



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:40 AM EDT

PDB ID : 8XIE / pdb_00008xie
Title : Archaeal exosome complex (Rrp4-Rrp41-Rrp42)
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Deposited on : 2023-12-19
Resolution : 3.50 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

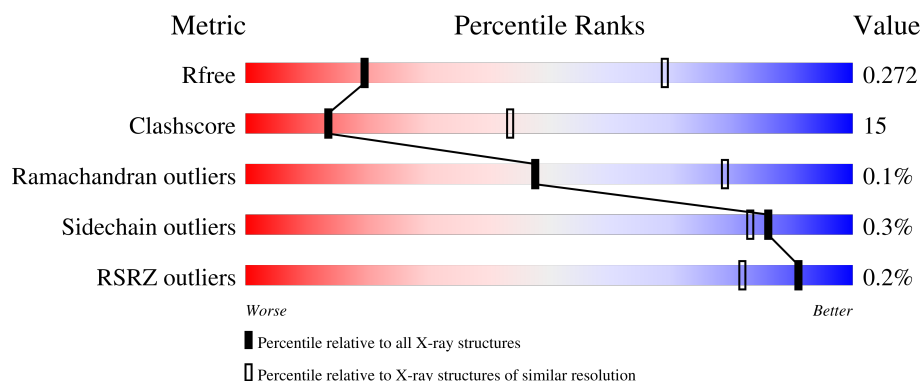
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	248	 65% 29% . .
1	C	248	 63% 30% 7%
1	D	248	 71% 21% 8%
2	B	260	 67% 25% 8%
2	E	260	 % 58% 33% 8%

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Mol	Chain	Length	Quality of chain
2	F	260	64% 28% 8%
3	G	237	69% 26% • •
3	H	237	64% 28% 8%
3	I	237	65% 31% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16183 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 Exosome complex component Rrp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1834	1145	317	359	13			
1	C	231	Total	C	N	O	S	0	0	0
			1788	1117	310	348	13			
1	D	230	Total	C	N	O	S	0	0	0
			1779	1111	308	347	13			

- Molecule 2 is a protein called Exosome complex component Rrp42.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1811	1146	308	351	6			
2	E	239	Total	C	N	O	S	0	0	0
			1820	1152	310	352	6			
2	F	239	Total	C	N	O	S	0	0	0
			1820	1152	310	352	6			

- Molecule 3 is a protein called Exosome complex component Rrp4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	227	Total	C	N	O	S	0	0	0
			1755	1138	285	321	11			
3	I	227	Total	C	N	O	S	0	0	0
			1752	1137	285	319	11			
3	H	219	Total	C	N	O	S	0	0	0
			1690	1096	275	309	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	ALA	-	expression tag	UNP Q9HIP3
I	0	ALA	-	expression tag	UNP Q9HIP3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	ALA	-	expression tag	UNP Q9HIP3

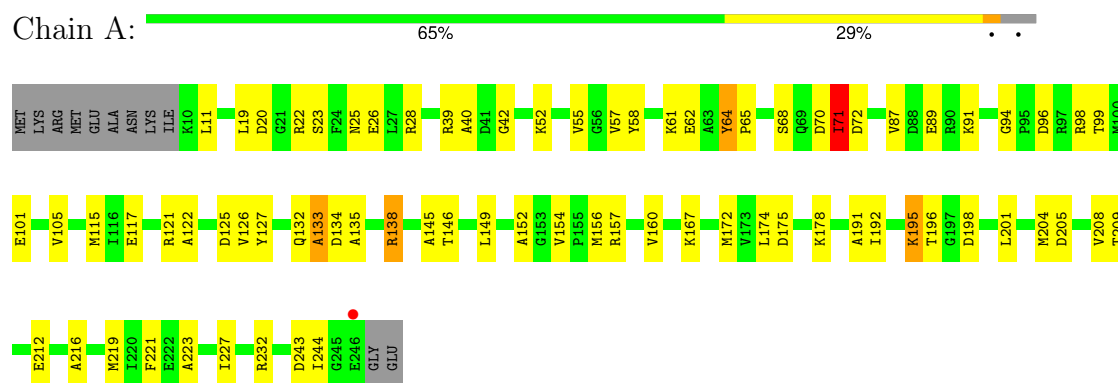
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	21	Total O 21 21	0	0
4	B	23	Total O 23 23	0	0
4	C	20	Total O 20 20	0	0
4	D	7	Total O 7 7	0	0
4	E	15	Total O 15 15	0	0
4	F	21	Total O 21 21	0	0
4	G	12	Total O 12 12	0	0
4	I	11	Total O 11 11	0	0
4	H	4	Total O 4 4	0	0

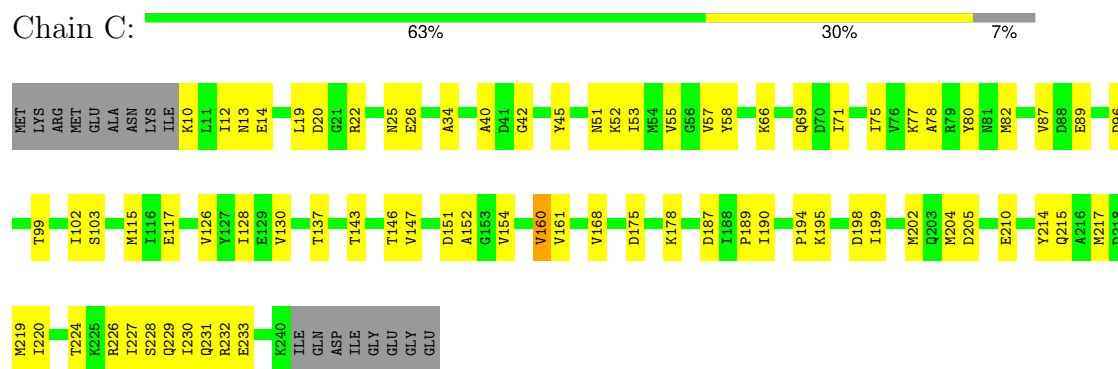
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

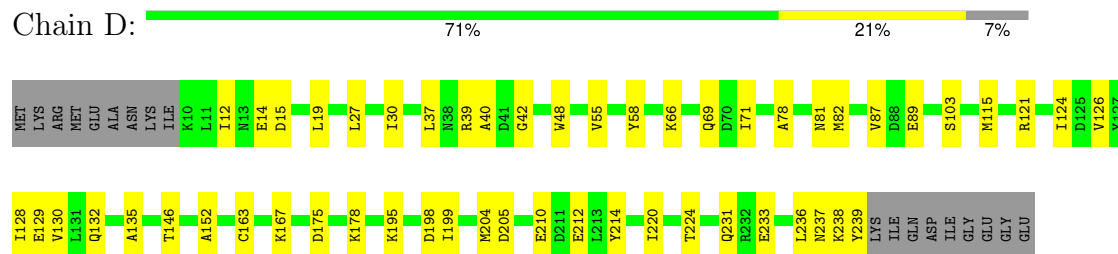
• Molecule 1: Exosome complex component Rrp41



