



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:24 PM GMT

PDB ID : 1AL0
Title : PROCAPSID OF BACTERIOPHAGE PHIX174
Authors : Rossmann, M.G.; Dokland, T.
Deposited on : 1997-06-06
Resolution : 3.50 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

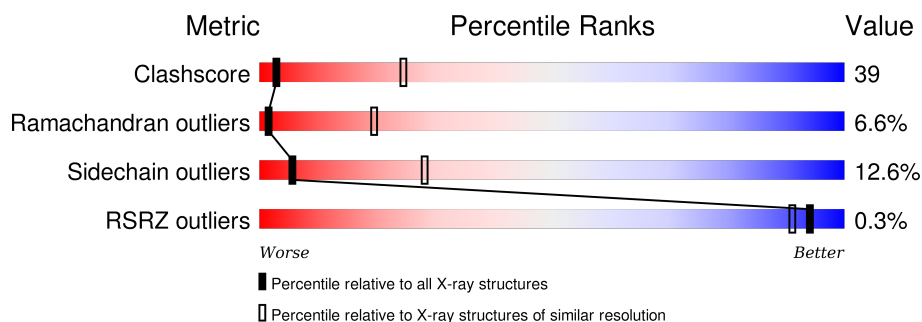
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	1	152	<div> <div>45%</div> <div>42%</div> <div>7%</div> <div>6%</div> </div>
1	2	152	<div> <div>36%</div> <div>36%</div> <div>14%</div> <div>13%</div> </div>
1	3	152	<div> <div>40%</div> <div>39%</div> <div>12%</div> <div>8%</div> </div>
1	4	152	<div> <div>46%</div> <div>38%</div> <div>10%</div> <div>•</div> </div>
2	F	426	<div> <div>35%</div> <div>46%</div> <div>14%</div> <div>•</div> </div>
3	G	175	<div> <div>57%</div> <div>34%</div> <div>7%</div> <div>•</div> </div>
4	B	120	<div> <div>2%</div> <div>8%</div> <div>18%</div> <div>9%</div> <div>5%</div> <div>59%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9521 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 SCAFFOLDING PROTEIN GPD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	143	Total	C	N	O	S	0	0	0
			1125	716	194	211	4			
1	2	133	Total	C	N	O	S	0	0	0
			1039	665	175	195	4			
1	3	140	Total	C	N	O	S	0	0	0
			1099	699	187	209	4			
1	4	146	Total	C	N	O	S	0	0	0
			1145	728	197	215	5			

- Molecule 2 is a protein called CAPSID PROTEIN GPF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	418	Total	C	N	O	S	0	0	0
			3358	2139	581	625	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	216	ARG	HIS	CONFLICT	UNP P03641

- Molecule 3 is a protein called SPIKE PROTEIN GPG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	175	Total	C	N	O	S	0	0	0
			1340	856	221	255	8			

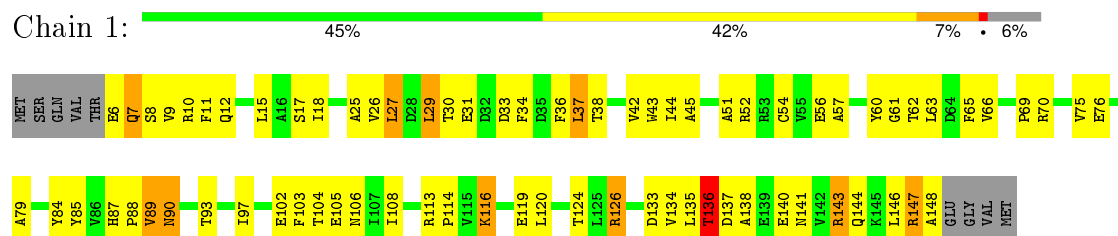
- Molecule 4 is a protein called SCAFFOLDING PROTEIN GPB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	49	Total	C	N	O	S	0	0	0
			415	262	71	80	2			

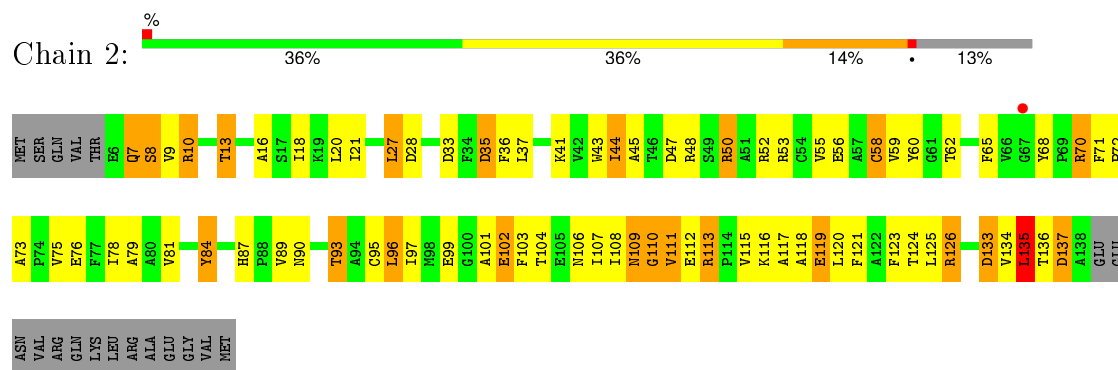
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

