



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:29 PM UTC

PDB ID : 3AXG / pdb_00003axg
Title : Structure of 6-aminohexanoate-oligomer hydrolase
Authors : Negoro, S.; Shibata, N.; Tanaka, Y.; Yasuhira, K.; Shibata, H.; Hashimoto, H.; Lee, Y.H.; Ohshima, S.; Santa, R.; Mochiji, K.; Goto, Y.; Ikegami, T.; Nagai, K.; Kato, D.; Takeo, M.; Higuchi, Y.
Deposited on : 2011-04-04
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
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

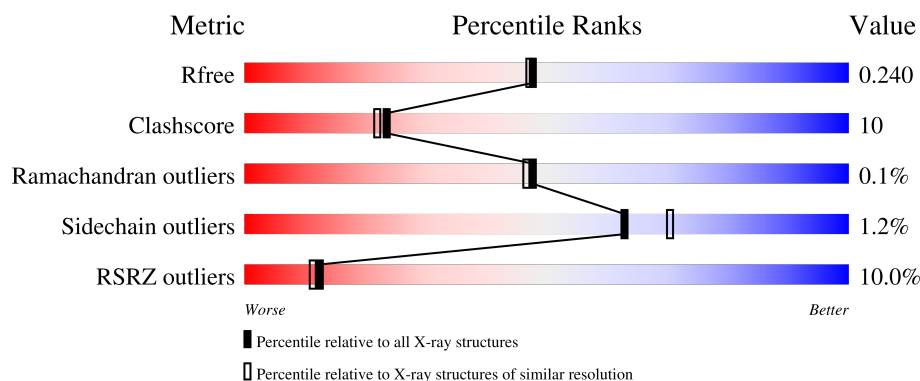
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	355	7% 81% 15% ..
1	B	355	20% 73% 23% ..
1	C	355	8% 80% 15% ..
1	D	355	6% 78% 18% ..
1	E	355	18% 78% 18% ..

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Mol	Chain	Length	Quality of chain
1	F	355	
1	G	355	
1	H	355	
1	I	355	
1	J	355	
1	K	355	
1	L	355	
1	M	355	
1	N	355	
1	O	355	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 40681 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 Endotype 6-aminohexanoat-oligomer hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2522	1578	451	485	8			
1	B	344	Total	C	N	O	S	0	0	0
			2522	1578	451	485	8			
1	C	344	Total	C	N	O	S	0	0	0
			2522	1578	451	485	8			
1	D	344	Total	C	N	O	S	0	0	0
			2522	1578	451	485	8			
1	E	344	Total	C	N	O	S	0	0	0
			2522	1578	451	485	8			
1	F	344	Total	C	N	O	S	0	0	0
			2522	1578	451	485	8			
1	G	344	Total	C	N	O	S	0	0	0
			2522	1578	451	485	8			
1	H	344	Total	C	N	O	S	0	0	0
			2522	1578	451	485	8			
1	I	344	Total	C	N	O	S	0	0	0
			2522	1578	451	485	8			
1	J	344	Total	C	N	O	S	0	0	0
			2522	1578	451	485	8			
1	K	342	Total	C	N	O	S	0	0	0
			2511	1571	449	483	8			
1	L	344	Total	C	N	O	S	0	0	0
			2522	1578	451	485	8			
1	M	344	Total	C	N	O	S	0	0	0
			2522	1578	451	485	8			
1	N	344	Total	C	N	O	S	0	0	0
			2522	1578	451	485	8			
1	O	344	Total	C	N	O	S	0	0	0
			2522	1578	451	485	8			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	K	1	Total Na 1 1	0	0
2	L	1	Total Na 1 1	0	0
2	M	1	Total Na 1 1	0	0
2	N	1	Total Na 1 1	0	0
2	O	1	Total Na 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	188	Total O 188 188	0	0
3	B	104	Total O 104 104	0	0
3	C	194	Total O 194 194	0	0
3	D	165	Total O 165 165	0	0
3	E	99	Total O 99 99	0	0
3	F	182	Total O 182 182	0	0
3	G	161	Total O 161 161	0	0
3	H	116	Total O 116 116	0	0
3	I	117	Total O 117 117	0	0
3	J	170	Total O 170 170	0	0
3	K	217	Total O 217 217	0	0
3	L	174	Total O 174 174	0	0
3	M	333	Total O 333 333	0	0
3	N	318	Total O 318 318	0	0

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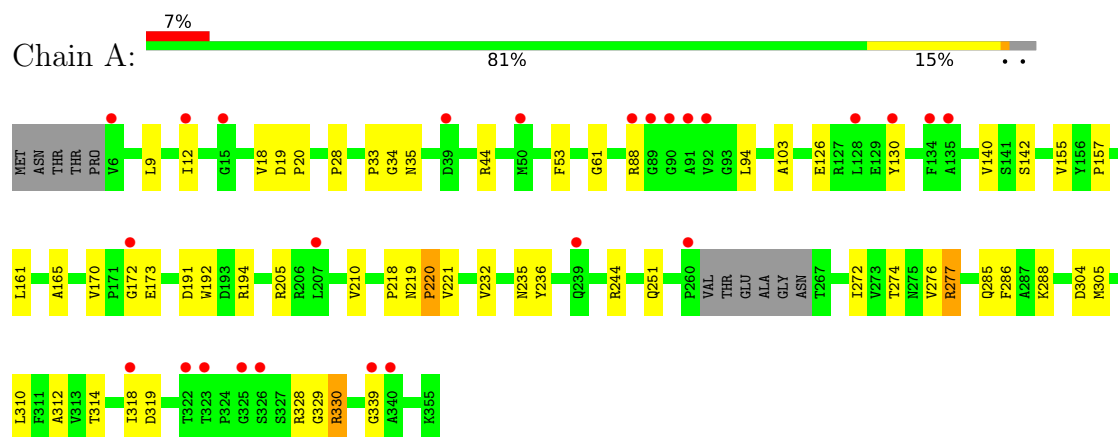
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	318	Total 318	O 318	0	0

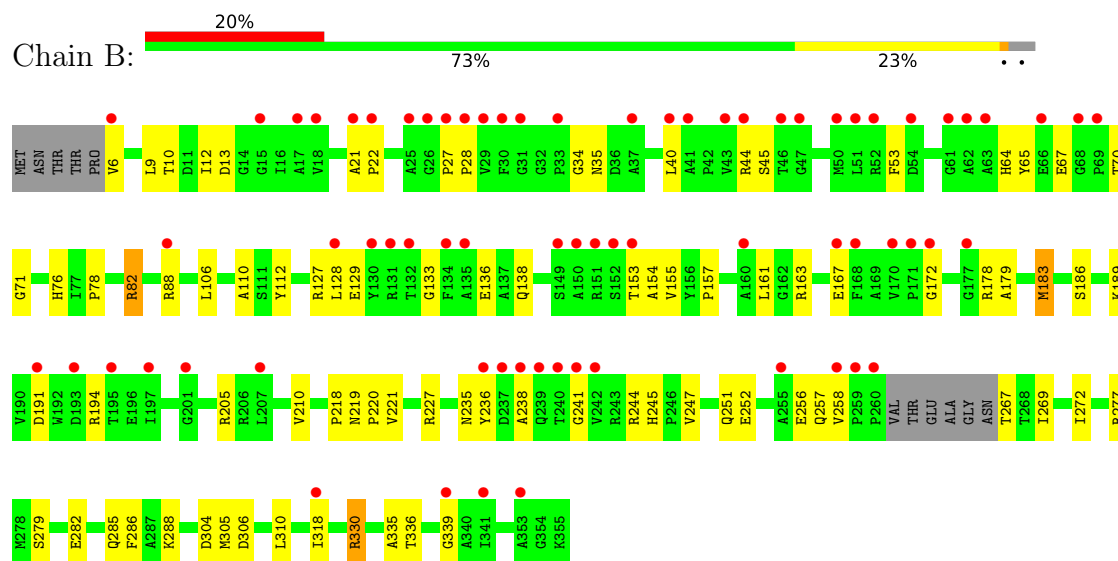
3 Residue-property plots [i](#)

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.

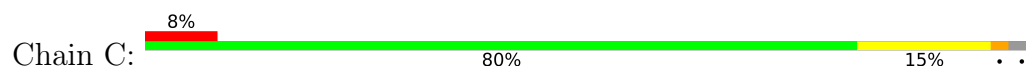
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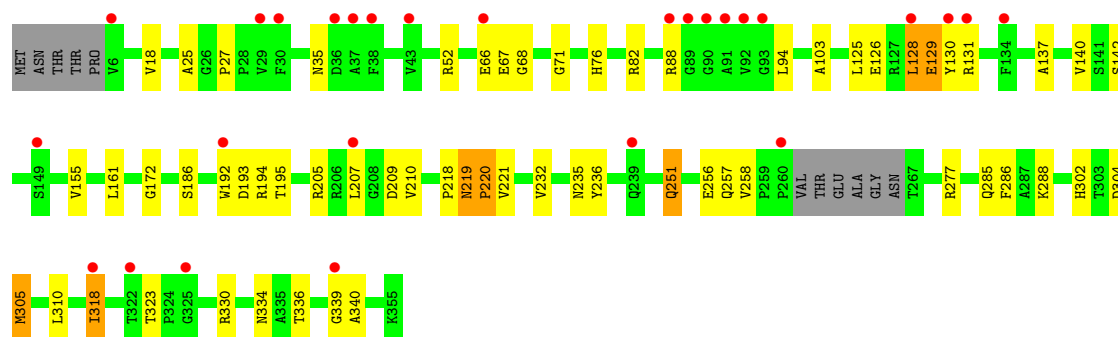


- Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

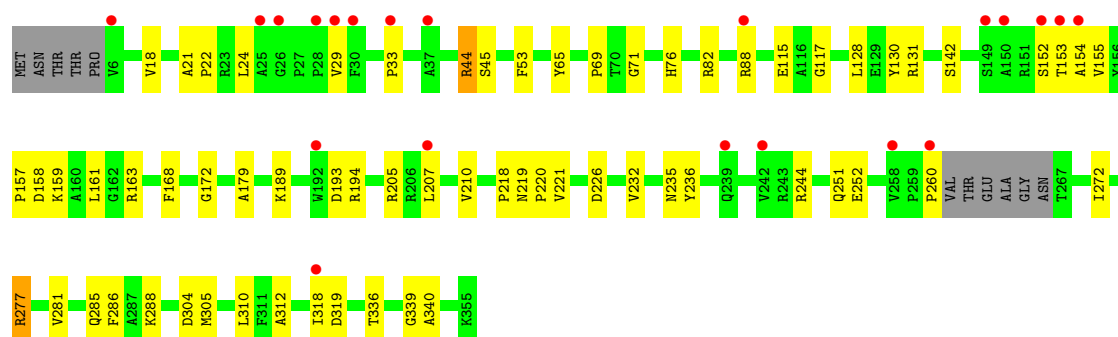
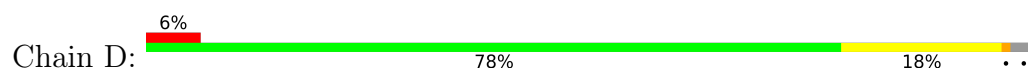


- Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

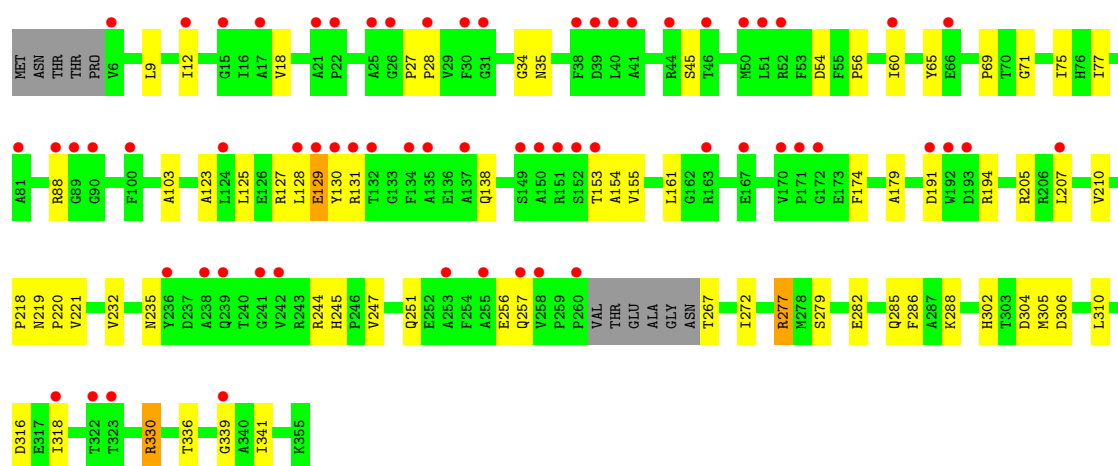
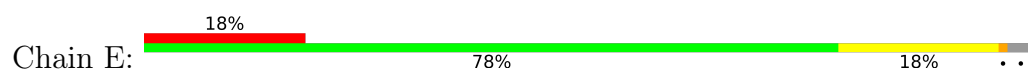




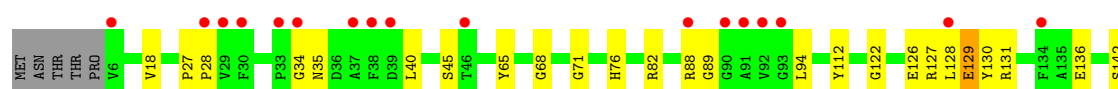
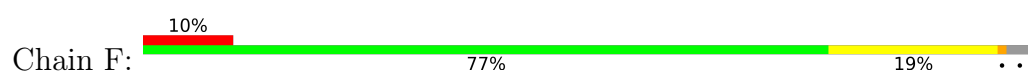
• Molecule 1: Endotype 6-aminoheptanoat-oligomer hydrolase

