21 (0%)	84	82	41, 77, 136, 190	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	123	ILE	3.5
1	E	450	THR	3.3
1	E	363	LEU	2.8
1	E	421	GLY	2.7
1	E	132	ILE	2.5
1	C	485	GLY	2.5
1	F	153	GLY	2.4
1	F	242	VAL	2.4
1	F	100	LEU	2.4
1	F	55	PRO	2.3
1	F	539	ASN	2.3
1	C	381	GLY	2.3
1	D	41	TYR	2.3
1	F	396	SER	2.2
1	F	101	ILE	2.2
1	C	49	ALA	2.1
1	F	135	ASN	2.1
1	F	331	ASN	2.1
1	E	540	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	526	THR	2.1
1	E	560	GLY	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
2	GOL	F	601	6/6	0.95	0.07	74,86,91,92	0
2	GOL	B	602	6/6	0.97	0.09	71,75,80,82	0
2	GOL	B	601	6/6	0.98	0.10	51,61,64,69	0
2	GOL	A	601	6/6	0.98	0.08	45,51,55,58	0
2	GOL	C	601	6/6	0.98	0.09	59,62,66,75	0
2	GOL	C	602	6/6	0.98	0.08	50,52,63,68	0
2	GOL	D	601	6/6	0.98	0.08	51,57,61,68	0
2	GOL	A	602	6/6	0.98	0.09	71,79,86,91	0
2	GOL	D	602	6/6	0.99	0.06	40,52,58,60	0
2	GOL	A	603	6/6	0.99	0.07	59,70,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.