



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:39 PM UTC

PDB ID : 4J4X / pdb_00004j4x
Title : Crystal structure of GraVN
Authors : Jiao, L.; Ouyang, S.; Liang, M.; Niu, F.; Shaw, N.; Wu, W.; Ding, W.; Jin, C.;
Zhu, Y.; Zhang, F.; Wang, T.; Li, C.; Zuo, X.; Luan, C.H.; Li, D.; Liu, Z.J.
Deposited on : 2013-02-07
Resolution : 2.51 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:

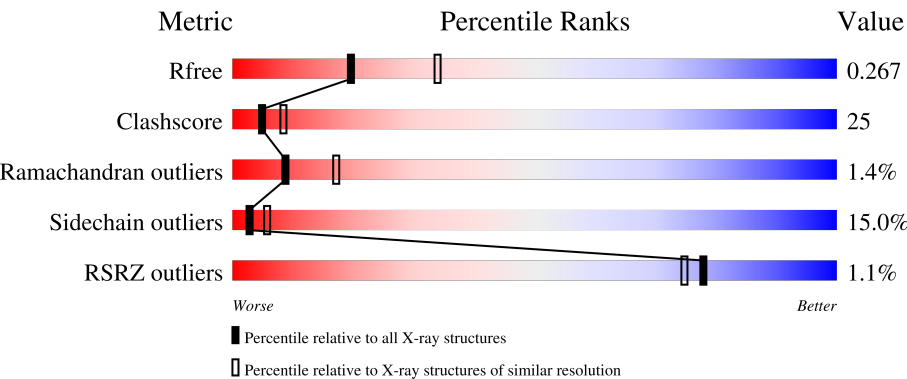
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	257	60%31%7%.
1	B	257	63%27%6%.
1	C	257	3% 49%33%11%. .
1	D	257	58%32%7%.
1	E	257	2% 48%37%11%. .

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Mol	Chain	Length	Quality of chain
1	F	257	% 60% 32% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11737 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 NP protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1938	1230	332	362	14			
1	B	248	Total	C	N	O	S	0	0	0
			1921	1220	329	358	14			
1	C	246	Total	C	N	O	S	0	0	0
			1910	1213	327	356	14			
1	D	249	Total	C	N	O	S	0	0	0
			1930	1226	331	359	14			
1	E	250	Total	C	N	O	S	0	0	0
			1938	1229	331	364	14			
1	F	248	Total	C	N	O	S	0	0	0
			1921	1220	329	358	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP E2DQZ4
A	-1	ASN	-	expression tag	UNP E2DQZ4
A	0	ALA	-	expression tag	UNP E2DQZ4
B	-2	SER	-	expression tag	UNP E2DQZ4
B	-1	ASN	-	expression tag	UNP E2DQZ4
B	0	ALA	-	expression tag	UNP E2DQZ4
C	-2	SER	-	expression tag	UNP E2DQZ4
C	-1	ASN	-	expression tag	UNP E2DQZ4
C	0	ALA	-	expression tag	UNP E2DQZ4
D	-2	SER	-	expression tag	UNP E2DQZ4
D	-1	ASN	-	expression tag	UNP E2DQZ4
D	0	ALA	-	expression tag	UNP E2DQZ4
E	-2	SER	-	expression tag	UNP E2DQZ4
E	-1	ASN	-	expression tag	UNP E2DQZ4
E	0	ALA	-	expression tag	UNP E2DQZ4
F	-2	SER	-	expression tag	UNP E2DQZ4
F	-1	ASN	-	expression tag	UNP E2DQZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP E2DQZ4

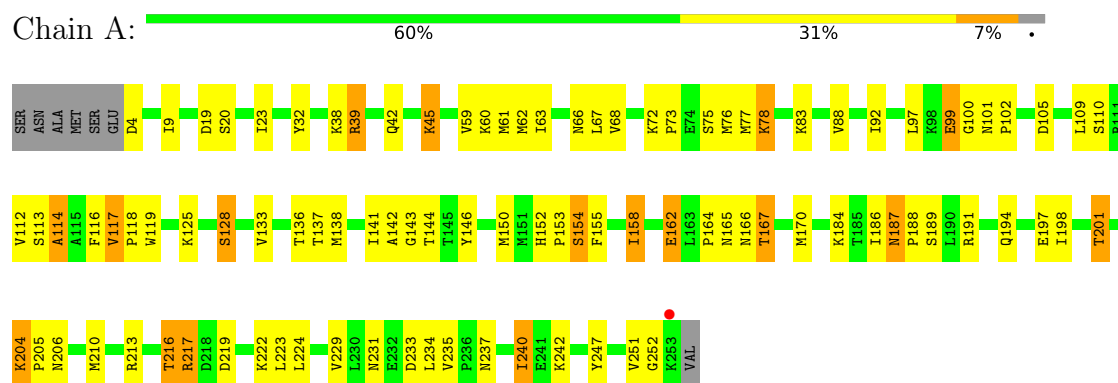
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	47	Total O 47 47	0	0
2	B	40	Total O 40 40	0	0
2	C	19	Total O 19 19	0	0
2	D	27	Total O 27 27	0	0
2	E	23	Total O 23 23	0	0
2	F	23	Total O 23 23	0	0

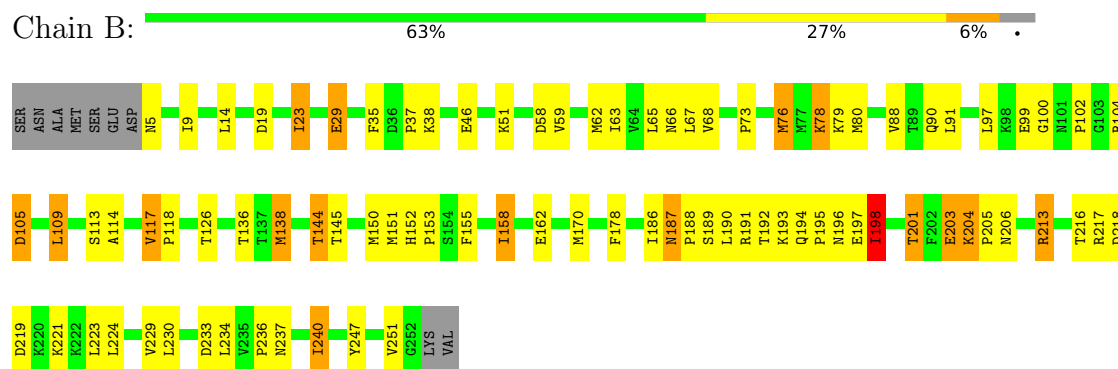
3 Residue-property plots

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 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.

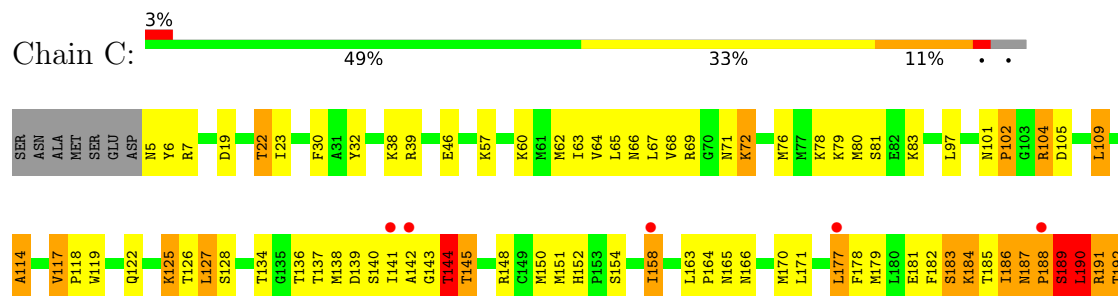
• Molecule 1: NP protein



• Molecule 1: NP protein



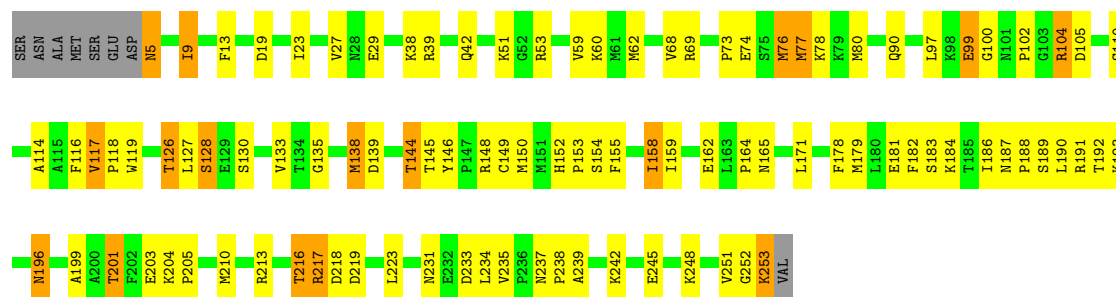
• Molecule 1: NP protein





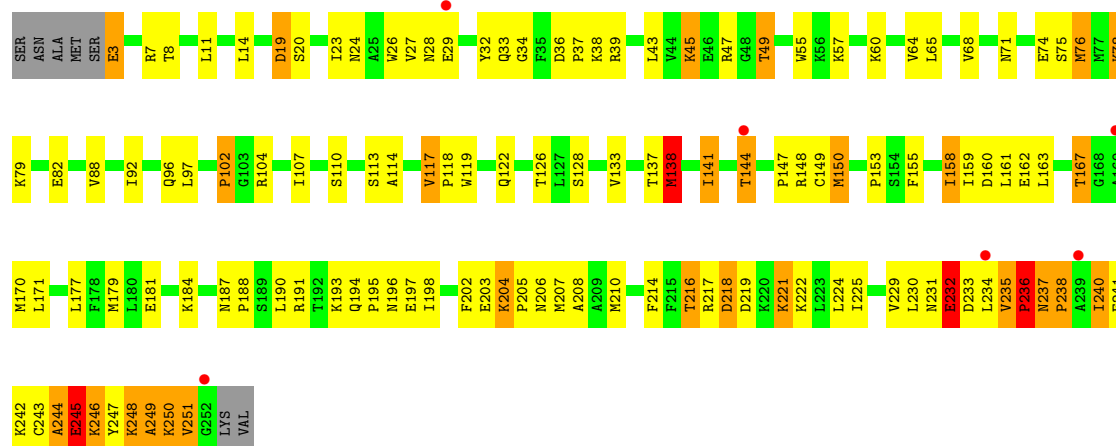
• Molecule 1: NP protein

Chain D: .



