Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2021 – 04:04 am BST

PDB ID	:	7NL4
Title	:	OsNIP2;1 silicon transporter from rice
Authors	:	van den Berg, B.
Deposited on	:	2021-02-22
Resolution	:	3.00 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:

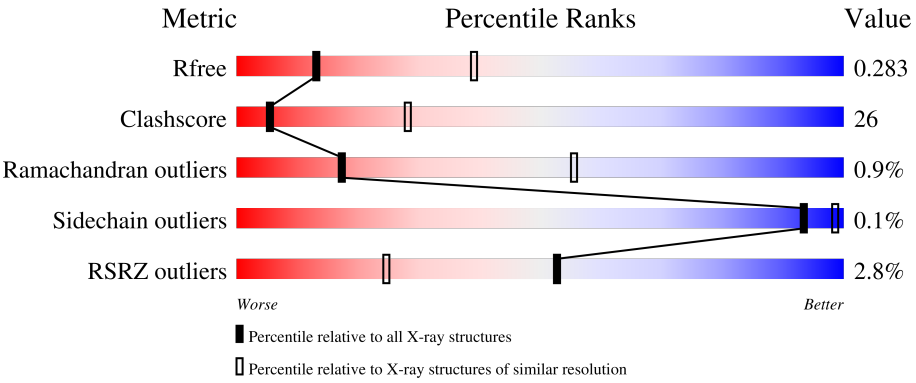
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	227	6% 52% 41% 5%
1	B	227	% 51% 42% 5%
1	C	227	% 54% 38% 6%
1	D	227	2% 56% 35% 5%
1	E	227	% 56% 36% 5%

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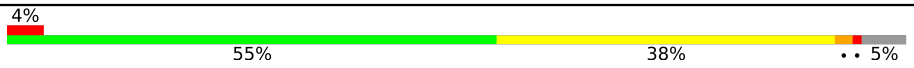
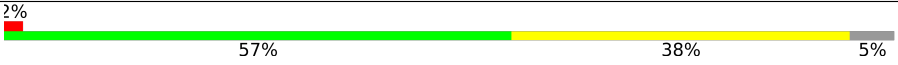
Mol	Chain	Length	Quality of chain
1	F	227	
1	G	227	
1	H	227	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12829 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 Aquaporin NIP2-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1605	1057	262	276	10			
1	B	216	Total	C	N	O	S	0	0	0
			1605	1057	262	276	10			
1	C	214	Total	C	N	O	S	0	0	0
			1585	1043	260	272	10			
1	D	216	Total	C	N	O	S	0	0	0
			1605	1057	262	276	10			
1	E	216	Total	C	N	O	S	0	0	0
			1605	1057	262	276	10			
1	F	216	Total	C	N	O	S	0	0	0
			1605	1057	262	276	10			
1	G	216	Total	C	N	O	S	0	0	0
			1605	1057	262	276	10			
1	H	216	Total	C	N	O	S	0	0	0
			1605	1057	262	276	10			

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cd	0	0
			1	1		
2	B	1	Total	Cd	0	0
			1	1		
2	C	1	Total	Cd	0	0
			1	1		
2	D	3	Total	Cd	0	0
			3	3		
2	F	1	Total	Cd	0	0
			1	1		
2	G	1	Total	Cd	0	0
			1	1		

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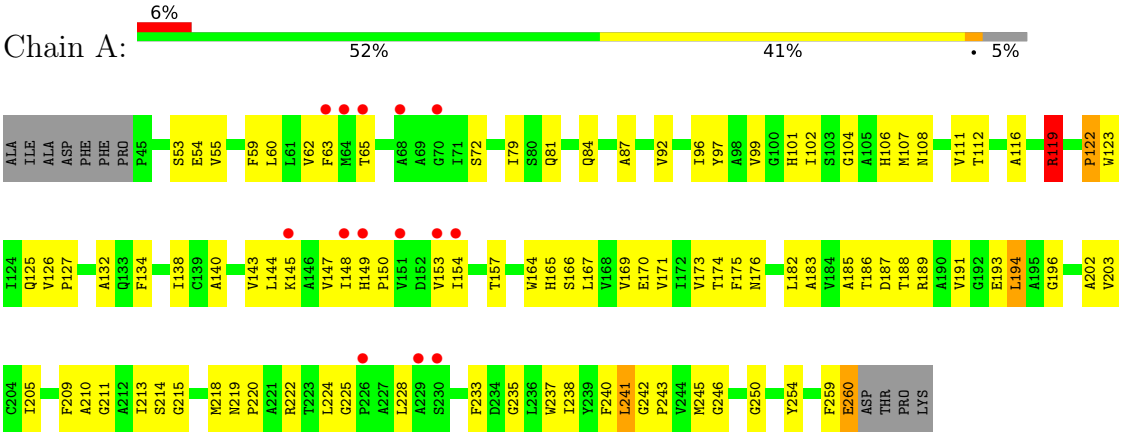
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	1	Total	Cd	0	0
			1	1		

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.

