



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:20 PM UTC

PDB ID : 3M85 / pdb_00003m85
Title : Archaeoglobus fulgidus exosome y70a with RNA bound to the active site
Authors : Hartung, S.; Hopfner, K.-P.
Deposited on : 2010-03-17
Resolution : 3.00 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

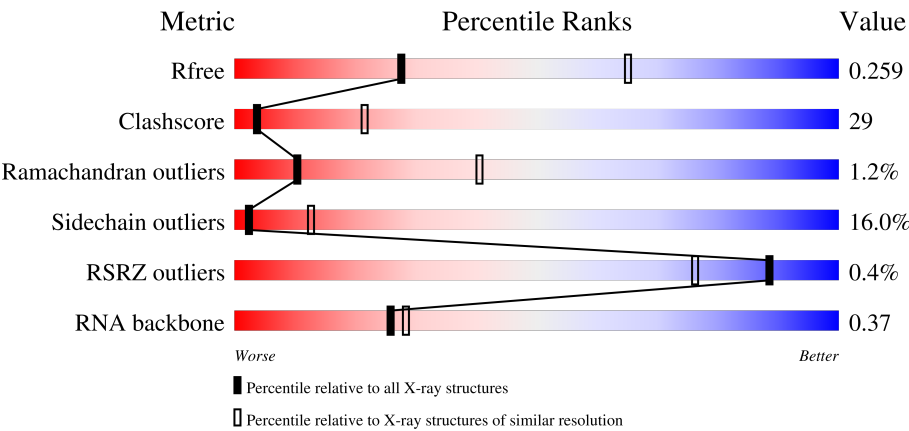
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	179	51%42%6%
1	B	179	2% 45%42%13%
1	C	179	53%41%6%
2	D	258	41%44%9%6%

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Mol	Chain	Length	Quality of chain
2	E	258	47%37%10%5%
2	F	258	51%38%7%5%
3	G	259	% 42%47%9% .
3	H	259	% 47%41%12%
3	I	259	58%36%6%
4	X	6	17%33%17%33%
4	Y	6	17%33%17%33%
4	Z	6	33%17%17%33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16110 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 Putative uncharacterized protein AF_0206.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	18	0	0
			1371	855	242	266	8			
1	B	179	Total	C	N	O	S	61	0	0
			1371	855	242	266	8			
1	C	179	Total	C	N	O	S	16	0	0
			1371	855	242	266	8			

- Molecule 2 is a protein called Probable exosome complex exonuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	243	Total	C	N	O	S	33	0	0
			1902	1198	334	357	13			
2	E	245	Total	C	N	O	S	48	0	0
			1920	1209	337	361	13			
2	F	246	Total	C	N	O	S	14	0	0
			1926	1213	337	363	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	65	GLU	ARG	engineered mutation	UNP O29757
E	65	GLU	ARG	engineered mutation	UNP O29757
F	65	GLU	ARG	engineered mutation	UNP O29757

- Molecule 3 is a protein called Probable exosome complex exonuclease 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	258	Total	C	N	O	S	77	0	0
			1997	1259	331	401	6			
3	H	258	Total	C	N	O	S	46	0	0
			1997	1259	331	401	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	259	Total	C	N	O	S	62	0	0
			2006	1265	332	403	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	70	ALA	TYR	engineered mutation	UNP O29756
H	70	ALA	TYR	engineered mutation	UNP O29756
I	70	ALA	TYR	engineered mutation	UNP O29756

- Molecule 4 is a RNA chain called 5'-R(*CP*UP*CP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	X	4	Total	C	N	O	P	1	0	0
			80	36	12	28	4			
4	Y	4	Total	C	N	O	P	1	0	0
			80	36	12	28	4			
4	Z	4	Total	C	N	O	P	1	0	0
			80	36	12	28	4			

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		

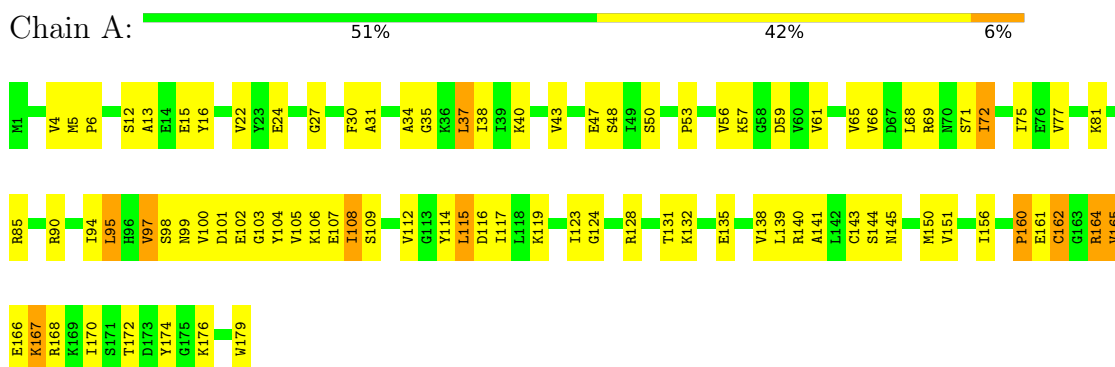
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	O	0	0
			1	1		
6	F	5	Total	O	0	0
			5	5		

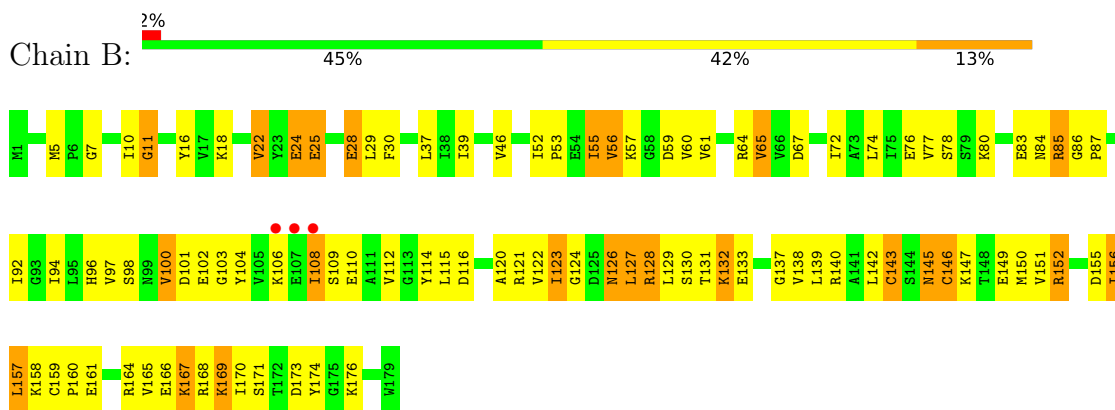
3 Residue-property plots

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.

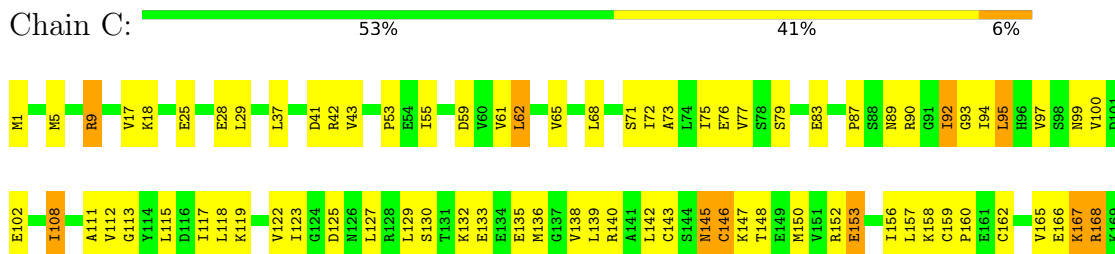
• Molecule 1: Putative uncharacterized protein AF_0206



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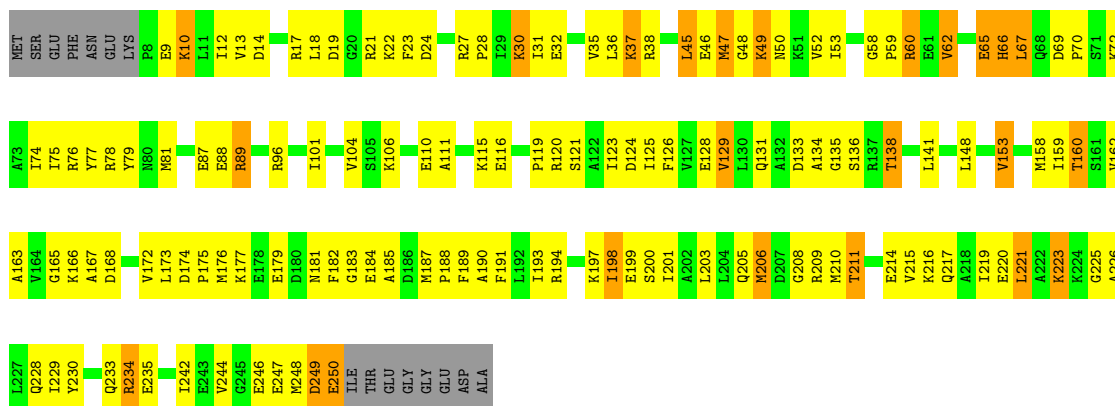
• Molecule 1: Putative uncharacterized protein AF_0206





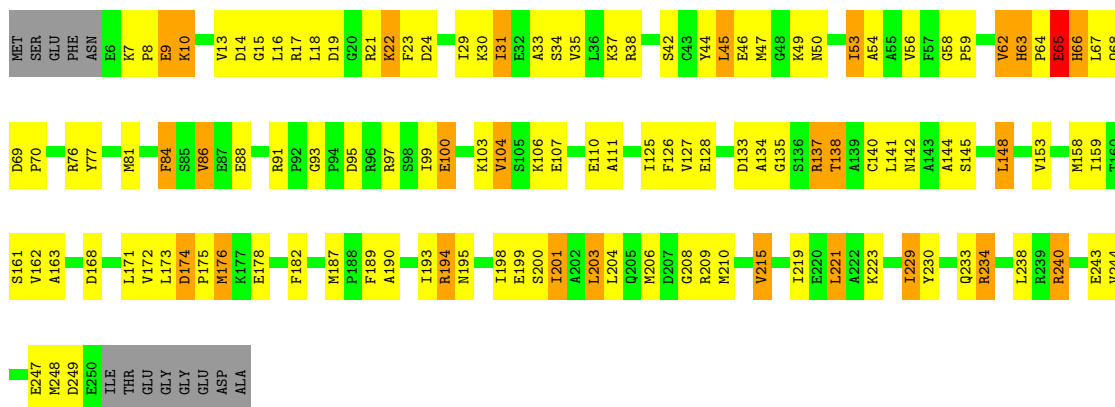
• Molecule 2: Probable exosome complex exonuclease 1

Chain D: 41% 44% 9% 6%



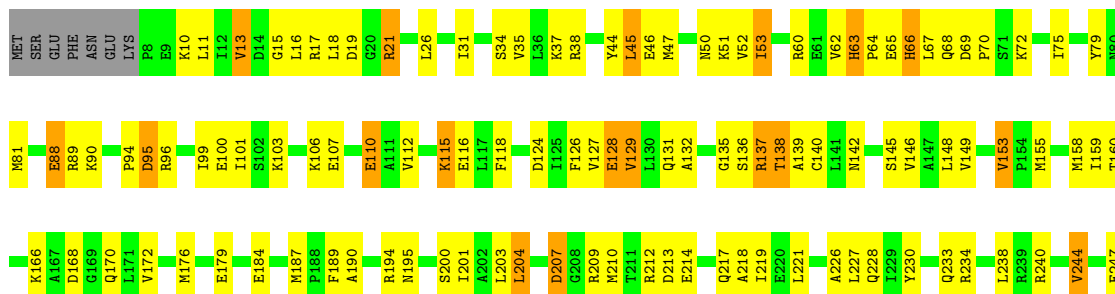
• Molecule 2: Probable exosome complex exonuclease 1

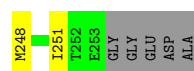
Chain E: 47% 37% 10% 5%



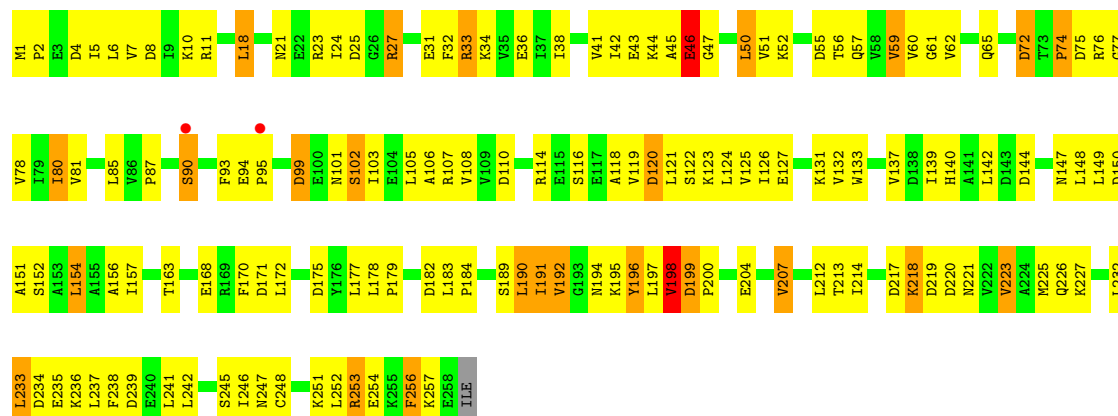
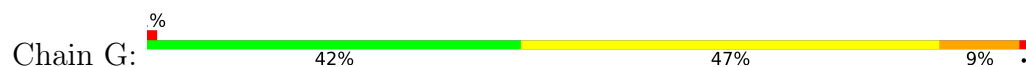
• Molecule 2: Probable exosome complex exonuclease 1

