



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 01:54 pm BST

PDB ID : 2Q9Q
Title : The crystal structure of full length human GINS complex
Authors : Chang, Y.P.; Wang, G.; Chen, X.S.
Deposited on : 2007-06-13
Resolution : 2.36 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

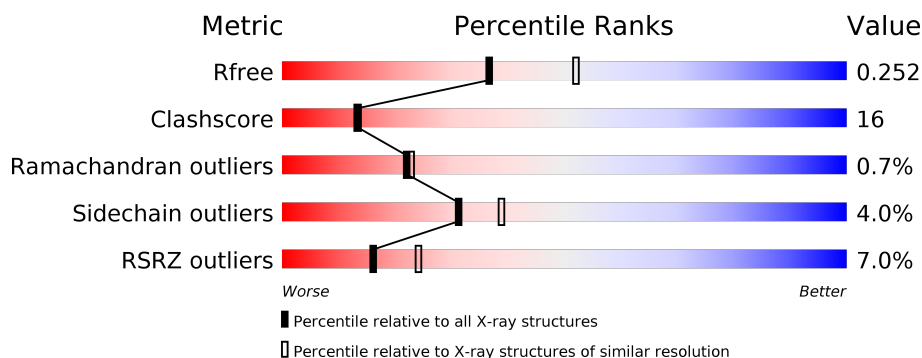
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 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	191	<div> <div>2%</div> <div> <div>60%</div> <div>28%</div> <div>8%</div> </div> </div>
1	E	191	<div> <div>3%</div> <div> <div>58%</div> <div>33%</div> <div>8%</div> </div> </div>
2	B	223	<div> <div>5%</div> <div> <div>57%</div> <div>29%</div> <div>12%</div> </div> </div>
2	F	223	<div> <div>5%</div> <div> <div>59%</div> <div>28%</div> <div>12%</div> </div> </div>
3	C	196	<div> <div>9%</div> <div> <div>52%</div> <div>20%</div> <div>26%</div> </div> </div>
3	G	196	<div> <div>5%</div> <div> <div>52%</div> <div>21%</div> <div>26%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	220	<div><div>8%</div><div><div></div><div>58%</div><div>25%</div><div>•</div><div>15%</div></div></div>
4	H	220	<div><div>10%</div><div><div></div><div>59%</div><div>22%</div><div>• •</div><div>15%</div></div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11883 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 DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	1	0	0
			1424	911	241	263	9			
1	E	175	Total	C	N	O	S	1	0	0
			1424	911	241	263	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	CLONING ARTIFACT	UNP Q9Y248
A	-4	PRO	-	CLONING ARTIFACT	UNP Q9Y248
A	-3	LEU	-	CLONING ARTIFACT	UNP Q9Y248
A	-2	GLY	-	CLONING ARTIFACT	UNP Q9Y248
A	-1	SER	-	CLONING ARTIFACT	UNP Q9Y248
A	0	ASN	-	CLONING ARTIFACT	UNP Q9Y248
E	-5	GLY	-	CLONING ARTIFACT	UNP Q9Y248
E	-4	PRO	-	CLONING ARTIFACT	UNP Q9Y248
E	-3	LEU	-	CLONING ARTIFACT	UNP Q9Y248
E	-2	GLY	-	CLONING ARTIFACT	UNP Q9Y248
E	-1	SER	-	CLONING ARTIFACT	UNP Q9Y248
E	0	ASN	-	CLONING ARTIFACT	UNP Q9Y248

- Molecule 2 is a protein called GINS complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	196	Total	C	N	O	S	0	0	0
			1614	1027	273	304	10			
2	F	196	Total	C	N	O	S	0	0	0
			1614	1027	273	304	10			

- Molecule 3 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	145	Total 1188	C 744	N 217	O 217	S 10	0	0	0
3	G	145	Total 1188	C 744	N 217	O 217	S 10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	97	ILE	VAL	VARIANT	UNP Q14691
G	97	ILE	VAL	VARIANT	UNP Q14691

- Molecule 4 is a protein called GINS complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	186	Total 1489	C 944	N 256	O 283	S 6	0	0	0
4	H	186	Total 1489	C 944	N 256	O 283	S 6	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	CLONING ARTIFACT	UNP Q9BRX5
D	-2	PRO	-	CLONING ARTIFACT	UNP Q9BRX5
D	-1	GLY	-	CLONING ARTIFACT	UNP Q9BRX5
D	0	GLY	-	CLONING ARTIFACT	UNP Q9BRX5
D	1	GLY	-	CLONING ARTIFACT	UNP Q9BRX5
H	-3	GLY	-	CLONING ARTIFACT	UNP Q9BRX5
H	-2	PRO	-	CLONING ARTIFACT	UNP Q9BRX5
H	-1	GLY	-	CLONING ARTIFACT	UNP Q9BRX5
H	0	GLY	-	CLONING ARTIFACT	UNP Q9BRX5
H	1	GLY	-	CLONING ARTIFACT	UNP Q9BRX5

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	68	Total 68	O 68	0	0
5	B	69	Total 69	O 69	0	0
5	C	47	Total 47	O 47	0	0

Continued on next page...

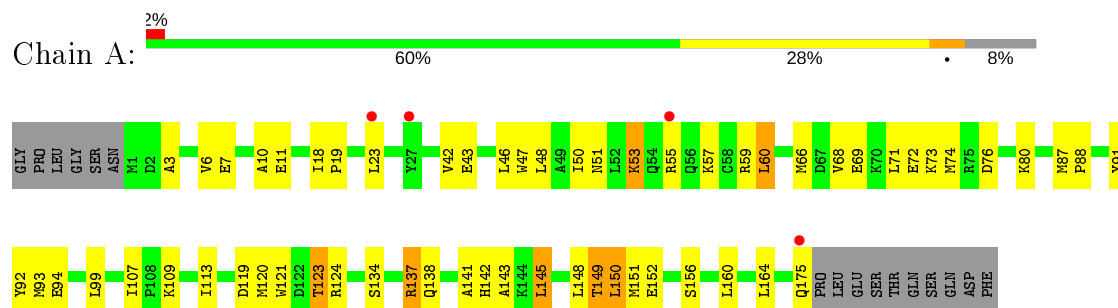
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	47	Total 47	O 47	0	0
5	E	53	Total 53	O 53	0	0
5	F	77	Total 77	O 77	0	0
5	G	45	Total 45	O 45	0	0
5	H	47	Total 47	O 47	0	0

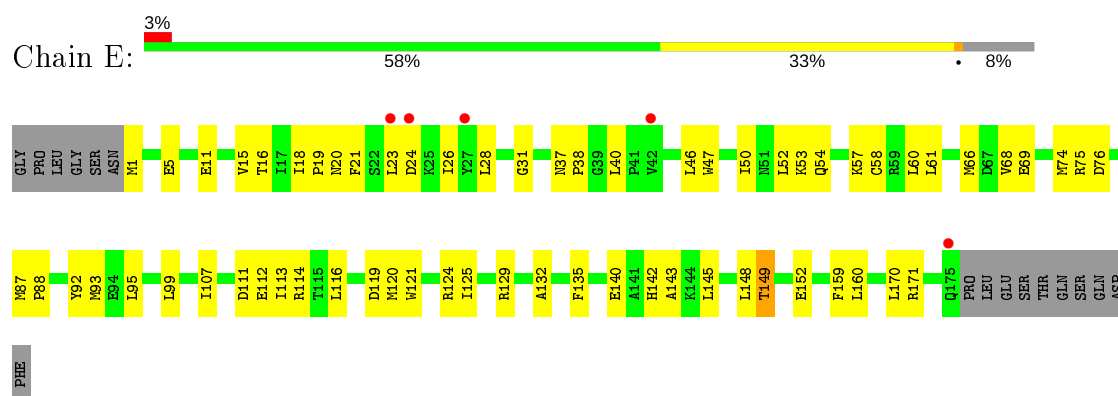
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

