



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:04 AM UTC

PDB ID : 7YLD / pdb_00007yld
Title : Two monobodies recognizing the conserved epitopes of SARS-CoV-2 N antigen applicable to the broad COVID-19 diagnosis
Authors : Hu, M.; Du, Y.; Sun, R.; Hao, Q.
Deposited on : 2022-07-26
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

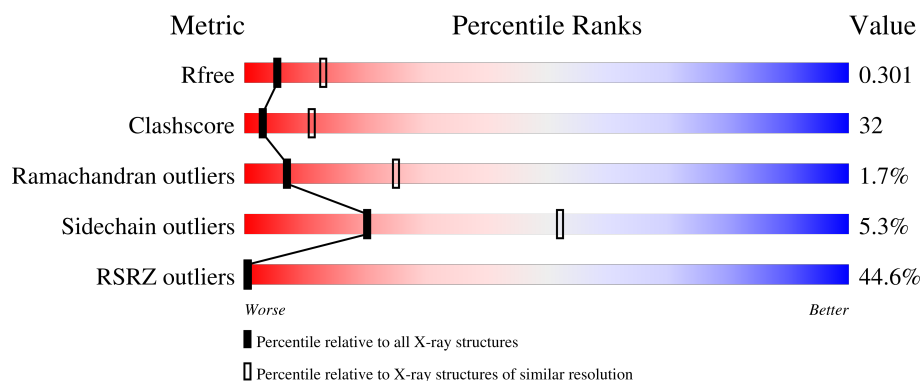
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	132	23% 52% 33% 15%
1	B	132	29% 43% 39% 17%
1	C	132	17% 49% 30% 18%
1	D	132	41% 33% 45% 22%
2	E	94	61% 49% 35% 11%

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Mol	Chain	Length	Quality of chain
2	F	94	55% 45% 39% 12%
2	G	94	45% 33% 38% 24%
2	I	94	45% 49% 37% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5989 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 Nucleoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	0	0	0
			872	559	151	162			
1	B	110	Total	C	N	O	0	0	0
			856	549	149	158			
1	C	108	Total	C	N	O	0	0	0
			845	544	146	155			
1	D	103	Total	C	N	O	0	0	0
			807	521	139	147			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	GLY	-	expression tag	UNP P0DTC9
A	44	SER	-	expression tag	UNP P0DTC9
A	45	GLY	-	expression tag	UNP P0DTC9
A	46	THR	-	expression tag	UNP P0DTC9
B	43	GLY	-	expression tag	UNP P0DTC9
B	44	SER	-	expression tag	UNP P0DTC9
B	45	GLY	-	expression tag	UNP P0DTC9
B	46	THR	-	expression tag	UNP P0DTC9
C	43	GLY	-	expression tag	UNP P0DTC9
C	44	SER	-	expression tag	UNP P0DTC9
C	45	GLY	-	expression tag	UNP P0DTC9
C	46	THR	-	expression tag	UNP P0DTC9
D	43	GLY	-	expression tag	UNP P0DTC9
D	44	SER	-	expression tag	UNP P0DTC9
D	45	GLY	-	expression tag	UNP P0DTC9
D	46	THR	-	expression tag	UNP P0DTC9

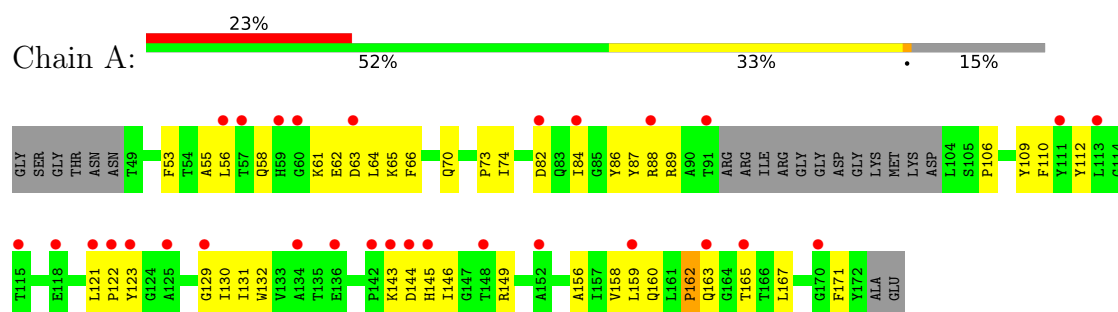
- Molecule 2 is a protein called NN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	84	Total	C	N	O	S	0	0	0
			674	439	110	124	1			
2	I	84	Total	C	N	O	S	0	0	0
			677	442	110	124	1			
2	F	83	Total	C	N	O	S	0	0	0
			669	435	109	124	1			
2	G	71	Total	C	N	O	S	0	0	0
			589	385	95	108	1			

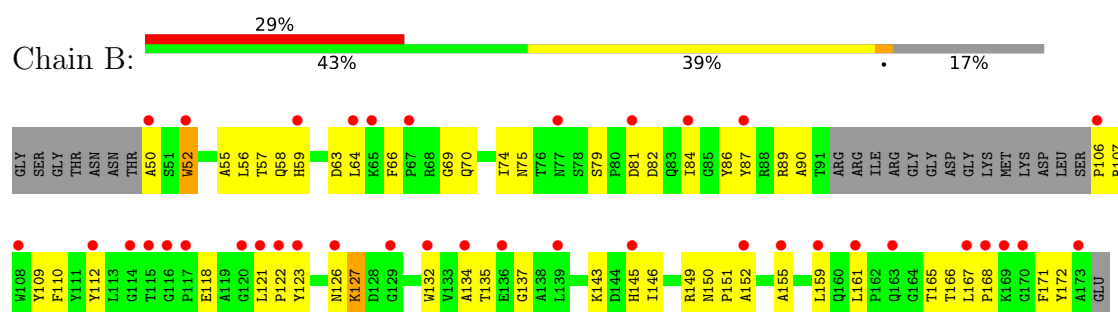
3 Residue-property plots [i](#)

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.

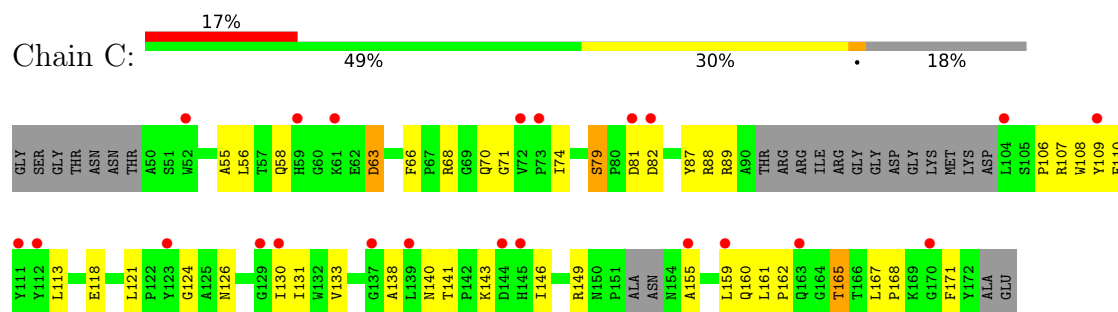
• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein

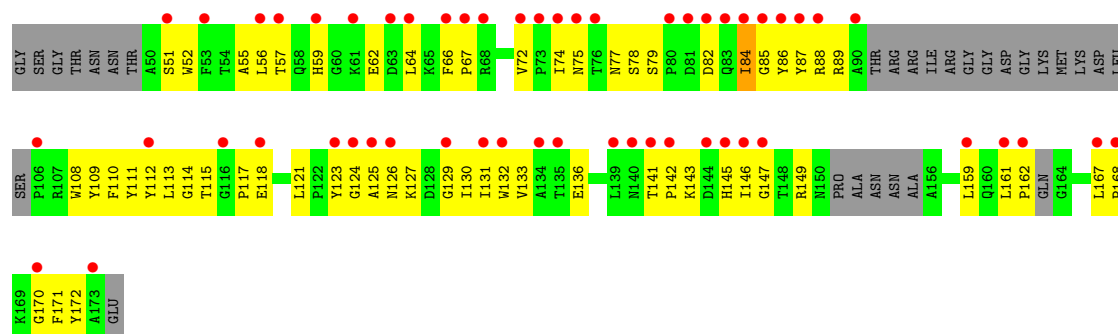


• Molecule 1: Nucleoprotein

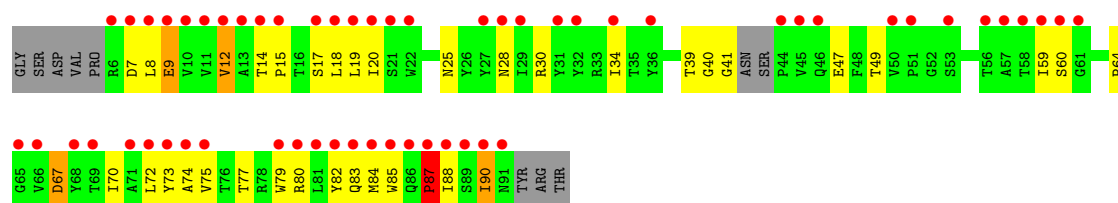


• Molecule 1: Nucleoprotein

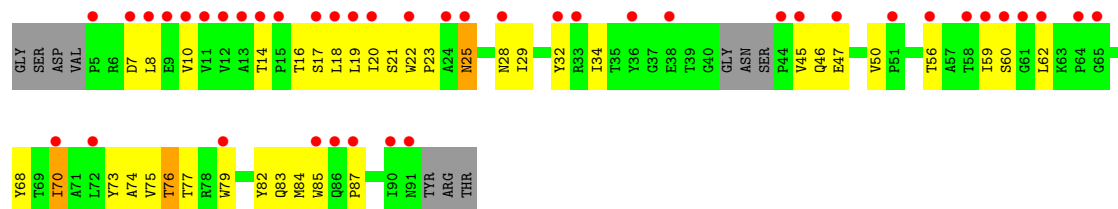
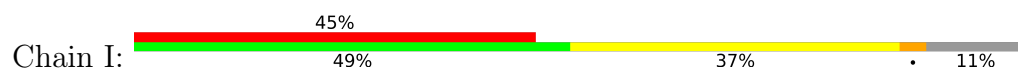




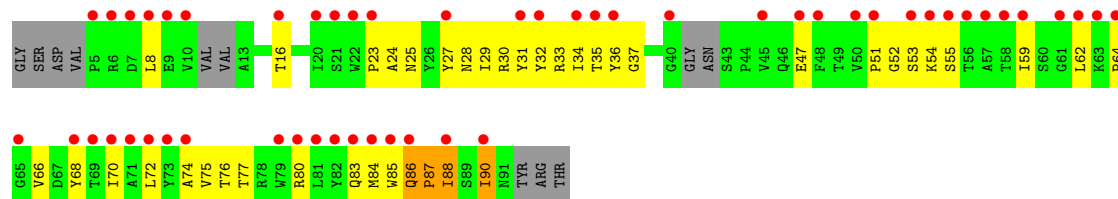
• Molecule 2: NN2



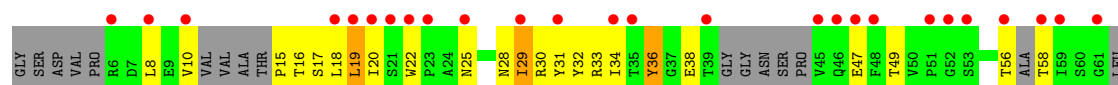
• Molecule 2: NN2



• Molecule 2: NN2



• Molecule 2: NN2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.55Å 74.30Å 87.45Å 108.51° 104.22° 96.67°	Depositor
Resolution (Å)	49.34 – 2.80 49.34 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (49.34-2.80) 90.5 (49.34-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.286 , 0.343 0.294 , 0.301	Depositor DCC
R_{free} test set	1999 reflections (5.71%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	1.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5989	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% 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	0.61	0/899	0.80	0/1228
1	B	0.50	0/883	0.70	0/1205
1	C	0.47	0/871	0.66	0/1187
1	D	0.38	0/831	0.62	0/1129
2	E	0.59	0/693	0.86	2/949 (0.2%)
2	F	0.45	0/688	0.70	0/941
2	G	0.65	0/604	0.96	0/821
2	I	0.57	0/697	0.77	0/955
All	All	0.53	0/6166	0.76	2/8415 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	87	PRO	CB-CA-C	-7.35	99.43	111.56
2	E	87	PRO	N-CA-C	5.33	123.44	112.47

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	872	0	839	49	0
1	B	856	0	822	50	0
1	C	845	0	813	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	807	0	776	67	0
2	E	674	0	669	34	0
2	F	669	0	659	62	0
2	G	589	0	573	53	0
2	I	677	0	674	36	0
All	All	5989	0	5825	375	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 32.