• Molecule 1: Exosome complex component Rrp41

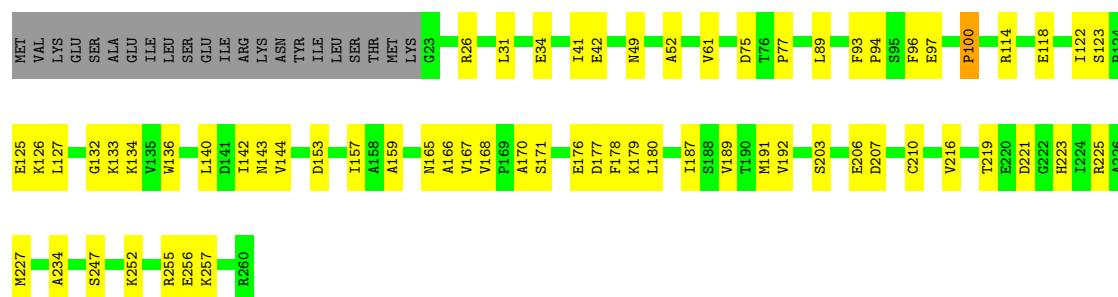


• Molecule 1: Exosome complex component Rrp41



• Molecule 2: Exosome complex component Rrp42

Chain B: 



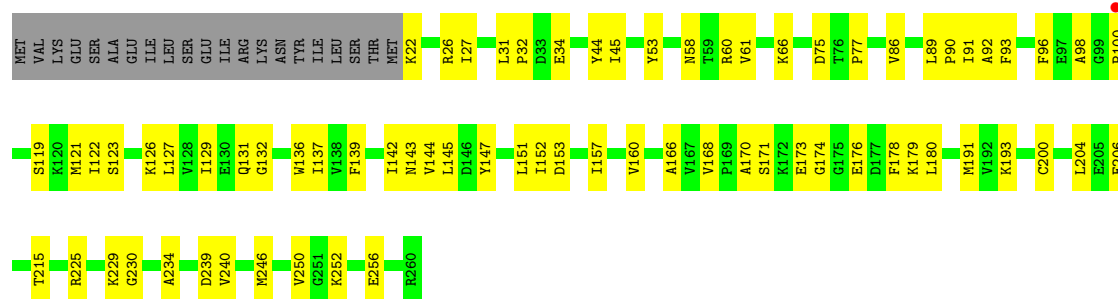
• Molecule 2: Exosome complex component Rrp42

Chain E: 



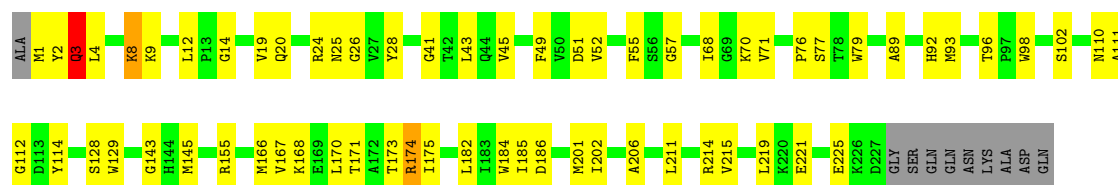
• Molecule 2: Exosome complex component Rrp42

Chain F: 



• Molecule 3: Exosome complex component Rrp4

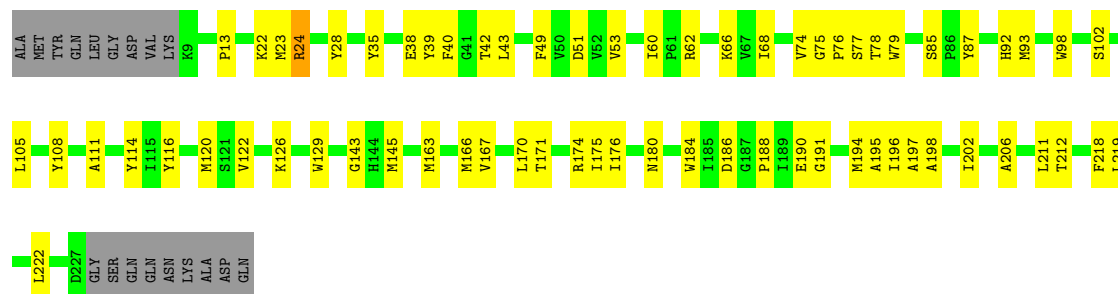
Chain G: 



• Molecule 3: Exosome complex component Rrp4

E216	N110	A0
L219	A111	M1
	I115	Y2
K226	V122	Q3
ASP	K126	L4
GLY	E127	V7
SER	S128	K8
GLN	W129	K9
GLN	G143	L12
ASN	H144	P13
LYS	M145	I17
ALA	I148	K22
ASP	R152	M23
GLN	R155	R24
	V156	V27
	V164	Y28
	V167	Y35
	K168	G41
	E169	T42
	L170	L43
	T171	F49
	A172	Y50
	T173	D51
	R174	P54
	M180	F55
	G181	Y59
	L182	I60
	I183	P61
	W184	R62
	I185	I68
	L186	P76
	G187	S77
	I188	T78
	E189	W79
	G191	F88
	V192	A89
	T193	H92
	I196	M93
	A197	W98
	A198	S102
	E203	L105
	A206	I106
	E209	T107
	G210	L108
	T211	I109

Chain H: 64% 28% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	240.82Å 240.82Å 216.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.43 – 3.50 49.43 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.4 (49.43-3.50) 94.5 (49.43-3.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.229 , 0.273 0.229 , 0.272	Depositor DCC
R_{free} test set	1986 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 106.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	0.178 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	16183	wwPDB-VP
Average B, all atoms (Å ²)	86.0	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 [i](#)

5.1 Standard geometry [i](#)

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	0.94	1/1859 (0.1%)	1.24	12/2506 (0.5%)
1	C	0.87	0/1813	1.05	0/2444
1	D	0.81	0/1804	0.99	0/2433
2	B	0.86	0/1839	1.01	0/2491
2	E	0.75	0/1848	0.97	0/2502
2	F	0.79	0/1848	0.99	0/2502
3	G	0.67	0/1788	0.96	4/2403 (0.2%)
3	H	0.67	0/1722	0.88	0/2315
3	I	0.70	0/1785	0.97	0/2399
All	All	0.79	1/16306 (0.0%)	1.01	16/21995 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
2	B	0	1
2	E	0	2
2	F	0	2
3	H	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	ILE	CG1-CD1	-7.37	1.23	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ILE	CA-CB-CG1	-11.08	91.56	110.40
1	A	71	ILE	N-CA-CB	-9.34	102.94	112.28
1	A	243	ASP	CA-C-N	7.08	134.72	121.97
1	A	243	ASP	C-N-CA	7.08	134.72	121.97
3	G	3	GLN	CA-C-N	6.39	133.37	122.12
3	G	3	GLN	C-N-CA	6.39	133.37	122.12
1	A	138	ARG	CG-CD-NE	-6.32	98.10	112.00
1	A	23	SER	N-CA-CB	6.09	118.53	110.25
3	G	57	GLY	N-CA-C	-5.99	100.62	111.16
1	A	71	ILE	CB-CG1-CD1	5.81	126.00	113.80
3	G	8	LYS	CB-CG-CD	-5.73	98.12	111.30
1	A	133	ALA	CA-C-N	5.64	132.05	122.12
1	A	133	ALA	C-N-CA	5.64	132.05	122.12
1	A	23	SER	CB-CA-C	-5.25	99.60	111.30
1	A	68	SER	N-CA-C	-5.09	105.44	113.02
1	A	195	LYS	CB-CG-CD	-5.01	99.78	111.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	ALA	Peptide
1	A	71	ILE	Peptide
2	B	100	PRO	Peptide
1	C	160	VAL	Mainchain
1	C	226	ARG	Sidechain
2	E	100	PRO	Peptide
2	E	98	ALA	Peptide
2	F	100	PRO	Peptide
2	F	98	ALA	Peptide
3	H	39	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1834	0	1837	65	0
1	C	1788	0	1794	58	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1779	0	1781	44	0
2	B	1811	0	1852	49	0
2	E	1820	0	1865	65	0
2	F	1820	0	1865	58	0
3	G	1755	0	1756	56	0
3	H	1690	0	1687	52	0
3	I	1752	0	1757	69	1
4	A	21	0	0	5	0
4	B	23	0	0	2	0
4	C	20	0	0	7	0
4	D	7	0	0	0	0
4	E	15	0	0	2	0
4	F	21	0	0	3	0
4	G	12	0	0	2	0
4	H	4	0	0	0	0
4	I	11	0	0	1	0
All	All	16183	0	16194	470	1

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 15.