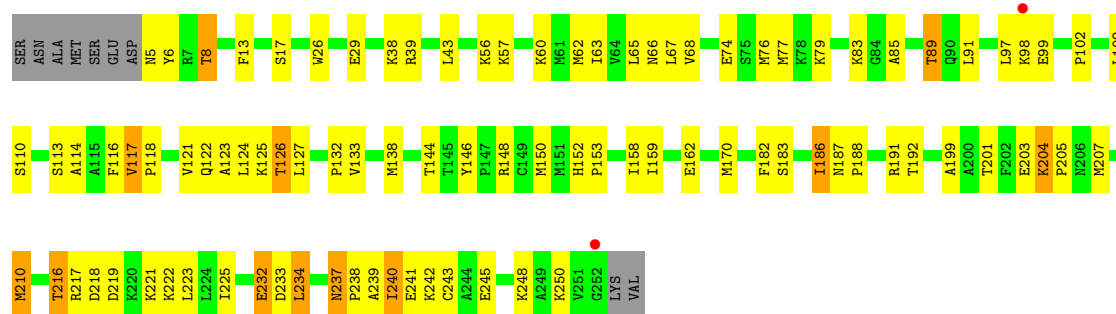
• Molecule 1: NP protein

Chain E: . .



• Molecule 1: NP protein

Chain F: .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.29Å 96.34Å 100.80Å 64.57° 81.72° 85.10°	Depositor
Resolution (Å)	49.59 – 2.51 49.59 – 2.51	Depositor EDS
% Data completeness (in resolution range)	96.8 (49.59-2.51) 97.2 (49.59-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.195 , 0.266 0.194 , 0.267	Depositor DCC
R_{free} test set	2996 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11737	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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

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	1.79	4/1973 (0.2%)	1.09	7/2664 (0.3%)
1	B	1.75	5/1956 (0.3%)	1.08	7/2642 (0.3%)
1	C	1.63	5/1945 (0.3%)	1.13	13/2627 (0.5%)
1	D	1.64	0/1965	1.04	3/2653 (0.1%)
1	E	1.50	3/1973 (0.2%)	1.08	9/2665 (0.3%)
1	F	1.66	1/1956 (0.1%)	1.07	4/2642 (0.2%)
All	All	1.66	18/11768 (0.2%)	1.08	43/15893 (0.3%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	144	THR	CA-C	-6.07	1.48	1.52
1	C	195	PRO	N-CD	5.56	1.55	1.47
1	B	109	LEU	C-O	-5.52	1.17	1.24
1	C	205	PRO	N-CD	5.44	1.55	1.47
1	E	236	PRO	N-CD	5.43	1.55	1.47
1	E	238	PRO	N-CD	5.31	1.55	1.47
1	B	88	VAL	C-O	-5.26	1.18	1.24
1	A	187	ASN	C-O	-5.25	1.20	1.25
1	C	109	LEU	C-O	-5.24	1.18	1.24
1	C	204	LYS	C-N	5.23	1.40	1.34
1	A	184	LYS	C-O	-5.15	1.18	1.24
1	B	59	VAL	C-O	-5.08	1.18	1.24
1	E	113	SER	C-O	-5.07	1.18	1.24
1	B	187	ASN	N-CA	-5.06	1.42	1.46
1	F	187	ASN	C-O	-5.04	1.20	1.25
1	A	72	LYS	C-O	-5.02	1.18	1.24
1	B	113	SER	C-O	-5.00	1.18	1.24
1	A	68	VAL	C-O	-5.00	1.18	1.24

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	VAL	N-CA-C	9.51	119.47	110.53
1	B	105	ASP	N-CA-C	8.52	120.65	111.36
1	B	68	VAL	N-CA-C	8.25	118.29	110.53
1	F	68	VAL	N-CA-C	7.70	118.50	110.72
1	C	198	ILE	N-CA-C	-7.66	103.39	110.82
1	C	245	GLU	N-CA-C	-7.38	103.23	111.28
1	C	114	ALA	N-CA-C	7.22	118.94	111.14
1	E	28	ASN	N-CA-C	7.02	119.02	111.36
1	A	114	ALA	N-CA-C	6.93	118.62	111.14
1	B	203	GLU	N-CA-C	6.39	117.91	111.07
1	A	100	GLY	N-CA-C	6.38	122.89	111.02
1	A	153	PRO	CA-C-N	6.16	129.15	120.28
1	A	153	PRO	C-N-CA	6.16	129.15	120.28
1	E	68	VAL	N-CA-C	6.12	116.90	110.72
1	C	71	ASN	N-CA-C	6.10	121.47	113.30
1	C	68	VAL	N-CA-C	6.03	116.19	110.53
1	A	142	ALA	N-CA-C	5.89	117.78	111.36
1	C	204	LYS	CA-C-N	-5.70	112.64	118.85
1	C	204	LYS	C-N-CA	-5.70	112.64	118.85
1	C	234	LEU	CA-C-N	-5.69	117.80	123.04
1	C	234	LEU	C-N-CA	-5.69	117.80	123.04
1	A	252	GLY	N-CA-C	-5.65	99.80	113.18
1	D	100	GLY	N-CA-C	5.62	121.48	111.02
1	F	126	THR	N-CA-C	5.61	117.47	111.36
1	E	237	ASN	N-CA-C	-5.59	103.13	110.39
1	D	217	ARG	N-CA-C	-5.57	105.20	111.28
1	B	100	GLY	N-CA-C	5.57	121.38	111.02
1	F	6	TYR	N-CA-C	5.57	117.35	111.28
1	C	187	ASN	CA-C-N	-5.49	112.98	119.84
1	C	187	ASN	C-N-CA	-5.49	112.98	119.84
1	C	134	THR	N-CA-C	5.42	117.87	110.55
1	B	221	LYS	N-CA-C	-5.41	105.38	111.28
1	B	23	ILE	CB-CA-C	-5.40	105.06	111.97
1	E	122	GLN	N-CA-C	5.38	117.22	111.36
1	E	237	ASN	CA-C-N	-5.31	113.20	119.84
1	E	237	ASN	C-N-CA	-5.31	113.20	119.84
1	E	208	ALA	N-CA-C	-5.28	105.53	111.28
1	E	138	MET	N-CA-C	-5.17	105.64	111.28
1	D	128	SER	N-CA-C	5.14	116.89	111.28
1	B	198	ILE	CB-CA-C	-5.12	105.22	112.14
1	E	71	ASN	N-CA-C	5.09	118.80	112.59
1	C	69	ARG	N-CA-C	5.03	119.37	112.88
1	F	186	ILE	CB-CA-C	-5.03	105.42	112.02

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	1938	0	1990	64	1
1	B	1921	0	1973	65	0
1	C	1910	0	1959	151	1
1	D	1930	0	1985	88	0
1	E	1938	0	1983	162	0
1	F	1921	0	1970	80	0
2	A	47	0	0	5	0
2	B	40	0	0	2	0
2	C	19	0	0	5	0
2	D	27	0	0	4	0
2	E	23	0	0	12	0
2	F	23	0	0	3	0
All	All	11737	0	11860	592	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 25.