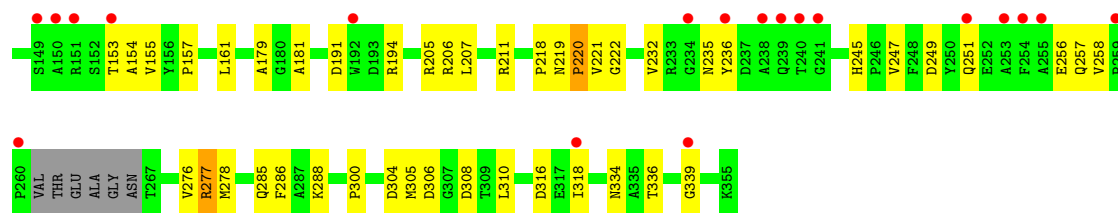


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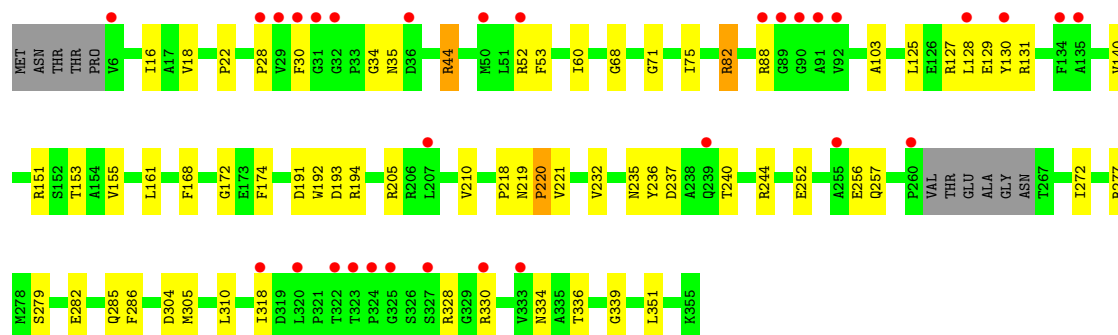
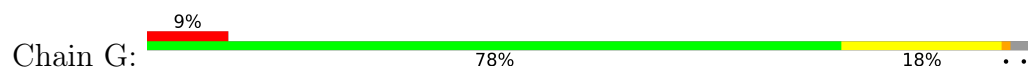


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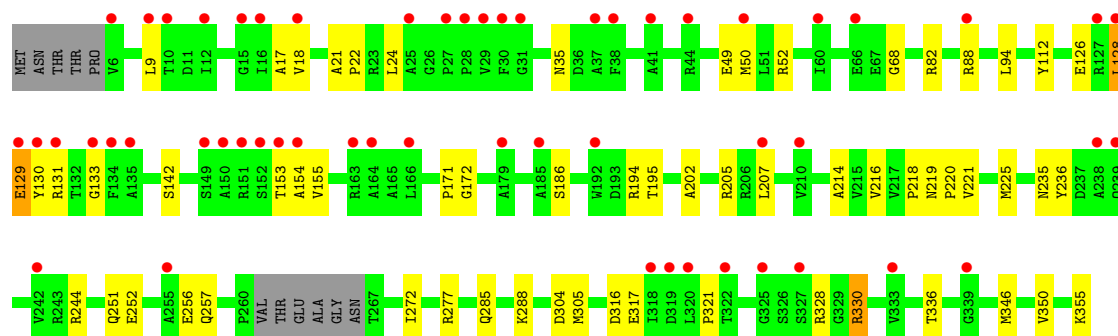
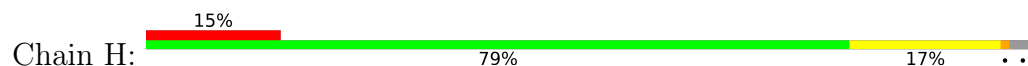




• Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase



• Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

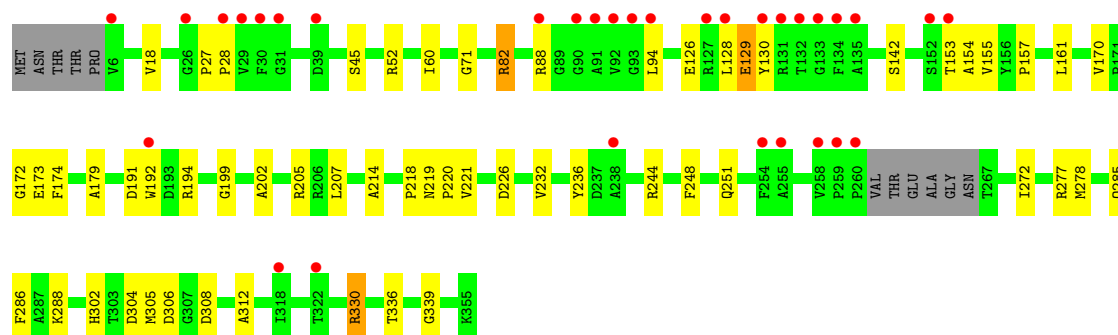
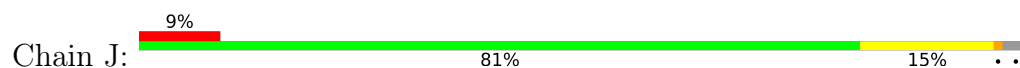


• Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

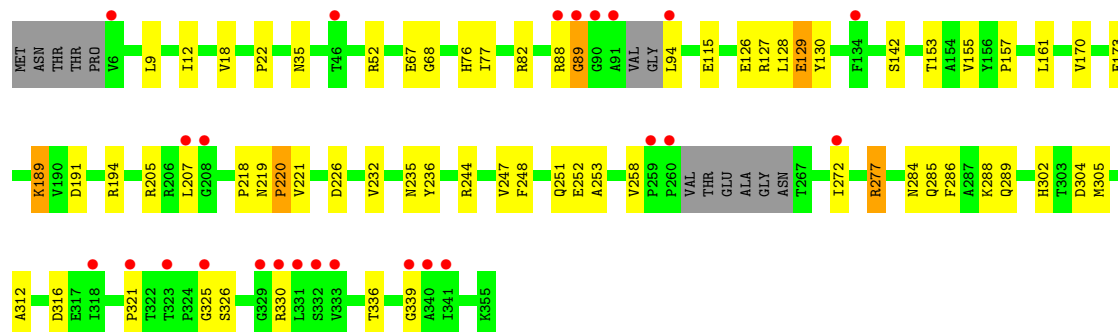
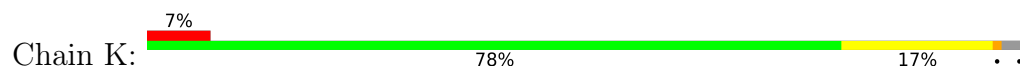




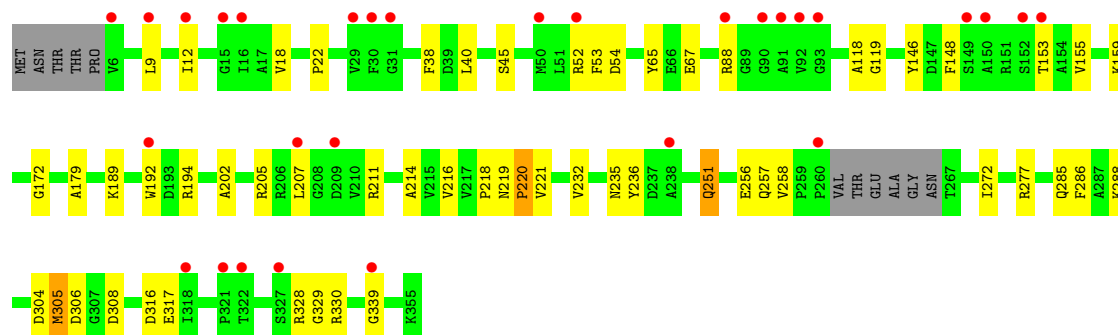
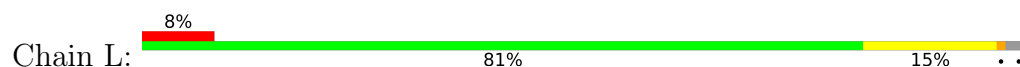
- Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase



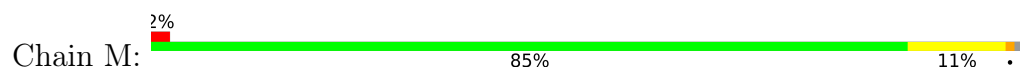
- Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

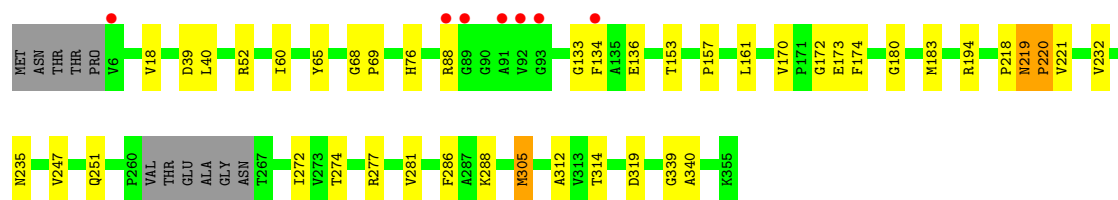


- Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

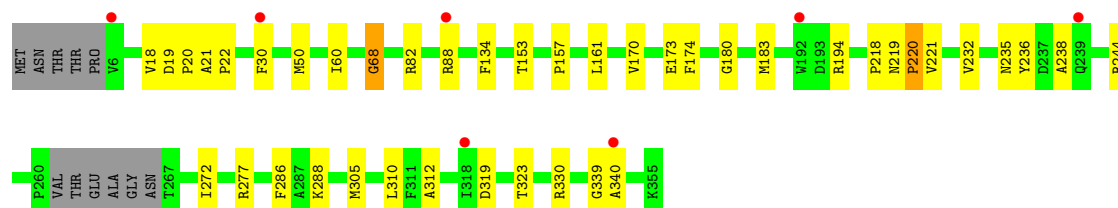
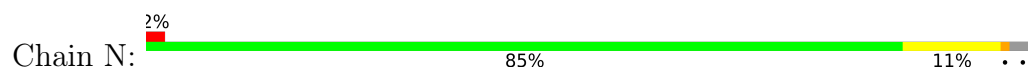


- Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

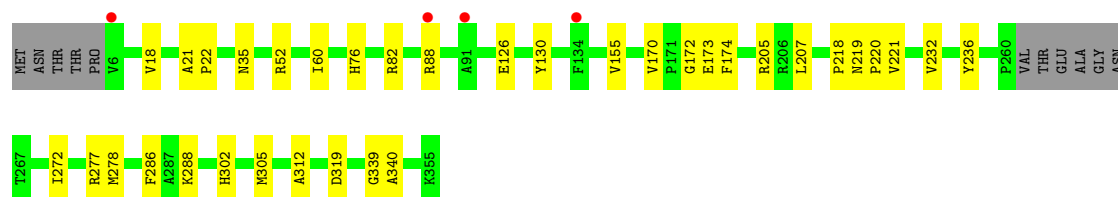
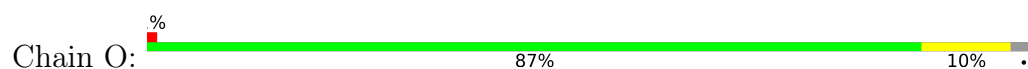




- Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase



- Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	155.86Å 214.45Å 478.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 2.00 49.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.1 (49.99-2.00) 94.2 (49.99-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.240 0.211 , 0.240	Depositor DCC
R_{free} test set	50323 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	40681	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.35% 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

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	0.40	0/2576	0.76	1/3505 (0.0%)
1	B	0.37	0/2576	0.75	0/3505
1	C	0.42	1/2576 (0.0%)	0.77	5/3505 (0.1%)
1	D	0.40	1/2576 (0.0%)	0.75	0/3505
1	E	0.37	0/2576	0.77	2/3505 (0.1%)
1	F	0.39	0/2576	0.76	1/3505 (0.0%)
1	G	0.39	0/2576	0.72	1/3505 (0.0%)
1	H	0.39	0/2576	0.75	0/3505
1	I	0.37	0/2576	0.75	3/3505 (0.1%)
1	J	0.40	0/2576	0.75	0/3505
1	K	0.39	0/2564	0.76	3/3487 (0.1%)
1	L	0.40	0/2576	0.74	1/3505 (0.0%)
1	M	0.48	2/2576 (0.1%)	0.78	3/3505 (0.1%)
1	N	0.48	1/2576 (0.0%)	0.78	1/3505 (0.0%)
1	O	0.46	1/2576 (0.0%)	0.76	0/3505
All	All	0.41	6/38628 (0.0%)	0.76	21/52557 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	340	ALA	CA-CB	6.56	1.63	1.53
1	M	340	ALA	CA-CB	5.89	1.62	1.53
1	O	340	ALA	CA-CB	5.65	1.62	1.53
1	C	340	ALA	CA-CB	5.40	1.62	1.53
1	D	340	ALA	CA-CB	5.15	1.61	1.53
1	M	340	ALA	CA-C	5.13	1.59	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	77	ILE	CA-C-N	5.92	126.07	119.32
1	K	77	ILE	C-N-CA	5.92	126.07	119.32
1	M	220	PRO	N-CA-C	5.92	120.37	111.14
1	C	323	THR	CA-C-N	5.76	126.51	120.12
1	C	323	THR	C-N-CA	5.76	126.51	120.12
1	G	220	PRO	N-CA-C	5.70	120.03	111.14
1	C	219	ASN	CA-C-N	5.43	125.36	119.76
1	C	219	ASN	C-N-CA	5.43	125.36	119.76
1	I	219	ASN	CA-C-N	5.43	125.37	119.78
1	I	219	ASN	C-N-CA	5.43	125.37	119.78
1	K	220	PRO	N-CA-C	5.42	119.59	111.14
1	M	219	ASN	CA-C-N	5.41	125.33	119.76
1	M	219	ASN	C-N-CA	5.41	125.33	119.76
1	A	220	PRO	N-CA-C	5.25	119.33	111.14
1	C	220	PRO	N-CA-C	5.24	119.31	111.14
1	N	220	PRO	N-CA-C	5.20	119.26	111.14
1	F	220	PRO	N-CA-C	5.15	119.39	111.21
1	I	220	PRO	N-CA-C	5.09	119.31	111.21
1	E	77	ILE	CA-C-N	5.07	126.17	119.84
1	E	77	ILE	C-N-CA	5.07	126.17	119.84
1	L	220	PRO	N-CA-C	5.06	119.26	111.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2522	0	2454	58	0
1	B	2522	0	2454	78	0
1	C	2522	0	2454	58	0
1	D	2522	0	2454	63	0
1	E	2522	0	2454	66	0
1	F	2522	0	2454	66	0
1	G	2522	0	2454	62	0
1	H	2522	0	2454	67	0
1	I	2522	0	2454	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2522	0	2454	62	0
1	K	2511	0	2441	68	0
1	L	2522	0	2454	51	0
1	M	2522	0	2454	33	0
1	N	2522	0	2454	33	0
1	O	2522	0	2454	29	0
2	A	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
3	A	188	0	0	3	0
3	B	104	0	0	3	0
3	C	194	0	0	2	0
3	D	165	0	0	7	0
3	E	99	0	0	1	0
3	F	182	0	0	3	0
3	G	161	0	0	3	0
3	H	116	0	0	3	0
3	I	117	0	0	5	0
3	J	170	0	0	2	0
3	K	217	0	0	6	0
3	L	174	0	0	1	0
3	M	333	0	0	7	0
3	N	318	0	0	3	0
3	O	318	0	0	4	0
All	All	40681	0	36797	758	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 10.