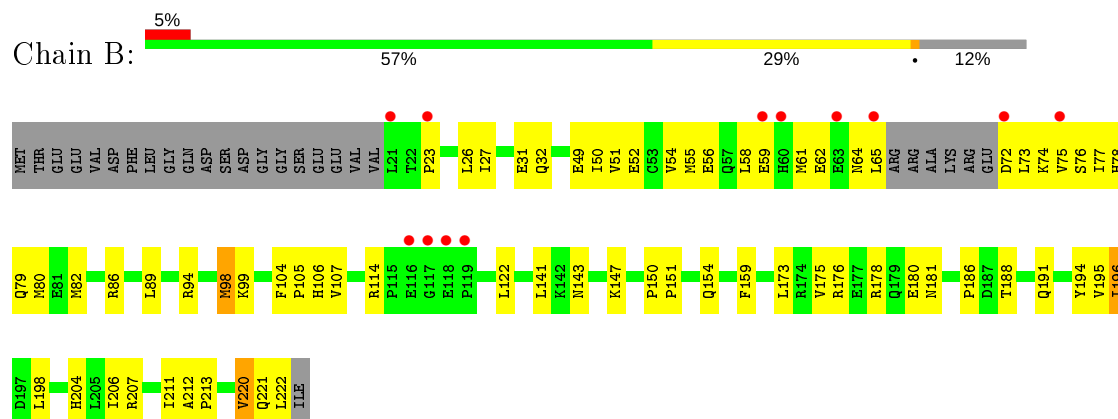
- Molecule 1: DNA replication complex GINS protein PSF2



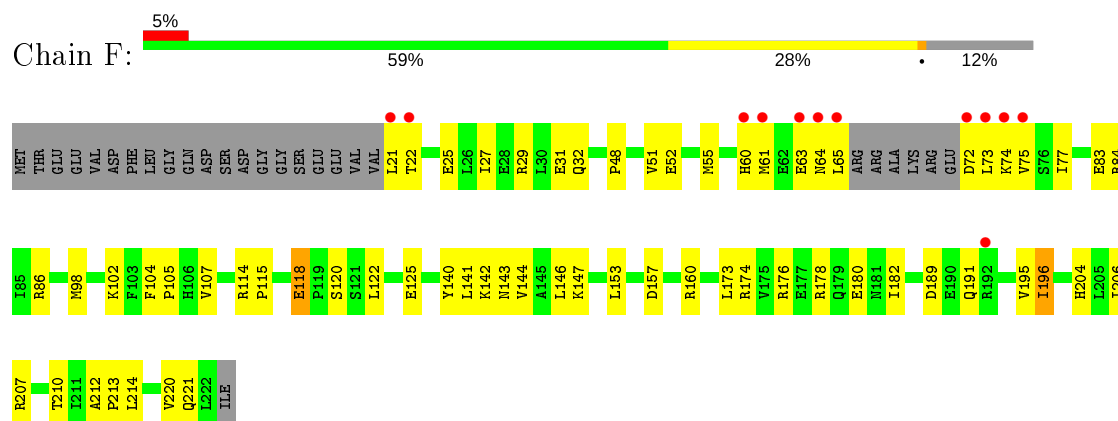
- Molecule 1: DNA replication complex GINS protein PSF2



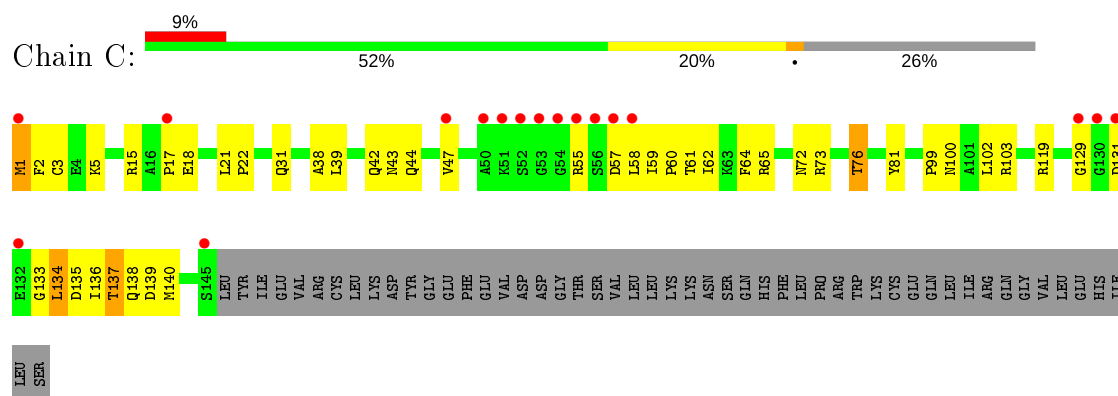
- Molecule 2: GINS complex subunit 4



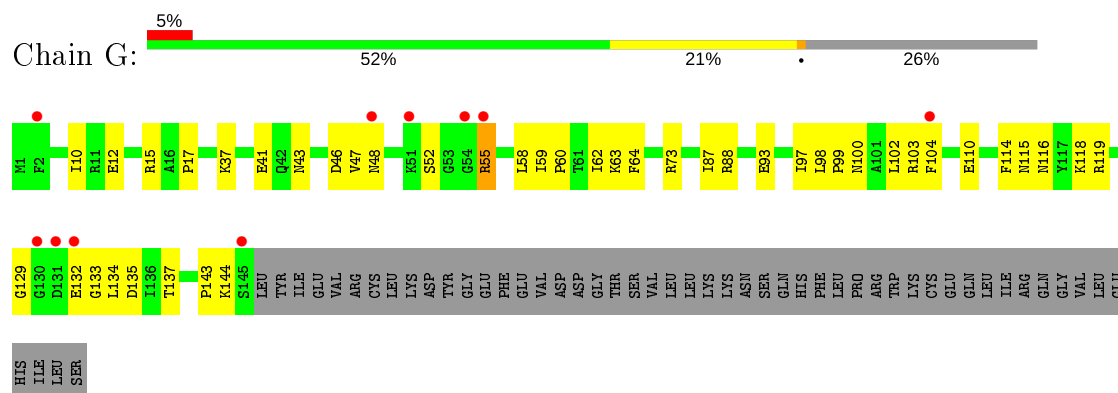
- Molecule 2: GINS complex subunit 4



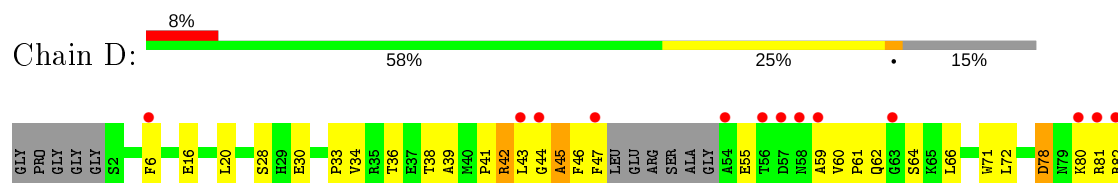
- Molecule 3: DNA replication complex GINS protein PSF1



