



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2017 – 08:26 AM EDT

PDB ID : 3FIJ
Title : Crystal structure of a uncharacterized protein lin1909
Authors : Sugadev, R.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center
for Structural Genomics (NYSGXRC)
Deposited on : unknown
Resolution : 2.30 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

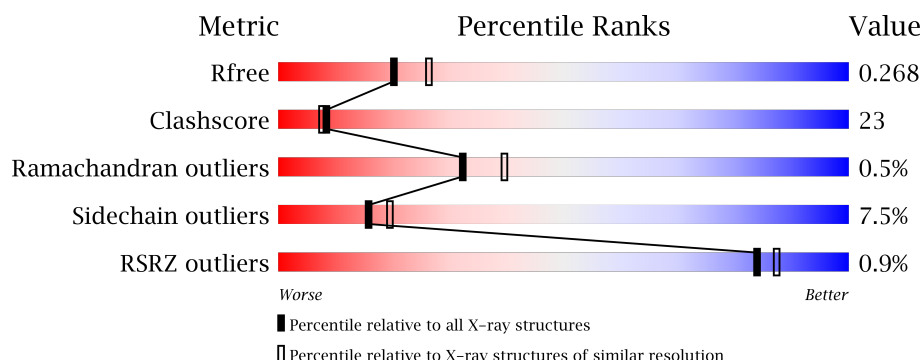
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	254	
1	B	254	
1	C	254	
1	D	254	
1	E	254	

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Mol	Chain	Length	Quality of chain
1	F	254	 52%31%•12%
1	G	254	 2%47%36%•13%
1	H	254	 56%30%•12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14467 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 Lin1909 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	Se	0	0	0
			1739	1110	292	332	1	4			
1	B	222	Total	C	N	O	S	Se	0	0	0
			1722	1100	289	329	1	3			
1	C	221	Total	C	N	O	S	Se	0	0	0
			1715	1095	288	328	1	3			
1	D	223	Total	C	N	O	S	Se	0	0	0
			1731	1105	291	331	1	3			
1	E	224	Total	C	N	O	S	Se	0	0	0
			1739	1110	292	332	1	4			
1	F	223	Total	C	N	O	S	Se	0	0	0
			1731	1105	291	331	1	3			
1	G	222	Total	C	N	O	S	Se	0	0	0
			1723	1100	290	329	1	3			
1	H	224	Total	C	N	O	S	Se	0	0	0
			1739	1110	292	332	1	4			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q92AL3
A	2	SER	-	expression tag	UNP Q92AL3
A	3	LEU	-	expression tag	UNP Q92AL3
A	247	GLU	-	expression tag	UNP Q92AL3
A	248	GLY	-	expression tag	UNP Q92AL3
A	249	HIS	-	expression tag	UNP Q92AL3
A	250	HIS	-	expression tag	UNP Q92AL3
A	251	HIS	-	expression tag	UNP Q92AL3
A	252	HIS	-	expression tag	UNP Q92AL3
A	253	HIS	-	expression tag	UNP Q92AL3
A	254	HIS	-	expression tag	UNP Q92AL3
B	1	MSE	-	expression tag	UNP Q92AL3
B	2	SER	-	expression tag	UNP Q92AL3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	LEU	-	expression tag	UNP Q92AL3
B	247	GLU	-	expression tag	UNP Q92AL3
B	248	GLY	-	expression tag	UNP Q92AL3
B	249	HIS	-	expression tag	UNP Q92AL3
B	250	HIS	-	expression tag	UNP Q92AL3
B	251	HIS	-	expression tag	UNP Q92AL3
B	252	HIS	-	expression tag	UNP Q92AL3
B	253	HIS	-	expression tag	UNP Q92AL3
B	254	HIS	-	expression tag	UNP Q92AL3
C	1	MSE	-	expression tag	UNP Q92AL3
C	2	SER	-	expression tag	UNP Q92AL3
C	3	LEU	-	expression tag	UNP Q92AL3
C	247	GLU	-	expression tag	UNP Q92AL3
C	248	GLY	-	expression tag	UNP Q92AL3
C	249	HIS	-	expression tag	UNP Q92AL3
C	250	HIS	-	expression tag	UNP Q92AL3
C	251	HIS	-	expression tag	UNP Q92AL3
C	252	HIS	-	expression tag	UNP Q92AL3
C	253	HIS	-	expression tag	UNP Q92AL3
C	254	HIS	-	expression tag	UNP Q92AL3
D	1	MSE	-	expression tag	UNP Q92AL3
D	2	SER	-	expression tag	UNP Q92AL3
D	3	LEU	-	expression tag	UNP Q92AL3
D	247	GLU	-	expression tag	UNP Q92AL3
D	248	GLY	-	expression tag	UNP Q92AL3
D	249	HIS	-	expression tag	UNP Q92AL3
D	250	HIS	-	expression tag	UNP Q92AL3
D	251	HIS	-	expression tag	UNP Q92AL3
D	252	HIS	-	expression tag	UNP Q92AL3
D	253	HIS	-	expression tag	UNP Q92AL3
D	254	HIS	-	expression tag	UNP Q92AL3
E	1	MSE	-	expression tag	UNP Q92AL3
E	2	SER	-	expression tag	UNP Q92AL3
E	3	LEU	-	expression tag	UNP Q92AL3
E	247	GLU	-	expression tag	UNP Q92AL3
E	248	GLY	-	expression tag	UNP Q92AL3
E	249	HIS	-	expression tag	UNP Q92AL3
E	250	HIS	-	expression tag	UNP Q92AL3
E	251	HIS	-	expression tag	UNP Q92AL3
E	252	HIS	-	expression tag	UNP Q92AL3
E	253	HIS	-	expression tag	UNP Q92AL3
E	254	HIS	-	expression tag	UNP Q92AL3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MSE	-	expression tag	UNP Q92AL3
F	2	SER	-	expression tag	UNP Q92AL3
F	3	LEU	-	expression tag	UNP Q92AL3
F	247	GLU	-	expression tag	UNP Q92AL3
F	248	GLY	-	expression tag	UNP Q92AL3
F	249	HIS	-	expression tag	UNP Q92AL3
F	250	HIS	-	expression tag	UNP Q92AL3
F	251	HIS	-	expression tag	UNP Q92AL3
F	252	HIS	-	expression tag	UNP Q92AL3
F	253	HIS	-	expression tag	UNP Q92AL3
F	254	HIS	-	expression tag	UNP Q92AL3
G	1	MSE	-	expression tag	UNP Q92AL3
G	2	SER	-	expression tag	UNP Q92AL3
G	3	LEU	-	expression tag	UNP Q92AL3
G	247	GLU	-	expression tag	UNP Q92AL3
G	248	GLY	-	expression tag	UNP Q92AL3
G	249	HIS	-	expression tag	UNP Q92AL3
G	250	HIS	-	expression tag	UNP Q92AL3
G	251	HIS	-	expression tag	UNP Q92AL3
G	252	HIS	-	expression tag	UNP Q92AL3
G	253	HIS	-	expression tag	UNP Q92AL3
G	254	HIS	-	expression tag	UNP Q92AL3
H	1	MSE	-	expression tag	UNP Q92AL3
H	2	SER	-	expression tag	UNP Q92AL3
H	3	LEU	-	expression tag	UNP Q92AL3
H	247	GLU	-	expression tag	UNP Q92AL3
H	248	GLY	-	expression tag	UNP Q92AL3
H	249	HIS	-	expression tag	UNP Q92AL3
H	250	HIS	-	expression tag	UNP Q92AL3
H	251	HIS	-	expression tag	UNP Q92AL3
H	252	HIS	-	expression tag	UNP Q92AL3
H	253	HIS	-	expression tag	UNP Q92AL3
H	254	HIS	-	expression tag	UNP Q92AL3

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0
2	A	1	Total 1	Mn 1	0	0
2	F	1	Total 1	Mn 1	0	0

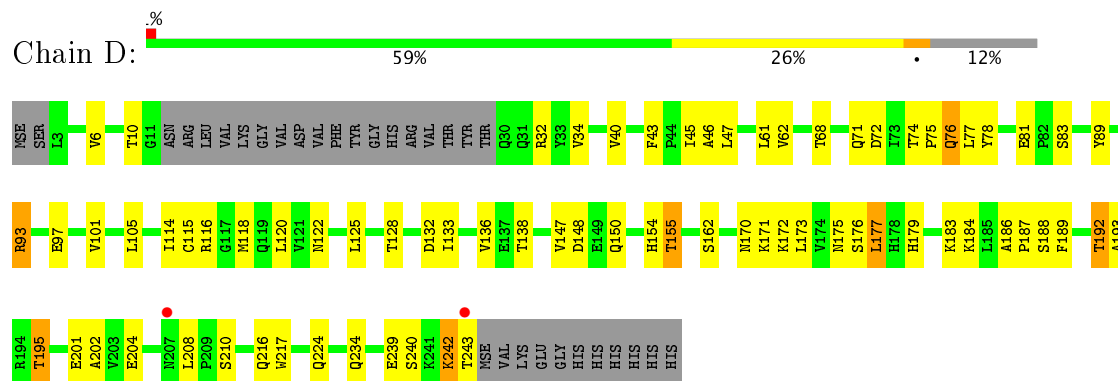
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total 100	O 100	0	0
3	B	85	Total 85	O 85	0	0
3	C	85	Total 85	O 85	0	0
3	D	92	Total 92	O 92	0	0
3	E	72	Total 72	O 72	0	0
3	F	73	Total 73	O 73	0	0
3	G	56	Total 56	O 56	0	0
3	H	57	Total 57	O 57	0	0

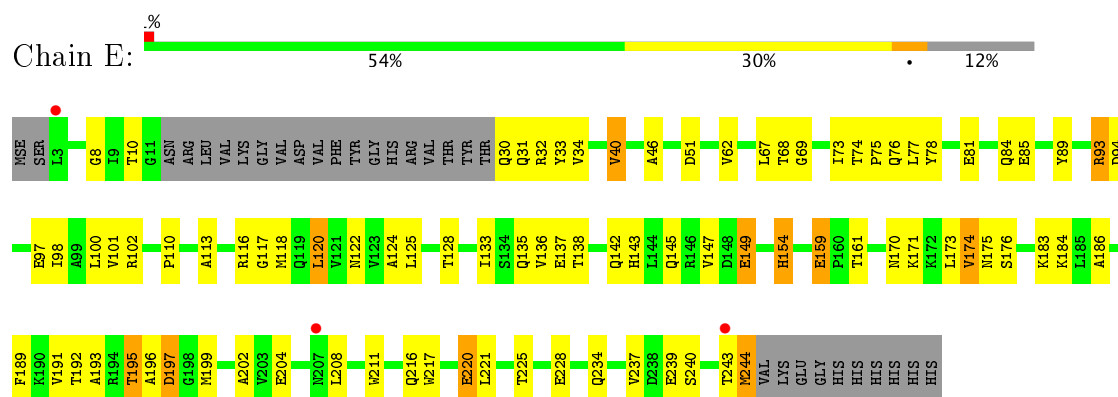
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($\text{RSRZ} > 2$). 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.