All (758) 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:153:THR:HG22	1:E:155:VAL:H	1.29	0.95
1:J:153:THR:HG22	1:J:155:VAL:H	1.32	0.95
1:M:221:VAL:HG11	1:M:305:MET:HE3	1.46	0.94
1:I:257:GLN:HE21	1:K:326:SER:HA	1.31	0.93
1:F:276:VAL:HG22	1:F:318:ILE:HD11	1.52	0.92
1:N:88:ARG:HH12	1:N:288:LYS:HB3	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:153:THR:HG22	1:I:155:VAL:H	1.31	0.91
1:I:285:GLN:HG2	1:K:304:ASP:HA	1.53	0.90
1:H:153:THR:HG22	1:H:155:VAL:H	1.38	0.88
1:M:88:ARG:HH12	1:M:288:LYS:HB3	1.37	0.88
1:E:305:MET:HE2	1:G:334:ASN:HD21	1.40	0.86
1:A:221:VAL:HG11	1:A:305:MET:HE3	1.57	0.86
1:I:305:MET:HE2	1:K:336:THR:HG21	1.57	0.86
1:I:221:VAL:HG11	1:I:305:MET:HE3	1.59	0.85
1:D:128:LEU:HD22	1:D:131:ARG:HE	1.42	0.85
1:F:153:THR:HG22	1:F:155:VAL:H	1.41	0.84
1:B:186:SER:H	1:B:219:ASN:HD22	1.24	0.84
1:C:221:VAL:HG21	1:C:305:MET:HB2	1.60	0.84
1:D:153:THR:HG22	1:D:155:VAL:H	1.40	0.83
1:B:153:THR:HG22	1:B:155:VAL:H	1.45	0.81
1:J:82:ARG:HG2	1:J:82:ARG:HH11	1.45	0.80
1:J:194:ARG:HG3	1:J:236:TYR:O	1.81	0.80
1:J:304:ASP:HA	1:L:285:GLN:HG2	1.63	0.80
1:A:304:ASP:HA	1:B:285:GLN:HG2	1.63	0.80
1:F:256:GLU:HG2	1:F:257:GLN:HE21	1.47	0.79
1:G:68:GLY:HA2	1:G:153:THR:HG21	1.65	0.78
1:I:9:LEU:O	1:I:12:ILE:HG22	1.82	0.78
1:D:88:ARG:HH12	1:D:288:LYS:HB3	1.47	0.78
1:G:221:VAL:HG11	1:G:305:MET:HE3	1.64	0.78
1:K:189:LYS:HG3	1:K:221:VAL:HA	1.64	0.77
1:F:285:GLN:HG2	1:H:304:ASP:HA	1.66	0.77
1:C:336:THR:HB	1:D:305:MET:HE3	1.66	0.77
1:L:205:ARG:NH2	1:L:207:LEU:HD21	1.99	0.77
1:E:244:ARG:HD3	3:E:1360:HOH:O	1.84	0.76
1:D:221:VAL:HG21	1:D:305:MET:HB2	1.66	0.76
1:F:82:ARG:HD3	3:F:2804:HOH:O	1.84	0.76
1:G:221:VAL:HG21	1:G:305:MET:HB2	1.68	0.75
1:J:221:VAL:HG11	1:J:305:MET:HE3	1.68	0.75
1:A:305:MET:HE1	3:A:357:HOH:O	1.85	0.75
1:K:153:THR:HG22	1:K:155:VAL:H	1.50	0.75
1:F:88:ARG:HH12	1:F:288:LYS:HB3	1.52	0.74
1:O:205:ARG:NH2	1:O:207:LEU:HD21	2.02	0.74
1:E:285:GLN:HG2	1:G:304:ASP:HA	1.71	0.73
1:H:205:ARG:NH2	1:H:207:LEU:HD21	2.03	0.73
1:C:210:VAL:HG22	1:C:318:ILE:HD11	1.71	0.73
1:B:9:LEU:O	1:B:12:ILE:HG22	1.88	0.72
1:H:216:VAL:HG22	1:H:218:PRO:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:304:ASP:HA	1:H:285:GLN:HG2	1.72	0.72
1:L:205:ARG:HH21	1:L:207:LEU:HD21	1.53	0.72
1:C:66:GLU:HG3	3:K:2456:HOH:O	1.87	0.71
1:J:94:LEU:HD12	1:J:142:SER:O	1.90	0.71
1:N:221:VAL:HG21	1:N:305:MET:HB2	1.72	0.71
1:C:304:ASP:HA	1:D:285:GLN:HG2	1.73	0.71
1:I:205:ARG:HE	1:I:207:LEU:HD21	1.53	0.71
1:J:336:THR:HB	1:L:305:MET:HE2	1.73	0.71
1:C:305:MET:HE2	1:D:336:THR:HB	1.74	0.70
1:I:330:ARG:HD3	1:K:191:ASP:OD2	1.91	0.70
1:I:87:ALA:HB1	1:I:92:VAL:HG21	1.74	0.70
1:H:205:ARG:HH21	1:H:207:LEU:HD21	1.56	0.70
1:L:153:THR:HG22	1:L:155:VAL:H	1.55	0.69
1:A:285:GLN:HG2	1:B:304:ASP:HA	1.73	0.69
1:I:88:ARG:NH1	1:I:288:LYS:HB3	2.08	0.69
1:C:285:GLN:HG2	1:D:304:ASP:HA	1.74	0.69
1:I:221:VAL:HG11	1:I:305:MET:CE	2.23	0.69
1:H:128:LEU:HD22	1:H:131:ARG:HE	1.58	0.69
1:A:191:ASP:OD2	1:B:330:ARG:HD3	1.92	0.68
1:I:88:ARG:HH11	1:I:288:LYS:HB3	1.58	0.68
1:O:88:ARG:HH12	1:O:288:LYS:HB3	1.58	0.68
1:H:328:ARG:HA	1:H:328:ARG:NH1	2.09	0.68
1:M:221:VAL:HG21	1:M:305:MET:HB2	1.76	0.68
1:L:88:ARG:HH12	1:L:288:LYS:HB3	1.58	0.67
1:L:328:ARG:NH1	1:L:328:ARG:HA	2.09	0.67
1:B:45:SER:HB3	1:B:179:ALA:HB1	1.76	0.67
1:I:244:ARG:HD3	3:I:1377:HOH:O	1.95	0.67
1:I:304:ASP:HA	1:K:285:GLN:HG2	1.77	0.67
1:H:88:ARG:HH12	1:H:288:LYS:HB3	1.60	0.67
1:J:221:VAL:HG21	1:J:305:MET:HB2	1.77	0.67
1:L:18:VAL:HG11	1:L:232:VAL:HB	1.76	0.67
1:I:285:GLN:HG2	1:K:304:ASP:CA	2.24	0.67
1:B:256:GLU:HG2	1:B:257:GLN:NE2	2.10	0.67
1:A:18:VAL:HG11	1:A:232:VAL:HB	1.76	0.66
1:D:44:ARG:HD2	3:D:739:HOH:O	1.94	0.66
1:F:205:ARG:NH2	1:F:207:LEU:HD21	2.11	0.66
1:E:205:ARG:CZ	1:E:207:LEU:HD21	2.25	0.66
1:J:128:LEU:O	1:J:129:GLU:HG2	1.96	0.66
1:G:305:MET:HE1	3:G:617:HOH:O	1.94	0.65
1:I:205:ARG:NE	1:I:207:LEU:HD21	2.11	0.65
1:E:305:MET:CE	1:G:334:ASN:HD21	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:LEU:HD22	1:E:12:ILE:HG21	1.77	0.65
1:E:330:ARG:HD3	1:G:191:ASP:OD2	1.96	0.65
1:G:244:ARG:NH2	1:G:252:GLU:OE2	2.28	0.65
1:A:305:MET:HE2	1:B:336:THR:HG21	1.78	0.65
1:F:18:VAL:HG11	1:F:232:VAL:HB	1.79	0.64
1:B:88:ARG:HH12	1:B:288:LYS:HB3	1.63	0.64
1:D:157:PRO:HB3	1:D:161:LEU:HD23	1.79	0.64
1:H:128:LEU:O	1:H:129:GLU:HG2	1.97	0.64
1:D:205:ARG:NE	1:D:207:LEU:HD21	2.12	0.64
1:J:272:ILE:HG22	1:J:312:ALA:HA	1.78	0.64
1:C:286:PHE:CE1	1:C:339:GLY:HA2	2.32	0.64
1:L:221:VAL:HG21	1:L:305:MET:HB2	1.78	0.64
1:D:205:ARG:NH2	1:D:207:LEU:HD21	2.12	0.64
1:D:18:VAL:HG11	1:D:232:VAL:HB	1.79	0.64
1:E:191:ASP:OD2	1:G:330:ARG:HD3	1.97	0.64
1:C:334:ASN:ND2	1:D:305:MET:HE2	2.13	0.64
1:E:221:VAL:HG21	1:E:305:MET:HB2	1.79	0.63
1:B:189:LYS:HE2	1:B:220:PRO:O	1.99	0.63
1:I:205:ARG:HH21	1:I:207:LEU:HD21	1.64	0.63
1:K:128:LEU:O	1:K:129:GLU:HG2	1.98	0.62
1:B:157:PRO:HB3	1:B:161:LEU:HD23	1.80	0.62
1:N:60:ILE:HD13	1:N:174:PHE:HD1	1.65	0.62
1:N:218:PRO:C	1:N:220:PRO:HD3	2.24	0.62
1:E:205:ARG:NE	1:E:207:LEU:HD21	2.13	0.62
1:B:88:ARG:NH1	1:B:288:LYS:HB3	2.13	0.62
1:B:256:GLU:HG2	1:B:257:GLN:HE21	1.63	0.62
1:C:334:ASN:HD21	1:D:305:MET:CE	2.13	0.62
1:I:128:LEU:O	1:I:129:GLU:HG2	1.98	0.62
1:G:128:LEU:C	1:G:129:GLU:HG2	2.24	0.62
1:M:218:PRO:C	1:M:220:PRO:HD3	2.25	0.61
1:N:82:ARG:HH11	1:N:82:ARG:HG2	1.64	0.61
1:D:205:ARG:CZ	1:D:207:LEU:HD21	2.30	0.61
1:D:194:ARG:HB3	1:D:235:ASN:HA	1.81	0.61
1:G:244:ARG:HD3	3:G:456:HOH:O	2.01	0.61
1:M:52:ARG:HG2	1:M:173:GLU:HG2	1.82	0.61
1:N:18:VAL:HG11	1:N:232:VAL:HB	1.82	0.61
1:J:88:ARG:NH1	1:J:288:LYS:HB3	2.15	0.61
1:M:170:VAL:HG23	1:M:173:GLU:HB2	1.83	0.61
1:C:128:LEU:CD2	1:C:131:ARG:HE	2.14	0.60
1:K:284:ASN:HB2	3:K:1426:HOH:O	2.00	0.60
1:E:128:LEU:O	1:E:129:GLU:HG2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:128:LEU:O	1:G:129:GLU:HG2	2.01	0.60
1:D:281:VAL:HG23	3:D:1479:HOH:O	2.01	0.60
1:M:18:VAL:HG11	1:M:232:VAL:HB	1.82	0.60
1:E:336:THR:HB	1:G:305:MET:HE2	1.84	0.60
1:G:30:PHE:CD1	1:H:133:GLY:HA2	2.35	0.60
1:I:52:ARG:HH12	1:I:173:GLU:HG2	1.65	0.60
1:A:205:ARG:HH22	1:B:251:GLN:CG	2.14	0.60
1:F:194:ARG:HB3	1:F:235:ASN:HA	1.83	0.60
1:C:218:PRO:C	1:C:220:PRO:HD3	2.27	0.60
1:F:256:GLU:HG2	1:F:257:GLN:NE2	2.17	0.60
1:E:304:ASP:HA	1:G:285:GLN:HG2	1.83	0.60
1:F:277:ARG:HD3	1:F:316:ASP:C	2.27	0.60
1:E:251:GLN:CG	1:G:205:ARG:HH22	2.15	0.59
1:F:128:LEU:C	1:F:129:GLU:HG2	2.25	0.59
1:G:286:PHE:CE1	1:G:339:GLY:HA2	2.37	0.59
1:K:272:ILE:HG22	1:K:312:ALA:HA	1.83	0.59
1:M:134:PHE:HB3	3:M:2653:HOH:O	2.02	0.59
1:C:192:TRP:CZ3	1:C:193:ASP:OD1	2.55	0.59
1:J:330:ARG:NH2	1:L:192:TRP:HB2	2.16	0.59
1:K:221:VAL:HG11	1:K:305:MET:HE3	1.84	0.59
1:C:256:GLU:HG2	1:C:257:GLN:HE21	1.66	0.59
1:M:88:ARG:HH12	1:M:288:LYS:CB	2.13	0.59
1:I:205:ARG:NH2	1:I:207:LEU:HD21	2.17	0.59
1:J:285:GLN:HG2	1:L:304:ASP:HA	1.85	0.59
1:K:205:ARG:NH2	1:K:207:LEU:HD21	2.18	0.59
1:E:286:PHE:CE1	1:E:339:GLY:HA2	2.38	0.59
1:K:153:THR:CG2	1:K:155:VAL:H	2.15	0.59
1:K:194:ARG:HB3	1:K:235:ASN:HA	1.85	0.59
1:C:126:GLU:HG2	1:C:130:TYR:OH	2.03	0.58
1:F:286:PHE:CE1	1:F:339:GLY:HA2	2.38	0.58
1:F:336:THR:HB	1:H:305:MET:HE2	1.84	0.58
1:I:15:GLY:HA2	3:I:2379:HOH:O	2.02	0.58
1:F:131:ARG:HB3	1:F:136:GLU:OE2	2.04	0.58
1:F:88:ARG:HD3	1:H:88:ARG:NH1	2.18	0.58
1:I:245:HIS:ND1	1:I:247:VAL:HG12	2.19	0.58
1:C:336:THR:CB	1:D:305:MET:HE3	2.33	0.58
1:C:194:ARG:HB3	1:C:235:ASN:HA	1.86	0.58
1:D:286:PHE:CE1	1:D:339:GLY:HA2	2.39	0.58
1:B:236:TYR:OH	1:B:241:GLY:HA2	2.03	0.58
1:L:189:LYS:HD2	1:L:192:TRP:CZ3	2.39	0.58
1:N:277:ARG:HD2	1:N:319:ASP:OD1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLY:HA3	1:C:130:TYR:CD1	2.38	0.57
1:E:130:TYR:CD1	1:F:34:GLY:HA3	2.39	0.57
1:K:286:PHE:CE1	1:K:339:GLY:HA2	2.39	0.57
1:O:221:VAL:HG21	1:O:305:MET:HB2	1.86	0.57
1:B:154:ALA:CB	1:C:130:TYR:HB3	2.35	0.57
1:E:88:ARG:NH1	1:E:288:LYS:HB3	2.18	0.57
1:B:13:ASP:HB2	1:B:227:ARG:HD2	1.86	0.57
1:A:88:ARG:HH11	1:A:288:LYS:HB3	1.69	0.57
1:I:305:MET:HE2	1:K:336:THR:CG2	2.32	0.57
1:O:88:ARG:HD2	1:O:302:HIS:CE1	2.40	0.57
1:I:219:ASN:N	1:I:220:PRO:CD	2.67	0.57
1:C:76:HIS:HD2	3:C:2294:HOH:O	1.86	0.57
1:E:305:MET:HE2	1:G:334:ASN:ND2	2.14	0.57
1:F:191:ASP:OD2	1:H:330:ARG:HD3	2.04	0.56
1:K:277:ARG:HD2	3:K:2625:HOH:O	2.05	0.56
1:I:18:VAL:HG11	1:I:232:VAL:HB	1.86	0.56
1:O:218:PRO:C	1:O:220:PRO:HD3	2.30	0.56
1:O:272:ILE:HG22	1:O:312:ALA:HA	1.87	0.56
1:F:221:VAL:HG11	1:F:305:MET:HE3	1.87	0.56
1:J:128:LEU:C	1:J:129:GLU:HG2	2.31	0.56
1:K:205:ARG:HH21	1:K:207:LEU:HD21	1.70	0.56
1:B:34:GLY:HA3	1:C:130:TYR:CE1	2.41	0.56
1:G:130:TYR:HB3	1:H:154:ALA:CB	2.35	0.56
1:A:194:ARG:HB3	1:A:235:ASN:HA	1.88	0.56
1:A:304:ASP:CA	1:B:285:GLN:HG2	2.33	0.56
1:H:128:LEU:C	1:H:129:GLU:HG2	2.31	0.56
1:K:18:VAL:HG11	1:K:232:VAL:HB	1.88	0.56
1:D:189:LYS:HE2	1:D:220:PRO:O	2.05	0.55
1:D:210:VAL:HA	1:D:318:ILE:HD11	1.87	0.55
1:D:277:ARG:HH21	1:D:319:ASP:CG	2.13	0.55
1:F:128:LEU:O	1:F:129:GLU:HG2	2.06	0.55
1:D:218:PRO:C	1:D:220:PRO:HD3	2.31	0.55
1:I:34:GLY:HA3	1:J:130:TYR:CD1	2.42	0.55
1:O:88:ARG:HH12	1:O:288:LYS:CB	2.19	0.55
1:J:82:ARG:NH1	1:J:278:MET:O	2.39	0.55
1:A:330:ARG:HD3	1:B:191:ASP:OD2	2.06	0.55
1:J:305:MET:HE1	3:J:1897:HOH:O	2.06	0.55
1:C:18:VAL:HG11	1:C:232:VAL:HB	1.88	0.55
1:H:244:ARG:HD3	3:H:2066:HOH:O	2.07	0.55
1:O:205:ARG:HH21	1:O:207:LEU:HD21	1.72	0.55
1:F:205:ARG:HH21	1:F:207:LEU:HD21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ARG:HH22	1:B:251:GLN:HG3	1.71	0.54
1:B:35:ASN:OD1	1:B:155:VAL:HA	2.06	0.54
1:F:205:ARG:CZ	1:F:207:LEU:HD21	2.38	0.54
1:F:205:ARG:HH22	1:H:251:GLN:HG2	1.71	0.54
1:K:128:LEU:C	1:K:129:GLU:HG2	2.32	0.54
1:A:286:PHE:CE1	1:A:339:GLY:HA2	2.42	0.54
1:E:88:ARG:HH21	1:E:302:HIS:CE1	2.24	0.54
1:K:218:PRO:C	1:K:220:PRO:HD3	2.32	0.54
1:I:257:GLN:NE2	1:K:326:SER:HA	2.13	0.54
1:J:170:VAL:CG2	1:J:173:GLU:HB2	2.37	0.54
1:N:219:ASN:N	1:N:220:PRO:CD	2.71	0.54
1:C:128:LEU:HD22	1:C:131:ARG:HE	1.72	0.54
1:E:128:LEU:CD2	1:E:131:ARG:HH21	2.21	0.54
1:E:245:HIS:ND1	1:E:247:VAL:HG12	2.23	0.54
1:G:18:VAL:HG11	1:G:232:VAL:HB	1.89	0.54
1:J:205:ARG:HH22	1:L:251:GLN:CD	2.16	0.54
1:J:218:PRO:C	1:J:220:PRO:HD3	2.33	0.54
1:B:110:ALA:HB1	3:B:1482:HOH:O	2.07	0.54
1:C:27:PRO:HB3	1:C:192:TRP:CZ3	2.43	0.54
1:F:276:VAL:HA	1:F:318:ILE:HG13	1.89	0.54
1:J:82:ARG:HG2	1:J:82:ARG:NH1	2.20	0.54
1:D:128:LEU:HD23	1:D:131:ARG:HH21	1.73	0.54
1:K:94:LEU:HD12	1:K:142:SER:O	2.08	0.54
1:N:272:ILE:HG22	1:N:312:ALA:HA	1.90	0.54
1:A:221:VAL:HG11	1:A:305:MET:CE	2.33	0.53
1:A:276:VAL:HG22	1:A:318:ILE:HD11	1.91	0.53
1:A:328:ARG:HA	1:A:328:ARG:NH1	2.23	0.53
1:B:286:PHE:CE1	1:B:339:GLY:HA2	2.43	0.53
1:C:142:SER:HB3	3:C:2072:HOH:O	2.08	0.53
1:D:128:LEU:CD2	1:D:131:ARG:HH21	2.20	0.53
1:H:221:VAL:HG21	1:H:305:MET:HB2	1.90	0.53
1:A:157:PRO:HB3	1:A:161:LEU:HD23	1.91	0.53
1:D:205:ARG:HE	1:D:207:LEU:HD21	1.74	0.53
1:D:244:ARG:HD3	3:D:1459:HOH:O	2.07	0.53
1:J:205:ARG:NE	1:J:207:LEU:HD21	2.23	0.53
1:A:210:VAL:HG22	1:A:318:ILE:HD11	1.90	0.53
1:O:60:ILE:HD13	1:O:174:PHE:HD1	1.73	0.53
1:C:35:ASN:OD1	1:C:155:VAL:HA	2.08	0.53
1:E:247:VAL:O	1:E:251:GLN:HB2	2.08	0.53
1:I:128:LEU:C	1:I:129:GLU:HG2	2.34	0.53
1:I:310:LEU:C	1:I:310:LEU:HD23	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:VAL:HG11	1:E:232:VAL:HB	1.91	0.53
1:G:34:GLY:HA3	1:H:130:TYR:CD1	2.42	0.53
1:I:88:ARG:HH11	1:I:288:LYS:CB	2.19	0.53
1:M:251:GLN:HG2	3:M:905:HOH:O	2.07	0.53