- Molecule 3: DNA replication complex GINS protein PSF1

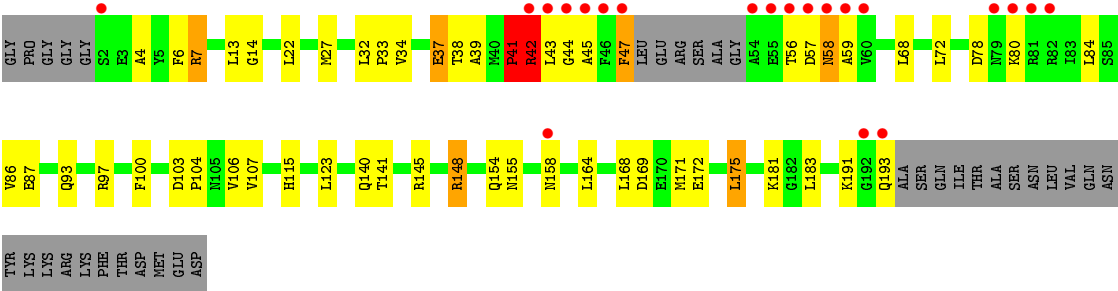


- Molecule 4: GINS complex subunit 3





● Molecule 4: GINS complex subunit 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.27Å 89.10Å 103.80Å 105.02° 103.58° 95.07°	Depositor
Resolution (Å)	29.58 – 2.36 43.60 – 2.36	Depositor EDS
% Data completeness (in resolution range)	90.6 (29.58-2.36) 96.0 (43.60-2.36)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.37Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.248 0.215 , 0.252	Depositor DCC
R_{free} test set	12899 reflections (8.38%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 66.3	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	0.93	EDS
Total number of atoms	11883	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/1454	0.53	0/1969
1	E	0.34	0/1454	0.54	0/1969
2	B	0.34	0/1645	0.56	0/2219
2	F	0.41	0/1645	0.59	0/2219
3	C	0.36	0/1211	0.53	0/1626
3	G	0.36	0/1211	0.55	0/1626
4	D	0.38	0/1523	0.60	2/2055 (0.1%)
4	H	0.37	0/1523	0.62	0/2055
All	All	0.37	0/11666	0.57	2/15738 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	6	PHE	CB-CG-CD2	-7.72	115.39	120.80
4	D	6	PHE	CB-CG-CD1	5.53	124.67	120.80

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	1424	0	1449	57	0
1	E	1424	0	1449	60	0
2	B	1614	0	1625	62	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1614	0	1625	49	0
3	C	1188	0	1180	49	0
3	G	1188	0	1180	34	0
4	D	1489	0	1436	51	0
4	H	1489	0	1436	55	0
5	A	68	0	0	1	0
5	B	69	0	0	4	0
5	C	47	0	0	4	0
5	D	47	0	0	3	0
5	E	53	0	0	4	0
5	F	77	0	0	1	0
5	G	45	0	0	3	0
5	H	47	0	0	1	0
All	All	11883	0	11380	369	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 16.