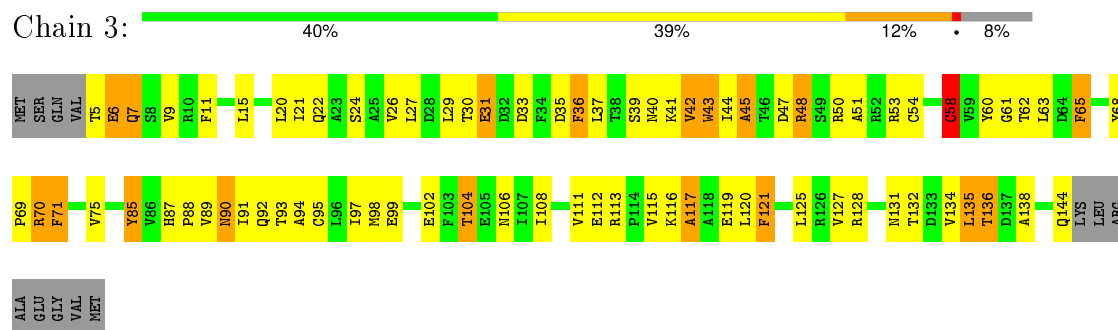
• Molecule 1: SCAFFOLDING PROTEIN GPD



• Molecule 1: SCAFFOLDING PROTEIN GPD

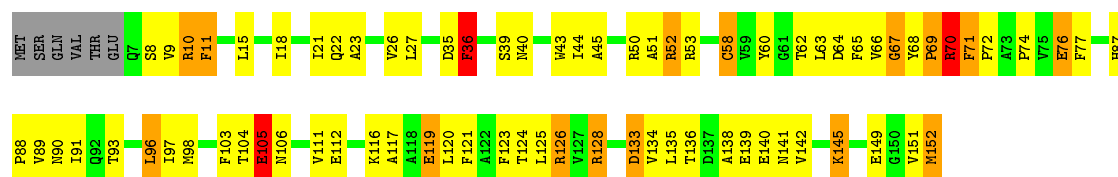


• Molecule 1: SCAFFOLDING PROTEIN GPD



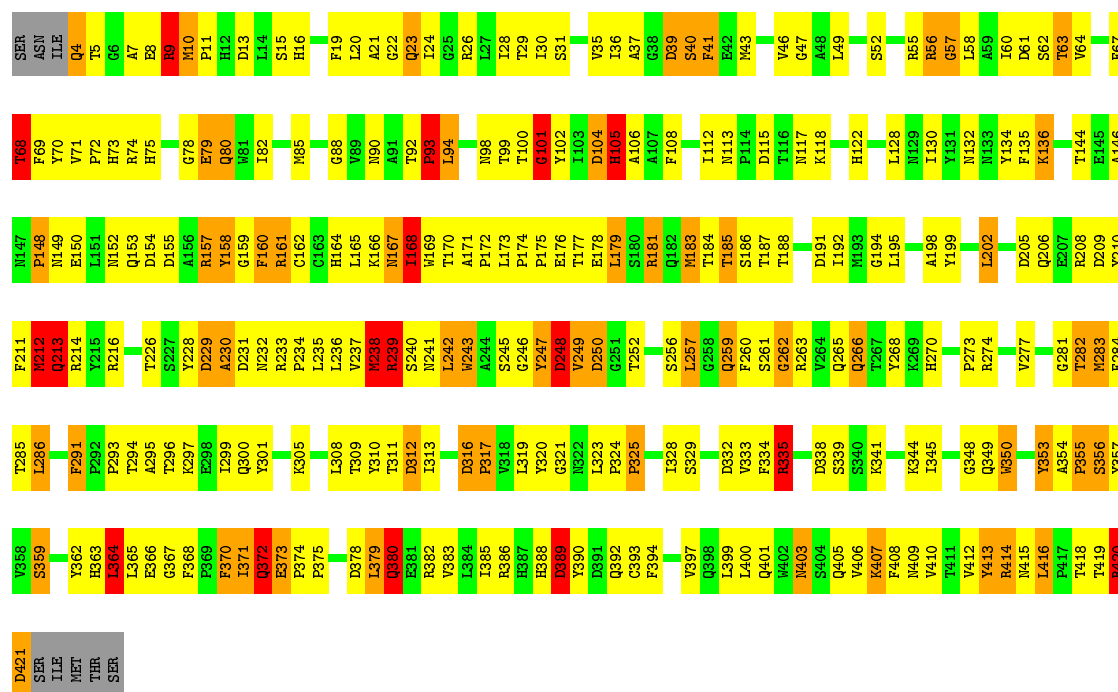
• Molecule 1: SCAFFOLDING PROTEIN GPD





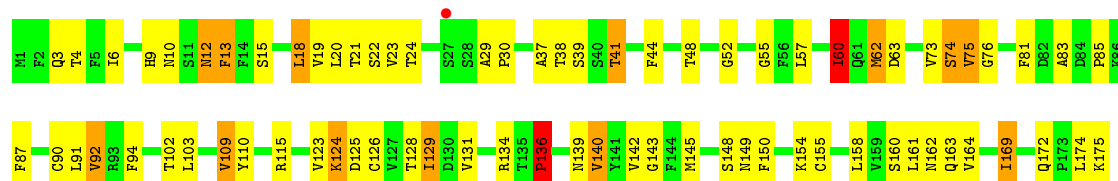
• Molecule 2: CAPSID PROTEIN GPF

Chain F: 35% 46% 14%



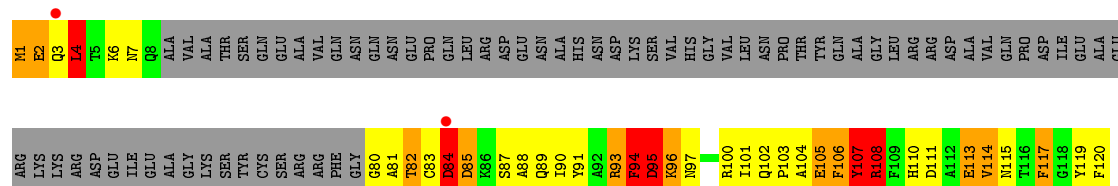
• Molecule 3: SPIKE PROTEIN GPG

Chain G: 57% 34% 7%



• Molecule 4: SCAFFOLDING PROTEIN GPB

Chain B: 2% 8% 18% 9% 5% 59%



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	774.00Å 774.00Å 774.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.50 44.54 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.50) 55.2 (44.54-3.50)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.25	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.48Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.316 , (Not available) 0.486 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 0.8	EDS
Estimated twinning fraction	0.004 for -l,-k,-h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	8 of 526777 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.16	EDS
Total number of atoms	9521	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	1.15	2/1145 (0.2%)	1.06	5/1557 (0.3%)
1	2	1.06	1/1059 (0.1%)	1.08	5/1443 (0.3%)
1	3	1.18	1/1119 (0.1%)	1.16	6/1524 (0.4%)
1	4	1.11	2/1165 (0.2%)	1.08	6/1582 (0.4%)
2	F	1.13	3/3454 (0.1%)	1.20	36/4702 (0.8%)
3	G	0.91	1/1372 (0.1%)	1.01	10/1872 (0.5%)
4	B	1.30	2/425 (0.5%)	1.41	9/569 (1.6%)
All	All	1.11	12/9739 (0.1%)	1.14	77/13249 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	3	0	1
1	4	0	1
2	F	0	1
4	B	0	3
All	All	0	6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	112	GLU	CG-CD	6.46	1.61	1.51
2	F	19	PHE	CB-CG	-6.21	1.40	1.51
2	F	162	CYS	CB-SG	-5.90	1.72	1.81
1	1	140	GLU	CG-CD	5.80	1.60	1.51
4	B	80	GLY	N-CA	5.72	1.54	1.46
1	1	6	GLU	CG-CD	5.65	1.60	1.51
4	B	84	ASP	CB-CG	5.46	1.63	1.51
1	3	58	CYS	CB-SG	-5.45	1.73	1.81
3	G	175	LYS	C-OXT	5.18	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	58	CYS	CB-SG	-5.12	1.73	1.81
1	2	58	CYS	CB-SG	-5.08	1.73	1.81
2	F	40	SER	C-O	5.03	1.32	1.23

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	95	ASP	N-CA-C	-9.58	85.14	111.00
2	F	421	ASP	N-CA-CB	8.85	126.53	110.60
1	1	136	THR	N-CA-C	-8.79	87.27	111.00
1	4	70	ARG	NE-CZ-NH2	7.87	124.23	120.30
1	3	48	ARG	NE-CZ-NH2	7.77	124.18	120.30
1	3	70	ARG	NE-CZ-NH2	7.59	124.09	120.30
2	F	420	ARG	NE-CZ-NH2	7.49	124.04	120.30
1	2	135	LEU	N-CA-C	7.15	130.31	111.00
2	F	157	ARG	NE-CZ-NH2	6.85	123.72	120.30
2	F	4	GLN	O-C-N	6.79	133.56	122.70
2	F	9	ARG	NE-CZ-NH2	6.79	123.69	120.30
3	G	74	SER	N-CA-C	6.71	129.12	111.00
2	F	421	ASP	CA-CB-CG	-6.62	98.84	113.40
2	F	356	SER	N-CA-C	-6.36	93.83	111.00
1	2	137	ASP	N-CA-C	6.28	127.96	111.00
1	4	36	PHE	CB-CA-C	-6.21	97.99	110.40
2	F	101	GLY	N-CA-C	6.20	128.59	113.10
2	F	93	PRO	N-CA-C	6.16	128.12	112.10
4	B	107	TYR	N-CA-C	6.16	127.62	111.00
2	F	168	ILE	CG1-CB-CG2	-6.14	97.89	111.40
2	F	392	GLN	CB-CA-C	-6.12	98.16	110.40
2	F	420	ARG	O-C-N	6.11	132.47	122.70
2	F	80	GLN	N-CA-C	-6.09	94.57	111.00
4	B	1	MET	CG-SD-CE	6.08	109.92	100.20
1	4	9	VAL	N-CA-C	-6.07	94.61	111.00
1	2	70	ARG	NE-CZ-NH2	6.02	123.31	120.30
2	F	10	MET	CG-SD-CE	5.98	109.76	100.20
1	1	143	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	4	152	MET	CG-SD-CE	5.97	109.75	100.20
2	F	4	GLN	CB-CA-C	5.92	122.23	110.40
1	3	144	GLN	N-CA-C	5.89	126.92	111.00
3	G	62	MET	CG-SD-CE	5.88	109.61	100.20
1	1	136	THR	N-CA-CB	5.86	121.44	110.30
2	F	43	MET	CG-SD-CE	5.82	109.52	100.20
3	G	145	MET	CG-SD-CE	5.80	109.48	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	98	MET	CG-SD-CE	5.80	109.48	100.20
3	G	172	GLN	N-CA-C	-5.74	95.49	111.00
2	F	40	SER	CA-C-N	5.72	129.78	117.20
2	F	4	GLN	N-CA-C	-5.69	95.63	111.00
2	F	364	LEU	CA-CB-CG	5.68	128.37	115.30
2	F	238	MET	N-CA-C	5.61	126.13	111.00
2	F	380	GLN	N-CA-C	-5.58	95.94	111.00
2	F	335	ARG	NE-CZ-NH1	-5.57	117.51	120.30
2	F	283	MET	CG-SD-CE	5.54	109.07	100.20
1	2	110	GLY	N-CA-C	-5.50	99.35	113.10
3	G	92	VAL	CB-CA-C	-5.47	101.01	111.40
1	3	90	ASN	N-CA-C	5.46	125.73	111.00
2	F	407	LYS	N-CA-CB	-5.46	100.78	110.60
2	F	291	PHE	N-CA-C	-5.45	96.28	111.00
2	F	416	LEU	N-CA-C	-5.42	96.37	111.00
2	F	85	MET	CG-SD-CE	5.38	108.81	100.20
4	B	111	ASP	N-CA-C	-5.38	96.47	111.00
2	F	403	ASN	CB-CA-C	-5.38	99.65	110.40
3	G	76	GLY	N-CA-C	-5.37	99.67	113.10
3	G	129	ILE	CB-CA-C	-5.37	100.87	111.60
4	B	107	TYR	CB-CA-C	-5.36	99.69	110.40
2	F	161	ARG	N-CA-C	5.35	125.44	111.00
2	F	13	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	1	148	ALA	N-CA-C	5.26	125.21	111.00
3	G	139	ASN	N-CA-C	-5.25	96.82	111.00
4	B	105	GLU	N-CA-C	-5.25	96.83	111.00
2	F	106	ALA	N-CA-C	-5.21	96.92	111.00
2	F	243	TRP	N-CA-C	-5.19	96.99	111.00
1	2	133	ASP	CB-CG-OD1	5.19	122.97	118.30
1	4	104	THR	CB-CA-C	-5.17	97.64	111.60
2	F	39	ASP	N-CA-C	5.17	124.95	111.00
1	3	42	VAL	CB-CA-C	-5.16	101.60	111.40
2	F	56	ARG	CG-CD-NE	-5.12	101.04	111.80
3	G	124	LYS	N-CA-C	-5.11	97.21	111.00
3	G	60	ILE	N-CA-C	-5.07	97.30	111.00
4	B	93	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	4	69	PRO	N-CA-C	-5.07	98.92	112.10
2	F	252	THR	N-CA-C	5.05	124.64	111.00
4	B	4	LEU	CA-CB-CG	5.05	126.92	115.30
1	1	89	VAL	N-CA-C	-5.04	97.39	111.00
4	B	113	GLU	N-CA-C	-5.03	97.42	111.00
2	F	40	SER	O-C-N	-5.03	114.66	122.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	3	68	TYR	Sidechain
1	4	36	PHE	Sidechain
4	B	107	TYR	Sidechain
4	B	119	TYR	Sidechain
4	B	82	THR	Mainchain
2	F	160	PHE	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1125	0	1121	75	0
1	2	1039	0	1031	102	0
1	3	1099	0	1086	95	0
1	4	1145	0	1142	94	0
2	F	3358	0	3242	306	0
3	G	1340	0	1323	64	0
4	B	415	0	376	73	0
All	All	9521	0	9321	742	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 39.