Chain F: 51% 38% 7% 5%

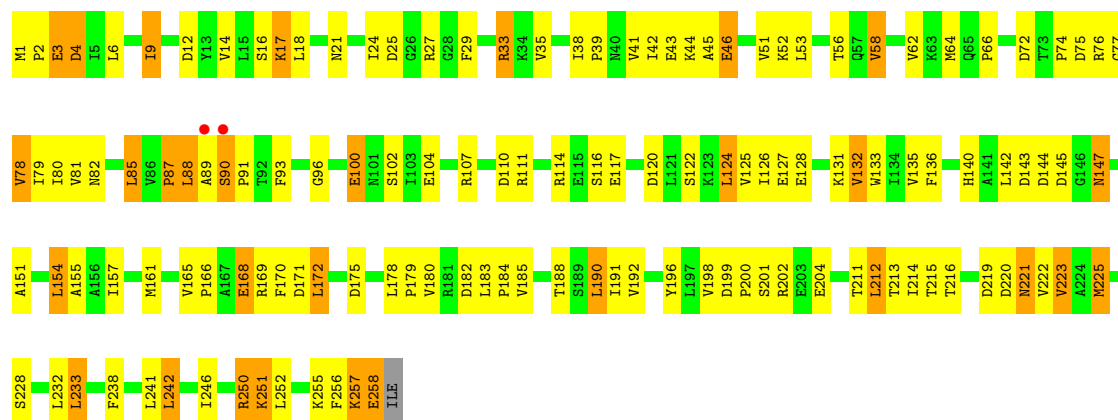




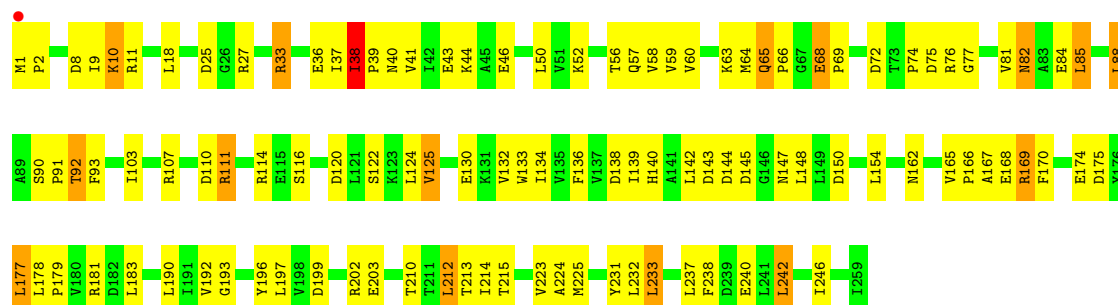
• Molecule 3: Probable exosome complex exonuclease 2



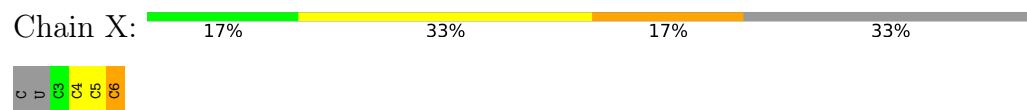
• Molecule 3: Probable exosome complex exonuclease 2



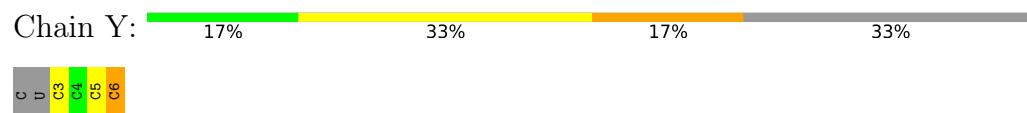
• Molecule 3: Probable exosome complex exonuclease 2



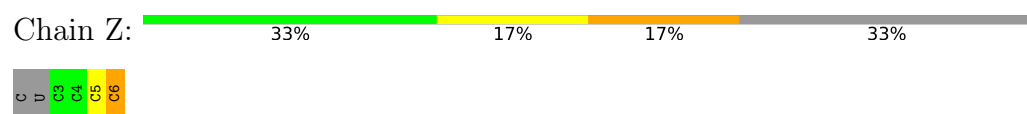
- Molecule 4: 5'-R(*CP*UP*CP*CP*CP*C)-3'



- Molecule 4: 5'-R(*CP*UP*CP*CP*CP*C)-3'



- Molecule 4: 5'-R(*CP*UP*CP*CP*CP*C)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	138.02Å 138.02Å 262.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.00 19.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-3.00) 99.4 (19.98-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 2.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_129)	Depositor
R, R_{free}	0.191 , 0.278 0.177 , 0.259	Depositor DCC
R_{free} test set	5167 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.8	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	16110	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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:
ZN

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	0.50	0/1385	0.93	1/1855 (0.1%)
1	B	0.47	0/1385	0.88	0/1855
1	C	0.48	0/1385	0.87	1/1855 (0.1%)
2	D	0.60	0/1929	0.96	0/2588
2	E	0.59	0/1947	0.97	8/2612 (0.3%)
2	F	0.66	0/1953	0.97	3/2621 (0.1%)
3	G	0.51	0/2025	0.95	7/2748 (0.3%)
3	H	0.62	0/2025	1.01	5/2748 (0.2%)
3	I	0.62	0/2034	0.98	5/2759 (0.2%)
4	X	0.86	0/87	1.51	2/132 (1.5%)
4	Y	0.73	0/87	1.21	1/132 (0.8%)
4	Z	0.84	0/87	1.28	1/132 (0.8%)
All	All	0.58	0/16329	0.96	34/22037 (0.2%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	78	VAL	N-CA-C	8.35	121.58	108.89
2	E	93	GLY	CA-C-N	8.28	128.77	119.83
2	E	93	GLY	C-N-CA	8.28	128.77	119.83
3	H	96	GLY	CA-C-N	7.22	127.81	120.38
3	H	96	GLY	C-N-CA	7.22	127.81	120.38
4	X	6	C	C4'-C3'-C2'	-7.15	95.45	102.60
2	E	248	MET	N-CA-C	6.95	121.92	112.68
4	Z	6	C	C4'-C3'-C2'	-6.83	95.77	102.60
2	E	174	ASP	CA-C-N	6.51	126.47	119.76
2	E	174	ASP	C-N-CA	6.51	126.47	119.76
3	G	198	VAL	CA-C-N	6.24	132.93	121.70
3	G	198	VAL	C-N-CA	6.24	132.93	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	118	PHE	CA-C-N	6.14	126.11	119.78
2	F	118	PHE	C-N-CA	6.14	126.11	119.78
4	Y	6	C	C4'-C3'-C2'	-6.00	96.60	102.60
3	G	227	LYS	N-CA-C	-5.90	102.74	110.53
3	G	199	ASP	N-CA-C	5.77	127.14	111.00
2	E	62	VAL	N-CA-C	5.74	116.88	107.24
3	G	191	ILE	N-CA-C	5.69	116.14	108.17
1	A	170	ILE	N-CA-C	5.56	115.80	107.51
3	H	211	THR	N-CA-C	5.47	117.73	109.41
3	G	90	SER	N-CA-C	5.42	113.10	108.22
1	C	92	ILE	N-CA-C	5.37	115.05	106.88
3	H	255	LYS	N-CA-C	-5.29	106.95	113.41
2	E	63	HIS	N-CA-C	-5.25	103.06	110.31
4	X	4	C	C4'-C3'-C2'	-5.22	97.38	102.60
3	I	65	GLN	CA-C-N	5.15	124.91	119.76
3	I	65	GLN	C-N-CA	5.15	124.91	119.76
3	I	90	SER	CA-C-N	5.14	124.80	119.56
3	I	90	SER	C-N-CA	5.14	124.80	119.56
3	G	74	PRO	N-CA-C	-5.12	107.53	114.80
2	F	137	ARG	N-CA-C	-5.07	105.19	111.33
2	E	66	HIS	N-CA-C	-5.06	106.37	112.54
3	I	38	ILE	N-CA-C	5.02	112.52	107.55

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	1371	0	1408	72	0
1	B	1371	0	1410	91	0
1	C	1371	0	1409	75	0
2	D	1902	0	1948	129	0
2	E	1920	0	1966	125	0
2	F	1926	0	1972	106	0
3	G	1997	0	2021	160	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1997	0	2021	144	0
3	I	2006	0	2032	86	0
4	X	80	0	45	1	0
4	Y	80	0	45	2	0
4	Z	80	0	45	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	5	0	0	0	0
All	All	16110	0	16322	914	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 29.