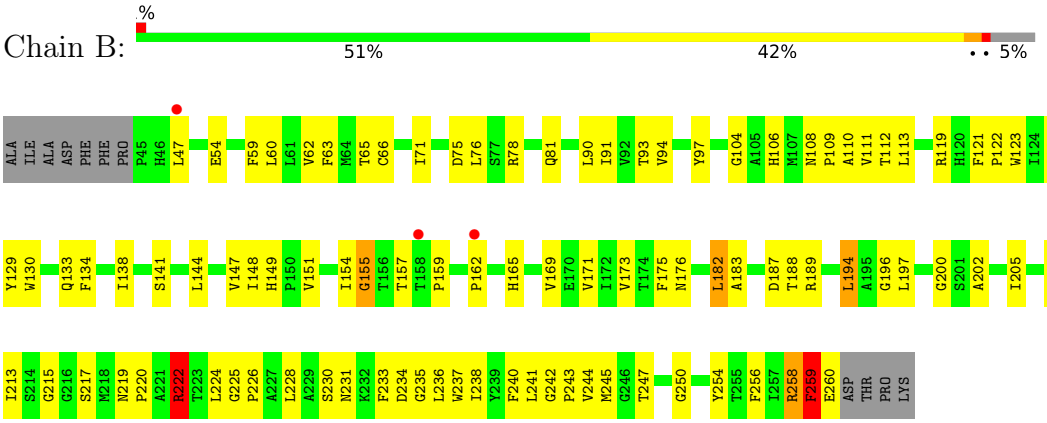
• Molecule 1: Aquaporin NIP2-1

Chain A:



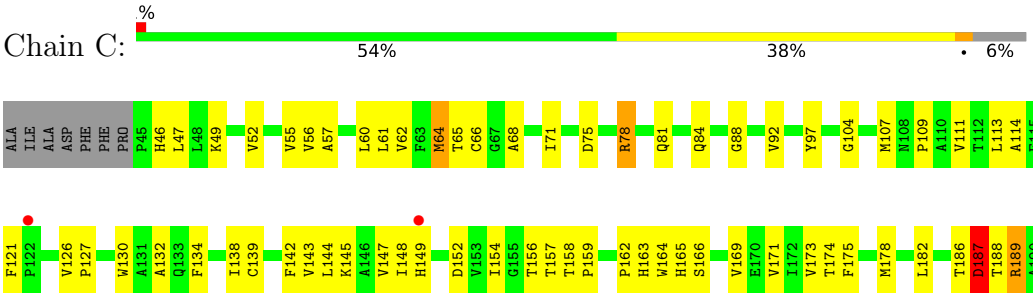
• Molecule 1: Aquaporin NIP2-1

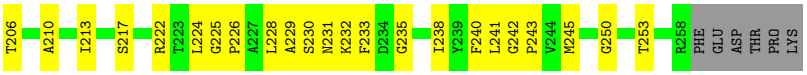
Chain B:



• Molecule 1: Aquaporin NIP2-1

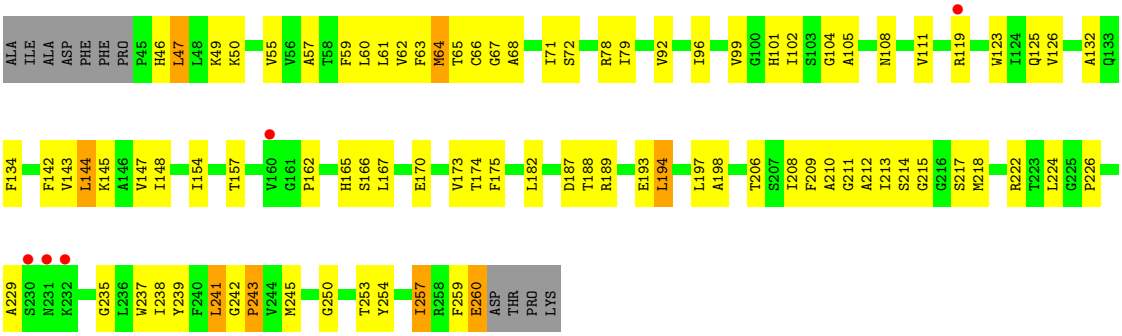
Chain C:





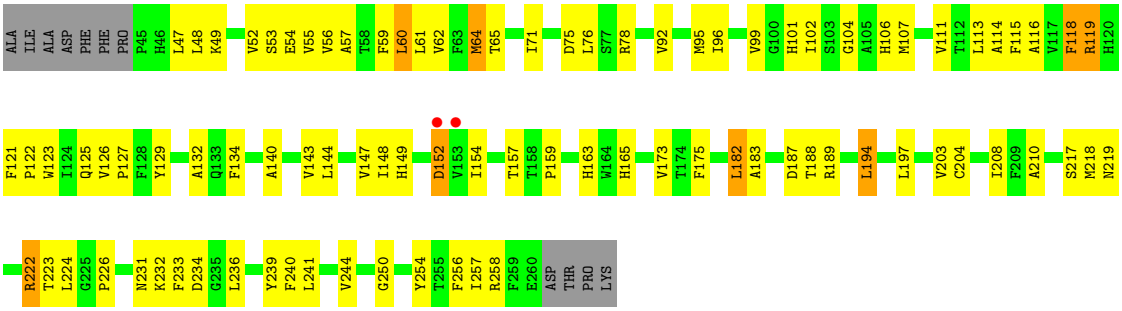
• Molecule 1: Aquaporin NIP2-1

Chain D:



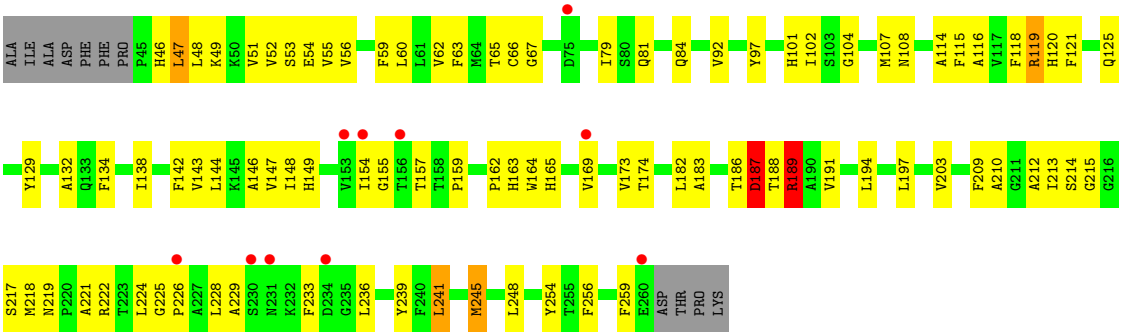
• Molecule 1: Aquaporin NIP2-1

Chain E:



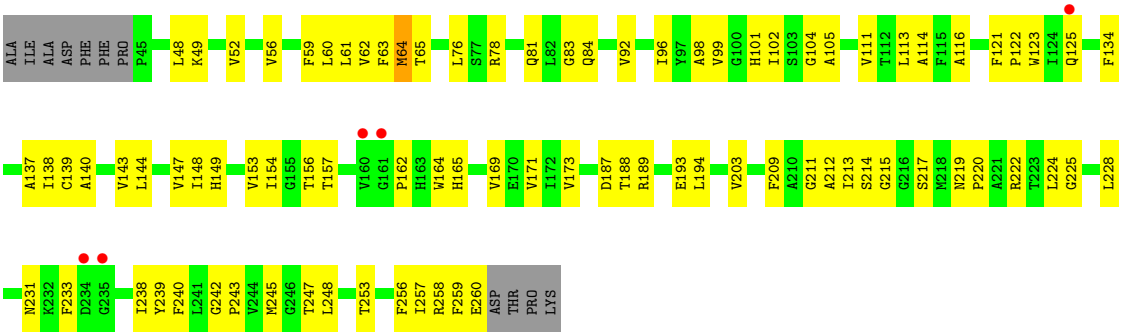
• Molecule 1: Aquaporin NIP2-1

Chain F:



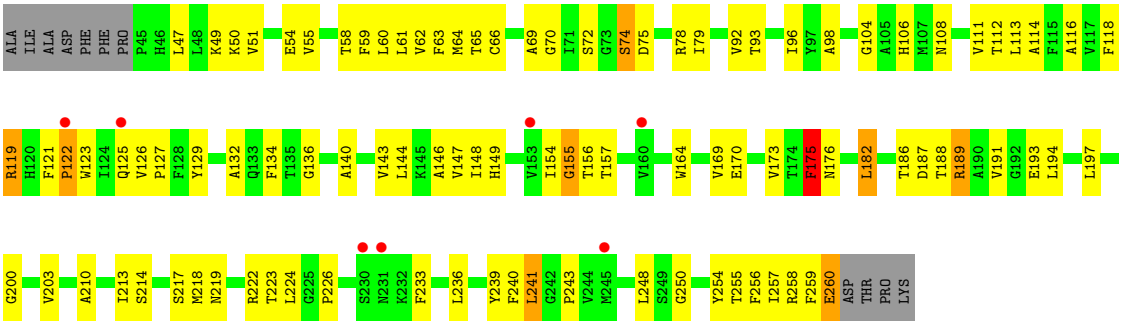
• Molecule 1: Aquaporin NIP2-1

Chain G:



• Molecule 1: Aquaporin NIP2-1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	94.89Å 96.69Å 99.79Å 63.91° 71.16° 65.07°	Depositor
Resolution (Å)	48.78 – 3.00 88.33 – 2.62	Depositor EDS
% Data completeness (in resolution range)	78.9 (48.78-3.00) 56.8 (88.33-2.62)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.62Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.238 , 0.282 0.238 , 0.283	Depositor DCC
R_{free} test set	2369 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	64.8	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	12829	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.60	0/1650	0.98	8/2256 (0.4%)
1	B	0.58	0/1650	0.93	6/2256 (0.3%)
1	C	0.60	1/1629 (0.1%)	0.91	6/2228 (0.3%)
1	D	0.58	0/1650	1.31	10/2256 (0.4%)
1	E	0.71	2/1650 (0.1%)	2.49	18/2256 (0.8%)
1	F	0.62	2/1650 (0.1%)	1.02	11/2256 (0.5%)
1	G	0.57	0/1650	0.87	9/2256 (0.4%)
1	H	0.58	0/1650	1.30	11/2256 (0.5%)
All	All	0.61	5/13179 (0.0%)	1.33	79/18020 (0.4%)

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	A	0	2
1	B	0	1
1	D	0	1
1	E	0	3
1	F	0	2
1	H	0	1
All	All	0	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	204	CYS	CB-SG	-7.00	1.70	1.82
1	E	119	ARG	CB-CG	6.83	1.71	1.52
1	F	119	ARG	CB-CG	-5.56	1.37	1.52
1	F	119	ARG	CZ-NH1	-5.51	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	191	VAL	CB-CG1	-5.34	1.41	1.52