All (592) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:194:GLN:CB	1:E:197:GLU:OE2	1.71	1.39
1:C:139:ASP:OD2	1:C:148:ARG:NH1	1.60	1.34
1:E:194:GLN:HB2	1:E:197:GLU:OE2	1.15	1.32
1:C:250:LYS:O	2:C:315:HOH:O	1.52	1.26
1:E:20:SER:O	1:E:24:ASN:ND2	1.65	1.25
1:B:104:ARG:NH1	1:C:80:MET:O	1.71	1.22
1:F:133:VAL:HG11	1:F:138:MET:HE1	1.23	1.17
1:C:194:GLN:O	1:C:197:GLU:OE2	1.62	1.15
1:B:194:GLN:O	1:B:197:GLU:HB2	1.49	1.13
1:A:62:MET:CE	1:A:97:LEU:HD11	1.79	1.12
1:E:38:LYS:HG2	1:E:214:PHE:CE1	1.84	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:ALA:O	1:F:126:THR:OG1	1.65	1.10
1:E:217:ARG:O	1:E:221:LYS:HG3	1.50	1.09
1:C:213:ARG:HH11	1:C:213:ARG:HB3	1.18	1.08
1:A:152:HIS:HD2	1:A:154:SER:HB2	1.18	1.07
1:C:197:GLU:OE2	1:C:197:GLU:N	1.87	1.06
1:C:188:PRO:HG3	1:C:191:ARG:HD2	1.40	1.04
1:E:194:GLN:N	1:E:197:GLU:OE2	1.90	1.04
1:E:229:VAL:O	1:E:230:LEU:HD23	1.58	1.04
1:C:138:MET:HE2	1:C:178:PHE:HA	1.40	1.04
1:B:198:ILE:O	1:B:201:THR:HB	1.58	1.03
1:C:104:ARG:NH1	1:D:80:MET:O	1.92	1.02
1:F:182:PHE:O	1:F:186:ILE:HG12	1.60	1.01
1:E:231:ASN:OD1	1:E:232:GLU:N	1.93	1.01
1:F:132:PRO:HD3	2:F:307:HOH:O	1.59	1.00
1:E:247:TYR:O	1:E:251:VAL:HG23	1.62	0.99
1:C:237:ASN:OD1	1:C:239:ALA:N	1.95	0.99
1:D:152:HIS:HD2	1:D:154:SER:HB2	1.26	0.99
1:C:231:ASN:HD21	1:C:235:VAL:CB	1.76	0.99
1:B:62:MET:HE2	1:B:97:LEU:HD11	1.46	0.97
1:A:62:MET:HE2	1:A:97:LEU:HD11	1.42	0.97
1:E:216:THR:HG22	1:E:219:ASP:H	1.30	0.96
1:C:231:ASN:HD21	1:C:235:VAL:CG2	1.79	0.96
1:C:231:ASN:ND2	1:C:235:VAL:HB	1.81	0.96
1:C:194:GLN:HB2	1:C:197:GLU:OE1	1.63	0.95
1:D:182:PHE:O	1:D:186:ILE:HG12	1.63	0.95
1:B:62:MET:CE	1:B:97:LEU:HD11	1.97	0.95
1:C:179:MET:O	1:C:183:SER:OG	1.86	0.94
1:B:65:LEU:HD11	1:B:76:MET:HE1	1.50	0.94
1:C:194:GLN:O	1:C:197:GLU:CD	2.11	0.94
1:E:155:PHE:HE2	1:E:159:ILE:HD11	1.32	0.93
1:E:194:GLN:CA	1:E:197:GLU:OE2	2.16	0.93
1:E:147:PRO:HB2	1:E:150:MET:HG3	1.48	0.93
1:F:216:THR:HB	1:F:219:ASP:OD2	1.68	0.92
1:E:38:LYS:HG2	1:E:214:PHE:HE1	1.33	0.92
1:A:152:HIS:CD2	1:A:154:SER:HB2	2.04	0.92
1:C:213:ARG:HB3	1:C:213:ARG:NH1	1.83	0.91
1:B:188:PRO:HA	1:B:191:ARG:HE	1.36	0.91
1:E:170:MET:CE	1:E:240:ILE:HG22	2.02	0.90
1:C:62:MET:HE3	1:C:97:LEU:HD11	1.50	0.90
1:C:164:PRO:O	1:C:165:ASN:HB2	1.70	0.90
1:D:237:ASN:OD1	1:D:239:ALA:N	2.03	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLU:OE1	1:C:81:SER:OG	1.90	0.89
1:E:231:ASN:HB3	1:E:235:VAL:HG11	1.54	0.89
1:C:188:PRO:CG	1:C:191:ARG:HD2	2.01	0.89
1:F:133:VAL:HG11	1:F:138:MET:CE	2.03	0.89
1:F:133:VAL:CG1	1:F:138:MET:HE1	2.01	0.89
1:E:194:GLN:HB2	1:E:197:GLU:CD	1.97	0.89
1:F:237:ASN:ND2	1:F:239:ALA:H	1.70	0.88
1:E:244:ALA:O	1:E:246:LYS:N	2.08	0.87
1:C:242:LYS:O	1:C:246:LYS:CG	2.23	0.87
1:C:140:SER:OG	2:C:312:HOH:O	1.90	0.87
1:C:188:PRO:HG3	1:C:191:ARG:CD	2.05	0.87
1:C:188:PRO:HB3	1:C:191:ARG:HB2	1.55	0.87
1:E:170:MET:HE2	1:E:240:ILE:HG22	1.55	0.87
1:C:138:MET:CE	1:C:178:PHE:HA	2.04	0.87
1:D:231:ASN:ND2	1:D:235:VAL:HB	1.91	0.86
1:F:237:ASN:HB3	1:F:240:ILE:HD12	1.58	0.86
1:F:98:LYS:HE3	1:F:98:LYS:HA	1.56	0.86
1:E:231:ASN:HB3	1:E:235:VAL:CG1	2.05	0.86
1:E:170:MET:HE2	1:E:240:ILE:CG2	2.06	0.85
1:B:216:THR:HG22	1:B:218:ASP:H	1.41	0.85
1:E:43:LEU:O	1:E:47:ARG:HB2	1.75	0.85
1:F:114:ALA:O	1:F:117:VAL:CG2	2.25	0.84
1:F:133:VAL:CG1	1:F:138:MET:CE	2.55	0.84
1:C:231:ASN:HD21	1:C:235:VAL:HG23	1.41	0.84
1:D:62:MET:CE	1:D:97:LEU:HD11	2.08	0.84
1:E:65:LEU:HD21	1:E:76:MET:HE1	1.59	0.83
1:E:149:CYS:SG	2:E:321:HOH:O	2.38	0.82
1:F:207:MET:HA	1:F:210:MET:HE2	1.60	0.82
1:C:187:ASN:O	1:C:190:LEU:HD12	1.79	0.82
1:E:137:THR:O	1:E:141:ILE:HG12	1.80	0.82
1:A:128:SER:OG	2:A:331:HOH:O	1.97	0.82
1:C:188:PRO:HA	1:C:190:LEU:N	1.95	0.81
1:D:135:GLY:O	1:D:139:ASP:OD1	1.99	0.81
1:C:72:LYS:O	1:C:76:MET:HG3	1.80	0.81
1:F:237:ASN:HD22	1:F:238:PRO:N	1.79	0.81
1:F:188:PRO:O	1:F:191:ARG:HG3	1.81	0.81
1:E:155:PHE:CE2	1:E:159:ILE:HD11	2.15	0.80
1:E:187:ASN:HB3	1:E:190:LEU:HD12	1.64	0.80
1:F:237:ASN:HD22	1:F:239:ALA:H	1.29	0.79
1:E:45:LYS:O	1:E:49:THR:OG1	2.00	0.79
1:D:149:CYS:SG	2:D:307:HOH:O	2.39	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LYS:HD3	2:A:347:HOH:O	1.81	0.79
1:E:33:GLN:OE1	2:E:304:HOH:O	2.01	0.79
1:E:194:GLN:H	1:E:197:GLU:CD	1.91	0.78
1:C:231:ASN:ND2	1:C:235:VAL:CB	2.42	0.78
1:C:62:MET:CE	1:C:97:LEU:HD11	2.14	0.78
1:D:216:THR:HG23	2:D:315:HOH:O	1.83	0.78
1:B:19:ASP:O	1:B:23:ILE:HG12	1.84	0.77
1:D:152:HIS:CD2	1:D:154:SER:HB2	2.16	0.77
1:E:170:MET:HE3	1:E:241:GLU:HA	1.66	0.77
1:C:148:ARG:HD2	1:C:151:MET:CE	2.15	0.76
1:E:170:MET:HE3	1:E:241:GLU:CA	2.14	0.76
1:D:231:ASN:HD21	1:D:235:VAL:HB	1.48	0.76
1:E:229:VAL:C	1:E:230:LEU:HD23	2.09	0.76
1:D:153:PRO:HG3	1:D:179:MET:HE1	1.68	0.76
1:E:114:ALA:O	1:E:117:VAL:HG22	1.85	0.76
1:A:63:ILE:HD11	1:A:112:VAL:HG12	1.67	0.76
1:A:204:LYS:HB3	1:A:205:PRO:HD3	1.68	0.76
1:B:138:MET:HG2	1:B:151:MET:HE3	1.67	0.76
1:E:144:THR:HG21	1:E:242:LYS:HE3	1.68	0.75
1:E:217:ARG:O	1:E:221:LYS:CG	2.32	0.75
1:C:181:GLU:O	1:C:184:LYS:HB2	1.87	0.75
1:D:248:LYS:O	1:D:252:GLY:N	2.19	0.75
1:D:62:MET:HE2	1:D:97:LEU:HD11	1.66	0.75
1:E:216:THR:CG2	1:E:218:ASP:CG	2.60	0.75