All (470) 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)
2:E:166:ALA:HB1	2:E:180:LEU:HB3	1.35	1.06
1:D:115:MET:HE3	3:H:38:GLU:HG3	1.38	1.01
1:A:98:ARG:HH12	1:A:138:ARG:HH12	1.04	0.98
2:B:166:ALA:HB1	2:B:180:LEU:HB3	1.49	0.95
2:F:166:ALA:HB1	2:F:180:LEU:HB3	1.51	0.92
3:H:198:ALA:HB2	3:H:219:LEU:HD21	1.54	0.90
2:F:31:LEU:HB2	2:F:34:GLU:HG3	1.53	0.89
1:A:98:ARG:NH1	1:A:138:ARG:HH12	1.73	0.87
1:A:71:ILE:HG13	1:A:71:ILE:O	1.76	0.86
2:F:61:VAL:HG12	2:F:144:VAL:HA	1.59	0.84
1:C:232:ARG:HD2	3:G:12:LEU:CD1	2.08	0.83
1:C:232:ARG:HD2	3:G:12:LEU:HD13	1.64	0.80
1:C:22:ARG:NH2	1:C:175:ASP:O	2.15	0.79
3:H:175:ILE:HD11	3:H:195:ALA:HB1	1.62	0.79
1:C:217:MET:HE1	2:E:240:VAL:HG11	1.64	0.79
1:A:146:THR:HG21	1:A:160:VAL:H	1.49	0.78
3:H:24:ARG:HB3	3:H:51:ASP:OD1	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:GLU:HA	2:B:100:PRO:HG3	1.66	0.77
2:B:143:ASN:ND2	4:B:301:HOH:O	2.18	0.76
3:I:24:ARG:HD2	3:I:49:PHE:CD2	2.20	0.76
3:I:93:MET:HE1	3:I:102:SER:HA	1.67	0.75
1:C:146:THR:HG21	1:C:160:VAL:H	1.52	0.75
2:F:126:LYS:O	4:F:301:HOH:O	2.05	0.74
3:G:145:MET:HE1	3:G:184:TRP:HD1	1.52	0.74
1:C:14:GLU:OE1	4:C:301:HOH:O	2.04	0.74
2:B:77:PRO:HB2	2:B:132:GLY:HA2	1.70	0.74
3:I:129:TRP:CZ3	3:I:129:TRP:CZ2	2.75	0.73
3:G:79:TRP:CZ2	3:G:79:TRP:CZ3	2.72	0.73
3:I:79:TRP:CZ2	3:I:79:TRP:CZ3	2.75	0.72
2:F:22:LYS:NZ	3:I:190:GLU:O	2.23	0.72
1:A:94:GLY:O	4:A:301:HOH:O	2.06	0.72
1:A:71:ILE:CD1	3:G:112:GLY:HA3	2.19	0.72
1:D:12:ILE:HG23	1:D:19:LEU:HG	1.72	0.72
3:G:25:ASN:OD1	4:G:301:HOH:O	2.09	0.71
3:H:129:TRP:CZ2	3:H:129:TRP:CZ3	2.77	0.71
3:H:79:TRP:CZ2	3:H:79:TRP:CZ3	2.76	0.71
3:I:41:GLY:HA2	3:I:55:PHE:CD1	2.25	0.71
3:I:98:TRP:CZ2	3:I:98:TRP:CZ3	2.77	0.71
1:C:10:LYS:O	4:C:302:HOH:O	2.09	0.71
3:H:163:MET:SD	3:H:212:THR:OG1	2.48	0.71
2:E:166:ALA:HB1	2:E:180:LEU:CB	2.18	0.70
1:C:146:THR:HG21	1:C:160:VAL:N	2.05	0.70
2:B:61:VAL:HG12	2:B:144:VAL:HA	1.74	0.69
1:D:238:LYS:HZ3	1:D:239:TYR:HD2	1.40	0.69
3:G:98:TRP:CZ2	3:G:98:TRP:CZ3	2.77	0.69
1:D:199:ILE:HD12	2:F:240:VAL:HG21	1.75	0.69
3:H:98:TRP:CZ2	3:H:98:TRP:CZ3	2.78	0.68
1:D:204:MET:HE2	1:D:205:ASP:O	1.92	0.68
2:E:26:ARG:NH2	2:E:200:CYS:O	2.26	0.68
1:A:71:ILE:HD12	3:G:111:ALA:O	1.93	0.67
2:B:127:LEU:HB3	2:B:136:TRP:HB2	1.76	0.67
1:C:40:ALA:HA	1:C:58:TYR:CE1	2.30	0.67
2:E:31:LEU:HB2	2:E:34:GLU:HG3	1.77	0.66
2:F:22:LYS:HE3	3:I:190:GLU:HB3	1.77	0.66
3:G:129:TRP:CZ2	3:G:129:TRP:CZ3	2.80	0.66
3:I:22:LYS:HD3	3:I:49:PHE:CE1	2.31	0.65
1:C:51:ASN:OD1	1:C:137:THR:HG23	1.96	0.65
3:I:41:GLY:HA2	3:I:55:PHE:HD1	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:NZ	3:I:28:TYR:CZ	2.65	0.65
1:A:146:THR:HG21	1:A:160:VAL:N	2.12	0.65
3:H:43:LEU:HD12	3:H:51:ASP:O	1.96	0.65
2:F:127:LEU:HB3	2:F:136:TRP:HB2	1.76	0.65
1:A:20:ASP:OD2	1:A:22:ARG:NH1	2.25	0.64
2:F:121:MET:HE1	2:F:160:VAL:HG13	1.77	0.64
2:E:110:ARG:NH2	4:E:301:HOH:O	2.21	0.64
1:D:135:ALA:HB2	1:D:178:LYS:HA	1.79	0.64
2:E:22:LYS:HG2	3:H:190:GLU:HB3	1.80	0.64
3:I:60:ILE:HD12	3:I:61:PRO:HD2	1.78	0.64
2:B:97:GLU:H	2:B:100:PRO:HB3	1.63	0.64
1:C:220:ILE:O	1:C:224:THR:HG23	1.98	0.64
2:E:170:ALA:HB3	2:E:176:GLU:O	1.98	0.64
2:F:131:GLN:NE2	4:F:302:HOH:O	2.32	0.63
3:I:22:LYS:NZ	4:I:301:HOH:O	2.30	0.63
1:D:82:MET:HA	1:D:130:VAL:HG13	1.79	0.63
2:B:166:ALA:HB3	2:B:179:LYS:HG3	1.81	0.63
1:D:210:GLU:HG2	1:D:214:TYR:CE2	2.34	0.63
1:C:10:LYS:HG3	4:C:302:HOH:O	1.99	0.62
3:H:188:PRO:HD2	3:H:191:GLY:HA3	1.81	0.62
1:D:14:GLU:HG2	1:D:15:ASP:N	2.13	0.62
2:F:166:ALA:HB1	2:F:180:LEU:N	2.13	0.62
3:H:171:THR:HA	3:H:194:MET:HE2	1.81	0.62
1:A:52:LYS:HE3	2:F:44:TYR:O	2.00	0.62
1:A:132:GLN:HB2	2:F:45:ILE:HG23	1.82	0.62
1:C:229:GLN:HG3	1:C:233:GLU:OE2	1.99	0.62
2:F:26:ARG:HD2	2:F:206:GLU:OE2	2.00	0.62
3:H:166:MET:O	3:H:170:LEU:HG	2.00	0.62
3:H:22:LYS:HD3	3:H:49:PHE:HE1	1.65	0.62
3:H:166:MET:HE2	3:H:212:THR:HG23	1.82	0.62
3:H:77:SER:HA	3:H:93:MET:HE2	1.82	0.61
1:C:232:ARG:HD2	3:G:12:LEU:HD12	1.82	0.61
2:F:152:ILE:HG21	2:F:215:THR:HG21	1.81	0.61
2:B:31:LEU:HB2	2:B:34:GLU:HG3	1.82	0.61
3:G:167:VAL:O	3:G:171:THR:HG22	2.00	0.61
1:A:96:ASP:OD1	1:A:99:THR:HG23	2.01	0.61
3:G:1:MET:O	3:G:2:TYR:HD1	1.82	0.61
3:I:188:PRO:HD2	3:I:191:GLY:HA3	1.83	0.61
1:A:42:GLY:HA3	1:A:152:ALA:HB2	1.82	0.60
3:G:43:LEU:HD12	3:G:51:ASP:O	2.01	0.60
2:B:140:LEU:HD21	2:B:159:ALA:HB1	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:166:ALA:HB3	2:E:179:LYS:HG3	1.83	0.60
2:F:168:VAL:HG11	2:F:178:PHE:CZ	2.37	0.59
1:A:204:MET:HE2	1:A:205:ASP:O	2.01	0.59
2:B:166:ALA:HB1	2:B:180:LEU:CB	2.30	0.59
3:H:68:ILE:HD11	3:H:176:ILE:HG22	1.85	0.59
3:H:68:ILE:O	3:H:180:ASN:ND2	2.27	0.59
3:I:155:ARG:HE	3:I:211:LEU:HD12	1.67	0.59
1:C:20:ASP:OD2	1:C:22:ARG:NH1	2.28	0.59
2:F:31:LEU:HB2	2:F:34:GLU:CG	2.30	0.58
1:A:204:MET:HE2	1:A:205:ASP:C	2.27	0.58
1:C:190:ILE:HD11	1:C:202:MET:HE3	1.84	0.58
1:D:40:ALA:HA	1:D:58:TYR:CE1	2.37	0.58
3:G:24:ARG:HD2	3:G:49:PHE:CD1	2.38	0.58
3:G:155:ARG:HG2	3:G:206:ALA:HB1	1.84	0.58
1:A:55:VAL:HG11	1:A:145:ALA:HA	1.84	0.58
1:C:25:ASN:ND2	4:C:305:HOH:O	2.24	0.58
1:D:40:ALA:HA	1:D:58:TYR:CZ	2.38	0.58
1:D:39:ARG:HH12	2:E:204:LEU:HD23	1.68	0.57