All (914) 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)
3:G:23:ARG:HH22	3:G:198:VAL:HG13	1.13	1.14
1:B:128:ARG:HG2	1:B:128:ARG:HH21	1.19	1.04
3:G:23:ARG:HH12	3:G:198:VAL:HG21	1.22	1.04
3:H:75:ASP:O	3:H:76:ARG:HG2	1.58	1.03
2:F:18:LEU:H	2:F:18:LEU:HD12	1.17	1.01
3:G:23:ARG:NH2	3:G:198:VAL:HG13	1.77	1.00
2:F:81:MET:HB2	2:F:90:LYS:HE2	1.44	1.00
1:B:156:ILE:HD11	1:B:167:LYS:HA	1.41	0.97
1:C:65:VAL:HG21	1:C:112:VAL:HG11	1.44	0.96
3:G:23:ARG:HH12	3:G:198:VAL:CG2	1.79	0.96
3:G:198:VAL:HB	3:G:199:ASP:C	1.92	0.95
2:F:131:GLN:NE2	3:H:44:LYS:H	1.65	0.94
2:F:131:GLN:HE21	3:H:44:LYS:H	1.08	0.93
1:B:143:CYS:HB3	1:B:146:CYS:SG	2.08	0.93
1:A:40:LYS:O	1:A:43:VAL:HG12	1.69	0.92
3:G:198:VAL:HB	3:G:199:ASP:CA	2.00	0.92
3:G:1:MET:N	3:G:4:ASP:HB3	1.85	0.92
3:G:124:LEU:HB3	3:G:133:TRP:HB2	1.50	0.91
2:D:198:ILE:HD12	2:D:223:LYS:HB3	1.50	0.91
2:F:18:LEU:HD12	2:F:18:LEU:N	1.84	0.90
2:D:210:MET:HE2	2:D:215:VAL:HG22	1.53	0.89
2:D:160:THR:HG23	2:D:233:GLN:HE22	1.37	0.89
1:B:145:ASN:H	1:B:145:ASN:HD22	0.93	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:VAL:HG22	1:C:108:ILE:HG23	1.55	0.88
2:D:160:THR:HG23	2:D:233:GLN:NE2	1.87	0.88
3:G:234:ASP:HB3	3:G:237:LEU:HD13	1.54	0.88
2:E:161:SER:HB2	2:E:189:PHE:O	1.74	0.87
3:H:257:LYS:N	3:H:257:LYS:HD2	1.91	0.86
1:C:119:LYS:HB2	1:C:139:LEU:HD11	1.57	0.86
1:B:128:ARG:HH21	1:B:128:ARG:CG	1.88	0.86
1:C:65:VAL:HG21	1:C:112:VAL:CG1	2.05	0.85
1:A:97:VAL:HG13	1:A:108:ILE:HB	1.59	0.85
1:B:145:ASN:HD22	1:B:145:ASN:N	1.74	0.84
3:G:23:ARG:HH22	3:G:198:VAL:CG1	1.90	0.84
3:I:225:MET:HE1	3:I:238:PHE:CE1	2.12	0.84
3:H:64:MET:HE3	3:H:135:VAL:HG22	1.60	0.84
3:I:91:PRO:HD2	3:I:202:ARG:HH12	1.41	0.84
3:H:250:ARG:HH21	3:H:250:ARG:HG3	1.44	0.83
3:G:1:MET:H3	3:G:4:ASP:HB3	1.43	0.83
3:G:144:ASP:HA	3:G:148:LEU:HD21	1.60	0.83
2:F:38:ARG:HH11	3:H:202:ARG:HD2	1.44	0.82
3:G:27:ARG:NH1	3:G:198:VAL:HG11	1.93	0.82
2:D:208:GLY:O	3:G:223:VAL:HA	1.79	0.82
2:E:10:LYS:HA	2:E:10:LYS:NZ	1.94	0.82
3:G:218:LYS:HG2	3:G:219:ASP:N	1.94	0.82
3:H:72:ASP:O	3:H:74:PRO:HD3	1.80	0.81
1:A:99:ASN:HA	1:A:132:LYS:HE3	1.61	0.81
2:E:56:VAL:HG21	2:E:148:LEU:HD13	1.62	0.80
1:C:65:VAL:HG22	1:C:75:ILE:HG12	1.64	0.80
3:G:139:ILE:HD13	3:G:152:SER:HB3	1.62	0.79
2:D:206:MET:CG	3:G:225:MET:HG3	2.12	0.79
1:B:57:LYS:HE2	1:B:124:GLY:HA2	1.64	0.79
2:F:18:LEU:H	2:F:18:LEU:CD1	1.94	0.79
2:F:112:VAL:HG21	2:F:159:ILE:HD11	1.64	0.79
1:B:173:ASP:HA	1:B:176:LYS:HD3	1.64	0.78
1:C:153:GLU:HG3	1:C:158:LYS:HE2	1.66	0.78
1:C:65:VAL:HG23	1:C:118:LEU:HD13	1.64	0.77
3:G:196:TYR:HD1	3:G:241:LEU:HD13	1.47	0.77
1:A:119:LYS:HB2	1:A:139:LEU:HD11	1.66	0.77
2:E:15:GLY:O	2:E:16:LEU:HD23	1.84	0.77
2:F:66:HIS:H	2:F:66:HIS:CD2	1.98	0.77
3:G:80:ILE:HD12	4:Y:3:C:H1'	1.65	0.77
2:E:63:HIS:CD2	2:E:64:PRO:HA	2.20	0.77
3:G:196:TYR:H	3:G:196:TYR:HD2	1.30	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:GLU:HG2	3:I:140:HIS:CE1	2.21	0.76
3:I:225:MET:HE1	3:I:238:PHE:CZ	2.19	0.76
1:B:16:TYR:CE2	1:B:39:ILE:HD13	2.21	0.76
3:G:23:ARG:NH1	3:G:198:VAL:CG2	2.48	0.76
1:B:145:ASN:H	1:B:145:ASN:ND2	1.72	0.76
3:I:59:VAL:CG2	3:I:142:LEU:HD11	2.17	0.75
3:I:177:LEU:H	3:I:177:LEU:HD22	1.50	0.75
1:C:108:ILE:HD13	1:C:108:ILE:H	1.51	0.75
2:E:128:GLU:HG2	3:G:140:HIS:CE1	2.21	0.75
3:H:191:ILE:HD11	3:H:212:LEU:HB2	1.68	0.75
3:G:168:GLU:HB2	3:G:175:ASP:OD1	1.87	0.75
2:D:67:LEU:H	2:D:67:LEU:HD22	1.52	0.74
2:E:209:ARG:HH12	3:H:117:GLU:HG3	1.51	0.74
3:I:110:ASP:OD2	3:I:114:ARG:NH2	2.20	0.74
3:G:157:ILE:HG23	3:G:256:PHE:CZ	2.21	0.74
2:E:111:ALA:HB1	3:H:232:LEU:HG	1.70	0.74
3:G:27:ARG:CZ	3:G:198:VAL:HG11	2.18	0.74
3:I:43:GLU:CD	3:I:43:GLU:H	1.96	0.73
3:G:25:ASP:OD1	3:G:27:ARG:HB2	1.87	0.73
2:D:206:MET:HG2	3:G:225:MET:HG3	1.70	0.73
3:H:90:SER:HA	3:H:202:ARG:HH12	1.53	0.73
1:A:164:ARG:HG3	1:A:165:VAL:H	1.53	0.73
3:G:23:ARG:NH1	3:G:198:VAL:HG21	1.99	0.73
3:H:1:MET:N	3:H:2:PRO:HD3	2.04	0.72
1:B:22:VAL:HG23	1:B:46:VAL:HG23	1.72	0.72
3:G:196:TYR:CD1	3:G:241:LEU:HD13	2.24	0.72
2:F:145:SER:HB3	2:F:158:MET:HE1	1.71	0.72
2:F:19:ASP:OD2	2:F:21:ARG:HD3	1.90	0.72
3:G:41:VAL:HG21	3:G:50:LEU:HB3	1.70	0.72
3:H:196:TYR:CD2	3:H:241:LEU:HD13	2.25	0.72
2:E:206:MET:CE	3:H:222:VAL:HG12	2.20	0.71
2:F:145:SER:OG	2:F:159:ILE:HB	1.91	0.71
1:A:65:VAL:HG21	1:A:112:VAL:HG12	1.72	0.71
2:D:210:MET:HE2	2:D:215:VAL:CG2	2.19	0.71
3:H:27:ARG:NH1	3:H:199:ASP:O	2.16	0.71
3:I:168:GLU:O	3:I:169:ARG:HB3	1.91	0.71
2:E:209:ARG:NH1	3:H:117:GLU:HG3	2.05	0.71
3:G:72:ASP:O	3:G:74:PRO:HD3	1.89	0.71
2:E:203:LEU:C	2:E:203:LEU:HD23	2.16	0.71
2:D:17:ARG:CZ	2:D:172:VAL:HB	2.21	0.71
3:G:62:VAL:HG22	3:G:137:VAL:HG22	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ARG:HG2	1:B:128:ARG:NH2	1.97	0.70
1:A:30:PHE:CE2	2:D:194:ARG:HD3	2.26	0.70
1:B:126:ASN:HB2	1:B:128:ARG:NH2	2.07	0.70
2:E:219:ILE:HD11	3:H:238:PHE:CE2	2.27	0.70
3:H:46:GLU:HG2	3:H:166:PRO:HG3	1.73	0.69
1:A:69:ARG:HB2	1:A:72:ILE:HG22	1.73	0.69
1:C:173:ASP:HA	1:C:176:LYS:HE2	1.74	0.69
2:F:129:VAL:HG21	2:F:132:ALA:HB2	1.75	0.69
2:D:19:ASP:OD1	2:D:21:ARG:HG3	1.91	0.69
3:G:120:ASP:OD1	3:G:123:LYS:HG3	1.92	0.69
1:C:90:ARG:NH1	3:H:2:PRO:HB2	2.07	0.69
2:F:17:ARG:HD2	2:F:179:GLU:OE1	1.91	0.69
3:I:38:ILE:HD13	3:I:38:ILE:N	2.06	0.69
1:C:75:ILE:HD13	1:C:118:LEU:HD22	1.73	0.69
3:H:124:LEU:HB2	3:H:133:TRP:HB2	1.74	0.69
1:C:117:ILE:HD13	1:C:140:ARG:HD2	1.74	0.69
3:H:191:ILE:CD1	3:H:212:LEU:HB2	2.23	0.69
3:G:56:THR:HG23	3:G:148:LEU:HD23	1.75	0.68
3:I:59:VAL:HG23	3:I:142:LEU:HD11	1.73	0.68
3:G:225:MET:HE1	3:G:238:PHE:CZ	2.28	0.68
2:D:198:ILE:HD12	2:D:223:LYS:CB	2.22	0.68
3:G:36:GLU:HG2	3:G:38:ILE:HD11	1.75	0.68
3:H:168:GLU:HG3	3:H:175:ASP:CG	2.18	0.68
1:B:143:CYS:CB	1:B:146:CYS:SG	2.81	0.68
1:A:5:MET:HG3	2:D:234:ARG:HG3	1.76	0.68
1:B:16:TYR:CE2	1:B:39:ILE:HG21	2.29	0.68
1:B:55:ILE:HG22	1:B:122:VAL:HG21	1.76	0.68
2:F:213:ASP:O	2:F:217:GLN:HG3	1.94	0.68
3:H:125:VAL:HA	3:H:132:VAL:CG2	2.23	0.68
3:H:1:MET:H2	3:H:2:PRO:HD3	1.57	0.67
3:H:89:ALA:HB1	3:H:144:ASP:H	1.59	0.67
2:E:50:ASN:ND2	2:E:133:ASP:HB3	2.09	0.67
1:B:151:VAL:HG12	1:B:158:LYS:O	1.94	0.67
3:I:25:ASP:OD2	3:I:27:ARG:HD3	1.95	0.67
3:G:43:GLU:HG2	3:G:44:LYS:H	1.59	0.67
1:C:76:GLU:O	1:C:76:GLU:HG3	1.95	0.67
2:D:62:VAL:HG22	2:D:67:LEU:HD23	1.77	0.67
2:F:10:LYS:HD2	2:F:168:ASP:OD1	1.95	0.67
3:G:196:TYR:O	3:G:197:LEU:HD12	1.95	0.66
3:H:87:PRO:HA	3:H:93:PHE:HB2	1.76	0.66
3:I:37:ILE:C	3:I:38:ILE:HD13	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:7:LYS:HB3	2:E:182:PHE:CE2	2.30	0.66
3:I:125:VAL:HA	3:I:132:VAL:HG23	1.78	0.66
2:E:206:MET:HE2	3:H:222:VAL:HG12	1.77	0.66
3:G:157:ILE:HG23	3:G:256:PHE:HZ	1.59	0.66
2:F:34:SER:HB2	2:F:240:ARG:HD3	1.78	0.66
3:G:59:VAL:HG22	3:G:142:LEU:HD11	1.77	0.65
2:E:10:LYS:HA	2:E:10:LYS:HZ3	1.61	0.65
3:G:60:VAL:HG11	3:G:156:ALA:HA	1.77	0.65
2:F:38:ARG:NH1	3:H:202:ARG:HD2	2.11	0.65
2:E:190:ALA:HB3	2:E:203:LEU:HB3	1.77	0.65
2:F:89:ARG:HD2	3:H:136:PHE:CG	2.32	0.65
3:G:46:GLU:H	3:G:46:GLU:CD	2.03	0.65
1:B:57:LYS:HE2	1:B:124:GLY:CA	2.27	0.65
2:D:67:LEU:HD22	2:D:67:LEU:N	2.10	0.65
2:D:163:ALA:O	2:D:175:PRO:HD3	1.97	0.65
1:A:65:VAL:HG21	1:A:112:VAL:CG1	2.27	0.64
2:D:17:ARG:HH12	2:D:173:LEU:H	1.45	0.64
2:E:135:GLY:HA2	2:E:137:ARG:NH1	2.12	0.64
1:C:93:GLY:HA2	1:C:127:LEU:HB2	1.80	0.64
3:G:254:GLU:C	3:G:256:PHE:H	2.04	0.64
1:B:159:CYS:SG	1:B:161:GLU:N	2.70	0.64
3:I:68:GLU:CD	3:I:68:GLU:H	2.05	0.64
2:D:173:LEU:HD13	2:D:221:LEU:HD13	1.79	0.64
2:E:47:MET:HE1	2:E:142:ASN:HD22	1.61	0.64
3:G:196:TYR:C	3:G:197:LEU:HD12	2.22	0.64
3:H:89:ALA:HB1	3:H:144:ASP:N	2.11	0.64
1:B:173:ASP:HA	1:B:176:LYS:CD	2.28	0.64
3:H:125:VAL:HA	3:H:132:VAL:HG23	1.79	0.64
3:G:212:LEU:HD23	3:G:213:THR:H	1.63	0.64
1:B:109:SER:O	1:B:110:GLU:HB3	1.97	0.64
1:B:10:ILE:O	1:B:11:GLY:O	2.16	0.64
3:I:225:MET:HE1	3:I:238:PHE:HE1	1.63	0.64
2:E:187:MET:HE2	2:E:189:PHE:CE2	2.34	0.63
2:D:78:ARG:HB3	2:D:126:PHE:HD2	1.63	0.63
3:G:18:LEU:HD22	3:G:195:LYS:HD2	1.78	0.63
1:B:65:VAL:HG11	1:B:116:ASP:OD2	1.97	0.63
3:H:42:ILE:HG22	3:H:42:ILE:O	1.99	0.63
1:C:53:PRO:HB3	1:C:83:GLU:OE2	1.98	0.63
2:D:111:ALA:HB1	3:G:232:LEU:HG	1.80	0.63
2:D:131:GLN:HE22	3:I:43:GLU:HB2	1.64	0.63
1:B:96:HIS:HD2	1:B:98:SER:H	1.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:46:GLU:HG2	3:I:166:PRO:HG3	1.80	0.63
1:A:167:LYS:HD3	1:A:168:ARG:N	2.14	0.63
3:I:10:LYS:HE3	3:I:203:GLU:OE2	1.99	0.63
1:C:73:ALA:HB3	1:C:95:LEU:HB3	1.79	0.62
3:H:256:PHE:C	3:H:258:GLU:H	2.07	0.62
1:C:75:ILE:HD12	1:C:129:LEU:HD12	1.81	0.62
2:F:66:HIS:CD2	2:F:66:HIS:N	2.68	0.62
2:F:137:ARG:HH11	2:F:137:ARG:HG2	1.65	0.62
1:A:119:LYS:HE2	1:A:179:TRP:OXT	1.99	0.62
1:C:145:ASN:O	1:C:146:CYS:HB3	2.00	0.62
2:F:116:GLU:H	2:F:116:GLU:CD	2.06	0.62
3:I:196:TYR:C	3:I:197:LEU:HD12	2.24	0.62
1:B:24:GLU:HG2	1:B:25:GLU:N	2.15	0.62
1:B:143:CYS:O	1:B:147:LYS:HD2	2.00	0.62
2:F:15:GLY:O	2:F:16:LEU:HD23	1.99	0.62
2:F:66:HIS:H	2:F:66:HIS:HD2	1.45	0.62
3:G:11:ARG:HG3	3:G:207:VAL:HA	1.82	0.62
2:F:149:VAL:CG2	2:F:155:MET:HE1	2.30	0.61
1:C:133:GLU:HB2	1:C:136:MET:HG2	1.81	0.61
3:G:218:LYS:HG2	3:G:219:ASP:H	1.65	0.61
1:A:116:ASP:OD1	1:A:168:ARG:NH1	2.34	0.61
1:B:142:LEU:HD23	1:B:149:GLU:HA	1.82	0.61
1:C:146:CYS:SG	1:C:148:THR:HG23	2.40	0.61
3:H:242:LEU:O	3:H:246:ILE:HG13	2.00	0.61
3:I:147:ASN:ND2	3:I:150:ASP:H	1.99	0.61
2:E:219:ILE:HD11	3:H:238:PHE:HE2	1.64	0.61
1:C:99:ASN:HA	1:C:132:LYS:HE3	1.82	0.61
2:E:45:LEU:C	2:E:45:LEU:HD12	2.25	0.61
2:F:230:TYR:HA	2:F:233:GLN:HE21	1.66	0.61
3:H:127:GLU:OE2	3:H:131:LYS:HD3	2.00	0.61
3:G:85:LEU:O	3:G:93:PHE:HB3	2.00	0.61
3:H:89:ALA:HB2	3:H:142:LEU:O	2.01	0.61
3:G:196:TYR:HD2	3:G:196:TYR:N	1.96	0.60
3:G:214:ILE:HG12	3:G:225:MET:CE	2.30	0.60
1:C:111:ALA:O	1:C:168:ARG:HB3	2.00	0.60
2:D:188:PRO:HD2	2:D:205:GLN:O	2.00	0.60
2:D:135:GLY:O	2:D:138:THR:HG22	2.01	0.60
2:E:193:ILE:HD12	2:E:230:TYR:HB2	1.81	0.60
2:D:22:LYS:HG2	2:D:23:PHE:H	1.66	0.60
2:E:44:TYR:CE2	2:E:46:GLU:HG3	2.37	0.60
3:G:147:ASN:ND2	3:G:150:ASP:H	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:203:LEU:C	2:D:203:LEU:HD23	2.27	0.60
2:F:131:GLN:HE21	3:H:44:LYS:N	1.90	0.60
2:F:128:GLU:HG2	3:H:140:HIS:NE2	2.17	0.60
1:C:150:MET:HE1	1:C:166:GLU:HB2	1.84	0.60
2:D:190:ALA:HB3	2:D:203:LEU:HB3	1.82	0.60
2:E:10:LYS:O	2:E:10:LYS:HD3	2.01	0.60
3:H:214:ILE:HG12	3:H:225:MET:HE2	1.84	0.60
1:B:110:GLU:O	1:B:168:ARG:HD3	2.02	0.60
2:F:101:ILE:HD13	2:F:137:ARG:HG3	1.84	0.60
2:F:149:VAL:HG22	2:F:155:MET:CE	2.32	0.60
1:C:167:LYS:O	1:C:167:LYS:HG3	2.02	0.59
1:A:117:ILE:HG21	3:I:9:ILE:HD11	1.84	0.59
1:B:16:TYR:HE2	1:B:39:ILE:HG21	1.67	0.59
3:H:161:MET:HG2	3:H:180:VAL:HG11	1.84	0.59
1:A:164:ARG:CG	1:A:165:VAL:N	2.65	0.59
3:H:25:ASP:OD2	3:H:27:ARG:HD3	2.02	0.59
2:E:10:LYS:HA	2:E:10:LYS:HZ2	1.66	0.59
3:G:219:ASP:O	3:G:220:ASP:HB2	2.03	0.59
3:H:110:ASP:OD2	3:H:114:ARG:NH2	2.35	0.59
1:C:93:GLY:CA	1:C:127:LEU:HB2	2.33	0.59
1:A:144:SER:HB2	1:A:166:GLU:OE1	2.02	0.59
2:D:87:GLU:O	3:I:63:LYS:HE2	2.03	0.59
2:F:103:LYS:O	2:F:107:GLU:HG3	2.02	0.59
2:F:127:VAL:HG11	2:F:140:CYS:HB3	1.83	0.58
2:F:210:MET:HE2	2:F:214:GLU:HB3	1.84	0.58
3:G:170:PHE:O	3:G:172:LEU:HD12	2.03	0.58
1:C:61:VAL:HG11	1:C:77:VAL:CG1	2.33	0.58
3:G:27:ARG:NH1	3:G:199:ASP:O	2.36	0.58
1:B:100:VAL:O	1:B:169:LYS:CD	2.52	0.58
2:F:96:ARG:NH1	3:I:82:ASN:OD1	2.37	0.58
3:G:242:LEU:HD23	3:G:242:LEU:O	2.04	0.58
2:E:8:PRO:C	2:E:10:LYS:H	2.12	0.58
3:H:127:GLU:HB2	3:H:131:LYS:H	1.68	0.58
2:D:247:GLU:O	2:D:250:GLU:HG2	2.03	0.58
3:G:198:VAL:HB	3:G:199:ASP:O	2.03	0.58
3:H:196:TYR:CG	3:H:241:LEU:HD13	2.39	0.58
1:C:159:CYS:SG	1:C:162:CYS:HB3	2.44	0.58
2:E:206:MET:HB3	3:H:225:MET:HG3	1.85	0.58
2:E:95:ASP:O	2:E:99:ILE:HG13	2.04	0.58
3:I:43:GLU:CD	3:I:43:GLU:N	2.60	0.58
2:D:216:LYS:HE2	3:G:239:ASP:CG	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1:MET:H1	3:G:5:ILE:HD12	1.68	0.57
3:G:25:ASP:OD1	3:G:27:ARG:HD3	2.04	0.57
1:B:53:PRO:HG2	1:B:85:ARG:O	2.04	0.57
1:C:75:ILE:CD1	1:C:118:LEU:HD22	2.33	0.57
2:E:22:LYS:HD3	2:E:24:ASP:OD1	2.04	0.57
2:F:38:ARG:HG3	3:H:202:ARG:NH1	2.19	0.57
3:G:214:ILE:HG12	3:G:225:MET:HE3	1.85	0.57
1:C:9:ARG:HG2	1:C:9:ARG:NH2	2.19	0.57
2:E:100:GLU:O	2:E:104:VAL:HG22	2.04	0.57
2:F:31:ILE:HG12	2:F:45:LEU:HD22	1.86	0.57
2:F:126:PHE:CE2	3:H:87:PRO:HG2	2.39	0.57
4:Y:5:C:H2'	4:Y:6:C:O4'	2.03	0.57
1:B:76:GLU:O	1:B:76:GLU:HG3	2.03	0.57
2:F:219:ILE:HD11	3:I:238:PHE:CE2	2.38	0.57
3:I:177:LEU:HD22	3:I:177:LEU:N	2.18	0.57
3:G:237:LEU:O	3:G:238:PHE:C	2.45	0.57
1:A:101:ASP:OD1	1:A:102:GLU:N	2.37	0.57
2:E:243:GLU:O	2:E:247:GLU:HG2	2.05	0.57
2:F:69:ASP:HB3	2:F:72:LYS:O	2.05	0.57
3:I:214:ILE:HG12	3:I:225:MET:HE3	1.87	0.57
2:D:76:ARG:HG3	2:D:124:ASP:OD2	2.04	0.57
2:D:165:GLY:HA3	2:D:175:PRO:HG3	1.86	0.57
2:F:149:VAL:HG22	2:F:155:MET:HE1	1.86	0.57
3:H:250:ARG:HG3	3:H:250:ARG:NH2	2.19	0.57
1:A:13:ALA:N	1:A:27:GLY:O	2.37	0.57
2:D:18:LEU:HD12	2:D:18:LEU:H	1.69	0.57
2:E:63:HIS:HD2	2:E:64:PRO:O	1.87	0.57
1:C:117:ILE:HG21	3:H:9:ILE:HD11	1.87	0.57
1:C:119:LYS:HB2	1:C:139:LEU:CD1	2.33	0.57
2:D:209:ARG:HD3	3:G:221:ASN:HD22	1.69	0.57
2:E:128:GLU:HG2	3:G:140:HIS:HE1	1.67	0.57
3:G:254:GLU:C	3:G:256:PHE:N	2.63	0.57
2:F:138:THR:HG22	2:F:139:ALA:N	2.20	0.56
1:A:53:PRO:HG2	1:A:85:ARG:O	2.05	0.56
2:E:203:LEU:HD23	2:E:204:LEU:N	2.19	0.56
2:D:242:ILE:O	2:D:246:GLU:HG3	2.06	0.56