[illegible][illegible][illegible]

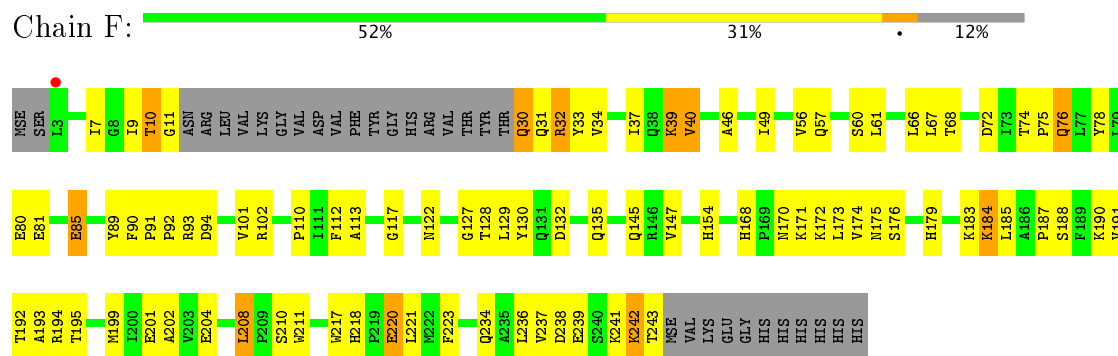
- Molecule 1: Lin1909 protein



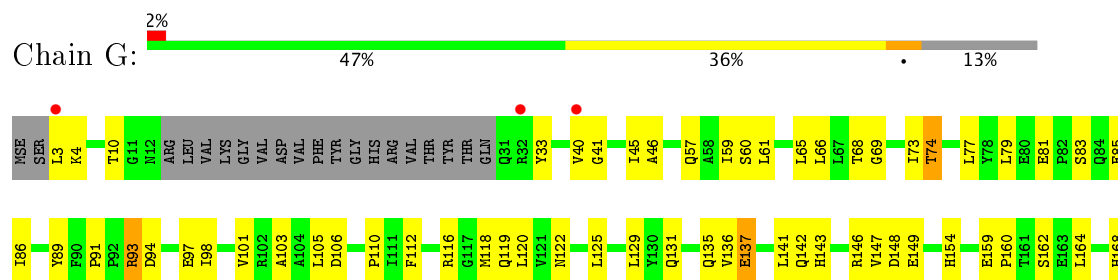
- Molecule 1: Lin1909 protein

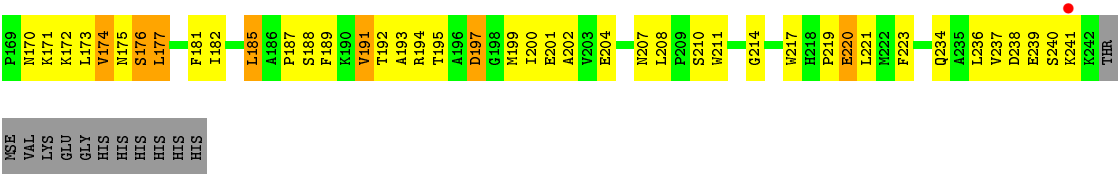


- Molecule 1: Lin1909 protein

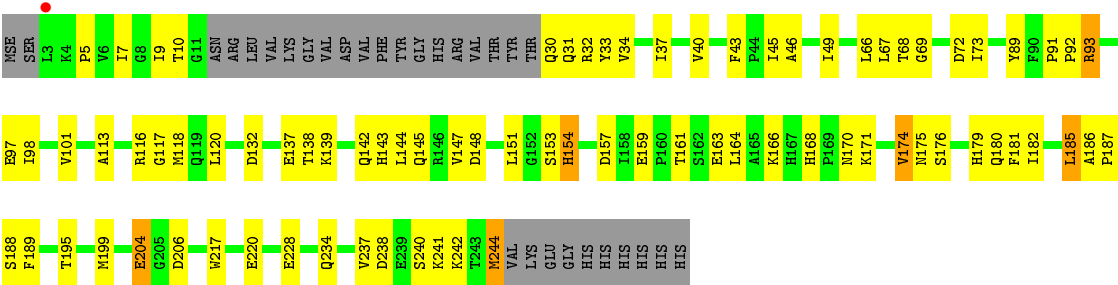


- Molecule 1: Lin1909 protein





● Molecule 1: Lin1909 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.06Å 131.21Å 93.29Å 90.00° 108.79° 90.00°	Depositor
Resolution (Å)	43.10 – 2.30 43.10 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.4 (43.10-2.30) 95.2 (43.10-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.269 0.217 , 0.268	Depositor DCC
R_{free} test set	3520 reflections (4.01%)	DCC
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14467	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.38	0/1772	0.68	0/2402
1	B	0.36	0/1756	0.65	0/2383
1	C	0.38	0/1749	0.66	0/2374
1	D	0.36	0/1765	0.65	0/2395
1	E	0.37	0/1772	0.67	0/2402
1	F	0.35	0/1765	0.63	0/2395
1	G	0.39	0/1757	0.66	2/2384 (0.1%)
1	H	0.34	0/1772	0.63	0/2402
All	All	0.37	0/14108	0.65	2/19137 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	177	LEU	N-CA-CB	5.82	122.05	110.40
1	G	176	SER	CB-CA-C	-5.29	100.04	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1739	0	1739	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1722	0	1723	60	0
1	C	1715	0	1710	92	0
1	D	1731	0	1730	66	0
1	E	1739	0	1739	75	0
1	F	1731	0	1730	104	0
1	G	1723	0	1721	102	0
1	H	1739	0	1739	83	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	100	0	0	10	0
3	B	85	0	0	5	0
3	C	85	0	0	9	0
3	D	92	0	0	2	0
3	E	72	0	0	3	0
3	F	73	0	0	7	0
3	G	56	0	0	4	0
3	H	57	0	0	2	0
All	All	14467	0	13831	638	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 23.