1:C:13:ASN:O	4:C:303:HOH:O	2.17	0.57
1:A:71:ILE:HD12	3:G:112:GLY:HA3	1.85	0.57
2:B:153:ASP:O	2:B:157:ILE:HG12	2.04	0.57
2:E:27:ILE:HG23	3:H:196:ILE:HG21	1.86	0.57
3:G:168:LYS:HD3	3:G:175:ILE:H	1.69	0.57
3:H:114:TYR:CD2	3:H:145:MET:HE3	2.40	0.57
1:C:42:GLY:HA2	1:C:151:ASP:OD2	2.05	0.56
1:D:14:GLU:OE1	1:D:14:GLU:N	2.32	0.56
1:C:57:VAL:HG22	1:C:126:VAL:HG22	1.87	0.56
2:E:153:ASP:O	2:E:157:ILE:HG12	2.06	0.56
3:I:68:ILE:O	3:I:182:LEU:HD12	2.06	0.56
1:A:244:ILE:HD12	1:A:244:ILE:H	1.71	0.56
1:A:91:LYS:NZ	4:A:301:HOH:O	2.39	0.55
2:B:192:VAL:HB	2:B:210:CYS:SG	2.46	0.55
3:I:89:ALA:HB2	3:I:128:SER:HB2	1.89	0.55
1:C:161:VAL:HG12	1:C:194:PRO:HG3	1.88	0.55
1:D:66:LYS:O	1:D:69:GLN:HB2	2.05	0.55
1:D:204:MET:HE2	1:D:205:ASP:C	2.31	0.55
1:A:98:ARG:NH1	1:A:138:ARG:NH1	2.50	0.55
2:B:75:ASP:OD1	2:B:75:ASP:N	2.34	0.55
1:C:77:LYS:NZ	4:C:308:HOH:O	2.39	0.55
1:D:55:VAL:HG22	1:D:128:ILE:HG12	1.89	0.55
2:F:86:VAL:HG22	2:F:142:ILE:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3:GLN:N	3:I:3:GLN:OE1	2.40	0.55
3:I:198:ALA:HB2	3:I:219:LEU:HD21	1.88	0.55
3:G:3:GLN:HG3	3:G:9:LYS:HD3	1.89	0.54
3:I:167:VAL:O	3:I:171:THR:HG22	2.07	0.54
1:A:201:LEU:HD23	1:A:201:LEU:C	2.32	0.54
1:D:82:MET:HA	1:D:130:VAL:CG1	2.37	0.54
2:F:193:LYS:HE3	2:F:239:ASP:OD2	2.08	0.54
2:B:26:ARG:HD2	2:B:206:GLU:OE2	2.06	0.54
3:H:75:GLY:O	3:H:105:LEU:HD22	2.07	0.54
3:H:202:ILE:O	3:H:206:ALA:N	2.40	0.54
2:F:166:ALA:HB1	2:F:180:LEU:CB	2.30	0.54
3:H:176:ILE:HB	3:H:184:TRP:HB3	1.89	0.54
3:G:202:ILE:HG23	3:G:211:LEU:HD21	1.89	0.53
1:D:69:GLN:OE1	1:D:121:ARG:NE	2.36	0.53
3:G:8:LYS:NZ	3:G:19:VAL:HG21	2.23	0.53
3:G:20:GLN:N	4:G:302:HOH:O	2.21	0.53
1:A:70:ASP:OD1	1:A:70:ASP:C	2.51	0.53
2:B:166:ALA:HB1	2:B:180:LEU:N	2.23	0.53
3:I:170:LEU:HD11	3:I:216:GLU:HG3	1.91	0.53
1:C:34:ALA:HB2	1:C:147:VAL:CG1	2.38	0.53
1:A:62:GLU:HB3	3:I:88:PHE:CE2	2.43	0.53
2:B:133:LYS:O	2:B:134:LYS:HD3	2.09	0.53
2:E:185:THR:HB	2:E:255:ARG:HD3	1.90	0.53
1:D:198:ASP:HB3	2:F:234:ALA:HB1	1.91	0.52
3:H:202:ILE:HA	3:H:211:LEU:HD21	1.90	0.52
2:B:93:PHE:CD1	2:B:94:PRO:HD2	2.44	0.52
1:D:66:LYS:HG3	1:D:69:GLN:NE2	2.24	0.52
1:C:204:MET:HE2	1:C:205:ASP:O	2.09	0.52
3:G:92:HIS:HB2	3:G:129:TRP:CZ3	2.44	0.52
3:I:93:MET:HE2	3:I:105:LEU:HD11	1.91	0.52
2:E:39:THR:OG1	2:E:55:ALA:HB3	2.10	0.52
2:B:89:LEU:HD11	2:B:143:ASN:OD1	2.09	0.52
1:C:198:ASP:HB3	2:E:234:ALA:HB1	1.90	0.52
3:I:4:LEU:HB2	3:I:7:VAL:O	2.10	0.52
2:B:187:ILE:HG12	2:B:255:ARG:HH11	1.75	0.52
1:C:22:ARG:HB3	1:C:26:GLU:HB3	1.91	0.52
1:C:55:VAL:HG22	1:C:128:ILE:HG12	1.91	0.52
2:F:92:ALA:HA	2:F:145:LEU:O	2.09	0.52
3:G:201:MET:HE2	3:G:214:ARG:CZ	2.40	0.52
3:G:143:GLY:HA3	3:G:186:ASP:HB2	1.92	0.52
1:C:195:LYS:NZ	3:G:28:TYR:CZ	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:122:ILE:O	2:F:123:SER:HB3	2.10	0.51
3:I:22:LYS:HB3	3:I:49:PHE:CD1	2.45	0.51
2:E:164:ARG:O	2:E:179:LYS:NZ	2.43	0.51
3:G:4:LEU:HG	3:G:8:LYS:O	2.10	0.51
1:A:71:ILE:HD11	3:G:112:GLY:HA3	1.91	0.51
2:E:129:ILE:HD11	2:E:136:TRP:CE2	2.45	0.51
2:F:193:LYS:HE3	2:F:239:ASP:CG	2.36	0.51
3:G:24:ARG:HB2	3:G:51:ASP:OD1	2.10	0.51
3:I:92:HIS:HB2	3:I:129:TRP:CZ3	2.46	0.51
1:A:28:ARG:NH1	1:A:134:ASP:OD2	2.42	0.51
2:E:58:ASN:OD1	2:E:60:ARG:NH2	2.43	0.51
1:A:121:ARG:HH12	3:G:110:ASN:HB3	1.75	0.51
2:B:170:ALA:HB3	2:B:176:GLU:O	2.11	0.51
1:C:40:ALA:HA	1:C:58:TYR:CZ	2.45	0.51
1:D:220:ILE:O	1:D:224:THR:HG23	2.10	0.51
3:H:93:MET:HE1	3:H:102:SER:HA	1.93	0.51
2:F:58:ASN:OD1	2:F:60:ARG:NH2	2.44	0.50
3:I:62:ARG:HA	3:I:122:VAL:HG21	1.92	0.50
1:A:101:GLU:OE2	2:B:114:ARG:NH2	2.45	0.50
1:A:156:MET:HE3	3:I:13:PRO:HG2	1.93	0.50
2:F:168:VAL:HG12	2:F:178:PHE:O	2.11	0.50
3:H:74:VAL:HG13	3:H:79:TRP:NE1	2.26	0.50
2:E:89:LEU:HD12	2:E:145:LEU:HD23	1.93	0.50
2:F:166:ALA:HB1	2:F:180:LEU:H	1.76	0.50
3:I:79:TRP:NE1	3:I:109:LEU:HB2	2.26	0.50
1:A:57:VAL:HG22	1:A:126:VAL:HG22	1.92	0.50
1:A:172:MET:HE2	1:A:216:ALA:HB2	1.92	0.50
1:C:199:ILE:HD12	2:E:240:VAL:HG21	1.92	0.50
2:B:168:VAL:HG11	2:B:178:PHE:CE2	2.47	0.50
2:F:90:PRO:HA	2:F:96:PHE:HB3	1.93	0.50
1:A:115:MET:HE3	1:A:157:ARG:NH2	2.27	0.49
2:E:93:PHE:CD1	2:E:94:PRO:HD2	2.47	0.49
2:E:121:MET:HE1	2:E:160:VAL:HG13	1.94	0.49
2:E:236:THR:O	2:E:240:VAL:HG23	2.12	0.49
3:I:79:TRP:CE2	3:I:109:LEU:HB2	2.47	0.49
3:I:89:ALA:CB	3:I:128:SER:HB2	2.42	0.49
1:C:45:TYR:OH	1:C:52:LYS:HD3	2.13	0.49
2:F:129:ILE:HD13	2:F:173:GLU:HG3	1.95	0.49
1:C:53:ILE:HD11	1:C:137:THR:HG22	1.95	0.49
3:G:26:GLY:HA3	3:G:52:VAL:HG23	1.94	0.49
3:I:77:SER:HA	3:I:93:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:LYS:NZ	3:H:28:TYR:CZ	2.79	0.49
2:E:88:LEU:HD22	2:E:105:ALA:HB2	1.95	0.49
2:E:90:PRO:HA	2:E:96:PHE:HB3	1.95	0.49
3:I:59:TYR:CZ	3:I:61:PRO:HA	2.47	0.49
1:C:34:ALA:HB2	1:C:147:VAL:HG12	1.94	0.49
2:F:26:ARG:NH2	2:F:200:CYS:O	2.45	0.49
3:H:143:GLY:HA3	3:H:186:ASP:HB2	1.94	0.49
3:I:24:ARG:HB2	3:I:51:ASP:OD1	2.12	0.49
2:F:170:ALA:HB3	2:F:176:GLU:O	2.13	0.49
3:H:78:THR:HG22	3:H:92:HIS:HA	1.95	0.49
3:H:197:ALA:HB1	3:H:218:PHE:CZ	2.48	0.49
2:B:216:VAL:HG22	2:B:227:MET:HE3	1.94	0.48
1:D:71:ILE:HG21	3:I:111:ALA:O	2.12	0.48