1:J:205:ARG:NH2	1:J:207:LEU:HD21	2.24	0.53
1:J:286:PHE:CE1	1:J:339:GLY:HA2	2.44	0.53
1:M:272:ILE:HG22	1:M:312:ALA:HA	1.90	0.53
1:A:210:VAL:HG22	1:A:318:ILE:CD1	2.39	0.53
3:F:1474:HOH:O	1:H:305:MET:HE1	2.08	0.53
1:I:128:LEU:HD22	1:I:131:ARG:HE	1.74	0.53
1:I:178:ARG:NH1	1:I:197:ILE:HG21	2.24	0.53
1:A:251:GLN:HG3	1:B:205:ARG:HH22	1.72	0.53
1:B:153:THR:CG2	1:B:155:VAL:HG23	2.40	0.53
1:G:218:PRO:C	1:G:220:PRO:HD3	2.33	0.53
1:H:88:ARG:NH1	1:H:288:LYS:HB3	2.24	0.53
1:J:60:ILE:HD13	1:J:174:PHE:HD1	1.73	0.52
1:B:244:ARG:HD3	3:B:1480:HOH:O	2.07	0.52
1:C:128:LEU:C	1:C:129:GLU:HG2	2.33	0.52
1:A:88:ARG:NH1	1:A:288:LYS:HB3	2.23	0.52
1:A:305:MET:HE2	1:B:336:THR:CB	2.40	0.52
1:B:178:ARG:HB3	1:B:183:MET:HE3	1.90	0.52
1:C:82:ARG:HG2	1:C:82:ARG:HH11	1.73	0.52
1:C:336:THR:HB	1:D:305:MET:CE	2.36	0.52
1:B:236:TYR:CE1	1:B:238:ALA:HA	2.45	0.52
1:D:82:ARG:HD2	3:D:2788:HOH:O	2.09	0.52
1:F:76:HIS:HE1	3:F:2336:HOH:O	1.91	0.52
1:L:218:PRO:C	1:L:220:PRO:HD3	2.35	0.52
1:B:53:PHE:CE1	1:B:172:GLY:HA2	2.45	0.52
1:E:153:THR:CG2	1:E:155:VAL:H	2.14	0.52
1:N:244:ARG:HD3	3:N:397:HOH:O	2.08	0.52
1:E:272:ILE:HG23	1:E:272:ILE:O	2.09	0.52
1:H:256:GLU:HG2	1:H:257:GLN:HE21	1.74	0.52
1:M:286:PHE:CE1	1:M:339:GLY:HA2	2.44	0.52
1:A:221:VAL:HG21	1:A:305:MET:HB2	1.90	0.52
1:F:251:GLN:CG	1:H:205:ARG:HH22	2.23	0.52
1:B:194:ARG:HB3	1:B:235:ASN:HA	1.90	0.52
1:I:52:ARG:NH1	1:I:173:GLU:HG2	2.25	0.52
1:I:127:ARG:C	1:I:129:GLU:H	2.17	0.52
1:B:9:LEU:HD22	1:B:12:ILE:HG21	1.92	0.52
1:I:286:PHE:CE1	1:I:339:GLY:HA2	2.45	0.52
1:N:157:PRO:HB3	1:N:161:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:MET:HE2	1:B:336:THR:CG2	2.40	0.52
1:D:244:ARG:NH2	1:D:252:GLU:OE2	2.35	0.52
1:F:247:VAL:O	1:F:251:GLN:HB2	2.10	0.52
1:H:128:LEU:CD2	1:H:131:ARG:HH21	2.23	0.52
1:I:226:ASP:OD1	1:I:230:THR:HB	2.10	0.52
1:N:272:ILE:HG21	1:N:286:PHE:HE2	1.74	0.52
1:B:71:GLY:HA2	1:B:161:LEU:HD21	1.90	0.51
1:L:328:ARG:HA	1:L:328:ARG:HH11	1.75	0.51
1:E:9:LEU:O	1:E:12:ILE:HG22	2.10	0.51
1:K:9:LEU:O	1:K:12:ILE:HG22	2.10	0.51
1:E:277:ARG:HG3	1:E:316:ASP:OD2	2.09	0.51
1:G:128:LEU:HD22	1:G:131:ARG:HH21	1.74	0.51
1:L:194:ARG:HB3	1:L:235:ASN:HA	1.91	0.51
1:M:219:ASN:N	1:M:220:PRO:CD	2.73	0.51
1:D:226:ASP:HB2	3:D:835:HOH:O	2.11	0.51
1:H:35:ASN:OD1	1:H:155:VAL:HA	2.11	0.51
1:A:218:PRO:C	1:A:220:PRO:HD3	2.36	0.51
1:E:153:THR:HG22	1:E:154:ALA:N	2.24	0.51
1:I:198:THR:OG1	1:I:199:GLY:N	2.42	0.51
1:O:286:PHE:CE1	1:O:339:GLY:HA2	2.45	0.51
1:I:64:HIS:HB2	1:I:70:THR:O	2.10	0.51
1:C:209:ASP:OD2	1:D:260:PRO:HA	2.10	0.51
1:H:244:ARG:HH22	1:H:252:GLU:CD	2.19	0.51
1:N:88:ARG:NH1	1:N:288:LYS:HB3	2.14	0.51
1:F:94:LEU:HD12	1:F:142:SER:O	2.09	0.51
1:J:191:ASP:OD2	1:L:330:ARG:HD3	2.10	0.51
1:A:34:GLY:HA3	1:D:130:TYR:CD1	2.46	0.51
1:D:44:ARG:HD3	1:D:168:PHE:HB3	1.93	0.51
1:H:219:ASN:N	1:H:220:PRO:CD	2.74	0.51
1:E:218:PRO:C	1:E:220:PRO:HD3	2.36	0.51
1:G:210:VAL:HG22	1:G:318:ILE:HD11	1.92	0.51
1:I:104:ILE:HD11	1:I:313:VAL:HG21	1.93	0.51
1:K:219:ASN:N	1:K:220:PRO:CD	2.74	0.51
1:M:52:ARG:HA	1:M:172:GLY:O	2.11	0.51
1:C:256:GLU:HG2	1:C:257:GLN:NE2	2.26	0.50
1:G:127:ARG:C	1:G:129:GLU:H	2.19	0.50
1:L:22:PRO:HG3	1:L:236:TYR:CZ	2.45	0.50
1:F:35:ASN:OD1	1:F:155:VAL:HA	2.11	0.50
1:F:218:PRO:C	1:F:220:PRO:HD3	2.36	0.50
1:L:9:LEU:HD22	1:L:12:ILE:HG21	1.93	0.50
1:E:207:LEU:HD11	1:E:341:ILE:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:222:GLY:HA2	1:F:300:PRO:HD2	1.94	0.50
1:I:106:LEU:HB3	1:I:269:ILE:CD1	2.40	0.50
1:L:40:LEU:HB3	1:L:65:TYR:CE1	2.47	0.50
1:M:76:HIS:HD2	3:M:372:HOH:O	1.94	0.50
1:C:205:ARG:HH22	1:D:251:GLN:CG	2.24	0.50
1:E:267:THR:N	1:E:306:ASP:OD2	2.43	0.50
1:H:225:MET:HE2	3:H:2091:HOH:O	2.11	0.50
1:K:244:ARG:HD3	3:K:535:HOH:O	2.10	0.50
1:J:205:ARG:CZ	1:J:207:LEU:HD21	2.41	0.50
1:K:88:ARG:HH21	1:K:302:HIS:CE1	2.30	0.50
1:L:305:MET:HE1	3:L:363:HOH:O	2.11	0.50
1:F:205:ARG:NE	1:F:207:LEU:HD21	2.27	0.50
1:H:17:ALA:O	1:H:355:LYS:HE3	2.12	0.50
1:A:219:ASN:N	1:A:220:PRO:CD	2.74	0.50
1:E:305:MET:HE1	3:G:1308:HOH:O	2.12	0.50
1:I:304:ASP:CA	1:K:285:GLN:HG2	2.41	0.50
1:A:35:ASN:OD1	1:A:155:VAL:HA	2.12	0.50
1:C:334:ASN:HD21	1:D:305:MET:HE1	1.75	0.50
1:I:218:PRO:C	1:I:220:PRO:HD3	2.37	0.50
1:K:127:ARG:C	1:K:129:GLU:H	2.19	0.50
1:A:194:ARG:HG3	1:A:236:TYR:O	2.11	0.49
1:J:157:PRO:HB3	1:J:161:LEU:HD23	1.93	0.49
1:D:45:SER:HB3	1:D:179:ALA:HB1	1.93	0.49
1:H:202:ALA:HA	1:H:214:ALA:O	2.11	0.49
1:K:126:GLU:HG2	1:K:130:TYR:CE2	2.47	0.49
1:M:153:THR:HG23	3:M:721:HOH:O	2.13	0.49
1:B:267:THR:N	1:B:306:ASP:OD2	2.45	0.49
1:K:277:ARG:HD3	1:K:316:ASP:C	2.38	0.49
1:O:76:HIS:HD2	3:O:778:HOH:O	1.94	0.49
1:C:88:ARG:HD2	1:C:302:HIS:CE1	2.47	0.49
1:D:76:HIS:HE1	3:D:1413:HOH:O	1.94	0.49
1:F:310:LEU:C	1:F:310:LEU:HD23	2.38	0.49
1:O:219:ASN:N	1:O:220:PRO:CD	2.76	0.49
1:H:153:THR:CG2	1:H:155:VAL:HG23	2.43	0.49
1:J:88:ARG:HD2	1:L:88:ARG:NH1	2.27	0.49
1:A:94:LEU:HD12	1:A:142:SER:O	2.13	0.49
1:A:251:GLN:CG	1:B:205:ARG:HH22	2.26	0.49
1:D:128:LEU:HD22	1:D:131:ARG:NE	2.20	0.49
1:G:125:LEU:HB2	1:H:112:TYR:CE1	2.48	0.49
1:H:218:PRO:C	1:H:220:PRO:HD3	2.38	0.49
1:A:126:GLU:HG2	1:A:130:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TYR:HB3	1:D:154:ALA:CB	2.43	0.49
1:H:346:MET:O	1:H:350:VAL:HG23	2.13	0.49
1:N:219:ASN:N	1:N:220:PRO:HD3	2.28	0.49
1:N:286:PHE:CE1	1:N:339:GLY:HA2	2.48	0.49
1:O:35:ASN:OD1	1:O:155:VAL:HA	2.12	0.49
1:I:205:ARG:CZ	1:I:207:LEU:HD21	2.42	0.49
1:I:219:ASN:N	1:I:220:PRO:HD3	2.28	0.49
1:I:284:ASN:OD1	1:I:288:LYS:HE3	2.12	0.49
1:K:67:GLU:O	1:K:153:THR:HG21	2.13	0.49
1:K:157:PRO:HB3	1:K:161:LEU:HD23	1.94	0.49
1:A:28:PRO:HD3	1:A:192:TRP:HB3	1.95	0.48
1:G:194:ARG:HB3	1:G:235:ASN:HA	1.94	0.48
1:B:210:VAL:HA	1:B:318:ILE:HD11	1.95	0.48
1:E:194:ARG:HB3	1:E:235:ASN:HA	1.94	0.48
1:H:277:ARG:HD2	1:H:316:ASP:C	2.37	0.48
1:I:71:GLY:HA2	1:I:161:LEU:HD21	1.94	0.48
1:M:194:ARG:HB3	1:M:235:ASN:HA	1.95	0.48
1:A:33:PRO:HD2	1:N:170:VAL:HG12	1.96	0.48
1:G:44:ARG:HD3	1:G:168:PHE:HB3	1.94	0.48
1:M:68:GLY:HA2	1:M:153:THR:OG1	2.14	0.48
1:E:45:SER:HB3	1:E:179:ALA:HB1	1.95	0.48
1:F:318:ILE:HD12	1:F:318:ILE:C	2.38	0.48
1:B:106:LEU:HD22	1:B:269:ILE:HD12	1.96	0.48
1:D:71:GLY:HA2	1:D:161:LEU:HD21	1.95	0.48
1:E:35:ASN:OD1	1:E:155:VAL:HA	2.14	0.48
1:C:128:LEU:HD23	1:C:131:ARG:HH21	1.78	0.48
1:E:88:ARG:HD2	1:G:88:ARG:NH1	2.28	0.48
1:G:28:PRO:HG3	1:G:192:TRP:CG	2.48	0.48
1:L:146:TYR:CZ	1:L:148:PHE:HB2	2.49	0.48
1:C:94:LEU:HD12	1:C:142:SER:O	2.14	0.48
1:G:191:ASP:OD1	1:G:193:ASP:HB2	2.14	0.48
1:D:82:ARG:HH11	1:D:82:ARG:HG2	1.79	0.48
1:E:336:THR:CB	1:G:305:MET:HE2	2.43	0.48
1:F:82:ARG:NH1	1:F:278:MET:O	2.47	0.48
1:H:171:PRO:HB3	3:H:2370:HOH:O	2.13	0.48
1:L:256:GLU:HG2	1:L:257:GLN:NE2	2.29	0.48
1:M:60:ILE:HD13	1:M:174:PHE:HD1	1.78	0.48
1:O:88:ARG:HH12	1:O:288:LYS:CG	2.27	0.48
1:A:9:LEU:O	1:A:12:ILE:HG22	2.14	0.48
1:B:244:ARG:NH2	1:B:252:GLU:OE2	2.37	0.48
1:D:33:PRO:O	1:D:153:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:ARG:NH1	1:H:88:ARG:HD2	2.29	0.48
1:H:244:ARG:NH2	1:H:252:GLU:OE2	2.46	0.48
1:I:186:SER:O	1:I:219:ASN:HA	2.13	0.47
3:B:2121:HOH:O	1:C:137:ALA:HB2	2.14	0.47
1:I:333:VAL:HG22	1:K:253:ALA:HB1	1.96	0.47
1:N:88:ARG:HH12	1:N:288:LYS:CB	2.16	0.47
1:B:128:LEU:HD12	1:B:138:GLN:HG2	1.94	0.47
1:J:192:TRP:HB2	1:L:330:ARG:NH2	2.29	0.47
1:L:219:ASN:N	1:L:220:PRO:CD	2.77	0.47
1:H:126:GLU:O	1:H:129:GLU:N	2.47	0.47
1:I:48:ARG:HG3	1:I:48:ARG:HH11	1.79	0.47
1:I:272:ILE:O	1:I:272:ILE:HG23	2.14	0.47
1:J:199:GLY:O	1:J:218:PRO:HD2	2.14	0.47
1:B:236:TYR:CZ	1:B:241:GLY:HA2	2.49	0.47
1:C:219:ASN:N	1:C:220:PRO:CD	2.78	0.47
1:F:306:ASP:HB3	1:F:308:ASP:OD1	2.15	0.47
1:M:69:PRO:HB2	1:M:183:MET:HE2	1.97	0.47
1:D:194:ARG:HG3	1:D:236:TYR:O	2.14	0.47
1:J:170:VAL:HG23	1:J:173:GLU:HB2	1.97	0.47
1:O:277:ARG:HD2	1:O:319:ASP:OD1	2.15	0.47
1:A:272:ILE:HG22	1:A:312:ALA:HA	1.95	0.47
1:B:153:THR:HG22	1:B:154:ALA:N	2.30	0.47
1:D:88:ARG:HH12	1:D:288:LYS:CB	2.24	0.47
1:E:205:ARG:NH2	1:E:207:LEU:HD21	2.30	0.47
1:J:304:ASP:CA	1:L:285:GLN:HG2	2.38	0.47
1:M:194:ARG:HD3	3:M:871:HOH:O	2.14	0.47
1:N:194:ARG:HB3	1:N:235:ASN:HA	1.97	0.47
1:N:218:PRO:C	1:N:220:PRO:CD	2.88	0.47
1:O:82:ARG:HG2	1:O:82:ARG:HH11	1.79	0.47
1:O:305:MET:HE1	3:O:389:HOH:O	2.14	0.47
1:A:277:ARG:HH21	1:A:319:ASP:CG	2.23	0.47
1:B:218:PRO:C	1:B:220:PRO:HD3	2.40	0.47
1:G:53:PHE:CZ	1:G:172:GLY:HA2	2.50	0.47
1:L:216:VAL:HG22	1:L:218:PRO:HD3	1.97	0.47
1:C:305:MET:HE2	1:D:336:THR:CB	2.45	0.47
1:D:205:ARG:HH21	1:D:207:LEU:HD21	1.76	0.47
1:I:52:ARG:HH12	1:I:173:GLU:CG	2.26	0.47
1:B:6:VAL:HB	1:B:10:THR:OG1	2.15	0.47
1:J:205:ARG:HH22	1:L:251:GLN:HG2	1.80	0.47
1:M:281:VAL:HG23	3:M:377:HOH:O	2.15	0.47
1:M:247:VAL:O	1:M:251:GLN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:ILE:HG22	1:D:312:ALA:HA	1.96	0.46
1:I:106:LEU:HB3	1:I:269:ILE:HD12	1.97	0.46
1:I:346:MET:O	1:I:350:VAL:HG23	2.15	0.46
1:L:272:ILE:O	1:L:272:ILE:HG23	2.14	0.46
1:L:277:ARG:HH21	1:L:317:GLU:C	2.23	0.46
1:M:219:ASN:N	1:M:220:PRO:HD3	2.30	0.46
1:E:153:THR:HG22	1:E:155:VAL:N	2.13	0.46
1:I:52:ARG:HA	1:I:172:GLY:O	2.16	0.46
1:K:272:ILE:HG23	1:K:272:ILE:O	2.15	0.46
1:F:127:ARG:C	1:F:129:GLU:H	2.24	0.46
1:G:151:ARG:HH11	1:G:153:THR:CG2	2.28	0.46
1:L:9:LEU:O	1:L:12:ILE:HG22	2.16	0.46
1:M:170:VAL:CG2	1:M:173:GLU:HB2	2.45	0.46
1:E:219:ASN:N	1:E:220:PRO:CD	2.79	0.46
1:I:258:VAL:HG22	1:K:321:PRO:HD3	1.97	0.46
1:D:163:ARG:HD3	3:D:1234:HOH:O	2.14	0.46
1:F:157:PRO:HB3	1:F:161:LEU:HD23	1.98	0.46
1:G:153:THR:OG1	1:G:155:VAL:HG23	2.14	0.46
1:G:279:SER:OG	1:G:282:GLU:HG3	2.16	0.46
1:I:205:ARG:HH22	1:K:251:GLN:CG	2.28	0.46
1:F:285:GLN:HG2	1:H:304:ASP:CA	2.42	0.46
1:G:219:ASN:N	1:G:220:PRO:CD	2.79	0.46
1:N:82:ARG:HG2	1:N:82:ARG:NH1	2.29	0.46
1:D:24:LEU:HD22	1:D:193:ASP:O	2.15	0.46
1:C:251:GLN:HG2	1:D:205:ARG:HH22	1.80	0.46
1:F:245:HIS:CD2	1:H:9:LEU:HD21	2.50	0.46
1:H:205:ARG:CZ	1:H:207:LEU:HD21	2.46	0.46
1:J:153:THR:CG2	1:J:155:VAL:HG23	2.46	0.46
1:B:27:PRO:HA	1:B:28:PRO:HD3	1.79	0.45
1:F:153:THR:HG22	1:F:154:ALA:N	2.30	0.45
1:F:194:ARG:HG3	1:F:236:TYR:O	2.17	0.45
1:N:134:PHE:HB3	3:N:1448:HOH:O	2.15	0.45
1:O:22:PRO:HG3	1:O:236:TYR:CZ	2.51	0.45
1:E:60:ILE:HD13	1:E:174:PHE:HD1	1.80	0.45
1:O:207:LEU:HD23	3:O:419:HOH:O	2.15	0.45
1:I:303:THR:HG22	1:K:289:GLN:CD	2.41	0.45
1:J:244:ARG:HD3	3:J:1890:HOH:O	2.16	0.45
1:B:67:GLU:O	1:B:153:THR:HG21	2.17	0.45
1:C:25:ALA:O	1:K:52:ARG:HD3	2.16	0.45
1:E:34:GLY:HA3	1:F:130:TYR:CD1	2.52	0.45
1:F:194:ARG:NH2	1:F:249:ASP:OD2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:27:PRO:HA	1:J:28:PRO:HD3	1.90	0.45
1:K:244:ARG:NH2	1:K:252:GLU:OE2	2.32	0.45
1:E:123:ALA:O	1:E:127:ARG:HG3	2.16	0.45
1:I:45:SER:HB3	1:I:179:ALA:HB1	1.97	0.45
1:J:18:VAL:HG11	1:J:232:VAL:HB	1.98	0.45
1:K:22:PRO:HG3	1:K:236:TYR:CZ	2.51	0.45
1:A:170:VAL:HG23	1:A:173:GLU:HB2	1.99	0.45
1:A:274:THR:O	1:A:314:THR:HA	2.17	0.45
1:B:247:VAL:O	1:B:251:GLN:HB2	2.16	0.45
1:G:60:ILE:HD13	1:G:174:PHE:HD1	1.80	0.45
1:G:82:ARG:HG2	1:G:82:ARG:HH11	1.82	0.45
1:H:277:ARG:NH1	1:H:317:GLU:O	2.50	0.45
1:I:226:ASP:HB2	3:I:1661:HOH:O	2.16	0.45
1:A:244:ARG:HD3	3:A:486:HOH:O	2.16	0.45
1:E:285:GLN:HG2	1:G:304:ASP:CA	2.44	0.45
1:K:115:GLU:HG3	1:L:118:ALA:HB1	1.98	0.45
1:K:189:LYS:CG	1:K:221:VAL:HA	2.40	0.45
1:L:277:ARG:HG3	1:L:316:ASP:OD2	2.17	0.45
1:A:191:ASP:OD2	1:B:330:ARG:CD	2.62	0.45
1:G:125:LEU:HD11	1:G:130:TYR:HA	1.99	0.45