All (375) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:68:TYR:HE1	2:G:70:ILE:CD1	1.39	1.30
2:G:68:TYR:CE1	2:G:70:ILE:CD1	2.27	1.18
2:F:88:ILE:HD12	2:F:90:ILE:CD1	1.75	1.17
2:G:68:TYR:CE1	2:G:70:ILE:HD11	1.81	1.16
1:D:57:THR:HG22	1:D:172:TYR:O	1.53	1.08
2:F:88:ILE:HD12	2:F:90:ILE:HD12	1.16	1.07
2:F:8:LEU:CD1	2:F:72:LEU:HD21	1.85	1.06
2:I:8:LEU:HD13	2:I:85:TRP:HB2	1.36	1.05
1:B:149:ARG:NH1	1:B:151:PRO:HA	1.68	1.05
1:A:143:LYS:HD2	1:A:146:ILE:HD12	1.41	0.99
2:G:68:TYR:HE1	2:G:70:ILE:HD12	1.26	0.96
1:B:118:GLU:HB3	1:B:121:LEU:HD13	1.47	0.93
2:F:8:LEU:HD21	2:F:87:PRO:HD3	1.48	0.93
1:B:149:ARG:HH11	1:B:151:PRO:HA	1.33	0.92
1:D:57:THR:HG21	1:D:59:HIS:HE1	1.35	0.91
2:F:88:ILE:CD1	2:F:90:ILE:CD1	2.48	0.89
2:F:88:ILE:CD1	2:F:90:ILE:HD12	2.03	0.88
2:F:8:LEU:HD12	2:F:72:LEU:HD21	1.54	0.88
1:B:149:ARG:NH1	1:B:151:PRO:CA	2.38	0.87
2:I:29:ILE:HD12	2:I:74:ALA:HB1	1.56	0.87
2:G:25:ASN:HD21	2:G:28:ASN:HB2	1.40	0.86
1:D:88:ARG:CZ	1:D:117:PRO:HG2	2.05	0.86
1:C:56:LEU:HD11	1:C:159:LEU:HD22	1.57	0.86
1:A:82:ASP:HA	1:A:143:LYS:HE3	1.58	0.85
2:G:19:LEU:HD12	2:G:56:THR:CG2	2.06	0.85
1:D:57:THR:CG2	1:D:59:HIS:CE1	2.60	0.85
1:A:82:ASP:CA	1:A:143:LYS:HE3	2.06	0.84
1:B:82:ASP:HA	1:B:143:LYS:HE3	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:19:LEU:CD1	2:G:56:THR:CG2	2.58	0.82
2:F:8:LEU:HD13	2:F:72:LEU:HD21	1.58	0.82
2:G:19:LEU:HD12	2:G:56:THR:HG23	1.61	0.82
1:D:57:THR:HG21	1:D:59:HIS:CE1	2.16	0.80
1:A:89:ARG:HD2	1:D:172:TYR:CE2	2.18	0.79
2:F:8:LEU:CD1	2:F:72:LEU:CD2	2.61	0.79
2:G:68:TYR:CD1	2:G:70:ILE:HG13	2.18	0.78
2:E:70:ILE:O	2:E:87:PRO:HD2	1.84	0.78
1:A:82:ASP:CB	1:A:143:LYS:HE3	2.14	0.77
2:E:18:LEU:HD11	2:E:59:ILE:HD12	1.67	0.77
1:D:52:TRP:HA	1:D:149:ARG:HE	1.48	0.77
1:A:112:TYR:HB3	1:A:143:LYS:HG3	1.67	0.76
2:F:24:ALA:HB2	2:F:55:SER:HB3	1.66	0.75
1:D:89:ARG:HG3	1:D:108:TRP:CH2	2.22	0.75
2:I:8:LEU:CD1	2:I:85:TRP:HB2	2.16	0.75
1:B:84:ILE:HG13	1:B:134:ALA:HB2	1.69	0.75
2:F:33:ARG:NH1	2:F:47:GLU:OE2	2.20	0.74
1:D:84:ILE:HG22	1:D:143:LYS:HZ2	1.52	0.74
2:I:8:LEU:HD13	2:I:85:TRP:CB	2.18	0.74
2:F:8:LEU:HD22	2:F:85:TRP:HB3	1.70	0.73
2:I:25:ASN:HD21	2:I:28:ASN:HB3	1.53	0.73
1:C:70:GLN:HB3	1:C:165:THR:HG22	1.71	0.73
1:D:88:ARG:NE	1:D:117:PRO:HG2	2.04	0.73
2:I:17:SER:HB2	2:I:60:SER:HA	1.71	0.72
1:B:87:TYR:CE1	1:B:110:PHE:HB2	2.25	0.72
1:B:149:ARG:HH12	1:B:151:PRO:CB	2.04	0.71
1:B:161:LEU:HD22	1:B:165:THR:HG21	1.74	0.70
1:A:63:ASP:OD2	1:D:59:HIS:CD2	2.44	0.70
1:D:75:ASN:ND2	1:D:77:ASN:OD1	2.23	0.70
1:D:57:THR:O	1:D:57:THR:HG23	1.92	0.70
2:I:18:LEU:HD11	2:I:20:ILE:HG23	1.73	0.70
1:A:58:GLN:NE2	1:A:62:GLU:O	2.24	0.70
1:B:149:ARG:HH12	1:B:151:PRO:HB3	1.57	0.70
1:A:58:GLN:HE22	1:A:63:ASP:HA	1.54	0.69
1:A:167:LEU:HD22	1:A:171:PHE:HB3	1.73	0.69
1:A:82:ASP:OD1	1:A:145:HIS:NE2	2.23	0.69
1:B:52:TRP:CE3	1:B:149:ARG:HB3	2.28	0.69
1:D:82:ASP:HB3	1:D:146:ILE:HD11	1.74	0.69
1:A:66:PHE:HE2	1:A:87:TYR:HE2	1.37	0.69
2:I:17:SER:HB2	2:I:59:ILE:O	1.94	0.68
2:F:30:ARG:NH1	2:F:77:THR:HA	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:THR:HG23	1:B:107:ARG:HG2	1.75	0.68
2:G:68:TYR:HD1	2:G:70:ILE:HG13	1.58	0.68
1:B:149:ARG:HH12	1:B:151:PRO:HA	1.60	0.67
2:G:19:LEU:CD1	2:G:56:THR:HG22	2.25	0.67
1:B:149:ARG:HH12	1:B:151:PRO:CA	2.08	0.67
1:A:87:TYR:CE1	1:A:110:PHE:HB2	2.30	0.67
1:D:89:ARG:HG3	1:D:108:TRP:CZ3	2.30	0.66
2:F:8:LEU:HD22	2:F:85:TRP:CB	2.25	0.66
2:I:25:ASN:HD21	2:I:28:ASN:CB	2.07	0.66
1:D:123:TYR:HE2	2:F:23:PRO:HG3	1.59	0.66
1:D:74:ILE:HG12	1:D:162:PRO:HD3	1.77	0.66
1:D:57:THR:HG23	1:D:59:HIS:ND1	2.10	0.66
2:G:68:TYR:CE1	2:G:70:ILE:CG1	2.78	0.66
2:F:53:SER:O	2:F:54:LYS:HD3	1.96	0.65
2:E:73:TYR:HA	2:E:83:GLN:HA	1.78	0.65
2:I:70:ILE:O	2:I:87:PRO:HD2	1.96	0.65
2:F:33:ARG:HD2	2:F:47:GLU:OE2	1.96	0.65
2:F:83:GLN:NE2	2:F:86:GLN:NE2	2.44	0.65
1:D:52:TRP:CE3	1:D:149:ARG:HD3	2.32	0.64
2:F:83:GLN:HE21	2:F:86:GLN:CD	2.05	0.64
1:A:88:ARG:HA	1:A:129:GLY:O	1.98	0.64
1:D:57:THR:CG2	1:D:59:HIS:HE1	2.01	0.64
2:E:12:VAL:HG22	2:E:19:LEU:HB2	1.80	0.64
2:E:73:TYR:CE1	2:E:83:GLN:HB3	2.33	0.64
1:D:62:GLU:N	1:D:62:GLU:OE2	2.31	0.63
2:E:25:ASN:HD21	2:E:28:ASN:HB3	1.63	0.63