2:F:166:ALA:HB3	2:F:179:LYS:HG3	1.94	0.48
3:G:77:SER:HA	3:G:93:MET:HE2	1.94	0.48
1:C:66:LYS:O	1:C:69:GLN:HB2	2.13	0.48
1:C:215:GLN:O	1:C:219:MET:HG3	2.14	0.48
3:G:76:PRO:HG2	3:H:76:PRO:HG2	1.94	0.48
1:C:178:LYS:HB3	4:C:314:HOH:O	2.12	0.48
2:E:166:ALA:HB1	2:E:180:LEU:N	2.27	0.48
3:I:77:SER:HA	3:I:93:MET:CE	2.43	0.48
2:F:119:SER:HA	2:F:225:ARG:NH1	2.28	0.48
3:G:41:GLY:HA2	3:G:55:PHE:CD1	2.48	0.48
2:F:153:ASP:O	2:F:157:ILE:HG12	2.14	0.48
3:G:171:THR:HG23	3:G:173:THR:HB	1.96	0.48
1:A:172:MET:CE	1:A:216:ALA:HB2	2.43	0.48
1:C:25:ASN:ND2	1:C:25:ASN:H	2.11	0.48
2:E:122:ILE:HD11	2:E:163:LEU:HD22	1.95	0.48
1:A:98:ARG:HH12	1:A:138:ARG:NH1	1.88	0.48
1:D:132:GLN:OE1	2:E:47:ARG:HB2	2.13	0.48
3:G:24:ARG:HD3	3:G:49:PHE:HB3	1.95	0.48
2:E:122:ILE:O	2:E:123:SER:HB3	2.14	0.48
3:G:76:PRO:HG2	3:I:76:PRO:HG2	1.96	0.48
1:A:192:ILE:HG21	1:A:221:PHE:HE1	1.79	0.48
2:F:191:MET:HE3	2:F:191:MET:HB2	1.76	0.48
2:B:219:THR:HG23	2:B:225:ARG:HG3	1.96	0.47
2:E:85:ASN:ND2	2:E:87:GLU:OE2	2.45	0.47
2:F:246:MET:O	2:F:250:VAL:HG13	2.13	0.47
3:G:68:ILE:O	3:G:182:LEU:HD12	2.13	0.47
3:H:42:THR:HB	3:H:53:VAL:HG23	1.96	0.47
1:A:198:ASP:HB3	2:B:234:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:140:LEU:HD21	2:E:159:ALA:HB1	1.96	0.47
2:E:252:LYS:HA	2:E:255:ARG:NH1	2.29	0.47
1:D:233:GLU:O	1:D:236:LEU:HB2	2.15	0.47
2:E:219:THR:HG23	2:E:225:ARG:HG3	1.96	0.47
1:A:149:LEU:HD22	1:A:154:VAL:HG11	1.96	0.47
2:F:229:LYS:HE2	2:F:230:GLY:O	2.14	0.47
3:H:22:LYS:HD3	3:H:49:PHE:CE1	2.48	0.47
1:A:191:ALA:HB3	1:A:201:LEU:HB3	1.97	0.47
2:E:92:ALA:HA	2:E:145:LEU:O	2.15	0.47
2:F:75:ASP:N	2:F:75:ASP:OD1	2.46	0.47
2:E:97:GLU:H	2:E:100:PRO:HB3	1.79	0.47
1:A:167:LYS:HD2	1:A:212:GLU:OE2	2.14	0.46
1:C:82:MET:HA	1:C:130:VAL:HG13	1.96	0.46
3:I:41:GLY:HA3	3:I:54:PRO:HA	1.97	0.46
3:H:79:TRP:CE2	3:H:105:LEU:HD23	2.50	0.46
2:E:89:LEU:HD11	2:E:143:ASN:ND2	2.29	0.46
1:A:232:ARG:HG2	3:I:12:LEU:HD13	1.98	0.46
2:B:227:MET:HB3	2:B:227:MET:HE2	1.66	0.46
2:E:125:GLU:HG2	2:E:126:LYS:N	2.31	0.46
3:H:62:ARG:HA	3:H:122:VAL:HG21	1.98	0.46
1:D:78:ALA:O	1:D:103:SER:HB3	2.16	0.46
2:E:168:VAL:HG11	2:E:178:PHE:CE2	2.51	0.46
1:A:71:ILE:CD1	3:G:111:ALA:O	2.63	0.46
1:C:12:ILE:HD12	1:C:168:VAL:HG13	1.97	0.46
1:A:208:VAL:HG22	1:A:212:GLU:HB2	1.97	0.46
1:C:71:ILE:HD11	3:H:111:ALA:HB3	1.97	0.46
3:I:182:LEU:HA	3:I:182:LEU:HD23	1.70	0.46
2:E:26:ARG:HD3	2:E:199:VAL:HG11	1.97	0.45
2:F:147:TYR:CE1	2:F:151:LEU:HG	2.51	0.45
1:A:22:ARG:HB3	1:A:26:GLU:HB3	1.99	0.45
2:B:219:THR:OG1	2:B:221:ASP:OD1	2.29	0.45
1:D:81:ASN:O	1:D:130:VAL:HG12	2.16	0.45
3:G:8:LYS:NZ	3:G:45:VAL:HG21	2.31	0.45
2:E:135:VAL:HG23	2:E:137:ILE:HD13	1.97	0.45
1:A:64:TYR:HA	4:A:317:HOH:O	2.14	0.45
1:A:117:GLU:H	1:A:117:GLU:CD	2.24	0.45
1:D:48:TRP:HE1	1:D:175:ASP:CG	2.24	0.45
3:G:76:PRO:CG	3:I:76:PRO:HG2	2.47	0.45
1:A:20:ASP:OD1	1:A:22:ARG:HG3	2.16	0.45
1:A:174:LEU:HD21	1:A:223:ALA:HB2	1.98	0.45
1:C:161:VAL:HG11	1:C:228:SER:OG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:186:PRO:O	2:E:187:ILE:HD13	2.16	0.45
2:F:27:ILE:HD13	3:I:196:ILE:HG21	1.97	0.45
3:G:8:LYS:HZ1	3:G:19:VAL:HG11	1.81	0.45
3:I:209:GLU:N	3:I:209:GLU:OE1	2.49	0.45
2:B:191:MET:HE3	2:B:191:MET:HB2	1.77	0.45
2:E:54:VAL:HG21	2:E:158:ALA:CA	2.47	0.45
2:F:166:ALA:CB	2:F:180:LEU:HB3	2.36	0.45
3:I:145:MET:HE1	3:I:184:TRP:HD1	1.82	0.45
3:H:66:LYS:HB3	3:H:116:TYR:CZ	2.51	0.45
2:B:171:SER:N	2:B:177:ASP:OD1	2.46	0.45
3:H:60:ILE:HD11	3:H:126:LYS:HD3	1.99	0.45
1:C:80:TYR:CG	1:C:102:ILE:HG21	2.51	0.44
1:C:227:ILE:O	1:C:230:ILE:N	2.49	0.44
2:E:61:VAL:HG12	2:E:144:VAL:HA	1.99	0.44
2:E:170:ALA:HB3	2:E:176:GLU:C	2.42	0.44
3:G:89:ALA:HB2	3:G:128:SER:HB2	1.98	0.44
3:G:173:THR:HG22	3:G:174:ARG:N	2.31	0.44
1:A:62:GLU:O	1:A:62:GLU:HG3	2.16	0.44
1:A:72:ASP:HA	4:A:314:HOH:O	2.17	0.44
2:E:129:ILE:HD11	2:E:136:TRP:CD2	2.52	0.44
2:E:131:GLN:CD	2:E:131:GLN:H	2.24	0.44
2:F:89:LEU:HD11	2:F:143:ASN:OD1	2.16	0.44
3:G:70:LYS:HB2	3:G:114:TYR:CE2	2.52	0.44
1:D:78:ALA:HA	1:D:126:VAL:O	2.17	0.44
1:D:146:THR:OG1	1:D:231:GLN:NE2	2.50	0.44
3:G:71:VAL:O	3:G:112:GLY:N	2.36	0.44
3:I:164:VAL:O	3:I:168:LYS:HG3	2.17	0.44
2:B:42:GLU:HB3	2:B:165:ASN:HD21	1.82	0.44
1:D:236:LEU:HD23	1:D:236:LEU:HA	1.65	0.44
3:G:170:LEU:HB2	3:G:219:LEU:HD13	1.99	0.44
2:E:131:GLN:H	2:E:131:GLN:NE2	2.16	0.44
2:E:192:VAL:HG22	2:E:202:PRO:HB3	1.99	0.44
2:B:216:VAL:O	2:B:247:SER:OG	2.35	0.44
1:C:195:LYS:HE2	3:G:14:GLY:CA	2.47	0.44
3:I:17:ILE:HD12	3:I:27:VAL:HG22	1.98	0.44
3:H:167:VAL:HG21	3:H:202:ILE:HD11	2.00	0.44
1:A:87:VAL:HG23	1:A:89:GLU:O	2.18	0.44
2:B:125:GLU:HG2	2:B:126:LYS:N	2.33	0.44
1:C:71:ILE:CD1	3:H:111:ALA:HB3	2.47	0.44
3:I:23:MET:HE3	3:I:35:TYR:CD2	2.52	0.44
1:A:22:ARG:NH2	1:A:175:ASP:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:NH1	2:F:204:LEU:HD23	2.32	0.44
2:B:142:ILE:HD11	2:B:159:ALA:HB2	2.00	0.44
1:D:37:LEU:HD23	1:D:37:LEU:HA	1.66	0.44
2:E:206:GLU:O	2:E:209:ILE:HG22	2.18	0.44
3:G:79:TRP:CZ3	3:G:96:THR:HG21	2.53	0.44
3:I:206:ALA:HA	3:I:211:LEU:HD11	1.99	0.44
2:B:203:SER:O	2:B:207:ASP:HB2	2.18	0.43
2:F:66:LYS:HB2	2:F:139:PHE:HB2	1.99	0.43
