



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:51 AM UTC

PDB ID : 2BA1 / pdb_00002ba1
Title : Archaeal exosome core
Authors : Hopfner, K.P.; Buttner, K.; Wenig, K.
Deposited on : 2005-10-13
Resolution : 2.70 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

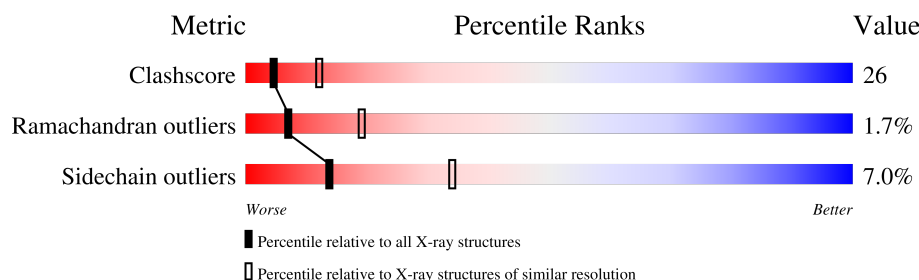
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	179	
1	B	179	
1	C	179	
2	D	258	
2	E	258	
2	F	258	
3	G	259	
3	H	259	

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Mol	Chain	Length	Quality of chain
3	I	259	 A horizontal bar chart showing the quality of chain I. The bar is divided into four segments: green (57%), yellow (33%), orange (5%), and grey (5%). 57% 33% 5% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15740 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 Archaeal exosome RNA binding protein CSL4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1371	855	242	266	8			
1	C	179	Total	C	N	O	S	19	0	0
			1371	855	242	266	8			
1	B	179	Total	C	N	O	S	23	0	0
			1371	855	242	266	8			

- Molecule 2 is a protein called Archaeal exosome complex exonuclease RRP41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	245	Total	C	N	O	S	0	0	0
			1921	1209	339	360	13			
2	D	245	Total	C	N	O	S	3	0	0
			1921	1209	339	360	13			
2	F	245	Total	C	N	O	S	9	0	0
			1921	1209	339	360	13			

- Molecule 3 is a protein called Archaeal exosome complex exonuclease RRP42.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	247	Total	C	N	O	S	3	0	0
			1926	1213	320	387	6			
3	G	247	Total	C	N	O	S	21	0	0
			1926	1213	320	387	6			
3	I	247	Total	C	N	O	S	14	0	0
			1926	1213	320	387	6			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

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

- Molecule 5 is water.

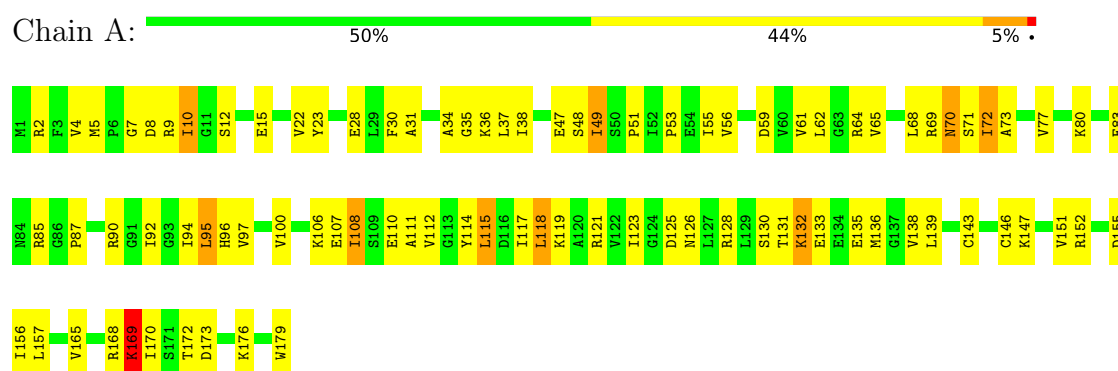
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	O 1	0	0
5	C	2	Total 2	O 2	0	0
5	E	8	Total 8	O 8	0	0
5	D	9	Total 9	O 9	0	0
5	F	22	Total 22	O 22	0	0
5	H	13	Total 13	O 13	0	0
5	G	5	Total 5	O 5	0	0
5	I	23	Total 23	O 23	0	0

3 Residue-property plots

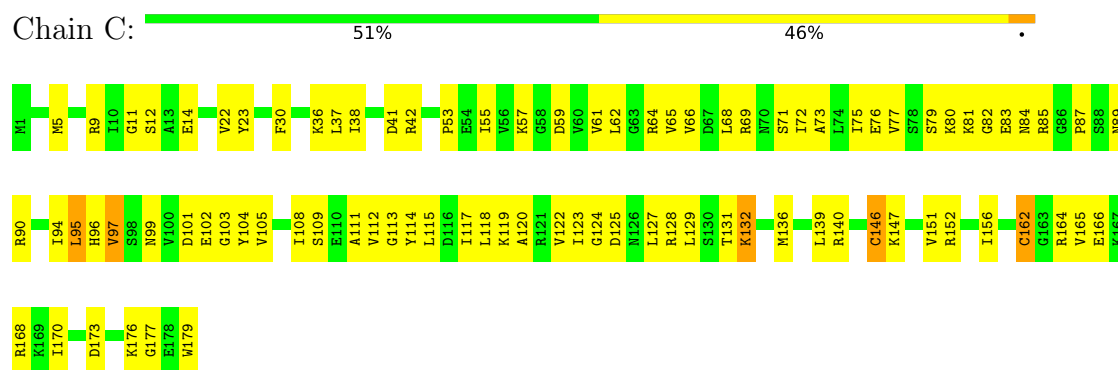
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

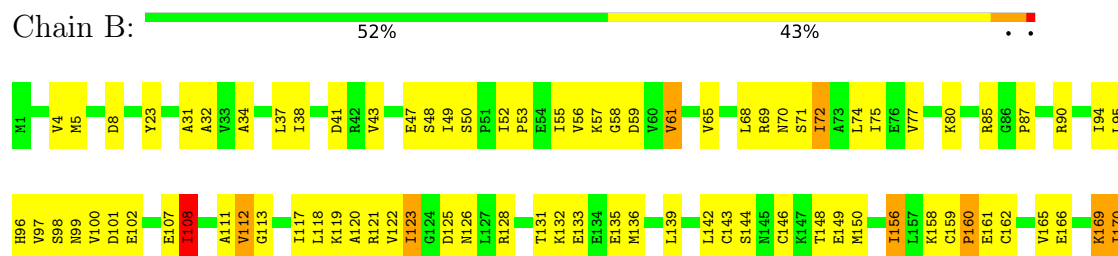
• Molecule 1: Archaeal exosome RNA binding protein CSL4



• Molecule 1: Archaeal exosome RNA binding protein CSL4



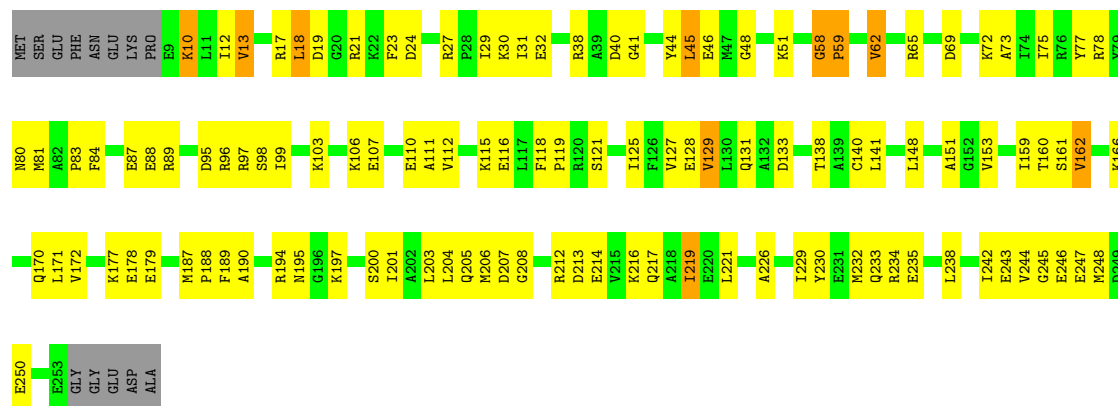
• Molecule 1: Archaeal exosome RNA binding protein CSL4





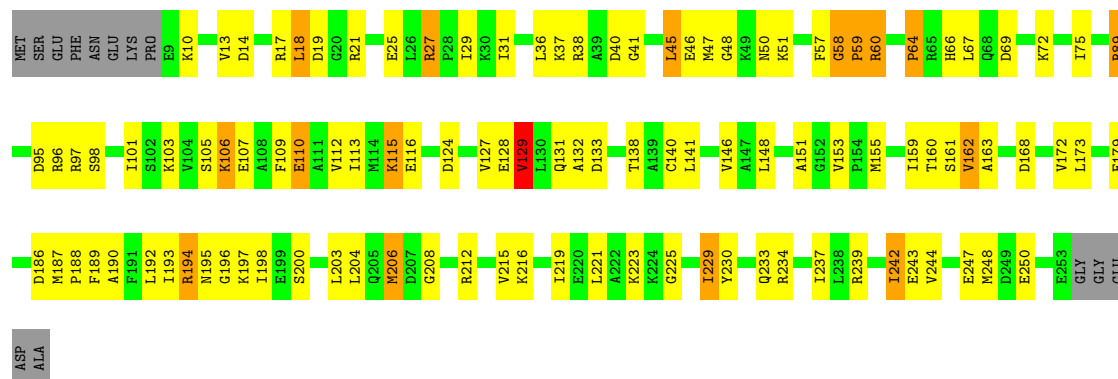
• Molecule 2: Archaeal exosome complex exonuclease RRP41

Chain E: 50% 41% 5%



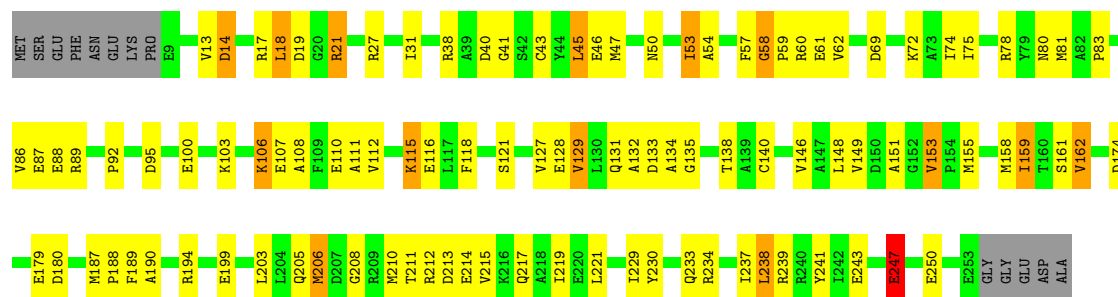
• Molecule 2: Archaeal exosome complex exonuclease RRP41