1:J:251:GLN:HG2	1:L:205:ARG:HH22	1.82	0.45
1:N:180:GLY:O	1:N:183:MET:HG2	2.16	0.45
1:E:54:ASP:OD1	1:E:56:PRO:HD3	2.16	0.45
1:J:205:ARG:HH22	1:L:251:GLN:CG	2.30	0.45
1:L:258:VAL:HG12	1:L:258:VAL:O	2.17	0.45
1:M:218:PRO:C	1:M:220:PRO:CD	2.90	0.45
1:B:133:GLY:HA3	1:B:136:GLU:OE2	2.17	0.45
1:B:163:ARG:O	1:B:167:GLU:HG3	2.17	0.45
1:D:65:TYR:O	1:D:69:PRO:HA	2.16	0.45
1:F:122:GLY:O	1:F:126:GLU:HG3	2.17	0.45
1:K:76:HIS:HD2	3:K:1557:HOH:O	2.00	0.45
1:C:218:PRO:C	1:C:220:PRO:CD	2.90	0.44
1:I:28:PRO:HG3	1:I:192:TRP:CG	2.52	0.44
1:K:272:ILE:CG2	1:K:312:ALA:HA	2.47	0.44
1:N:194:ARG:HG2	1:N:236:TYR:C	2.43	0.44
1:B:245:HIS:ND1	1:B:247:VAL:HG12	2.32	0.44
1:C:88:ARG:HH12	1:C:288:LYS:HB3	1.82	0.44
1:E:279:SER:OG	1:E:282:GLU:HG3	2.17	0.44
1:G:52:ARG:HB3	1:G:52:ARG:NH1	2.32	0.44
1:K:219:ASN:N	1:K:220:PRO:HD3	2.32	0.44
1:N:272:ILE:HG21	1:N:286:PHE:CE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:TYR:O	1:E:69:PRO:HA	2.18	0.44
1:F:45:SER:HB3	1:F:179:ALA:HB1	1.99	0.44
1:F:88:ARG:NE	1:H:88:ARG:NE	2.66	0.44
1:G:22:PRO:HG3	1:G:236:TYR:CZ	2.52	0.44
1:I:277:ARG:HE	1:I:277:ARG:HB2	1.49	0.44
1:A:88:ARG:CZ	1:B:88:ARG:NE	2.81	0.44
1:A:329:GLY:HA3	1:B:191:ASP:HB2	1.98	0.44
1:B:183:MET:HE3	1:B:183:MET:HA	1.99	0.44
1:E:88:ARG:CZ	1:G:88:ARG:NH2	2.80	0.44
1:G:103:ALA:HB3	1:G:140:VAL:HG22	1.99	0.44
1:A:61:GLY:HA3	1:A:165:ALA:O	2.18	0.44
1:A:88:ARG:HD2	1:B:88:ARG:HH11	1.82	0.44
1:B:221:VAL:HG21	1:B:305:MET:HB2	1.99	0.44
1:J:330:ARG:H	1:J:330:ARG:HD3	1.82	0.44
1:F:219:ASN:N	1:F:220:PRO:CD	2.80	0.44
1:B:310:LEU:C	1:B:310:LEU:HD23	2.42	0.44
1:E:128:LEU:HD12	1:E:138:GLN:HG2	1.99	0.44
1:F:40:LEU:HB3	1:F:65:TYR:CE1	2.53	0.44
1:I:88:ARG:HG3	1:I:302:HIS:CE1	2.53	0.44
1:L:286:PHE:CE1	1:L:339:GLY:HA2	2.52	0.44
1:C:27:PRO:HA	1:C:192:TRP:CE3	2.52	0.44
1:C:71:GLY:HA2	1:C:161:LEU:HD21	2.00	0.44
1:C:334:ASN:ND2	1:D:305:MET:CE	2.75	0.44
1:O:170:VAL:CG2	1:O:173:GLU:HB2	2.48	0.44
1:H:272:ILE:O	1:H:272:ILE:HG23	2.17	0.44
1:K:68:GLY:HA2	1:K:153:THR:HG21	1.99	0.44
1:O:219:ASN:N	1:O:220:PRO:HD3	2.33	0.44
1:D:53:PHE:CE1	1:D:172:GLY:HA2	2.52	0.43
1:D:153:THR:CG2	1:D:155:VAL:H	2.22	0.43
1:H:52:ARG:HA	1:H:172:GLY:O	2.18	0.43
1:H:194:ARG:HB3	1:H:235:ASN:HA	2.00	0.43
1:J:45:SER:HB3	1:J:179:ALA:HB1	2.00	0.43
1:M:68:GLY:H	1:M:69:PRO:HA	1.84	0.43
1:N:68:GLY:HA2	1:N:153:THR:OG1	2.18	0.43
1:C:126:GLU:HG2	1:C:130:TYR:CZ	2.53	0.43
1:D:115:GLU:OE1	1:D:158:ASP:HB2	2.17	0.43
1:I:295:HIS:O	1:I:295:HIS:ND1	2.44	0.43
1:E:12:ILE:HG13	1:E:12:ILE:O	2.18	0.43
1:E:75:ILE:O	1:E:103:ALA:HA	2.18	0.43
1:G:128:LEU:HD22	1:G:131:ARG:NH2	2.33	0.43
1:G:328:ARG:NE	1:G:328:ARG:HA	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:153:THR:HG22	1:H:154:ALA:N	2.33	0.43
1:L:54:ASP:O	1:L:211:ARG:NE	2.46	0.43
1:O:82:ARG:NH1	1:O:278:MET:O	2.47	0.43
1:I:333:VAL:CG2	1:K:253:ALA:HB1	2.48	0.43
1:C:194:ARG:HG3	1:C:236:TYR:O	2.18	0.43
1:F:27:PRO:HA	1:F:28:PRO:HD3	1.90	0.43
1:I:61:GLY:HA3	1:I:165:ALA:O	2.19	0.43
3:I:518:HOH:O	1:K:305:MET:HE1	2.18	0.43
1:J:226:ASP:C	1:J:226:ASP:OD2	2.61	0.43
1:L:45:SER:HB3	1:L:179:ALA:HB1	1.99	0.43
1:L:277:ARG:HE	1:L:277:ARG:HB2	1.58	0.43
1:A:285:GLN:HG2	1:B:304:ASP:CA	2.43	0.43
1:D:310:LEU:C	1:D:310:LEU:HD23	2.44	0.43
1:E:153:THR:CG2	1:E:154:ALA:N	2.81	0.43
1:H:49:GLU:HG2	1:H:50:MET:N	2.34	0.43
1:I:218:PRO:C	1:I:220:PRO:CD	2.91	0.43
1:J:219:ASN:N	1:J:220:PRO:CD	2.82	0.43
1:C:103:ALA:HB3	1:C:140:VAL:HG22	2.00	0.43
1:E:128:LEU:C	1:E:129:GLU:HG2	2.43	0.43
1:E:153:THR:CG2	1:E:155:VAL:HG23	2.49	0.43
1:I:303:THR:OG1	1:I:306:ASP:OD1	2.29	0.43
1:B:219:ASN:N	1:B:220:PRO:CD	2.81	0.43
1:F:221:VAL:HG21	1:F:305:MET:HB2	2.01	0.43
1:F:334:ASN:HD21	1:H:305:MET:CE	2.32	0.43
1:M:133:GLY:HA3	1:M:136:GLU:OE2	2.19	0.43
1:E:71:GLY:HA2	1:E:161:LEU:HD21	2.01	0.43
1:E:310:LEU:C	1:E:310:LEU:HD23	2.43	0.43
1:F:71:GLY:O	1:F:181:ALA:HA	2.18	0.43
1:F:336:THR:HG21	1:H:305:MET:HE3	1.99	0.43
1:J:306:ASP:HB3	1:J:308:ASP:OD1	2.19	0.43
1:F:336:THR:HB	1:H:305:MET:CE	2.48	0.43
1:H:18:VAL:HG13	1:H:355:LYS:HA	2.01	0.43
1:I:321:PRO:HD3	1:K:258:VAL:HG22	2.00	0.43
1:N:19:ASP:HA	1:N:20:PRO:HD3	1.91	0.43
1:O:126:GLU:HG2	1:O:130:TYR:CE2	2.53	0.43
1:B:76:HIS:O	1:B:78:PRO:HD3	2.18	0.42
1:D:159:LYS:HE2	1:D:163:ARG:HH21	1.84	0.42
1:H:128:LEU:HD22	1:H:131:ARG:NE	2.29	0.42
1:A:88:ARG:HH11	1:A:288:LYS:CB	2.31	0.42
1:B:82:ARG:HB3	1:B:82:ARG:HH21	1.84	0.42
1:G:151:ARG:NH1	1:G:153:THR:HG23	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:GLU:CG	1:B:257:GLN:HE21	2.30	0.42
1:B:279:SER:OG	1:B:282:GLU:HG3	2.19	0.42
1:G:35:ASN:OD1	1:G:155:VAL:HA	2.19	0.42
1:K:35:ASN:OD1	1:K:155:VAL:HA	2.18	0.42
1:M:40:LEU:HB3	1:M:65:TYR:CE1	2.54	0.42
1:A:103:ALA:HB3	1:A:140:VAL:HG22	2.01	0.42
1:B:82:ARG:HH21	1:B:82:ARG:CB	2.32	0.42
1:F:258:VAL:HG22	1:H:321:PRO:HD3	2.02	0.42
1:J:126:GLU:HG2	1:J:130:TYR:CE2	2.53	0.42
1:J:157:PRO:HA	1:J:161:LEU:HD23	2.01	0.42
1:J:191:ASP:HB2	1:L:329:GLY:HA3	2.02	0.42
1:K:277:ARG:HA	1:K:316:ASP:OD2	2.19	0.42
1:C:128:LEU:C	1:C:129:GLU:CG	2.93	0.42
1:C:186:SER:HB2	1:C:195:THR:HG22	2.00	0.42
1:E:210:VAL:HA	1:E:318:ILE:HD11	2.01	0.42
1:K:247:VAL:O	1:K:251:GLN:HB2	2.20	0.42
1:O:52:ARG:HA	1:O:172:GLY:O	2.20	0.42
1:D:219:ASN:N	1:D:220:PRO:CD	2.82	0.42
1:E:221:VAL:HG21	1:E:305:MET:CB	2.46	0.42
1:I:153:THR:CG2	1:I:155:VAL:HG23	2.49	0.42
1:A:19:ASP:HA	1:A:20:PRO:HD3	1.91	0.42
1:B:112:TYR:CE1	1:C:125:LEU:HB2	2.54	0.42
1:B:186:SER:O	1:B:219:ASN:HA	2.20	0.42
1:C:52:ARG:HA	1:C:172:GLY:O	2.19	0.42
1:G:125:LEU:CD1	1:G:130:TYR:HA	2.49	0.42
1:J:194:ARG:HG3	1:J:236:TYR:C	2.44	0.42
1:K:88:ARG:O	1:K:89:GLY:O	2.36	0.42
1:G:310:LEU:C	1:G:310:LEU:HD23	2.45	0.42
1:I:202:ALA:HA	1:I:214:ALA:O	2.20	0.42
1:K:126:GLU:HG2	1:K:130:TYR:CZ	2.55	0.42
1:B:127:ARG:C	1:B:129:GLU:H	2.27	0.42
1:F:88:ARG:NH1	1:H:88:ARG:CD	2.82	0.42
1:F:277:ARG:HG3	1:F:316:ASP:OD2	2.20	0.42
1:K:170:VAL:HG23	1:K:173:GLU:HB2	2.02	0.42
1:K:272:ILE:HG21	1:K:286:PHE:HE2	1.85	0.42
1:M:157:PRO:HB3	1:M:161:LEU:HD23	2.02	0.42
1:B:21:ALA:HA	1:B:22:PRO:HD3	1.97	0.42
1:E:305:MET:CE	1:G:336:THR:HB	2.50	0.42
1:I:281:VAL:HG23	3:I:838:HOH:O	2.20	0.42
1:A:328:ARG:HA	1:A:328:ARG:CZ	2.50	0.41
1:B:210:VAL:HA	1:B:318:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:VAL:O	1:C:258:VAL:HG12	2.19	0.41
1:D:117:GLY:HA3	1:D:142:SER:OG	2.20	0.41
1:H:218:PRO:C	1:H:220:PRO:CD	2.93	0.41
1:I:244:ARG:NH2	1:I:252:GLU:OE2	2.50	0.41
1:K:52:ARG:HG2	1:K:173:GLU:HG2	2.02	0.41
1:A:219:ASN:N	1:A:220:PRO:HD3	2.35	0.41
1:C:310:LEU:HD23	1:C:310:LEU:C	2.45	0.41
1:E:256:GLU:HG2	1:E:257:GLN:HE21	1.85	0.41
1:G:34:GLY:HA3	1:H:130:TYR:CG	2.55	0.41
1:H:94:LEU:HD12	1:H:142:SER:O	2.20	0.41
1:I:305:MET:CE	1:K:336:THR:HG21	2.40	0.41
1:J:170:VAL:HG21	1:J:173:GLU:HB2	2.02	0.41
1:L:219:ASN:N	1:L:220:PRO:HD3	2.35	0.41
1:B:157:PRO:CB	1:B:161:LEU:HD23	2.49	0.41
1:G:75:ILE:O	1:G:103:ALA:HA	2.20	0.41
1:L:38:PHE:CD2	1:L:67:GLU:HG2	2.55	0.41
1:L:202:ALA:HA	1:L:214:ALA:O	2.20	0.41
1:A:53:PHE:CE1	1:A:172:GLY:HA2	2.56	0.41
1:F:256:GLU:CG	1:F:257:GLN:HE21	2.25	0.41
1:G:272:ILE:O	1:G:272:ILE:HG23	2.20	0.41
1:I:88:ARG:HD2	1:K:88:ARG:NH1	2.35	0.41
1:L:53:PHE:CE1	1:L:172:GLY:HA2	2.55	0.41
1:G:71:GLY:HA2	1:G:161:LEU:HD21	2.03	0.41
1:H:21:ALA:HA	1:H:22:PRO:HD3	1.79	0.41
1:J:88:ARG:HH11	1:J:288:LYS:HB3	1.83	0.41
1:J:244:ARG:NH2	1:J:248:PHE:HB3	2.35	0.41
1:M:277:ARG:HD2	1:M:319:ASP:OD1	2.20	0.41
1:O:82:ARG:HD2	3:O:2738:HOH:O	2.20	0.41
1:F:206:ARG:CZ	1:F:211:ARG:NH2	2.84	0.41
1:J:277:ARG:HE	1:J:277:ARG:HB2	1.70	0.41
1:J:285:GLN:HG2	1:L:304:ASP:CA	2.50	0.41
1:K:88:ARG:NH1	1:K:288:LYS:HB3	2.36	0.41
1:L:12:ILE:O	1:L:12:ILE:HG13	2.20	0.41
1:L:119:GLY:HA2	1:L:159:LYS:HG3	2.02	0.41
1:L:256:GLU:HG2	1:L:257:GLN:HE21	1.84	0.41
1:M:180:GLY:O	1:M:183:MET:HG2	2.21	0.41
1:O:82:ARG:HG2	1:O:82:ARG:NH1	2.36	0.41
1:A:310:LEU:HD23	1:A:310:LEU:C	2.46	0.41
1:J:88:ARG:HH21	1:J:302:HIS:CE1	2.39	0.41
1:N:236:TYR:CE1	1:N:238:ALA:HA	2.56	0.41
1:A:272:ILE:HG23	1:A:272:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:ALA:HA	1:D:22:PRO:HD3	1.87	0.41
1:E:218:PRO:C	1:E:220:PRO:CD	2.94	0.41
1:O:170:VAL:HG23	1:O:173:GLU:HB2	2.02	0.41
1:A:272:ILE:O	1:A:272:ILE:CG2	2.69	0.41
1:B:40:LEU:HD13	1:B:65:TYR:CE2	2.56	0.41
1:B:64:HIS:HB2	1:B:70:THR:O	2.20	0.41
1:E:251:GLN:HG3	1:G:205:ARG:HH22	1.86	0.41
1:G:256:GLU:HG2	1:G:257:GLN:NE2	2.35	0.41
1:M:274:THR:O	1:M:314:THR:HA	2.21	0.41
1:O:18:VAL:HG11	1:O:232:VAL:HB	2.01	0.41
1:B:272:ILE:O	1:B:272:ILE:HG23	2.20	0.41
1:D:29:VAL:HB	1:D:152:SER:OG	2.20	0.41
1:E:125:LEU:HB2	1:F:112:TYR:CE1	2.56	0.41
1:E:128:LEU:HD23	1:E:131:ARG:HH21	1.86	0.41
1:H:128:LEU:HD23	1:H:128:LEU:HA	1.90	0.41
1:K:82:ARG:HH11	1:K:82:ARG:HG2	1.86	0.41
1:N:21:ALA:HA	1:N:22:PRO:HD3	1.93	0.41
1:F:305:MET:HE2	1:H:336:THR:CB	2.51	0.40
1:H:24:LEU:HD21	1:H:236:TYR:HD1	1.86	0.40
1:J:153:THR:HG22	1:J:154:ALA:N	2.36	0.40
1:K:226:ASP:HB2	3:K:692:HOH:O	2.20	0.40
1:L:306:ASP:HB3	1:L:308:ASP:OD1	2.21	0.40
1:N:194:ARG:CG	1:N:236:TYR:O	2.68	0.40
1:N:323:THR:HB	3:N:1595:HOH:O	2.21	0.40
1:E:27:PRO:HA	1:E:28:PRO:HD3	1.98	0.40
1:G:16:ILE:HD12	1:G:351:LEU:HB2	2.03	0.40
1:G:237:ASP:HB3	1:G:240:THR:OG1	2.21	0.40
1:I:69:PRO:HB2	1:I:183:MET:HE2	2.03	0.40
1:I:205:ARG:HE	1:I:207:LEU:CD2	2.27	0.40
1:I:205:ARG:HH22	1:K:251:GLN:HG3	1.84	0.40
1:J:82:ARG:NH1	1:J:82:ARG:CG	2.80	0.40
1:J:202:ALA:HA	1:J:214:ALA:O	2.21	0.40
1:J:205:ARG:HE	1:J:207:LEU:HD21	1.86	0.40
1:K:248:PHE:O	1:K:252:GLU:HG3	2.21	0.40
3:M:822:HOH:O	1:N:30:PHE:HB3	2.21	0.40
1:N:310:LEU:HD23	1:N:310:LEU:C	2.46	0.40
1:A:218:PRO:C	1:A:220:PRO:CD	2.94	0.40
3:A:1249:HOH:O	1:B:335:ALA:HB3	2.21	0.40
1:C:67:GLU:OE2	1:C:67:GLU:N	2.49	0.40
1:C:219:ASN:N	1:C:220:PRO:HD3	2.35	0.40
1:F:128:LEU:HD23	1:F:128:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:128:LEU:HD23	1:H:131:ARG:HH21	1.86	0.40
1:J:52:ARG:HA	1:J:172:GLY:O	2.21	0.40
1:K:218:PRO:C	1:K:220:PRO:CD	2.95	0.40
1:B:258:VAL:O	1:B:258:VAL:HG12	2.22	0.40
1:G:256:GLU:HG2	1:G:257:GLN:HE21	1.86	0.40
1:H:186:SER:HB2	1:H:195:THR:HG22	2.03	0.40
1:I:236:TYR:HA	1:I:243:ARG:HG2	2.03	0.40
1:J:71:GLY:HA2	1:J:161:LEU:HD21	2.04	0.40
1:J:88:ARG:NH1	1:J:288:LYS:CB	2.84	0.40
1:C:82:ARG:HG2	1:C:82:ARG:NH1	2.35	0.40
1:F:305:MET:HE2	1:H:336:THR:HB	2.02	0.40
1:I:257:GLN:HG3	1:K:325:GLY:O	2.22	0.40
1:N:50:MET:CG	1:N:173:GLU:HG2	2.51	0.40
1:O:21:ALA:HA	1:O:22:PRO:HD3	1.91	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	340/355 (96%)	326 (96%)	14 (4%)	0	100	100
1	B	340/355 (96%)	324 (95%)	16 (5%)	0	100	100
1	C	340/355 (96%)	327 (96%)	12 (4%)	1 (0%)	36	35
1	D	340/355 (96%)	329 (97%)	11 (3%)	0	100	100
1	E	340/355 (96%)	321 (94%)	19 (6%)	0	100	100
1	F	340/355 (96%)	327 (96%)	11 (3%)	2 (1%)	21	17
1	G	340/355 (96%)	327 (96%)	13 (4%)	0	100	100
1	H	340/355 (96%)	322 (95%)	17 (5%)	1 (0%)	36	35
1	I	340/355 (96%)	326 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	340/355 (96%)	320 (94%)	20 (6%)	0	100	100
1	K	336/355 (95%)	319 (95%)	16 (5%)	1 (0%)	36	35
1	L	340/355 (96%)	322 (95%)	18 (5%)	0	100	100
1	M	340/355 (96%)	327 (96%)	13 (4%)	0	100	100
1	N	340/355 (96%)	326 (96%)	13 (4%)	1 (0%)	36	35
1	O	340/355 (96%)	326 (96%)	14 (4%)	0	100	100
All	All	5096/5325 (96%)	4869 (96%)	221 (4%)	6 (0%)	48	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	89	GLY
1	C	68	GLY
1	F	68	GLY
1	F	89	GLY
1	N	68	GLY
1	H	68	GLY