All (742) 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:F:7:ALA:CB	4:B:100:ARG:CD	1.79	1.58
2:F:7:ALA:HB3	4:B:100:ARG:CD	1.42	1.41
2:F:7:ALA:CB	4:B:100:ARG:HD2	1.44	1.32
1:4:151:VAL:O	1:4:152:MET:HG2	1.13	1.29
2:F:7:ALA:CB	4:B:100:ARG:HD3	1.51	1.23
1:4:10:ARG:NH2	1:4:139:GLU:HB2	1.60	1.14
1:4:10:ARG:NH1	1:4:11:PHE:HB2	1.63	1.13
2:F:274:ARG:HH22	4:B:96:LYS:HA	1.07	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:151:VAL:O	1:4:152:MET:CG	1.99	1.11
2:F:157:ARG:NE	2:F:158:TYR:OH	1.84	1.10
2:F:7:ALA:HB1	4:B:100:ARG:CB	1.81	1.09
2:F:181:ARG:HG3	2:F:202:LEU:HD21	1.33	1.09
2:F:7:ALA:HB1	4:B:100:ARG:CD	1.60	1.08
2:F:341:LYS:HB3	2:F:382:ARG:HH22	1.13	1.07
2:F:68:THR:HG22	2:F:285:THR:HG22	1.37	1.05
2:F:154:ASP:O	2:F:158:TYR:HD1	1.36	1.04
2:F:154:ASP:HA	2:F:158:TYR:CE1	1.93	1.03
2:F:7:ALA:HB1	4:B:100:ARG:HD3	1.20	1.02
1:4:126:ARG:HH11	1:4:126:ARG:HG3	1.25	1.00
1:2:52:ARG:HH21	1:2:101:ALA:HA	1.26	1.00
1:3:43:TRP:HE1	1:3:90:ASN:HB3	1.25	0.99
2:F:7:ALA:HB1	4:B:100:ARG:HA	1.44	0.98
2:F:7:ALA:CA	4:B:100:ARG:HD3	1.93	0.98
2:F:7:ALA:HB1	4:B:100:ARG:CA	1.95	0.96
1:3:43:TRP:HE1	1:3:90:ASN:CB	1.78	0.96
2:F:157:ARG:CG	2:F:158:TYR:CE1	2.49	0.96
4:B:6:LYS:HG2	4:B:83:CYS:SG	2.06	0.95
1:3:58:CYS:SG	1:3:85:TYR:CD2	2.59	0.94
2:F:154:ASP:O	2:F:158:TYR:CD1	2.19	0.94
4:B:113:GLU:O	4:B:114:VAL:HB	1.66	0.94
3:G:60:ILE:HD13	3:G:161:LEU:HB2	1.50	0.93
2:F:153:GLN:O	2:F:157:ARG:HG2	1.69	0.92
2:F:157:ARG:HG3	2:F:158:TYR:CE1	2.04	0.92
2:F:7:ALA:HB1	4:B:100:ARG:CG	1.99	0.92
1:1:15:LEU:HA	1:1:18:ILE:HD12	1.51	0.92
2:F:7:ALA:C	4:B:100:ARG:HD3	1.90	0.92
1:2:27:LEU:HD23	1:2:27:LEU:H	1.35	0.92
1:4:10:ARG:HH11	1:4:11:PHE:H	1.12	0.91
2:F:212:MET:SD	2:F:213:GLN:N	2.44	0.90
2:F:157:ARG:HG3	2:F:158:TYR:CZ	2.05	0.90
3:G:169:ILE:HD13	3:G:169:ILE:H	1.36	0.90
4:B:7:ASN:HA	4:B:110:HIS:O	1.73	0.89
2:F:154:ASP:HA	2:F:158:TYR:HE1	1.37	0.87
2:F:72:PRO:HD2	2:F:75:HIS:ND1	1.89	0.87
3:G:38:THR:HG23	3:G:163:GLN:HE21	1.40	0.87
1:2:52:ARG:NH2	1:2:101:ALA:HA	1.88	0.87
4:B:3:GLN:HG2	4:B:87:SER:HB2	1.56	0.86
2:F:274:ARG:NH2	4:B:96:LYS:HA	1.89	0.86
1:3:60:TYR:CD2	1:3:70:ARG:HD3	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:16:ALA:HB1	1:3:42:VAL:HG21	1.59	0.85
3:G:15:SER:HA	3:G:41:THR:HG23	1.56	0.84
2:F:309:THR:HG22	2:F:310:TYR:H	1.40	0.84
1:2:87:HIS:HD2	1:2:89:VAL:HB	1.42	0.84
1:2:13:THR:HG23	1:3:89:VAL:O	1.77	0.84
2:F:297:LYS:HG2	2:F:335:ARG:HB3	1.60	0.84
2:F:166:LYS:HG2	4:B:117:PHE:CE2	2.13	0.83
2:F:70:TYR:CE2	2:F:72:PRO:HG3	2.14	0.82
1:1:134:VAL:HG12	1:1:136:THR:N	1.92	0.82
1:2:73:ALA:O	1:2:104:THR:HG22	1.78	0.82
3:G:39:SER:HB2	3:G:162:ASN:HD22	1.44	0.82
2:F:341:LYS:CB	2:F:382:ARG:HH22	1.92	0.82
2:F:247:TYR:HD1	2:F:248:ASP:H	1.25	0.81
4:B:6:LYS:HE2	4:B:83:CYS:SG	2.20	0.81
1:1:7:GLN:HG3	1:1:126:ARG:NH1	1.96	0.81
2:F:341:LYS:HB3	2:F:382:ARG:NH2	1.95	0.81
2:F:309:THR:HG22	2:F:310:TYR:N	1.96	0.80
2:F:414:ARG:HB3	2:F:414:ARG:NH1	1.96	0.80
2:F:157:ARG:HG2	2:F:158:TYR:CE1	2.16	0.80
2:F:256:SER:HB2	2:F:259:GLN:HB2	1.61	0.79
1:4:35:ASP:O	1:4:39:SER:HB3	1.82	0.79
2:F:250:ASP:HA	2:F:260:PHE:HD1	1.48	0.79
2:F:35:VAL:HG11	2:F:277:VAL:HG21	1.64	0.79
2:F:75:HIS:CD2	2:F:232:ASN:HA	2.18	0.78
1:4:128:ARG:HH11	1:4:128:ARG:CG	1.95	0.78
2:F:68:THR:CG2	2:F:285:THR:HG22	2.11	0.78
2:F:311:THR:HG22	2:F:319:LEU:HD13	1.64	0.78
2:F:68:THR:HA	2:F:285:THR:HA	1.65	0.78
1:3:121:PHE:CE1	1:3:125:LEU:HD11	2.19	0.78
4:B:4:LEU:HB2	4:B:110:HIS:HE1	1.49	0.77
2:F:20:LEU:HD11	2:F:30:ILE:HG12	1.64	0.77
2:F:256:SER:O	2:F:257:LEU:HB2	1.84	0.77
3:G:83:ALA:O	3:G:85:PRO:HD3	1.84	0.77
1:1:30:THR:HA	1:1:147:ARG:NE	1.99	0.77
2:F:7:ALA:O	4:B:100:ARG:HD3	1.82	0.77
1:2:87:HIS:CD2	1:2:89:VAL:H	2.03	0.77
1:1:31:GLU:N	1:1:147:ARG:HH21	1.82	0.77
1:3:43:TRP:HE1	1:3:90:ASN:CG	1.87	0.77
1:2:99:GLU:HB2	1:2:117:ALA:HB2	1.66	0.76
1:2:44:ILE:HG12	1:2:45:ALA:N	1.98	0.76
1:2:44:ILE:HG12	1:2:45:ALA:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:7:ALA:CB	4:B:100:ARG:CB	2.60	0.76
1:3:43:TRP:NE1	1:3:90:ASN:HB3	2.00	0.76
4:B:3:GLN:HG2	4:B:87:SER:CB	2.15	0.76
1:4:10:ARG:HH11	1:4:11:PHE:N	1.82	0.76
2:F:208:ARG:HA	2:F:212:MET:HG3	1.67	0.75
1:2:84:TYR:CE1	1:2:135:LEU:HB2	2.21	0.75
1:3:115:VAL:HG13	1:3:119:GLU:HB3	1.68	0.75
2:F:135:PHE:O	2:F:136:LYS:HB3	1.86	0.75
4:B:6:LYS:CG	4:B:83:CYS:SG	2.75	0.75
2:F:7:ALA:C	4:B:100:ARG:CD	2.55	0.74
4:B:106:PHE:O	4:B:107:TYR:HB2	1.83	0.74
3:G:143:GLY:HA2	3:G:161:LEU:HD21	1.70	0.74
2:F:363:HIS:O	2:F:364:LEU:HG	1.87	0.74
3:G:38:THR:HG23	3:G:163:GLN:NE2	2.03	0.73
2:F:250:ASP:HA	2:F:260:PHE:CD1	2.23	0.73
1:2:10:ARG:HG2	1:2:10:ARG:HH11	1.54	0.73
1:1:143:ARG:HA	1:1:146:LEU:HG	1.71	0.73
1:2:68:TYR:HE1	1:3:93:THR:HG22	1.53	0.73
1:1:69:PRO:HG2	1:2:96:LEU:HD11	1.71	0.73
2:F:212:MET:SD	2:F:213:GLN:CA	2.77	0.72
2:F:30:ILE:CG2	2:F:408:PHE:HZ	2.02	0.72
2:F:273:PRO:HD2	4:B:107:TYR:OH	1.88	0.72
2:F:247:TYR:CE2	2:F:263:ARG:HD3	2.23	0.72
2:F:328:ILE:HG22	2:F:329:SER:H	1.55	0.72
1:2:84:TYR:CE1	1:2:133:ASP:HA	2.24	0.72
2:F:7:ALA:CB	4:B:100:ARG:CG	2.63	0.72
1:3:89:VAL:HG12	1:3:90:ASN:OD1	1.88	0.72
2:F:30:ILE:HG22	2:F:408:PHE:HZ	1.53	0.72
1:4:151:VAL:C	1:4:152:MET:HG2	2.07	0.72
2:F:49:LEU:HD23	2:F:64:VAL:HG21	1.70	0.71
1:3:44:ILE:HG22	1:3:45:ALA:H	1.55	0.71
2:F:75:HIS:HD2	2:F:232:ASN:HA	1.55	0.71
1:1:66:VAL:HG11	1:2:44:ILE:HA	1.72	0.71
3:G:90:CYS:SG	3:G:109:VAL:HG22	2.29	0.71
2:F:9:ARG:NH2	2:F:40:SER:HB2	2.06	0.71
3:G:12:ASN:HD22	3:G:13:PHE:N	1.88	0.71
2:F:64:VAL:HB	2:F:242:LEU:HD12	1.72	0.71
1:3:102:GLU:OE1	1:3:112:GLU:HA	1.90	0.71
1:2:10:ARG:HH11	1:2:10:ARG:CG	2.05	0.70
1:2:71:PHE:HB3	1:2:72:PRO:HD3	1.72	0.70
1:1:79:ALA:HA	1:1:124:THR:HG22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:67:GLY:O	1:4:69:PRO:HD3	1.90	0.70
4:B:3:GLN:HG2	4:B:87:SER:HA	1.71	0.70
1:3:106:ASN:HB3	1:3:111:VAL:O	1.92	0.70
2:F:15:SER:HB3	2:F:410:VAL:H	1.57	0.70
1:3:71:PHE:CE1	1:4:96:LEU:HG	2.27	0.70
2:F:414:ARG:CG	2:F:414:ARG:HH11	2.05	0.69
1:1:7:GLN:HA	1:1:10:ARG:HD2	1.74	0.69
1:4:74:PRO:HD2	1:4:77:PHE:CD2	2.27	0.69
2:F:7:ALA:CB	4:B:100:ARG:HA	2.20	0.69
1:4:10:ARG:HH12	1:4:11:PHE:HB2	1.53	0.69
4:B:3:GLN:CG	4:B:87:SER:HA	2.22	0.69
2:F:414:ARG:HH11	2:F:414:ARG:HB3	1.57	0.69
2:F:181:ARG:CG	2:F:202:LEU:HD21	2.20	0.69
2:F:406:VAL:HG12	2:F:407:LYS:N	2.08	0.69
1:2:56:GLU:HG2	1:2:103:PHE:CZ	2.28	0.69
1:4:128:ARG:HH11	1:4:128:ARG:HG2	1.55	0.69
3:G:158:LEU:H	3:G:158:LEU:HD23	1.58	0.69
2:F:57:GLY:HA2	2:F:261:SER:O	1.93	0.69
1:2:107:ILE:HG23	1:2:110:GLY:O	1.93	0.69
4:B:3:GLN:HG2	4:B:87:SER:CA	2.23	0.68
2:F:301:TYR:HE1	2:F:328:ILE:HG23	1.58	0.68
2:F:7:ALA:CA	4:B:100:ARG:CD	2.59	0.68
2:F:309:THR:CG2	2:F:310:TYR:H	2.06	0.68
1:2:16:ALA:HB1	1:3:42:VAL:CG2	2.24	0.68
1:2:21:ILE:HD11	1:2:62:THR:HA	1.74	0.68
1:1:108:ILE:HG23	1:2:123:PHE:CE1	2.29	0.68
2:F:295:ALA:HA	2:F:371:ILE:HG22	1.74	0.68
1:2:27:LEU:HD23	1:2:27:LEU:N	2.08	0.68
1:4:126:ARG:NH1	1:4:126:ARG:HG3	1.97	0.67
1:2:10:ARG:HH12	1:2:76:GLU:CD	1.97	0.67
2:F:82:ILE:N	2:F:82:ILE:HD12	2.10	0.67
3:G:169:ILE:HD13	3:G:169:ILE:N	2.09	0.67
2:F:166:LYS:HG2	4:B:117:PHE:CZ	2.29	0.67
2:F:9:ARG:NH1	4:B:101:ILE:HG13	2.09	0.67
1:4:10:ARG:NH1	1:4:11:PHE:CB	2.53	0.67
2:F:30:ILE:HG22	2:F:408:PHE:CZ	2.30	0.67
1:4:133:ASP:HB2	2:F:118:LYS:NZ	2.09	0.67
2:F:211:PHE:O	2:F:212:MET:HB3	1.95	0.66
1:4:105:GLU:CG	1:4:106:ASN:H	2.08	0.66
2:F:7:ALA:CB	4:B:100:ARG:HB3	2.25	0.66
1:2:18:ILE:HG21	1:2:84:TYR:CD2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:413:TYR:CD1	2:F:413:TYR:N	2.64	0.66
1:4:27:LEU:HD13	1:4:58:CYS:SG	2.35	0.66
2:F:414:ARG:HH11	2:F:414:ARG:CB	2.09	0.66
2:F:79:GLU:HA	2:F:82:ILE:HD13	1.76	0.66
2:F:247:TYR:CD2	2:F:263:ARG:HD3	2.30	0.66
2:F:158:TYR:CD1	2:F:158:TYR:N	2.65	0.65
3:G:12:ASN:HD22	3:G:13:PHE:H	1.44	0.65
1:3:127:VAL:CG1	1:3:131:ASN:HD21	2.10	0.65
1:4:10:ARG:NH1	1:4:11:PHE:H	1.88	0.65
1:4:10:ARG:CZ	1:4:139:GLU:HB2	2.25	0.65
1:3:60:TYR:CE2	1:3:70:ARG:HD3	2.31	0.65
1:1:108:ILE:HG12	1:2:123:PHE:HE1	1.61	0.65
1:3:27:LEU:HD11	1:3:85:TYR:HE2	1.62	0.65
4:B:6:LYS:HE3	4:B:82:THR:HA	1.77	0.65
1:1:135:LEU:HB2	1:1:137:ASP:HB2	1.77	0.65
3:G:74:SER:O	3:G:125:ASP:O	2.15	0.64
3:G:63:ASP:H	3:G:163:GLN:HE22	1.45	0.64
1:1:31:GLU:H	1:1:147:ARG:HH21	1.44	0.64
1:4:44:ILE:HG22	1:4:45:ALA:N	2.13	0.64
1:4:124:THR:O	1:4:128:ARG:HB2	1.98	0.64
2:F:328:ILE:HG22	2:F:332:ASP:HB2	1.80	0.64
4:B:105:GLU:O	4:B:106:PHE:HB2	1.98	0.64
4:B:95:ASP:C	4:B:97:ASN:N	2.50	0.64
2:F:29:THR:HA	2:F:286:LEU:HD23	1.79	0.64
2:F:320:TYR:HH	2:F:350:TRP:HZ3	1.43	0.63
1:3:63:LEU:HD23	1:4:93:THR:HG22	1.80	0.63
1:3:121:PHE:HE1	1:3:125:LEU:HD11	1.63	0.63
1:2:93:THR:O	1:2:97:ILE:HG13	1.98	0.63
2:F:418:THR:HG22	2:F:419:THR:N	2.13	0.63
1:3:87:HIS:CG	1:3:88:PRO:HD2	2.34	0.63
2:F:328:ILE:HD11	2:F:345:ILE:HG21	1.81	0.63
2:F:308:LEU:HD13	2:F:313:ILE:HD11	1.80	0.63
2:F:9:ARG:HA	2:F:415:ASN:HD22	1.64	0.62
2:F:41:PHE:HA	2:F:412:VAL:HG13	1.81	0.62
1:2:108:ILE:O	1:2:111:VAL:HG22	1.99	0.62
2:F:418:THR:HG22	2:F:419:THR:H	1.64	0.62
1:2:78:ILE:CD1	1:2:104:THR:HG21	2.29	0.62
1:3:42:VAL:HG12	1:3:43:TRP:N	2.14	0.62
2:F:40:SER:OG	2:F:274:ARG:HG2	1.99	0.62
1:4:10:ARG:NH2	1:4:139:GLU:CB	2.52	0.62
1:3:5:THR:O	1:3:6:GLU:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:228:TYR:CZ	2:F:230:ALA:HB3	2.35	0.62
1:1:116:LYS:NZ	1:1:119:GLU:HB2	2.15	0.62
1:1:66:VAL:CG1	1:2:44:ILE:HA	2.30	0.62
1:4:10:ARG:HH21	1:4:139:GLU:HB2	1.54	0.61
1:3:26:VAL:HG13	1:3:65:PHE:CD2	2.35	0.61
1:4:67:GLY:O	1:4:68:TYR:C	2.36	0.61
1:1:30:THR:HA	1:1:147:ARG:HE	1.61	0.61
2:F:274:ARG:HB3	4:B:105:GLU:HG2	1.83	0.61
2:F:414:ARG:HD3	2:F:416:LEU:HG	1.83	0.61
1:1:9:VAL:HG21	1:2:7:GLN:OE1	1.99	0.61
1:2:113:ARG:NH2	1:2:119:GLU:CD	2.53	0.61
1:3:37:LEU:HD21	1:3:58:CYS:SG	2.40	0.61
1:1:30:THR:HB	1:1:147:ARG:NH2	2.16	0.61
1:2:18:ILE:HG21	1:2:84:TYR:HD2	1.64	0.61
1:3:36:PHE:CE2	1:3:50:ARG:HB2	2.36	0.61
1:3:43:TRP:NE1	1:3:90:ASN:CG	2.55	0.60
1:4:93:THR:O	1:4:97:ILE:HG13	2.01	0.60
1:1:108:ILE:HG12	1:2:123:PHE:CE1	2.36	0.60
1:3:26:VAL:HG13	1:3:65:PHE:HD2	1.67	0.60
4:B:87:SER:OG	4:B:88:ALA:N	2.35	0.60
1:1:134:VAL:HG12	1:1:136:THR:H	1.65	0.60
2:F:206:GLN:O	2:F:210:TYR:HD1	1.85	0.60
2:F:309:THR:CG2	2:F:310:TYR:N	2.63	0.60
1:4:21:ILE:O	1:4:23:ALA:N	2.34	0.60
1:4:68:TYR:OH	1:4:139:GLU:OE2	2.19	0.60
2:F:285:THR:O	2:F:286:LEU:HB2	2.01	0.60
2:F:69:PHE:CE1	2:F:134:TYR:CD2	2.89	0.60
3:G:60:ILE:CD1	3:G:161:LEU:HB2	2.30	0.60
1:3:71:PHE:CE1	1:4:117:ALA:HB1	2.37	0.60
1:2:109:ASN:O	1:2:111:VAL:HG13	2.01	0.60
1:4:66:VAL:O	1:4:66:VAL:HG12	2.01	0.60
1:4:116:LYS:HD2	1:4:119:GLU:OE1	2.02	0.60
2:F:169:TRP:CZ3	2:F:375:PRO:HG3	2.37	0.60
1:3:27:LEU:HD13	1:3:29:LEU:HD12	1.83	0.59
2:F:49:LEU:HD22	2:F:64:VAL:HG11	1.83	0.59
1:4:68:TYR:OH	1:4:139:GLU:CD	2.40	0.59