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	119	ARG	NE-CZ-NH1	-64.95	87.82	120.30
1	E	152	ASP	CB-CG-OD1	49.72	163.04	118.30
1	E	119	ARG	NE-CZ-NH2	42.58	141.59	120.30
1	E	152	ASP	CB-CG-OD2	-38.32	83.81	118.30
1	D	260	GLU	OE1-CD-OE2	-37.57	78.22	123.30
1	H	260	GLU	OE1-CD-OE2	-34.20	82.26	123.30
1	E	119	ARG	NH1-CZ-NH2	-27.80	88.82	119.40
1	E	152	ASP	OD1-CG-OD2	-23.00	79.59	123.30
1	H	260	GLU	CG-CD-OE1	21.42	161.13	118.30
1	D	260	GLU	CG-CD-OE2	-19.28	79.73	118.30
1	H	260	GLU	CG-CD-OE2	-17.79	82.73	118.30
1	E	119	ARG	CD-NE-CZ	17.50	148.09	123.60
1	D	260	GLU	CG-CD-OE1	16.85	152.00	118.30
1	A	119	ARG	NE-CZ-NH1	-15.80	112.40	120.30
1	A	119	ARG	CD-NE-CZ	13.60	142.63	123.60
1	F	119	ARG	NE-CZ-NH1	-12.02	114.29	120.30
1	E	118	PHE	C-N-CA	-10.51	95.42	121.70
1	F	118	PHE	C-N-CA	-10.02	96.65	121.70
1	E	119	ARG	CA-CB-CG	-9.39	92.74	113.40
1	B	222	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	F	119	ARG	NH1-CZ-NH2	8.88	129.17	119.40
1	E	119	ARG	N-CA-CB	8.71	126.27	110.60
1	D	47	LEU	CB-CG-CD2	-8.59	96.39	111.00
1	A	119	ARG	CB-CG-CD	-8.37	89.84	111.60
1	F	119	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	H	175	PHE	CB-CG-CD2	-7.21	115.75	120.80
1	C	119	ARG	CG-CD-NE	6.96	126.42	111.80
1	D	241	LEU	CB-CG-CD2	-6.95	99.18	111.00
1	B	194	LEU	CA-CB-CG	6.77	130.88	115.30
1	E	182	LEU	CB-CG-CD1	-6.76	99.51	111.00
1	H	241	LEU	CB-CG-CD2	-6.74	99.55	111.00
1	B	222	ARG	CD-NE-CZ	6.61	132.86	123.60
1	A	260	GLU	CG-CD-OE2	-6.61	105.09	118.30
1	H	119	ARG	CG-CD-NE	6.52	125.50	111.80
1	G	76	LEU	CB-CG-CD1	-6.49	99.97	111.00
1	C	64	MET	CA-CB-CG	-6.48	102.28	113.30
1	H	194	LEU	CA-CB-CG	6.40	130.02	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	189	ARG	CB-CG-CD	-6.39	94.97	111.60
1	F	194	LEU	CB-CG-CD2	6.38	121.85	111.00
1	G	194	LEU	CA-CB-CG	6.34	129.89	115.30
1	G	78	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	D	194	LEU	CA-CB-CG	6.20	129.57	115.30
1	F	245	MET	CA-CB-CG	6.18	123.81	113.30
1	G	258	ARG	CG-CD-NE	-6.18	98.82	111.80
1	F	119	ARG	CG-CD-NE	6.13	124.66	111.80
1	E	194	LEU	CB-CG-CD1	-6.06	100.70	111.00
1	C	189	ARG	CB-CG-CD	-6.04	95.90	111.60
1	F	47	LEU	CA-CB-CG	6.01	129.13	115.30
1	D	47	LEU	CA-CB-CG	5.98	129.06	115.30
1	E	119	ARG	CB-CA-C	-5.98	98.44	110.40
1	E	119	ARG	N-CA-C	-5.93	94.98	111.00
1	H	182	LEU	CB-CG-CD1	-5.92	100.93	111.00
1	C	187	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	B	182	LEU	CB-CG-CD1	-5.89	100.98	111.00
1	H	175	PHE	CB-CG-CD1	5.87	124.91	120.80
1	E	76	LEU	CB-CG-CD1	-5.84	101.07	111.00
1	G	228	LEU	CB-CG-CD2	-5.81	101.12	111.00
1	G	76	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	241	LEU	CA-CB-CG	-5.70	102.18	115.30
1	E	60	LEU	CB-CG-CD2	5.69	120.67	111.00
1	C	78	ARG	CG-CD-NE	-5.64	99.96	111.80
1	G	76	LEU	CB-CG-CD2	-5.55	101.56	111.00
1	F	120	HIS	C-N-CA	-5.45	108.08	121.70
1	D	119	ARG	CG-CD-NE	5.45	123.24	111.80
1	G	64	MET	CA-CB-CG	-5.37	104.18	113.30
1	C	189	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	A	260	GLU	CG-CD-OE1	5.31	128.92	118.30
1	E	194	LEU	CA-CB-CG	5.28	127.45	115.30
1	D	144	LEU	CB-CG-CD2	5.26	119.94	111.00
1	G	258	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	H	119	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	258	ARG	C-N-CA	5.17	134.62	121.70
1	A	260	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	A	194	LEU	CA-CB-CG	5.16	127.16	115.30
1	E	64	MET	CA-CB-CG	-5.09	104.65	113.30
1	D	64	MET	CA-CB-CG	-5.06	104.70	113.30
1	H	189	ARG	CB-CG-CD	-5.03	98.53	111.60
1	F	241	LEU	CA-CB-CG	-5.02	103.75	115.30
1	B	259	PHE	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	ARG	Sidechain
1	A	260	GLU	Sidechain
1	B	222	ARG	Sidechain
1	D	260	GLU	Sidechain
1	E	118	PHE	Peptide
1	E	119	ARG	Sidechain,Mainchain
1	F	187	ASP	Sidechain
1	F	189	ARG	Sidechain
1	H	175	PHE	Sidechain

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	1605	0	1629	95	0
1	B	1605	0	1629	99	0
1	C	1585	0	1614	91	0
1	D	1605	0	1629	102	0
1	E	1605	0	1629	91	0
1	F	1605	0	1629	105	0
1	G	1605	0	1629	84	0
1	H	1605	0	1629	107	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	3	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
All	All	12829	0	13017	672	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 26.