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	252/261 (97%)	249 (99%)	3 (1%)	63	70
1	B	252/261 (97%)	247 (98%)	5 (2%)	48	54
1	C	252/261 (97%)	244 (97%)	8 (3%)	34	35
1	D	252/261 (97%)	250 (99%)	2 (1%)	73	80
1	E	252/261 (97%)	249 (99%)	3 (1%)	63	70
1	F	252/261 (97%)	250 (99%)	2 (1%)	73	80
1	G	252/261 (97%)	249 (99%)	3 (1%)	63	70
1	H	252/261 (97%)	248 (98%)	4 (2%)	55	62
1	I	252/261 (97%)	248 (98%)	4 (2%)	55	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	252/261 (97%)	249 (99%)	3 (1%)	63	70
1	K	251/261 (96%)	247 (98%)	4 (2%)	55	62
1	L	252/261 (97%)	249 (99%)	3 (1%)	63	70
1	M	252/261 (97%)	250 (99%)	2 (1%)	73	80
1	N	252/261 (97%)	251 (100%)	1 (0%)	84	89
1	O	252/261 (97%)	252 (100%)	0	100	100
All	All	3779/3915 (96%)	3732 (99%)	47 (1%)	63	70

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	277	ARG
1	A	330	ARG
1	B	44	ARG
1	B	82	ARG
1	B	183	MET
1	B	277	ARG
1	B	330	ARG
1	C	128	LEU
1	C	129	GLU
1	C	207	LEU
1	C	251	GLN
1	C	277	ARG
1	C	305	MET
1	C	318	ILE
1	C	330	ARG
1	D	44	ARG
1	D	277	ARG
1	E	129	GLU
1	E	277	ARG
1	E	330	ARG
1	F	129	GLU
1	F	277	ARG
1	G	44	ARG
1	G	82	ARG
1	G	277	ARG
1	H	82	ARG
1	H	128	LEU
1	H	129	GLU