All (638) 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:128:THR:HG22	1:C:183:LYS:HB3	1.28	1.15
1:A:241:LYS:HA	1:A:244:MSE:HE3	1.11	1.05
1:G:182:ILE:HD12	1:G:200:ILE:HD11	1.41	1.00
1:A:241:LYS:HA	1:A:244:MSE:CE	1.92	1.00
1:G:176:SER:O	1:G:177:LEU:HG	1.62	0.99
1:D:40:VAL:HG11	1:D:234:GLN:HA	1.44	0.99
1:F:199:MSE:HE3	1:F:199:MSE:HA	1.46	0.97
1:D:32:ARG:HH21	1:D:224:GLN:NE2	1.63	0.95
1:E:159:GLU:OE1	1:E:161:THR:HG22	1.67	0.94
1:G:46:ALA:HB3	1:H:46:ALA:HB3	1.48	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:GLU:HG3	1:E:135:GLN:HE21	1.40	0.85
1:G:181:PHE:CG	1:G:199:MSE:HE3	2.12	0.84
1:B:10:THR:HG23	1:B:68:THR:HG22	1.59	0.83
1:G:220:GLU:OE1	1:G:221:LEU:HG	1.79	0.83
1:G:176:SER:O	1:G:177:LEU:CG	2.27	0.82
1:A:94:ASP:O	1:A:98:ILE:HG12	1.80	0.81
1:H:5:PRO:HG3	1:H:241:LYS:HB3	1.61	0.80
1:A:10:THR:HG22	1:A:68:THR:H	1.44	0.80
1:C:8:GLY:H	1:C:62:VAL:HG21	1.44	0.80
1:D:133:ILE:O	1:D:136:VAL:HG12	1.80	0.79
1:E:84:GLN:HA	1:G:142:GLN:HB2	1.63	0.79
1:C:8:GLY:N	1:C:62:VAL:HG21	1.97	0.79
1:F:11:GLY:HA2	1:F:30:GLN:HE22	1.47	0.79
1:D:184:LYS:HE3	3:D:381:HOH:O	1.82	0.78
1:A:5:PRO:HG3	1:A:244:MSE:HE1	1.65	0.78
1:H:148:ASP:HB3	1:H:151:LEU:HD13	1.66	0.78
1:D:40:VAL:CG1	1:D:234:GLN:HA	2.15	0.77
1:A:93:ARG:HD2	1:A:116:ARG:NH2	2.00	0.76
1:G:182:ILE:CD1	1:G:200:ILE:HD11	2.15	0.76
1:F:33:TYR:CE2	1:F:220:GLU:HG2	2.20	0.76
1:D:132:ASP:OD1	1:D:179:HIS:HD2	1.68	0.76
3:A:584:HOH:O	1:C:54:THR:HB	1.86	0.76
1:A:243:THR:HB	3:A:266:HOH:O	1.85	0.75
1:H:241:LYS:HA	1:H:244:MSE:CG	2.16	0.75
1:A:74:THR:OG1	1:A:77:LEU:HD13	1.86	0.75
1:E:94:ASP:O	1:E:98:ILE:HG12	1.87	0.75
1:C:128:THR:HG22	1:C:183:LYS:CB	2.15	0.75
1:E:89:TYR:O	1:G:147:VAL:HG13	1.87	0.75
1:F:10:THR:HG22	1:F:68:THR:H	1.53	0.74
1:C:74:THR:HG23	1:C:94:ASP:OD1	1.86	0.74
1:A:33:TYR:CE2	1:A:220:GLU:HG2	2.21	0.74
1:E:145:GLN:NE2	1:E:176:SER:H	1.86	0.74
1:G:40:VAL:HG12	1:G:237:VAL:HG21	1.69	0.73
1:F:220:GLU:OE2	1:F:221:LEU:HG	1.87	0.73
1:B:172:LYS:HE2	1:B:228:GLU:OE1	1.87	0.73
1:C:119:GLN:HE21	1:C:216:GLN:HE22	1.35	0.73
1:A:46:ALA:HB3	1:C:46:ALA:HB3	1.70	0.72
1:F:208:LEU:H	1:F:208:LEU:HD12	1.54	0.72
1:A:191:VAL:HG11	1:A:194:ARG:NH2	2.06	0.71
1:A:10:THR:CG2	1:A:68:THR:H	2.03	0.71
1:E:85:GLU:HG3	1:E:135:GLN:NE2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:THR:HG23	1:F:81:GLU:OE2	1.91	0.70
1:C:159:GLU:HB2	1:C:162:SER:OG	1.91	0.70
1:D:122:ASN:HD21	1:D:186:ALA:H	1.38	0.70
1:E:159:GLU:HG2	3:E:539:HOH:O	1.89	0.70
1:E:33:TYR:CE2	1:E:220:GLU:HG2	2.27	0.70
1:H:132:ASP:OD1	1:H:179:HIS:HD2	1.73	0.70
1:A:219:PRO:HA	1:A:222:MSE:HE2	1.73	0.70
1:G:33:TYR:CE2	1:G:220:GLU:HG2	2.26	0.70
1:H:181:PHE:CG	1:H:199:MSE:HE3	2.26	0.70
1:F:76:GLN:HE21	1:F:76:GLN:H	1.39	0.70
1:C:122:ASN:HD21	1:C:186:ALA:H	1.38	0.69
1:D:40:VAL:HG13	1:D:234:GLN:NE2	2.07	0.69
1:G:181:PHE:CD1	1:G:199:MSE:HE3	2.26	0.69
1:B:193:ALA:HB3	1:B:202:ALA:HB3	1.74	0.69
1:C:119:GLN:O	1:C:123:VAL:HG12	1.92	0.69
1:G:136:VAL:HG21	1:G:199:MSE:HE2	1.75	0.69
1:C:225:THR:HG22	3:C:266:HOH:O	1.93	0.69
1:H:181:PHE:CB	1:H:199:MSE:HE3	2.23	0.69
1:G:40:VAL:HG11	1:G:234:GLN:HA	1.75	0.69
1:B:40:VAL:HG22	1:B:234:GLN:NE2	2.08	0.68
1:H:91:PRO:HB2	1:H:92:PRO:HD3	1.73	0.68
1:E:145:GLN:HE22	1:E:175:ASN:HA	1.59	0.68
1:F:147:VAL:HG13	1:H:89:TYR:O	1.94	0.68
1:F:241:LYS:C	1:F:243:THR:H	1.96	0.68
1:B:147:VAL:HG13	1:C:89:TYR:O	1.93	0.68
1:C:190:LYS:HZ2	1:C:191:VAL:HG22	1.58	0.68
1:E:192:THR:HG21	1:E:204:GLU:OE2	1.93	0.68
1:D:32:ARG:NH2	1:D:224:GLN:NE2	2.41	0.67
1:D:40:VAL:HG13	1:D:234:GLN:CD	2.14	0.67
1:E:122:ASN:HD21	1:E:186:ALA:H	1.42	0.67
1:A:33:TYR:CD2	1:A:220:GLU:HG2	2.30	0.67
1:G:191:VAL:HG11	1:G:194:ARG:HH12	1.58	0.67
1:D:10:THR:HG22	1:D:68:THR:H	1.60	0.67
1:F:241:LYS:O	1:F:243:THR:N	2.24	0.66
1:F:76:GLN:H	1:F:76:GLN:NE2	1.93	0.66
1:C:97:GLU:OE1	1:C:116:ARG:NH1	2.28	0.66
1:F:168:HIS:HD2	1:F:172:LYS:HG2	1.60	0.66
1:G:136:VAL:HG21	1:G:199:MSE:CE	2.26	0.66
1:E:10:THR:CG2	1:E:68:THR:H	2.09	0.66
1:C:195:THR:C	1:C:197:ASP:H	1.97	0.66
1:A:133:ILE:HG12	1:A:181:PHE:CE1	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:THR:HG23	1:G:81:GLU:OE2	1.96	0.65
1:H:187:PRO:O	1:H:188:SER:HB2	1.95	0.65
1:G:40:VAL:CG1	1:G:234:GLN:HA	2.27	0.65
1:F:31:GLN:O	1:F:34:VAL:HG22	1.97	0.65
1:B:71:GLN:HG2	3:B:375:HOH:O	1.96	0.65
1:C:131:GLN:HB2	1:C:135:GLN:HE22	1.62	0.65
1:F:242:LYS:HB2	3:F:422:HOH:O	1.97	0.65
1:C:68:THR:CG2	1:C:69:GLY:N	2.59	0.64
1:G:93:ARG:HD2	1:G:116:ARG:NH2	2.12	0.64
1:H:9:ILE:HD11	1:H:37:ILE:HD12	1.78	0.64
1:A:74:THR:HG23	1:A:94:ASP:OD2	1.96	0.64
1:C:81:GLU:HG3	1:C:82:PRO:HD2	1.79	0.64
1:F:199:MSE:CE	1:F:199:MSE:HA	2.24	0.64
1:G:159:GLU:HB3	1:G:162:SER:OG	1.98	0.64
1:A:147:VAL:HG13	1:D:89:TYR:O	1.97	0.64
1:C:101:VAL:O	1:C:105:LEU:HD13	1.97	0.64
1:C:51:ASP:O	1:C:54:THR:HG22	1.98	0.64
1:B:137:GLU:CD	1:B:137:GLU:H	2.01	0.64
1:D:10:THR:CG2	1:D:68:THR:H	2.11	0.64
1:A:222:MSE:HE3	1:A:229:SER:OG	1.99	0.63
1:A:122:ASN:ND2	1:A:186:ALA:H	1.97	0.63
1:E:74:THR:HB	1:E:77:LEU:HD13	1.81	0.63
1:G:105:LEU:HD23	1:G:210:SER:OG	1.97	0.63
1:A:122:ASN:HD21	1:A:186:ALA:H	1.47	0.63
1:C:70:GLY:N	1:C:116:ARG:HG2	2.13	0.63
1:A:97:GLU:OE1	1:A:120:LEU:HD13	1.98	0.63
1:E:195:THR:C	1:E:197:ASP:H	2.02	0.63
1:A:5:PRO:CG	1:A:244:MSE:HE1	2.28	0.62
1:A:193:ALA:HB3	1:A:202:ALA:HB3	1.81	0.62
1:B:187:PRO:O	1:B:188:SER:HB3	1.98	0.62
1:H:159:GLU:OE2	1:H:161:THR:HG23	1.99	0.62
1:C:6:VAL:HG12	1:C:62:VAL:HG23	1.82	0.62
1:C:10:THR:CG2	1:C:68:THR:H	2.13	0.62
1:H:98:ILE:O	1:H:101:VAL:HG22	2.00	0.62
1:H:31:GLN:O	1:H:34:VAL:HG22	1.98	0.62
1:D:72:ASP:OD2	1:D:179:HIS:HE1	1.83	0.62
1:B:93:ARG:NH1	1:B:97:GLU:OE1	2.32	0.61
1:H:139:LYS:HB3	1:H:139:LYS:NZ	2.16	0.61
1:H:37:ILE:HD11	1:H:66:LEU:HD22	1.82	0.61
1:C:147:VAL:HG13	1:G:89:TYR:O	2.00	0.61
1:F:239:GLU:O	1:F:242:LYS:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:LEU:HD23	1:D:210:SER:OG	2.00	0.61
1:D:32:ARG:HH21	1:D:224:GLN:HE22	1.46	0.61
1:C:191:VAL:HG21	1:C:194:ARG:HH12	1.65	0.60
1:C:10:THR:CG2	1:C:67:LEU:HA	2.31	0.60
1:H:241:LYS:HA	1:H:244:MSE:HG2	1.81	0.60
1:H:30:GLN:HA	1:H:33:TYR:HD1	1.66	0.60
1:A:150:GLN:HG3	1:A:221:LEU:O	2.02	0.60
1:A:241:LYS:CA	1:A:244:MSE:HE3	2.07	0.60
1:B:215:VAL:HG13	1:B:217:TRP:CD2	2.36	0.60
1:A:176:SER:C	1:A:177:LEU:HD22	2.22	0.60
1:F:33:TYR:CD2	1:F:68:THR:HG22	2.36	0.60
1:G:159:GLU:HB3	1:G:162:SER:HG	1.67	0.60
1:D:172:LYS:HD3	1:D:173:LEU:H	1.66	0.60
1:F:10:THR:CG2	1:F:68:THR:H	2.15	0.59
1:G:116:ARG:NH1	3:G:376:HOH:O	2.36	0.59
1:A:58:ALA:O	1:A:61:LEU:HD22	2.02	0.59
1:D:32:ARG:HH22	1:D:150:GLN:HE21	1.48	0.59
1:E:128:THR:HB	1:E:184:LYS:HB3	1.85	0.59
1:H:137:GLU:H	1:H:137:GLU:CD	2.04	0.59
1:C:116:ARG:HD3	3:C:257:HOH:O	2.02	0.59
1:E:243:THR:O	1:E:244:MSE:HB3	2.00	0.59
1:E:195:THR:C	1:E:197:ASP:N	2.54	0.59
1:F:191:VAL:HG11	1:F:194:ARG:HH21	1.68	0.59
1:G:197:ASP:HB3	1:G:199:MSE:HG2	1.85	0.59
1:B:50:ASP:HB3	1:B:54:THR:HG21	1.85	0.59
1:E:31:GLN:O	1:E:34:VAL:HG22	2.02	0.59
1:A:211:TRP:CG	1:A:239:GLU:HG2	2.38	0.58
1:A:91:PRO:HB2	1:A:92:PRO:HD3	1.85	0.58