1:F:85:ALA:O	1:F:89:THR:OG1	2.04	0.75
1:C:148:ARG:HA	1:C:151:MET:CE	2.17	0.75
1:E:181:GLU:OE2	1:E:184:LYS:NZ	2.20	0.75
1:C:229:VAL:O	1:C:230:LEU:HD23	1.87	0.75
1:E:216:THR:HG21	1:E:218:ASP:OD2	1.86	0.74
1:E:194:GLN:CG	1:E:197:GLU:OE2	2.34	0.74
1:F:62:MET:HE2	1:F:97:LEU:HD21	1.69	0.74
1:B:114:ALA:O	1:B:117:VAL:HG22	1.87	0.74
1:D:133:VAL:HG11	1:D:138:MET:CE	2.17	0.74
1:C:231:ASN:OD1	1:C:233:ASP:N	2.21	0.73
1:F:62:MET:HE2	1:F:97:LEU:HD11	1.71	0.73
1:E:234:LEU:HD23	1:E:234:LEU:O	1.89	0.73
1:C:138:MET:HE2	1:C:178:PHE:CA	2.18	0.73
1:A:125:LYS:O	2:A:331:HOH:O	2.06	0.72
1:E:38:LYS:CG	1:E:214:PHE:CE1	2.69	0.72
1:E:233:ASP:H	1:E:235:VAL:HG12	1.53	0.72
1:B:194:GLN:O	1:B:197:GLU:CB	2.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ASP:O	1:D:234:LEU:HB2	1.87	0.72
1:F:117:VAL:N	1:F:118:PRO:CD	2.52	0.71
1:E:3:GLU:CG	2:E:318:HOH:O	2.38	0.71
1:E:138:MET:HE2	1:E:138:MET:CA	2.19	0.71
1:C:188:PRO:CB	1:C:191:ARG:HB2	2.21	0.71
1:B:65:LEU:HD11	1:B:76:MET:CE	2.20	0.71
1:C:62:MET:CE	1:C:97:LEU:HD21	2.21	0.71
1:C:188:PRO:HA	1:C:190:LEU:H	1.53	0.71
1:C:152:HIS:ND1	1:C:154:SER:HB2	2.06	0.70
1:C:142:ALA:O	1:C:144:THR:N	2.23	0.70
1:C:148:ARG:HA	1:C:151:MET:HE2	1.71	0.70
1:D:74:GLU:HA	1:D:77:MET:HE2	1.73	0.70
1:B:158:ILE:HD11	1:B:223:LEU:HD13	1.73	0.70
1:E:60:LYS:HG2	1:E:119:TRP:CE2	2.26	0.70
1:C:188:PRO:HB3	1:C:190:LEU:C	2.16	0.70
1:C:165:ASN:O	1:C:166:ASN:HB2	1.92	0.69
1:E:38:LYS:CG	1:E:214:PHE:CD1	2.75	0.69
1:C:139:ASP:OD2	1:C:148:ARG:CZ	2.41	0.69
1:D:117:VAL:N	1:D:118:PRO:CD	2.55	0.69
1:E:3:GLU:HG2	2:E:318:HOH:O	1.93	0.68
1:D:216:THR:HB	1:D:219:ASP:OD2	1.93	0.68
1:F:237:ASN:HD22	1:F:237:ASN:C	2.01	0.68
1:C:137:THR:O	1:C:141:ILE:HG12	1.93	0.68
1:C:194:GLN:CB	1:C:197:GLU:OE1	2.39	0.68
1:C:216:THR:HG22	1:C:219:ASP:H	1.58	0.68
1:D:146:TYR:O	1:D:148:ARG:NH1	2.27	0.68
1:D:117:VAL:HG23	1:D:118:PRO:HD3	1.75	0.68
1:F:114:ALA:O	1:F:117:VAL:HG22	1.93	0.68
1:A:66:ASN:HB2	1:A:109:LEU:HB3	1.75	0.67
1:B:5:ASN:O	1:B:9:ILE:HG13	1.94	0.67
1:C:62:MET:HE1	1:C:97:LEU:HD21	1.77	0.67
1:E:160:ASP:HB3	1:E:163:LEU:HG	1.76	0.67
1:E:38:LYS:HG2	1:E:214:PHE:CD1	2.28	0.67
1:E:188:PRO:HA	2:E:320:HOH:O	1.95	0.67
1:E:216:THR:HB	1:E:219:ASP:OD2	1.95	0.67
1:C:60:LYS:O	1:C:64:VAL:HG23	1.94	0.67
1:E:242:LYS:O	1:E:246:LYS:HD2	1.95	0.67
1:F:62:MET:CE	1:F:97:LEU:HD21	2.24	0.66
1:D:9:ILE:CD1	1:E:55:TRP:HH2	2.08	0.66
1:C:195:PRO:O	1:C:197:GLU:N	2.28	0.66
1:D:158:ILE:HD11	1:D:223:LEU:HD13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:ARG:HG2	2:E:304:HOH:O	1.95	0.66
1:E:170:MET:HE1	1:E:241:GLU:HB2	1.76	0.66
1:D:188:PRO:O	1:D:191:ARG:CG	2.44	0.65
1:A:165:ASN:O	1:A:166:ASN:HB2	1.96	0.65
1:A:198:ILE:O	1:A:201:THR:HB	1.97	0.65
1:C:242:LYS:O	1:C:246:LYS:HG3	1.95	0.65
1:B:233:ASP:O	1:B:234:LEU:HB2	1.96	0.65
1:C:144:THR:O	1:C:145:THR:OG1	2.11	0.65
1:E:204:LYS:N	1:E:205:PRO:CD	2.58	0.65
1:D:158:ILE:HD11	1:D:223:LEU:CD1	2.26	0.64
1:C:194:GLN:N	1:C:197:GLU:OE1	2.31	0.64
1:D:216:THR:HG22	1:D:218:ASP:N	2.11	0.64
1:C:63:ILE:O	1:C:67:LEU:HG	1.96	0.64
1:F:152:HIS:CD2	1:F:153:PRO:HD2	2.33	0.64
1:C:195:PRO:O	1:C:198:ILE:N	2.27	0.64
1:D:117:VAL:HG13	1:D:154:SER:OG	1.98	0.64
1:F:133:VAL:HG12	1:F:138:MET:CE	2.26	0.64
1:B:194:GLN:O	1:B:197:GLU:N	2.31	0.63
1:A:133:VAL:HG11	1:A:138:MET:CE	2.28	0.63
1:E:216:THR:HG22	1:E:219:ASP:N	2.09	0.63
1:A:75:SER:HA	1:A:78:LYS:HE3	1.79	0.63
1:B:158:ILE:HG23	1:B:224:LEU:HD21	1.81	0.63
1:E:247:TYR:O	1:E:251:VAL:CG2	2.41	0.63
1:E:153:PRO:HD3	1:E:179:MET:HE1	1.79	0.63
1:F:233:ASP:O	1:F:234:LEU:HB2	1.98	0.63
1:E:104:ARG:NH1	1:E:104:ARG:HB2	2.13	0.62
1:B:216:THR:HG22	1:B:218:ASP:N	2.13	0.62
1:C:65:LEU:HD21	1:C:76:MET:HE1	1.82	0.62
1:E:202:PHE:C	1:E:205:PRO:HD2	2.24	0.62
1:E:216:THR:CG2	1:E:218:ASP:OD2	2.48	0.62
1:A:63:ILE:HD12	1:A:113:SER:HA	1.81	0.62
1:B:65:LEU:CD1	1:B:76:MET:HE1	2.27	0.62
1:C:148:ARG:HD2	1:C:151:MET:HE1	1.80	0.62
1:C:194:GLN:C	1:C:197:GLU:OE2	2.41	0.62
1:E:177:LEU:HD22	1:E:243:CYS:HB3	1.80	0.62
1:E:191:ARG:NE	2:E:320:HOH:O	2.33	0.62
1:A:63:ILE:CD1	1:A:112:VAL:HG12	2.30	0.62
1:E:230:LEU:HD22	1:E:236:PRO:HA	1.81	0.62
1:F:98:LYS:HE3	1:F:98:LYS:CA	2.30	0.61
1:A:62:MET:HE2	1:A:97:LEU:CD1	2.25	0.61
1:C:141:ILE:CD1	2:C:312:HOH:O	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ASN:HB3	1:C:240:ILE:HD13	1.81	0.61
1:E:97:LEU:HD23	1:E:107:ILE:HG22	1.82	0.61
1:E:170:MET:HE3	1:E:240:ILE:HG22	1.81	0.61
1:C:142:ALA:C	1:C:144:THR:H	2.08	0.61
1:E:133:VAL:HG11	1:E:138:MET:HE1	1.81	0.61
1:B:216:THR:HB	1:B:219:ASP:CG	2.26	0.61
1:C:237:ASN:HB3	1:C:240:ILE:CD1	2.30	0.61
1:E:19:ASP:OD2	1:E:19:ASP:N	2.15	0.61
1:E:188:PRO:O	1:E:191:ARG:HG3	2.00	0.61
1:C:186:ILE:O	1:C:187:ASN:HB3	1.99	0.60
1:D:188:PRO:HA	1:D:191:ARG:HE	1.66	0.60
1:E:138:MET:HE2	1:E:138:MET:HA	1.83	0.60
1:A:114:ALA:O	1:A:117:VAL:HG22	2.01	0.60
1:E:147:PRO:CB	1:E:150:MET:HG3	2.28	0.60
1:E:236:PRO:O	2:E:316:HOH:O	2.15	0.60
1:C:191:ARG:HH11	1:C:191:ARG:CG	2.14	0.60
1:E:245:GLU:O	1:E:249:ALA:N	2.26	0.60
1:C:19:ASP:OD2	1:C:22:THR:OG1	2.18	0.60
1:F:221:LYS:O	1:F:225:ILE:HG13	2.02	0.60
1:E:19:ASP:OD2	2:E:302:HOH:O	2.16	0.60