1:2:78:ILE:HD11	1:2:104:THR:HG21	1.83	0.59
1:2:78:ILE:HD11	1:2:104:THR:CG2	2.32	0.59
1:3:116:LYS:HG3	1:3:117:ALA:H	1.67	0.59
2:F:238:MET:SD	2:F:238:MET:C	2.80	0.59
1:4:67:GLY:O	1:4:69:PRO:CD	2.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:87:HIS:CD2	1:2:89:VAL:HB	2.31	0.59
1:1:87:HIS:CG	1:1:88:PRO:HD2	2.37	0.59
1:4:68:TYR:C	1:4:69:PRO:O	2.35	0.59
2:F:67:PHE:O	2:F:68:THR:HG23	2.03	0.59
3:G:9:HIS:HD2	3:G:74:SER:OG	1.85	0.59
4:B:114:VAL:HG12	4:B:115:ASN:N	2.17	0.59
2:F:212:MET:SD	2:F:212:MET:C	2.81	0.59
3:G:13:PHE:N	3:G:13:PHE:HD1	2.01	0.58
2:F:36:ILE:HG22	2:F:37:ALA:N	2.16	0.58
1:4:10:ARG:NH1	1:4:139:GLU:OE2	2.36	0.58
2:F:354:ALA:HB1	2:F:355:PRO:HD2	1.85	0.58
3:G:81:PHE:CD1	3:G:155:CYS:HB3	2.37	0.58
1:1:141:ASN:O	1:1:144:GLN:HB2	2.02	0.58
2:F:202:LEU:HD13	2:F:206:GLN:NE2	2.19	0.58
2:F:397:VAL:HG12	2:F:397:VAL:O	2.03	0.58
3:G:13:PHE:CD1	3:G:13:PHE:N	2.72	0.58
1:1:108:ILE:HG23	1:2:123:PHE:HE1	1.69	0.58
2:F:168:ILE:HG13	2:F:353:TYR:CD2	2.39	0.58
1:4:145:LYS:NZ	1:4:149:GLU:HB2	2.18	0.58
2:F:154:ASP:CA	2:F:158:TYR:HE1	2.14	0.58
1:3:60:TYR:HD2	1:3:70:ARG:HD3	1.63	0.58
1:3:87:HIS:CD2	1:3:88:PRO:HD2	2.38	0.58
1:2:71:PHE:O	1:2:73:ALA:N	2.37	0.58
2:F:24:ILE:HD11	2:F:291:PHE:HD2	1.68	0.58
2:F:414:ARG:HH11	2:F:414:ARG:HG2	1.69	0.57
2:F:35:VAL:HG21	2:F:283:MET:HG3	1.86	0.57
2:F:73:HIS:ND1	2:F:281:GLY:HA2	2.19	0.57
1:1:84:TYR:HE1	1:1:134:VAL:HB	1.69	0.57
1:2:71:PHE:HB3	1:2:72:PRO:CD	2.33	0.57
2:F:49:LEU:CD2	2:F:64:VAL:HG21	2.33	0.57
1:1:79:ALA:CB	1:1:124:THR:HG22	2.34	0.57
2:F:26:ARG:HD3	2:F:159:GLY:O	2.05	0.57
2:F:249:VAL:O	2:F:249:VAL:HG12	2.04	0.57
2:F:240:SER:OG	2:F:270:HIS:HD2	1.86	0.57
3:G:74:SER:O	3:G:75:VAL:HG12	2.05	0.57
3:G:110:TYR:CE2	3:G:129:ILE:HD12	2.40	0.57
2:F:104:ASP:O	2:F:105:HIS:HB2	2.04	0.57
1:1:8:SER:O	1:1:12:GLN:HG2	2.04	0.57
1:2:7:GLN:HE22	1:2:126:ARG:HH21	1.52	0.57
1:2:68:TYR:CE1	1:3:93:THR:HG22	2.36	0.57
2:F:23:GLN:HE22	2:F:401:GLN:NE2	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:328:ILE:HG22	2:F:329:SER:N	2.19	0.57
2:F:23:GLN:NE2	2:F:24:ILE:HG22	2.20	0.57
1:4:71:PHE:CD2	1:4:72:PRO:O	2.57	0.57
1:3:43:TRP:N	1:3:43:TRP:CD1	2.71	0.56
1:1:133:ASP:O	1:1:134:VAL:HG23	2.05	0.56
1:3:36:PHE:HE2	1:3:50:ARG:HB2	1.70	0.56
3:G:44:PHE:O	3:G:44:PHE:HD1	1.87	0.56
1:4:64:ASP:OD1	1:4:70:ARG:NH2	2.36	0.56
2:F:239:ARG:O	2:F:239:ARG:HG3	1.96	0.56
1:2:20:LEU:HD13	1:2:65:PHE:HE1	1.70	0.56
2:F:39:ASP:O	2:F:40:SER:HB3	2.04	0.56
3:G:41:THR:HB	3:G:160:SER:HB2	1.86	0.56
2:F:320:TYR:HE2	2:F:348:GLY:HA2	1.70	0.56
1:3:71:PHE:CZ	1:4:117:ALA:HB1	2.40	0.56
2:F:167:ASN:OD1	2:F:168:ILE:N	2.38	0.56
1:1:31:GLU:H	1:1:147:ARG:NH2	2.03	0.56
3:G:158:LEU:N	3:G:158:LEU:HD23	2.19	0.56
2:F:152:ASN:HB2	2:F:155:ASP:HB2	1.87	0.56
1:3:7:GLN:HB3	1:3:11:PHE:CD1	2.40	0.56
1:3:127:VAL:HG13	1:3:131:ASN:HD21	1.69	0.56
4:B:1:MET:O	4:B:2:GLU:HB2	2.06	0.56
1:3:71:PHE:HE1	1:4:96:LEU:HG	1.71	0.56
1:2:36:PHE:HZ	1:2:47:ASP:HB3	1.70	0.56
2:F:7:ALA:HB3	4:B:100:ARG:HD2	0.63	0.55
2:F:26:ARG:HB3	2:F:159:GLY:O	2.06	0.55
1:2:7:GLN:C	1:2:9:VAL:H	2.09	0.55
2:F:263:ARG:HH21	2:F:265:GLN:NE2	2.03	0.55
1:3:127:VAL:HG12	1:3:131:ASN:ND2	2.22	0.55
2:F:36:ILE:CG2	2:F:37:ALA:N	2.69	0.55
1:1:38:THR:HG22	1:1:85:TYR:O	2.07	0.55
2:F:212:MET:SD	2:F:213:GLN:HA	2.47	0.55
1:2:56:GLU:HG2	1:2:103:PHE:CE1	2.41	0.55
1:1:76:GLU:OE1	1:1:104:THR:HG23	2.06	0.55
1:2:35:ASP:HB3	1:2:41:LYS:NZ	2.22	0.55
2:F:353:TYR:OH	2:F:355:PRO:HA	2.07	0.55
2:F:367:GLY:O	2:F:368:PHE:CG	2.60	0.55
1:1:25:ALA:HB3	1:1:62:THR:CG2	2.37	0.55
2:F:8:GLU:N	4:B:100:ARG:NH1	2.55	0.54
1:2:111:VAL:CG2	1:2:111:VAL:O	2.55	0.54
4:B:85:ASP:O	4:B:89:GLN:HG3	2.07	0.54
2:F:154:ASP:CA	2:F:158:TYR:CE1	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:3:GLN:NE2	4:B:90:ILE:HB	2.22	0.54
1:3:44:ILE:HG22	1:3:45:ALA:N	2.21	0.54
1:3:75:VAL:HG23	1:3:102:GLU:C	2.28	0.54
1:4:76:GLU:OE1	1:4:123:PHE:HE2	1.91	0.54
2:F:157:ARG:CG	2:F:158:TYR:CZ	2.80	0.54
1:4:36:PHE:CE2	1:4:50:ARG:HB2	2.41	0.54
2:F:102:TYR:HD2	2:F:105:HIS:CE1	2.26	0.54
3:G:94:PHE:CD2	3:G:103:LEU:HD12	2.43	0.54
3:G:90:CYS:SG	3:G:109:VAL:CG2	2.95	0.54
1:4:43:TRP:CZ3	1:4:51:ALA:HB1	2.43	0.54
2:F:386:ARG:HG3	2:F:389:ASP:OD2	2.08	0.54
2:F:56:ARG:HH22	2:F:366:GLU:H	1.55	0.54
1:3:26:VAL:HB	1:3:62:THR:HG22	1.90	0.54
2:F:236:LEU:O	2:F:238:MET:N	2.40	0.54
2:F:78:GLY:O	2:F:80:GLN:N	2.40	0.54
1:4:138:ALA:O	1:4:142:VAL:HG23	2.08	0.54
1:1:79:ALA:CA	1:1:124:THR:HG22	2.36	0.54
1:2:113:ARG:HH21	1:2:119:GLU:CD	2.11	0.54
3:G:38:THR:HG23	3:G:163:GLN:HB3	1.90	0.54
1:4:67:GLY:O	1:4:69:PRO:N	2.41	0.53
1:3:29:LEU:HD22	1:3:33:ASP:HB3	1.88	0.53
1:2:60:TYR:CD1	1:2:70:ARG:HD3	2.43	0.53
1:3:42:VAL:HG12	1:3:43:TRP:H	1.74	0.53
2:F:259:GLN:O	2:F:260:PHE:CD1	2.61	0.53
1:2:20:LEU:HD13	1:2:65:PHE:CE1	2.43	0.53
3:G:15:SER:CA	3:G:41:THR:HG23	2.33	0.53
1:4:145:LYS:HZ3	1:4:149:GLU:HB2	1.74	0.53
2:F:195:LEU:O	2:F:198:ALA:HB3	2.08	0.53
1:1:43:TRP:CZ3	1:1:51:ALA:HB1	2.43	0.53
2:F:56:ARG:NH2	2:F:366:GLU:H	2.07	0.53
2:F:202:LEU:HD13	2:F:206:GLN:HE21	1.73	0.53
2:F:285:THR:O	2:F:286:LEU:CB	2.55	0.53
1:2:106:ASN:HB2	1:2:115:VAL:HG22	1.89	0.53
2:F:199:TYR:O	2:F:202:LEU:HB2	2.08	0.53
1:3:60:TYR:O	1:3:63:LEU:HB2	2.09	0.53
1:1:119:GLU:HG3	3:G:134:ARG:O	2.09	0.53
2:F:98:ASN:O	2:F:148:PRO:HD2	2.09	0.53
2:F:55:ARG:HH12	2:F:366:GLU:CD	2.12	0.53
1:1:90:ASN:HD22	1:1:90:ASN:C	2.12	0.53
2:F:357:TYR:CE1	2:F:359:SER:HA	2.43	0.53
2:F:35:VAL:CG2	2:F:283:MET:HG3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:413:TYR:H	2:F:413:TYR:HD1	1.56	0.52
1:4:139:GLU:O	1:4:142:VAL:HB	2.09	0.52
2:F:175:PRO:HG2	2:F:176:GLU:HG3	1.91	0.52
1:3:69:PRO:O	1:4:96:LEU:HD11	2.09	0.52
3:G:44:PHE:O	3:G:44:PHE:CD1	2.61	0.52
1:3:58:CYS:SG	1:3:85:TYR:CE2	2.93	0.52
1:3:75:VAL:O	1:3:75:VAL:HG12	2.09	0.52
1:3:36:PHE:HE2	1:3:50:ARG:HD2	1.75	0.52
2:F:362:TYR:HD1	2:F:368:PHE:CE2	2.27	0.52
2:F:56:ARG:HH12	2:F:365:LEU:HB3	1.74	0.52
4:B:113:GLU:O	4:B:114:VAL:CB	2.48	0.52
3:G:41:THR:CB	3:G:160:SER:HB2	2.40	0.52
2:F:413:TYR:HD1	2:F:413:TYR:N	2.04	0.52
2:F:23:GLN:HE22	2:F:401:GLN:CD	2.13	0.52
1:1:116:LYS:HZ2	1:1:119:GLU:HB2	1.75	0.52
2:F:153:GLN:HB3	2:F:157:ARG:HD3	1.91	0.52
2:F:157:ARG:NE	2:F:158:TYR:CZ	2.64	0.52
2:F:414:ARG:NH1	2:F:414:ARG:CB	2.69	0.51
2:F:238:MET:SD	2:F:238:MET:O	2.69	0.51
2:F:235:LEU:N	2:F:235:LEU:HD23	2.25	0.51
2:F:112:ILE:HD12	2:F:112:ILE:N	2.24	0.51
1:1:102:GLU:HG2	1:1:113:ARG:O	2.10	0.51
1:1:87:HIS:CE1	1:1:88:PRO:HG2	2.45	0.51
2:F:239:ARG:NH1	4:B:120:PHE:CD1	2.78	0.51
1:3:33:ASP:OD2	1:3:53:ARG:NH2	2.42	0.51
1:4:128:ARG:HH11	1:4:128:ARG:HG3	1.76	0.51
1:2:58:CYS:HB2	1:2:81:VAL:HG11	1.92	0.51
2:F:311:THR:HG22	2:F:319:LEU:CD1	2.37	0.51
1:3:115:VAL:CG1	1:3:119:GLU:HB3	2.39	0.51
2:F:406:VAL:CG1	2:F:407:LYS:N	2.73	0.51
2:F:69:PHE:CE1	2:F:134:TYR:HD2	2.28	0.51
2:F:363:HIS:O	2:F:364:LEU:CG	2.58	0.51
1:3:26:VAL:CG1	1:3:65:PHE:CD2	2.94	0.51
1:1:29:LEU:HD21	1:1:57:ALA:HB3	1.92	0.51
1:2:10:ARG:NH1	1:2:76:GLU:HG2	2.25	0.51
2:F:242:LEU:HD21	2:F:268:TYR:HB2	1.93	0.51
1:4:133:ASP:CB	2:F:118:LYS:NZ	2.73	0.51
1:3:116:LYS:CG	1:3:117:ALA:N	2.74	0.51
2:F:8:GLU:HA	4:B:100:ARG:CZ	2.41	0.51
1:2:107:ILE:HG12	1:2:112:GLU:HG2	1.92	0.51
4:B:95:ASP:C	4:B:97:ASN:H	2.12	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:7:GLN:HE22	1:2:126:ARG:NH2	2.08	0.51
1:1:134:VAL:HG13	1:1:138:ALA:HB3	1.93	0.51
1:1:116:LYS:HZ1	1:1:119:GLU:CD	2.14	0.51
2:F:179:LEU:HD21	2:F:344:LYS:HD3	1.92	0.51
2:F:420:ARG:C	2:F:421:ASP:O	2.45	0.51
1:4:145:LYS:HD3	1:4:145:LYS:C	2.32	0.51
4:B:102:GLN:O	4:B:105:GLU:HB2	2.11	0.50
1:3:29:LEU:HD21	1:3:54:CYS:HA	1.93	0.50
2:F:23:GLN:HE22	2:F:24:ILE:HG22	1.75	0.50
3:G:3:GLN:HE21	3:G:4:THR:N	2.08	0.50
1:4:87:HIS:CE1	1:4:88:PRO:HG2	2.47	0.50
1:1:106:ASN:HD21	1:1:113:ARG:HD3	1.77	0.50
1:1:26:VAL:HG11	1:1:65:PHE:HB2	1.94	0.50
1:4:62:THR:O	1:4:65:PHE:HB3	2.12	0.50
3:G:62:MET:SD	3:G:131:VAL:HG12	2.51	0.50
2:F:60:ILE:HD11	2:F:370:PHE:CE1	2.46	0.50
1:4:87:HIS:CE1	1:4:89:VAL:HG23	2.46	0.50
2:F:173:LEU:HD12	2:F:325:PRO:CG	2.41	0.50
2:F:8:GLU:CA	4:B:100:ARG:CZ	2.90	0.50
1:1:42:VAL:HG12	1:1:43:TRP:N	2.26	0.50
2:F:104:ASP:O	2:F:105:HIS:CB	2.59	0.50
3:G:18:LEU:HD22	3:G:20:LEU:H	1.77	0.50
1:3:135:LEU:O	1:3:136:THR:C	2.51	0.49
2:F:333:VAL:O	2:F:333:VAL:HG12	2.12	0.49
2:F:247:TYR:CD1	2:F:248:ASP:N	2.77	0.49
2:F:299:ILE:HG22	2:F:300:GLN:N	2.27	0.49
1:4:121:PHE:CZ	1:4:125:LEU:HD11	2.47	0.49
1:3:35:ASP:O	1:3:39:SER:N	2.45	0.49
2:F:7:ALA:O	4:B:100:ARG:CD	2.55	0.49
2:F:8:GLU:N	4:B:100:ARG:CZ	2.76	0.49
3:G:75:VAL:HG13	3:G:75:VAL:O	2.12	0.49
3:G:48:THR:HG22	3:G:154:LYS:HG2	1.94	0.49
2:F:187:THR:C	2:F:188:THR:HG23	2.32	0.49
4:B:94:PHE:CE1	4:B:104:ALA:HB3	2.48	0.49
4:B:93:ARG:O	4:B:94:PHE:HB2	2.10	0.49
2:F:157:ARG:CZ	2:F:158:TYR:OH	2.57	0.49
1:1:30:THR:O	1:1:31:GLU:C	2.50	0.49
2:F:320:TYR:OH	2:F:350:TRP:HZ3	1.96	0.49
2:F:23:GLN:NE2	2:F:401:GLN:NE2	2.59	0.49
2:F:8:GLU:O	2:F:8:GLU:CG	2.57	0.49
1:2:7:GLN:HG2	1:2:7:GLN:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:191:ASP:O	2:F:194:GLY:N	2.43	0.49
1:3:127:VAL:O	1:3:131:ASN:ND2	2.46	0.49
2:F:172:PRO:HG2	2:F:379:LEU:HD13	1.95	0.49
2:F:40:SER:O	2:F:41:PHE:C	2.51	0.49
4:B:4:LEU:HB3	4:B:108:ARG:HB3	1.95	0.49
1:3:125:LEU:O	1:3:128:ARG:HB3	2.13	0.49
1:3:75:VAL:HG23	1:3:102:GLU:O	2.13	0.48
1:2:113:ARG:NH2	1:2:119:GLU:OE1	2.45	0.48
1:3:87:HIS:CE1	1:3:89:VAL:HG23	2.47	0.48
1:4:133:ASP:HA	1:4:136:THR:OG1	2.13	0.48
1:3:127:VAL:HG12	1:3:131:ASN:HD21	1.77	0.48
1:3:65:PHE:CD1	1:3:65:PHE:C	2.87	0.48
2:F:239:ARG:CG	2:F:239:ARG:O	2.59	0.48
3:G:62:MET:HG3	3:G:131:VAL:HG12	1.95	0.48
2:F:24:ILE:HG23	2:F:24:ILE:O	2.12	0.48
3:G:87:PHE:CB	3:G:148:SER:HB2	2.43	0.48
1:1:60:TYR:CD2	1:1:70:ARG:HD3	2.48	0.48
2:F:378:ASP:O	2:F:380:GLN:N	2.47	0.48
3:G:62:MET:SD	3:G:131:VAL:CG1	3.02	0.48
1:3:48:ARG:O	1:3:51:ALA:HB3	2.14	0.48
1:2:10:ARG:NH1	1:2:76:GLU:CD	2.64	0.48
1:2:106:ASN:HD22	1:2:113:ARG:HH21	1.60	0.48
1:1:52:ARG:O	1:1:56:GLU:HB2	2.14	0.48
2:F:296:THR:HB	2:F:363:HIS:HB2	1.95	0.48
1:1:44:ILE:HG22	1:1:45:ALA:N	2.28	0.48
3:G:12:ASN:ND2	3:G:13:PHE:N	2.58	0.48
2:F:72:PRO:HD2	2:F:75:HIS:CE1	2.47	0.47
1:4:27:LEU:CD1	1:4:58:CYS:SG	3.02	0.47
1:2:43:TRP:H	1:2:90:ASN:HD21	1.62	0.47
4:B:94:PHE:HA	4:B:102:GLN:OE1	2.14	0.47
4:B:105:GLU:O	4:B:106:PHE:CB	2.59	0.47
2:F:397:VAL:CG1	2:F:397:VAL:O	2.62	0.47
3:G:131:VAL:O	3:G:140:VAL:HG11	2.15	0.47
3:G:9:HIS:HB2	3:G:74:SER:HB2	1.96	0.47
3:G:38:THR:HG22	3:G:38:THR:O	2.13	0.47
2:F:265:GLN:O	2:F:266:GLN:C	2.51	0.47
1:1:116:LYS:NZ	1:1:119:GLU:CD	2.67	0.47
1:1:75:VAL:HG11	1:1:103:PHE:HE1	1.78	0.47
1:1:34:PHE:C	1:1:36:PHE:H	2.16	0.47
1:2:75:VAL:HG12	1:2:123:PHE:CD2	2.50	0.47