1:G:137:GLU:H	1:G:137:GLU:CD	2.05	0.58
1:C:10:THR:HG22	1:C:67:LEU:HA	1.85	0.58
1:C:40:VAL:O	1:C:40:VAL:HG13	2.03	0.58
1:E:73:ILE:HD13	1:E:120:LEU:HA	1.84	0.58
1:E:149:GLU:HB3	1:E:221:LEU:HD13	1.85	0.58
1:F:195:THR:HG23	1:F:201:GLU:HG3	1.84	0.58
1:C:190:LYS:NZ	1:C:191:VAL:HG22	2.18	0.58
1:E:128:THR:HG22	1:E:183:LYS:HB3	1.84	0.58
1:F:30:GLN:O	1:F:30:GLN:HG3	2.03	0.58
1:F:211:TRP:CG	1:F:239:GLU:HG2	2.39	0.58
1:F:191:VAL:HG11	1:F:194:ARG:NH2	2.18	0.58
1:G:195:THR:C	1:G:197:ASP:H	2.07	0.58
1:A:5:PRO:CB	1:A:244:MSE:HE1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:VAL:HG21	1:H:89:TYR:CZ	2.38	0.57
1:F:40:VAL:HG22	1:F:234:GLN:NE2	2.19	0.57
1:C:195:THR:C	1:C:197:ASP:N	2.57	0.57
1:C:86:ILE:HG23	1:C:131:GLN:HB3	1.85	0.57
1:H:40:VAL:CG1	1:H:234:GLN:HA	2.33	0.57
1:F:37:ILE:HD11	1:F:66:LEU:HD22	1.86	0.57
1:F:74:THR:HG23	1:F:94:ASP:OD1	2.04	0.57
1:G:195:THR:HG23	1:G:201:GLU:HG3	1.85	0.57
1:G:202:ALA:HA	1:G:214:GLY:O	2.05	0.57
1:E:10:THR:CG2	1:E:67:LEU:HA	2.35	0.57
1:H:185:LEU:HD22	1:H:186:ALA:O	2.05	0.57
1:A:133:ILE:HG12	1:A:181:PHE:HE1	1.67	0.57
1:H:181:PHE:CG	1:H:199:MSE:CE	2.88	0.57
1:A:72:ASP:OD2	1:A:179:HIS:HE1	1.88	0.56
1:C:191:VAL:HG21	1:C:194:ARG:NH1	2.19	0.56
1:H:40:VAL:HG12	1:H:237:VAL:HG21	1.86	0.56
1:C:193:ALA:HB3	1:C:202:ALA:HB3	1.87	0.56
1:F:7:ILE:HG21	1:F:37:ILE:HD13	1.86	0.56
1:E:125:LEU:HD22	1:E:189:PHE:CE2	2.39	0.56
1:E:243:THR:O	1:E:244:MSE:CB	2.52	0.56
1:C:129:LEU:HD23	1:C:182:ILE:HA	1.88	0.56
1:F:128:THR:HG22	1:F:129:LEU:N	2.21	0.56
1:G:141:LEU:H	1:G:197:ASP:CG	2.09	0.56
1:G:74:THR:HG22	1:G:94:ASP:OD1	2.06	0.56
1:H:220:GLU:OE2	1:H:220:GLU:N	2.36	0.56
1:E:10:THR:HG22	1:E:67:LEU:HA	1.88	0.56
1:E:145:GLN:NE2	1:E:176:SER:N	2.53	0.56
1:E:32:ARG:HG2	1:E:221:LEU:HD23	1.88	0.56
1:H:7:ILE:HG21	1:H:37:ILE:CD1	2.36	0.56
1:H:175:ASN:OD1	1:H:217:TRP:HB2	2.04	0.56
1:F:9:ILE:HD11	1:F:37:ILE:HD12	1.86	0.56
1:F:241:LYS:C	1:F:243:THR:N	2.58	0.55
1:B:56:VAL:HG13	3:B:512:HOH:O	2.06	0.55
1:C:122:ASN:ND2	1:C:186:ALA:H	2.03	0.55
1:D:162:SER:HB2	1:D:204:GLU:OE1	2.07	0.55
1:E:225:THR:O	1:E:225:THR:HG22	2.06	0.55
1:G:182:ILE:HD12	1:G:200:ILE:CD1	2.28	0.55
1:H:145:GLN:NE2	1:H:176:SER:H	2.04	0.55
1:B:193:ALA:HB3	1:B:202:ALA:CB	2.37	0.55
1:C:30:GLN:N	3:C:410:HOH:O	2.40	0.55
1:A:155:THR:HG23	1:D:81:GLU:CD	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ALA:HB3	3:A:307:HOH:O	2.07	0.55
1:C:215:VAL:HG13	1:C:217:TRP:CD2	2.42	0.55
1:A:122:ASN:HD21	1:A:185:LEU:HA	1.72	0.54
1:H:154:HIS:NE2	1:H:176:SER:HB2	2.21	0.54
1:C:50:ASP:HB3	1:C:54:THR:HG21	1.89	0.54
1:E:183:LYS:HD3	3:E:282:HOH:O	2.06	0.54
1:F:175:ASN:OD1	1:F:217:TRP:HB2	2.07	0.54
1:H:174:VAL:HG21	1:H:217:TRP:CE2	2.41	0.54
1:H:174:VAL:HG21	1:H:217:TRP:CD2	2.43	0.54
1:H:181:PHE:CE2	1:H:199:MSE:HG3	2.41	0.54
1:C:86:ILE:HG23	1:C:131:GLN:OE1	2.07	0.54
1:H:185:LEU:HD21	1:H:189:PHE:HB2	1.88	0.54
1:B:187:PRO:O	1:B:188:SER:CB	2.55	0.54
1:F:39:LYS:O	1:F:39:LYS:HD3	2.06	0.54
1:H:145:GLN:NE2	1:H:153:SER:OG	2.41	0.54
1:C:228:GLU:HG3	3:C:283:HOH:O	2.08	0.54
1:D:240:SER:O	1:D:243:THR:HG22	2.08	0.54
1:D:32:ARG:NH2	1:D:224:GLN:HE22	2.04	0.54
1:G:195:THR:C	1:G:197:ASP:N	2.61	0.54
1:A:187:PRO:O	1:A:188:SER:HB2	2.07	0.54
1:D:125:LEU:HD22	1:D:189:PHE:CZ	2.43	0.54
1:D:93:ARG:HD2	1:D:116:ARG:NH2	2.22	0.54
1:A:207:ASN:HA	3:A:444:HOH:O	2.07	0.53
1:B:93:ARG:HH11	1:B:93:ARG:HG2	1.74	0.53
1:A:158:ILE:HD12	1:A:169:PRO:O	2.08	0.53
1:A:5:PRO:HB3	1:A:244:MSE:HE1	1.90	0.53
1:E:40:VAL:HG22	1:E:234:GLN:NE2	2.23	0.53
1:F:40:VAL:CG1	1:F:237:VAL:HG21	2.38	0.53
1:F:56:VAL:HG23	1:F:57:GLN:N	2.23	0.53
1:A:149:GLU:HB2	1:A:221:LEU:HD13	1.91	0.53
1:B:97:GLU:OE2	1:B:120:LEU:HD13	2.09	0.53
1:G:191:VAL:HG21	1:G:194:ARG:NH1	2.23	0.53
1:C:187:PRO:O	1:C:188:SER:HB2	2.09	0.53
1:G:177:LEU:N	3:G:262:HOH:O	2.24	0.53
1:F:187:PRO:O	1:F:188:SER:HB2	2.07	0.53
1:A:40:VAL:HG12	1:A:237:VAL:HG21	1.91	0.53
1:A:74:THR:HG21	1:A:91:PRO:HA	1.90	0.53
1:C:73:ILE:HG21	1:C:123:VAL:HG11	1.91	0.53
1:E:211:TRP:CG	1:E:239:GLU:HG2	2.44	0.53
1:F:39:LYS:HD2	3:F:289:HOH:O	2.09	0.53
1:G:149:GLU:HG3	1:G:221:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40:VAL:HG13	1:H:234:GLN:HA	1.90	0.53
1:D:122:ASN:ND2	1:D:186:ALA:H	2.05	0.53
1:F:56:VAL:HG23	1:F:57:GLN:H	1.74	0.53
1:F:208:LEU:HD11	3:F:273:HOH:O	2.08	0.52
1:G:189:PHE:CE2	1:G:208:LEU:HD11	2.45	0.52
1:A:191:VAL:HG12	3:A:269:HOH:O	2.09	0.52
1:D:76:GLN:HE21	1:D:76:GLN:H	1.57	0.52
1:A:122:ASN:ND2	1:A:185:LEU:HD12	2.25	0.52
1:A:93:ARG:HD2	1:A:116:ARG:HH21	1.74	0.52
1:H:163:GLU:HA	1:H:166:LYS:HE2	1.92	0.52
1:H:49:ILE:HD12	1:H:93:ARG:HA	1.92	0.52
1:H:43:PHE:HE2	1:H:45:ILE:HD11	1.73	0.52
1:G:110:PRO:HG2	1:G:240:SER:HA	1.91	0.52
1:E:195:THR:O	1:E:197:ASP:N	2.43	0.52
1:E:113:ALA:HB1	1:E:117:GLY:C	2.30	0.52
1:E:98:ILE:O	1:E:101:VAL:HG22	2.09	0.52
1:F:74:THR:HG22	1:F:89:TYR:HD1	1.74	0.52
1:A:191:VAL:HG11	1:A:194:ARG:HH21	1.73	0.52
1:A:57:GLN:O	1:A:61:LEU:HD13	2.10	0.52
1:C:97:GLU:O	1:C:101:VAL:HG13	2.09	0.52
1:F:72:ASP:OD2	1:F:179:HIS:HE1	1.93	0.52
1:G:83:SER:O	1:G:86:ILE:HG22	2.10	0.52
1:B:10:THR:CG2	1:B:68:THR:H	2.23	0.52
1:B:93:ARG:NH1	1:B:97:GLU:CD	2.63	0.52
1:F:32:ARG:HD2	3:F:269:HOH:O	2.10	0.52
1:G:73:ILE:HD12	1:G:129:LEU:HD11	1.92	0.52
1:F:193:ALA:HB3	1:F:202:ALA:HB3	1.92	0.51
1:A:175:ASN:OD1	1:A:217:TRP:HB2	2.11	0.51
1:B:3:LEU:N	1:B:3:LEU:HD13	2.25	0.51
1:E:93:ARG:HD2	1:E:116:ARG:NH2	2.25	0.51
1:E:40:VAL:O	1:E:40:VAL:CG1	2.59	0.51
1:E:33:TYR:CD2	1:E:220:GLU:HG2	2.46	0.51
1:F:67:LEU:HD12	1:F:113:ALA:HB2	1.92	0.51
1:H:241:LYS:HA	1:H:244:MSE:HG3	1.90	0.51
1:H:10:THR:CG2	1:H:68:THR:H	2.24	0.51
1:D:76:GLN:NE2	1:D:76:GLN:H	2.08	0.51
1:F:145:GLN:HG2	1:F:176:SER:O	2.10	0.51
1:B:91:PRO:HB2	1:B:92:PRO:HD3	1.93	0.51
1:E:197:ASP:HB3	1:E:199:MSE:H	1.75	0.51
1:F:110:PRO:HB3	1:F:239:GLU:HG3	1.92	0.51
1:H:157:ASP:OD1	1:H:171:LYS:NZ	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:THR:HG23	1:D:201:GLU:HG3	1.93	0.51
1:E:193:ALA:HB3	1:E:202:ALA:HB3	1.92	0.51
1:A:155:THR:HG23	1:D:81:GLU:OE2	2.10	0.51
1:F:220:GLU:OE2	1:F:221:LEU:N	2.44	0.51
1:A:30:GLN:N	3:A:283:HOH:O	2.42	0.51
1:A:74:THR:HG21	1:A:91:PRO:HG3	1.93	0.51
1:E:122:ASN:ND2	1:E:186:ALA:H	2.06	0.51
1:F:39:LYS:HA	1:F:39:LYS:HZ2	1.75	0.51
1:F:74:THR:HG21	1:F:91:PRO:HA	1.92	0.51
1:A:174:VAL:HG13	1:A:217:TRP:CB	2.42	0.50
1:D:32:ARG:NH2	1:D:150:GLN:HE21	2.09	0.50
1:D:147:VAL:HG21	1:F:89:TYR:CZ	2.46	0.50
1:B:162:SER:O	1:B:165:ALA:HB3	2.11	0.50
1:C:68:THR:HG22	1:C:69:GLY:N	2.27	0.50
1:F:192:THR:HG21	1:F:204:GLU:OE2	2.11	0.50
1:G:69:GLY:HA2	1:G:116:ARG:HB3	1.93	0.50
1:B:10:THR:HG22	1:B:67:LEU:HA	1.93	0.50
1:B:89:TYR:CZ	1:E:147:VAL:HG21	2.46	0.50
1:D:136:VAL:HG13	1:D:138:THR:O	2.10	0.50
1:H:164:LEU:HD11	1:H:168:HIS:HD2	1.76	0.50
1:C:147:VAL:HG21	1:G:89:TYR:CZ	2.47	0.50
1:F:172:LYS:HD3	3:F:337:HOH:O	2.10	0.50
1:H:7:ILE:HG21	1:H:37:ILE:HD13	1.94	0.50
1:C:74:THR:HG21	1:C:91:PRO:HA	1.94	0.50
1:B:54:THR:HG22	1:B:96:TYR:HE1	1.77	0.50
1:C:195:THR:HG23	1:C:201:GLU:HG3	1.92	0.50