Chain D: 53% 35% 6% 5%

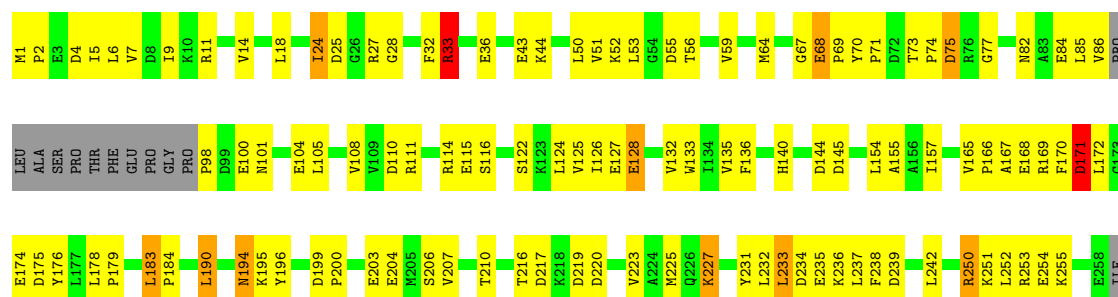


• Molecule 2: Archaeal exosome complex exonuclease RRP41

Chain F: 55% 34% 5% 5%

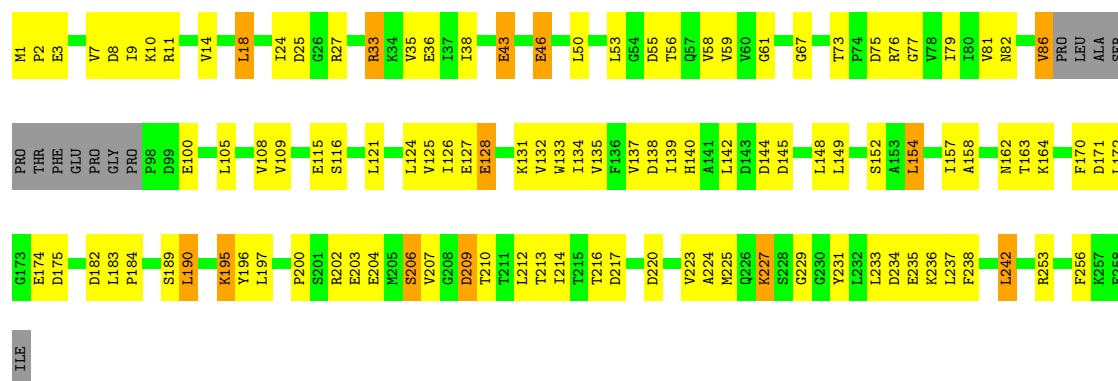


Chain H:  51% 40% 5% 5%



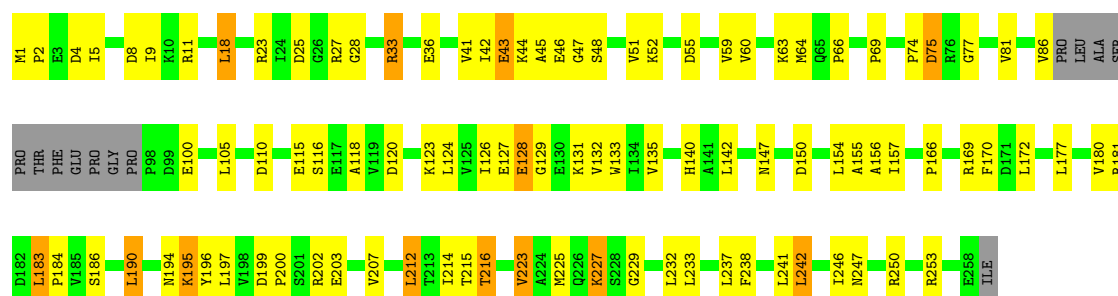
• Molecule 3: Archaeal exosome complex exonuclease RRP42

Chain G:  53% 37% 5% 5%



• Molecule 3: Archaeal exosome complex exonuclease RRP42

Chain I:  57% 33% 5% 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	137.46 Å 137.46 Å 261.01 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15740	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

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	0.39	0/1385	0.89	1/1855 (0.1%)
1	B	0.34	0/1385	0.80	2/1855 (0.1%)
1	C	0.37	0/1385	0.86	2/1855 (0.1%)
2	D	0.51	1/1947 (0.1%)	1.00	6/2612 (0.2%)
2	E	0.48	0/1947	0.99	3/2612 (0.1%)
2	F	0.53	0/1947	1.02	3/2612 (0.1%)
3	G	0.44	0/1949	0.92	3/2638 (0.1%)
3	H	0.50	0/1949	0.94	5/2638 (0.2%)
3	I	0.51	0/1949	0.95	2/2638 (0.1%)
All	All	0.47	1/15843 (0.0%)	0.94	27/21315 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	129	VAL	CA-CB	5.16	1.60	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	43	GLU	N-CA-C	8.98	121.00	111.03
2	D	133	ASP	N-CA-C	-6.40	100.38	108.45
2	F	133	ASP	N-CA-C	-6.39	100.40	108.45
2	D	192	LEU	N-CA-C	-6.25	99.08	109.46
2	D	96	ARG	N-CA-C	-6.17	104.46	111.07
2	F	115	LYS	N-CA-C	5.98	118.58	111.71
3	H	33	ARG	N-CA-C	-5.95	102.86	110.53
1	A	10	ILE	N-CA-C	-5.82	106.80	111.81
2	E	219	ILE	N-CA-C	-5.82	104.84	110.42
1	C	69	ARG	N-CA-C	-5.79	103.29	110.41
3	H	28	GLY	N-CA-C	-5.71	103.94	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	GLU	CB-CA-C	-5.59	109.62	117.23
2	E	133	ASP	N-CA-C	-5.45	101.59	108.45
2	F	247	GLU	N-CA-C	-5.41	105.49	112.68
3	H	255	LYS	N-CA-C	-5.37	106.73	113.28
2	D	115	LYS	N-CA-C	5.36	118.04	111.82
1	C	177	GLY	N-CA-C	-5.27	108.00	115.43
3	G	256	PHE	N-CA-C	-5.21	106.94	113.72
2	D	25	GLU	N-CA-C	5.17	116.95	108.52
3	I	28	GLY	N-CA-C	-5.17	104.80	113.02
3	H	68	GLU	N-CA-C	5.16	121.21	109.81
3	I	75	ASP	N-CA-C	-5.12	106.98	113.23
2	D	27	ARG	N-CA-C	-5.08	102.65	110.07
3	G	206	SER	N-CA-C	-5.07	106.93	113.01
1	B	32	ALA	N-CA-C	-5.06	107.16	113.38
2	E	96	ARG	N-CA-C	-5.05	105.96	111.82
3	H	24	ILE	CB-CA-C	-5.03	105.45	111.88

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	92	0
1	B	1371	0	1409	109	0
1	C	1371	0	1408	84	0
2	D	1921	0	1971	112	0
2	E	1921	0	1971	115	0
2	F	1921	0	1971	85	0
3	G	1926	0	1951	118	0
3	H	1926	0	1951	107	0
3	I	1926	0	1951	100	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	2	0	0	0	0
5	D	9	0	0	1	0
5	E	8	0	0	0	0
5	F	22	0	0	0	0
5	G	5	0	0	0	0
5	H	13	0	0	1	0
5	I	23	0	0	3	0
All	All	15740	0	15991	818	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 26.