2:E:64:PRO:HG2	2:E:67:LEU:HB2	1.87	0.56
2:F:44:TYR:OH	2:F:51:LYS:HD3	2.06	0.56
2:F:95:ASP:N	2:F:95:ASP:OD2	2.38	0.56
3:H:190:LEU:HD13	3:H:192:VAL:HG23	1.86	0.56
1:B:150:MET:HE1	1:B:159:CYS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:207:ASP:OD1	3:I:111:ARG:HG2	2.06	0.56
3:H:33:ARG:HD3	3:H:199:ASP:OD1	2.05	0.56
1:C:71:SER:O	1:C:97:VAL:HG23	2.05	0.56
3:G:225:MET:HE1	3:G:238:PHE:CE1	2.40	0.56
1:A:119:LYS:NZ	1:A:135:GLU:HG2	2.21	0.56
2:F:17:ARG:HD3	2:F:172:VAL:HG11	1.86	0.56
2:D:31:ILE:HG12	2:D:45:LEU:HD22	1.87	0.56
3:H:214:ILE:HD13	3:H:242:LEU:HD23	1.86	0.56
3:I:242:LEU:O	3:I:246:ILE:HG13	2.06	0.56
1:A:97:VAL:HA	1:A:100:VAL:HG23	1.87	0.56
2:E:95:ASP:OD2	2:E:97:ARG:HB3	2.06	0.56
3:G:59:VAL:CG2	3:G:142:LEU:HD11	2.35	0.56
3:I:27:ARG:NH1	3:I:199:ASP:O	2.39	0.56
3:H:87:PRO:HA	3:H:93:PHE:CB	2.36	0.56
3:H:185:VAL:O	3:H:215:THR:HG23	2.06	0.56
1:B:96:HIS:CD2	1:B:98:SER:H	2.24	0.56
1:B:60:VAL:CG2	1:B:121:ARG:HH11	2.19	0.55
2:E:34:SER:HB3	2:E:240:ARG:HD3	1.88	0.55
1:C:119:LYS:HE2	1:C:135:GLU:HG2	1.89	0.55
1:A:75:ILE:HD13	1:A:95:LEU:HB2	1.87	0.55
2:D:200:SER:CB	3:G:232:LEU:HB3	2.36	0.55
2:F:89:ARG:HD2	3:H:136:PHE:CD1	2.42	0.55
2:F:128:GLU:HG2	3:H:140:HIS:CE1	2.40	0.55
3:G:99:ASP:O	3:G:103:ILE:HG12	2.07	0.55
2:F:248:MET:O	2:F:251:ILE:HG22	2.07	0.55
3:G:23:ARG:NH1	3:G:198:VAL:HG22	2.22	0.55
3:G:33:ARG:HD2	3:G:199:ASP:OD1	2.06	0.55
2:E:208:GLY:O	3:H:223:VAL:HA	2.07	0.55
2:F:209:ARG:HH22	3:I:116:SER:C	2.14	0.55
1:B:161:GLU:OE2	1:B:161:GLU:HA	2.06	0.55
1:B:169:LYS:NZ	1:B:169:LYS:HB3	2.22	0.55
2:D:17:ARG:NH1	2:D:173:LEU:H	2.04	0.55
2:D:206:MET:HG3	3:G:225:MET:HG3	1.88	0.55
1:C:87:PRO:HD2	1:C:90:ARG:HD2	1.89	0.55
3:H:190:LEU:HB2	3:H:200:PRO:HG3	1.88	0.55
1:B:100:VAL:O	1:B:169:LYS:HD2	2.07	0.54
1:B:114:TYR:O	1:B:115:LEU:HB2	2.07	0.54
2:E:103:LYS:HE2	2:E:107:GLU:OE2	2.06	0.54
1:A:141:ALA:CB	1:A:168:ARG:HH12	2.20	0.54
1:C:112:VAL:HG12	1:C:113:GLY:N	2.22	0.54
3:H:251:LYS:HD2	3:H:251:LYS:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:VAL:HG12	1:C:62:LEU:N	2.22	0.54
3:H:116:SER:OG	3:H:184:PRO:HG3	2.07	0.54
1:A:5:MET:HG3	2:D:234:ARG:CG	2.38	0.54
1:B:156:ILE:HG13	1:B:157:LEU:H	1.72	0.54
2:E:13:VAL:O	2:E:14:ASP:C	2.50	0.54
1:B:56:VAL:HG13	1:B:57:LYS:N	2.21	0.54
1:C:9:ARG:HD3	2:F:195:ASN:HD21	1.72	0.54
3:G:198:VAL:CB	3:G:199:ASP:C	2.75	0.54
3:H:75:ASP:C	3:H:76:ARG:HG2	2.31	0.54
1:C:138:VAL:O	1:C:171:SER:HB3	2.08	0.54
2:F:45:LEU:HB3	2:F:52:VAL:HG22	1.89	0.54
2:F:94:PRO:HB2	2:F:99:ILE:HD11	1.89	0.54
2:F:131:GLN:NE2	3:H:44:LYS:N	2.47	0.54
3:G:38:ILE:N	3:G:38:ILE:HD12	2.23	0.54
3:G:46:GLU:O	3:G:163:THR:HA	2.08	0.54
3:H:77:GLY:HA2	3:H:132:VAL:HG11	1.90	0.54
2:E:153:VAL:HG23	2:E:153:VAL:O	2.08	0.53
1:C:90:ARG:HH12	3:H:2:PRO:HB2	1.73	0.53
1:C:152:ARG:HA	1:C:157:LEU:HD23	1.90	0.53
2:D:220:GLU:OE2	2:D:220:GLU:HA	2.08	0.53
3:I:166:PRO:O	3:I:170:PHE:HD1	1.91	0.53
1:C:143:CYS:SG	1:C:145:ASN:O	2.66	0.53
2:F:47:MET:SD	2:F:138:THR:CG2	2.97	0.53
3:G:76:ARG:HB3	3:G:121:LEU:HB3	1.90	0.53
1:A:97:VAL:HG12	1:A:105:VAL:HG13	1.89	0.53
1:B:10:ILE:HG22	1:B:11:GLY:N	2.23	0.53
2:D:35:VAL:HG23	2:D:36:LEU:HG	1.90	0.53
1:A:141:ALA:HB1	1:A:168:ARG:HH12	1.74	0.53
2:F:45:LEU:HB3	2:F:52:VAL:CG2	2.39	0.53
3:I:215:THR:HB	3:I:224:ALA:HB3	1.89	0.53
1:A:100:VAL:O	1:A:131:THR:HB	2.08	0.53
2:E:8:PRO:O	2:E:9:GLU:HG2	2.08	0.53
3:G:46:GLU:N	3:G:46:GLU:OE1	2.40	0.53
3:H:76:ARG:HA	3:H:122:SER:HA	1.90	0.53
3:H:188:THR:OG1	3:H:213:THR:HG23	2.09	0.53
2:E:158:MET:CE	2:E:233:GLN:NE2	2.72	0.53
3:H:66:PRO:HD3	3:H:133:TRP:CZ3	2.44	0.53
1:A:164:ARG:CG	1:A:165:VAL:H	2.21	0.53
1:C:62:LEU:HD12	1:C:118:LEU:O	2.08	0.53
2:E:135:GLY:HA2	2:E:137:ARG:HH12	1.72	0.53
1:A:117:ILE:HD12	1:A:140:ARG:HH21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ALA:HB1	1:B:129:LEU:HB3	1.91	0.52
1:B:123:ILE:O	1:B:128:ARG:HB2	2.09	0.52
3:H:85:LEU:O	3:H:93:PHE:CD1	2.61	0.52
1:C:123:ILE:HG13	1:C:130:SER:HB2	1.90	0.52
2:F:19:ASP:OD1	2:F:21:ARG:HG2	2.09	0.52
3:I:69:PRO:CD	3:I:130:GLU:HA	2.39	0.52
2:E:10:LYS:HD3	2:E:10:LYS:C	2.34	0.52
2:E:19:ASP:OD1	2:E:21:ARG:HG3	2.09	0.52
3:H:53:LEU:O	3:H:56:THR:HB	2.09	0.52
3:I:39:PRO:O	3:I:40:ASN:HB2	2.09	0.52
1:B:145:ASN:ND2	1:B:146:CYS:SG	2.83	0.52
2:D:13:VAL:O	2:D:14:ASP:HB2	2.09	0.52
3:H:42:ILE:HG22	3:H:45:ALA:CB	2.39	0.52
1:C:5:MET:HG3	2:F:234:ARG:HG3	1.91	0.52
2:E:106:LYS:HE2	2:E:110:GLU:OE1	2.10	0.52
2:E:201:ILE:CD1	2:E:204:LEU:HB2	2.40	0.52
3:H:81:VAL:HB	3:H:110:ASP:HB2	1.92	0.52
1:A:143:CYS:SG	1:A:145:ASN:HB3	2.50	0.52
1:C:61:VAL:HG13	1:C:79:SER:O	2.10	0.52
3:H:90:SER:CA	3:H:202:ARG:HH12	2.21	0.52
1:C:9:ARG:HG2	1:C:9:ARG:HH21	1.74	0.52
2:D:249:ASP:O	2:D:250:GLU:C	2.52	0.52
2:F:110:GLU:CG	2:F:115:LYS:HE2	2.40	0.52
2:D:167:ALA:O	2:D:168:ASP:C	2.53	0.52
2:E:37:LYS:HD2	3:G:55:ASP:OD1	2.09	0.52
2:F:81:MET:HA	2:F:129:VAL:HG13	1.92	0.52
1:B:169:LYS:HB3	1:B:169:LYS:HZ2	1.75	0.52
1:C:95:LEU:HD23	1:C:129:LEU:HB2	1.92	0.52
2:D:158:MET:HE3	2:D:233:GLN:NE2	2.25	0.52
2:E:64:PRO:O	2:E:65:GLU:HB3	2.08	0.52
2:F:244:VAL:O	2:F:247:GLU:HG2	2.10	0.52
2:D:160:THR:CG2	2:D:233:GLN:NE2	2.69	0.51
1:A:81:LYS:HB2	1:A:179:TRP:CZ3	2.45	0.51
2:E:31:ILE:HG12	2:E:45:LEU:HD22	1.93	0.51
2:E:128:GLU:CG	3:G:140:HIS:CE1	2.92	0.51
3:G:212:LEU:HD23	3:G:213:THR:N	2.24	0.51
3:G:1:MET:H2	3:G:4:ASP:HB3	1.73	0.51
3:G:196:TYR:HB3	3:G:241:LEU:HD22	1.91	0.51
3:I:60:VAL:HG22	3:I:139:ILE:HA	1.92	0.51
2:D:21:ARG:CZ	2:D:27:ARG:HG3	2.41	0.51
2:D:191:PHE:CG	2:D:198:ILE:HD13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:45:ALA:O	3:G:47:GLY:N	2.44	0.51
3:G:105:LEU:HD11	3:G:149:LEU:HA	1.93	0.51
1:C:177:GLY:O	3:H:9:ILE:HG23	2.11	0.51
3:H:72:ASP:OD1	3:H:72:ASP:C	2.54	0.51
1:C:112:VAL:CG1	1:C:113:GLY:N	2.74	0.51
3:G:1:MET:N	3:G:5:ILE:HD12	2.25	0.51
1:A:75:ILE:HD12	1:A:75:ILE:N	2.25	0.50
2:E:21:ARG:NH1	2:E:174:ASP:O	2.44	0.50
3:H:9:ILE:O	3:H:12:ASP:HB2	2.10	0.50
3:H:220:ASP:OD2	3:H:250:ARG:NH2	2.43	0.50
1:B:5:MET:HG3	2:E:234:ARG:HG3	1.92	0.50
2:E:103:LYS:O	2:E:107:GLU:HG3	2.10	0.50
1:A:48:SER:C	1:A:50:SER:H	2.18	0.50
2:E:210:MET:CE	2:E:215:VAL:HA	2.42	0.50
1:B:126:ASN:O	1:B:127:LEU:HB2	2.11	0.50
3:G:77:GLY:HA2	3:G:132:VAL:CG2	2.41	0.50
3:I:69:PRO:HD2	3:I:130:GLU:HA	1.94	0.50
1:A:162:CYS:SG	1:A:164:ARG:HB3	2.52	0.50
1:B:5:MET:HG3	2:E:234:ARG:CG	2.41	0.50
2:E:163:ALA:O	2:E:175:PRO:HD3	2.12	0.50
3:G:31:GLU:O	3:G:198:VAL:HG12	2.12	0.50
3:I:196:TYR:C	3:I:196:TYR:CD1	2.89	0.50
3:I:132:VAL:HG22	3:I:133:TRP:N	2.25	0.50
1:A:150:MET:HE1	1:A:166:GLU:HB2	1.93	0.50
3:G:192:VAL:HG22	3:G:192:VAL:O	2.12	0.50
3:H:219:ASP:O	3:H:220:ASP:HB2	2.10	0.50
1:B:77:VAL:HG21	1:B:127:LEU:HD13	1.93	0.49
1:B:150:MET:HA	1:B:150:MET:HE2	1.93	0.49
2:D:89:ARG:O	2:D:89:ARG:HG2	2.12	0.49
2:D:209:ARG:HD3	3:G:221:ASN:ND2	2.27	0.49
2:E:19:ASP:CG	2:E:21:ARG:HG3	2.37	0.49
3:H:250:ARG:HH21	3:H:250:ARG:CG	2.15	0.49
2:E:206:MET:CB	3:H:225:MET:HG3	2.42	0.49
3:G:198:VAL:HB	3:G:199:ASP:CB	2.42	0.49
2:D:17:ARG:NH1	2:D:172:VAL:HB	2.26	0.49
2:D:30:LYS:HE3	2:D:46:GLU:OE2	2.12	0.49
2:E:84:PHE:CD1	3:G:61:GLY:HA3	2.47	0.49
2:F:63:HIS:HA	2:F:64:PRO:C	2.37	0.49
3:H:89:ALA:HB2	3:H:142:LEU:C	2.37	0.49
1:A:6:PRO:HA	1:A:31:ALA:O	2.12	0.49
2:D:198:ILE:HD11	2:D:226:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:144:ALA:O	2:E:148:LEU:HD22	2.13	0.49
3:H:250:ARG:NH2	3:H:250:ARG:CG	2.74	0.49
3:H:257:LYS:HD2	3:H:257:LYS:H	1.75	0.49
1:A:22:VAL:HG13	1:A:30:PHE:O	2.12	0.49
2:D:46:GLU:HA	2:D:50:ASN:O	2.12	0.49
2:E:50:ASN:HD22	2:E:50:ASN:H	1.60	0.49
2:F:129:VAL:CG2	2:F:132:ALA:HB2	2.42	0.49
2:F:212:ARG:HG2	3:I:242:LEU:HD13	1.94	0.49
3:G:126:ILE:HB	3:G:131:LYS:C	2.37	0.49
3:H:120:ASP:OD2	3:H:122:SER:OG	2.24	0.49
1:A:123:ILE:HD12	1:A:124:GLY:N	2.27	0.49
1:B:67:ASP:HB3	1:B:74:LEU:HB2	1.95	0.49
1:C:76:GLU:O	1:C:76:GLU:CG	2.60	0.49
3:H:168:GLU:HG3	3:H:175:ASP:OD2	2.12	0.49
3:I:33:ARG:NH2	3:I:199:ASP:OD2	2.45	0.49
1:A:119:LYS:HB2	1:A:139:LEU:CD1	2.41	0.49
1:B:156:ILE:HD11	1:B:167:LYS:CA	2.28	0.49
2:D:193:ILE:CD1	2:D:198:ILE:HG12	2.43	0.49
3:H:38:ILE:HD12	3:H:38:ILE:N	2.27	0.49
2:D:10:LYS:HD3	2:D:168:ASP:OD1	2.11	0.49
2:E:64:PRO:O	2:E:65:GLU:CB	2.61	0.49
2:E:203:LEU:C	2:E:203:LEU:CD2	2.84	0.49
3:G:23:ARG:NH2	3:G:198:VAL:HG22	2.28	0.49
3:G:32:PHE:CE1	3:G:199:ASP:HB2	2.48	0.49
2:E:133:ASP:OD2	2:E:134:ALA:N	2.46	0.48
2:F:176:MET:HG2	2:F:179:GLU:OE2	2.13	0.48
1:B:121:ARG:HD2	1:B:133:GLU:OE1	2.13	0.48
2:D:77:TYR:C	2:D:77:TYR:CD2	2.90	0.48
2:D:184:GLU:O	2:D:185:ALA:HB2	2.13	0.48
2:F:11:LEU:HA	2:F:18:LEU:HD11	1.94	0.48
2:F:137:ARG:H	2:F:137:ARG:HD3	1.77	0.48
3:G:77:GLY:O	3:G:121:LEU:HD23	2.13	0.48
3:I:103:ILE:O	3:I:107:ARG:HG3	2.13	0.48
1:A:104:TYR:HD2	1:A:105:VAL:H	1.61	0.48
2:D:17:ARG:HH12	2:D:173:LEU:N	2.09	0.48
3:G:110:ASP:OD2	3:G:114:ARG:NH2	2.45	0.48
2:D:166:LYS:HB3	2:D:185:ALA:HB3	1.95	0.48
2:E:141:LEU:HD11	2:E:203:LEU:CD1	2.44	0.48
1:B:61:VAL:HB	1:B:77:VAL:HG13	1.95	0.48
2:F:60:ARG:NH1	3:H:91:PRO:HB3	2.29	0.48
2:D:163:ALA:O	2:D:175:PRO:CD	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:8:PRO:O	2:E:10:LYS:N	2.45	0.48
3:I:36:GLU:HB2	3:I:52:LYS:HB2	1.95	0.48
1:A:71:SER:O	1:A:97:VAL:HG22	2.14	0.48
1:C:123:ILE:CG1	1:C:130:SER:HB2	2.43	0.48
3:G:23:ARG:NH2	3:G:198:VAL:CG1	2.61	0.48
2:F:64:PRO:CB	2:F:66:HIS:CD2	2.97	0.48
3:H:21:ASN:CG	3:H:21:ASN:O	2.57	0.48
1:A:4:VAL:O	1:A:34:ALA:HA	2.14	0.48
1:B:18:LYS:HG2	1:B:22:VAL:O	2.14	0.48
2:F:47:MET:SD	2:F:138:THR:HG22	2.54	0.48
3:I:74:PRO:O	3:I:75:ASP:HB3	2.13	0.48
1:C:152:ARG:HD2	1:C:170:ILE:HG21	1.96	0.47
2:D:69:ASP:OD1	2:D:70:PRO:CD	2.62	0.47
2:F:75:ILE:HG22	2:F:106:LYS:HG3	1.95	0.47
3:H:157:ILE:HG23	3:H:256:PHE:HE1	1.77	0.47
1:A:150:MET:CE	1:A:166:GLU:HB2	2.44	0.47
1:B:10:ILE:HG22	1:B:11:GLY:H	1.78	0.47
2:D:189:PHE:CE2	2:D:219:ILE:HG12	2.49	0.47
2:D:217:GLN:O	2:D:220:GLU:N	2.44	0.47
2:E:210:MET:HE2	2:E:215:VAL:HG22	1.95	0.47
3:G:51:VAL:O	3:G:57:GLN:HA	2.14	0.47
3:H:154:LEU:O	3:H:157:ILE:HG22	2.15	0.47
1:A:119:LYS:HD2	1:A:139:LEU:HD21	1.96	0.47
2:E:30:LYS:C	2:E:31:ILE:HG13	2.39	0.47
2:E:86:VAL:HG11	4:Z:6:C:C2	2.49	0.47
2:F:50:ASN:OD1	2:F:136:SER:HB3	2.14	0.47
2:F:60:ARG:NH2	2:F:124:ASP:OD1	2.47	0.47
2:D:65:GLU:OE2	2:D:66:HIS:N	2.45	0.47
2:D:69:ASP:OD1	2:D:70:PRO:HD2	2.14	0.47
3:G:196:TYR:N	3:G:196:TYR:CD2	2.69	0.47
3:H:214:ILE:HG12	3:H:225:MET:CE	2.43	0.47
3:I:77:GLY:HA2	3:I:132:VAL:CG2	2.45	0.47
3:I:174:GLU:HG2	3:I:175:ASP:N	2.29	0.47
2:F:69:ASP:CG	2:F:72:LYS:HG2	2.39	0.47
3:G:75:ASP:O	3:G:76:ARG:HG2	2.15	0.47
3:G:77:GLY:HA2	3:G:132:VAL:HG21	1.97	0.47
1:B:102:GLU:HB2	1:B:132:LYS:HB3	1.94	0.47
2:D:81:MET:HA	2:D:129:VAL:HG22	1.97	0.47
2:F:53:ILE:HG23	3:H:88:LEU:HD21	1.95	0.47
3:H:51:VAL:HG23	3:H:155:ALA:HB2	1.96	0.47
1:B:164:ARG:HG2	1:B:165:VAL:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ARG:HH21	1:C:9:ARG:CG	2.27	0.47
2:D:205:GLN:HE21	3:G:226:GLN:HE22	1.62	0.47
2:E:42:SER:HA	2:E:54:ALA:O	2.15	0.47
2:E:187:MET:HE2	2:E:189:PHE:CZ	2.49	0.47
3:G:24:ILE:HD11	3:G:204:GLU:HG3	1.96	0.47
3:G:234:ASP:OD1	3:G:234:ASP:C	2.58	0.47
3:G:242:LEU:HD23	3:G:242:LEU:C	2.40	0.47
3:H:1:MET:N	3:H:2:PRO:CD	2.76	0.47
3:H:3:GLU:CD	3:H:3:GLU:H	2.22	0.47
3:I:41:VAL:HG21	3:I:50:LEU:HB2	1.95	0.47
3:I:196:TYR:CD1	3:I:196:TYR:O	2.68	0.47
1:B:64:ARG:CZ	3:G:5:ILE:HG13	2.45	0.47
2:D:210:MET:CE	2:D:215:VAL:HA	2.44	0.47
2:F:110:GLU:HG2	2:F:115:LYS:HE2	1.97	0.47
1:B:55:ILE:CG2	1:B:122:VAL:HG21	2.44	0.47
2:E:219:ILE:O	2:E:223:LYS:HG3	2.15	0.47
3:H:2:PRO:HD2	3:H:3:GLU:CD	2.40	0.47
3:H:38:ILE:HA	3:H:39:PRO:HD3	1.73	0.47
3:I:1:MET:HB2	3:I:2:PRO:HD3	1.97	0.47
3:I:147:ASN:HD21	3:I:150:ASP:H	1.63	0.47
1:A:56:VAL:HG22	1:A:59:ASP:OD1	2.15	0.47
3:G:23:ARG:CZ	3:G:198:VAL:HG22	2.44	0.47
1:C:150:MET:HE3	1:C:157:LEU:CB	2.45	0.46
2:E:138:THR:HG22	2:E:161:SER:OG	2.15	0.46
3:H:127:GLU:O	3:H:128:GLU:C	2.57	0.46
2:E:53:ILE:HG23	2:E:128:GLU:HB3	1.97	0.46
2:F:145:SER:HB3	2:F:158:MET:CE	2.44	0.46
2:F:187:MET:HE2	2:F:204:LEU:HD21	1.98	0.46
3:G:118:ALA:HA	3:G:182:ASP:H	1.80	0.46
1:C:55:ILE:O	1:C:89:ASN:ND2	2.48	0.46
3:H:35:VAL:HA	3:H:52:LYS:O	2.15	0.46
3:H:157:ILE:HG23	3:H:256:PHE:CE1	2.50	0.46
2:D:52:VAL:CG1	2:D:53:ILE:N	2.78	0.46
3:G:65:GLN:HA	3:G:133:TRP:HZ3	1.81	0.46
1:A:138:VAL:O	1:A:174:TYR:HD1	1.99	0.46
2:D:211:THR:HG23	2:D:214:GLU:HB2	1.98	0.46
2:D:181:ASN:O	2:D:182:PHE:CD2	2.68	0.46
2:E:8:PRO:O	2:E:9:GLU:CG	2.62	0.46
2:E:23:PHE:CE2	2:E:24:ASP:HB3	2.50	0.46
2:F:126:PHE:CD2	3:H:87:PRO:HB2	2.51	0.46
1:A:114:TYR:O	1:A:115:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:VAL:HG23	1:B:169:LYS:HD2	1.98	0.46
1:B:131:THR:HG21	1:B:137:GLY:HA2	1.97	0.46
1:C:28:GLU:O	1:C:29:LEU:HD23	2.16	0.46
2:D:47:MET:O	2:D:48:GLY:C	2.57	0.46
2:F:190:ALA:HB3	2:F:203:LEU:HB3	1.97	0.46
3:G:1:MET:O	3:G:1:MET:HG3	2.15	0.46
1:B:59:ASP:OD2	1:B:80:LYS:HE3	2.16	0.46
2:F:95:ASP:O	2:F:99:ILE:HG12	2.16	0.46
3:H:25:ASP:OD2	3:H:27:ARG:CD	2.64	0.46
3:I:92:THR:O	3:I:92:THR:HG23	2.15	0.46
1:A:160:PRO:O	1:A:161:GLU:C	2.58	0.46
1:C:68:LEU:HD22	1:C:108:ILE:CG1	2.46	0.46
2:D:89:ARG:HD3	3:I:136:PHE:CG	2.51	0.46
2:D:200:SER:HB3	3:G:232:LEU:HB3	1.96	0.46
2:E:49:LYS:HA	2:E:49:LYS:HD3	1.62	0.46
1:C:41:ASP:C	1:C:43:VAL:H	2.23	0.46
2:D:58:GLY:HA2	2:D:60:ARG:HG2	1.97	0.46
2:D:79:TYR:CD2	2:D:79:TYR:O	2.69	0.46
2:E:194:ARG:O	2:E:195:ASN:HB3	2.15	0.46