1:B:89:TYR:CE1	1:E:147:VAL:HG21	2.47	0.50
1:F:74:THR:HG21	1:F:91:PRO:HG3	1.93	0.50
1:G:74:THR:HG21	1:G:91:PRO:HA	1.93	0.50
1:H:142:GLN:NE2	3:H:256:HOH:O	2.29	0.50
1:D:40:VAL:CG1	1:D:40:VAL:O	2.59	0.50
1:G:187:PRO:O	1:G:188:SER:HB2	2.11	0.50
1:B:193:ALA:CB	1:B:202:ALA:HB3	2.41	0.50
1:D:74:THR:HB	1:D:77:LEU:HD13	1.93	0.50
1:C:241:LYS:HE3	3:C:520:HOH:O	2.12	0.49
1:F:40:VAL:HG13	1:F:40:VAL:O	2.11	0.49
1:F:60:SER:HA	3:F:413:HOH:O	2.12	0.49
1:G:182:ILE:HB	1:G:200:ILE:HD11	1.93	0.49
1:B:194:ARG:NH2	3:B:385:HOH:O	2.44	0.49
1:F:66:LEU:HD12	1:F:112:PHE:O	2.12	0.49
1:G:40:VAL:CG1	1:G:40:VAL:O	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:69:GLY:HA2	1:H:116:ARG:HB3	1.93	0.49
1:C:162:SER:OG	1:C:192:THR:HG23	2.12	0.49
1:E:97:GLU:HB3	1:E:120:LEU:HD22	1.93	0.49
1:H:159:GLU:HG2	1:H:161:THR:HG22	1.94	0.49
1:B:46:ALA:HB3	1:D:46:ALA:HB3	1.94	0.49
1:G:176:SER:O	1:G:177:LEU:CD2	2.60	0.49
1:H:10:THR:CG2	1:H:67:LEU:HA	2.42	0.49
1:E:30:GLN:OE1	1:E:30:GLN:HA	2.12	0.49
1:G:192:THR:HG21	1:G:204:GLU:OE1	2.12	0.49
1:A:155:THR:HB	1:A:173:LEU:HD12	1.95	0.49
1:B:93:ARG:HH12	1:B:97:GLU:CD	2.16	0.49
1:C:145:GLN:HG2	1:C:176:SER:O	2.13	0.49
1:F:238:ASP:O	1:F:241:LYS:HB3	2.12	0.49
1:G:125:LEU:HD12	1:G:189:PHE:CZ	2.47	0.49
1:G:182:ILE:HB	1:G:200:ILE:CD1	2.42	0.49
1:A:110:PRO:HG3	1:A:240:SER:CA	2.42	0.49
1:A:193:ALA:HB3	1:A:202:ALA:CB	2.42	0.49
1:H:185:LEU:CD2	1:H:189:PHE:HB2	2.42	0.49
1:H:168:HIS:CE1	1:H:228:GLU:HB3	2.47	0.49
1:D:71:GLN:HB2	3:D:367:HOH:O	2.13	0.49
1:F:75:PRO:HB2	1:F:80:GLU:O	2.12	0.49
1:H:118:MSE:HE3	1:H:182:ILE:CD1	2.43	0.49
1:C:6:VAL:O	1:C:62:VAL:HG22	2.13	0.48
1:F:40:VAL:HG22	1:F:234:GLN:CD	2.33	0.48
1:D:147:VAL:HG12	1:D:148:ASP:N	2.29	0.48
1:C:112:PHE:HB2	1:C:236:LEU:HD13	1.95	0.48
1:E:154:HIS:CE1	1:E:174:VAL:HG12	2.48	0.48
1:F:112:PHE:HB3	1:F:236:LEU:HD22	1.95	0.48
1:G:174:VAL:HG21	1:G:217:TRP:CD2	2.48	0.48
1:G:98:ILE:O	1:G:101:VAL:HG12	2.13	0.48
1:D:43:PHE:CE2	1:D:45:ILE:HD11	2.48	0.48
1:D:147:VAL:HG21	1:F:89:TYR:CE1	2.48	0.48
1:D:75:PRO:HA	1:D:78:TYR:CE2	2.48	0.48
1:B:56:VAL:HG23	1:B:57:GLN:N	2.28	0.48
1:D:118:MSE:HE1	1:D:216:GLN:HB2	1.95	0.48
1:G:45:ILE:HG23	1:H:45:ILE:HG23	1.96	0.48
1:C:59:ILE:HG13	1:C:103:ALA:HB3	1.96	0.48
1:F:78:TYR:OH	1:F:129:LEU:HD11	2.13	0.48
1:D:175:ASN:OD1	1:D:217:TRP:HB2	2.14	0.48
1:G:162:SER:OG	1:G:192:THR:HG23	2.14	0.48
1:G:33:TYR:CD2	1:G:68:THR:HG22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:ASP:OD2	1:H:179:HIS:HE1	1.97	0.48
1:C:195:THR:O	1:C:197:ASP:N	2.46	0.47
1:B:159:GLU:O	1:B:165:ALA:HB2	2.14	0.47
1:G:60:SER:HA	3:G:563:HOH:O	2.14	0.47
1:H:7:ILE:CG2	1:H:37:ILE:HD13	2.44	0.47
1:D:125:LEU:HD22	1:D:189:PHE:CE2	2.49	0.47
1:F:39:LYS:HA	1:F:39:LYS:NZ	2.28	0.47
1:G:195:THR:OG1	1:G:197:ASP:HB2	2.14	0.47
1:G:172:LYS:HG2	1:G:173:LEU:N	2.29	0.47
1:G:174:VAL:HG21	1:G:217:TRP:CE2	2.49	0.47
1:A:243:THR:O	1:A:244:MSE:HG3	2.15	0.47
1:B:51:ASP:O	1:B:54:THR:HG22	2.14	0.47
1:E:40:VAL:O	1:E:40:VAL:HG13	2.15	0.47
1:E:33:TYR:CE2	1:E:68:THR:HG22	2.50	0.47
1:G:185:LEU:HD22	1:G:189:PHE:HB2	1.97	0.47
1:B:124:ALA:C	1:B:125:LEU:HD12	2.35	0.47
1:C:68:THR:HG23	1:C:69:GLY:H	1.78	0.47
1:F:129:LEU:HA	1:F:183:LYS:H	1.79	0.47
1:F:7:ILE:CG2	1:F:37:ILE:HD13	2.44	0.47
1:B:40:VAL:HG21	1:B:234:GLN:CA	2.45	0.47
1:E:145:GLN:HE22	1:E:175:ASN:CA	2.25	0.47
1:E:33:TYR:CD2	1:E:68:THR:HG22	2.49	0.47
1:F:32:ARG:HD3	1:F:221:LEU:CD2	2.45	0.47
1:C:224:GLN:HB2	3:C:260:HOH:O	2.14	0.47
1:C:68:THR:HG22	1:C:69:GLY:O	2.14	0.47
1:D:192:THR:HG22	1:D:202:ALA:HB3	1.97	0.47
1:A:142:GLN:HB2	1:D:83:SER:O	2.15	0.47
1:E:137:GLU:CD	1:E:137:GLU:H	2.18	0.47
1:F:199:MSE:HE3	1:F:199:MSE:CA	2.29	0.47
1:G:119:GLN:HG2	1:G:129:LEU:HD22	1.97	0.47
1:A:174:VAL:HG11	1:A:217:TRP:CE3	2.49	0.46
1:G:112:PHE:HB3	1:G:236:LEU:HD22	1.97	0.46
1:A:49:ILE:HD11	1:A:93:ARG:HG3	1.96	0.46
1:A:83:SER:O	1:H:142:GLN:HB2	2.16	0.46
1:C:189:PHE:CE2	1:C:208:LEU:HD11	2.50	0.46
1:C:62:VAL:HG22	1:C:64:GLY:H	1.79	0.46
1:A:219:PRO:HA	1:A:222:MSE:CE	2.45	0.46
1:B:215:VAL:HG22	1:B:217:TRP:CH2	2.50	0.46
1:E:136:VAL:HG23	1:E:138:THR:O	2.16	0.46
1:F:208:LEU:HD13	1:F:210:SER:O	2.15	0.46
1:C:40:VAL:O	1:C:40:VAL:CG1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:PHE:CE1	1:D:208:LEU:HD11	2.50	0.46
1:F:39:LYS:HB2	1:F:39:LYS:HZ3	1.81	0.46
1:G:195:THR:O	1:G:197:ASP:N	2.49	0.46
1:H:238:ASP:O	1:H:242:LYS:HB2	2.15	0.46
1:C:159:GLU:HG3	3:C:589:HOH:O	2.16	0.46
1:A:98:ILE:CD1	1:A:124:ALA:HB2	2.46	0.46
1:G:116:ARG:HG2	1:G:116:ARG:HH11	1.80	0.45
1:G:159:GLU:OE2	1:G:160:PRO:HD2	2.15	0.45
1:H:145:GLN:HE22	1:H:175:ASN:HA	1.80	0.45
1:H:40:VAL:HG11	1:H:234:GLN:HA	1.98	0.45
1:A:138:THR:HG21	3:A:277:HOH:O	2.15	0.45
1:E:125:LEU:HD22	1:E:189:PHE:HE2	1.80	0.45
1:E:225:THR:CG2	1:E:225:THR:O	2.64	0.45
1:A:72:ASP:OD2	1:A:179:HIS:CE1	2.68	0.45
1:F:174:VAL:HG13	1:F:217:TRP:CB	2.47	0.45
1:C:157:ASP:OD2	1:C:171:LYS:HE3	2.16	0.45
1:E:75:PRO:HA	1:E:78:TYR:CE2	2.51	0.45
1:F:7:ILE:HG21	1:F:37:ILE:CD1	2.46	0.45
1:G:164:LEU:HD11	1:G:168:HIS:HD2	1.81	0.45
1:E:174:VAL:HG13	1:E:217:TRP:HB3	1.99	0.45
1:F:33:TYR:CD2	1:F:220:GLU:HG2	2.50	0.45
1:G:182:ILE:CB	1:G:200:ILE:HD11	2.46	0.45
1:D:176:SER:O	1:D:177:LEU:HD13	2.16	0.45
1:D:187:PRO:O	1:D:188:SER:HB2	2.16	0.45
1:E:33:TYR:CE2	1:E:220:GLU:CG	2.96	0.45
1:E:110:PRO:HG3	1:E:240:SER:HA	1.99	0.45
1:A:110:PRO:HG3	1:A:240:SER:HA	1.98	0.45
1:C:10:THR:HG21	1:C:67:LEU:HA	1.99	0.45
1:G:59:ILE:HG13	1:G:103:ALA:HB3	1.99	0.45
1:G:93:ARG:HD3	1:G:97:GLU:OE2	2.17	0.45
1:A:40:VAL:HG13	1:A:40:VAL:O	2.16	0.45
1:D:32:ARG:HH21	1:D:224:GLN:HE21	1.53	0.45
1:D:43:PHE:HE2	1:D:45:ILE:HD11	1.82	0.45
1:G:45:ILE:HG23	1:H:45:ILE:CG2	2.46	0.45
1:C:73:ILE:N	1:C:73:ILE:HD12	2.32	0.45
1:G:66:LEU:HD12	1:G:112:PHE:O	2.17	0.45
1:A:40:VAL:O	1:A:40:VAL:CG1	2.65	0.45
1:B:3:LEU:HD22	1:B:3:LEU:N	2.32	0.45
1:D:239:GLU:HA	1:D:242:LYS:HZ3	1.81	0.45
1:F:242:LYS:O	1:F:243:THR:OG1	2.30	0.45
1:H:185:LEU:HD21	1:H:189:PHE:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASN:O	1:B:171:LYS:HB2	2.16	0.44
1:B:40:VAL:O	1:B:40:VAL:HG13	2.17	0.44
1:C:192:THR:CG2	1:C:192:THR:O	2.65	0.44
1:E:118:MSE:HE1	1:E:216:GLN:HB2	1.99	0.44
1:C:50:ASP:HB3	1:C:54:THR:CG2	2.47	0.44
1:C:74:THR:HG21	1:C:91:PRO:HG3	2.00	0.44
1:F:130:TYR:HA	3:F:322:HOH:O	2.17	0.44
1:F:74:THR:HG22	1:F:89:TYR:CD1	2.52	0.44
1:G:191:VAL:HG11	1:G:194:ARG:NH1	2.29	0.44
1:H:174:VAL:HG22	1:H:217:TRP:CD1	2.53	0.44
1:A:155:THR:HG23	1:D:81:GLU:OE1	2.18	0.44
1:B:31:GLN:HA	1:B:34:VAL:CG1	2.47	0.44
1:C:191:VAL:CG2	1:C:194:ARG:HH12	2.30	0.44
1:E:69:GLY:HA2	1:E:116:ARG:HB3	1.99	0.44
1:E:40:VAL:HG12	1:E:237:VAL:HG21	1.99	0.44
1:F:40:VAL:HG21	1:F:234:GLN:CA	2.47	0.44
1:C:68:THR:HG23	1:C:69:GLY:N	2.32	0.44
1:G:118:MSE:HE3	1:G:182:ILE:CD1	2.48	0.44
1:G:141:LEU:N	1:G:197:ASP:OD1	2.50	0.44
1:A:193:ALA:CB	1:A:202:ALA:HB3	2.46	0.44
1:B:125:LEU:HD12	1:B:125:LEU:N	2.33	0.44
1:C:228:GLU:O	1:C:231:GLN:HB2	2.18	0.44
1:E:124:ALA:C	1:E:125:LEU:HD12	2.38	0.44
1:A:74:THR:HG21	1:A:91:PRO:CA	2.48	0.44
1:C:159:GLU:HB2	1:C:162:SER:HG	1.79	0.44