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Mol	Chain	Res	Type
1	H	330	ARG
1	I	52	ARG
1	I	176	GLN
1	I	277	ARG
1	I	330	ARG
1	J	82	ARG
1	J	129	GLU
1	J	330	ARG
1	K	129	GLU
1	K	189	LYS
1	K	277	ARG
1	K	330	ARG
1	L	52	ARG
1	L	251	GLN
1	L	305	MET
1	M	39	ASP
1	M	305	MET
1	N	330	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	219	ASN
1	B	257	GLN
1	B	284	ASN
1	C	138	GLN
1	C	257	GLN
1	C	284	ASN
1	D	284	ASN
1	E	257	GLN
1	F	76	HIS
1	F	257	GLN
1	F	284	ASN
1	G	257	GLN
1	G	334	ASN
1	H	257	GLN
1	H	284	ASN
1	H	285	GLN
1	I	176	GLN
1	I	257	GLN
1	J	138	GLN
1	J	257	GLN

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Mol	Chain	Res	Type
1	L	257	GLN
1	L	284	ASN
1	M	76	HIS
1	M	251	GLN
1	O	76	HIS
1	O	101	ASN
1	O	251	GLN
1	O	284	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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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	344/355 (96%)	0.43	25 (7%) 21 19	18, 31, 50, 71	0
1	B	344/355 (96%)	1.09	71 (20%) 2 2	22, 40, 60, 70	0
1	C	344/355 (96%)	0.43	27 (7%) 19 18	18, 30, 51, 64	0
1	D	344/355 (96%)	0.42	21 (6%) 27 26	18, 32, 53, 74	0
1	E	344/355 (96%)	1.13	64 (18%) 3 3	21, 39, 60, 83	0
1	F	344/355 (96%)	0.73	36 (10%) 11 10	21, 32, 54, 77	0
1	G	344/355 (96%)	0.43	31 (9%) 15 14	18, 31, 53, 69	0
1	H	344/355 (96%)	1.12	55 (15%) 5 4	20, 37, 59, 74	0
1	I	344/355 (96%)	1.36	82 (23%) 2 2	25, 38, 55, 67	0
1	J	344/355 (96%)	0.51	32 (9%) 14 13	19, 30, 56, 71	0
1	K	342/355 (96%)	0.45	25 (7%) 21 19	19, 30, 49, 64	0
1	L	344/355 (96%)	0.51	29 (8%) 17 15	20, 32, 51, 63	0
1	M	344/355 (96%)	-0.44	7 (2%) 65 64	10, 18, 35, 57	0
1	N	344/355 (96%)	-0.51	7 (2%) 65 64	10, 19, 33, 49	0
1	O	344/355 (96%)	-0.41	4 (1%) 76 76	13, 21, 34, 45	0
All	All	5158/5325 (96%)	0.48	516 (10%) 12 11	10, 31, 54, 83	0