2:F:386:ARG:O	2:F:388:HIS:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:185:THR:HG22	2:F:186:SER:O	2.14	0.47
2:F:7:ALA:C	4:B:100:ARG:NE	2.67	0.47
4:B:94:PHE:O	4:B:95:ASP:HB2	2.14	0.47
2:F:29:THR:HG22	2:F:286:LEU:CD2	2.45	0.47
2:F:20:LEU:HD22	2:F:30:ILE:HG23	1.97	0.47
1:2:135:LEU:HD13	1:2:136:THR:N	2.30	0.47
2:F:406:VAL:C	2:F:407:LYS:HG3	2.35	0.47
1:3:65:PHE:C	1:3:65:PHE:HD1	2.18	0.47
2:F:169:TRP:HZ3	2:F:375:PRO:HG3	1.77	0.47
1:4:98:MET:HB2	1:4:120:LEU:HD13	1.95	0.47
1:3:60:TYR:CD1	1:3:60:TYR:N	2.79	0.47
1:1:134:VAL:HG12	1:1:135:LEU:N	2.30	0.47
2:F:11:PRO:HG2	2:F:11:PRO:O	2.13	0.47
2:F:284:PHE:N	2:F:284:PHE:CD1	2.82	0.47
2:F:372:GLN:O	2:F:373:GLU:HB2	2.15	0.47
2:F:202:LEU:O	2:F:205:ASP:N	2.48	0.47
2:F:380:GLN:H	2:F:382:ARG:H	1.62	0.47
2:F:128:LEU:HD23	2:F:160:PHE:HZ	1.79	0.47
2:F:135:PHE:O	2:F:136:LYS:CB	2.55	0.47
1:1:87:HIS:ND1	1:1:89:VAL:HB	2.30	0.47
3:G:73:VAL:HG11	3:G:142:VAL:HG11	1.97	0.47
3:G:161:LEU:HD12	3:G:161:LEU:N	2.29	0.46
1:2:106:ASN:ND2	1:2:119:GLU:OE1	2.48	0.46
1:3:116:LYS:CG	1:3:117:ALA:H	2.28	0.46
2:F:178:GLU:C	2:F:179:LEU:HD23	2.36	0.46
2:F:263:ARG:HH21	2:F:265:GLN:HE22	1.63	0.46
1:2:95:CYS:SG	1:2:121:PHE:HA	2.56	0.46
2:F:247:TYR:HD1	2:F:248:ASP:N	2.03	0.46
2:F:406:VAL:C	2:F:407:LYS:CG	2.83	0.46
2:F:82:ILE:HD12	2:F:82:ILE:H	1.76	0.46
2:F:418:THR:HG21	2:F:420:ARG:HD3	1.97	0.46
1:2:79:ALA:HA	1:2:124:THR:HG22	1.97	0.46
1:4:35:ASP:O	1:4:36:PHE:C	2.54	0.46
1:4:44:ILE:CG2	1:4:45:ALA:N	2.78	0.46
1:2:116:LYS:HB2	1:2:119:GLU:OE2	2.16	0.46
2:F:390:TYR:O	2:F:394:PHE:CD2	2.69	0.46
2:F:320:TYR:CE2	2:F:348:GLY:HA2	2.51	0.46
2:F:403:ASN:HB3	2:F:405:GLN:HE22	1.81	0.46
1:4:151:VAL:C	1:4:152:MET:CG	2.76	0.46
1:2:71:PHE:CB	1:2:72:PRO:CD	2.93	0.46
1:2:68:TYR:N	1:2:68:TYR:CD1	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:100:THR:HG23	2:F:149:ASN:HA	1.98	0.46
2:F:98:ASN:HB2	2:F:149:ASN:HD21	1.80	0.46
3:G:20:LEU:HG	3:G:21:THR:N	2.31	0.46
2:F:92:THR:HA	2:F:93:PRO:HD2	1.49	0.46
1:4:151:VAL:O	1:4:152:MET:SD	2.74	0.46
1:4:68:TYR:O	1:4:69:PRO:C	2.53	0.45
2:F:15:SER:HB3	2:F:409:ASN:HA	1.99	0.45
2:F:390:TYR:O	2:F:394:PHE:HD2	2.00	0.45
3:G:87:PHE:HB3	3:G:148:SER:HB2	1.97	0.45
1:4:68:TYR:HH	1:4:139:GLU:CD	2.16	0.45
2:F:41:PHE:CA	2:F:412:VAL:HG13	2.45	0.45
3:G:13:PHE:HD1	3:G:13:PHE:H	1.65	0.45
1:2:97:ILE:H	1:2:97:ILE:HG13	1.57	0.45
2:F:128:LEU:CD2	2:F:160:PHE:HZ	2.29	0.45
1:4:90:ASN:O	1:4:91:ILE:C	2.54	0.45
2:F:241:ASN:OD1	2:F:241:ASN:C	2.54	0.45
2:F:63:THR:HG23	2:F:243:TRP:CE2	2.51	0.45
2:F:152:ASN:HB2	2:F:155:ASP:H	1.81	0.45
2:F:334:PHE:CD2	2:F:374:PRO:HB3	2.51	0.45
4:B:82:THR:OG1	4:B:91:TYR:CD2	2.59	0.45
2:F:418:THR:CG2	2:F:419:THR:N	2.79	0.45
2:F:39:ASP:OD2	2:F:414:ARG:NH2	2.50	0.45
2:F:152:ASN:O	2:F:153:GLN:C	2.54	0.45
1:2:68:TYR:N	1:2:68:TYR:HD1	2.13	0.45
2:F:229:ASP:O	2:F:231:ASP:N	2.50	0.45
2:F:30:ILE:HG21	2:F:408:PHE:HZ	1.79	0.45
2:F:167:ASN:OD1	2:F:167:ASN:C	2.54	0.45
3:G:4:THR:HG22	3:G:6:ILE:H	1.82	0.45
3:G:164:VAL:HG12	3:G:164:VAL:O	2.16	0.45
1:3:104:THR:O	1:3:108:ILE:HG13	2.17	0.45
2:F:20:LEU:O	2:F:21:ALA:HB2	2.17	0.45
1:1:33:ASP:O	1:1:36:PHE:HB3	2.17	0.45
1:4:60:TYR:HD1	1:4:63:LEU:HD12	1.81	0.45
1:3:24:SER:HA	1:4:89:VAL:HG22	1.99	0.45
2:F:183:MET:HG3	2:F:184:THR:N	2.32	0.45
2:F:172:PRO:HG2	2:F:379:LEU:CD1	2.47	0.45
2:F:245:SER:OG	2:F:246:GLY:N	2.48	0.45
2:F:174:PRO:HD2	2:F:177:THR:CG2	2.47	0.45
1:4:140:GLU:O	1:4:141:ASN:C	2.55	0.44
2:F:295:ALA:HA	2:F:371:ILE:CG2	2.44	0.44
1:3:62:THR:HG21	1:4:89:VAL:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:29:ALA:O	3:G:102:THR:HA	2.17	0.44
1:1:90:ASN:O	1:1:90:ASN:ND2	2.49	0.44
1:3:104:THR:CB	1:4:126:ARG:HH12	2.30	0.44
1:2:71:PHE:CD1	1:2:71:PHE:C	2.90	0.44
1:3:92:GLN:HG3	1:3:121:PHE:CD2	2.52	0.44
2:F:329:SER:HB2	2:F:339:SER:HA	2.00	0.44
1:1:79:ALA:HB1	1:1:124:THR:HG22	1.98	0.44
1:2:35:ASP:HB3	1:2:41:LYS:HZ1	1.81	0.44
1:4:98:MET:HB2	1:4:120:LEU:CD1	2.48	0.44
4:B:102:GLN:HB3	4:B:103:PRO:HD2	1.99	0.44
2:F:363:HIS:O	2:F:364:LEU:CB	2.66	0.44
1:3:91:ILE:O	1:3:94:ALA:HB3	2.18	0.44
4:B:3:GLN:HE22	4:B:90:ILE:CG2	2.30	0.44
1:4:123:PHE:CD2	1:4:134:VAL:HG11	2.53	0.44
2:F:60:ILE:HG22	2:F:61:ASP:H	1.82	0.44
1:4:50:ARG:HH11	1:4:53:ARG:HH11	1.66	0.44
1:2:20:LEU:HB3	1:2:65:PHE:CZ	2.52	0.44
1:4:123:PHE:CE2	1:4:134:VAL:CG1	3.01	0.44
1:2:121:PHE:CE2	1:2:125:LEU:HD22	2.53	0.44
2:F:399:LEU:HD13	2:F:403:ASN:OD1	2.17	0.44
1:1:93:THR:O	1:1:97:ILE:HG23	2.17	0.44
4:B:6:LYS:CE	4:B:83:CYS:SG	2.99	0.44
1:4:105:GLU:CG	1:4:106:ASN:N	2.79	0.44
2:F:69:PHE:CD2	2:F:130:ILE:HD13	2.53	0.44
1:1:37:LEU:HG	1:1:54:CYS:HB3	1.99	0.44
2:F:388:HIS:O	2:F:390:TYR:N	2.51	0.43
1:3:131:ASN:O	1:3:135:LEU:N	2.50	0.43
2:F:74:ARG:NH2	2:F:229:ASP:HB2	2.33	0.43
1:2:124:THR:C	1:2:126:ARG:H	2.21	0.43
2:F:79:GLU:CA	2:F:82:ILE:HD13	2.46	0.43
2:F:122:HIS:CD2	2:F:282:THR:HG21	2.54	0.43
1:2:9:VAL:HG13	1:3:88:PRO:HB3	2.00	0.43
1:2:110:GLY:O	1:2:111:VAL:C	2.56	0.43
4:B:87:SER:O	4:B:91:TYR:CD2	2.71	0.43
1:3:115:VAL:HG13	1:3:119:GLU:CB	2.45	0.43
1:4:71:PHE:CE2	1:4:72:PRO:O	2.71	0.43
1:2:7:GLN:C	1:2:9:VAL:N	2.72	0.43
1:3:121:PHE:HE1	1:3:125:LEU:HD21	1.84	0.43
2:F:191:ASP:O	2:F:192:ILE:C	2.57	0.43
2:F:88:GLY:O	2:F:90:ASN:N	2.51	0.43
2:F:273:PRO:CD	4:B:107:TYR:OH	2.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:75:VAL:HA	3:G:160:SER:O	2.18	0.43
1:1:120:LEU:O	1:1:124:THR:HG23	2.19	0.43
2:F:195:LEU:HD23	2:F:195:LEU:HA	1.76	0.43
1:2:125:LEU:HD12	1:2:125:LEU:HA	1.84	0.43
1:2:52:ARG:O	1:2:53:ARG:C	2.57	0.43
2:F:418:THR:CG2	2:F:419:THR:H	2.29	0.43
1:1:113:ARG:NH2	3:G:136:PRO:CG	2.82	0.43
3:G:19:VAL:HG13	3:G:20:LEU:N	2.33	0.43
2:F:146:ALA:HB3	2:F:150:GLU:OE2	2.18	0.43
1:2:55:VAL:O	1:2:59:VAL:HG23	2.19	0.43
1:2:78:ILE:HD12	1:2:104:THR:HG21	2.00	0.43
1:4:52:ARG:O	1:4:53:ARG:C	2.56	0.43
1:1:31:GLU:H	1:1:147:ARG:HE	1.65	0.43
1:2:48:ARG:HG2	1:2:97:ILE:HG23	2.00	0.43
2:F:73:HIS:CE1	2:F:281:GLY:HA2	2.53	0.43
2:F:239:ARG:NH1	4:B:120:PHE:HD1	2.16	0.43
2:F:293:PRO:O	2:F:294:THR:HG23	2.19	0.43
2:F:46:VAL:HG12	2:F:47:GLY:N	2.33	0.43
1:3:29:LEU:HD22	1:3:33:ASP:CB	2.49	0.42
2:F:261:SER:OG	2:F:262:GLY:N	2.48	0.42
1:2:108:ILE:O	1:2:111:VAL:HG13	2.19	0.42
1:4:23:ALA:HB1	1:4:26:VAL:HG23	2.01	0.42
1:3:116:LYS:O	1:3:117:ALA:C	2.57	0.42
1:1:87:HIS:ND1	1:1:89:VAL:N	2.61	0.42
1:2:36:PHE:HB2	1:2:50:ARG:NH1	2.34	0.42
2:F:60:ILE:HG22	2:F:61:ASP:N	2.34	0.42
2:F:305:LYS:NZ	2:F:312:ASP:CG	2.73	0.42
1:1:11:PHE:CE1	1:1:15:LEU:HD11	2.54	0.42
1:4:87:HIS:CG	1:4:88:PRO:HD2	2.54	0.42
2:F:168:ILE:HD13	2:F:168:ILE:HG21	1.63	0.42
2:F:173:LEU:HD12	2:F:325:PRO:HG2	1.99	0.42
1:2:43:TRP:H	1:2:90:ASN:ND2	2.17	0.42
2:F:216:ARG:HH21	2:F:229:ASP:HA	1.84	0.42
1:4:44:ILE:HG22	1:4:45:ALA:H	1.84	0.42
1:4:15:LEU:HD23	1:4:62:THR:HG21	2.01	0.42
1:3:48:ARG:O	1:3:51:ALA:N	2.52	0.42
3:G:123:VAL:HG22	3:G:124:LYS:N	2.34	0.42
2:F:319:LEU:C	2:F:321:GLY:N	2.72	0.42
2:F:79:GLU:H	2:F:82:ILE:HD13	1.84	0.42
3:G:52:GLY:O	3:G:150:PHE:N	2.52	0.42
1:4:40:ASN:O	1:4:40:ASN:OD1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:328:ILE:CG2	2:F:332:ASP:HB2	2.47	0.42
1:4:62:THR:HA	1:4:65:PHE:HB3	2.01	0.42
1:4:65:PHE:HD2	1:4:66:VAL:HG23	1.83	0.42
2:F:209:ASP:O	2:F:213:GLN:NE2	2.53	0.42
1:2:135:LEU:HD22	1:2:135:LEU:HA	1.78	0.42
1:2:108:ILE:HG22	1:2:109:ASN:ND2	2.35	0.42
1:3:87:HIS:HE1	1:3:89:VAL:HG23	1.85	0.42
1:2:18:ILE:HA	1:2:21:ILE:HD12	2.01	0.42
2:F:100:THR:OG1	2:F:105:HIS:CD2	2.73	0.42
1:1:113:ARG:NH2	3:G:136:PRO:HG2	2.34	0.42
2:F:379:LEU:HD12	2:F:383:VAL:CG2	2.50	0.42
2:F:323:LEU:HA	2:F:324:PRO:HD2	1.90	0.42
1:3:21:ILE:O	1:3:22:GLN:C	2.57	0.42
1:1:25:ALA:HB3	1:1:62:THR:HG22	2.02	0.42
1:1:60:TYR:O	1:1:63:LEU:HB2	2.18	0.42
2:F:71:VAL:HG22	2:F:234:PRO:HB3	2.02	0.42
1:2:120:LEU:HD23	1:2:120:LEU:HA	1.67	0.42
1:2:113:ARG:NH2	1:2:119:GLU:OE2	2.53	0.41
1:2:33:ASP:O	1:2:36:PHE:HB3	2.19	0.41
3:G:158:LEU:N	3:G:158:LEU:CD2	2.82	0.41
2:F:69:PHE:HE1	2:F:134:TYR:CD2	2.36	0.41
2:F:362:TYR:CD1	2:F:368:PHE:CZ	3.08	0.41
2:F:273:PRO:O	2:F:274:ARG:C	2.58	0.41
4:B:83:CYS:O	4:B:84:ASP:HB2	2.21	0.41
2:F:338:ASP:OD1	2:F:338:ASP:C	2.58	0.41
4:B:93:ARG:HD2	4:B:93:ARG:H	1.85	0.41
1:3:87:HIS:ND1	1:3:89:VAL:HB	2.35	0.41
1:2:18:ILE:HG21	1:2:84:TYR:CE2	2.56	0.41
1:2:8:SER:C	1:2:10:ARG:N	2.69	0.41
2:F:24:ILE:CD1	2:F:291:PHE:HD2	2.34	0.41
2:F:294:THR:HG1	2:F:370:PHE:HD1	1.69	0.41
2:F:171:ALA:N	2:F:172:PRO:HD3	2.36	0.41
1:1:134:VAL:CG1	1:1:135:LEU:N	2.83	0.41
1:3:135:LEU:HD22	1:3:135:LEU:O	2.21	0.41
1:3:47:ASP:O	1:3:48:ARG:C	2.58	0.41
3:G:30:PRO:O	3:G:57:LEU:HD23	2.20	0.41
2:F:22:GLY:HA3	2:F:28:ILE:HD12	2.03	0.41
1:3:20:LEU:HD21	1:4:91:ILE:HD12	2.03	0.41
2:F:161:ARG:HD2	2:F:385:ILE:O	2.21	0.41
1:2:36:PHE:CZ	1:2:50:ARG:HD2	2.55	0.41
1:2:121:PHE:O	1:2:125:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:399:LEU:HD23	2:F:399:LEU:HA	1.89	0.41
1:3:30:THR:O	1:3:31:GLU:C	2.59	0.41
1:4:128:ARG:NH1	1:4:128:ARG:HG2	2.27	0.41
1:3:15:LEU:CD2	1:3:131:ASN:OD1	2.69	0.41
2:F:78:GLY:C	2:F:80:GLN:H	2.23	0.41
1:1:27:LEU:HD22	1:1:29:LEU:CD1	2.51	0.41
4:B:93:ARG:O	4:B:94:PHE:CB	2.69	0.41
1:1:108:ILE:HG23	1:2:123:PHE:CZ	2.56	0.41
1:1:25:ALA:HB3	1:1:62:THR:HG21	2.02	0.41
1:1:29:LEU:H	1:1:29:LEU:HG	1.24	0.41
2:F:93:PRO:O	2:F:94:LEU:HB2	2.21	0.41
3:G:29:ALA:CB	3:G:55:GLY:O	2.69	0.41
2:F:316:ASP:HA	2:F:317:PRO:HD2	1.84	0.41
1:2:10:ARG:NH1	1:2:10:ARG:CG	2.70	0.41
1:3:44:ILE:CG2	1:3:45:ALA:H	2.29	0.41
1:4:128:ARG:NH1	1:4:128:ARG:CG	2.65	0.40
2:F:170:THR:C	2:F:172:PRO:HD3	2.41	0.40
1:3:20:LEU:CD2	1:4:91:ILE:HD12	2.51	0.40
1:1:114:PRO:O	1:1:114:PRO:HG2	2.21	0.40
2:F:99:THR:HB	2:F:113:ASN:HD21	1.84	0.40
3:G:160:SER:C	3:G:161:LEU:HD12	2.42	0.40
3:G:9:HIS:HD2	3:G:74:SER:CB	2.35	0.40
1:1:135:LEU:HD23	1:1:135:LEU:HA	1.84	0.40
1:1:30:THR:O	1:1:33:ASP:N	2.54	0.40
2:F:132:ASN:HA	2:F:136:LYS:HD2	2.03	0.40
1:4:18:ILE:CD1	1:4:26:VAL:HG11	2.51	0.40
3:G:19:VAL:CG1	3:G:20:LEU:N	2.85	0.40
2:F:101:GLY:HA2	2:F:117:ASN:OD1	2.21	0.40
2:F:40:SER:O	2:F:41:PHE:O	2.39	0.40
2:F:82:ILE:N	2:F:82:ILE:CD1	2.80	0.40
2:F:174:PRO:HD2	2:F:177:THR:HG21	2.02	0.40
2:F:16:HIS:CG	2:F:16:HIS:O	2.74	0.40
1:3:95:CYS:C	1:3:97:ILE:N	2.75	0.40
2:F:165:LEU:HA	2:F:165:LEU:HD23	1.90	0.40
1:3:85:TYR:N	1:3:85:TYR:CD1	2.89	0.40
1:4:71:PHE:HB2	1:4:72:PRO:HD2	2.03	0.40
1:4:135:LEU:HA	1:4:135:LEU:HD23	1.83	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	1	141/152 (93%)	125 (89%)	14 (10%)	2 (1%)	14	58
1	2	131/152 (86%)	103 (79%)	20 (15%)	8 (6%)	2	21
1	3	138/152 (91%)	114 (83%)	13 (9%)	11 (8%)	1	13
1	4	144/152 (95%)	112 (78%)	26 (18%)	6 (4%)	3	32
2	F	416/426 (98%)	331 (80%)	47 (11%)	38 (9%)	1	11
3	G	173/175 (99%)	152 (88%)	18 (10%)	3 (2%)	11	54
4	B	45/120 (38%)	25 (56%)	9 (20%)	11 (24%)	0	1
All	All	1188/1329 (89%)	962 (81%)	147 (12%)	79 (7%)	1	19