All (818) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ILE:HG21	3:H:9:ILE:HD11	1.29	1.09
2:E:112:VAL:HG21	2:E:159:ILE:HD11	1.10	1.05
2:D:31:ILE:HG12	2:D:45:LEU:HD22	1.43	1.00
3:G:76:ARG:HH21	3:G:121:LEU:HD12	1.26	0.94
2:E:201:ILE:HG12	3:H:233:LEU:HB3	1.45	0.94
3:G:18:LEU:HD22	3:G:195:LYS:HE3	1.47	0.93
3:I:77:GLY:HA2	3:I:132:VAL:CG1	2.00	0.92
3:I:216:THR:HG22	3:I:253:ARG:HH22	1.33	0.91
3:G:14:VAL:HG22	3:G:24:ILE:HD11	1.51	0.90
3:I:216:THR:CG2	3:I:253:ARG:HH22	1.84	0.89
1:A:119:LYS:HB2	1:A:139:LEU:HD11	1.54	0.89
2:E:112:VAL:HG21	2:E:159:ILE:CD1	2.01	0.89
2:D:127:VAL:HG11	2:D:140:CYS:HB3	1.55	0.88
3:G:124:LEU:HB3	3:G:133:TRP:HB2	1.57	0.87
1:A:12:SER:HB3	1:A:15:GLU:HG3	1.58	0.85
1:B:170:ILE:HD12	1:B:170:ILE:H	1.41	0.84
1:A:135:GLU:OE1	1:A:136:MET:HE3	1.76	0.84
2:D:112:VAL:HG21	2:D:159:ILE:HD11	1.60	0.83
3:I:77:GLY:HA2	3:I:132:VAL:HG11	1.60	0.82
2:F:110:GLU:HG2	2:F:115:LYS:NZ	1.95	0.82
1:B:53:PRO:HG2	1:B:87:PRO:HA	1.62	0.81
2:D:148:LEU:HD22	2:D:153:VAL:HG21	1.62	0.81
1:A:64:ARG:HH11	1:A:117:ILE:HD11	1.46	0.80
1:B:5:MET:HE2	2:E:234:ARG:HA	1.62	0.80
2:D:131:GLN:HE22	3:I:43:GLU:HG2	1.47	0.80
1:C:64:ARG:HH12	3:H:4:ASP:HB2	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:201:ILE:HD12	2:E:204:LEU:HB2	1.62	0.80
1:B:65:VAL:HG12	1:B:75:ILE:HG13	1.65	0.79
3:G:225:MET:HE1	3:G:238:PHE:HE1	1.48	0.78
2:E:31:ILE:HG12	2:E:45:LEU:HD22	1.66	0.78
3:G:214:ILE:HG12	3:G:225:MET:HE3	1.66	0.78
1:C:118:LEU:HD21	1:C:131:THR:HG21	1.66	0.78
3:G:77:GLY:HA2	3:G:132:VAL:CG1	2.14	0.78
3:G:225:MET:HE1	3:G:238:PHE:CE1	2.18	0.77
2:F:127:VAL:HG11	2:F:140:CYS:HB3	1.64	0.77
2:E:78:ARG:HH11	3:G:86:VAL:HG13	1.50	0.76
2:D:141:LEU:HD11	2:D:203:LEU:HD13	1.67	0.76
2:E:110:GLU:HG2	2:E:115:LYS:NZ	2.01	0.76
2:E:112:VAL:CG2	2:E:159:ILE:HD11	2.05	0.76
3:H:216:THR:HG21	5:H:270:HOH:O	1.86	0.75
2:D:127:VAL:HG11	2:D:140:CYS:CB	2.17	0.75
2:D:239:ARG:O	2:D:243:GLU:HG3	1.87	0.75
3:I:33:ARG:HD3	3:I:199:ASP:OD1	1.87	0.75
3:I:183:LEU:HD13	3:I:253:ARG:HG3	1.69	0.75
2:F:127:VAL:HG11	2:F:140:CYS:CB	2.16	0.74
1:C:68:LEU:HD13	1:C:109:SER:HA	1.69	0.74
2:D:38:ARG:NH2	3:I:202:ARG:HG2	2.02	0.74
1:A:4:VAL:HG13	1:A:8:ASP:HB2	1.70	0.74
1:C:101:ASP:HA	1:C:132:LYS:HA	1.68	0.74
1:B:139:LEU:HD11	1:B:179:TRP:HB3	1.68	0.74
3:I:46:GLU:HG2	3:I:166:PRO:HD3	1.70	0.73
1:B:90:ARG:NH1	3:G:2:PRO:HB2	2.04	0.73
2:E:110:GLU:HG2	2:E:115:LYS:HZ3	1.52	0.73
2:E:95:ASP:O	2:E:99:ILE:HG12	1.89	0.73
3:I:69:PRO:HB3	3:I:132:VAL:HG21	1.71	0.73
2:F:31:ILE:HG12	2:F:45:LEU:HD22	1.69	0.73
2:F:128:GLU:HG2	3:H:140:HIS:CE1	2.24	0.73
2:D:17:ARG:HD2	2:D:179:GLU:OE1	1.89	0.72
3:I:157:ILE:HD13	3:I:184:PRO:HD2	1.71	0.72
1:A:97:VAL:HG22	1:A:108:ILE:HG13	1.71	0.72
1:B:65:VAL:HG11	1:B:112:VAL:CG1	2.19	0.72
1:C:72:ILE:HG23	1:C:94:ILE:HG23	1.72	0.72
2:F:131:GLN:NE2	3:H:44:LYS:H	1.89	0.71
1:B:131:THR:HB	1:B:169:LYS:NZ	2.05	0.71
1:B:158:LYS:HG3	1:B:165:VAL:HG22	1.73	0.70
2:F:230:TYR:HA	2:F:233:GLN:HE21	1.57	0.70
3:G:115:GLU:HB2	3:G:223:VAL:HG13	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ARG:NH1	3:H:2:PRO:HB2	2.07	0.69
1:A:87:PRO:HG2	1:A:90:ARG:HG2	1.74	0.69
1:C:36:LYS:HD2	1:C:38:ILE:HD11	1.74	0.69
2:F:190:ALA:HB3	2:F:203:LEU:HB3	1.75	0.69
3:H:124:LEU:HB3	3:H:133:TRP:HB2	1.75	0.69
2:E:247:GLU:O	2:E:250:GLU:HB3	1.93	0.68
3:H:172:LEU:N	3:H:172:LEU:HD12	2.09	0.68
3:I:126:ILE:HB	3:I:131:LYS:HB3	1.75	0.68
2:E:45:LEU:HD13	2:E:46:GLU:N	2.09	0.68
2:E:170:GLN:HE21	2:E:170:GLN:HA	1.59	0.68
1:B:87:PRO:HG2	1:B:90:ARG:HG2	1.75	0.68
2:D:106:LYS:HE2	2:D:110:GLU:OE2	1.94	0.68
1:C:119:LYS:HB2	1:C:139:LEU:HD11	1.73	0.68
2:F:103:LYS:HD2	3:I:100:GLU:CG	2.24	0.68
2:E:103:LYS:HD2	3:H:100:GLU:CG	2.24	0.68
1:B:99:ASN:HA	1:B:132:LYS:HE2	1.76	0.67
1:A:111:ALA:O	1:A:168:ARG:HB2	1.93	0.67
3:I:41:VAL:C	3:I:42:ILE:HD12	2.18	0.67
3:I:43:GLU:CD	3:I:43:GLU:H	2.01	0.67
1:C:173:ASP:HA	1:C:176:LYS:HD2	1.75	0.67
1:C:53:PRO:HB3	1:C:83:GLU:OE2	1.94	0.67
2:F:19:ASP:OD2	2:F:21:ARG:HD3	1.95	0.66
2:D:103:LYS:HD2	3:G:100:GLU:HG2	1.78	0.66
3:H:183:LEU:HD13	3:H:253:ARG:HG3	1.76	0.66
3:H:126:ILE:HD13	3:H:172:LEU:HD21	1.77	0.66
3:H:227:LYS:NZ	3:H:231:TYR:O	2.29	0.66
3:G:76:ARG:HH21	3:G:121:LEU:CD1	2.06	0.66
1:A:87:PRO:HG2	1:A:90:ARG:CG	2.26	0.66
2:F:31:ILE:HG12	2:F:45:LEU:CD2	2.25	0.66
1:A:34:ALA:HB3	1:A:49:ILE:HD12	1.76	0.66
3:H:116:SER:OG	3:H:184:PRO:HG3	1.96	0.66
1:B:87:PRO:HG2	1:B:90:ARG:CG	2.26	0.66
3:H:77:GLY:HA2	3:H:132:VAL:CG1	2.26	0.66
1:C:64:ARG:NH1	3:H:4:ASP:HB2	2.11	0.65
1:C:118:LEU:HD23	1:C:119:LYS:N	2.10	0.65
2:F:110:GLU:HG2	2:F:115:LYS:HZ2	1.61	0.65
3:G:126:ILE:HG22	3:G:127:GLU:HG3	1.79	0.65
3:I:212:LEU:HD23	3:I:227:LYS:HB3	1.77	0.65
3:G:190:LEU:HD23	3:G:210:THR:O	1.96	0.65
1:B:131:THR:HG23	1:B:136:MET:HB2	1.77	0.65
3:H:14:VAL:HG22	3:H:24:ILE:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:225:MET:HE1	3:H:238:PHE:CZ	2.31	0.65
2:D:230:TYR:HA	2:D:233:GLN:HE21	1.61	0.65
1:C:75:ILE:HD12	1:C:129:LEU:HD12	1.78	0.65
2:E:213:ASP:O	2:E:217:GLN:HG3	1.97	0.64
1:C:61:VAL:HG12	1:C:62:LEU:N	2.13	0.64
3:G:209:ASP:OD2	3:G:209:ASP:N	2.26	0.64
3:I:74:PRO:O	3:I:75:ASP:HB3	1.96	0.64
2:D:215:VAL:O	2:D:219:ILE:HD12	1.97	0.64
2:F:162:VAL:HG22	2:F:229:ILE:HD12	1.79	0.64
2:E:201:ILE:HD11	3:H:233:LEU:HD12	1.78	0.64
2:D:146:VAL:HG13	2:D:237:ILE:CD1	2.27	0.64
2:F:211:THR:OG1	2:F:214:GLU:HG3	1.98	0.64
2:E:188:PRO:HG2	2:E:205:GLN:HB2	1.78	0.64
3:I:116:SER:OG	3:I:184:PRO:HG3	1.99	0.63
3:I:147:ASN:ND2	3:I:150:ASP:H	1.96	0.63
1:C:90:ARG:HH12	3:H:2:PRO:HB2	1.61	0.63
1:C:168:ARG:O	1:C:170:ILE:HG13	1.97	0.63
1:A:49:ILE:HD13	1:A:49:ILE:H	1.64	0.63
1:C:117:ILE:HG21	3:H:9:ILE:CD1	2.19	0.63
2:F:110:GLU:HG2	2:F:115:LYS:HZ3	1.62	0.63
3:I:126:ILE:HD12	3:I:172:LEU:HD23	1.81	0.63
2:E:127:VAL:HG11	2:E:140:CYS:CB	2.29	0.63
2:E:189:PHE:CE2	2:E:219:ILE:HD13	2.34	0.63
3:I:196:TYR:C	3:I:197:LEU:HD12	2.24	0.63
1:A:117:ILE:HG21	3:I:9:ILE:HD11	1.80	0.63
1:C:55:ILE:HB	1:C:89:ASN:HD21	1.64	0.63
2:E:201:ILE:CG1	3:H:233:LEU:HB3	2.24	0.62
3:G:170:PHE:HB2	3:G:172:LEU:HD13	1.79	0.62
2:D:103:LYS:HD2	3:G:100:GLU:CG	2.29	0.62
1:A:2:ARG:NH2	1:A:38:ILE:HD13	2.13	0.62
2:F:81:MET:HA	2:F:129:VAL:HG13	1.80	0.62
2:E:81:MET:HA	2:E:129:VAL:HG13	1.82	0.62
2:E:141:LEU:HD11	2:E:203:LEU:HD13	1.82	0.62
2:E:166:LYS:HZ2	2:E:214:GLU:CD	2.07	0.62
2:D:128:GLU:HG2	3:I:140:HIS:CE1	2.35	0.62
1:B:85:ARG:HH12	2:E:58:GLY:HA3	1.64	0.62
1:C:61:VAL:CG1	1:C:77:VAL:HG13	2.29	0.62
3:G:212:LEU:HD23	3:G:227:LYS:HB3	1.81	0.61
1:B:118:LEU:HD23	1:B:119:LYS:N	2.14	0.61
2:E:243:GLU:O	2:E:247:GLU:HB2	2.00	0.61
1:C:119:LYS:HE2	1:C:136:MET:CE	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:19:ASP:OD2	2:E:21:ARG:HG3	2.00	0.61
2:F:213:ASP:O	2:F:217:GLN:HG3	1.99	0.61
2:D:242:ILE:N	2:D:242:ILE:HD13	2.14	0.61
2:F:127:VAL:HG11	2:F:140:CYS:SG	2.40	0.61
1:C:65:VAL:HG21	1:C:112:VAL:CG1	2.31	0.61
1:C:119:LYS:HE3	1:C:179:TRP:OXT	2.00	0.61
3:H:216:THR:CG2	3:H:220:ASP:HA	2.31	0.61
1:C:59:ASP:OD1	1:C:80:LYS:HE3	2.01	0.61
2:E:162:VAL:HG22	2:E:229:ILE:HD12	1.82	0.61
2:D:173:LEU:HD21	2:D:225:GLY:HA3	1.82	0.61
2:F:132:ALA:O	3:H:44:LYS:HE3	2.00	0.61
3:G:115:GLU:CB	3:G:223:VAL:HG13	2.31	0.61
2:D:206:MET:HG2	3:G:225:MET:HG3	1.83	0.61
2:E:194:ARG:O	2:E:195:ASN:HB3	1.99	0.61
1:C:66:VAL:CG2	1:C:76:GLU:HB2	2.31	0.60
2:E:81:MET:HG2	2:E:129:VAL:CG1	2.32	0.60
1:A:125:ASP:O	1:A:126:ASN:HB2	2.01	0.60
3:G:116:SER:OG	3:G:184:PRO:HG3	2.01	0.60
1:B:112:VAL:HG12	1:B:113:GLY:N	2.17	0.60
2:F:187:MET:HE2	2:F:189:PHE:CZ	2.36	0.60
2:E:128:GLU:HG2	3:G:140:HIS:CE1	2.36	0.60
2:D:146:VAL:HG13	2:D:237:ILE:HD11	1.83	0.60
3:H:33:ARG:HD3	3:H:199:ASP:OD1	2.02	0.60
3:I:120:ASP:HA	3:I:181:ARG:NH2	2.15	0.60
2:F:189:PHE:CE2	2:F:219:ILE:HD13	2.37	0.60
1:A:111:ALA:HA	1:A:168:ARG:HA	1.84	0.60
1:A:22:VAL:HG13	1:A:30:PHE:O	2.02	0.60
1:B:38:ILE:HD11	1:B:47:GLU:OE2	2.02	0.60
1:A:61:VAL:CG1	1:A:77:VAL:HG13	2.32	0.59
2:E:131:GLN:HE22	3:G:43:GLU:H	1.50	0.59
3:I:25:ASP:OD2	3:I:27:ARG:HD3	2.01	0.59
1:A:119:LYS:HE3	1:A:179:TRP:OXT	2.03	0.59
1:A:168:ARG:O	1:A:170:ILE:HG13	2.02	0.59
2:E:127:VAL:HG11	2:E:140:CYS:HB3	1.83	0.59
2:F:57:PHE:O	2:F:58:GLY:O	2.21	0.59
1:C:119:LYS:HB2	1:C:139:LEU:CD1	2.32	0.59
2:D:132:ALA:O	3:I:44:LYS:HE3	2.02	0.59
1:B:131:THR:HG23	1:B:136:MET:CB	2.33	0.59
3:I:5:ILE:HD12	3:I:5:ILE:H	1.67	0.59
1:A:59:ASP:CG	1:A:80:LYS:HE3	2.27	0.59
2:E:106:LYS:HE2	2:E:110:GLU:OE2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:212:ARG:HG2	3:H:242:LEU:CD1	2.33	0.59
2:D:45:LEU:HD13	2:D:46:GLU:N	2.18	0.59
2:F:131:GLN:HE21	3:H:44:LYS:H	1.50	0.59
1:B:74:LEU:C	1:B:75:ILE:HD12	2.28	0.59
2:F:17:ARG:HD2	2:F:179:GLU:OE1	2.02	0.59
3:G:183:LEU:HD13	3:G:253:ARG:HG3	1.84	0.59
3:G:214:ILE:HD13	3:G:242:LEU:HD23	1.84	0.59
1:B:131:THR:HB	1:B:169:LYS:HZ1	1.66	0.59
2:E:87:GLU:HG2	2:E:177:LYS:NZ	2.18	0.59
2:E:190:ALA:HB3	2:E:203:LEU:HB3	1.85	0.59
1:B:131:THR:CB	1:B:169:LYS:HZ1	2.16	0.58
2:E:216:LYS:HE3	3:H:239:ASP:OD1	2.03	0.58
2:D:31:ILE:HG12	2:D:45:LEU:CD2	2.26	0.58
3:I:64:MET:HE3	3:I:135:VAL:HG22	1.84	0.58
1:B:61:VAL:HG21	1:B:77:VAL:CG1	2.33	0.58
3:G:115:GLU:HB2	3:G:223:VAL:CG1	2.33	0.58
2:E:78:ARG:NH2	2:E:80:ASN:HB2	2.17	0.58
2:D:75:ILE:O	2:D:106:LYS:HD2	2.03	0.58
2:F:41:GLY:HA3	2:F:151:ALA:HB2	1.85	0.58
3:G:38:ILE:N	3:G:38:ILE:HD12	2.19	0.58
1:C:85:ARG:HH11	2:F:58:GLY:HA3	1.68	0.58
2:D:13:VAL:O	2:D:13:VAL:HG23	2.03	0.58
3:G:79:ILE:HG12	3:G:135:VAL:HB	1.86	0.58
1:B:139:LEU:CD1	1:B:179:TRP:HB3	2.34	0.58
3:G:36:GLU:HG2	3:G:38:ILE:HD11	1.84	0.58
1:C:5:MET:HE2	2:F:234:ARG:HA	1.85	0.58
1:C:146:CYS:SG	1:C:162:CYS:HB3	2.44	0.58
3:G:131:LYS:O	3:G:132:VAL:HG23	2.03	0.58
1:A:97:VAL:HA	1:A:100:VAL:HG23	1.86	0.57
1:B:53:PRO:HG3	1:B:85:ARG:O	2.03	0.57
2:D:57:PHE:O	2:D:58:GLY:O	2.21	0.57
2:D:109:PHE:HB3	2:D:113:ILE:HD13	1.85	0.57
2:F:78:ARG:NH2	2:F:80:ASN:HB2	2.18	0.57
3:G:10:LYS:HD2	3:G:203:GLU:CD	2.29	0.57
1:A:119:LYS:HG2	1:A:136:MET:CE	2.34	0.57
2:E:40:ASP:OD2	2:E:58:GLY:N	2.38	0.57
3:G:77:GLY:HA2	3:G:132:VAL:HG11	1.87	0.57
3:I:225:MET:HE1	3:I:238:PHE:CE1	2.38	0.57
3:I:242:LEU:O	3:I:246:ILE:HG12	2.05	0.57
2:D:38:ARG:CZ	3:I:202:ARG:HG2	2.34	0.57
2:E:19:ASP:CG	2:E:21:ARG:HG3	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:81:MET:HG2	2:E:129:VAL:HG11	1.86	0.57
3:G:35:VAL:HG22	3:G:53:LEU:HD13	1.87	0.57
3:G:196:TYR:C	3:G:197:LEU:HD12	2.30	0.57
1:C:82:GLY:O	1:C:83:GLU:HG3	2.05	0.56
2:D:198:ILE:HD12	2:D:223:LYS:HB3	1.85	0.56
2:F:127:VAL:CG1	2:F:140:CYS:SG	2.92	0.56
1:A:119:LYS:HE2	1:A:136:MET:CE	2.35	0.56
1:A:30:PHE:CE2	2:D:194:ARG:HD2	2.40	0.56
1:C:61:VAL:HG11	1:C:77:VAL:HG13	1.86	0.56
1:A:61:VAL:HG13	1:A:77:VAL:HG13	1.87	0.56
1:C:73:ALA:HB3	1:C:95:LEU:HB3	1.88	0.56
1:B:150:MET:HE1	1:B:166:GLU:HG3	1.87	0.56
2:D:17:ARG:CZ	2:D:172:VAL:HB	2.35	0.56
2:F:106:LYS:HE2	2:F:110:GLU:OE2	2.05	0.56
1:C:112:VAL:HG12	1:C:113:GLY:H	1.71	0.56
1:B:85:ARG:NH1	2:E:58:GLY:HA3	2.21	0.56
1:B:135:GLU:HB3	1:B:136:MET:HE2	1.88	0.56
2:E:187:MET:HE2	2:E:189:PHE:CZ	2.41	0.56
1:A:85:ARG:HH11	2:D:59:PRO:HD2	1.70	0.56
1:A:155:ASP:O	1:A:156:ILE:HD13	2.05	0.56
1:C:61:VAL:HG12	1:C:62:LEU:H	1.69	0.56
1:B:53:PRO:HG2	1:B:87:PRO:CA	2.33	0.56
2:E:17:ARG:HD2	2:E:179:GLU:OE1	2.05	0.56
3:G:234:ASP:OD1	3:G:236:LYS:HB3	2.06	0.56
1:C:117:ILE:HD13	1:C:140:ARG:HD2	1.87	0.55
2:F:46:GLU:HA	2:F:50:ASN:O	2.06	0.55
3:H:55:ASP:HB2	3:H:145:ASP:OD1	2.06	0.55
3:G:24:ILE:HD13	3:G:203:GLU:OE2	2.05	0.55
3:I:18:LEU:HD22	3:I:195:LYS:HE3	1.89	0.55
2:E:125:ILE:CD1	2:E:148:LEU:HD21	2.37	0.55
3:H:64:MET:HG2	3:H:135:VAL:HG22	1.88	0.55
1:C:87:PRO:HG2	1:C:90:ARG:HG3	1.88	0.55
1:B:65:VAL:O	1:B:65:VAL:HG23	2.06	0.55
2:E:10:LYS:HE3	2:E:12:ILE:O	2.07	0.55
3:H:77:GLY:HA2	3:H:132:VAL:HG11	1.86	0.55
3:G:77:GLY:HA2	3:G:132:VAL:HG13	1.88	0.55
3:I:225:MET:HE1	3:I:238:PHE:CZ	2.41	0.55
1:A:92:ILE:N	1:A:92:ILE:HD12	2.22	0.55
2:E:103:LYS:O	2:E:107:GLU:HG3	2.05	0.55
1:C:114:TYR:O	1:C:115:LEU:HB2	2.05	0.55
2:D:190:ALA:HB3	2:D:203:LEU:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:78:ARG:HH11	3:G:86:VAL:CG1	2.18	0.55