1:D:126:ASN:HB2	2:F:83:GLN:HB3	1.79	0.63
1:A:82:ASP:HA	1:A:143:LYS:CE	2.29	0.63
2:F:8:LEU:HD21	2:F:87:PRO:CD	2.25	0.62
1:A:89:ARG:O	1:A:89:ARG:HG2	1.99	0.62
1:C:58:GLN:HE21	1:C:106:PRO:CG	2.13	0.62
2:F:30:ARG:HG3	2:F:30:ARG:HH11	1.65	0.62
1:A:82:ASP:HB3	1:A:143:LYS:HE3	1.80	0.61
1:D:57:THR:HG23	1:D:59:HIS:CE1	2.33	0.61
2:F:83:GLN:NE2	2:F:86:GLN:CD	2.59	0.61
2:E:67:ASP:HB2	2:E:90:ILE:HG13	1.83	0.61
1:A:66:PHE:HE2	1:A:87:TYR:CE2	2.17	0.61
2:I:8:LEU:HG	2:I:8:LEU:O	1.99	0.61
2:G:10:VAL:HG12	2:G:20:ILE:HG22	1.81	0.61
1:D:124:GLY:HA2	2:F:85:TRP:CZ2	2.36	0.61
2:G:19:LEU:HD11	2:G:56:THR:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:TYR:CD2	1:D:146:ILE:HG21	2.36	0.60
2:F:66:VAL:O	2:F:68:TYR:CE2	2.54	0.60
1:D:88:ARG:NH2	1:D:117:PRO:HG2	2.15	0.60
1:A:58:GLN:HB3	1:A:106:PRO:HG2	1.81	0.60
2:E:70:ILE:HB	2:E:87:PRO:HG2	1.83	0.60
1:A:66:PHE:CE2	1:A:87:TYR:HE2	2.19	0.60
2:E:74:ALA:N	2:E:82:TYR:O	2.21	0.60
1:D:52:TRP:CZ3	1:D:149:ARG:HB3	2.36	0.60
2:F:8:LEU:HD12	2:F:72:LEU:CD2	2.29	0.60
2:E:75:VAL:HA	2:E:80:ARG:O	2.02	0.59
1:B:149:ARG:NH1	1:B:151:PRO:CB	2.65	0.59
2:G:56:THR:HG22	2:G:56:THR:O	2.03	0.59
1:B:58:GLN:HG3	1:B:171:PHE:HE1	1.68	0.59
1:C:58:GLN:HE21	1:C:106:PRO:HG2	1.67	0.58
1:C:113:LEU:HD11	1:C:140:ASN:OD1	2.04	0.58
2:G:68:TYR:CE1	2:G:70:ILE:HG13	2.37	0.58
2:I:70:ILE:HB	2:I:87:PRO:HG2	1.83	0.58
2:F:36:TYR:HB3	2:F:70:ILE:HG23	1.83	0.58
2:G:36:TYR:N	2:G:36:TYR:CD2	2.72	0.58
1:D:52:TRP:CA	1:D:149:ARG:HE	2.16	0.58
2:G:22:TRP:CH2	2:G:56:THR:C	2.82	0.57
2:G:36:TYR:HA	2:G:69:THR:O	2.04	0.57
1:B:150:ASN:ND2	1:B:152:ALA:HB3	2.20	0.57
2:G:68:TYR:CE1	2:G:70:ILE:HD12	2.16	0.57
1:C:71:GLY:HA3	1:C:133:VAL:HG21	1.86	0.56
1:D:126:ASN:ND2	2:F:85:TRP:H	2.03	0.56
2:F:36:TYR:HB2	2:F:70:ILE:HG12	1.86	0.56
1:B:123:TYR:HE1	1:B:132:TRP:HB3	1.70	0.56
1:D:127:LYS:HB3	1:D:130:ILE:HG12	1.85	0.56
2:G:75:VAL:HA	2:G:80:ARG:O	2.05	0.56
2:F:25:ASN:HD21	2:F:28:ASN:HB2	1.70	0.56
2:I:16:THR:O	2:I:62:LEU:HB2	2.05	0.56
2:I:18:LEU:HD12	2:I:19:LEU:N	2.20	0.56
1:C:58:GLN:NE2	1:C:108:TRP:HE1	2.03	0.55
1:C:124:GLY:HA3	2:G:85:TRP:CZ2	2.41	0.55
1:C:113:LEU:HD22	1:C:141:THR:O	2.07	0.55
2:E:30:ARG:HE	2:E:77:THR:HA	1.72	0.55
1:D:79:SER:O	1:D:82:ASP:N	2.39	0.55
1:D:129:GLY:C	1:D:130:ILE:HD13	2.32	0.55
1:D:52:TRP:HA	1:D:149:ARG:NE	2.21	0.54
1:D:168:PRO:HG2	1:D:171:PHE:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:70:ILE:O	2:G:87:PRO:HB3	2.07	0.54
1:B:55:ALA:HB2	1:B:109:TYR:CE2	2.43	0.54
1:C:162:PRO:O	1:C:165:THR:OG1	2.24	0.54
1:A:163:GLN:NE2	1:B:155:ALA:HB2	2.22	0.54
1:C:118:GLU:HB3	1:C:121:LEU:HD13	1.88	0.54
2:G:34:ILE:O	2:G:47:GLU:HA	2.07	0.54
1:B:52:TRP:CZ3	1:B:149:ARG:HB3	2.42	0.53
2:E:18:LEU:HD13	2:E:20:ILE:HG13	1.89	0.53
1:A:58:GLN:NE2	1:A:63:ASP:HA	2.22	0.53
1:A:87:TYR:HE1	1:A:110:PHE:HB2	1.71	0.53
1:B:123:TYR:CE1	1:B:132:TRP:HB3	2.43	0.53
1:C:74:ILE:HG12	1:C:160:GLN:O	2.08	0.53
2:I:17:SER:CB	2:I:60:SER:HA	2.38	0.53
2:G:25:ASN:ND2	2:G:29:ILE:HD13	2.24	0.53
2:E:70:ILE:O	2:E:87:PRO:CD	2.56	0.53
1:B:52:TRP:HE3	1:B:149:ARG:HB3	1.71	0.53
1:B:112:TYR:CD2	1:B:146:ILE:HG21	2.43	0.53
1:A:144:ASP:OD1	1:A:145:HIS:N	2.42	0.53
1:C:167:LEU:HD12	1:C:171:PHE:CB	2.39	0.53
1:D:161:LEU:HD12	1:D:167:LEU:HD21	1.90	0.53
1:D:84:ILE:CG2	1:D:143:LYS:HZ2	2.21	0.52
2:G:31:TYR:HE1	2:G:33:ARG:HD3	1.73	0.52
2:G:84:MET:HB3	2:G:85:TRP:CE3	2.43	0.52
2:F:66:VAL:O	2:F:68:TYR:CD2	2.63	0.52
2:G:72:LEU:HD22	2:G:84:MET:HG3	1.91	0.52
1:A:55:ALA:HB2	1:A:109:TYR:CE1	2.45	0.52
1:B:172:TYR:CE2	1:C:89:ARG:HD2	2.44	0.52
2:G:8:LEU:HD13	2:G:85:TRP:CE3	2.44	0.52
1:A:63:ASP:OD2	1:D:59:HIS:HD2	1.93	0.52
2:G:22:TRP:CZ3	2:G:56:THR:C	2.88	0.52
1:C:167:LEU:HD12	1:C:171:PHE:HB3	1.92	0.51
2:G:31:TYR:CE1	2:G:33:ARG:HD3	2.45	0.51
1:A:89:ARG:HD2	1:D:172:TYR:CZ	2.44	0.51
2:G:74:ALA:HB3	2:G:84:MET:HE3	1.92	0.51
1:B:87:TYR:CD1	1:B:110:PHE:HB2	2.45	0.51
1:D:51:SER:O	1:D:149:ARG:HG2	2.11	0.51
2:F:33:ARG:HH11	2:F:33:ARG:HB3	1.75	0.51
1:B:84:ILE:HG22	1:B:143:LYS:HE2	1.92	0.51
1:D:113:LEU:HD12	1:D:114:GLY:H	1.75	0.51
1:A:123:TYR:CE1	1:A:132:TRP:HB3	2.46	0.51