3:G:18:LEU:HD23	3:G:18:LEU:HA	1.80	0.46
3:G:190:LEU:HD13	3:G:190:LEU:C	2.41	0.46
3:H:79:ILE:HG12	3:H:135:VAL:HB	1.98	0.46
3:H:221:ASN:N	3:H:221:ASN:HD22	2.14	0.46
1:A:143:CYS:C	1:A:145:ASN:H	2.24	0.45
2:E:134:ALA:O	2:E:135:GLY:C	2.58	0.45
3:G:25:ASP:C	3:G:27:ARG:H	2.24	0.45
3:G:251:LYS:HB2	3:G:251:LYS:HE3	1.77	0.45
1:B:57:LYS:HA	1:B:122:VAL:HG12	1.99	0.45
1:B:120:ALA:CB	1:B:129:LEU:HB3	2.46	0.45
2:D:148:LEU:HD22	2:D:153:VAL:HG21	1.98	0.45
2:E:56:VAL:HG22	2:E:125:ILE:HG12	1.98	0.45
2:F:149:VAL:HG23	2:F:155:MET:HE1	1.98	0.45
3:H:85:LEU:HD22	3:H:102:SER:HA	1.98	0.45
1:A:12:SER:O	1:A:15:GLU:HB3	2.17	0.45
1:B:28:GLU:C	1:B:29:LEU:HD23	2.40	0.45
1:B:110:GLU:HG2	1:B:167:LYS:O	2.16	0.45
3:H:58:VAL:HG11	3:H:151:ALA:HB1	1.98	0.45
3:I:57:GLN:HG2	3:I:143:ASP:HB3	1.99	0.45
1:B:152:ARG:HH11	1:B:170:ILE:HD12	1.81	0.45
2:D:179:GLU:O	2:D:183:GLY:HA3	2.16	0.45
2:E:23:PHE:C	2:E:23:PHE:CD2	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:64:PRO:HB3	2:F:66:HIS:CD2	2.52	0.45
3:G:197:LEU:C	3:G:198:VAL:CG2	2.89	0.45
3:H:3:GLU:OE1	3:H:4:ASP:OD1	2.35	0.45
2:D:74:ILE:C	2:D:75:ILE:HD13	2.41	0.45
2:D:176:MET:HE3	2:D:179:GLU:OE1	2.16	0.45
3:G:25:ASP:CG	3:G:27:ARG:HB2	2.41	0.45
3:G:183:LEU:HD13	3:G:253:ARG:HG2	1.98	0.45
2:D:173:LEU:HD12	2:D:173:LEU:HA	1.81	0.45
2:E:141:LEU:CD1	2:E:203:LEU:HD13	2.47	0.45
2:E:229:ILE:O	2:E:230:TYR:C	2.60	0.45
2:F:79:TYR:CD2	2:F:79:TYR:C	2.95	0.45
3:H:125:VAL:HA	3:H:132:VAL:HG22	1.96	0.45
3:I:144:ASP:HB2	3:I:148:LEU:HD11	1.98	0.45
1:C:125:ASP:C	1:C:127:LEU:N	2.73	0.45
2:D:77:TYR:HA	2:D:125:ILE:O	2.17	0.45
2:E:69:ASP:OD1	2:E:69:ASP:C	2.59	0.45
2:E:107:GLU:HA	2:E:110:GLU:HG3	1.99	0.45
3:H:124:LEU:O	3:H:132:VAL:HG22	2.17	0.45
2:D:77:TYR:HB3	2:D:106:LYS:HB2	1.99	0.45
2:E:201:ILE:HG23	3:H:233:LEU:O	2.17	0.44
1:A:35:GLY:HA3	1:A:47:GLU:O	2.18	0.44
3:G:45:ALA:C	3:G:47:GLY:N	2.75	0.44
3:G:116:SER:CB	3:G:184:PRO:HG3	2.47	0.44
3:H:251:LYS:HD2	3:H:251:LYS:H	1.82	0.44
2:D:10:LYS:HE2	2:D:12:ILE:O	2.17	0.44
2:D:96:ARG:HD3	3:G:103:ILE:HD12	1.99	0.44
1:A:24:GLU:C	1:A:24:GLU:CD	2.85	0.44
1:A:164:ARG:HG3	1:A:165:VAL:N	2.21	0.44
2:D:135:GLY:O	2:D:136:SER:C	2.61	0.44
3:G:1:MET:N	3:G:2:PRO:HA	2.32	0.44
3:H:17:LYS:HD2	3:H:17:LYS:HA	1.67	0.44
3:I:65:GLN:HA	3:I:133:TRP:HZ3	1.82	0.44
3:I:210:THR:HB	3:I:231:TYR:CD2	2.52	0.44
2:F:135:GLY:O	2:F:138:THR:HB	2.17	0.44
3:I:63:LYS:HB3	3:I:63:LYS:HE3	1.89	0.44
1:A:97:VAL:HA	1:A:100:VAL:CG2	2.47	0.44
2:D:225:GLY:O	2:D:229:ILE:HG13	2.17	0.44
2:F:45:LEU:HD13	2:F:46:GLU:N	2.32	0.44
3:G:122:SER:O	3:G:125:VAL:HG23	2.18	0.44
1:B:86:GLY:HA2	1:B:87:PRO:HD3	1.87	0.44
2:D:37:LYS:HD3	2:D:37:LYS:HA	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:211:THR:HG23	2:D:214:GLU:CG	2.48	0.44
1:A:13:ALA:HB2	1:A:27:GLY:O	2.18	0.44
1:B:56:VAL:CG1	1:B:57:LYS:N	2.81	0.44
2:D:75:ILE:HD12	2:D:123:ILE:HB	2.00	0.44
3:G:225:MET:HE1	3:G:238:PHE:HZ	1.78	0.44
3:H:2:PRO:HD2	3:H:3:GLU:H	1.83	0.44
3:I:81:VAL:HB	3:I:110:ASP:HB2	2.00	0.44
1:A:108:ILE:O	1:A:108:ILE:CG1	2.66	0.44
2:D:72:LYS:O	2:D:119:PRO:HA	2.18	0.44
2:E:67:LEU:HD23	2:E:67:LEU:HA	1.82	0.44
2:F:110:GLU:HG3	2:F:115:LYS:HE2	2.00	0.44
3:H:169:ARG:HD2	3:H:170:PHE:CE2	2.53	0.44
3:I:232:LEU:HD23	3:I:232:LEU:HA	1.82	0.44
2:D:45:LEU:HD12	2:D:45:LEU:C	2.43	0.43
2:D:47:MET:HE3	2:D:47:MET:HB3	1.58	0.43
2:E:33:ALA:HB3	2:E:240:ARG:HG2	1.99	0.43
3:G:32:PHE:CD1	3:G:199:ASP:HB2	2.53	0.43
3:I:41:VAL:HG21	3:I:50:LEU:CB	2.48	0.43
3:I:165:VAL:HA	3:I:166:PRO:HD3	1.88	0.43
1:B:157:LEU:HD21	1:B:168:ARG:HB2	2.01	0.43
2:D:131:GLN:NE2	3:I:44:LYS:H	2.16	0.43
2:D:219:ILE:HG21	3:G:235:GLU:OE2	2.17	0.43
2:E:221:LEU:HD23	2:E:221:LEU:HA	1.72	0.43
2:F:127:VAL:HG11	2:F:140:CYS:CB	2.48	0.43
3:H:14:VAL:HG21	3:H:204:GLU:HA	2.00	0.43
3:H:170:PHE:O	3:H:171:ASP:C	2.61	0.43
1:B:52:ILE:HA	1:B:53:PRO:HD3	1.89	0.43
2:D:110:GLU:O	2:D:115:LYS:HE2	2.17	0.43
2:E:63:HIS:HA	2:E:64:PRO:C	2.43	0.43
2:F:51:LYS:HG3	2:F:131:GLN:HB3	2.01	0.43
2:F:81:MET:HB2	2:F:90:LYS:CE	2.31	0.43
2:D:58:GLY:HA2	2:D:59:PRO:C	2.44	0.43
2:D:62:VAL:HG22	2:D:67:LEU:CD2	2.45	0.43
2:E:45:LEU:C	2:E:45:LEU:CD1	2.91	0.43
2:F:13:VAL:O	2:F:13:VAL:HG22	2.18	0.43
3:G:144:ASP:CG	3:G:148:LEU:HD11	2.43	0.43
2:E:81:MET:CE	2:E:86:VAL:HG13	2.49	0.43
3:G:2:PRO:HA	3:G:5:ILE:CD1	2.48	0.43
3:G:46:GLU:HG2	3:G:62:VAL:O	2.19	0.43
3:G:108:VAL:HG11	3:G:149:LEU:HD11	2.00	0.43
3:H:46:GLU:CG	3:H:166:PRO:HG3	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:201:SER:HB2	3:H:204:GLU:H	1.83	0.43
1:C:159:CYS:HA	1:C:160:PRO:HD3	1.76	0.43
2:D:30:LYS:C	2:D:31:ILE:HG13	2.43	0.43
2:E:141:LEU:HD11	2:E:203:LEU:HD13	2.00	0.43
3:G:1:MET:H1	3:G:5:ILE:CD1	2.30	0.43
1:B:121:ARG:HG3	1:B:122:VAL:N	2.33	0.43
1:C:59:ASP:O	1:C:122:VAL:HG23	2.18	0.43
2:D:133:ASP:O	2:D:134:ALA:C	2.62	0.43
2:F:209:ARG:NH2	3:I:116:SER:HA	2.34	0.43
3:G:170:PHE:O	3:G:171:ASP:HB2	2.19	0.43
3:H:168:GLU:O	3:H:169:ARG:C	2.61	0.43
3:I:64:MET:HG3	3:I:166:PRO:HD3	2.00	0.43
1:A:99:ASN:O	1:A:132:LYS:HG3	2.19	0.43
1:B:138:VAL:HG21	1:B:168:ARG:HD2	1.99	0.43
2:E:29:ILE:CD1	2:E:229:ILE:HD13	2.48	0.43
3:G:178:LEU:HD23	3:G:179:PRO:N	2.33	0.43
3:H:165:VAL:HA	3:H:166:PRO:HD3	1.78	0.43
2:D:219:ILE:O	2:D:223:LYS:HG2	2.18	0.43
3:G:144:ASP:CA	3:G:148:LEU:HD21	2.40	0.43
3:H:242:LEU:HD23	3:H:242:LEU:HA	1.78	0.43
3:I:225:MET:HE1	3:I:238:PHE:HZ	1.80	0.43
3:I:237:LEU:O	3:I:237:LEU:HD23	2.18	0.43
1:A:38:ILE:HD11	1:A:47:GLU:OE2	2.19	0.42
1:A:68:LEU:HD11	1:A:112:VAL:O	2.18	0.42
1:B:121:ARG:O	1:B:129:LEU:HA	2.19	0.42
1:C:68:LEU:HD22	1:C:108:ILE:HG13	2.00	0.42
1:C:77:VAL:HG23	1:C:93:GLY:H	1.84	0.42
2:E:127:VAL:HG11	2:E:140:CYS:HB3	2.01	0.42
3:G:77:GLY:HA2	3:G:132:VAL:HB	2.01	0.42
3:G:101:ASN:O	3:G:102:SER:C	2.62	0.42
3:H:190:LEU:HB2	3:H:200:PRO:CG	2.48	0.42
1:B:65:VAL:HG12	1:B:116:ASP:O	2.19	0.42
2:D:60:ARG:H	2:D:60:ARG:HG3	1.72	0.42
2:F:88:GLU:O	2:F:89:ARG:C	2.61	0.42
3:G:107:ARG:O	3:G:108:VAL:C	2.61	0.42
1:B:150:MET:HB2	1:B:174:TYR:OH	2.19	0.42
1:C:142:LEU:HD22	1:C:147:LYS:O	2.19	0.42
2:E:53:ILE:CG2	2:E:128:GLU:HB3	2.49	0.42
2:F:210:MET:HE1	2:F:218:ALA:HB2	2.01	0.42
3:G:110:ASP:OD2	3:G:110:ASP:C	2.62	0.42
3:G:236:LYS:O	3:G:239:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:107:ARG:HH11	4:Z:5:C:P	2.43	0.42
3:I:57:GLN:HG2	3:I:143:ASP:CB	2.49	0.42
3:I:77:GLY:HA2	3:I:132:VAL:HG22	2.00	0.42
1:A:99:ASN:HA	1:A:132:LYS:CE	2.41	0.42
1:A:101:ASP:HA	1:A:132:LYS:HA	2.01	0.42
1:B:103:GLY:O	1:B:104:TYR:HB2	2.20	0.42
3:G:150:ASP:O	3:G:151:ALA:C	2.62	0.42
3:H:190:LEU:HD13	3:H:192:VAL:CG2	2.49	0.42
1:B:128:ARG:CG	1:B:128:ARG:NH2	2.58	0.42
1:C:108:ILE:H	1:C:108:ILE:CD1	2.27	0.42
2:D:187:MET:HE2	2:D:189:PHE:CZ	2.55	0.42
2:E:47:MET:HE1	2:E:142:ASN:ND2	2.32	0.42
2:F:26:LEU:HD12	2:F:228:GLN:HE21	1.85	0.42
2:F:142:ASN:O	2:F:146:VAL:HG23	2.19	0.42
3:G:214:ILE:HG12	3:G:225:MET:HE2	2.00	0.42
3:H:124:LEU:H	3:H:124:LEU:HG	1.48	0.42
1:A:56:VAL:HG23	1:A:57:LYS:O	2.19	0.42
1:B:22:VAL:HG23	1:B:46:VAL:CG2	2.47	0.42
2:D:24:ASP:HB3	2:D:221:LEU:HD21	2.01	0.42
2:D:69:ASP:HA	2:D:70:PRO:HD3	1.83	0.42
2:D:194:ARG:NH2	2:D:199:GLU:OE2	2.53	0.42
3:G:81:VAL:O	3:G:106:ALA:HB1	2.19	0.42
3:G:178:LEU:HA	3:G:179:PRO:HD3	1.83	0.42
1:C:179:TRP:CE3	1:C:179:TRP:OXT	2.73	0.42
2:D:77:TYR:HE2	2:D:79:TYR:HB2	1.83	0.42
2:D:129:VAL:O	2:D:129:VAL:CG2	2.68	0.42
2:D:210:MET:CE	2:D:215:VAL:HG22	2.38	0.42
2:E:17:ARG:NH2	2:E:21:ARG:NH1	2.68	0.42
2:E:22:LYS:H	2:E:22:LYS:HG3	1.63	0.42
2:D:17:ARG:NH1	2:D:23:PHE:O	2.52	0.42
2:E:187:MET:HE3	2:E:204:LEU:HD21	2.01	0.42
3:G:191:ILE:HD12	3:G:191:ILE:N	2.35	0.42
3:H:89:ALA:HB2	3:H:143:ASP:HA	2.01	0.42
3:I:120:ASP:HA	3:I:181:ARG:NH2	2.34	0.42
3:I:178:LEU:HG	3:I:179:PRO:HD2	2.02	0.42
1:A:72:ILE:O	1:A:72:ILE:CG2	2.65	0.42
1:B:7:GLY:O	1:B:30:PHE:HD2	2.03	0.42
1:B:55:ILE:H	1:B:55:ILE:HG12	1.47	0.42
2:D:101:ILE:O	2:D:104:VAL:HG12	2.20	0.42
2:E:66:HIS:CD2	2:E:66:HIS:C	2.97	0.42
2:E:77:TYR:HA	2:E:125:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:176:MET:HE2	2:E:176:MET:HB2	1.94	0.42
2:E:210:MET:HE2	2:E:215:VAL:CG2	2.49	0.42
2:F:37:LYS:HE2	3:H:145:ASP:OD1	2.19	0.42
1:B:101:ASP:O	1:B:102:GLU:HB3	2.20	0.42
1:B:157:LEU:O	1:B:165:VAL:HG13	2.20	0.42
2:D:165:GLY:HA3	2:D:175:PRO:CG	2.48	0.42
3:G:198:VAL:HB	3:G:199:ASP:HB3	2.02	0.42
2:D:197:LYS:HD3	2:D:197:LYS:HA	1.91	0.41
2:E:53:ILE:HG13	2:E:54:ALA:N	2.33	0.41
2:F:96:ARG:HD3	3:I:103:ILE:HD13	2.02	0.41
3:H:178:LEU:HA	3:H:179:PRO:HD3	1.88	0.41
1:B:131:THR:HG22	1:B:131:THR:O	2.19	0.41
1:C:53:PRO:HG2	1:C:87:PRO:HA	2.01	0.41
2:D:148:LEU:HA	2:D:148:LEU:HD23	1.66	0.41
2:E:198:ILE:H	2:E:198:ILE:HG12	1.52	0.41
2:F:148:LEU:HD23	2:F:153:VAL:HG11	2.01	0.41
3:G:126:ILE:H	3:G:132:VAL:HA	1.85	0.41
3:I:212:LEU:HD22	3:I:213:THR:N	2.35	0.41
1:A:77:VAL:O	1:A:90:ARG:HB2	2.20	0.41
1:A:115:LEU:HD21	2:F:70:PRO:HB2	2.02	0.41
2:D:119:PRO:C	2:D:120:ARG:HG2	2.45	0.41
2:E:84:PHE:C	2:E:84:PHE:CD2	2.98	0.41
1:A:15:GLU:HG2	1:A:16:TYR:CD1	2.55	0.41
1:A:167:LYS:HD3	1:A:167:LYS:C	2.45	0.41
3:G:198:VAL:CB	3:G:199:ASP:CA	2.87	0.41
3:H:41:VAL:HG23	3:H:42:ILE:HD13	2.02	0.41
3:H:89:ALA:O	3:H:93:PHE:CD1	2.73	0.41
3:H:100:GLU:H	3:H:100:GLU:HG3	1.68	0.41
3:H:170:PHE:O	3:H:172:LEU:HD13	2.20	0.41
3:I:39:PRO:HB3	3:I:162:ASN:ND2	2.35	0.41
3:H:29:PHE:O	3:H:198:VAL:HG23	2.21	0.41
3:H:257:LYS:O	3:H:258:GLU:C	2.64	0.41
3:I:85:LEU:O	3:I:93:PHE:CG	2.72	0.41
1:C:152:ARG:HH21	1:C:170:ILE:CG2	2.33	0.41
2:D:49:LYS:HE3	2:D:49:LYS:HA	2.01	0.41
2:D:229:ILE:O	2:D:230:TYR:C	2.64	0.41
2:E:126:PHE:CE2	3:G:87:PRO:HG2	2.55	0.41
2:F:64:PRO:CB	2:F:66:HIS:HD2	2.33	0.41
3:G:127:GLU:HG2	3:G:131:LYS:HB2	2.02	0.41
1:A:48:SER:C	1:A:50:SER:N	2.78	0.41
1:B:157:LEU:HD12	1:B:166:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:248:MET:O	2:D:250:GLU:CG	2.69	0.41
2:E:35:VAL:N	2:E:42:SER:OG	2.54	0.41
2:E:58:GLY:HA2	2:E:59:PRO:C	2.46	0.41
2:E:158:MET:HE3	2:E:233:GLN:NE2	2.35	0.41
3:G:8:ASP:O	3:G:11:ARG:HB3	2.20	0.41
1:C:17:VAL:O	1:C:18:LYS:C	2.64	0.41
1:C:97:VAL:HG22	1:C:108:ILE:CG2	2.39	0.41
2:E:201:ILE:HD13	2:E:204:LEU:HB2	2.02	0.41
3:G:194:ASN:HA	3:G:237:LEU:HD21	2.03	0.41
3:G:199:ASP:HA	3:G:200:PRO:HD2	1.97	0.41
3:I:59:VAL:HG23	3:I:142:LEU:CD1	2.47	0.41
3:I:192:VAL:O	3:I:193:GLY:C	2.61	0.41
1:B:150:MET:CE	1:B:159:CYS:HB2	2.50	0.41
1:C:115:LEU:HD11	2:E:70:PRO:HB2	2.02	0.41
2:D:67:LEU:N	2:D:67:LEU:CD2	2.80	0.41
2:D:158:MET:CE	2:D:233:GLN:NE2	2.84	0.41
2:F:166:LYS:HE3	2:F:214:GLU:OE1	2.20	0.41
2:F:187:MET:HE2	2:F:189:PHE:CZ	2.56	0.41
3:G:38:ILE:HD13	3:G:50:LEU:HD23	2.03	0.41
3:G:182:ASP:CG	3:G:217:ASP:HB2	2.46	0.41
3:H:216:THR:HG21	3:H:246:ILE:HG23	2.03	0.41
3:H:256:PHE:C	3:H:258:GLU:N	2.75	0.41
3:G:27:ARG:NE	3:G:33:ARG:HG3	2.36	0.41
3:H:6:LEU:HD23	3:H:6:LEU:HA	1.88	0.41
3:H:88:LEU:HD12	3:H:88:LEU:HA	1.78	0.41
1:A:37:LEU:C	1:A:37:LEU:CD2	2.94	0.40
1:A:104:TYR:HD2	1:A:105:VAL:N	2.18	0.40
1:A:167:LYS:HD3	1:A:168:ARG:H	1.83	0.40
1:B:96:HIS:O	1:B:100:VAL:HG12	2.20	0.40
2:D:27:ARG:HB3	2:D:28:PRO:CD	2.51	0.40
2:D:166:LYS:HD2	2:D:214:GLU:OE2	2.21	0.40
2:E:38:ARG:HA	2:E:38:ARG:HD3	1.87	0.40
2:E:201:ILE:HD11	2:E:204:LEU:HB2	2.02	0.40
2:F:201:ILE:HB	3:I:233:LEU:HB3	2.03	0.40
3:G:118:ALA:O	3:G:119:VAL:HG23	2.21	0.40
3:H:78:VAL:HG12	3:H:79:ILE:N	2.36	0.40
3:I:122:SER:C	3:I:124:LEU:H	2.28	0.40
3:I:225:MET:HE2	3:I:225:MET:HB3	1.72	0.40
1:B:22:VAL:O	1:B:22:VAL:HG12	2.22	0.40
1:C:125:ASP:C	1:C:127:LEU:H	2.27	0.40
2:E:10:LYS:O	2:E:168:ASP:OD1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:173:LEU:O	2:E:174:ASP:C	2.64	0.40
2:E:187:MET:HG2	2:E:189:PHE:CE1	2.56	0.40
2:E:210:MET:HE3	2:E:215:VAL:HA	2.02	0.40
2:F:19:ASP:OD1	2:F:21:ARG:CG	2.69	0.40
2:F:160:THR:HG21	2:F:226:ALA:O	2.21	0.40
3:G:212:LEU:CD1	3:G:233:LEU:HD11	2.51	0.40
3:I:169:ARG:O	3:I:169:ARG:HG2	2.20	0.40
1:B:159:CYS:HA	1:B:160:PRO:HD3	1.90	0.40
2:D:27:ARG:HH11	2:D:174:ASP:CG	2.29	0.40
2:D:81:MET:HB3	2:D:81:MET:HE3	1.82	0.40
2:D:217:GLN:O	2:D:220:GLU:HB2	2.21	0.40
2:E:17:ARG:CZ	2:E:172:VAL:HB	2.52	0.40
2:E:50:ASN:HD21	2:E:133:ASP:HB3	1.85	0.40
3:G:154:LEU:HD12	3:G:154:LEU:HA	1.89	0.40
3:G:248:CYS:O	3:G:252:LEU:HG	2.22	0.40
3:H:147:ASN:HD22	3:H:147:ASN:HA	1.68	0.40
3:I:8:ASP:O	3:I:11:ARG:HB3	2.21	0.40
3:I:68:GLU:HA	3:I:69:PRO:HD3	1.95	0.40
1:A:123:ILE:HD12	1:A:123:ILE:C	2.47	0.40
1:C:5:MET:HE3	1:C:5:MET:HB3	1.89	0.40
1:C:76:GLU:HA	1:C:92:ILE:HD13	2.03	0.40
1:C:102:GLU:HG2	1:C:132:LYS:HD3	2.03	0.40
3:I:33:ARG:NH1	3:I:145:ASP:O	2.55	0.40
3:I:65:GLN:HA	3:I:66:PRO:HD3	1.83	0.40
3:I:107:ARG:HH12	4:X:5:C:P	2.43	0.40
2:D:166:LYS:HE2	2:D:184:GLU:OE1	2.22	0.40
2:E:69:ASP:HA	2:E:70:PRO:HD3	1.99	0.40
2:F:53:ILE:CG2	3:H:88:LEU:HD21	2.51	0.40
3:H:43:GLU:C	3:H:45:ALA:H	2.30	0.40
3:H:252:LEU:HD23	3:H:252:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	177/179 (99%)	158 (89%)	16 (9%)	3 (2%)	7	32
1	B	177/179 (99%)	148 (84%)	23 (13%)	6 (3%)	3	17
1	C	177/179 (99%)	158 (89%)	17 (10%)	2 (1%)	11	43
2	D	241/258 (93%)	212 (88%)	28 (12%)	1 (0%)	30	65
2	E	243/258 (94%)	224 (92%)	16 (7%)	3 (1%)	10	40
2	F	244/258 (95%)	236 (97%)	7 (3%)	1 (0%)	30	65
3	G	256/259 (99%)	215 (84%)	37 (14%)	4 (2%)	7	34
3	H	256/259 (99%)	229 (90%)	25 (10%)	2 (1%)	16	50
3	I	257/259 (99%)	236 (92%)	19 (7%)	2 (1%)	16	50
All	All	2028/2088 (97%)	1816 (90%)	188 (9%)	24 (1%)	10	40