All (369) 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:A:51:ASN:HD21	1:A:55:ARG:HH21	1.13	0.90
1:A:119:ASP:O	1:A:123:THR:HG22	1.69	0.90
4:H:44:GLY:N	4:H:58:ASN:HB3	1.87	0.90
3:G:15:ARG:HD3	5:G:199:HOH:O	1.73	0.89
1:E:129:ARG:HH11	4:H:154:GLN:HE21	1.21	0.87
4:H:44:GLY:H	4:H:58:ASN:HB3	1.38	0.87
4:D:45:ALA:HB3	4:D:47:PHE:HD2	1.42	0.85
1:A:74:MET:SD	1:A:88:PRO:HG3	2.16	0.85
1:E:129:ARG:HH11	4:H:154:GLN:NE2	1.75	0.84
2:B:114:ARG:HB3	2:B:114:ARG:HH11	1.44	0.83
4:H:34:VAL:HG12	4:H:86:VAL:HG12	1.59	0.82
1:E:74:MET:SD	1:E:88:PRO:HG3	2.21	0.81
4:D:33:PRO:HB2	4:D:87:GLU:HB2	1.62	0.80
1:A:137:ARG:HH11	1:A:137:ARG:HB2	1.47	0.79
4:H:38:THR:HG22	4:H:39:ALA:H	1.48	0.78
1:A:156:SER:HB3	4:D:154:GLN:HE22	1.47	0.78
4:D:78:ASP:OD2	4:D:82:ARG:HG2	1.84	0.78
2:F:65:LEU:HD22	2:F:75:VAL:HG23	1.63	0.78
4:D:173:ARG:O	4:D:177:GLN:HG2	1.85	0.77
1:E:121:TRP:O	1:E:125:ILE:HG12	1.85	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:ASN:OD1	3:C:65:ARG:HD2	1.84	0.77
1:A:149:THR:HG22	1:A:152:GLU:HG3	1.65	0.76
2:F:72:ASP:O	2:F:75:VAL:HG12	1.86	0.76
4:H:42:ARG:H	4:H:42:ARG:HD2	1.50	0.76
4:H:56:THR:HG22	4:H:56:THR:O	1.85	0.75
3:C:131:ASP:HA	5:C:229:HOH:O	1.86	0.75
3:C:135:ASP:OD1	3:C:137:THR:HB	1.86	0.74
1:A:120:MET:O	1:A:124:ARG:HG3	1.88	0.74
3:G:64:PHE:CE1	4:H:72:LEU:HD21	2.23	0.74
3:G:99:PRO:HD2	3:G:102:LEU:HD12	1.70	0.74
4:D:30:GLU:OE2	4:D:115:HIS:HD2	1.72	0.73
4:D:34:VAL:HG12	4:D:86:VAL:HG12	1.69	0.73
4:H:103:ASP:O	4:H:106:VAL:HG22	1.88	0.72
1:E:142:HIS:HE1	2:F:204:HIS:ND1	1.89	0.71
1:E:132:ALA:HB1	1:E:160:LEU:HD21	1.73	0.70
3:G:58:LEU:O	3:G:62:ILE:HG13	1.91	0.70
1:E:66:MET:HG2	1:E:113:ILE:HD13	1.73	0.70
2:B:65:LEU:HD13	2:B:79:GLN:HE21	1.56	0.70
1:A:51:ASN:ND2	1:A:55:ARG:HH21	1.89	0.69
4:D:45:ALA:HB3	4:D:47:PHE:CD2	2.25	0.69
4:D:36:THR:HB	4:D:64:SER:H	1.58	0.69
4:D:36:THR:HG22	4:D:38:THR:H	1.58	0.69
3:C:72:ASN:O	3:C:76:THR:HG23	1.91	0.69
4:D:107:VAL:O	4:D:145:ARG:NH2	2.26	0.69
2:B:173:LEU:HD13	2:B:220:VAL:CG2	2.22	0.68
4:D:81:ARG:HD2	4:D:85:SER:HB3	1.75	0.68
1:A:149:THR:HG22	1:A:152:GLU:CG	2.23	0.68
2:B:178:ARG:HH12	2:B:180:GLU:CD	1.98	0.67
4:H:107:VAL:O	4:H:145:ARG:NH2	2.27	0.67
2:B:94:ARG:NH1	3:C:140:MET:HA	2.10	0.67
2:F:29:ARG:HG3	2:F:29:ARG:HH11	1.59	0.67
3:G:88:ARG:NH1	4:H:4:ALA:HB1	2.10	0.67
4:H:7:ARG:HH22	4:H:22:LEU:HB2	1.61	0.66
4:H:44:GLY:HA3	4:H:58:ASN:O	1.96	0.65
2:F:143:ASN:HA	2:F:147:LYS:HD2	1.79	0.65
2:F:104:PHE:CG	2:F:105:PRO:HD3	2.32	0.65
1:A:156:SER:HB3	4:D:154:GLN:NE2	2.12	0.65
2:B:194:TYR:CE1	2:B:196:ILE:HD13	2.32	0.64
4:H:32:LEU:HD23	4:H:68:LEU:O	1.97	0.64
3:G:55:ARG:H	3:G:55:ARG:HD2	1.61	0.64
2:F:22:THR:OG1	2:F:25:GLU:HG3	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:38:THR:HG22	4:H:39:ALA:N	2.13	0.64
3:G:100:ASN:HB3	3:G:104:PHE:CE1	2.33	0.63
3:G:37:LYS:O	3:G:41:GLU:HG2	1.97	0.63
3:C:1:MET:HG2	4:D:47:PHE:HA	1.79	0.63
1:E:149:THR:HG21	5:E:191:HOH:O	1.98	0.63
4:D:38:THR:N	4:D:62:GLN:HG3	2.15	0.62
1:A:142:HIS:HD2	5:B:265:HOH:O	1.83	0.62
3:C:61:THR:HG23	4:D:43:LEU:HG	1.81	0.62
3:C:61:THR:HA	4:D:43:LEU:HD11	1.81	0.62
4:H:100:PHE:O	4:H:104:PRO:HG3	2.00	0.61
1:A:71:LEU:HD22	1:A:120:MET:CE	2.30	0.61
3:C:137:THR:HG22	3:C:138:GLN:NE2	2.15	0.61
1:A:42:VAL:HG22	5:A:224:HOH:O	1.99	0.60
2:F:107:VAL:HG12	2:F:122:LEU:HD11	1.81	0.60
3:G:98:LEU:HB2	3:G:103:ARG:HD3	1.82	0.60
2:B:212:ALA:HB3	2:B:213:PRO:HD3	1.83	0.60
4:H:42:ARG:H	4:H:42:ARG:CD	2.14	0.60
2:F:84:ARG:HA	3:G:143:PRO:HG3	1.84	0.60
2:B:32:GLN:HG3	2:B:221:GLN:OE1	2.01	0.60
3:G:132:GLU:HB2	5:G:226:HOH:O	2.02	0.59
2:B:73:LEU:O	2:B:77:ILE:HG12	2.03	0.59
1:A:46:LEU:O	1:A:50:ILE:HG12	2.02	0.59
3:G:135:ASP:OD1	3:G:137:THR:HB	2.02	0.59
3:G:73:ARG:HD2	5:G:198:HOH:O	2.00	0.59
4:H:7:ARG:HH21	4:H:22:LEU:HD12	1.68	0.59
4:D:155:ASN:HD21	4:D:158:ASN:HA	1.67	0.59
4:D:38:THR:O	4:D:62:GLN:HA	2.02	0.59
2:F:182:ILE:HB	2:F:196:ILE:HG22	1.85	0.59
4:H:7:ARG:NH2	4:H:22:LEU:HB2	2.17	0.59
3:C:100:ASN:ND2	3:C:103:ARG:HH22	2.01	0.58
1:A:175:GLN:HG3	2:B:188:THR:HG21	1.85	0.58
3:C:44:GLN:HE21	3:C:44:GLN:HA	1.66	0.58