3:H:219:ASP:O	3:H:220:ASP:HB2	2.07	0.55
3:G:105:LEU:C	3:G:105:LEU:HD23	2.32	0.55
1:A:100:VAL:O	1:A:131:THR:HB	2.07	0.55
3:G:1:MET:N	3:G:2:PRO:HD2	2.22	0.55
2:F:103:LYS:HD2	3:I:100:GLU:HG3	1.88	0.55
1:C:65:VAL:HG21	1:C:112:VAL:HG12	1.87	0.55
2:D:97:ARG:O	2:D:101:ILE:HG12	2.07	0.55
2:D:204:LEU:HB3	3:G:227:LYS:HG2	1.87	0.55
2:F:13:VAL:O	2:F:13:VAL:HG23	2.07	0.55
1:B:111:ALA:HB1	1:B:169:LYS:HD3	1.89	0.54
2:E:41:GLY:HA3	2:E:151:ALA:HB2	1.89	0.54
2:D:27:ARG:HD2	2:D:48:GLY:HA3	1.88	0.54
2:F:40:ASP:HB2	2:F:58:GLY:H	1.72	0.54
3:I:177:LEU:HD12	3:I:177:LEU:N	2.22	0.54
1:B:156:ILE:N	1:B:156:ILE:HD12	2.21	0.54
2:D:29:ILE:CD1	2:D:229:ILE:HD13	2.37	0.54
2:F:128:GLU:HG2	3:H:140:HIS:NE2	2.21	0.54
3:H:25:ASP:OD2	3:H:27:ARG:HD3	2.07	0.54
2:F:118:PHE:O	2:F:121:SER:HB2	2.07	0.54
3:H:64:MET:HE3	3:H:135:VAL:HG22	1.88	0.54
1:B:143:CYS:HA	1:B:166:GLU:OE1	2.07	0.54
3:H:194:ASN:C	3:H:237:LEU:HD12	2.33	0.54
1:C:81:LYS:HB2	1:C:179:TRP:CZ3	2.42	0.54
1:B:55:ILE:HD11	1:B:87:PRO:HG3	1.89	0.54
1:B:100:VAL:HG22	1:B:169:LYS:CD	2.37	0.54
3:H:237:LEU:HD23	3:H:237:LEU:C	2.33	0.54
2:D:138:THR:HG21	2:D:162:VAL:HA	1.89	0.54
2:F:89:ARG:HD2	3:H:136:PHE:CD2	2.42	0.54
2:F:189:PHE:CZ	2:F:219:ILE:HD13	2.43	0.54
1:B:52:ILE:HD13	2:E:59:PRO:HG3	1.89	0.54
1:B:112:VAL:HG12	1:B:113:GLY:H	1.72	0.54
3:I:43:GLU:C	3:I:45:ALA:H	2.15	0.54
1:B:55:ILE:CD1	1:B:80:LYS:HB2	2.38	0.54
1:B:69:ARG:HB2	1:B:72:ILE:HG23	1.90	0.54
2:D:116:GLU:CD	2:D:116:GLU:H	2.16	0.54
1:C:101:ASP:HA	1:C:132:LYS:CA	2.37	0.54
1:C:156:ILE:HG21	1:C:165:VAL:HB	1.90	0.54
1:B:99:ASN:HA	1:B:132:LYS:CE	2.38	0.54
2:D:17:ARG:HD3	2:D:172:VAL:HG11	1.90	0.54
2:D:95:ASP:H	2:D:98:SER:HB2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:124:LEU:HB3	3:I:133:TRP:HB2	1.89	0.54
1:B:117:ILE:HG21	3:G:9:ILE:HD11	1.90	0.53
1:B:118:LEU:HD21	1:B:120:ALA:HB2	1.90	0.53
2:E:242:ILE:O	2:E:246:GLU:HG2	2.08	0.53
2:E:29:ILE:HB	2:E:232:MET:SD	2.48	0.53
3:I:60:VAL:HG11	3:I:156:ALA:HA	1.89	0.53
3:G:197:LEU:HD12	3:G:197:LEU:N	2.23	0.53
1:C:23:TYR:OH	2:F:194:ARG:HD3	2.09	0.53
3:H:67:GLY:O	3:H:69:PRO:HD3	2.09	0.53
2:F:188:PRO:HG2	2:F:205:GLN:HB2	1.91	0.53
3:H:194:ASN:O	3:H:237:LEU:HD12	2.09	0.53
2:E:201:ILE:O	2:E:201:ILE:HG13	2.09	0.53
3:H:71:PRO:O	3:H:74:PRO:HD3	2.09	0.53
3:I:127:GLU:O	3:I:129:GLY:N	2.41	0.53
1:B:48:SER:C	1:B:50:SER:H	2.15	0.53
3:H:216:THR:HG23	3:H:220:ASP:HA	1.91	0.53
2:E:103:LYS:HD2	3:H:100:GLU:HG3	1.91	0.53
2:F:13:VAL:O	2:F:14:ASP:HB2	2.08	0.53
3:G:183:LEU:HD13	3:G:253:ARG:CG	2.39	0.53
1:A:73:ALA:HB2	1:A:108:ILE:HD13	1.91	0.52
1:A:87:PRO:O	1:A:90:ARG:HG3	2.09	0.52
1:B:61:VAL:HG21	1:B:77:VAL:HG13	1.90	0.52
2:F:212:ARG:HG2	3:I:242:LEU:HD13	1.90	0.52
2:F:78:ARG:HH11	3:H:86:VAL:HG13	1.73	0.52
2:D:153:VAL:O	2:D:155:MET:HG3	2.10	0.52
3:G:59:VAL:CG2	3:G:142:LEU:HD11	2.39	0.52
3:G:145:ASP:C	3:G:202:ARG:HB2	2.35	0.52
3:I:194:ASN:O	3:I:237:LEU:HD12	2.09	0.52
1:A:23:TYR:OH	2:D:194:ARG:HD3	2.09	0.52
1:B:119:LYS:HD2	1:B:179:TRP:HB2	1.92	0.52
2:E:189:PHE:HE2	2:E:219:ILE:HD13	1.74	0.52
3:H:251:LYS:O	3:H:254:GLU:HG2	2.09	0.52
3:G:10:LYS:HD2	3:G:203:GLU:CG	2.40	0.52
1:B:156:ILE:HG22	1:B:166:GLU:O	2.10	0.52
2:D:127:VAL:CG1	2:D:140:CYS:SG	2.98	0.52
2:F:53:ILE:HD13	2:F:54:ALA:N	2.24	0.52
2:F:239:ARG:O	2:F:243:GLU:HG3	2.09	0.52
3:I:203:GLU:HG2	5:I:261:HOH:O	2.09	0.52
1:A:123:ILE:HG12	1:A:130:SER:HB2	1.92	0.52
1:B:159:CYS:SG	1:B:162:CYS:SG	3.05	0.52
1:C:102:GLU:OE1	1:C:102:GLU:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ILE:HD12	1:B:75:ILE:N	2.24	0.52
3:H:104:GLU:O	3:H:108:VAL:HG23	2.10	0.52
3:H:183:LEU:HD13	3:H:253:ARG:CG	2.40	0.52
1:B:59:ASP:OD1	1:B:80:LYS:NZ	2.39	0.52
3:H:127:GLU:O	3:H:128:GLU:C	2.53	0.52
1:A:49:ILE:HD13	1:A:49:ILE:N	2.23	0.51
2:E:17:ARG:CZ	2:E:172:VAL:HB	2.40	0.51
2:D:19:ASP:OD2	2:D:21:ARG:HG3	2.10	0.51
2:D:131:GLN:HE21	3:I:44:LYS:H	1.56	0.51
1:A:131:THR:HG22	1:A:169:LYS:NZ	2.26	0.51
1:B:8:ASP:CG	2:E:234:ARG:HH22	2.17	0.51
3:G:50:LEU:HD12	3:G:58:VAL:O	2.09	0.51
1:A:119:LYS:HB2	1:A:139:LEU:CD1	2.33	0.51
1:C:79:SER:OG	3:H:6:LEU:HD11	2.09	0.51
3:H:50:LEU:HD13	3:H:59:VAL:CG2	2.40	0.51
1:B:131:THR:HB	1:B:169:LYS:HZ2	1.73	0.51
3:H:1:MET:N	3:H:2:PRO:HD2	2.26	0.51
3:G:164:LYS:HE2	3:G:175:ASP:OD2	2.10	0.51
3:G:216:THR:CG2	3:G:220:ASP:HA	2.41	0.51
3:I:237:LEU:C	3:I:237:LEU:HD23	2.36	0.51
2:F:78:ARG:HH22	2:F:80:ASN:CG	2.19	0.51
3:H:24:ILE:HD13	3:H:203:GLU:OE2	2.11	0.51
3:G:237:LEU:C	3:G:237:LEU:HD23	2.36	0.51
2:E:23:PHE:CE2	2:E:24:ASP:HB3	2.46	0.51
2:E:201:ILE:CD1	3:H:233:LEU:HD12	2.41	0.51
3:H:43:GLU:H	3:H:43:GLU:CD	2.18	0.51
3:H:234:ASP:OD1	3:H:236:LYS:HB3	2.11	0.51
3:I:47:GLY:O	3:I:48:SER:HB3	2.10	0.51
3:I:197:LEU:HD12	3:I:197:LEU:N	2.26	0.51
2:D:153:VAL:O	2:D:153:VAL:HG23	2.11	0.51
2:F:215:VAL:O	2:F:219:ILE:HG12	2.11	0.51
3:G:154:LEU:O	3:G:157:ILE:HG22	2.11	0.51
1:B:65:VAL:HG21	1:B:113:GLY:O	2.11	0.50
1:B:97:VAL:HG23	1:B:98:SER:N	2.27	0.50
1:B:158:LYS:HG2	1:B:159:CYS:N	2.26	0.50
1:A:117:ILE:HG23	3:I:5:ILE:HG23	1.94	0.50
3:H:166:PRO:O	3:H:170:PHE:HD2	1.94	0.50
1:C:87:PRO:HG2	1:C:90:ARG:CG	2.42	0.50
1:B:68:LEU:HD11	1:B:113:GLY:O	2.11	0.50
3:H:5:ILE:HD12	3:H:5:ILE:N	2.26	0.50
3:I:105:LEU:C	3:I:105:LEU:HD23	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:69:ASP:HB3	2:E:72:LYS:O	2.12	0.50
2:D:17:ARG:NH2	2:D:172:VAL:HB	2.27	0.50
1:C:57:LYS:HE3	1:C:123:ILE:O	2.12	0.50
2:E:138:THR:HG22	2:E:161:SER:OG	2.11	0.50
3:G:7:VAL:HG13	3:G:206:SER:HB2	1.94	0.50
3:I:1:MET:O	3:I:4:ASP:HB2	2.11	0.50
2:E:230:TYR:HA	2:E:233:GLN:HE21	1.76	0.50
2:F:203:LEU:HD23	2:F:203:LEU:C	2.37	0.50
3:I:203:GLU:HG3	5:I:270:HOH:O	2.11	0.50
1:A:65:VAL:HG21	1:A:112:VAL:HG13	1.94	0.49
1:A:131:THR:HG22	1:A:131:THR:O	2.12	0.49
3:H:170:PHE:O	3:H:171:ASP:HB2	2.12	0.49
2:E:131:GLN:HE22	3:G:43:GLU:N	2.10	0.49
2:D:40:ASP:OD2	2:D:58:GLY:N	2.46	0.49
3:I:126:ILE:HD12	3:I:172:LEU:CD2	2.41	0.49
2:F:107:GLU:CD	3:I:229:GLY:H	2.20	0.49
2:D:69:ASP:HB3	2:D:72:LYS:O	2.13	0.49
2:D:148:LEU:HD22	2:D:153:VAL:CG2	2.37	0.49
2:F:21:ARG:NH1	2:F:174:ASP:HB3	2.28	0.49
3:H:64:MET:HE3	3:H:135:VAL:CG2	2.42	0.49
3:I:120:ASP:OD2	3:I:123:LYS:HG3	2.11	0.49
1:A:131:THR:HG22	1:A:169:LYS:HZ1	1.78	0.49
1:A:131:THR:CG2	1:A:169:LYS:HG3	2.42	0.49
1:B:100:VAL:HG22	1:B:169:LYS:HD3	1.95	0.49
3:H:7:VAL:HG13	3:H:206:SER:HB2	1.94	0.49
3:G:59:VAL:HG23	3:G:142:LEU:HD11	1.93	0.49
3:G:202:ARG:O	3:G:202:ARG:HD3	2.11	0.49
1:B:5:MET:HE2	2:E:234:ARG:CA	2.38	0.49
3:H:178:LEU:HD12	3:H:179:PRO:HD2	1.94	0.49
3:I:196:TYR:C	3:I:196:TYR:CD1	2.90	0.49
1:C:147:LYS:HG3	2:E:116:GLU:HB3	1.94	0.49
2:D:127:VAL:HG12	2:D:140:CYS:SG	2.53	0.49
1:B:85:ARG:NH2	2:E:151:ALA:O	2.45	0.49
3:G:144:ASP:HB2	3:G:148:LEU:HD11	1.93	0.49
3:I:77:GLY:HA2	3:I:132:VAL:HG12	1.90	0.49
1:C:119:LYS:HG2	1:C:136:MET:CE	2.43	0.49
3:G:67:GLY:HA3	3:G:134:ILE:CD1	2.43	0.49
3:I:59:VAL:CG2	3:I:142:LEU:HD11	2.42	0.49
1:A:69:ARG:O	1:A:70:ASN:C	2.55	0.48
3:I:216:THR:CG2	3:I:253:ARG:NH2	2.66	0.48
1:A:4:VAL:HG11	1:A:31:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:VAL:HG12	1:B:57:LYS:N	2.28	0.48
2:E:111:ALA:HB1	3:H:232:LEU:HG	1.95	0.48
1:A:146:CYS:O	1:A:147:LYS:HB2	2.13	0.48
2:E:128:GLU:CD	3:G:140:HIS:NE2	2.71	0.48
2:F:74:ILE:C	2:F:75:ILE:HD12	2.38	0.48
1:A:73:ALA:HB3	1:A:95:LEU:HB3	1.95	0.48
2:E:203:LEU:C	2:E:203:LEU:HD23	2.37	0.48
3:H:14:VAL:CG2	3:H:24:ILE:HD11	2.42	0.48
3:H:225:MET:HE1	3:H:238:PHE:HZ	1.75	0.48
1:B:58:GLY:O	1:B:121:ARG:NH2	2.47	0.48
1:B:173:ASP:HA	1:B:176:LYS:HD2	1.96	0.48
3:H:190:LEU:HB2	3:H:200:PRO:HB3	1.94	0.48
1:C:118:LEU:HD23	1:C:119:LYS:H	1.79	0.48
1:B:142:LEU:HD23	1:B:149:GLU:HA	1.96	0.48
2:F:111:ALA:HB1	3:I:232:LEU:HG	1.94	0.48
2:F:194:ARG:HB2	2:F:199:GLU:HG3	1.95	0.48
3:H:11:ARG:HG3	3:H:207:VAL:HA	1.96	0.48
3:G:125:VAL:HA	3:G:132:VAL:HG22	1.94	0.48
1:A:71:SER:HA	1:A:97:VAL:CG2	2.44	0.48
1:C:112:VAL:HG12	1:C:113:GLY:N	2.29	0.48
2:D:45:LEU:HD11	2:D:47:MET:HG3	1.94	0.48
1:C:156:ILE:CG2	1:C:165:VAL:HB	2.44	0.48
3:G:170:PHE:O	3:G:171:ASP:HB2	2.14	0.48
3:I:126:ILE:HB	3:I:131:LYS:O	2.14	0.48
3:I:183:LEU:HD13	3:I:253:ARG:CG	2.42	0.48
2:D:206:MET:HG3	3:G:225:MET:N	2.29	0.47
2:F:78:ARG:NH1	3:H:86:VAL:HG13	2.29	0.47
3:G:76:ARG:NH2	3:G:121:LEU:HD12	2.10	0.47
1:A:53:PRO:HB3	1:A:83:GLU:OE1	2.13	0.47
1:A:65:VAL:HG21	1:A:112:VAL:CG1	2.43	0.47
1:B:41:ASP:C	1:B:43:VAL:H	2.21	0.47
2:D:248:MET:C	2:D:250:GLU:H	2.22	0.47
2:E:103:LYS:HD2	3:H:100:GLU:HG2	1.95	0.47
2:D:89:ARG:HB2	3:I:63:LYS:CB	2.45	0.47
2:D:107:GLU:CD	3:G:229:GLY:H	2.22	0.47
2:D:206:MET:HG3	3:G:224:ALA:HA	1.97	0.47
1:B:8:ASP:OD2	2:E:234:ARG:NH2	2.46	0.47
1:B:90:ARG:HH12	3:G:2:PRO:HB2	1.78	0.47
2:E:75:ILE:O	2:E:106:LYS:HD2	2.14	0.47
3:G:139:ILE:HD13	3:G:152:SER:HB3	1.96	0.47
2:D:160:THR:O	2:D:190:ALA:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:216:THR:HG22	3:G:217:ASP:N	2.28	0.47
2:E:212:ARG:HG2	3:H:242:LEU:HD11	1.96	0.47
2:F:103:LYS:HD2	3:I:100:GLU:HG2	1.96	0.47
3:G:237:LEU:HD23	3:G:237:LEU:O	2.14	0.47
3:I:118:ALA:O	3:I:180:VAL:HA	2.14	0.47
3:I:120:ASP:HA	3:I:181:ARG:HH21	1.79	0.47
1:C:9:ARG:HH11	1:C:11:GLY:HA2	1.78	0.47
1:C:136:MET:HE2	1:C:136:MET:HA	1.96	0.47
1:B:55:ILE:HD13	1:B:80:LYS:HB2	1.95	0.47
1:B:87:PRO:HG2	1:B:90:ARG:HG3	1.96	0.47
1:B:126:ASN:N	1:B:126:ASN:HD22	2.11	0.47
1:B:133:GLU:OE2	1:B:136:MET:HE3	2.15	0.47
2:E:87:GLU:CD	2:E:87:GLU:H	2.23	0.47
2:D:129:VAL:HG21	2:D:132:ALA:HB2	1.96	0.47
2:E:188:PRO:HD2	2:E:205:GLN:O	2.15	0.47
2:F:95:ASP:N	2:F:95:ASP:OD2	2.48	0.47
3:H:105:LEU:HD23	3:H:105:LEU:C	2.40	0.47
3:H:210:THR:CG2	3:H:231:TYR:HB3	2.45	0.47
3:I:186:SER:HA	3:I:215:THR:HA	1.97	0.47
3:H:74:PRO:O	3:H:75:ASP:HB2	2.14	0.47
3:H:167:ALA:N	3:H:175:ASP:OD1	2.48	0.47
3:G:25:ASP:OD2	3:G:27:ARG:HD3	2.13	0.47
1:A:48:SER:O	1:A:51:PRO:HD3	2.15	0.46
2:F:208:GLY:H	3:I:115:GLU:HG3	1.80	0.46
1:A:49:ILE:H	1:A:49:ILE:CD1	2.26	0.46
1:A:55:ILE:HD13	1:A:77:VAL:HG11	1.95	0.46
2:E:125:ILE:HD11	2:E:148:LEU:HD21	1.96	0.46
2:D:163:ALA:HA	2:D:188:PRO:HA	1.97	0.46
3:H:25:ASP:OD2	3:H:27:ARG:CD	2.62	0.46
3:G:242:LEU:O	3:G:242:LEU:HD22	2.16	0.46
1:A:90:ARG:NH1	3:I:2:PRO:HB2	2.30	0.46
1:A:97:VAL:HA	1:A:100:VAL:CG2	2.45	0.46
1:B:4:VAL:HG11	1:B:31:ALA:HB2	1.97	0.46
2:E:245:GLY:C	2:E:247:GLU:H	2.23	0.46
2:D:19:ASP:CG	2:D:21:ARG:HG3	2.41	0.46
3:G:190:LEU:HB2	3:G:200:PRO:HB3	1.96	0.46
3:I:25:ASP:CG	3:I:27:ARG:HD3	2.40	0.46
1:B:128:ARG:HH21	1:B:128:ARG:HG3	1.80	0.46
2:E:204:LEU:HD23	2:E:204:LEU:C	2.40	0.46
3:G:202:ARG:HD3	3:G:202:ARG:C	2.40	0.46
1:A:173:ASP:HA	1:A:176:LYS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:SER:O	1:B:132:LYS:NZ	2.48	0.46
2:E:88:GLU:O	2:E:89:ARG:C	2.58	0.46
2:D:51:LYS:HE3	3:I:43:GLU:OE2	2.16	0.46
2:D:109:PHE:HB3	2:D:113:ILE:CD1	2.45	0.46
3:H:5:ILE:HD12	3:H:5:ILE:H	1.81	0.46
3:G:149:LEU:HD21	3:G:213:THR:HG21	1.97	0.46
1:C:65:VAL:HG21	1:C:112:VAL:HG11	1.97	0.46
1:B:52:ILE:HG12	1:B:85:ARG:NH2	2.30	0.46
1:B:61:VAL:CG2	1:B:77:VAL:HG13	2.46	0.46
2:F:110:GLU:O	2:F:115:LYS:HE2	2.16	0.46
3:H:110:ASP:OD1	3:H:114:ARG:NH2	2.48	0.46
1:B:59:ASP:CG	1:B:80:LYS:HZ1	2.22	0.46
1:B:131:THR:CG2	1:B:169:LYS:HZ1	2.28	0.46
2:D:212:ARG:HG2	3:G:242:LEU:CD1	2.45	0.46
3:I:147:ASN:HD21	3:I:150:ASP:H	1.63	0.46
1:A:108:ILE:C	1:A:110:GLU:H	2.23	0.46
1:C:22:VAL:HG13	1:C:30:PHE:O	2.15	0.46
1:C:120:ALA:HB3	1:C:129:LEU:HD22	1.98	0.46
2:E:131:GLN:NE2	3:G:43:GLU:H	2.11	0.46
2:E:190:ALA:CB	2:E:203:LEU:HB3	2.46	0.46
2:D:131:GLN:NE2	3:I:44:LYS:H	2.14	0.46
2:F:38:ARG:HG3	3:H:144:ASP:O	2.16	0.46
3:I:11:ARG:HG3	3:I:207:VAL:HA	1.98	0.46
2:E:207:ASP:OD2	3:H:111:ARG:HG2	2.16	0.46
2:D:95:ASP:HB3	2:D:98:SER:H	1.81	0.46
3:G:10:LYS:O	3:G:14:VAL:HG23	2.15	0.46
3:G:108:VAL:O	3:G:109:VAL:C	2.57	0.46
1:A:119:LYS:HG2	1:A:136:MET:HE1	1.97	0.45
2:F:106:LYS:HB3	2:F:106:LYS:NZ	2.30	0.45
3:I:59:VAL:HG23	3:I:142:LEU:CD1	2.46	0.45
1:B:123:ILE:O	1:B:128:ARG:HB3	2.15	0.45
1:B:148:THR:HG22	1:B:149:GLU:N	2.31	0.45
2:E:197:LYS:HG3	2:E:197:LYS:O	2.15	0.45