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	11	GLY
1	B	108	ILE
3	G	72	ASP
3	I	88	LEU
1	A	160	PRO
1	A	164	ARG
1	B	126	ASN
1	B	155	ASP
2	E	65	GLU
3	G	46	GLU
3	G	95	PRO
3	I	167	ALA
1	C	42	ARG
3	G	198	VAL
3	H	90	SER
2	D	177	LYS
2	E	9	GLU
2	F	65	GLU
3	H	87	PRO
1	A	103	GLY
1	B	123	ILE
1	B	156	ILE
1	C	100	VAL

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Mol	Chain	Res	Type
2	E	31	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	149/149 (100%)	128 (86%)	21 (14%)	3	16
1	B	149/149 (100%)	115 (77%)	34 (23%)	1	5
1	C	149/149 (100%)	133 (89%)	16 (11%)	6	26
2	D	202/214 (94%)	165 (82%)	37 (18%)	2	9
2	E	204/214 (95%)	167 (82%)	37 (18%)	2	9
2	F	205/214 (96%)	176 (86%)	29 (14%)	3	16
3	G	225/226 (100%)	188 (84%)	37 (16%)	2	12
3	H	225/226 (100%)	186 (83%)	39 (17%)	2	10
3	I	226/226 (100%)	198 (88%)	28 (12%)	4	20
All	All	1734/1767 (98%)	1456 (84%)	278 (16%)	2	12