1:E:149:THR:HG23	5:E:207:HOH:O	2.03	0.58
4:H:44:GLY:CA	4:H:58:ASN:HB3	2.32	0.58
1:A:23:LEU:HD11	2:B:74:LYS:HE3	1.85	0.58
1:A:87:MET:HG2	1:A:92:TYR:CD2	2.38	0.58
4:H:155:ASN:OD1	4:H:158:ASN:HA	2.04	0.58
1:A:87:MET:HG3	1:A:88:PRO:HD2	1.86	0.58
4:D:80:LYS:HD2	4:D:82:ARG:HH12	1.69	0.58
3:C:61:THR:HG23	4:D:43:LEU:CG	2.34	0.57
4:H:56:THR:O	4:H:57:ASP:HB2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:HIS:O	2:B:82:MET:HG3	2.04	0.57
3:G:43:ASN:O	3:G:47:VAL:HG23	2.04	0.57
1:A:149:THR:CG2	1:A:152:GLU:HG3	2.33	0.57
3:G:100:ASN:HB3	3:G:104:PHE:CZ	2.39	0.57
4:H:45:ALA:C	4:H:47:PHE:H	2.08	0.57
3:C:59:ILE:HA	3:C:62:ILE:HD12	1.87	0.57
1:A:145:LEU:HD13	1:A:148:LEU:HD12	1.84	0.57
2:F:21:LEU:HD12	2:F:21:LEU:N	2.20	0.56
1:A:142:HIS:HE1	2:B:204:HIS:ND1	2.03	0.56
4:D:44:GLY:C	4:D:46:PHE:H	2.07	0.56
4:D:44:GLY:O	4:D:46:PHE:N	2.37	0.56
2:F:174:ARG:HD3	5:F:292:HOH:O	2.05	0.56
3:C:55:ARG:HG2	3:C:55:ARG:HH11	1.70	0.56
3:C:58:LEU:HD21	4:D:42:ARG:HH12	1.70	0.56
3:C:55:ARG:HB2	3:C:57:ASP:OD2	2.05	0.56
2:B:191:GLN:HB3	5:B:262:HOH:O	2.06	0.56
1:E:93:MET:HE1	1:E:121:TRP:HB2	1.88	0.56
3:C:44:GLN:NE2	3:C:44:GLN:HA	2.20	0.56
1:E:23:LEU:HD12	2:F:73:LEU:HD23	1.88	0.56
1:E:46:LEU:HD22	1:E:95:LEU:HD22	1.87	0.56
1:A:71:LEU:HD22	1:A:120:MET:HE1	1.88	0.55
2:B:23:PRO:HD2	5:B:254:HOH:O	2.05	0.55
1:E:68:VAL:HG23	1:E:69:GLU:N	2.20	0.55
4:D:155:ASN:ND2	4:D:158:ASN:HA	2.21	0.55
4:H:41:PRO:O	4:H:43:LEU:N	2.39	0.55
1:E:53:LYS:HG2	1:E:60:LEU:HD13	1.88	0.55
1:E:26:ILE:HG12	2:F:74:LYS:HZ2	1.72	0.54
1:E:92:TYR:CE1	1:E:93:MET:HE2	2.43	0.54
2:B:173:LEU:HD13	2:B:220:VAL:HG21	1.88	0.54
1:E:111:ASP:HA	1:E:114:ARG:HH12	1.72	0.54
2:F:32:GLN:HG3	2:F:221:GLN:OE1	2.07	0.54
3:G:10:ILE:HG23	4:H:22:LEU:HD22	1.89	0.54
4:H:42:ARG:HD2	4:H:42:ARG:N	2.19	0.54
2:B:76:SER:O	2:B:80:MET:HG3	2.07	0.54
1:E:21:PHE:CD2	1:E:57:LYS:HE3	2.42	0.54
2:F:195:VAL:O	2:F:196:ILE:HD12	2.08	0.54
4:D:191:LYS:HG2	4:D:191:LYS:O	2.06	0.54
4:D:92:TYR:HA	5:D:249:HOH:O	2.07	0.53
2:F:189:ASP:OD2	2:F:191:GLN:HB3	2.08	0.53
4:H:33:PRO:HB2	4:H:87:GLU:HB2	1.89	0.53
3:C:59:ILE:HB	3:C:60:PRO:HD3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:115:ASN:HA	3:G:118:LYS:HG2	1.90	0.53
3:C:55:ARG:C	3:C:57:ASP:H	2.12	0.53
3:C:73:ARG:HD2	5:C:197:HOH:O	2.07	0.53
4:D:192:GLY:O	4:D:193:GLN:HB2	2.08	0.53
1:A:120:MET:O	1:A:124:ARG:CG	2.57	0.53
1:E:99:LEU:HB3	1:E:107:ILE:HD11	1.89	0.53
2:B:94:ARG:HH12	3:C:140:MET:HA	1.72	0.53
1:A:156:SER:CB	4:D:154:GLN:HE22	2.20	0.53
1:E:15:VAL:HG11	1:E:46:LEU:HD13	1.89	0.53
2:B:32:GLN:NE2	5:B:245:HOH:O	2.41	0.53
2:B:143:ASN:O	2:B:147:LYS:HE2	2.09	0.53
1:E:26:ILE:HA	2:F:74:LYS:HZ2	1.74	0.53
3:C:81:TYR:CD1	4:D:20:LEU:HD13	2.44	0.53
1:E:142:HIS:CE1	2:F:204:HIS:ND1	2.74	0.53
3:G:48:ASN:O	3:G:52:SER:HB2	2.09	0.53
4:D:91:ILE:HD13	4:D:112:MET:HB3	1.90	0.52
2:F:142:LYS:HA	2:F:146:LEU:HB2	1.91	0.52
4:H:164:LEU:C	4:H:164:LEU:HD23	2.29	0.52
2:B:104:PHE:CD2	2:B:105:PRO:HD3	2.45	0.52
2:F:182:ILE:HD11	2:F:214:LEU:HD11	1.91	0.52
2:F:206:ILE:HG12	2:F:207:ARG:N	2.24	0.52
2:B:107:VAL:CG1	2:B:122:LEU:HD11	2.40	0.52
3:C:5:LYS:HE3	3:C:31:GLN:OE1	2.09	0.52
1:E:23:LEU:HD23	1:E:24:ASP:N	2.24	0.52
4:H:32:LEU:N	4:H:32:LEU:HD23	2.25	0.52
2:F:140:TYR:CE1	2:F:144:VAL:HG21	2.45	0.52
2:F:115:PRO:HG2	2:F:118:GLU:HB2	1.92	0.52
1:E:111:ASP:HA	1:E:114:ARG:NH1	2.24	0.52
4:D:80:LYS:HD2	4:D:82:ARG:NH1	2.24	0.51
2:B:194:TYR:HE1	2:B:196:ILE:HD13	1.72	0.51
2:B:104:PHE:CG	2:B:105:PRO:HD3	2.45	0.51
1:A:53:LYS:CG	1:A:60:LEU:HD23	2.41	0.51
2:B:106:HIS:HE1	2:B:159:PHE:O	1.93	0.51
2:B:98:MET:HG3	2:B:99:LYS:N	2.25	0.51
1:E:129:ARG:NH1	4:H:154:GLN:HE21	2.00	0.51
1:A:93:MET:CE	1:A:121:TRP:HB2	2.41	0.51
1:A:93:MET:HE1	1:A:121:TRP:HB2	1.91	0.51
1:E:112:GLU:O	1:E:116:LEU:HG	2.11	0.51
2:B:65:LEU:HD13	2:B:79:GLN:NE2	2.25	0.50
2:B:61:MET:HA	2:B:64:ASN:HD22	1.76	0.50
2:F:83:GLU:HA	2:F:86:ARG:NH1	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LYS:HE2	2:B:73:LEU:HD22	1.94	0.50
2:F:48:PRO:O	2:F:52:GLU:HG3	2.10	0.50
4:D:30:GLU:OE2	4:D:115:HIS:CD2	2.58	0.50
3:C:119:ARG:HD3	5:C:211:HOH:O	2.11	0.50