1:A:114:TYR:O	1:A:115:LEU:HB2	2.15	0.45
1:C:80:LYS:O	1:C:81:LYS:C	2.59	0.45
2:E:83:PRO:HG2	3:G:138:ASP:CB	2.46	0.45
2:F:148:LEU:O	2:F:153:VAL:HG13	2.16	0.45
3:I:23:ARG:HA	5:I:260:HOH:O	2.16	0.45
1:A:64:ARG:NH1	3:I:8:ASP:OD1	2.49	0.45
2:D:41:GLY:HA3	2:D:151:ALA:HB2	1.98	0.45
2:D:64:PRO:HB2	2:D:66:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:216:THR:CG2	3:H:217:ASP:N	2.80	0.45
3:G:81:VAL:HG22	3:G:137:VAL:HB	1.99	0.45
1:B:5:MET:CE	2:E:234:ARG:HA	2.40	0.45
1:B:95:LEU:C	1:B:95:LEU:HD23	2.42	0.45
3:G:127:GLU:O	3:G:128:GLU:C	2.59	0.45
1:A:5:MET:HG3	2:D:234:ARG:HG3	1.99	0.45
1:A:118:LEU:CD1	1:A:138:VAL:HG22	2.46	0.45
1:B:97:VAL:HG12	1:B:108:ILE:CD1	2.46	0.45
2:E:84:PHE:CD1	3:G:61:GLY:HA3	2.51	0.45
2:E:170:GLN:HE21	2:E:170:GLN:CA	2.23	0.45
2:E:170:GLN:HA	2:E:170:GLN:NE2	2.30	0.45
2:D:216:LYS:HA	2:D:219:ILE:HD13	1.99	0.45
3:G:53:LEU:O	3:G:56:THR:HB	2.17	0.45
1:A:35:GLY:HA3	1:A:47:GLU:O	2.17	0.45
1:C:55:ILE:HD11	1:C:87:PRO:HG3	1.98	0.45
1:C:117:ILE:HD12	1:C:117:ILE:N	2.32	0.45
2:D:206:MET:CG	3:G:225:MET:HG3	2.46	0.45
1:A:4:VAL:HG13	1:A:8:ASP:CB	2.44	0.45
1:B:55:ILE:HG22	1:B:122:VAL:HG21	1.99	0.45
2:D:29:ILE:HD13	2:D:229:ILE:HD13	1.98	0.45
3:G:59:VAL:HG23	3:G:142:LEU:CD1	2.46	0.45
3:I:1:MET:N	3:I:2:PRO:HD2	2.32	0.45
3:I:190:LEU:HB2	3:I:200:PRO:HB3	1.99	0.45
1:A:157:LEU:HD12	1:A:168:ARG:HD2	1.98	0.45
1:C:168:ARG:HE	1:C:168:ARG:HB3	1.63	0.45
3:H:32:PHE:CE2	3:H:252:LEU:HD11	2.51	0.45
3:G:75:ASP:OD2	3:G:125:VAL:HG21	2.17	0.45
3:I:157:ILE:CD1	3:I:184:PRO:HD2	2.45	0.45
3:I:237:LEU:HD23	3:I:237:LEU:O	2.16	0.45
1:A:36:LYS:HD2	1:A:38:ILE:HD11	1.98	0.44
1:B:72:ILE:C	1:B:72:ILE:HD13	2.41	0.44
2:E:10:LYS:HG2	2:E:13:VAL:HG13	1.99	0.44
2:E:81:MET:HE2	2:E:97:ARG:HH21	1.82	0.44
2:E:81:MET:HE2	2:E:97:ARG:NH2	2.31	0.44
2:E:219:ILE:HG21	3:H:235:GLU:OE2	2.17	0.44
2:F:88:GLU:O	2:F:89:ARG:C	2.60	0.44
3:G:172:LEU:HD12	3:G:172:LEU:N	2.31	0.44
2:D:18:LEU:HB2	5:D:261:HOH:O	2.18	0.44
2:F:21:ARG:CZ	2:F:27:ARG:HG3	2.47	0.44
3:I:81:VAL:HB	3:I:110:ASP:HB2	1.98	0.44
1:C:53:PRO:HG2	1:C:87:PRO:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:VAL:O	1:C:114:TYR:HE1	2.00	0.44
1:B:55:ILE:CG2	1:B:122:VAL:HG21	2.48	0.44
1:B:170:ILE:HD12	1:B:170:ILE:N	2.21	0.44
2:D:208:GLY:H	3:G:115:GLU:HG3	1.81	0.44
2:F:74:ILE:HG12	2:F:121:SER:O	2.17	0.44
1:A:131:THR:O	1:A:132:LYS:C	2.60	0.44
1:C:84:ASN:N	1:C:84:ASN:HD22	2.15	0.44
1:B:143:CYS:SG	1:B:144:SER:N	2.90	0.44
3:I:115:GLU:HB2	3:I:223:VAL:HG13	1.98	0.44
1:A:10:ILE:HD12	1:A:10:ILE:N	2.33	0.44
1:A:143:CYS:O	1:A:147:LYS:HA	2.18	0.44
1:C:12:SER:C	1:C:14:GLU:H	2.25	0.44
2:E:73:ALA:HB2	2:E:118:PHE:O	2.18	0.44
2:E:131:GLN:NE2	3:G:43:GLU:N	2.66	0.44
3:H:220:ASP:OD2	3:H:250:ARG:NH2	2.51	0.44
3:G:105:LEU:HD23	3:G:105:LEU:O	2.18	0.44
2:E:44:TYR:OH	2:E:51:LYS:HD3	2.18	0.44
2:D:110:GLU:HG2	2:D:115:LYS:NZ	2.33	0.44
2:D:131:GLN:NE2	3:I:43:GLU:HG2	2.25	0.44
3:I:36:GLU:HB3	3:I:52:LYS:HB2	1.99	0.44
1:A:34:ALA:HB3	1:A:49:ILE:CD1	2.44	0.44
1:C:61:VAL:CG1	1:C:62:LEU:N	2.79	0.44
1:B:139:LEU:O	1:B:139:LEU:HD23	2.17	0.44
2:E:208:GLY:HA2	3:H:115:GLU:OE1	2.18	0.44
2:F:146:VAL:HG13	2:F:237:ILE:HD11	1.99	0.44
3:H:73:THR:O	3:H:75:ASP:N	2.48	0.44
3:H:84:GLU:C	3:H:85:LEU:HD12	2.43	0.44
3:H:165:VAL:HG21	3:H:176:TYR:CE2	2.52	0.44
3:I:43:GLU:CD	3:I:43:GLU:N	2.73	0.44
1:A:62:LEU:CD2	3:I:5:ILE:HG22	2.47	0.44
1:A:96:HIS:CE1	1:A:128:ARG:HH12	2.35	0.44
1:C:41:ASP:O	1:C:42:ARG:HB2	2.17	0.44
2:D:89:ARG:O	2:D:89:ARG:HD3	2.18	0.44
2:D:243:GLU:O	2:D:247:GLU:HB2	2.18	0.44
3:H:216:THR:HG21	3:H:220:ASP:HA	2.00	0.44
1:B:65:VAL:HA	1:B:75:ILE:HA	2.00	0.43
2:D:13:VAL:O	2:D:14:ASP:HB2	2.18	0.43
2:F:112:VAL:HG12	2:F:155:MET:HB3	1.99	0.43
1:A:119:LYS:HG2	1:A:136:MET:HE2	2.00	0.43
1:B:95:LEU:HD23	1:B:96:HIS:O	2.18	0.43
2:E:17:ARG:CD	2:E:179:GLU:OE1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:189:PHE:HA	2:D:203:LEU:O	2.17	0.43
1:A:85:ARG:HH11	2:D:58:GLY:HA3	1.83	0.43
1:C:71:SER:O	1:C:97:VAL:HG22	2.18	0.43
1:C:75:ILE:HD13	1:C:118:LEU:HD13	1.99	0.43
1:C:118:LEU:HD21	1:C:131:THR:CG2	2.41	0.43
2:D:109:PHE:O	2:D:113:ILE:HD13	2.17	0.43
3:H:36:GLU:HB3	3:H:52:LYS:HB2	1.99	0.43
3:H:122:SER:O	3:H:125:VAL:HG23	2.18	0.43
3:H:216:THR:HG22	3:H:217:ASP:O	2.17	0.43
1:A:108:ILE:C	1:A:110:GLU:N	2.75	0.43
2:E:212:ARG:HG2	3:H:242:LEU:HD12	2.00	0.43
3:H:216:THR:O	3:H:253:ARG:NH2	2.52	0.43
3:I:216:THR:HG23	3:I:253:ARG:HH22	1.73	0.43
1:A:95:LEU:HD13	1:A:112:VAL:HG21	2.01	0.43
1:C:62:LEU:HD22	1:C:179:TRP:CE2	2.54	0.43
1:C:128:ARG:HH21	1:C:128:ARG:HG3	1.82	0.43
2:E:10:LYS:CG	2:E:13:VAL:HG13	2.48	0.43
2:E:119:PRO:C	2:E:121:SER:H	2.27	0.43
2:D:60:ARG:HD2	2:D:124:ASP:OD1	2.19	0.43
3:H:27:ARG:NH1	3:H:199:ASP:HB3	2.33	0.43
3:I:126:ILE:HD11	3:I:133:TRP:CD1	2.53	0.43
1:C:101:ASP:C	1:C:103:GLY:H	2.26	0.43
2:D:212:ARG:HG2	3:G:242:LEU:HD13	1.99	0.43
2:D:64:PRO:HG2	2:D:67:LEU:HD12	2.01	0.43
2:D:212:ARG:HD3	2:D:212:ARG:C	2.44	0.43
2:F:238:LEU:O	2:F:241:TYR:HB3	2.19	0.43
3:H:50:LEU:HD13	3:H:59:VAL:HG23	2.00	0.43
3:H:51:VAL:CG2	3:H:155:ALA:HB2	2.48	0.43
3:I:5:ILE:HD12	3:I:5:ILE:N	2.30	0.43
1:A:53:PRO:HG2	1:A:87:PRO:HA	2.00	0.43
1:B:100:VAL:HG13	1:B:101:ASP:N	2.33	0.43
2:E:77:TYR:HB3	2:E:106:LYS:HB2	2.01	0.43
2:D:10:LYS:HG2	2:D:168:ASP:OD1	2.18	0.43
2:D:187:MET:HG2	2:D:189:PHE:CE1	2.54	0.43
2:D:216:LYS:HA	2:D:219:ILE:CD1	2.49	0.43
3:H:242:LEU:HD13	3:H:242:LEU:C	2.44	0.43
1:A:64:ARG:HH11	1:A:117:ILE:CD1	2.25	0.43
2:D:29:ILE:HA	2:D:46:GLU:O	2.18	0.43
2:F:138:THR:HG23	2:F:161:SER:C	2.44	0.43
1:B:65:VAL:HG12	1:B:75:ILE:CG1	2.40	0.43
2:D:105:SER:OG	2:D:141:LEU:HD21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:46:GLU:O	3:G:163:THR:HA	2.19	0.43
1:A:121:ARG:HE	1:A:133:GLU:CD	2.27	0.42
3:I:127:GLU:O	3:I:128:GLU:C	2.61	0.42
1:A:106:LYS:O	1:A:107:GLU:HB2	2.18	0.42
2:D:244:VAL:O	2:D:248:MET:HG3	2.19	0.42
2:F:108:ALA:O	2:F:159:ILE:HD11	2.19	0.42
1:C:61:VAL:CG1	1:C:62:LEU:H	2.32	0.42
1:B:23:TYR:OH	2:E:194:ARG:NH2	2.53	0.42
2:D:58:GLY:O	2:D:60:ARG:HG2	2.19	0.42
2:D:195:ASN:O	2:D:197:LYS:N	2.52	0.42
3:G:133:TRP:CZ2	3:G:172:LEU:HD22	2.53	0.42
1:C:125:ASP:C	1:C:127:LEU:N	2.76	0.42
1:B:99:ASN:HA	1:B:132:LYS:NZ	2.34	0.42
1:B:100:VAL:O	1:B:169:LYS:CE	2.67	0.42
2:E:95:ASP:H	2:E:98:SER:HB2	1.85	0.42
2:E:187:MET:HE2	2:E:189:PHE:CE2	2.55	0.42
3:G:204:GLU:O	3:G:207:VAL:HG23	2.19	0.42
2:D:115:LYS:H	2:D:115:LYS:HG2	1.65	0.42
1:A:131:THR:HG21	1:A:169:LYS:HG3	2.01	0.42
1:C:9:ARG:HG3	1:C:30:PHE:CE2	2.54	0.42
2:D:219:ILE:HG21	3:G:235:GLU:OE2	2.19	0.42
2:F:75:ILE:HD12	2:F:75:ILE:N	2.35	0.42
2:E:27:ARG:HD2	2:E:48:GLY:HA3	2.02	0.42
2:D:37:LYS:HE2	2:D:38:ARG:HH11	1.84	0.42
1:C:59:ASP:O	1:C:122:VAL:HG23	2.20	0.42
1:C:111:ALA:O	1:C:168:ARG:HB2	2.20	0.42
1:B:119:LYS:O	1:B:119:LYS:HG2	2.20	0.42
1:B:131:THR:HG21	1:B:169:LYS:HZ1	1.84	0.42
1:A:61:VAL:HG11	1:A:77:VAL:HG13	2.01	0.42
1:A:72:ILE:CD1	1:A:94:ILE:HG23	2.50	0.42
1:B:146:CYS:C	1:B:148:THR:H	2.27	0.42
1:B:173:ASP:O	1:B:176:LYS:HB2	2.19	0.42
3:G:55:ASP:HB2	3:G:145:ASP:OD1	2.19	0.42
1:A:56:VAL:HG22	1:A:59:ASP:OD1	2.19	0.42
1:B:4:VAL:O	1:B:34:ALA:HA	2.20	0.42
2:E:116:GLU:CD	2:E:116:GLU:H	2.28	0.42
1:C:82:GLY:C	1:C:83:GLU:HG3	2.44	0.41
2:D:128:GLU:CD	3:I:140:HIS:NE2	2.78	0.41
2:F:83:PRO:HG3	2:F:92:PRO:HB3	2.00	0.41
2:F:206:MET:HE3	2:F:210:MET:SD	2.60	0.41
3:G:197:LEU:N	3:G:197:LEU:CD1	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:225:MET:HE1	3:G:238:PHE:CZ	2.55	0.41
1:C:151:VAL:HG12	1:C:152:ARG:N	2.34	0.41
1:B:100:VAL:O	1:B:131:THR:O	2.38	0.41
1:B:146:CYS:C	1:B:148:THR:N	2.79	0.41
2:F:135:GLY:O	2:F:138:THR:HB	2.20	0.41
3:H:168:GLU:C	3:H:170:PHE:N	2.79	0.41
3:G:33:ARG:NH1	3:G:145:ASP:O	2.53	0.41
1:A:68:LEU:HD22	1:A:108:ILE:CG2	2.49	0.41
1:C:95:LEU:HD21	1:C:99:ASN:O	2.20	0.41
1:B:97:VAL:O	1:B:100:VAL:HG12	2.20	0.41
2:E:248:MET:C	2:E:250:GLU:H	2.26	0.41
2:D:190:ALA:CB	2:D:203:LEU:HB3	2.51	0.41
3:H:98:PRO:N	3:H:101:ASN:HD22	2.18	0.41
3:G:50:LEU:HD13	3:G:59:VAL:CG2	2.49	0.41
1:C:162:CYS:SG	1:C:164:ARG:HB3	2.61	0.41
1:B:117:ILE:HD11	3:G:8:ASP:CB	2.50	0.41
3:H:157:ILE:HD13	3:H:184:PRO:HD2	2.02	0.41
3:G:227:LYS:NZ	3:G:231:TYR:O	2.54	0.41
3:I:51:VAL:CG2	3:I:155:ALA:HB2	2.50	0.41
3:I:181:ARG:HE	3:I:181:ARG:HB3	1.74	0.41
3:I:247:ASN:OD1	3:I:250:ARG:NH1	2.53	0.41
1:A:9:ARG:CZ	1:A:28:GLU:OE2	2.68	0.41
1:B:65:VAL:HA	1:B:74:LEU:O	2.20	0.41
1:B:117:ILE:HD11	3:G:8:ASP:HB2	2.02	0.41
1:B:126:ASN:N	1:B:126:ASN:ND2	2.68	0.41
2:D:131:GLN:HE22	3:I:43:GLU:CG	2.24	0.41
3:H:53:LEU:O	3:H:56:THR:HB	2.21	0.41
3:H:200:PRO:HA	3:H:204:GLU:OE2	2.21	0.41
3:G:8:ASP:O	3:G:11:ARG:HB3	2.19	0.41
3:G:216:THR:CG2	3:G:217:ASP:N	2.83	0.41
1:A:123:ILE:HD11	1:A:128:ARG:HG3	2.03	0.41
3:G:1:MET:N	3:G:2:PRO:CD	2.82	0.41
3:I:66:PRO:HD2	3:I:170:PHE:CE2	2.55	0.41
1:A:135:GLU:CD	1:A:136:MET:HE3	2.41	0.41
1:A:156:ILE:HG21	1:A:165:VAL:CG1	2.50	0.41
1:C:96:HIS:CD2	1:C:97:VAL:HG23	2.56	0.41
2:F:127:VAL:HG12	2:F:140:CYS:SG	2.60	0.41
2:F:149:VAL:HG21	2:F:158:MET:SD	2.60	0.41
3:H:225:MET:HE1	3:H:238:PHE:CE1	2.56	0.41
3:G:25:ASP:OD2	3:G:27:ARG:CD	2.68	0.41
2:D:89:ARG:HD3	2:D:89:ARG:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:112:VAL:CG2	2:D:159:ILE:HD11	2.40	0.41
2:D:138:THR:HG23	2:D:161:SER:C	2.46	0.41
2:D:212:ARG:NH1	2:D:216:LYS:NZ	2.69	0.41
2:F:129:VAL:HG21	2:F:132:ALA:HB2	2.03	0.41
2:F:134:ALA:HB1	2:F:180:ASP:OD2	2.21	0.41
3:G:154:LEU:HD12	3:G:154:LEU:HA	1.86	0.41
1:A:7:GLY:N	1:A:31:ALA:O	2.47	0.41
1:A:152:ARG:HH22	1:A:172:THR:HA	1.85	0.41
1:B:100:VAL:O	1:B:169:LYS:NZ	2.51	0.41
1:B:101:ASP:O	1:B:102:GLU:C	2.64	0.41
2:E:29:ILE:CG2	2:E:30:LYS:N	2.83	0.41
2:E:62:VAL:O	2:E:62:VAL:HG13	2.20	0.41
2:E:160:THR:HG21	2:E:226:ALA:O	2.21	0.41
2:E:194:ARG:O	2:E:195:ASN:CB	2.67	0.41
2:F:69:ASP:HB3	2:F:72:LYS:O	2.21	0.41
2:F:86:VAL:HG23	2:F:88:GLU:O	2.21	0.41
2:F:247:GLU:O	2:F:250:GLU:HB3	2.21	0.41
3:H:70:TYR:HB2	3:H:73:THR:OG1	2.21	0.41
3:H:172:LEU:N	3:H:172:LEU:CD1	2.78	0.41
3:G:216:THR:HG21	3:G:220:ASP:HA	2.02	0.41
3:I:194:ASN:C	3:I:237:LEU:HD12	2.46	0.41
3:G:214:ILE:CG1	3:G:225:MET:HE3	2.44	0.41
1:A:118:LEU:HD12	1:A:138:VAL:HA	2.03	0.40
1:A:123:ILE:C	1:A:123:ILE:HD12	2.47	0.40
1:C:55:ILE:HB	1:C:89:ASN:ND2	2.33	0.40
1:C:166:GLU:OE1	1:C:168:ARG:NH2	2.54	0.40
1:B:158:LYS:HG2	1:B:159:CYS:H	1.86	0.40
2:F:58:GLY:O	2:F:59:PRO:C	2.64	0.40
3:G:14:VAL:CG2	3:G:24:ILE:HD11	2.37	0.40
3:G:182:ASP:OD2	3:G:183:LEU:N	2.54	0.40
3:I:157:ILE:HG12	3:I:183:LEU:HD23	2.03	0.40
1:B:160:PRO:HG2	1:B:161:GLU:H	1.85	0.40
2:E:38:ARG:NH1	3:G:145:ASP:OD2	2.48	0.40
2:D:160:THR:OG1	2:D:193:ILE:HD12	2.21	0.40
2:F:190:ALA:CB	2:F:203:LEU:HB3	2.49	0.40
3:H:196:TYR:CD1	3:H:196:TYR:C	2.99	0.40
3:G:158:ALA:O	3:G:162:ASN:ND2	2.54	0.40
1:A:111:ALA:HA	1:A:168:ARG:CA	2.51	0.40
2:D:36:LEU:HD22	3:I:142:LEU:O	2.20	0.40
3:H:33:ARG:CD	3:H:199:ASP:OD1	2.69	0.40
3:G:126:ILE:HD13	3:G:172:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:GLU:HA	2:D:50:ASN:O	2.21	0.40
2:D:47:MET:O	2:D:50:ASN:HB2	2.21	0.40
2:D:153:VAL:O	2:D:153:VAL:CG2	2.69	0.40
2:F:17:ARG:O	2:F:19:ASP:N	2.54	0.40
2:F:75:ILE:O	2:F:106:LYS:HD2	2.21	0.40
3:H:43:GLU:OE1	3:H:43:GLU:N	2.41	0.40
3:G:225:MET:HE2	3:G:225:MET:HB3	1.95	0.40
3:I:214:ILE:HG12	3:I:225:MET:HE3	2.01	0.40
2:E:81:MET:CE	2:E:97:ARG:NH2	2.85	0.40
2:E:170:GLN:CA	2:E:170:GLN:NE2	2.85	0.40
2:D:37:LYS:HD2	3:I:55:ASP:OD1	2.21	0.40
2:F:62:VAL:O	2:F:62:VAL:HG13	2.20	0.40
3:G:73:THR:CB	3:G:76:ARG:HD3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	177/179 (99%)	159 (90%)	15 (8%)	3 (2%)	7	19
1	B	177/179 (99%)	143 (81%)	26 (15%)	8 (4%)	2	4
1	C	177/179 (99%)	154 (87%)	22 (12%)	1 (1%)	21	44
2	D	243/258 (94%)	227 (93%)	11 (4%)	5 (2%)	5	15
2	E	243/258 (94%)	223 (92%)	15 (6%)	5 (2%)	5	15
2	F	243/258 (94%)	233 (96%)	8 (3%)	2 (1%)	16	37
3	G	243/259 (94%)	219 (90%)	22 (9%)	2 (1%)	16	37
3	H	243/259 (94%)	224 (92%)	14 (6%)	5 (2%)	5	15
3	I	243/259 (94%)	228 (94%)	13 (5%)	2 (1%)	16	37
All	All	1989/2088 (95%)	1810 (91%)	146 (7%)	33 (2%)	7	19