1:D:40:VAL:O	1:D:40:VAL:HG12	2.17	0.44
1:F:122:ASN:OD1	1:F:127:GLY:HA3	2.17	0.44
1:H:113:ALA:HB1	1:H:117:GLY:C	2.38	0.44
1:A:170:ASN:O	1:A:171:LYS:HB2	2.17	0.44
1:E:170:ASN:O	1:E:171:LYS:HB2	2.17	0.44
1:F:154:HIS:NE2	1:F:176:SER:HB2	2.32	0.44
1:F:132:ASP:OD1	1:F:179:HIS:HD2	2.01	0.44
1:G:175:ASN:OD1	1:G:217:TRP:HB2	2.17	0.44
1:G:57:GLN:O	1:G:61:LEU:HG	2.18	0.44
1:A:133:ILE:O	1:A:136:VAL:HG22	2.18	0.43
1:B:129:LEU:HD12	1:B:182:ILE:HA	2.00	0.43
1:B:147:VAL:HG21	1:C:89:TYR:CZ	2.52	0.43
1:F:170:ASN:O	1:F:171:LYS:HB2	2.18	0.43
1:F:208:LEU:N	1:F:208:LEU:HD12	2.23	0.43
1:F:241:LYS:HE2	1:F:241:LYS:HB2	1.90	0.43
1:G:143:HIS:NE2	1:G:197:ASP:OD2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ASP:OD2	1:A:51:ASP:N	2.44	0.43
1:C:97:GLU:HB3	1:C:120:LEU:HD22	2.01	0.43
1:D:40:VAL:HG11	1:D:234:GLN:CA	2.31	0.43
1:F:122:ASN:ND2	1:F:185:LEU:HD12	2.33	0.43
1:H:30:GLN:HA	1:H:33:TYR:CD1	2.48	0.43
1:H:7:ILE:HB	1:H:37:ILE:HD13	2.00	0.43
1:A:174:VAL:HG13	1:A:217:TRP:HB3	2.00	0.43
1:D:128:THR:OG1	1:D:183:LYS:HB3	2.17	0.43
1:G:181:PHE:CD2	1:G:199:MSE:HE3	2.51	0.43
1:G:74:THR:HB	1:G:89:TYR:CD1	2.53	0.43
1:E:174:VAL:HG13	1:E:217:TRP:CB	2.47	0.43
1:F:113:ALA:HB1	1:F:117:GLY:C	2.39	0.43
1:F:130:TYR:CZ	1:F:183:LYS:HD3	2.53	0.43
1:H:7:ILE:HG21	1:H:37:ILE:HD11	2.00	0.43
1:H:93:ARG:O	1:H:97:GLU:HG3	2.19	0.43
1:G:147:VAL:HG12	1:G:148:ASP:N	2.32	0.43
1:G:211:TRP:CG	1:G:239:GLU:HG2	2.53	0.43
1:C:69:GLY:HA2	1:C:116:ARG:HG3	2.00	0.43
1:C:3:LEU:N	1:C:3:LEU:HD22	2.33	0.43
1:D:172:LYS:HD3	1:D:173:LEU:N	2.31	0.43
1:E:193:ALA:HB3	1:E:202:ALA:CB	2.47	0.43
1:E:76:GLN:NE2	1:E:81:GLU:HA	2.33	0.43
1:E:98:ILE:HD13	1:E:124:ALA:HB2	2.01	0.43
1:B:40:VAL:HG22	1:B:234:GLN:CD	2.38	0.43
1:G:217:TRP:CD1	1:G:219:PRO:HD3	2.54	0.43
1:H:151:LEU:N	1:H:151:LEU:HD12	2.33	0.43
1:H:43:PHE:CE2	1:H:45:ILE:HD11	2.54	0.43
1:A:93:ARG:HD3	1:A:97:GLU:CD	2.38	0.43
1:F:40:VAL:HG13	1:F:237:VAL:HG21	2.00	0.43
1:G:74:THR:CG2	1:G:94:ASP:OD1	2.67	0.43
1:G:97:GLU:HB3	1:G:120:LEU:HD22	2.01	0.43
1:A:30:GLN:HB3	3:A:379:HOH:O	2.19	0.43
1:B:31:GLN:O	1:B:34:VAL:HG13	2.18	0.43
1:A:98:ILE:HD13	1:A:124:ALA:HB2	2.00	0.42
1:E:143:HIS:O	1:E:176:SER:OG	2.37	0.42
1:G:40:VAL:O	1:G:40:VAL:HG12	2.18	0.42
1:C:184:LYS:HG2	3:C:467:HOH:O	2.18	0.42
1:F:147:VAL:HG21	1:H:89:TYR:CE1	2.54	0.42
1:G:77:LEU:CD1	1:G:94:ASP:HB3	2.49	0.42
1:C:86:ILE:CG2	1:C:131:GLN:OE1	2.67	0.42
1:E:142:GLN:NE2	1:E:145:GLN:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:THR:CG2	1:F:129:LEU:N	2.82	0.42
1:H:143:HIS:O	1:H:176:SER:OG	2.37	0.42
1:H:40:VAL:HG12	1:H:40:VAL:O	2.18	0.42
1:B:147:VAL:O	1:B:148:ASP:C	2.57	0.42
1:C:117:GLY:O	1:C:121:VAL:HG13	2.20	0.42
1:D:170:ASN:O	1:D:171:LYS:HB2	2.20	0.42
1:H:93:ARG:HG3	1:H:116:ARG:NH2	2.35	0.42
1:B:98:ILE:O	1:B:102:ARG:HG3	2.18	0.42
1:B:234:GLN:NE2	3:B:370:HOH:O	2.47	0.42
1:H:40:VAL:O	1:H:40:VAL:CG1	2.67	0.42
1:F:33:TYR:CE2	1:F:68:THR:HG22	2.54	0.42
1:G:4:LYS:HD2	1:G:41:GLY:O	2.17	0.42
1:F:74:THR:HG21	1:F:91:PRO:CA	2.49	0.42
1:B:215:VAL:HG13	1:B:217:TRP:CE3	2.55	0.42
1:B:40:VAL:CG1	1:B:237:VAL:HG21	2.49	0.42
1:C:199:MSE:HE2	1:C:199:MSE:HA	2.01	0.42
1:F:218:HIS:HB3	1:F:220:GLU:OE2	2.19	0.42
1:G:10:THR:HG22	1:G:68:THR:H	1.84	0.42
1:A:187:PRO:O	1:A:188:SER:CB	2.67	0.42
1:B:93:ARG:HH11	1:B:116:ARG:NH2	2.18	0.42
1:D:114:ILE:HG23	1:D:217:TRP:O	2.20	0.42
1:B:180:GLN:NE2	3:B:272:HOH:O	2.52	0.42
1:D:115:CYS:O	1:D:116:ARG:C	2.57	0.42
1:G:40:VAL:HG13	1:G:234:GLN:HA	2.02	0.42
1:G:40:VAL:HG12	1:G:237:VAL:CG2	2.46	0.42
1:D:193:ALA:HB3	1:D:202:ALA:HB3	2.01	0.41
1:G:136:VAL:CG2	1:G:199:MSE:HE1	2.50	0.41
1:A:59:ILE:N	1:A:59:ILE:HD12	2.34	0.41
1:E:173:LEU:HD23	1:E:173:LEU:HA	1.95	0.41
1:H:187:PRO:O	1:H:188:SER:CB	2.67	0.41
1:A:128:THR:HG21	3:A:271:HOH:O	2.19	0.41
1:B:145:GLN:HG2	1:B:176:SER:O	2.21	0.41
1:A:11:GLY:HA3	3:A:594:HOH:O	2.19	0.41
1:A:89:TYR:O	1:H:147:VAL:HG13	2.21	0.41
1:A:147:VAL:HG21	1:D:89:TYR:CZ	2.54	0.41
1:C:193:ALA:HB3	1:C:202:ALA:CB	2.50	0.41
1:C:8:GLY:N	1:C:62:VAL:CG2	2.78	0.41
1:E:228:GLU:HG3	3:E:484:HOH:O	2.21	0.41
1:G:122:ASN:ND2	1:G:185:LEU:HD23	2.36	0.41
1:F:76:GLN:NE2	1:F:76:GLN:N	2.66	0.41
1:H:170:ASN:O	1:H:171:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ALA:HA	1:C:197:ASP:OD1	2.19	0.41
1:C:224:GLN:HB3	3:C:266:HOH:O	2.19	0.41
1:F:75:PRO:HG2	1:F:76:GLN:NE2	2.36	0.41
1:G:125:LEU:HD12	1:G:189:PHE:HZ	1.86	0.41
1:G:238:ASP:O	1:G:241:LYS:HG2	2.20	0.41
1:A:89:TYR:CZ	1:H:147:VAL:HG21	2.56	0.41
1:B:93:ARG:NH1	1:B:116:ARG:NH2	2.69	0.41
1:F:101:VAL:HG23	1:F:102:ARG:N	2.35	0.41
1:E:46:ALA:HB3	1:F:46:ALA:HB3	2.03	0.41
1:C:147:VAL:CG2	1:G:89:TYR:CZ	3.04	0.41
1:B:10:THR:CG2	1:B:67:LEU:HA	2.50	0.41
1:D:97:GLU:O	1:D:101:VAL:HG23	2.21	0.41
1:E:189:PHE:CE1	1:E:208:LEU:HD11	2.56	0.41
1:F:9:ILE:HD12	1:F:34:VAL:HG12	2.01	0.41
1:A:136:VAL:HG23	1:A:138:THR:O	2.21	0.41
1:C:40:VAL:HG22	1:C:234:GLN:OE1	2.21	0.41
1:C:74:THR:HA	1:C:75:PRO:HD3	1.80	0.41
1:H:10:THR:HG22	1:H:68:THR:H	1.86	0.41
1:F:147:VAL:CG2	1:H:89:TYR:CZ	3.02	0.41
1:B:116:ARG:HG3	1:B:117:GLY:N	2.35	0.41
1:B:186:ALA:HA	1:B:187:PRO:HD3	1.93	0.41
1:B:54:THR:HG22	1:B:96:TYR:CE1	2.55	0.41
1:F:184:LYS:HE3	1:F:184:LYS:HB3	1.96	0.41
1:G:170:ASN:O	1:G:171:LYS:HB2	2.20	0.41
1:G:193:ALA:HB3	1:G:202:ALA:HB3	2.03	0.41
1:G:40:VAL:HG13	1:G:234:GLN:CD	2.41	0.41
1:H:73:ILE:N	1:H:73:ILE:HD12	2.35	0.41
1:B:68:THR:HG23	1:B:93:ARG:NH2	2.35	0.40
1:C:83:SER:O	1:C:86:ILE:HG13	2.19	0.40
1:D:125:LEU:N	1:D:125:LEU:HD12	2.36	0.40
1:H:10:THR:HG21	1:H:67:LEU:HA	2.03	0.40
1:H:72:ASP:HB3	1:H:180:GLN:OE1	2.21	0.40
1:B:131:GLN:O	1:B:180:GLN:HG2	2.21	0.40
1:C:98:ILE:O	1:C:101:VAL:HG22	2.22	0.40
1:G:131:GLN:HB2	1:G:135:GLN:OE1	2.20	0.40
1:G:97:GLU:OE1	1:G:116:ARG:NH1	2.54	0.40
1:A:71:GLN:HB3	1:A:88:ALA:O	2.21	0.40
1:B:71:GLN:HE21	1:B:71:GLN:HB3	1.69	0.40
1:C:166:LYS:HB3	1:C:166:LYS:NZ	2.36	0.40
1:D:6:VAL:HG12	1:D:62:VAL:HG12	2.03	0.40
1:A:147:VAL:CG2	1:D:89:TYR:CZ	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:GLN:HE21	1:E:176:SER:N	2.18	0.40
1:E:8:GLY:HA3	1:E:62:VAL:HG11	2.02	0.40
1:G:199:MSE:HA	3:G:268:HOH:O	2.21	0.40
1:A:10:THR:HG22	1:A:68:THR:N	2.22	0.40
1:F:129:LEU:HA	1:F:183:LYS:N	2.35	0.40
1:F:237:VAL:O	1:F:241:LYS:N	2.51	0.40
1:F:85:GLU:HG2	1:F:135:GLN:NE2	2.36	0.40
1:G:40:VAL:HG13	1:G:234:GLN:NE2	2.36	0.40
1:H:240:SER:C	1:H:242:LYS:H	2.23	0.40
1:A:218:HIS:HB3	1:A:220:GLU:OE2	2.20	0.40
1:F:172:LYS:HD2	1:F:173:LEU:H	1.85	0.40
1:F:90:PHE:CD1	1:F:92:PRO:HD2	2.57	0.40
1:H:204:GLU:HG3	3:H:263:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	220/254 (87%)	208 (94%)	9 (4%)	3 (1%)	13	13
1	B	218/254 (86%)	211 (97%)	6 (3%)	1 (0%)	32	39
1	C	217/254 (85%)	208 (96%)	9 (4%)	0	100	100
1	D	219/254 (86%)	207 (94%)	11 (5%)	1 (0%)	32	39
1	E	220/254 (87%)	210 (96%)	8 (4%)	2 (1%)	20	23
1	F	219/254 (86%)	208 (95%)	10 (5%)	1 (0%)	32	39
1	G	218/254 (86%)	206 (94%)	12 (6%)	0	100	100
1	H	220/254 (87%)	210 (96%)	10 (4%)	0	100	100
All	All	1751/2032 (86%)	1668 (95%)	75 (4%)	8 (0%)	32	39