1:E:171:ARG:HH11	1:E:171:ARG:HG3	1.77	0.50
3:C:43:ASN:OD1	3:C:62:ILE:HA	2.11	0.49
1:A:134:SER:O	1:A:138:GLN:HG3	2.13	0.49
2:F:104:PHE:CD2	2:F:105:PRO:HD3	2.47	0.49
1:A:137:ARG:NH1	1:A:137:ARG:HB2	2.22	0.49
3:G:88:ARG:HH11	4:H:4:ALA:HB1	1.78	0.49
2:B:50:ILE:O	2:B:54:VAL:HG23	2.12	0.49
5:E:205:HOH:O	4:H:14:GLY:HA2	2.12	0.49
4:D:34:VAL:HG22	4:D:66:LEU:O	2.13	0.49
3:G:129:GLY:HA3	3:G:133:GLY:HA2	1.94	0.49
3:G:116:ASN:HA	3:G:119:ARG:NH1	2.28	0.49
1:A:18:ILE:HB	1:A:59:ARG:HB3	1.93	0.49
1:E:50:ILE:O	1:E:54:GLN:HG3	2.13	0.48
4:H:168:LEU:HB3	4:H:172:GLU:HB2	1.94	0.48
3:C:1:MET:SD	3:C:2:PHE:N	2.81	0.48
2:B:191:GLN:CD	4:H:181:LYS:HD2	2.34	0.48
3:C:44:GLN:CA	3:C:44:GLN:HE21	2.23	0.48
1:E:135:PHE:CE1	1:E:143:ALA:HB2	2.49	0.48
4:D:16:GLU:HB2	5:D:233:HOH:O	2.14	0.48
1:A:66:MET:HG2	1:A:113:ILE:HD13	1.96	0.48
2:B:55:MET:HE3	3:C:129:GLY:CA	2.44	0.48
1:A:99:LEU:HB3	1:A:107:ILE:HD11	1.95	0.48
2:F:60:HIS:O	2:F:63:GLU:HB3	2.13	0.48
1:E:170:LEU:HD21	4:H:13:LEU:HD22	1.95	0.48
2:F:107:VAL:CG1	2:F:122:LEU:HD11	2.44	0.48
3:G:15:ARG:O	3:G:17:PRO:HD3	2.13	0.48
3:C:1:MET:HG2	4:D:47:PHE:CA	2.43	0.47
3:G:97:ILE:N	3:G:97:ILE:HD12	2.29	0.47
1:A:175:GLN:HG3	2:B:188:THR:CB	2.44	0.47
4:D:41:PRO:C	4:D:43:LEU:H	2.18	0.47
1:E:93:MET:CE	1:E:121:TRP:HB2	2.45	0.47
2:F:27:ILE:O	2:F:31:GLU:HG3	2.14	0.47
4:D:142:PHE:HZ	4:D:175:LEU:HD11	1.79	0.47
4:D:38:THR:HA	4:D:62:GLN:HE21	1.79	0.47
4:H:44:GLY:H	4:H:58:ASN:CB	2.20	0.47
4:H:78:ASP:OD2	4:H:80:LYS:HB2	2.14	0.47
1:A:11:GLU:HA	1:A:46:LEU:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:THR:HB	1:E:152:GLU:OE1	2.15	0.47
1:A:71:LEU:HD22	1:A:120:MET:HE3	1.97	0.47
2:B:49:GLU:CD	2:B:49:GLU:H	2.18	0.47
2:B:54:VAL:O	2:B:58:LEU:HG	2.15	0.47
1:E:16:THR:HG22	1:E:61:LEU:HD22	1.97	0.47
2:B:72:ASP:O	2:B:75:VAL:HB	2.14	0.47
1:A:76:ASP:O	1:A:80:LYS:HG3	2.16	0.46
2:B:195:VAL:O	2:B:196:ILE:HD12	2.15	0.46
4:H:37:GLU:HA	4:H:37:GLU:OE1	2.16	0.46
4:D:41:PRO:HA	4:D:59:ALA:HB2	1.96	0.46
1:E:87:MET:HE2	1:E:92:TYR:CE1	2.50	0.46
2:F:176:ARG:HD2	2:F:221:GLN:HB2	1.98	0.46
1:A:11:GLU:HB3	1:A:47:TRP:HB3	1.97	0.46
4:H:148:ARG:HG2	4:H:148:ARG:HH11	1.81	0.46
2:B:114:ARG:CB	2:B:114:ARG:HH11	2.23	0.46
1:E:1:MET:HA	1:E:5:GLU:OE2	2.15	0.46
1:E:75:ARG:HD2	1:E:76:ASP:N	2.31	0.46
2:B:181:ASN:HA	2:B:195:VAL:CG1	2.45	0.46
2:B:55:MET:HE3	3:C:129:GLY:HA2	1.97	0.46
1:A:69:GLU:HG2	1:A:73:LYS:NZ	2.31	0.46
1:E:53:LYS:O	1:E:53:LYS:HD3	2.15	0.46
1:A:19:PRO:HG2	1:A:42:VAL:HG21	1.98	0.45
1:A:7:GLU:CD	4:D:189:TRP:HE1	2.20	0.45
3:C:99:PRO:HD2	3:C:102:LEU:HD12	1.98	0.45
1:E:37:ASN:CB	1:E:40:LEU:HD13	2.46	0.45
1:E:75:ARG:HG3	1:E:119:ASP:OD2	2.16	0.45
1:E:92:TYR:CE1	1:E:93:MET:CE	2.99	0.45
2:B:62:GLU:N	2:B:82:MET:HE1	2.31	0.45
1:E:120:MET:O	1:E:124:ARG:CG	2.65	0.45
2:B:107:VAL:HG12	2:B:122:LEU:HD11	1.99	0.45
3:C:134:LEU:HD23	3:C:134:LEU:HA	1.80	0.45
4:H:45:ALA:C	4:H:47:PHE:N	2.68	0.45
1:A:3:ALA:HB1	1:A:151:MET:HE3	1.98	0.45
2:B:27:ILE:O	2:B:31:GLU:HG3	2.16	0.45
1:E:87:MET:HE2	1:E:92:TYR:CZ	2.52	0.45
2:F:153:LEU:HA	3:G:73:ARG:HH21	1.82	0.45
3:G:114:PHE:O	3:G:118:LYS:HG2	2.17	0.45
3:G:59:ILE:HB	3:G:60:PRO:HD3	1.99	0.45
4:H:103:ASP:CG	4:H:106:VAL:HG13	2.37	0.45
4:H:141:THR:O	4:H:145:ARG:HG3	2.16	0.45
2:B:211:ILE:C	2:B:211:ILE:HD12	2.37	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:ILE:CD1	1:E:61:LEU:HD11	2.46	0.45
2:B:178:ARG:NH1	2:B:180:GLU:CD	2.69	0.45
3:C:44:GLN:C	3:C:47:VAL:HG12	2.36	0.45
1:E:57:LYS:O	1:E:58:CYS:HB3	2.16	0.45
2:F:178:ARG:NH1	2:F:180:GLU:OE2	2.50	0.45
2:F:29:ARG:HG3	2:F:29:ARG:NH1	2.30	0.45
3:C:15:ARG:O	3:C:17:PRO:HD3	2.17	0.44
3:G:88:ARG:HD3	3:G:88:ARG:C	2.38	0.44
1:A:160:LEU:O	1:A:164:LEU:HG	2.16	0.44
3:G:12:GLU:HA	3:G:15:ARG:HH21	1.82	0.44
1:E:149:THR:HG22	1:E:152:GLU:H	1.81	0.44
1:E:93:MET:HE3	1:E:121:TRP:HE3	1.82	0.44
2:F:142:LYS:O	2:F:147:LYS:HB3	2.17	0.44
1:A:53:LYS:HD3	1:A:53:LYS:O	2.16	0.44
1:E:20:ASN:HD21	1:E:57:LYS:HA	1.82	0.44
2:F:61:MET:HA	2:F:64:ASN:HD22	1.81	0.44
1:A:74:MET:SD	1:A:88:PRO:CG	2.99	0.44
3:C:55:ARG:HG2	3:C:55:ARG:NH1	2.32	0.44
4:H:57:ASP:O	4:H:58:ASN:CG	2.56	0.44