1:A:195:LYS:HB2	1:A:196:THR:HG23	1.99	0.43
2:E:120:LYS:NZ	4:E:303:HOH:O	2.50	0.43
3:I:143:GLY:HA3	3:I:186:ASP:HB2	2.00	0.43
1:A:61:LYS:O	1:A:122:ALA:HA	2.18	0.43
1:D:30:ILE:HD11	1:D:48:TRP:CE2	2.54	0.43
1:D:121:ARG:NH1	3:I:110:ASN:HB3	2.32	0.43
2:E:127:LEU:HB3	2:E:136:TRP:HB2	1.99	0.43
3:I:152:ARG:O	3:I:156:VAL:HG23	2.18	0.43
3:H:74:VAL:HG13	3:H:79:TRP:HE1	1.83	0.43
3:H:85:SER:OG	3:H:87:TYR:O	2.35	0.43
2:B:31:LEU:HD23	2:B:31:LEU:HA	1.85	0.43
2:E:133:LYS:O	2:E:134:LYS:HD3	2.18	0.43
3:I:2:TYR:O	3:I:9:LYS:HD3	2.18	0.43
3:H:23:MET:HE3	3:H:35:TYR:CD2	2.53	0.43
3:H:163:MET:HE2	3:H:163:MET:HB2	1.59	0.43
2:F:123:SER:OG	2:F:126:LYS:HG3	2.19	0.43
3:G:185:ILE:HG21	3:G:185:ILE:HD13	1.79	0.43
1:C:115:MET:HE2	1:C:117:GLU:OE2	2.18	0.43
2:E:54:VAL:HG21	2:E:158:ALA:HA	2.01	0.43
3:G:77:SER:CB	3:G:93:MET:HE3	2.49	0.43
3:I:41:GLY:HA2	3:I:55:PHE:CE1	2.53	0.43
3:I:60:ILE:HD13	3:I:126:LYS:HE2	2.00	0.43
1:D:237:ASN:O	1:D:238:LYS:C	2.60	0.43
2:F:137:ILE:HD12	2:F:137:ILE:HG23	1.74	0.43
3:I:1:MET:CG	3:I:2:TYR:H	2.32	0.43
3:H:120:MET:N	3:H:129:TRP:O	2.44	0.43
2:B:140:LEU:HD21	2:B:159:ALA:CB	2.48	0.42
3:G:166:MET:O	3:G:170:LEU:HG	2.19	0.42
3:G:221:GLU:O	3:G:225:GLU:HG3	2.19	0.42
1:A:135:ALA:HB2	1:A:178:LYS:HA	2.01	0.42
1:D:163:CYS:HB3	1:D:220:ILE:HG23	2.00	0.42
1:A:25:ASN:HB3	1:A:219:MET:HE3	2.00	0.42
2:B:61:VAL:CG1	2:B:144:VAL:HG22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:LYS:O	2:B:256:GLU:HG2	2.19	0.42
2:B:257:LYS:NZ	4:B:306:HOH:O	2.52	0.42
2:E:53:TYR:OH	2:E:60:ARG:HD3	2.18	0.42
2:E:192:VAL:HB	2:E:210:CYS:SG	2.59	0.42
2:F:252:LYS:O	2:F:256:GLU:HG2	2.20	0.42
3:G:3:GLN:HE21	3:G:9:LYS:NZ	2.18	0.42
1:C:152:ALA:HB3	1:C:154:VAL:HG23	2.02	0.42
2:E:67:ILE:HG12	2:E:138:VAL:HG22	2.00	0.42
2:E:89:LEU:HD11	2:E:143:ASN:HD22	1.84	0.42
3:I:22:LYS:HD3	3:I:49:PHE:HE1	1.83	0.42
1:C:87:VAL:HG23	1:C:89:GLU:O	2.19	0.42
1:A:58:TYR:OH	2:F:91:ILE:O	2.32	0.42
1:A:125:ASP:HB3	1:A:127:TYR:CZ	2.54	0.42
1:C:210:GLU:HG2	1:C:214:TYR:CE2	2.54	0.42
1:A:11:LEU:N	4:A:304:HOH:O	2.51	0.42
1:D:81:ASN:HB3	1:D:129:GLU:OE1	2.20	0.42
1:D:124:ILE:HG21	1:D:124:ILE:HD13	1.77	0.42
2:B:122:ILE:O	2:B:123:SER:HB3	2.19	0.42
2:B:187:ILE:HG12	2:B:255:ARG:NH1	2.35	0.42
3:I:59:TYR:CE1	3:I:61:PRO:HA	2.54	0.42
3:I:190:GLU:HG3	3:I:226:LYS:NZ	2.35	0.42
3:H:171:THR:OG1	3:H:195:ALA:N	2.52	0.42
3:H:198:ALA:CB	3:H:219:LEU:HD11	2.50	0.42
2:B:118:GLU:O	2:B:225:ARG:NH1	2.52	0.42
1:C:19:LEU:HD23	1:C:19:LEU:HA	1.87	0.42
2:F:66:LYS:HA	2:F:66:LYS:HD2	1.90	0.42
3:G:8:LYS:HE3	3:G:45:VAL:HG21	2.02	0.42
3:I:60:ILE:HG23	3:I:60:ILE:O	2.20	0.42
1:D:27:LEU:HD23	1:D:175:ASP:HB2	2.02	0.41
3:I:148:ILE:HB	3:I:203:GLU:CD	2.45	0.41
1:A:40:ALA:HA	1:A:58:TYR:CE2	2.55	0.41
2:B:49:ASN:O	2:B:167:VAL:HB	2.20	0.41
1:C:25:ASN:HB3	1:C:219:MET:CE	2.50	0.41
1:C:143:THR:HG23	1:C:231:GLN:NE2	2.34	0.41
1:D:42:GLY:HA3	1:D:152:ALA:HB2	2.01	0.41
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.69	0.41
2:E:168:VAL:HG12	2:E:178:PHE:O	2.20	0.41
2:F:171:SER:HA	2:F:174:GLY:O	2.20	0.41
3:H:218:PHE:CZ	3:H:222:LEU:HD11	2.55	0.41
2:E:124:PRO:HA	2:E:127:LEU:HG	2.02	0.41
2:E:129:ILE:HD13	2:E:173:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:42:GLU:HB3	2:E:165:ASN:HD21	1.86	0.41
3:I:68:ILE:O	3:I:180:ASN:ND2	2.54	0.41
2:F:77:PRO:HB2	2:F:132:GLY:HA2	2.03	0.41
3:I:12:LEU:HA	3:I:12:LEU:HD23	1.81	0.41
3:H:175:ILE:HA	3:H:184:TRP:O	2.20	0.41
1:D:233:GLU:O	1:D:236:LEU:N	2.54	0.41
2:E:150:ASN:ND2	2:E:201:ASP:HA	2.35	0.41
2:E:166:ALA:HB1	2:E:180:LEU:CA	2.50	0.41
3:H:98:TRP:HB3	3:H:108:TYR:CD1	2.56	0.41
2:F:93:PHE:O	2:F:96:PHE:HB2	2.21	0.41
3:I:168:LYS:O	3:I:172:ALA:N	2.53	0.41
1:A:105:VAL:HG12	1:A:201:LEU:CD1	2.51	0.41
1:A:209:THR:HG22	2:B:223:HIS:CE1	2.56	0.41
2:B:93:PHE:HB3	2:B:96:PHE:CD1	2.55	0.41
1:D:87:VAL:HG23	1:D:89:GLU:O	2.21	0.41
2:E:229:LYS:NZ	2:E:233:GLY:O	2.50	0.41
2:F:53:TYR:CD1	2:F:53:TYR:C	2.99	0.41
3:G:93:MET:HE1	3:G:102:SER:HB3	2.03	0.41
3:G:166:MET:HE1	3:G:215:VAL:HB	2.02	0.41
2:B:41:ILE:O	2:B:52:ALA:HA	2.21	0.41
2:B:166:ALA:HB1	2:B:180:LEU:H	1.83	0.41
2:B:189:VAL:O	2:B:191:MET:HE2	2.21	0.41
2:F:22:LYS:NZ	3:I:193:THR:HB	2.35	0.41
2:F:22:LYS:HZ2	3:I:193:THR:HB	1.86	0.41
2:F:26:ARG:NH1	2:F:206:GLU:OE1	2.53	0.41
3:I:68:ILE:HA	3:I:115:ILE:O	2.21	0.41
1:C:187:ASP:OD2	1:C:189:PRO:HD3	2.21	0.40
1:C:204:MET:HE2	1:C:205:ASP:C	2.46	0.40
1:D:167:LYS:HD2	1:D:212:GLU:OE2	2.21	0.40
2:F:32:PRO:HB2	4:F:304:HOH:O	2.19	0.40
1:A:223:ALA:O	1:A:227:ILE:HG13	2.22	0.40
1:C:96:ASP:OD1	1:C:99:THR:HG23	2.21	0.40
1:D:121:ARG:HH12	3:I:110:ASN:HB3	1.85	0.40
2:E:26:ARG:HD2	2:E:206:GLU:OE2	2.21	0.40
2:F:166:ALA:CB	2:F:179:LYS:HG3	2.51	0.40
3:I:43:LEU:O	3:I:43:LEU:HG	2.21	0.40
3:H:114:TYR:CG	3:H:145:MET:HE3	2.57	0.40
1:C:202:MET:HE1	1:C:217:MET:HE3	2.03	0.40
3:H:13:PRO:HD3	3:H:40:PHE:HB2	2.03	0.40
1:C:75:ILE:HG22	1:C:77:LYS:HG3	2.02	0.40
1:C:78:ALA:O	1:C:103:SER:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TYR:HB3	1:A:65:PRO:CD	2.51	0.40
3:I:152:ARG:HB2	3:I:203:GLU:HG3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LYS:NZ	3:I:2:TYR:OH[3_655]	2.08	0.12