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	SER
1	E	149	GLU
1	A	149	GLU
1	E	196	ALA
1	F	242	LYS
1	A	188	SER
1	A	196	ALA
1	D	242	LYS

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	190/212 (90%)	177 (93%)	13 (7%)	18	24
1	B	188/212 (89%)	172 (92%)	16 (8%)	12	15
1	C	187/212 (88%)	172 (92%)	15 (8%)	14	17
1	D	189/212 (89%)	178 (94%)	11 (6%)	23	31
1	E	190/212 (90%)	175 (92%)	15 (8%)	14	18
1	F	189/212 (89%)	174 (92%)	15 (8%)	14	18
1	G	188/212 (89%)	171 (91%)	17 (9%)	11	13
1	H	190/212 (90%)	178 (94%)	12 (6%)	21	28
All	All	1511/1696 (89%)	1397 (92%)	114 (8%)	16	19

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	10	THR
1	A	34	VAL
1	A	39	LYS
1	A	40	VAL
1	A	56	VAL

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Mol	Chain	Res	Type
1	A	61	LEU
1	A	93	ARG
1	A	154	HIS
1	A	155	THR
1	A	174	VAL
1	A	195	THR
1	A	220	GLU
1	B	3	LEU
1	B	34	VAL
1	B	40	VAL
1	B	47	LEU
1	B	54	THR
1	B	61	LEU
1	B	105	LEU
1	B	106	ASP
1	B	116	ARG
1	B	129	LEU
1	B	154	HIS
1	B	164	LEU
1	B	190	LYS
1	B	195	THR
1	B	213	LEU
1	B	223	PHE
1	C	3	LEU
1	C	39	LYS
1	C	74	THR
1	C	100	LEU
1	C	116	ARG
1	C	120	LEU
1	C	121	VAL
1	C	123	VAL
1	C	154	HIS
1	C	155	THR
1	C	164	LEU
1	C	171	LYS
1	C	195	THR
1	C	197	ASP
1	C	241	LYS
1	D	34	VAL
1	D	47	LEU
1	D	61	LEU
1	D	76	GLN