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	111	VAL
1	3	9	VAL
1	3	61	GLY
1	3	117	ALA
1	4	8	SER
1	4	22	GLN
1	4	70	ARG
2	F	5	THR
2	F	41	PHE
2	F	93	PRO
2	F	105	HIS
2	F	168	ILE
2	F	185	THR
2	F	212	MET
2	F	230	ALA
2	F	237	VAL
2	F	316	ASP
2	F	355	PRO

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Mol	Chain	Res	Type
2	F	356	SER
2	F	364	LEU
2	F	379	LEU
3	G	37	ALA
4	B	81	ALA
4	B	84	ASP
4	B	94	PHE
4	B	95	ASP
4	B	114	VAL
1	1	61	GLY
1	1	136	THR
1	2	137	ASP
1	3	6	GLU
1	4	105	GLU
2	F	101	GLY
2	F	213	GLN
2	F	380	GLN
3	G	75	VAL
4	B	2	GLU
4	B	96	LYS
4	B	106	PHE
4	B	108	ARG
1	2	8	SER
1	2	28	ASP
1	2	118	ALA
1	2	134	VAL
1	3	7	GLN
1	3	31	GLU
1	3	99	GLU
1	3	136	THR
1	3	138	ALA
2	F	94	LEU
2	F	266	GLN
2	F	371	ILE
2	F	372	GLN
2	F	373	GLU
2	F	389	ASP
4	B	117	PHE
1	3	132	THR
1	4	71	PHE
2	F	57	GLY
2	F	68	THR