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	235/248 (95%)	228 (97%)	6 (3%)	1 (0%)	30	62
1	C	229/248 (92%)	227 (99%)	2 (1%)	0	100	100
1	D	228/248 (92%)	228 (100%)	0	0	100	100
2	B	236/260 (91%)	234 (99%)	2 (1%)	0	100	100
2	E	237/260 (91%)	234 (99%)	3 (1%)	0	100	100
2	F	237/260 (91%)	235 (99%)	2 (1%)	0	100	100
3	G	225/237 (95%)	222 (99%)	2 (1%)	1 (0%)	30	62
3	H	217/237 (92%)	216 (100%)	1 (0%)	0	100	100
3	I	225/237 (95%)	219 (97%)	6 (3%)	0	100	100
All	All	2069/2235 (93%)	2043 (99%)	24 (1%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	TYR
3	G	3	GLN

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	195/204 (96%)	195 (100%)	0	100	100
1	C	190/204 (93%)	190 (100%)	0	100	100
1	D	189/204 (93%)	189 (100%)	0	100	100
2	B	199/220 (90%)	199 (100%)	0	100	100
2	E	200/220 (91%)	200 (100%)	0	100	100
2	F	200/220 (91%)	200 (100%)	0	100	100
3	G	192/199 (96%)	191 (100%)	1 (0%)	81	80
3	H	185/199 (93%)	183 (99%)	2 (1%)	65	74
3	I	191/199 (96%)	189 (99%)	2 (1%)	68	75
All	All	1741/1869 (93%)	1736 (100%)	5 (0%)	86	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	174	ARG
3	I	24	ARG
3	I	174	ARG
3	H	24	ARG
3	H	174	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	131	GLN
2	B	165	ASN
1	C	25	ASN
1	C	38	ASN
1	C	203	GLN
1	C	215	GLN
1	D	33	GLN
1	D	38	ASN