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	108	ILE
1	B	112	VAL
2	E	58	GLY
2	D	58	GLY
2	F	58	GLY
3	H	75	ASP
3	H	171	ASP
3	G	174	GLU
3	I	128	GLU
1	A	132	LYS
1	C	124	GLY
1	B	71	SER
1	B	169	LYS
2	E	18	LEU
2	E	65	ARG
2	D	196	GLY
2	F	18	LEU
3	H	128	GLU
1	A	70	ASN
1	B	70	ASN
2	E	10	LYS
2	E	59	PRO
2	D	89	ARG
1	A	169	LYS
3	H	169	ARG
3	G	128	GLU
3	I	169	ARG
3	H	174	GLU
1	B	123	ILE
1	B	160	PRO
2	D	59	PRO
2	D	64	PRO
1	B	49	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%)	140 (94%)	9 (6%)	17	41
1	B	149/149 (100%)	141 (95%)	8 (5%)	20	45
1	C	149/149 (100%)	140 (94%)	9 (6%)	17	41
2	D	204/214 (95%)	190 (93%)	14 (7%)	14	34
2	E	204/214 (95%)	188 (92%)	16 (8%)	11	29
2	F	204/214 (95%)	183 (90%)	21 (10%)	7	18
3	G	217/227 (96%)	203 (94%)	14 (6%)	15	37
3	H	217/227 (96%)	203 (94%)	14 (6%)	15	37
3	I	217/227 (96%)	202 (93%)	15 (7%)	14	34
All	All	1710/1770 (97%)	1590 (93%)	120 (7%)	14	34