1:C:240:ILE:HD12	1:C:240:ILE:N	2.17	0.59
1:C:213:ARG:HH11	1:C:213:ARG:CB	2.05	0.59
1:D:188:PRO:O	1:D:191:ARG:HG2	2.01	0.59
1:E:231:ASN:CA	1:E:235:VAL:HG13	2.32	0.59
1:C:101:ASN:N	1:C:102:PRO:CD	2.66	0.59
1:D:231:ASN:HD21	1:D:235:VAL:CB	2.13	0.59
1:F:114:ALA:O	1:F:117:VAL:HG23	2.02	0.59
1:B:237:ASN:HB3	1:B:240:ILE:HD12	1.84	0.59
1:C:242:LYS:O	1:C:246:LYS:HG2	2.01	0.59
1:F:63:ILE:O	1:F:67:LEU:HG	2.03	0.59
1:E:225:ILE:HA	1:E:230:LEU:O	2.03	0.59
1:B:204:LYS:HB3	1:B:205:PRO:HD3	1.85	0.59
1:A:216:THR:HB	1:A:219:ASP:OD2	2.02	0.58
1:C:170:MET:HG2	1:C:240:ILE:HG22	1.84	0.58
1:E:231:ASN:HB3	1:E:235:VAL:HG13	1.84	0.58
1:E:231:ASN:N	1:E:235:VAL:HG13	2.19	0.58
1:C:188:PRO:HB3	1:C:190:LEU:O	2.03	0.58
1:D:153:PRO:CG	1:D:179:MET:HE1	2.32	0.58
1:A:62:MET:HE3	1:A:97:LEU:HD11	1.80	0.58
1:A:117:VAL:N	1:A:118:PRO:CD	2.66	0.58
1:F:98:LYS:HA	1:F:98:LYS:CE	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:THR:HG22	1:B:145:THR:H	1.68	0.58
1:F:117:VAL:N	1:F:118:PRO:HD3	2.19	0.58
1:D:204:LYS:HB2	1:D:205:PRO:HD3	1.86	0.57
1:D:133:VAL:HG11	1:D:138:MET:HE2	1.85	0.57
1:A:237:ASN:HB3	1:A:240:ILE:HD12	1.87	0.57
1:B:192:THR:O	1:B:193:LYS:HD2	2.05	0.57
1:E:144:THR:CG2	1:E:242:LYS:HE3	2.33	0.57
1:E:230:LEU:CD2	1:E:236:PRO:HA	2.35	0.57
1:F:152:HIS:CG	1:F:153:PRO:HD2	2.39	0.57
1:F:239:ALA:O	1:F:243:CYS:SG	2.58	0.57
1:D:190:LEU:HD11	1:D:201:THR:HG21	1.87	0.57
1:E:188:PRO:O	1:E:191:ARG:CG	2.53	0.57
1:E:231:ASN:C	1:E:233:ASP:H	2.13	0.57
1:B:230:LEU:HD23	1:B:236:PRO:HA	1.87	0.57
1:C:148:ARG:HD2	1:C:151:MET:HE2	1.86	0.57
1:C:186:ILE:HG22	1:C:187:ASN:HD22	1.69	0.57
1:D:144:THR:HG22	1:D:145:THR:H	1.69	0.57
1:C:38:LYS:HG3	1:C:214:PHE:CE1	2.40	0.57
1:D:199:ALA:O	1:D:203:GLU:HG3	2.05	0.57
1:E:184:LYS:O	1:E:187:ASN:O	2.23	0.57
1:C:223:LEU:O	1:C:227:ILE:HG12	2.04	0.56
1:C:141:ILE:HD13	2:C:312:HOH:O	2.04	0.56
1:F:216:THR:HG22	1:F:218:ASP:N	2.19	0.56
1:D:116:PHE:C	1:D:118:PRO:HD2	2.30	0.56
1:D:182:PHE:CE2	1:D:186:ILE:HG13	2.40	0.56
1:B:117:VAL:N	1:B:118:PRO:CD	2.68	0.56
1:C:188:PRO:HG3	1:C:191:ARG:HB2	1.88	0.56
1:D:184:LYS:O	1:D:187:ASN:O	2.23	0.56
1:B:73:PRO:HA	1:B:76:MET:HG3	1.88	0.56
1:C:198:ILE:O	1:C:201:THR:HG22	2.06	0.56
1:E:104:ARG:HB2	1:E:104:ARG:HH11	1.71	0.56
1:E:159:ILE:HD12	1:E:171:LEU:HB3	1.87	0.56
1:F:159:ILE:HB	1:F:210:MET:HG2	1.87	0.56
1:E:231:ASN:O	1:E:233:ASP:N	2.38	0.55
1:F:97:LEU:O	1:F:98:LYS:HD2	2.06	0.55
1:E:206:ASN:O	1:E:210:MET:HG3	2.06	0.55
1:F:162:GLU:OE1	1:F:162:GLU:HA	2.07	0.55
1:E:159:ILE:CD1	1:E:171:LEU:HB3	2.36	0.55
1:A:247:TYR:O	1:A:251:VAL:HG22	2.07	0.55
1:E:153:PRO:CD	1:E:179:MET:HE1	2.36	0.55
1:E:216:THR:HG23	1:E:218:ASP:OD1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:CYS:C	1:E:244:ALA:O	2.45	0.55
1:F:170:MET:HE3	1:F:241:GLU:HA	1.88	0.55
1:D:188:PRO:O	1:D:191:ARG:HG3	2.06	0.55
1:E:3:GLU:HG3	2:E:318:HOH:O	2.05	0.55
1:C:190:LEU:C	1:C:192:THR:H	2.15	0.55
1:D:9:ILE:HD13	1:E:55:TRP:HH2	1.70	0.55
1:E:38:LYS:HG3	1:E:214:PHE:CD1	2.42	0.55
1:E:117:VAL:N	1:E:118:PRO:CD	2.70	0.55
1:F:225:ILE:HD13	1:F:232:GLU:HA	1.89	0.55
1:C:117:VAL:N	1:C:118:PRO:CD	2.70	0.54
1:A:158:ILE:HD11	1:A:223:LEU:HD13	1.89	0.54
1:C:101:ASN:N	1:C:102:PRO:HD3	2.22	0.54
1:C:188:PRO:HG2	1:C:191:ARG:HD2	1.89	0.54
1:C:248:LYS:O	1:C:248:LYS:HD3	2.07	0.54
1:D:231:ASN:HD21	1:D:235:VAL:CG2	2.20	0.54
1:E:233:ASP:N	1:E:235:VAL:HG12	2.21	0.54
1:C:231:ASN:HD22	1:C:235:VAL:HB	1.71	0.54
1:D:204:LYS:CB	1:D:205:PRO:HD3	2.38	0.54
1:F:62:MET:CE	1:F:97:LEU:HD11	2.36	0.54
1:D:216:THR:HG22	1:D:218:ASP:H	1.73	0.54
1:E:128:SER:HB3	1:E:148:ARG:HG3	1.89	0.54
1:A:231:ASN:OD1	1:A:233:ASP:HB2	2.07	0.54
1:A:143:GLY:O	1:A:144:THR:HG23	2.08	0.54
1:D:139:ASP:OD1	1:D:139:ASP:N	2.40	0.53
1:A:73:PRO:HA	1:A:76:MET:HG2	1.90	0.53
1:C:188:PRO:CG	1:C:191:ARG:HB2	2.39	0.53
1:A:164:PRO:O	1:A:167:THR:OG1	2.24	0.53
1:C:170:MET:HG2	1:C:240:ILE:CG2	2.38	0.53
1:B:192:THR:C	1:B:193:LYS:HD2	2.33	0.53
1:B:188:PRO:HA	1:B:191:ARG:NE	2.14	0.53
1:F:116:PHE:C	1:F:118:PRO:HD2	2.34	0.53
1:B:62:MET:HE1	1:B:97:LEU:HD21	1.90	0.53
1:C:142:ALA:C	1:C:144:THR:N	2.66	0.53
1:E:231:ASN:CB	1:E:235:VAL:CG1	2.85	0.53
1:B:158:ILE:HD11	1:B:223:LEU:CD1	2.39	0.53
1:E:104:ARG:CZ	1:E:104:ARG:HB3	2.37	0.53
1:A:144:THR:HG21	1:A:242:LYS:CD	2.40	0.52
1:C:139:ASP:CG	1:C:145:THR:HA	2.32	0.52
1:C:191:ARG:HH11	1:C:191:ARG:HG2	1.73	0.52
1:C:194:GLN:CA	1:C:197:GLU:OE1	2.58	0.52
1:F:216:THR:HG22	1:F:218:ASP:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ARG:NH2	1:C:105:ASP:OD2	2.24	0.52
1:C:177:LEU:HD13	1:C:243:CYS:O	2.10	0.52
1:A:152:HIS:HD2	1:A:154:SER:CB	2.05	0.52
1:A:231:ASN:OD1	1:A:233:ASP:N	2.33	0.52
1:B:63:ILE:O	1:B:67:LEU:HG	2.10	0.52
1:E:170:MET:HE3	1:E:241:GLU:N	2.24	0.52
1:E:195:PRO:HA	1:E:198:ILE:HD12	1.91	0.52
1:F:62:MET:HE3	1:F:91:LEU:HB3	1.92	0.52
1:B:204:LYS:CB	1:B:205:PRO:HD3	2.39	0.51
1:A:62:MET:HE1	1:A:97:LEU:HD21	1.92	0.51
1:A:143:GLY:C	1:A:144:THR:HG23	2.35	0.51
1:B:14:LEU:HD12	1:C:122:GLN:NE2	2.25	0.51
1:D:216:THR:HB	1:D:219:ASP:CG	2.35	0.51
1:D:216:THR:HG22	1:D:219:ASP:H	1.75	0.51
1:D:231:ASN:OD1	1:D:233:ASP:N	2.44	0.51
1:C:242:LYS:O	1:C:246:LYS:CB	2.57	0.51