2:B:176:ARG:HD2	2:B:221:GLN:HB2	2.00	0.44
2:F:173:LEU:HD13	2:F:220:VAL:HG22	2.00	0.44
3:C:58:LEU:O	3:C:62:ILE:HG13	2.17	0.44
4:D:28:SER:O	4:D:71:TRP:HD1	2.01	0.44
3:G:55:ARG:HH11	3:G:55:ARG:HG3	1.83	0.44
1:E:135:PHE:CE1	1:E:140:GLU:HB2	2.52	0.43
4:D:134:ILE:O	4:D:138:LEU:HG	2.19	0.43
3:C:64:PHE:HE1	4:D:72:LEU:HD21	1.83	0.43
1:E:1:MET:N	5:E:187:HOH:O	2.51	0.43
1:A:6:VAL:HG13	1:A:150:LEU:HD13	2.01	0.43
4:H:41:PRO:C	4:H:43:LEU:H	2.22	0.43
2:B:175:VAL:HG21	2:B:198:LEU:HB3	2.00	0.43
3:G:144:LYS:HE3	4:H:193:GLN:OE1	2.19	0.43
4:H:84:LEU:HD12	4:H:84:LEU:O	2.19	0.43
1:A:68:VAL:O	1:A:72:GLU:HB2	2.18	0.43
2:B:150:PRO:O	2:B:154:GLN:HG3	2.19	0.43
2:B:206:ILE:HG12	2:B:207:ARG:N	2.34	0.43
3:C:38:ALA:O	3:C:42:GLN:HG3	2.18	0.43
2:B:51:VAL:HG13	2:B:89:LEU:HD11	2.01	0.43
2:F:29:ARG:HH11	2:F:29:ARG:CG	2.29	0.43
3:G:87:ILE:HD13	3:G:110:GLU:HB3	2.00	0.43
1:A:10:ALA:HB2	1:A:91:TYR:CD2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:212:ALA:HB3	2:F:213:PRO:HD3	1.99	0.43
4:D:38:THR:OG1	4:D:39:ALA:N	2.51	0.42
4:H:44:GLY:HA3	4:H:58:ASN:HB3	2.01	0.42
2:F:125:GLU:CD	2:F:125:GLU:H	2.23	0.42
3:C:44:GLN:O	3:C:47:VAL:HG12	2.20	0.42
3:G:116:ASN:HA	3:G:119:ARG:HH12	1.84	0.42
3:C:3:CYS:HA	5:C:206:HOH:O	2.19	0.42
3:C:57:ASP:OD2	3:C:58:LEU:HD13	2.19	0.42
1:E:68:VAL:CG2	1:E:69:GLU:N	2.83	0.42
2:F:114:ARG:HD2	2:F:120:SER:HA	2.00	0.42
2:B:173:LEU:C	2:B:173:LEU:HD12	2.39	0.42
4:D:44:GLY:C	4:D:46:PHE:N	2.73	0.42
4:D:83:ILE:HG22	4:D:84:LEU:HD22	2.01	0.42
2:F:51:VAL:O	2:F:55:MET:HG3	2.19	0.42
2:F:102:LYS:HE3	4:H:6:PHE:HB3	2.01	0.42
1:A:175:GLN:HG3	2:B:188:THR:CG2	2.50	0.42
1:E:11:GLU:HB3	1:E:47:TRP:HB3	2.02	0.42
2:F:157:ASP:OD2	2:F:160:ARG:HD3	2.19	0.42
2:F:98:MET:HG3	4:H:6:PHE:CZ	2.55	0.42
1:E:28:LEU:HB2	1:E:31:GLY:O	2.20	0.42
2:B:61:MET:HB3	2:B:82:MET:CE	2.50	0.42
2:B:195:VAL:HG12	2:B:196:ILE:N	2.35	0.42
4:H:115:HIS:HE1	5:H:227:HOH:O	2.02	0.42
1:E:159:PHE:CE1	4:H:175:LEU:HD22	2.55	0.42
3:C:21:LEU:HA	3:C:22:PRO:HD2	1.99	0.41
1:E:38:PRO:O	1:E:40:LEU:HD12	2.20	0.41
2:B:150:PRO:HA	2:B:151:PRO:HD3	1.91	0.41
2:B:23:PRO:O	2:B:26:LEU:HB3	2.21	0.41
3:C:55:ARG:HB2	3:C:57:ASP:CG	2.41	0.41
4:D:41:PRO:O	4:D:43:LEU:N	2.53	0.41
4:D:83:ILE:HB	5:D:231:HOH:O	2.19	0.41
1:E:120:MET:O	1:E:124:ARG:HG3	2.19	0.41
1:A:3:ALA:HB1	1:A:151:MET:CE	2.51	0.41
2:B:55:MET:CE	3:C:129:GLY:HA3	2.51	0.41
4:H:84:LEU:HD12	4:H:84:LEU:C	2.41	0.41
1:A:142:HIS:CG	1:A:143:ALA:N	2.89	0.41
4:D:60:VAL:HA	4:D:61:PRO:HD3	1.97	0.41
1:A:6:VAL:HG12	1:A:94:GLU:OE1	2.20	0.41
3:C:134:LEU:HD13	3:C:136:ILE:CG2	2.51	0.41
1:E:148:LEU:HA	1:E:148:LEU:HD23	1.88	0.41
2:F:206:ILE:HG12	2:F:207:ARG:H	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ALA:CB	2:B:186:PRO:HA	2.51	0.41
2:B:55:MET:CE	3:C:129:GLY:CA	2.99	0.41
3:C:2:PHE:CE1	3:C:39:LEU:HD21	2.56	0.41
2:B:52:GLU:O	2:B:56:GLU:HG3	2.21	0.41
2:F:61:MET:O	2:F:65:LEU:HG	2.21	0.41
3:G:115:ASN:HA	3:G:118:LYS:CG	2.50	0.41
4:H:93:GLN:O	4:H:97:ARG:HG3	2.21	0.41
2:B:86:ARG:HD2	3:C:139:ASP:OD2	2.22	0.40
3:C:129:GLY:O	3:C:133:GLY:N	2.54	0.40
4:D:84:LEU:N	4:D:84:LEU:HD23	2.36	0.40
1:A:109:LYS:O	1:A:113:ILE:HG13	2.21	0.40
1:A:137:ARG:HH11	1:A:137:ARG:CB	2.24	0.40
1:E:26:ILE:HA	2:F:74:LYS:NZ	2.37	0.40
1:A:145:LEU:CD1	1:A:148:LEU:HD12	2.48	0.40
2:B:75:VAL:O	2:B:79:GLN:HG3	2.21	0.40
1:E:149:THR:HG22	1:E:152:GLU:HG3	2.03	0.40
1:E:19:PRO:O	1:E:38:PRO:HA	2.22	0.40
2:F:73:LEU:O	2:F:77:ILE:HG13	2.22	0.40
1:A:55:ARG:HB3	1:A:57:LYS:HG3	2.04	0.40
1:E:16:THR:CG2	1:E:61:LEU:HD22	2.52	0.40
3:G:46:ASP:OD2	4:H:42:ARG:NH1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	173/191 (91%)	168 (97%)	5 (3%)	0	100	100
1	E	173/191 (91%)	168 (97%)	5 (3%)	0	100	100
2	B	192/223 (86%)	185 (96%)	7 (4%)	0	100	100
2	F	192/223 (86%)	188 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	143/196 (73%)	136 (95%)	6 (4%)	1 (1%)	22	23
3	G	143/196 (73%)	135 (94%)	8 (6%)	0	100	100
4	D	182/220 (83%)	169 (93%)	10 (6%)	3 (2%)	9	8
4	H	182/220 (83%)	169 (93%)	8 (4%)	5 (3%)	5	2
All	All	1380/1660 (83%)	1318 (96%)	53 (4%)	9 (1%)	22	23