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Mol	Chain	Res	Type
2	F	79	GLU
2	F	136	LYS
2	F	239	ARG
2	F	248	ASP
2	F	257	LEU
2	F	325	PRO
2	F	370	PHE
1	2	102	GLU
1	3	45	ALA
2	F	167	ASN
2	F	286	LEU
2	F	400	LEU
3	G	136	PRO
4	B	107	TYR
1	2	7	GLN
1	4	67	GLY
2	F	262	GLY
2	F	249	VAL
2	F	317	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	119/127 (94%)	108 (91%)	11 (9%)	11	45
1	2	110/127 (87%)	94 (86%)	16 (14%)	4	23
1	3	117/127 (92%)	103 (88%)	14 (12%)	6	30
1	4	121/127 (95%)	107 (88%)	14 (12%)	7	33
2	F	364/372 (98%)	315 (86%)	49 (14%)	5	26
3	G	153/153 (100%)	133 (87%)	20 (13%)	5	27
4	B	42/101 (42%)	37 (88%)	5 (12%)	6	31
All	All	1026/1134 (90%)	897 (87%)	129 (13%)	5	28

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	7	GLN
1	1	17	SER
1	1	27	LEU
1	1	29	LEU
1	1	37	LEU
1	1	90	ASN
1	1	105	GLU
1	1	116	LYS
1	1	126	ARG
1	1	136	THR
1	1	147	ARG
1	2	10	ARG
1	2	13	THR
1	2	27	LEU
1	2	35	ASP
1	2	37	LEU
1	2	44	ILE
1	2	50	ARG
1	2	84	TYR
1	2	93	THR
1	2	96	LEU
1	2	102	GLU
1	2	109	ASN
1	2	113	ARG
1	2	119	GLU
1	2	126	ARG
1	2	135	LEU
1	3	36	PHE
1	3	40	ASN
1	3	41	LYS
1	3	43	TRP
1	3	58	CYS
1	3	65	PHE
1	3	71	PHE
1	3	85	TYR
1	3	104	THR
1	3	113	ARG
1	3	120	LEU
1	3	121	PHE
1	3	134	VAL
1	3	135	LEU
1	4	10	ARG
1	4	11	PHE