1:C:143:LYS:HB3	1:C:146:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:34:ILE:O	2:E:47:GLU:HB2	2.11	0.51
2:I:25:ASN:ND2	2:I:28:ASN:HB3	2.24	0.51
1:C:126:ASN:ND2	2:G:85:TRP:O	2.43	0.51
2:I:21:SER:HA	2:I:56:THR:HA	1.93	0.50
2:F:33:ARG:O	2:F:72:LEU:HA	2.11	0.50
2:F:36:TYR:HA	2:F:70:ILE:HA	1.93	0.50
2:I:29:ILE:CD1	2:I:74:ALA:HB1	2.36	0.50
1:A:84:ILE:HG22	1:A:143:LYS:HZ1	1.77	0.50
1:B:167:LEU:HD23	1:B:168:PRO:HD2	1.92	0.50
1:B:50:ALA:HB1	1:B:149:ARG:O	2.10	0.50
2:I:83:GLN:C	2:I:84:MET:HG2	2.37	0.50
2:G:29:ILE:HG21	2:G:32:TYR:CE1	2.46	0.50
1:D:57:THR:CG2	1:D:57:THR:O	2.59	0.50
1:D:115:THR:HG21	1:D:147:GLY:HA2	1.94	0.50
1:C:71:GLY:CA	1:C:133:VAL:HG21	2.41	0.50
2:E:30:ARG:NE	2:E:77:THR:HA	2.27	0.50
1:D:87:TYR:CE1	1:D:110:PHE:HD2	2.30	0.49
1:C:161:LEU:HD22	1:C:165:THR:HG21	1.94	0.49
2:G:36:TYR:N	2:G:36:TYR:HD2	2.10	0.49
1:A:87:TYR:HB2	1:A:131:ILE:HG13	1.94	0.49
1:A:82:ASP:O	1:A:143:LYS:HE2	2.13	0.49
1:B:150:ASN:HD21	1:B:152:ALA:HB3	1.77	0.49
1:B:58:GLN:HB3	1:B:106:PRO:HB2	1.94	0.49
1:D:51:SER:HA	1:D:111:TYR:CE1	2.48	0.49
2:E:18:LEU:HD12	2:E:18:LEU:O	2.12	0.48
2:F:29:ILE:HD12	2:F:75:VAL:O	2.12	0.48
1:C:55:ALA:HB1	1:C:107:ARG:HB3	1.96	0.48
2:F:34:ILE:N	2:F:34:ILE:HD12	2.29	0.48
1:B:59:HIS:NE2	1:C:63:ASP:OD1	2.46	0.48
1:B:82:ASP:OD1	1:B:145:HIS:NE2	2.44	0.48
1:D:78:SER:HB2	1:D:82:ASP:HB2	1.96	0.48
2:I:18:LEU:CD1	2:I:20:ILE:HG23	2.43	0.48
2:F:75:VAL:HA	2:F:80:ARG:O	2.13	0.48
2:F:88:ILE:HD12	2:F:90:ILE:HD11	1.83	0.48
2:E:79:TRP:HA	2:E:79:TRP:CE3	2.49	0.47
1:D:142:PRO:HD3	2:F:27:TYR:CE2	2.49	0.47
2:E:8:LEU:HB2	2:E:85:TRP:CE3	2.49	0.47
1:C:88:ARG:HG3	1:C:130:ILE:HD11	1.96	0.47
1:D:82:ASP:CG	1:D:145:HIS:HE2	2.23	0.47
1:D:108:TRP:HZ3	1:D:129:GLY:O	1.96	0.47
2:G:73:TYR:HD2	2:G:81:LEU:HD21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:PRO:HD3	2:F:27:TYR:CZ	2.49	0.47
2:I:62:LEU:HB3	2:I:68:TYR:CE2	2.50	0.47
2:G:19:LEU:HD11	2:G:58:THR:N	2.29	0.47
2:G:72:LEU:HB3	2:G:84:MET:HB2	1.95	0.47
1:D:55:ALA:HB2	1:D:109:TYR:CE1	2.50	0.47
2:I:21:SER:HB2	2:I:56:THR:HG22	1.96	0.47
1:D:126:ASN:HD21	2:F:85:TRP:H	1.62	0.47
2:E:15:PRO:O	2:E:64:PRO:HG3	2.15	0.47
2:F:30:ARG:HH11	2:F:30:ARG:CG	2.28	0.46
2:G:8:LEU:HD13	2:G:85:TRP:HE3	1.79	0.46
2:G:73:TYR:CD2	2:G:81:LEU:HD21	2.51	0.46
1:C:168:PRO:HD2	1:C:171:PHE:CD2	2.50	0.46
1:D:84:ILE:HG22	1:D:143:LYS:NZ	2.25	0.46
1:D:167:LEU:HB3	1:D:168:PRO:HD2	1.97	0.46
2:G:22:TRP:CH2	2:G:56:THR:N	2.83	0.46
2:E:14:THR:HG23	2:E:15:PRO:HD2	1.96	0.46
2:E:17:SER:HB3	2:E:60:SER:HA	1.98	0.46
2:G:8:LEU:HD22	2:G:85:TRP:HB2	1.96	0.46
1:C:58:GLN:CG	1:C:106:PRO:HG2	2.46	0.46
2:E:67:ASP:CB	2:E:90:ILE:HG13	2.45	0.46
1:B:63:ASP:OD2	1:B:89:ARG:NH2	2.49	0.46
1:D:126:ASN:HD21	2:F:85:TRP:N	2.14	0.46
2:G:30:ARG:HE	2:G:77:THR:HA	1.81	0.46
2:G:66:VAL:HG23	2:G:66:VAL:O	2.16	0.46
1:C:58:GLN:HG2	1:C:106:PRO:HG2	1.97	0.46
1:B:112:TYR:HB3	1:B:143:LYS:HG3	1.98	0.46
2:I:8:LEU:HA	2:I:21:SER:O	2.16	0.46
1:C:79:SER:OG	1:C:82:ASP:OD2	2.33	0.46
2:E:18:LEU:HD12	2:E:18:LEU:C	2.41	0.46
2:I:34:ILE:HD12	2:I:34:ILE:N	2.31	0.45
2:F:31:TYR:HA	2:F:52:GLY:N	2.31	0.45
1:D:74:ILE:CG1	1:D:162:PRO:HD3	2.45	0.45
1:B:56:LEU:CD1	1:B:159:LEU:HD13	2.46	0.45
1:B:86:TYR:HB3	1:B:132:TRP:CZ3	2.51	0.45
2:G:25:ASN:OD1	2:G:25:ASN:C	2.60	0.45
1:C:89:ARG:HB2	1:C:108:TRP:CE2	2.51	0.45
1:A:82:ASP:CA	1:A:143:LYS:CE	2.87	0.45
1:C:66:PHE:HE2	1:C:87:TYR:CE2	2.34	0.45
1:C:87:TYR:CE1	1:C:110:PHE:HB2	2.51	0.45
2:F:29:ILE:CD1	2:F:75:VAL:H	2.29	0.45
2:G:31:TYR:HD1	2:G:32:TYR:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:HD23	1:B:132:TRP:HZ2	1.82	0.45
2:I:7:ASP:O	2:I:22:TRP:HA	2.17	0.45
1:A:64:LEU:HD12	1:A:65:LYS:N	2.32	0.45
1:B:126:ASN:O	1:B:127:LYS:HG2	2.17	0.45
1:C:113:LEU:C	1:C:113:LEU:HD23	2.42	0.45
1:B:112:TYR:CE2	1:B:146:ILE:HG21	2.52	0.45
1:C:56:LEU:HD13	1:C:159:LEU:HD13	1.98	0.45
1:D:118:GLU:HB3	1:D:121:LEU:HD22	1.98	0.45
1:D:129:GLY:O	1:D:130:ILE:HD13	2.17	0.45
1:B:90:ALA:HB2	1:B:109:TYR:HD1	1.81	0.45
1:D:51:SER:OG	1:D:52:TRP:N	2.50	0.45
2:F:16:THR:HG22	2:F:64:PRO:HG3	1.99	0.45
1:A:70:GLN:OE1	1:A:165:THR:HA	2.16	0.44
1:C:55:ALA:HB2	1:C:109:TYR:CE2	2.52	0.44
1:D:131:ILE:HG12	1:D:132:TRP:N	2.32	0.44