1:C:32:TYR:CG	1:C:204:LYS:HE2	2.45	0.51
1:C:142:ALA:O	1:C:144:THR:OG1	2.25	0.51
1:E:104:ARG:CZ	1:E:104:ARG:CB	2.88	0.51
1:C:6:TYR:OH	1:D:42:GLN:HG3	2.10	0.51
1:E:245:GLU:O	1:E:248:LYS:N	2.44	0.51
1:F:74:GLU:HA	1:F:77:MET:HE2	1.91	0.51
1:B:76:MET:HE3	1:B:80:MET:HE1	1.92	0.51
1:E:104:ARG:NE	2:E:310:HOH:O	1.86	0.51
1:F:216:THR:HB	1:F:219:ASP:CG	2.33	0.51
1:C:242:LYS:C	1:C:246:LYS:HG3	2.35	0.51
1:D:19:ASP:HB2	2:D:311:HOH:O	2.11	0.51
1:D:114:ALA:O	1:D:117:VAL:HG22	2.10	0.51
1:D:216:THR:CG2	1:D:218:ASP:HB2	2.41	0.51
1:F:199:ALA:O	1:F:203:GLU:HG3	2.11	0.51
1:F:124:LEU:HD13	1:F:148:ARG:O	2.11	0.51
1:A:32:TYR:CD1	1:A:32:TYR:C	2.89	0.51
1:A:194:GLN:HB2	1:A:197:GLU:OE2	2.11	0.51
1:B:138:MET:CE	1:B:178:PHE:HA	2.41	0.51
1:E:104:ARG:NH1	1:E:104:ARG:CB	2.73	0.51
1:E:138:MET:HE2	1:E:138:MET:N	2.26	0.51
1:A:143:GLY:O	1:A:144:THR:CG2	2.58	0.50
1:E:60:LYS:HG2	1:E:119:TRP:CZ2	2.46	0.50
1:C:207:MET:HA	1:C:210:MET:HE2	1.93	0.50
1:B:62:MET:HE3	1:B:91:LEU:HB3	1.94	0.50
1:C:243:CYS:O	1:C:247:TYR:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ASN:ND2	1:C:235:VAL:HG23	2.19	0.50
1:D:164:PRO:O	1:D:165:ASN:HB2	2.11	0.50
1:D:216:THR:CG2	1:D:218:ASP:H	2.24	0.50
1:F:158:ILE:HG22	1:F:158:ILE:O	2.10	0.50
1:A:224:LEU:HD22	1:A:229:VAL:HG11	1.93	0.49
1:E:231:ASN:CB	1:E:235:VAL:HG13	2.41	0.49
1:C:196:ASN:OD1	1:C:196:ASN:N	2.45	0.49
1:E:75:SER:O	1:E:78:LYS:HG3	2.12	0.49
1:B:216:THR:N	1:B:219:ASP:OD2	2.31	0.49
1:C:60:LYS:HG2	1:C:119:TRP:CE2	2.47	0.49
1:B:152:HIS:CD2	1:B:153:PRO:HD2	2.47	0.49
1:C:242:LYS:O	1:C:246:LYS:N	2.34	0.49
1:E:144:THR:OG1	1:E:242:LYS:HD2	2.13	0.49
1:C:148:ARG:HA	1:C:151:MET:HE3	1.95	0.49
1:F:182:PHE:CZ	1:F:186:ILE:HD11	2.48	0.49
1:C:216:THR:HB	1:C:219:ASP:OD2	2.13	0.49
1:D:53:ARG:HH12	1:D:90:GLN:HG2	1.77	0.49
1:B:197:GLU:OE2	1:B:197:GLU:HA	2.13	0.49
1:B:187:ASN:HB3	1:B:190:LEU:HD12	1.94	0.48
1:E:34:GLY:HA2	1:F:79:LYS:HD3	1.94	0.48
1:C:163:LEU:HB3	1:C:164:PRO:HD2	1.94	0.48
1:E:231:ASN:C	1:E:235:VAL:CG1	2.86	0.48
1:A:144:THR:HG21	1:A:242:LYS:HD3	1.95	0.48
1:C:203:GLU:O	1:C:204:LYS:C	2.54	0.48
1:D:133:VAL:CG1	1:D:138:MET:HE2	2.43	0.48
1:F:65:LEU:HD11	1:F:76:MET:HE3	1.95	0.48
1:C:231:ASN:OD1	1:C:233:ASP:CA	2.61	0.48
1:F:182:PHE:O	1:F:186:ILE:CG1	2.46	0.48
1:A:62:MET:CE	1:A:97:LEU:CD1	2.72	0.48
1:A:138:MET:HG3	1:A:146:TYR:CG	2.48	0.48
1:E:43:LEU:HB3	1:E:107:ILE:HD11	1.95	0.48
1:C:141:ILE:HD13	1:C:141:ILE:N	2.29	0.47
1:F:186:ILE:O	2:F:321:HOH:O	2.20	0.47
1:D:69:ARG:HB3	1:D:76:MET:HG2	1.95	0.47
1:C:114:ALA:O	1:C:117:VAL:HG22	2.14	0.47
1:D:23:ILE:O	1:D:27:VAL:HG23	2.14	0.47
1:E:231:ASN:C	1:E:233:ASP:N	2.73	0.47
1:A:231:ASN:HD21	1:A:235:VAL:HB	1.80	0.47
1:D:138:MET:HE1	1:D:181:GLU:HG3	1.96	0.47
1:D:196:ASN:HD22	1:E:191:ARG:HB3	1.80	0.47
1:E:237:ASN:OD1	1:E:238:PRO:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:NH1	1:A:42:GLN:OE1	2.42	0.47
1:B:105:ASP:HB2	2:B:309:HOH:O	2.15	0.47
1:C:139:ASP:CG	1:C:148:ARG:NH1	2.61	0.47
1:C:229:VAL:C	1:C:230:LEU:HD23	2.39	0.47
1:D:159:ILE:HB	1:D:210:MET:HG2	1.97	0.47
1:C:38:LYS:HG3	1:C:214:PHE:HE1	1.78	0.47
1:E:161:LEU:CD1	1:E:207:MET:HE1	2.45	0.47
1:E:249:ALA:O	1:E:251:VAL:N	2.48	0.47
1:F:158:ILE:HD12	1:F:223:LEU:HD13	1.96	0.47
1:A:4:ASP:OD1	1:A:4:ASP:N	2.43	0.47
1:B:138:MET:HE2	1:B:178:PHE:HA	1.96	0.47
1:D:104:ARG:NH2	1:E:82:GLU:HG3	2.29	0.47
1:E:23:ILE:O	1:E:27:VAL:HG23	2.14	0.47
1:E:249:ALA:C	1:E:251:VAL:N	2.72	0.47
1:B:213:ARG:HG2	1:B:213:ARG:HH11	1.80	0.47
1:E:158:ILE:CG2	1:E:224:LEU:HD21	2.44	0.47
1:B:66:ASN:HB2	1:B:109:LEU:HB3	1.97	0.47
1:F:204:LYS:N	1:F:205:PRO:HD2	2.30	0.47
1:C:60:LYS:HG2	1:C:119:TRP:CZ2	2.50	0.46
1:E:7:ARG:O	1:E:11:LEU:HG	2.15	0.46
1:A:137:THR:O	1:A:141:ILE:HG12	2.15	0.46
1:B:233:ASP:O	1:B:234:LEU:CB	2.63	0.46
1:C:30:PHE:O	1:D:69:ARG:NH1	2.46	0.46
1:C:66:ASN:HB2	1:C:109:LEU:HB3	1.96	0.46
1:C:230:LEU:CD2	1:C:236:PRO:HA	2.46	0.46
1:A:170:MET:HG2	1:A:240:ILE:HG22	1.96	0.46
1:C:125:LYS:HG2	1:C:126:THR:N	2.29	0.46
1:C:158:ILE:HA	1:C:158:ILE:HD12	1.72	0.46
1:C:191:ARG:CG	1:C:191:ARG:NH1	2.73	0.46
1:D:138:MET:HE1	1:D:181:GLU:CB	2.45	0.46
1:E:88:VAL:O	1:E:92:ILE:HG13	2.15	0.46
1:F:116:PHE:C	1:F:118:PRO:CD	2.88	0.46
1:F:133:VAL:HG12	1:F:138:MET:HE2	1.96	0.46
1:A:59:VAL:O	1:A:63:ILE:HG12	2.15	0.46
1:B:58:ASP:O	1:B:62:MET:HG3	2.15	0.46
1:C:190:LEU:H	1:C:190:LEU:HG	1.60	0.46
1:C:231:ASN:ND2	1:C:235:VAL:H	2.14	0.46
1:C:158:ILE:HD11	1:C:223:LEU:HD13	1.98	0.46
1:D:150:MET:HG2	1:D:155:PHE:CZ	2.50	0.46
1:E:195:PRO:O	1:E:198:ILE:N	2.47	0.46
1:C:234:LEU:HD12	1:C:234:LEU:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:TRP:HB2	1:F:13:PHE:HB3	1.98	0.46
1:B:158:ILE:CG2	1:B:224:LEU:HD21	2.46	0.46
1:B:35:PHE:O	1:B:37:PRO:HD3	2.16	0.46
1:C:171:LEU:HD23	1:C:171:LEU:HA	1.75	0.45
1:E:97:LEU:CD2	1:E:107:ILE:HG22	2.46	0.45
1:A:233:ASP:O	1:A:234:LEU:HB2	2.17	0.45
1:C:6:TYR:CZ	1:D:42:GLN:HG3	2.52	0.45
1:C:188:PRO:CA	1:C:190:LEU:N	2.73	0.45
1:C:237:ASN:OD1	1:C:238:PRO:N	2.49	0.45
1:F:217:ARG:HB2	2:F:308:HOH:O	2.15	0.45
1:B:216:THR:HB	1:B:219:ASP:OD2	2.17	0.45
1:E:194:GLN:HB2	1:E:197:GLU:CG	2.47	0.45