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Mol	Chain	Res	Type
1	4	52	ARG
1	4	70	ARG
1	4	76	GLU
1	4	96	LEU
1	4	103	PHE
1	4	105	GLU
1	4	111	VAL
1	4	119	GLU
1	4	126	ARG
1	4	128	ARG
1	4	133	ASP
1	4	145	LYS
2	F	4	GLN
2	F	9	ARG
2	F	10	MET
2	F	23	GLN
2	F	31	SER
2	F	52	SER
2	F	58	LEU
2	F	62	SER
2	F	63	THR
2	F	68	THR
2	F	104	ASP
2	F	105	HIS
2	F	108	PHE
2	F	115	ASP
2	F	144	THR
2	F	148	PRO
2	F	158	TYR
2	F	164	HIS
2	F	179	LEU
2	F	181	ARG
2	F	183	MET
2	F	202	LEU
2	F	212	MET
2	F	213	GLN
2	F	214	ARG
2	F	226	THR
2	F	229	ASP
2	F	233	ARG
2	F	238	MET
2	F	239	ARG

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Mol	Chain	Res	Type
2	F	242	LEU
2	F	247	TYR
2	F	248	ASP
2	F	250	ASP
2	F	259	GLN
2	F	282	THR
2	F	312	ASP
2	F	335	ARG
2	F	349	GLN
2	F	350	TRP
2	F	353	TYR
2	F	359	SER
2	F	364	LEU
2	F	372	GLN
2	F	389	ASP
2	F	393	CYS
2	F	413	TYR
2	F	414	ARG
2	F	420	ARG
3	G	10	ASN
3	G	12	ASN
3	G	13	PHE
3	G	18	LEU
3	G	22	SER
3	G	23	VAL
3	G	24	THR
3	G	41	THR
3	G	60	ILE
3	G	91	LEU
3	G	92	VAL
3	G	109	VAL
3	G	115	ARG
3	G	126	CYS
3	G	128	THR
3	G	136	PRO
3	G	140	VAL
3	G	149	ASN
3	G	169	ILE
3	G	174	LEU
4	B	4	LEU
4	B	84	ASP
4	B	85	ASP

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Mol	Chain	Res	Type
4	B	94	PHE
4	B	108	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	90	ASN
1	1	106	ASN
1	1	141	ASN
1	2	87	HIS
1	2	90	ASN
1	2	109	ASN
1	3	131	ASN
2	F	23	GLN
2	F	75	HIS
2	F	105	HIS
2	F	149	ASN
2	F	206	GLN
2	F	232	ASN
2	F	265	GLN
2	F	270	HIS
2	F	387	HIS
2	F	405	GLN
2	F	415	ASN
3	G	3	GLN
3	G	9	HIS
3	G	10	ASN
3	G	12	ASN
3	G	70	ASN
3	G	149	ASN
3	G	162	ASN
3	G	163	GLN
4	B	3	GLN
4	B	110	HIS

5.3.3 RNA ⓘ

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	1	143/152 (94%)	-0.14	0 100 100	20, 20, 20, 20	0
1	2	133/152 (87%)	-0.12	1 (0%) 87 80	20, 20, 20, 20	0
1	3	140/152 (92%)	-0.21	0 100 100	20, 20, 20, 20	0
1	4	146/152 (96%)	-0.11	0 100 100	20, 20, 20, 20	0
2	F	418/426 (98%)	-0.00	0 100 100	20, 20, 20, 20	0
3	G	175/175 (100%)	0.18	1 (0%) 90 85	20, 20, 20, 20	0
4	B	49/120 (40%)	0.24	2 (4%) 41 32	20, 20, 20, 20	0
All	All	1204/1329 (90%)	-0.03	4 (0%) 94 91	20, 20, 20, 20	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	67	GLY	2.4
4	B	3	GLN	2.4
3	G	27	SER	2.3
4	B	84	ASP	2.3

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

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

6.3 Carbohydrates ⓘ

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.