2:I:34:ILE:O	2:I:47:GLU:HA	2.18	0.44
1:A:61:LYS:HD2	1:A:61:LYS:N	2.32	0.44
1:A:74:ILE:HD12	1:A:162:PRO:HD3	1.98	0.44
1:C:159:LEU:C	1:C:159:LEU:HD23	2.43	0.44
1:D:87:TYR:CE1	1:D:110:PHE:HB2	2.51	0.44
2:I:75:VAL:HG13	2:I:79:TRP:HA	1.99	0.44
2:F:25:ASN:HD21	2:F:28:ASN:CB	2.30	0.44
2:F:29:ILE:HD13	2:F:74:ALA:HB1	1.99	0.44
2:F:83:GLN:NE2	2:F:86:GLN:HE22	2.15	0.44
2:G:73:TYR:CE2	2:G:83:GLN:HG2	2.52	0.44
1:A:82:ASP:O	1:A:143:LYS:CE	2.66	0.44
1:A:149:ARG:NH2	1:A:156:ALA:HB2	2.33	0.44
1:B:64:LEU:HD11	1:B:66:PHE:CE2	2.52	0.44
1:C:68:ARG:H	1:C:68:ARG:HG3	1.46	0.44
2:E:72:LEU:HD23	2:E:84:MET:HB2	1.99	0.44
1:C:87:TYR:HB2	1:C:131:ILE:HG22	2.00	0.44
2:E:8:LEU:C	2:E:9:GLU:HG2	2.42	0.44
2:F:37:GLY:O	2:F:68:TYR:HA	2.18	0.44
2:F:34:ILE:HG21	2:F:59:ILE:HD11	1.99	0.44
1:C:71:GLY:C	1:C:133:VAL:HG21	2.41	0.44
2:G:19:LEU:HD11	2:G:56:THR:CG2	2.39	0.44
1:D:110:PHE:CD1	1:D:110:PHE:C	2.96	0.43
2:E:17:SER:HB2	2:E:59:ILE:O	2.18	0.43
2:E:17:SER:CB	2:E:60:SER:HA	2.48	0.43
2:F:32:TYR:CE1	2:F:52:GLY:HA2	2.53	0.43
2:F:35:THR:O	2:F:35:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PHE:HB2	1:A:159:LEU:HD12	2.00	0.43
1:A:73:PRO:HB3	1:A:159:LEU:HG	2.00	0.43
2:E:8:LEU:HD22	2:E:84:MET:O	2.17	0.43
2:F:76:THR:HG23	2:F:80:ARG:O	2.18	0.43
1:A:121:LEU:HD23	1:A:132:TRP:HZ2	1.83	0.43
2:I:45:VAL:C	2:I:46:GLN:HG3	2.43	0.43
1:C:141:THR:O	1:C:143:LYS:CE	2.67	0.43
2:I:22:TRP:HB2	2:I:23:PRO:HD2	2.00	0.43
1:A:149:ARG:CZ	1:A:156:ALA:HB2	2.49	0.43
1:B:81:ASP:HA	1:B:137:GLY:O	2.18	0.43
1:D:64:LEU:HD11	1:D:66:PHE:CE2	2.54	0.43
2:G:84:MET:HB3	2:G:85:TRP:HE3	1.83	0.43
1:D:62:GLU:N	1:D:62:GLU:CD	2.77	0.43
1:B:69:GLY:O	1:B:135:THR:HG22	2.19	0.43
1:C:149:ARG:HD2	1:C:155:ALA:C	2.44	0.42
2:I:14:THR:OG1	2:I:17:SER:O	2.20	0.42
1:A:158:VAL:O	1:A:160:GLN:HG3	2.19	0.42
2:F:8:LEU:HD13	2:F:72:LEU:CD2	2.36	0.42
2:F:16:THR:O	2:F:62:LEU:HD12	2.19	0.42
1:C:168:PRO:HD2	1:C:171:PHE:HD2	1.84	0.42
1:C:74:ILE:HD11	1:C:162:PRO:HD3	2.01	0.42
2:F:54:LYS:HD3	2:F:54:LYS:HA	1.62	0.42
1:C:58:GLN:OE1	1:C:63:ASP:HA	2.19	0.42
2:G:22:TRP:CZ3	2:G:56:THR:CA	3.03	0.42
1:D:86:TYR:CZ	1:D:111:TYR:HB2	2.54	0.42
2:F:32:TYR:HE2	2:F:84:MET:HE1	1.84	0.42
1:B:55:ALA:HB2	1:B:109:TYR:CZ	2.55	0.42
1:D:125:ALA:HB3	1:D:132:TRP:HZ2	1.84	0.42
1:D:56:LEU:HD21	1:D:159:LEU:HD22	2.02	0.41
1:A:86:TYR:HB3	1:A:132:TRP:CZ3	2.55	0.41
1:A:122:PRO:HD3	2:E:28:ASN:ND2	2.34	0.41
2:I:29:ILE:HG21	2:I:32:TYR:CE1	2.56	0.41
2:G:20:ILE:HG13	2:G:20:ILE:O	2.20	0.41
2:E:39:THR:O	2:E:41:GLY:N	2.53	0.41
1:A:73:PRO:HG3	1:A:110:PHE:CD2	2.55	0.41
1:B:82:ASP:CG	1:B:145:HIS:HE2	2.27	0.41
1:D:85:GLY:HA3	1:D:110:PHE:CZ	2.56	0.41
2:I:25:ASN:OD1	2:I:25:ASN:C	2.63	0.41
2:F:8:LEU:HD22	2:F:85:TRP:HB2	2.01	0.41
1:B:75:ASN:OD1	1:B:75:ASN:C	2.64	0.41
2:I:76:THR:HG21	2:I:82:TYR:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:GLY:HA3	2:G:85:TRP:CE2	2.56	0.41
2:E:7:ASP:OD1	2:E:8:LEU:N	2.47	0.41
2:E:14:THR:CG2	2:E:15:PRO:HD2	2.51	0.41
1:C:109:TYR:N	1:C:109:TYR:CD2	2.88	0.41
2:F:25:ASN:OD1	2:F:25:ASN:C	2.64	0.41
2:F:32:TYR:CE2	2:F:84:MET:HE1	2.56	0.41
1:A:64:LEU:HG	1:A:131:ILE:HD11	2.03	0.40
2:F:29:ILE:HD11	2:F:31:TYR:O	2.20	0.40
1:A:56:LEU:HD23	1:A:56:LEU:HA	1.90	0.40
1:A:129:GLY:C	1:A:130:ILE:HD12	2.47	0.40
1:B:70:GLN:OE1	1:B:166:THR:N	2.53	0.40
1:B:122:PRO:HG3	2:I:29:ILE:HD11	2.03	0.40
2:E:73:TYR:CD1	2:E:83:GLN:HB3	2.57	0.40
1:C:81:ASP:HA	1:C:138:ALA:HA	2.04	0.40
1:B:126:ASN:HB2	2:I:83:GLN:HG3	2.04	0.40
1:C:71:GLY:HA2	1:C:161:LEU:HD21	2.03	0.40
2:E:25:ASN:C	2:E:25:ASN:OD1	2.64	0.40
2:I:73:TYR:HA	2:I:83:GLN:HA	2.04	0.40
2:G:87:PRO:HB2	2:G:88:ILE:H	1.70	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	108/132 (82%)	95 (88%)	12 (11%)	1 (1%)	14	41
1	B	106/132 (80%)	95 (90%)	10 (9%)	1 (1%)	14	41
1	C	102/132 (77%)	95 (93%)	7 (7%)	0	100	100
1	D	95/132 (72%)	84 (88%)	8 (8%)	3 (3%)	3	11
2	E	80/94 (85%)	72 (90%)	6 (8%)	2 (2%)	4	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	77/94 (82%)	60 (78%)	13 (17%)	4 (5%)	1	5
2	G	61/94 (65%)	53 (87%)	7 (12%)	1 (2%)	7	27
2	I	80/94 (85%)	69 (86%)	11 (14%)	0	100	100
All	All	709/904 (78%)	623 (88%)	74 (10%)	12 (2%)	7	25