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Mol	Chain	Res	Type
1	D	237	ASN
2	E	131	GLN
2	E	143	ASN
2	F	131	GLN
3	G	3	GLN
3	I	58	GLN
3	I	94	ASN
3	H	25	ASN
3	H	44	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	237/248 (95%)	-1.33	1 (0%) 88 72	19, 53, 130, 197	0
1	C	231/248 (93%)	-1.46	0 100 100	26, 55, 108, 199	0
1	D	230/248 (92%)	-1.41	0 100 100	27, 64, 123, 206	0
2	B	238/260 (91%)	-1.40	0 100 100	23, 61, 124, 201	0
2	E	239/260 (91%)	-1.39	2 (0%) 82 60	31, 68, 136, 229	0
2	F	239/260 (91%)	-1.40	1 (0%) 88 72	25, 66, 133, 221	0
3	G	227/237 (95%)	-1.23	0 100 100	50, 105, 165, 216	0
3	H	219/237 (92%)	-0.73	0 100 100	71, 155, 223, 260	0
3	I	227/237 (95%)	-1.28	0 100 100	46, 99, 147, 182	0
All	All	2087/2235 (93%)	-1.30	4 (0%) 91 82	19, 75, 178, 260	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	100	PRO	3.8
2	E	100	PRO	2.6
2	E	95	SER	2.5
1	A	246	GLU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.