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	49	ILE
1	A	72	ILE
1	A	95	LEU
1	A	108	ILE
1	A	115	LEU
1	A	118	LEU
1	A	151	VAL
1	A	169	LYS
1	C	37	LEU
1	C	95	LEU
1	C	97	VAL
1	C	104	TYR
1	C	105	VAL
1	C	108	ILE
1	C	132	LYS
1	C	146	CYS
1	C	162	CYS
1	B	37	LEU
1	B	61	VAL
1	B	72	ILE
1	B	94	ILE
1	B	108	ILE
1	B	125	ASP
1	B	156	ILE
1	B	170	ILE

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Mol	Chain	Res	Type
2	E	13	VAL
2	E	18	LEU
2	E	32	GLU
2	E	45	LEU
2	E	62	VAL
2	E	129	VAL
2	E	153	VAL
2	E	162	VAL
2	E	171	LEU
2	E	178	GLU
2	E	200	SER
2	E	206	MET
2	E	221	LEU
2	E	235	GLU
2	E	238	LEU
2	E	244	VAL
2	D	18	LEU
2	D	45	LEU
2	D	60	ARG
2	D	106	LYS
2	D	110	GLU
2	D	129	VAL
2	D	162	VAL
2	D	186	ASP
2	D	194	ARG
2	D	200	SER
2	D	206	MET
2	D	221	LEU
2	D	229	ILE
2	D	242	ILE
2	F	14	ASP
2	F	18	LEU
2	F	21	ARG
2	F	43	CYS
2	F	45	LEU
2	F	47	MET
2	F	53	ILE
2	F	60	ARG
2	F	61	GLU
2	F	87	GLU
2	F	100	GLU
2	F	106	LYS