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	41	PRO
4	H	42	ARG
4	H	59	ALA
4	D	45	ALA
4	H	58	ASN
4	H	191	LYS
3	C	18	GLU
4	D	42	ARG
4	D	55	GLU

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	159/173 (92%)	150 (94%)	9 (6%)	20	22
1	E	159/173 (92%)	156 (98%)	3 (2%)	57	68
2	B	182/205 (89%)	176 (97%)	6 (3%)	38	46
2	F	182/205 (89%)	178 (98%)	4 (2%)	52	63
3	C	126/174 (72%)	122 (97%)	4 (3%)	39	47
3	G	126/174 (72%)	122 (97%)	4 (3%)	39	47
4	D	160/186 (86%)	153 (96%)	7 (4%)	28	34
4	H	160/186 (86%)	147 (92%)	13 (8%)	11	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1254/1476 (85%)	1204 (96%)	50 (4%)	31	39

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	48	LEU
1	A	53	LYS
1	A	60	LEU
1	A	123	THR
1	A	137	ARG
1	A	145	LEU
1	A	149	THR
1	A	150	LEU
2	B	59	GLU
2	B	98	MET
2	B	141	LEU
2	B	196	ILE
2	B	220	VAL
2	B	222	LEU
3	C	1	MET
3	C	76	THR
3	C	134	LEU
3	C	137	THR
4	D	78	ASP
4	D	94	GLU
4	D	125	HIS
4	D	127	ASP
4	D	159	GLU
4	D	169	ASP
4	D	193	GLN
1	E	52	LEU
1	E	145	LEU
1	E	149	THR
2	F	118	GLU
2	F	141	LEU
2	F	196	ILE
2	F	210	THR
3	G	55	ARG
3	G	63	LYS
3	G	93	GLU
3	G	134	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	7	ARG
4	H	27	MET
4	H	37	GLU
4	H	41	PRO
4	H	42	ARG
4	H	47	PHE
4	H	123	LEU
4	H	140	GLN
4	H	148	ARG
4	H	169	ASP
4	H	171	MET
4	H	175	LEU
4	H	183	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	51	ASN
1	A	54	GLN
1	A	101	ASN
1	A	142	HIS
1	A	147	ASN
1	A	166	HIS
2	B	32	GLN
2	B	57	GLN
2	B	64	ASN
2	B	79	GLN
2	B	143	ASN
2	B	154	GLN
3	C	20	GLN
3	C	44	GLN
3	C	100	ASN
3	C	138	GLN
4	D	62	GLN
4	D	93	GLN
4	D	115	HIS
4	D	155	ASN
4	D	187	GLN
1	E	37	ASN
1	E	54	GLN
1	E	56	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	142	HIS
1	E	154	ASN
1	E	162	GLN
1	E	175	GLN
2	F	32	GLN
2	F	64	ASN
2	F	154	GLN
3	G	20	GLN
4	H	62	GLN
4	H	115	HIS
4	H	136	GLN
4	H	140	GLN
4	H	154	GLN
4	H	187	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	175/191 (91%)	0.12	4 (2%) 60 70	16, 31, 61, 81	1 (0%)
1	E	175/191 (91%)	0.25	5 (2%) 51 62	17, 33, 61, 83	1 (0%)
2	B	196/223 (87%)	0.40	12 (6%) 21 31	13, 30, 66, 97	0
2	F	196/223 (87%)	0.09	12 (6%) 21 31	14, 25, 62, 90	0
3	C	145/196 (73%)	0.59	17 (11%) 4 7	16, 33, 87, 114	0
3	G	145/196 (73%)	0.34	10 (6%) 16 24	14, 34, 80, 117	0
4	D	186/220 (84%)	0.50	17 (9%) 9 14	12, 32, 83, 109	0
4	H	186/220 (84%)	0.56	21 (11%) 5 8	14, 31, 78, 113	0
All	All	1404/1660 (84%)	0.35	98 (6%) 16 24	12, 31, 74, 117	2 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	47	PHE	11.7
4	D	47	PHE	10.1
4	H	56	THR	9.7
3	G	131	ASP	8.7
3	C	131	ASP	8.3
3	G	55	ARG	7.6
4	H	193	GLN	7.5
3	C	129	GLY	6.8
4	H	57	ASP	6.0
2	B	65	LEU	5.8
3	C	54	GLY	5.6
3	C	132	GLU	5.5
4	D	57	ASP	5.2
3	G	132	GLU	5.1
3	C	55	ARG	5.1
4	D	193	GLN	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	H	54	ALA	4.9
3	G	104	PHE	4.9
3	C	50	ALA	4.9
4	H	80	LYS	4.8
4	D	56	THR	4.6
4	D	58	ASN	4.4
3	C	56	SER	4.4
3	C	51	LYS	4.2
4	D	54	ALA	4.2
4	D	44	GLY	4.1
4	H	55	GLU	4.1
2	F	63	GLU	3.8
2	B	116	GLU	3.8
2	B	21	LEU	3.7
2	F	65	LEU	3.6
2	F	75	VAL	3.6
4	H	59	ALA	3.5
2	B	75	VAL	3.5
3	C	53	GLY	3.4
1	A	27	TYR	3.4
3	C	1	MET	3.4
4	H	192	GLY	3.3
4	H	45	ALA	3.3
4	D	80	LYS	3.3
1	E	24	ASP	3.2
3	C	47	VAL	3.2
2	F	73	LEU	3.1
1	E	175	GLN	3.1
2	B	23	PRO	3.1
2	B	63	GLU	3.1
3	G	54	GLY	3.1
4	D	63	GLY	3.0
4	H	60	VAL	3.0
1	E	27	TYR	3.0
1	E	42	VAL	3.0
4	H	43	LEU	2.9
4	D	160	ASP	2.9
4	H	58	ASN	2.9
3	G	2	PHE	2.9
4	H	81	ARG	2.9
3	C	130	GLY	2.9
2	F	22	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	H	158	ASN	2.8
2	F	72	ASP	2.8
3	G	51	LYS	2.8
2	B	118	GLU	2.7
2	B	72	ASP	2.7
4	D	59	ALA	2.7
1	A	175	GLN	2.7
4	D	81	ARG	2.7
4	H	44	GLY	2.6
2	F	64	ASN	2.6
3	C	52	SER	2.5
3	C	58	LEU	2.5
2	B	119	PRO	2.5
2	F	74	LYS	2.5
3	C	145	SER	2.4
2	B	60	HIS	2.4
1	A	23	LEU	2.4
1	A	55	ARG	2.4
4	D	43	LEU	2.3
4	H	46	PHE	2.3
4	D	82	ARG	2.3
3	G	130	GLY	2.3
3	C	57	ASP	2.3
3	G	145	SER	2.3
4	D	6	PHE	2.2
4	H	2	SER	2.2
4	H	82	ARG	2.2
3	G	48	ASN	2.1
4	D	191	LYS	2.1
2	F	21	LEU	2.1
2	F	192	ARG	2.1
2	F	61	MET	2.1
3	C	17	PRO	2.1
4	H	42	ARG	2.1
4	D	192	GLY	2.1
1	E	23	LEU	2.1
4	H	79	ASN	2.1
2	B	117	GLY	2.1
2	F	60	HIS	2.0
2	B	59	GLU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.