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	136	GLU
1	B	127	LYS
2	E	87	PRO
1	D	170	GLY
2	G	87	PRO
1	D	67	PRO
2	F	51	PRO
2	F	86	GLN
2	F	87	PRO
2	E	40	GLY
1	A	162	PRO
2	F	88	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	89/103 (86%)	89 (100%)	0	100	100
1	B	86/103 (84%)	83 (96%)	3 (4%)	32	67
1	C	86/103 (84%)	83 (96%)	3 (4%)	32	67
1	D	81/103 (79%)	77 (95%)	4 (5%)	22	55
2	E	73/82 (89%)	67 (92%)	6 (8%)	10	33
2	F	73/82 (89%)	72 (99%)	1 (1%)	59	85
2	G	64/82 (78%)	54 (84%)	10 (16%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	74/82 (90%)	68 (92%)	6 (8%)	11	33
All	All	626/740 (85%)	593 (95%)	33 (5%)	20	52

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	52	TRP
1	B	74	ILE
1	B	79	SER
1	C	63	ASP
1	C	79	SER
1	C	165	THR
1	D	72	VAL
1	D	84	ILE
1	D	133	VAL
1	D	141	THR
2	E	9	GLU
2	E	12	VAL
2	E	49	THR
2	E	67	ASP
2	E	88	ILE
2	E	90	ILE
2	I	10	VAL
2	I	25	ASN
2	I	50	VAL
2	I	70	ILE
2	I	76	THR
2	I	77	THR
2	F	90	ILE
2	G	15	PRO
2	G	16	THR
2	G	17	SER
2	G	18	LEU
2	G	19	LEU
2	G	29	ILE
2	G	36	TYR
2	G	38	GLU
2	G	49	THR
2	G	67	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	C	58	GLN
1	D	59	HIS
2	F	83	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	112/132 (84%)	1.58	30 (26%) 1 1	37, 54, 79, 89	0
1	B	110/132 (83%)	1.73	38 (34%) 1 1	42, 63, 89, 97	0
1	C	108/132 (81%)	1.47	22 (20%) 3 2	54, 68, 90, 102	0
1	D	103/132 (78%)	2.31	54 (52%) 0 0	60, 86, 107, 122	0
2	E	84/94 (89%)	2.59	57 (67%) 0 0	38, 61, 93, 99	0
2	F	83/94 (88%)	2.64	52 (62%) 0 0	66, 114, 154, 165	0
2	G	71/94 (75%)	2.32	42 (59%) 0 0	53, 96, 160, 167	0
2	I	84/94 (89%)	2.28	42 (50%) 0 0	35, 66, 86, 98	0
All	All	755/904 (83%)	2.06	337 (44%) 0 0	35, 72, 136, 167	0