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Mol	Chain	Res	Type
2	F	116	GLU
2	F	129	VAL
2	F	153	VAL
2	F	159	ILE
2	F	162	VAL
2	F	206	MET
2	F	221	LEU
2	F	238	LEU
2	F	247	GLU
3	H	18	LEU
3	H	33	ARG
3	H	68	GLU
3	H	82	ASN
3	H	154	LEU
3	H	171	ASP
3	H	183	LEU
3	H	190	LEU
3	H	194	ASN
3	H	195	LYS
3	H	223	VAL
3	H	227	LYS
3	H	233	LEU
3	H	250	ARG
3	G	3	GLU
3	G	18	LEU
3	G	33	ARG
3	G	46	GLU
3	G	82	ASN
3	G	86	VAL
3	G	154	LEU
3	G	189	SER
3	G	190	LEU
3	G	195	LYS
3	G	209	ASP
3	G	227	LYS
3	G	233	LEU
3	G	242	LEU
3	I	18	LEU
3	I	33	ARG
3	I	43	GLU
3	I	86	VAL
3	I	154	LEU

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Mol	Chain	Res	Type
3	I	183	LEU
3	I	190	LEU
3	I	195	LYS
3	I	212	LEU
3	I	216	THR
3	I	223	VAL
3	I	227	LYS
3	I	233	LEU
3	I	241	LEU
3	I	242	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	96	HIS
1	A	126	ASN
1	C	84	ASN
1	C	126	ASN
1	B	70	ASN
1	B	84	ASN
1	B	96	HIS
1	B	126	ASN
2	E	131	GLN
2	E	170	GLN
2	E	195	ASN
2	E	228	GLN
2	E	233	GLN
2	D	66	HIS
2	D	80	ASN
2	D	131	GLN
2	D	170	GLN
2	D	195	ASN
2	D	228	GLN
2	D	233	GLN
2	F	131	GLN
2	F	170	GLN
2	F	233	GLN
3	H	147	ASN
3	H	194	ASN
3	G	21	ASN
3	G	57	GLN

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Mol	Chain	Res	Type
3	G	65	GLN
3	G	147	ASN
3	I	147	ASN
3	I	194	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.