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	61	VAL
1	A	66	VAL
1	A	72	ILE
1	A	94	ILE
1	A	95	LEU
1	A	97	VAL
1	A	98	SER
1	A	106	LYS
1	A	107	GLU
1	A	108	ILE
1	A	109	SER
1	A	115	LEU

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Mol	Chain	Res	Type
1	A	128	ARG
1	A	151	VAL
1	A	156	ILE
1	A	162	CYS
1	A	165	VAL
1	A	167	LYS
1	A	172	THR
1	A	176	LYS
1	B	22	VAL
1	B	24	GLU
1	B	25	GLU
1	B	28	GLU
1	B	37	LEU
1	B	55	ILE
1	B	56	VAL
1	B	65	VAL
1	B	72	ILE
1	B	78	SER
1	B	83	GLU
1	B	84	ASN
1	B	85	ARG
1	B	92	ILE
1	B	94	ILE
1	B	97	VAL
1	B	100	VAL
1	B	106	LYS
1	B	108	ILE
1	B	112	VAL
1	B	127	LEU
1	B	128	ARG
1	B	130	SER
1	B	132	LYS
1	B	139	LEU
1	B	140	ARG
1	B	143	CYS
1	B	145	ASN
1	B	146	CYS
1	B	152	ARG
1	B	157	LEU
1	B	167	LYS
1	B	169	LYS
1	B	171	SER