1:E:244:ALA:C	1:E:246:LYS:N	2.73	0.45
1:C:240:ILE:CD1	1:C:240:ILE:N	2.79	0.45
1:E:233:ASP:H	1:E:235:VAL:CG1	2.27	0.45
1:A:9:ILE:HG23	2:A:344:HOH:O	2.17	0.45
1:E:138:MET:CA	1:E:138:MET:CE	2.92	0.45
1:A:162:GLU:HB2	1:A:217:ARG:HH11	1.81	0.45
1:F:66:ASN:HB2	1:F:109:LEU:HB3	1.98	0.45
1:F:242:LYS:HE3	1:F:242:LYS:HB2	1.68	0.45
1:B:229:VAL:HG12	1:B:230:LEU:HG	1.99	0.44
1:C:5:ASN:ND2	2:C:317:HOH:O	2.49	0.44
1:D:237:ASN:CG	1:D:238:PRO:HD2	2.42	0.44
1:F:237:ASN:HB3	1:F:240:ILE:CD1	2.37	0.44
1:B:152:HIS:CG	1:B:153:PRO:HD2	2.52	0.44
1:D:116:PHE:C	1:D:118:PRO:CD	2.89	0.44
1:D:178:PHE:CE2	1:D:179:MET:HE2	2.53	0.44
1:D:248:LYS:O	1:D:253:LYS:N	2.46	0.44
1:E:170:MET:CE	1:E:241:GLU:HB2	2.46	0.44
1:E:240:ILE:N	1:E:240:ILE:CD1	2.81	0.44
1:A:116:PHE:C	1:A:118:PRO:HD2	2.43	0.44
1:A:234:LEU:N	1:A:234:LEU:CD1	2.80	0.44
1:B:195:PRO:HA	1:B:198:ILE:HG13	1.98	0.44
1:E:170:MET:CE	1:E:241:GLU:N	2.81	0.44
1:E:233:ASP:HB3	1:E:235:VAL:HB	1.99	0.44
1:D:60:LYS:HG2	1:D:119:TRP:CE2	2.53	0.44
1:E:65:LEU:HD11	1:E:76:MET:HE3	2.00	0.44
1:E:245:GLU:C	1:E:247:TYR:N	2.73	0.44
1:C:233:ASP:O	1:C:234:LEU:HB2	2.17	0.44
1:A:231:ASN:ND2	1:A:235:VAL:HB	2.33	0.44
1:B:158:ILE:HD12	1:B:158:ILE:HA	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:CG1	1:A:138:MET:CE	2.94	0.44
1:C:117:VAL:HG23	1:C:118:PRO:HD3	2.00	0.44
1:A:204:LYS:CB	1:A:205:PRO:HD3	2.45	0.43
1:E:7:ARG:NH1	1:F:219:ASP:OD1	2.50	0.43
1:E:231:ASN:O	1:E:235:VAL:HG12	2.17	0.43
1:F:204:LYS:HB2	1:F:204:LYS:HE2	1.80	0.43
1:C:62:MET:HE2	1:C:97:LEU:HD21	1.98	0.43
1:D:152:HIS:CD2	1:D:154:SER:H	2.35	0.43
1:E:32:TYR:CD2	1:E:204:LYS:HD2	2.53	0.43
1:B:78:LYS:HG2	1:B:79:LYS:HG2	1.99	0.43
1:D:193:LYS:HA	1:D:193:LYS:HD3	1.91	0.43
1:B:138:MET:HE2	1:B:178:PHE:HB2	2.00	0.43
1:D:73:PRO:HD2	1:D:99:GLU:HG2	2.01	0.43
1:B:158:ILE:HG23	1:B:224:LEU:CD2	2.47	0.43
1:C:165:ASN:O	1:C:166:ASN:CB	2.63	0.43
1:E:170:MET:CE	1:E:241:GLU:CA	2.90	0.43
1:F:146:TYR:OH	1:F:150:MET:HE2	2.18	0.43
1:D:148:ARG:N	1:D:148:ARG:HD2	2.34	0.43
1:C:188:PRO:CA	1:C:189:SER:C	2.92	0.43
1:C:234:LEU:N	1:C:234:LEU:CD1	2.82	0.43
1:B:216:THR:HG22	1:B:217:ARG:N	2.33	0.43
1:E:163:LEU:HD23	1:E:163:LEU:HA	1.78	0.43
1:F:62:MET:HE2	1:F:97:LEU:CD1	2.46	0.43
1:D:62:MET:HE1	1:D:97:LEU:HD21	2.00	0.42
1:E:202:PHE:O	1:E:205:PRO:HD2	2.18	0.42
1:F:43:LEU:HA	1:F:43:LEU:HD23	1.75	0.42
1:A:63:ILE:O	1:A:67:LEU:HG	2.19	0.42
1:B:5:ASN:HB3	2:B:326:HOH:O	2.19	0.42
1:C:164:PRO:O	1:C:165:ASN:CB	2.51	0.42
1:D:117:VAL:N	1:D:118:PRO:HD2	2.34	0.42
1:D:133:VAL:HG11	1:D:138:MET:HE3	1.97	0.42
1:D:138:MET:HB3	1:D:146:TYR:CB	2.48	0.42
1:D:139:ASP:HA	1:D:144:THR:O	2.20	0.42
1:D:204:LYS:N	1:D:205:PRO:CD	2.82	0.42
1:E:171:LEU:HD23	1:E:171:LEU:HA	1.75	0.42
1:C:158:ILE:O	1:C:158:ILE:HG23	2.19	0.42
1:D:5:ASN:N	2:D:323:HOH:O	2.51	0.42
1:E:233:ASP:O	1:E:234:LEU:HB3	2.19	0.42
1:D:9:ILE:HD11	1:E:55:TRP:HH2	1.81	0.42
1:A:99:GLU:H	1:A:99:GLU:HG2	1.70	0.42
1:C:76:MET:HE3	1:C:76:MET:HB2	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:GLU:O	1:C:184:LYS:N	2.53	0.42
1:E:38:LYS:HG3	1:E:214:PHE:HD1	1.85	0.42
1:F:5:ASN:ND2	1:F:8:THR:HB	2.34	0.42
1:A:206:ASN:O	1:A:210:MET:HG3	2.19	0.42
1:F:122:GLN:O	1:F:125:LYS:HG2	2.19	0.42
1:D:13:PHE:HB3	1:E:119:TRP:HB2	2.01	0.42
1:F:117:VAL:O	1:F:121:VAL:HG22	2.20	0.42
1:F:170:MET:HE2	1:F:170:MET:HB3	1.75	0.42
1:E:23:ILE:O	1:E:26:TRP:HB2	2.20	0.41
1:C:199:ALA:C	1:C:201:THR:N	2.77	0.41
1:D:62:MET:HE3	1:D:97:LEU:HD11	1.98	0.41
1:E:102:PRO:CB	2:E:307:HOH:O	2.68	0.41
1:B:247:TYR:O	1:B:251:VAL:HG22	2.20	0.41
1:C:185:THR:HA	1:C:191:ARG:NH2	2.36	0.41
1:E:190:LEU:HA	1:E:193:LYS:HE3	2.02	0.41
1:A:4:ASP:CB	2:A:336:HOH:O	2.68	0.41
1:A:187:ASN:HA	1:A:188:PRO:HD3	1.76	0.41
1:C:23:ILE:HG21	1:D:126:THR:OG1	2.21	0.41
1:C:127:LEU:C	1:C:127:LEU:HD12	2.45	0.41
1:C:150:MET:HE2	1:C:150:MET:HB3	1.93	0.41
1:C:181:GLU:O	1:C:182:PHE:C	2.64	0.41
1:B:204:LYS:CB	1:B:205:PRO:CD	2.98	0.41
1:F:56:LYS:O	1:F:60:LYS:HG3	2.20	0.41
1:F:182:PHE:CE2	1:F:186:ILE:HG13	2.55	0.41
1:C:188:PRO:HD2	1:C:188:PRO:O	2.20	0.41
1:E:92:ILE:HA	1:E:97:LEU:HD12	2.03	0.41
1:E:167:THR:O	1:E:170:MET:HB3	2.21	0.41
1:F:65:LEU:HD21	1:F:76:MET:HE1	2.02	0.41
1:F:170:MET:CE	1:F:240:ILE:HG22	2.51	0.41
1:A:61:MET:HE3	1:F:26:TRP:NE1	2.36	0.41
1:A:88:VAL:O	1:A:92:ILE:HG13	2.21	0.41
1:B:117:VAL:N	1:B:118:PRO:HD2	2.36	0.41
1:D:171:LEU:HD23	1:D:171:LEU:HA	1.79	0.41
1:F:62:MET:HE2	1:F:97:LEU:CD2	2.45	0.41
1:E:60:LYS:O	1:E:64:VAL:HG23	2.21	0.41
1:F:237:ASN:ND2	1:F:237:ASN:C	2.72	0.41
1:A:60:LYS:HG2	1:A:119:TRP:CE2	2.56	0.40
1:B:150:MET:HG2	1:B:155:PHE:CZ	2.57	0.40
1:E:153:PRO:CG	1:E:179:MET:HE1	2.51	0.40
1:F:65:LEU:HD11	1:F:76:MET:CE	2.51	0.40
1:E:141:ILE:HG12	1:E:141:ILE:H	1.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:VAL:HG12	1:E:230:LEU:CD2	2.51	0.40
1:A:150:MET:HG2	1:A:155:PHE:CZ	2.56	0.40
1:E:36:ASP:HA	1:E:37:PRO:HD2	1.89	0.40
1:E:92:ILE:O	1:E:96:GLN:N	2.54	0.40
1:E:133:VAL:HG11	1:E:138:MET:CE	2.48	0.40
1:D:242:LYS:O	1:D:245:GLU:HB2	2.22	0.40
1:E:204:LYS:N	1:E:205:PRO:HD2	2.36	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:A:19:ASP:OD2	1:C:7:ARG:NH2[1_654]	1.95	0.25