All (337) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	57	ALA	7.4
2	E	86	GLN	5.9
2	F	72	LEU	5.8
2	E	13	ALA	5.6
1	B	52	TRP	5.6
2	I	85	TRP	5.3
2	E	87	PRO	5.2
1	D	134	ALA	5.2
2	I	8	LEU	5.2
2	E	14	THR	5.2
2	E	17	SER	5.1
2	F	20	ILE	5.0
1	D	90	ALA	4.8
2	E	83	GLN	4.8
2	G	51	PRO	4.8
2	F	5	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
2	F	85	TRP	4.7
1	C	163	GLN	4.7
2	I	13	ALA	4.7
1	D	132	TRP	4.7
2	F	9	GLU	4.6
2	G	61	GLY	4.5
1	B	134	ALA	4.5
2	E	32	TYR	4.4
1	D	141	THR	4.4
2	F	58	THR	4.4
2	F	23	PRO	4.4
2	F	31	TYR	4.3
2	I	7	ASP	4.2
2	F	34	ILE	4.2
2	I	14	THR	4.2
2	F	36	TYR	4.2
1	B	173	ALA	4.2
2	E	18	LEU	4.2
2	F	45	VAL	4.1
2	G	10	VAL	4.1
1	A	143	LYS	4.1
2	F	8	LEU	4.1
2	F	22	TRP	4.1
1	A	129	GLY	4.1
2	I	61	GLY	4.1
1	D	162	PRO	4.1
1	D	84	ILE	4.0
1	D	129	GLY	4.0
2	I	11	VAL	4.0
2	G	58	THR	4.0
2	I	5	PRO	4.0
2	E	88	ILE	3.9
2	F	70	ILE	3.9
1	D	88	ARG	3.9
2	G	88	ILE	3.9
2	E	72	LEU	3.9
2	E	79	TRP	3.9
2	F	84	MET	3.9
1	D	80	PRO	3.9
1	A	123	TYR	3.9
2	F	32	TYR	3.9
2	G	18	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
2	E	85	TRP	3.8
2	I	12	VAL	3.8
2	G	68	TYR	3.8
2	I	17	SER	3.8
2	F	79	TRP	3.8
2	I	51	PRO	3.8
2	G	59	ILE	3.7
2	F	7	ASP	3.7
1	A	88	ARG	3.7
2	F	50	VAL	3.7
1	D	59	HIS	3.7
2	E	74	ALA	3.7
2	G	70	ILE	3.7
2	F	86	GLN	3.6
1	D	126	ASN	3.6
2	E	12	VAL	3.6
2	I	32	TYR	3.6
2	G	71	ALA	3.6
2	F	82	TYR	3.6
1	C	104	LEU	3.6
2	I	19	LEU	3.6
2	F	56	THR	3.6
2	I	20	ILE	3.5
2	I	10	VAL	3.5
1	D	76	THR	3.5
1	D	116	GLY	3.5
2	E	15	PRO	3.5
2	F	57	ALA	3.5
2	G	52	GLY	3.4
1	D	173	ALA	3.4
2	F	48	PHE	3.4
2	I	9	GLU	3.4
2	I	60	SER	3.4
1	A	84	ILE	3.4
2	F	59	ILE	3.4
1	A	163	GLN	3.4
1	B	129	GLY	3.4
1	D	125	ALA	3.4
1	B	84	ILE	3.3
2	I	90	ILE	3.3
1	D	82	ASP	3.3
2	E	66	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	61	LYS	3.3
2	G	8	LEU	3.3
2	F	55	SER	3.3
1	D	86	TYR	3.3
2	E	20	ILE	3.3
2	I	28	ASN	3.3
1	D	139	LEU	3.3
1	D	74	ILE	3.2
1	A	115	THR	3.2
2	I	22	TRP	3.2
1	A	111	TYR	3.2
1	C	82	ASP	3.2
1	D	167	LEU	3.2
2	G	72	LEU	3.2
1	A	144	ASP	3.2
1	D	75	ASN	3.2
2	F	6	ARG	3.2
1	D	73	PRO	3.2
1	D	81	ASP	3.2
2	G	19	LEU	3.2
1	A	118	GLU	3.2
2	I	18	LEU	3.1
2	F	40	GLY	3.1
2	E	19	LEU	3.1
1	D	140	ASN	3.1
1	D	147	GLY	3.1
2	G	65	GLY	3.1
2	F	90	ILE	3.1
1	C	112	TYR	3.1
2	I	45	VAL	3.1
2	E	65	GLY	3.1
2	F	21	SER	3.1
2	G	86	GLN	3.1
2	E	56	THR	3.1
2	G	23	PRO	3.0
1	C	155	ALA	3.0
2	F	10	VAL	3.0
2	G	75	VAL	3.0
1	D	66	PHE	3.0
1	D	87	TYR	3.0
2	F	27	TYR	3.0
1	D	146	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	63	ASP	3.0
2	E	59	ILE	3.0
1	D	144	ASP	3.0
2	E	7	ASP	3.0
1	A	142	PRO	3.0
1	B	50	ALA	3.0
2	E	84	MET	3.0
2	G	39	THR	3.0
2	E	22	TRP	2.9
2	E	82	TYR	2.9
1	A	82	ASP	2.9
2	E	21	SER	2.9
1	D	53	PHE	2.9
1	D	112	TYR	2.9
2	I	65	GLY	2.9
1	A	148	THR	2.9
2	F	35	THR	2.9
2	I	59	ILE	2.9
2	I	87	PRO	2.9
2	G	47	GLU	2.9
1	D	170	GLY	2.9
1	B	108	TRP	2.9
1	D	123	TYR	2.9
1	A	134	ALA	2.9
1	B	81	ASP	2.9
2	I	56	THR	2.9
1	D	67	PRO	2.8
2	E	11	VAL	2.8
1	B	77	ASN	2.8
2	E	89	SER	2.8
2	I	36	TYR	2.8
1	D	161	LEU	2.8
2	E	8	LEU	2.8
2	F	53	SER	2.8
1	D	106	PRO	2.8
2	E	80	ARG	2.7
2	G	6	ARG	2.7
2	E	50	VAL	2.7
1	A	60	GLY	2.7
2	E	44	PRO	2.7
2	F	88	ILE	2.7
2	G	81	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	112	TYR	2.7
2	E	91	ASN	2.7
1	C	81	ASP	2.7
2	I	44	PRO	2.7
2	F	51	PRO	2.7
1	D	72	VAL	2.7
2	E	45	VAL	2.7
1	C	130	ILE	2.7
2	G	73	TYR	2.7
2	G	35	THR	2.7
2	E	9	GLU	2.7
2	I	86	GLN	2.7
2	G	66	VAL	2.7
1	B	161	LEU	2.7
1	B	117	PRO	2.7
2	I	58	THR	2.7
1	C	145	HIS	2.6
1	B	116	GLY	2.6
1	A	159	LEU	2.6
2	E	46	GLN	2.6
1	C	59	HIS	2.6
2	G	85	TRP	2.6
2	E	36	TYR	2.6
1	B	168	PRO	2.6
1	D	124	GLY	2.6
1	D	64	LEU	2.6
1	B	152	ALA	2.6
1	C	170	GLY	2.6
1	D	168	PRO	2.6
2	F	64	PRO	2.6
2	F	65	GLY	2.6
1	D	85	GLY	2.6
1	D	131	ILE	2.6
2	E	75	VAL	2.6
2	E	71	ALA	2.6
1	A	59	HIS	2.5
1	B	64	LEU	2.5
1	C	109	TYR	2.5
1	B	65	LYS	2.5
2	E	29	ILE	2.5
2	E	90	ILE	2.5
1	C	123	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	G	31	TYR	2.5
2	I	47	GLU	2.5
1	B	126	ASN	2.5
2	I	64	PRO	2.5
1	C	137	GLY	2.5
2	I	70	ILE	2.5
2	F	71	ALA	2.5
1	D	145	HIS	2.5
1	D	56	LEU	2.5
2	G	20	ILE	2.5
2	G	21	SER	2.5
1	A	136	GLU	2.5
1	B	155	ALA	2.5
2	E	6	ARG	2.5
1	C	61	LYS	2.5
2	F	63	LYS	2.5
1	C	144	ASP	2.4
1	B	106	PRO	2.4
2	E	53	SER	2.4
2	I	24	ALA	2.4
1	B	59	HIS	2.4
2	F	80	ARG	2.4
1	C	52	TRP	2.4
2	F	68	TYR	2.4
1	B	139	LEU	2.4
2	F	47	GLU	2.4
2	G	48	PHE	2.4
1	A	125	ALA	2.4
2	E	34	ILE	2.4
2	G	34	ILE	2.4
2	G	64	PRO	2.4
2	F	54	LYS	2.4
1	C	139	LEU	2.4
2	I	15	PRO	2.4
1	B	170	GLY	2.3
2	E	60	SER	2.3
2	I	72	LEU	2.3
2	F	69	THR	2.3
2	F	73	TYR	2.3
2	F	83	GLN	2.3
1	C	159	LEU	2.3
2	F	62	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	33	ARG	2.3
2	E	81	LEU	2.3
1	A	91	THR	2.3
1	D	57	THR	2.3
1	D	135	THR	2.3
2	G	56	THR	2.3
1	B	120	GLY	2.3
2	F	74	ALA	2.3
1	A	121	LEU	2.3
1	D	83	GLN	2.3
2	G	22	TRP	2.3
2	G	45	VAL	2.3
1	C	129	GLY	2.3
2	I	25	ASN	2.2
2	I	91	ASN	2.2
1	B	169	LYS	2.2
2	G	78	ARG	2.2
1	B	132	TRP	2.2
2	I	79	TRP	2.2
1	B	123	TYR	2.2
1	D	51	SER	2.2
2	E	51	PRO	2.2
2	F	61	GLY	2.2
1	B	167	LEU	2.2
2	I	38	GLU	2.2
1	D	68	ARG	2.2
1	B	67	PRO	2.2
1	D	142	PRO	2.2
2	F	16	THR	2.2
1	B	87	TYR	2.2
2	E	31	TYR	2.2
1	A	170	GLY	2.2
2	F	81	LEU	2.2
1	A	145	HIS	2.2
1	A	56	LEU	2.2
1	D	118	GLU	2.2
2	E	61	GLY	2.2
1	B	115	THR	2.1
2	E	58	THR	2.1
1	A	113	LEU	2.1
1	B	159	LEU	2.1
1	D	159	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	53	SER	2.1
1	B	136	GLU	2.1
1	A	122	PRO	2.1
1	D	63	ASP	2.1
2	G	79	TRP	2.1
1	C	111	TYR	2.1
2	E	68	TYR	2.1
2	G	29	ILE	2.1
2	G	46	GLN	2.1
1	B	122	PRO	2.1
1	A	57	THR	2.1
1	C	72	VAL	2.1
1	C	73	PRO	2.1
2	G	87	PRO	2.1
1	B	114	GLY	2.1
2	E	69	THR	2.1
2	E	27	TYR	2.1
2	E	73	TYR	2.1
1	B	145	HIS	2.0
1	B	163	GLN	2.0
2	E	10	VAL	2.0
2	I	62	LEU	2.0
1	B	121	LEU	2.0
2	E	28	ASN	2.0
2	G	25	ASN	2.0
1	A	152	ALA	2.0
1	A	165	THR	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.