All (516) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	89	GLY	7.8
1	A	134	PHE	7.0
1	F	192	TRP	7.0
1	E	134	PHE	6.8
1	J	134	PHE	6.1
1	J	91	ALA	5.9
1	F	91	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	F	30	PHE	5.8
1	C	30	PHE	5.8
1	F	134	PHE	5.7
1	H	6	VAL	5.7
1	G	31	GLY	5.6
1	B	134	PHE	5.6
1	C	192	TRP	5.6
1	I	6	VAL	5.5
1	G	134	PHE	5.5
1	K	339	GLY	5.4
1	K	91	ALA	5.4
1	K	88	ARG	5.4
1	C	6	VAL	5.3
1	J	92	VAL	5.1
1	A	6	VAL	5.0
1	B	29	VAL	4.9
1	A	89	GLY	4.9
1	I	89	GLY	4.9
1	I	30	PHE	4.7
1	E	6	VAL	4.6
1	I	260	PRO	4.6
1	B	6	VAL	4.6
1	I	29	VAL	4.6
1	J	93	GLY	4.6
1	M	134	PHE	4.6
1	G	91	ALA	4.5
1	A	50	MET	4.5
1	J	133	GLY	4.5
1	M	91	ALA	4.5
1	C	130	TYR	4.5
1	H	134	PHE	4.5
1	D	192	TRP	4.4
1	N	192	TRP	4.4
1	K	90	GLY	4.4
1	F	153	THR	4.4
1	F	6	VAL	4.4
1	K	134	PHE	4.3
1	M	89	GLY	4.3
1	I	238	ALA	4.3
1	K	6	VAL	4.3
1	E	318	ILE	4.3
1	E	152	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	91	ALA	4.2
1	I	339	GLY	4.2
1	D	6	VAL	4.1
1	J	29	VAL	4.1
1	G	89	GLY	4.0
1	I	134	PHE	4.0
1	I	340	ALA	4.0
1	H	152	SER	4.0
1	A	88	ARG	4.0
1	E	253	ALA	3.9
1	G	6	VAL	3.9
1	H	29	VAL	3.9
1	J	6	VAL	3.9
1	B	69	PRO	3.9
1	G	90	GLY	3.9
1	E	150	ALA	3.9
1	L	152	SER	3.9
1	G	30	PHE	3.9
1	B	128	LEU	3.9
1	L	6	VAL	3.9
1	E	30	PHE	3.9
1	D	29	VAL	3.8
1	J	132	THR	3.8
1	D	30	PHE	3.8
1	H	30	PHE	3.8
1	L	31	GLY	3.8
1	E	50	MET	3.8
1	I	37	ALA	3.7
1	E	130	TYR	3.7
1	G	324	PRO	3.7
1	C	89	GLY	3.7
1	A	91	ALA	3.7
1	G	255	ALA	3.7
1	D	242	VAL	3.7
1	O	6	VAL	3.7
1	A	260	PRO	3.6
1	G	325	GLY	3.6
1	A	340	ALA	3.6
1	F	33	PRO	3.6
1	M	88	ARG	3.6
1	C	92	VAL	3.6
1	B	30	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	192	TRP	3.5
1	B	242	VAL	3.5
1	K	260	PRO	3.5
1	L	260	PRO	3.5
1	L	192	TRP	3.5
1	K	340	ALA	3.5
1	D	149	SER	3.5
1	I	258	VAL	3.5
1	C	93	GLY	3.5
1	J	260	PRO	3.4
1	J	31	GLY	3.4
1	L	93	GLY	3.4
1	B	236	TYR	3.4
1	H	153	THR	3.4
1	M	92	VAL	3.4
1	A	318	ILE	3.4
1	K	341	ILE	3.4
1	G	29	VAL	3.4
1	H	339	GLY	3.4
1	B	50	MET	3.4
1	M	6	VAL	3.4
1	N	6	VAL	3.4
1	E	191	ASP	3.3
1	F	92	VAL	3.3
1	I	177	GLY	3.3
1	G	52	ARG	3.3
1	H	44	ARG	3.3
1	I	88	ARG	3.3
1	B	240	THR	3.3
1	I	27	PRO	3.3
1	E	12	ILE	3.3
1	G	318	ILE	3.3
1	I	153	THR	3.3
1	A	90	GLY	3.3
1	G	32	GLY	3.3
1	H	135	ALA	3.3
1	J	128	LEU	3.3
1	E	239	GLN	3.3
1	L	322	THR	3.2
1	B	47	GLY	3.2
1	B	260	PRO	3.2
1	B	88	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	51	LEU	3.2
1	J	39	ASP	3.2
1	G	88	ARG	3.2
1	K	207	LEU	3.2
1	L	12	ILE	3.2
1	E	153	THR	3.2
1	E	172	GLY	3.2
1	L	92	VAL	3.1
1	B	318	ILE	3.1
1	E	193	ASP	3.1
1	E	88	ARG	3.1
1	B	172	GLY	3.1
1	C	260	PRO	3.1
1	I	28	PRO	3.1
1	K	259	PRO	3.1
1	I	40	LEU	3.1
1	F	236	TYR	3.1
1	F	39	ASP	3.1
1	L	91	ALA	3.1
1	E	128	LEU	3.1
1	F	339	GLY	3.0
1	I	236	TYR	3.0
1	B	51	LEU	3.0
1	E	242	VAL	3.0
1	I	18	VAL	3.0
1	D	152	SER	3.0
1	E	44	ARG	3.0
1	E	46	THR	3.0
1	E	192	TRP	3.0
1	L	153	THR	3.0
1	E	135	ALA	3.0
1	E	258	VAL	3.0
1	H	149	SER	3.0
1	J	258	VAL	3.0
1	H	88	ARG	3.0
1	A	322	THR	3.0
1	J	192	TRP	3.0
1	F	149	SER	3.0
1	I	25	ALA	3.0
1	F	29	VAL	3.0
1	J	318	ILE	3.0
1	I	50	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	N	88	ARG	2.9
1	B	37	ALA	2.9
1	B	41	ALA	2.9
1	A	325	GLY	2.9
1	H	318	ILE	2.9
1	I	12	ILE	2.9
1	E	167	GLU	2.9
1	L	29	VAL	2.9
1	F	88	ARG	2.9
1	J	130	TYR	2.9
1	L	149	SER	2.9
1	F	150	ALA	2.9
1	I	41	ALA	2.9
1	H	128	LEU	2.9
1	F	318	ILE	2.9
1	B	150	ALA	2.9
1	B	239	GLN	2.8
1	E	257	GLN	2.8
1	L	52	ARG	2.8
1	I	16	ILE	2.8
1	F	38	PHE	2.8
1	I	148	PHE	2.8
1	I	57	GLY	2.8
1	E	124	LEU	2.8
1	I	192	TRP	2.8
1	E	170	VAL	2.8
1	I	240	THR	2.8
1	C	318	ILE	2.8
1	L	318	ILE	2.8
1	C	88	ARG	2.8
1	O	134	PHE	2.8
1	I	146	TYR	2.8
1	H	25	ALA	2.8
1	B	40	LEU	2.8
1	D	153	THR	2.8
1	B	43	VAL	2.8
1	G	260	PRO	2.8
1	B	151	ARG	2.8
1	I	34	GLY	2.8
1	I	90	GLY	2.8
1	N	30	PHE	2.8
1	B	353	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	91	ALA	2.8
1	A	207	LEU	2.8
1	J	94	LEU	2.8
1	D	88	ARG	2.7
1	G	50	MET	2.7
1	F	93	GLY	2.7
1	L	15	GLY	2.7
1	I	207	LEU	2.7
1	B	46	THR	2.7
1	B	44	ARG	2.7
1	D	28	PRO	2.7
1	D	318	ILE	2.7
1	I	68	GLY	2.7
1	D	37	ALA	2.7
1	D	150	ALA	2.7
1	H	9	LEU	2.7
1	H	207	LEU	2.7
1	J	88	ARG	2.7
1	E	260	PRO	2.7
1	I	43	VAL	2.7
1	B	149	SER	2.7
1	F	90	GLY	2.7
1	H	31	GLY	2.7
1	I	31	GLY	2.7
1	M	93	GLY	2.7
1	E	151	ARG	2.7
1	H	151	ARG	2.7
1	L	88	ARG	2.7
1	F	255	ALA	2.7
1	I	24	LEU	2.7
1	B	193	ASP	2.7
1	E	52	ARG	2.7
1	I	151	ARG	2.7
1	J	26	GLY	2.7
1	E	137	ALA	2.6
1	H	129	GLU	2.6
1	H	238	ALA	2.6
1	B	168	PHE	2.6
1	F	46	THR	2.6
1	J	30	PHE	2.6
1	B	131	ARG	2.6
1	B	68	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	222	GLY	2.6
1	H	41	ALA	2.6
1	K	323	THR	2.6
1	B	207	LEU	2.6
1	C	134	PHE	2.6
1	E	40	LEU	2.6
1	I	56	PRO	2.6
1	H	327	SER	2.6
1	B	130	TYR	2.6
1	G	333	VAL	2.6
1	H	210	VAL	2.6
1	H	242	VAL	2.6
1	E	15	GLY	2.6
1	B	62	ALA	2.6
1	C	37	ALA	2.6
1	G	323	THR	2.6
1	H	37	ALA	2.6
1	H	154	ALA	2.6
1	I	165	ALA	2.6
1	J	259	PRO	2.6
1	B	191	ASP	2.6
1	G	36	ASP	2.6
1	L	30	PHE	2.6
1	B	170	VAL	2.6
1	C	43	VAL	2.6
1	G	130	TYR	2.6
1	H	130	TYR	2.6
1	I	242	VAL	2.6
1	K	318	ILE	2.6
1	N	318	ILE	2.6
1	I	15	GLY	2.6
1	F	37	ALA	2.6
1	D	260	PRO	2.6
1	A	12	ILE	2.5
1	I	131	ARG	2.5
1	F	238	ALA	2.5
1	J	135	ALA	2.5
1	B	15	GLY	2.5
1	B	201	GLY	2.5
1	C	339	GLY	2.5
1	H	12	ILE	2.5
1	I	170	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	90	GLY	2.5
1	K	329	GLY	2.5
1	B	195	THR	2.5
1	H	10	THR	2.5
1	I	198	THR	2.5
1	B	171	PRO	2.5
1	F	259	PRO	2.5
1	G	135	ALA	2.5
1	F	234	GLY	2.5
1	H	133	GLY	2.5
1	J	131	ARG	2.5
1	H	239	GLN	2.5
1	E	41	ALA	2.5
1	I	62	ALA	2.5
1	G	207	LEU	2.5
1	L	207	LEU	2.5
1	F	151	ARG	2.5
1	H	38	PHE	2.5
1	A	339	GLY	2.5
1	I	71	GLY	2.5
1	B	18	VAL	2.4
1	K	333	VAL	2.4
1	C	322	THR	2.4
1	I	46	THR	2.4
1	K	332	SER	2.4
1	G	28	PRO	2.4
1	I	33	PRO	2.4
1	B	17	ALA	2.4
1	I	17	ALA	2.4
1	H	320	LEU	2.4
1	O	88	ARG	2.4
1	B	61	GLY	2.4
1	E	90	GLY	2.4
1	I	26	GLY	2.4
1	A	239	GLN	2.4
1	E	149	SER	2.4
1	E	236	TYR	2.4
1	E	22	PRO	2.4
1	E	163	ARG	2.4
1	C	128	LEU	2.4
1	G	128	LEU	2.4
1	I	14	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	239	GLN	2.4
1	B	152	SER	2.4
1	C	149	SER	2.4
1	H	127	ARG	2.4
1	I	69	PRO	2.4
1	L	150	ALA	2.4
1	E	129	GLU	2.4
1	B	31	GLY	2.4
1	B	241	GLY	2.4
1	F	241	GLY	2.4
1	I	32	GLY	2.4
1	B	341	ILE	2.4
1	D	258	VAL	2.4
1	I	92	VAL	2.4
1	I	341	ILE	2.4
1	E	132	THR	2.4
1	A	130	TYR	2.3
1	B	135	ALA	2.3
1	B	167	GLU	2.3
1	E	25	ALA	2.3
1	I	239	GLN	2.3
1	I	172	GLY	2.3
1	I	208	GLY	2.3
1	L	90	GLY	2.3
1	I	193	ASP	2.3
1	C	38	PHE	2.3
1	I	52	ARG	2.3
1	F	240	THR	2.3
1	J	153	THR	2.3
1	K	46	THR	2.3
1	F	239	GLN	2.3
1	G	239	GLN	2.3
1	I	176	GLN	2.3
1	B	25	ALA	2.3
1	D	154	ALA	2.3
1	E	81	ALA	2.3
1	I	179	ALA	2.3
1	J	238	ALA	2.3
1	E	207	LEU	2.3
1	K	325	GLY	2.3
1	E	131	ARG	2.3
1	H	163	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	127	ARG	2.3
1	K	272	ILE	2.3
1	C	29	VAL	2.3
1	E	66	GLU	2.3
1	B	153	THR	2.3
1	I	259	PRO	2.3
1	D	25	ALA	2.3
1	E	17	ALA	2.3
1	I	353	ALA	2.3
1	C	325	GLY	2.3
1	L	9	LEU	2.3
1	L	339	GLY	2.3
1	H	50	MET	2.3
1	B	197	ILE	2.3
1	B	258	VAL	2.3
1	H	333	VAL	2.3
1	I	232	VAL	2.3
1	F	260	PRO	2.3
1	J	28	PRO	2.3
1	E	238	ALA	2.3
1	E	255	ALA	2.3
1	F	253	ALA	2.3
1	H	150	ALA	2.3
1	H	185	ALA	2.3
1	J	255	ALA	2.3
1	B	177	GLY	2.3
1	F	34	GLY	2.3
1	K	208	GLY	2.3
1	A	128	LEU	2.3
1	E	51	LEU	2.3
1	H	166	LEU	2.3
1	L	50	MET	2.3
1	I	152	SER	2.2
1	I	38	PHE	2.2
1	I	272	ILE	2.2
1	A	323	THR	2.2
1	E	322	THR	2.2
1	B	52	ARG	2.2
1	G	330	ARG	2.2
1	B	54	ASP	2.2
1	H	319	ASP	2.2
1	B	21	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	241	GLY	2.2
1	I	150	ALA	2.2
1	N	340	ALA	2.2
1	K	94	LEU	2.2
1	G	327	SER	2.2
1	A	39	ASP	2.2
1	E	339	GLY	2.2
1	H	15	GLY	2.2
1	B	255	ALA	2.2
1	H	179	ALA	2.2
1	H	27	PRO	2.2
1	H	28	PRO	2.2
1	A	92	VAL	2.2
1	G	92	VAL	2.2
1	A	172	GLY	2.2
1	E	89	GLY	2.2
1	I	354	GLY	2.2
1	B	63	ALA	2.2
1	F	251	GLN	2.2
1	N	239	GLN	2.2
1	G	320	LEU	2.2
1	A	326	SER	2.2
1	H	131	ARG	2.2
1	B	28	PRO	2.1
1	F	28	PRO	2.1
1	L	209	ASP	2.2
1	I	53	PHE	2.1
1	A	15	GLY	2.1
1	C	90	GLY	2.1
1	E	26	GLY	2.1
1	E	31	GLY	2.1
1	I	351	LEU	2.1
1	J	152	SER	2.1
1	E	39	ASP	2.1
1	B	22	PRO	2.1
1	G	322	THR	2.1
1	K	321	PRO	2.1
1	F	254	PHE	2.1
1	L	16	ILE	2.1
1	B	339	GLY	2.1
1	C	131	ARG	2.1
1	K	330	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	135	ALA	2.1
1	B	160	ALA	2.1
1	H	255	ALA	2.1
1	I	135	ALA	2.1
1	I	253	ALA	2.1
1	D	207	LEU	2.1
1	F	128	LEU	2.1
1	K	331	LEU	2.1
1	L	327	SER	2.1
1	I	305	MET	2.1
1	B	66	GLU	2.1
1	B	237	ASP	2.1
1	B	259	PRO	2.1
1	E	28	PRO	2.1
1	H	322	THR	2.1
1	J	322	THR	2.1
1	D	26	GLY	2.1
1	H	60	ILE	2.1
1	I	180	GLY	2.1
1	E	100	PHE	2.1
1	B	238	ALA	2.1
1	H	164	ALA	2.1
1	L	238	ALA	2.1
1	H	66	GLU	2.1
1	C	36	ASP	2.1
1	B	132	THR	2.1
1	D	33	PRO	2.1
1	E	323	THR	2.1
1	L	321	PRO	2.1
1	B	26	GLY	2.1
1	E	38	PHE	2.1
1	I	204	PHE	2.1
1	O	91	ALA	2.1
1	B	27	PRO	2.0
1	B	33	PRO	2.0
1	E	171	PRO	2.0
1	E	60	ILE	2.0
1	H	16	ILE	2.0
1	C	66	GLU	2.0
1	H	18	VAL	2.0
1	J	254	PHE	2.0
1	E	21	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	207	LEU	2.0
1	D	239	GLN	2.0
1	I	42	PRO	2.0
1	H	325	GLY	2.0
1	I	47	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($\text{\AA}^2$)	Q<0.9
2	NA	A	3005	1/1	0.95	0.07	32,32,32,32	0
2	NA	L	3006	1/1	0.95	0.08	44,44,44,44	0
2	NA	O	3004	1/1	0.95	0.06	34,34,34,34	0
2	NA	K	3001	1/1	0.96	0.06	28,28,28,28	0
2	NA	M	3003	1/1	0.97	0.06	32,32,32,32	0
2	NA	N	3002	1/1	0.99	0.05	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.