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Mol	Chain	Res	Type
1	C	1	MET
1	C	9	ARG
1	C	25	GLU
1	C	37	LEU
1	C	62	LEU
1	C	72	ILE
1	C	94	ILE
1	C	95	LEU
1	C	108	ILE
1	C	145	ASN
1	C	146	CYS
1	C	153	GLU
1	C	156	ILE
1	C	165	VAL
1	C	167	LYS
1	C	168	ARG
2	D	9	GLU
2	D	10	LYS
2	D	30	LYS
2	D	32	GLU
2	D	37	LYS
2	D	38	ARG
2	D	45	LEU
2	D	47	MET
2	D	49	LYS
2	D	60	ARG
2	D	62	VAL
2	D	65	GLU
2	D	66	HIS
2	D	67	LEU
2	D	88	GLU
2	D	89	ARG
2	D	116	GLU
2	D	121	SER
2	D	129	VAL
2	D	138	THR
2	D	141	LEU
2	D	153	VAL
2	D	159	ILE
2	D	160	THR
2	D	162	VAL
2	D	198	ILE

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Mol	Chain	Res	Type
2	D	201	ILE
2	D	206	MET
2	D	211	THR
2	D	221	LEU
2	D	223	LYS
2	D	228	GLN
2	D	234	ARG
2	D	235	GLU
2	D	244	VAL
2	D	249	ASP
2	D	250	GLU
2	E	10	LYS
2	E	18	LEU
2	E	22	LYS
2	E	45	LEU
2	E	53	ILE
2	E	62	VAL
2	E	65	GLU
2	E	68	GLN
2	E	76	ARG
2	E	84	PHE
2	E	86	VAL
2	E	88	GLU
2	E	91	ARG
2	E	100	GLU
2	E	104	VAL
2	E	137	ARG
2	E	138	THR
2	E	145	SER
2	E	148	LEU
2	E	159	ILE
2	E	162	VAL
2	E	171	LEU
2	E	176	MET
2	E	178	GLU
2	E	194	ARG
2	E	199	GLU
2	E	200	SER
2	E	201	ILE
2	E	203	LEU
2	E	215	VAL
2	E	221	LEU

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Mol	Chain	Res	Type
2	E	229	ILE
2	E	234	ARG
2	E	238	LEU
2	E	240	ARG
2	E	244	VAL
2	E	249	ASP
2	F	13	VAL
2	F	21	ARG
2	F	35	VAL
2	F	45	LEU
2	F	53	ILE
2	F	62	VAL
2	F	63	HIS
2	F	66	HIS
2	F	67	LEU
2	F	68	GLN
2	F	88	GLU
2	F	95	ASP
2	F	100	GLU
2	F	110	GLU
2	F	115	LYS
2	F	128	GLU
2	F	129	VAL
2	F	138	THR
2	F	153	VAL
2	F	170	GLN
2	F	184	GLU
2	F	194	ARG
2	F	200	SER
2	F	204	LEU
2	F	207	ASP
2	F	221	LEU
2	F	227	LEU
2	F	238	LEU
2	F	244	VAL
3	G	6	LEU
3	G	7	VAL
3	G	10	LYS
3	G	18	LEU
3	G	21	ASN
3	G	27	ARG
3	G	33	ARG

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Mol	Chain	Res	Type
3	G	34	LYS
3	G	42	ILE
3	G	46	GLU
3	G	50	LEU
3	G	52	LYS
3	G	59	VAL
3	G	78	VAL
3	G	80	ILE
3	G	90	SER
3	G	94	GLU
3	G	99	ASP
3	G	102	SER
3	G	120	ASP
3	G	154	LEU
3	G	177	LEU
3	G	189	SER
3	G	190	LEU
3	G	192	VAL
3	G	196	TYR
3	G	198	VAL
3	G	207	VAL
3	G	218	LYS
3	G	223	VAL
3	G	233	LEU
3	G	245	SER
3	G	246	ILE
3	G	247	ASN
3	G	253	ARG
3	G	256	PHE
3	G	257	LYS
3	H	3	GLU
3	H	4	ASP
3	H	9	ILE
3	H	16	SER
3	H	17	LYS
3	H	18	LEU
3	H	24	ILE
3	H	33	ARG
3	H	46	GLU
3	H	58	VAL
3	H	62	VAL
3	H	80	ILE

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Mol	Chain	Res	Type
3	H	82	ASN
3	H	85	LEU
3	H	88	LEU
3	H	100	GLU
3	H	104	GLU
3	H	111	ARG
3	H	124	LEU
3	H	126	ILE
3	H	132	VAL
3	H	147	ASN
3	H	154	LEU
3	H	168	GLU
3	H	172	LEU
3	H	182	ASP
3	H	183	LEU
3	H	190	LEU
3	H	212	LEU
3	H	221	ASN
3	H	223	VAL
3	H	225	MET
3	H	228	SER
3	H	233	LEU
3	H	242	LEU
3	H	250	ARG
3	H	251	LYS
3	H	257	LYS
3	H	258	GLU
3	I	10	LYS
3	I	18	LEU
3	I	33	ARG
3	I	38	ILE
3	I	56	THR
3	I	58	VAL
3	I	68	GLU
3	I	72	ASP
3	I	76	ARG
3	I	82	ASN
3	I	84	GLU
3	I	85	LEU
3	I	88	LEU
3	I	92	THR
3	I	111	ARG

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Mol	Chain	Res	Type
3	I	125	VAL
3	I	134	ILE
3	I	138	ASP
3	I	154	LEU
3	I	169	ARG
3	I	177	LEU
3	I	183	LEU
3	I	190	LEU
3	I	212	LEU
3	I	223	VAL
3	I	233	LEU
3	I	240	GLU
3	I	242	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	B	96	HIS
1	B	126	ASN
1	B	145	ASN
1	C	84	ASN
2	D	68	GLN
2	D	131	GLN
2	D	181	ASN
2	D	233	GLN
2	E	50	ASN
2	E	63	HIS
2	E	66	HIS
2	E	80	ASN
2	E	205	GLN
2	E	228	GLN
2	E	233	GLN
2	F	66	HIS
2	F	131	GLN
2	F	170	GLN
2	F	181	ASN
2	F	195	ASN
2	F	205	GLN
2	F	233	GLN
3	G	82	ASN
3	G	147	ASN

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Mol	Chain	Res	Type
3	G	221	ASN
3	H	147	ASN
3	H	162	ASN
3	I	147	ASN
3	I	162	ASN
3	I	247	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	X	3/6 (50%)	1 (33%)	0
4	Y	3/6 (50%)	0	0
4	Z	3/6 (50%)	0	0
All	All	9/18 (50%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	X	6	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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

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	179/179 (100%)	-0.56	0 100 100	31, 62, 94, 115	6 (3%)
1	B	179/179 (100%)	-0.16	3 (1%) 69 45	13, 77, 115, 136	15 (8%)
1	C	179/179 (100%)	-0.54	0 100 100	33, 69, 101, 133	8 (4%)
2	D	242/258 (93%)	-0.54	0 100 100	30, 54, 88, 119	7 (2%)
2	E	243/258 (94%)	-0.64	0 100 100	30, 48, 83, 108	9 (3%)
2	F	246/258 (95%)	-0.87	0 100 100	21, 38, 74, 104	4 (1%)
3	G	253/259 (97%)	-0.38	2 (0%) 82 64	32, 65, 107, 125	12 (4%)
3	H	258/259 (99%)	-0.72	2 (0%) 82 64	9, 41, 85, 95	10 (3%)
3	I	256/259 (98%)	-0.74	1 (0%) 88 76	17, 41, 88, 121	11 (4%)
4	X	4/6 (66%)	-0.22	0 100 100	75, 79, 81, 84	0
4	Y	4/6 (66%)	0.69	0 100 100	93, 104, 105, 109	0
4	Z	4/6 (66%)	0.17	0 100 100	90, 90, 93, 96	0
All	All	2047/2106 (97%)	-0.58	8 (0%) 88 76	9, 53, 99, 136	82 (4%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	107	GLU	8.3
1	B	106	LYS	3.0
3	H	89	ALA	3.0
3	H	90	SER	2.9
1	B	108	ILE	2.8
3	G	90	SER	2.5
3	G	95	PRO	2.5
3	I	1	MET	2.1

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
5	ZN	B	180	1/1	0.94	0.05	118,118,118,118	0
5	ZN	C	180	1/1	0.97	0.04	81,81,81,81	0
5	ZN	A	180	1/1	0.99	0.02	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.