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Mol	Chain	Res	Type
1	D	93	ARG
1	D	120	LEU
1	D	154	HIS
1	D	155	THR
1	D	177	LEU
1	D	192	THR
1	D	195	THR
1	E	40	VAL
1	E	51	ASP
1	E	93	ARG
1	E	100	LEU
1	E	102	ARG
1	E	120	LEU
1	E	133	ILE
1	E	154	HIS
1	E	159	GLU
1	E	174	VAL
1	E	191	VAL
1	E	195	THR
1	E	197	ASP
1	E	220	GLU
1	E	244	MSE
1	F	10	THR
1	F	30	GLN
1	F	32	ARG
1	F	39	LYS
1	F	40	VAL
1	F	49	ILE
1	F	61	LEU
1	F	76	GLN
1	F	85	GLU
1	F	93	ARG
1	F	184	LYS
1	F	190	LYS
1	F	208	LEU
1	F	220	GLU
1	F	223	PHE
1	G	3	LEU
1	G	65	LEU
1	G	74	THR
1	G	79	LEU
1	G	85	GLU

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Mol	Chain	Res	Type
1	G	93	ARG
1	G	106	ASP
1	G	137	GLU
1	G	146	ARG
1	G	154	HIS
1	G	174	VAL
1	G	185	LEU
1	G	191	VAL
1	G	197	ASP
1	G	207	ASN
1	G	220	GLU
1	G	223	PHE
1	H	32	ARG
1	H	93	ARG
1	H	120	LEU
1	H	138	THR
1	H	144	LEU
1	H	154	HIS
1	H	174	VAL
1	H	185	LEU
1	H	195	THR
1	H	204	GLU
1	H	206	ASP
1	H	244	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	38	GLN
1	A	57	GLN
1	A	71	GLN
1	A	119	GLN
1	A	122	ASN
1	A	150	GLN
1	A	179	HIS
1	A	207	ASN
1	B	38	GLN
1	B	71	GLN
1	B	180	GLN
1	B	234	GLN
1	C	122	ASN

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Mol	Chain	Res	Type
1	C	135	GLN
1	C	216	GLN
1	C	224	GLN
1	D	38	GLN
1	D	57	GLN
1	D	71	GLN
1	D	76	GLN
1	D	122	ASN
1	D	150	GLN
1	D	179	HIS
1	D	207	ASN
1	E	31	GLN
1	E	38	GLN
1	E	57	GLN
1	E	71	GLN
1	E	76	GLN
1	E	84	GLN
1	E	119	GLN
1	E	122	ASN
1	E	142	GLN
1	E	145	GLN
1	E	207	ASN
1	E	234	GLN
1	F	30	GLN
1	F	38	GLN
1	F	76	GLN
1	F	84	GLN
1	F	122	ASN
1	F	167	HIS
1	F	168	HIS
1	F	179	HIS
1	F	207	ASN
1	G	31	GLN
1	G	38	GLN
1	G	57	GLN
1	G	71	GLN
1	G	84	GLN
1	G	122	ASN
1	G	142	GLN
1	G	150	GLN
1	G	207	ASN
1	H	31	GLN

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Mol	Chain	Res	Type
1	H	38	GLN
1	H	119	GLN
1	H	145	GLN
1	H	150	GLN
1	H	179	HIS
1	H	234	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	220/254 (86%)	-0.17	1 (0%) 90 93	11, 21, 36, 53	0
1	B	219/254 (86%)	-0.15	1 (0%) 90 93	11, 20, 36, 51	0
1	C	218/254 (85%)	-0.00	3 (1%) 75 80	15, 22, 36, 43	0
1	D	220/254 (86%)	-0.18	2 (0%) 84 87	11, 20, 36, 57	0
1	E	220/254 (86%)	-0.08	3 (1%) 75 80	15, 24, 38, 59	0
1	F	220/254 (86%)	0.07	1 (0%) 90 93	15, 26, 41, 56	0
1	G	219/254 (86%)	0.10	4 (1%) 69 74	14, 31, 44, 60	0
1	H	220/254 (86%)	0.04	1 (0%) 90 93	12, 30, 43, 60	0
All	All	1756/2032 (86%)	-0.05	16 (0%) 84 87	11, 24, 41, 60	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	3	LEU	4.6
1	D	243	THR	3.9
1	F	3	LEU	3.2
1	H	3	LEU	2.8
1	G	40	VAL	2.6
1	E	243	THR	2.5
1	B	207	ASN	2.4
1	C	209	PRO	2.4
1	A	207	ASN	2.4
1	E	3	LEU	2.2
1	G	241	LYS	2.2
1	D	207	ASN	2.2
1	C	241	LYS	2.1
1	E	207	ASN	2.1
1	C	207	ASN	2.0
1	G	32	ARG	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MN	D	300	1/1	1.00	0.12	-0.02	15,15,15,15	0
2	MN	F	300	1/1	1.00	0.12	-0.07	19,19,19,19	0
2	MN	C	300	1/1	1.00	0.11	-0.45	16,16,16,16	0
2	MN	A	300	1/1	1.00	0.10	-1.04	15,15,15,15	0
2	MN	G	300	1/1	1.00	0.10	-1.08	18,18,18,18	0
2	MN	B	300	1/1	1.00	0.09	-1.24	16,16,16,16	0
2	MN	E	300	1/1	0.99	0.07	-2.82	17,17,17,17	0
2	MN	H	300	1/1	0.99	0.07	-5.78	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.