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	248/257 (96%)	245 (99%)	2 (1%)	1 (0%)	30	49
1	B	246/257 (96%)	242 (98%)	3 (1%)	1 (0%)	30	49
1	C	244/257 (95%)	224 (92%)	10 (4%)	10 (4%)	2	3
1	D	247/257 (96%)	242 (98%)	4 (2%)	1 (0%)	30	49
1	E	248/257 (96%)	234 (94%)	8 (3%)	6 (2%)	4	8
1	F	246/257 (96%)	241 (98%)	4 (2%)	1 (0%)	30	49
All	All	1479/1542 (96%)	1428 (97%)	31 (2%)	20 (1%)	9	17

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	145	THR

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Mol	Chain	Res	Type
1	C	190	LEU
1	C	196	ASN
1	C	203	GLU
1	C	143	GLY
1	E	250	LYS
1	C	189	SER
1	C	195	PRO
1	E	232	GLU
1	C	193	LYS
1	E	249	ALA
1	D	102	PRO
1	E	245	GLU
1	A	102	PRO
1	B	102	PRO
1	E	244	ALA
1	C	102	PRO
1	E	102	PRO
1	C	188	PRO
1	F	102	PRO

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	211/217 (97%)	182 (86%)	29 (14%)	3	7
1	B	209/217 (96%)	183 (88%)	26 (12%)	4	9
1	C	208/217 (96%)	175 (84%)	33 (16%)	2	5
1	D	210/217 (97%)	176 (84%)	34 (16%)	2	4
1	E	211/217 (97%)	172 (82%)	39 (18%)	1	3
1	F	209/217 (96%)	181 (87%)	28 (13%)	4	8
All	All	1258/1302 (97%)	1069 (85%)	189 (15%)	3	6

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	23	ILE
1	A	38	LYS
1	A	39	ARG
1	A	45	LYS
1	A	77	MET
1	A	78	LYS
1	A	83	LYS
1	A	99	GLU
1	A	101	ASN
1	A	105	ASP
1	A	110	SER
1	A	117	VAL
1	A	128	SER
1	A	136	THR
1	A	154	SER
1	A	158	ILE
1	A	162	GLU
1	A	167	THR
1	A	186	ILE
1	A	189	SER
1	A	191	ARG
1	A	201	THR
1	A	204	LYS
1	A	213	ARG
1	A	216	THR
1	A	217	ARG
1	A	222	LYS
1	A	240	ILE
1	B	29	GLU
1	B	38	LYS
1	B	46	GLU
1	B	51	LYS
1	B	76	MET
1	B	78	LYS
1	B	90	GLN
1	B	99	GLU
1	B	117	VAL
1	B	126	THR
1	B	136	THR
1	B	138	MET
1	B	144	THR
1	B	158	ILE

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Mol	Chain	Res	Type
1	B	162	GLU
1	B	170	MET
1	B	186	ILE
1	B	189	SER
1	B	196	ASN
1	B	198	ILE
1	B	201	THR
1	B	203	GLU
1	B	204	LYS
1	B	206	ASN
1	B	213	ARG
1	B	240	ILE
1	C	22	THR
1	C	46	GLU
1	C	57	LYS
1	C	72	LYS
1	C	78	LYS
1	C	79	LYS
1	C	83	LYS
1	C	104	ARG
1	C	117	VAL
1	C	125	LYS
1	C	127	LEU
1	C	128	SER
1	C	136	THR
1	C	144	THR
1	C	158	ILE
1	C	177	LEU
1	C	183	SER
1	C	184	LYS
1	C	186	ILE
1	C	189	SER
1	C	190	LEU
1	C	191	ARG
1	C	192	THR
1	C	193	LYS
1	C	195	PRO
1	C	196	ASN
1	C	197	GLU
1	C	198	ILE
1	C	210	MET
1	C	213	ARG

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Mol	Chain	Res	Type
1	C	216	THR
1	C	217	ARG
1	C	243	CYS
1	D	5	ASN
1	D	9	ILE
1	D	29	GLU
1	D	38	LYS
1	D	39	ARG
1	D	51	LYS
1	D	59	VAL
1	D	68	VAL
1	D	76	MET
1	D	77	MET
1	D	78	LYS
1	D	99	GLU
1	D	104	ARG
1	D	105	ASP
1	D	110	SER
1	D	117	VAL
1	D	126	THR
1	D	127	LEU
1	D	128	SER
1	D	130	SER
1	D	138	MET
1	D	144	THR
1	D	158	ILE
1	D	162	GLU
1	D	183	SER
1	D	189	SER
1	D	192	THR
1	D	196	ASN
1	D	201	THR
1	D	213	ARG
1	D	216	THR
1	D	217	ARG
1	D	251	VAL
1	D	253	LYS
1	E	3	GLU
1	E	8	THR
1	E	14	LEU
1	E	19	ASP
1	E	29	GLU

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Mol	Chain	Res	Type
1	E	39	ARG
1	E	45	LYS
1	E	49	THR
1	E	57	LYS
1	E	74	GLU
1	E	76	MET
1	E	78	LYS
1	E	79	LYS
1	E	110	SER
1	E	117	VAL
1	E	126	THR
1	E	138	MET
1	E	141	ILE
1	E	144	THR
1	E	150	MET
1	E	158	ILE
1	E	162	GLU
1	E	167	THR
1	E	196	ASN
1	E	203	GLU
1	E	204	LYS
1	E	216	THR
1	E	218	ASP
1	E	221	LYS
1	E	222	LYS
1	E	232	GLU
1	E	235	VAL
1	E	236	PRO
1	E	240	ILE
1	E	245	GLU
1	E	246	LYS
1	E	248	LYS
1	E	250	LYS
1	E	251	VAL
1	F	8	THR
1	F	17	SER
1	F	29	GLU
1	F	38	LYS
1	F	39	ARG
1	F	57	LYS
1	F	83	LYS
1	F	89	THR

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Mol	Chain	Res	Type
1	F	99	GLU
1	F	110	SER
1	F	113	SER
1	F	117	VAL
1	F	127	LEU
1	F	144	THR
1	F	183	SER
1	F	192	THR
1	F	201	THR
1	F	204	LYS
1	F	210	MET
1	F	216	THR
1	F	222	LYS
1	F	232	GLU
1	F	234	LEU
1	F	237	ASN
1	F	240	ILE
1	F	245	GLU
1	F	248	LYS
1	F	250	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	152	HIS
1	B	33	GLN
1	C	187	ASN
1	D	42	GLN
1	D	90	GLN
1	D	101	ASN
1	D	122	GLN
1	D	152	HIS
1	E	101	ASN
1	E	165	ASN
1	E	196	ASN
1	F	5	ASN
1	F	33	GLN
1	F	122	GLN
1	F	237	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](#)

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

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	250/257 (97%)	-0.21	1 (0%) 88 86	30, 47, 68, 96	0
1	B	248/257 (96%)	-0.13	0 100 100	30, 48, 74, 87	0
1	C	246/257 (95%)	0.28	7 (2%) 55 50	31, 60, 103, 120	0
1	D	249/257 (96%)	0.05	0 100 100	34, 59, 86, 95	0
1	E	250/257 (97%)	0.37	6 (2%) 59 55	37, 67, 104, 123	0
1	F	248/257 (96%)	0.02	2 (0%) 82 80	34, 58, 78, 91	0
All	All	1491/1542 (96%)	0.06	16 (1%) 78 75	30, 56, 91, 123	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	234	LEU	3.0
1	C	195	PRO	2.7
1	C	142	ALA	2.7
1	C	177	LEU	2.6
1	F	252	GLY	2.5
1	E	169	ALA	2.4
1	F	98	LYS	2.3
1	C	244	ALA	2.3
1	E	144	THR	2.2
1	C	141	ILE	2.2
1	E	29	GLU	2.2
1	A	253	LYS	2.2
1	E	252	GLY	2.1
1	C	158	ILE	2.1
1	E	239	ALA	2.0
1	C	188	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.