All (672) 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:F:187:ASP:OD1	1:F:189:ARG:NH2	1.84	1.10
1:A:149:HIS:HB2	1:D:165:HIS:HE1	1.13	1.10
1:A:149:HIS:HB2	1:D:165:HIS:CE1	1.92	1.04
1:D:104:GLY:HA3	1:D:189:ARG:HB3	1.43	1.00
1:H:157:THR:OG1	1:H:222:ARG:NH1	1.96	0.99
1:A:104:GLY:HA3	1:A:189:ARG:HB3	1.38	0.99
1:A:188:THR:HG23	1:A:191:VAL:HG21	1.54	0.89
1:D:157:THR:OG1	1:D:222:ARG:NH1	2.05	0.88
1:C:159:PRO:HG2	1:C:163:HIS:CD2	2.10	0.86
1:F:213:ILE:HD11	1:H:148:ILE:HG22	1.56	0.85
1:B:104:GLY:HA3	1:B:189:ARG:HB3	1.59	0.84
1:E:257:ILE:HA	1:G:49:LYS:HD2	1.59	0.84
1:F:182:LEU:HD23	1:F:254:TYR:HB3	1.58	0.84
1:G:104:GLY:CA	1:G:189:ARG:HB3	2.07	0.83
1:G:187:ASP:OD1	1:G:189:ARG:NH2	2.11	0.83
1:A:167:LEU:N	1:A:238:ILE:HD11	1.95	0.82
1:D:104:GLY:CA	1:D:189:ARG:HB3	2.10	0.82
1:D:182:LEU:HD23	1:D:254:TYR:HB3	1.62	0.82
1:F:157:THR:HG21	1:F:217:SER:HB2	1.62	0.81
1:H:175:PHE:CD1	1:H:250:GLY:HA2	2.15	0.81
1:A:104:GLY:CA	1:A:189:ARG:HB3	2.10	0.81
1:E:165:HIS:NE2	1:G:149:HIS:HB2	1.96	0.80
1:F:187:ASP:HA	1:F:189:ARG:NH2	1.96	0.79
1:F:187:ASP:HA	1:F:189:ARG:HH21	1.50	0.76
1:F:59:PHE:HD1	1:F:60:LEU:HD12	1.51	0.76
1:F:49:LYS:NZ	1:G:256:PHE:O	2.19	0.76
1:B:173:VAL:HA	1:D:64:MET:HE1	1.68	0.75
1:G:104:GLY:HA3	1:G:189:ARG:HB3	1.67	0.75
1:F:144:LEU:O	1:F:148:ILE:HG12	1.88	0.74
1:F:62:VAL:HA	1:F:65:THR:HG22	1.67	0.74
1:H:175:PHE:HD1	1:H:250:GLY:HA2	1.53	0.74
1:B:104:GLY:CA	1:B:189:ARG:HB3	2.17	0.74
1:B:188:THR:N	1:B:189:ARG:HA	2.02	0.73
1:H:187:ASP:HA	1:H:189:ARG:NH2	2.02	0.73
1:C:188:THR:N	1:C:189:ARG:HA	2.01	0.73
1:A:119:ARG:HH11	1:A:185:ALA:HB3	1.54	0.73
1:F:256:PHE:O	1:H:49:LYS:HE3	1.88	0.73
1:H:119:ARG:HD3	1:H:182:LEU:HD11	1.68	0.73
1:A:149:HIS:HB3	1:A:150:PRO:HD3	1.69	0.73
1:B:148:ILE:HG22	1:C:213:ILE:HD11	1.71	0.73
1:E:231:ASN:OD1	1:E:233:PHE:HE1	1.71	0.72
1:A:173:VAL:HA	1:C:64:MET:HE1	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:THR:OG1	1:F:222:ARG:NH2	2.22	0.72
1:D:59:PHE:HD1	1:D:60:LEU:HD12	1.55	0.72
1:D:187:ASP:OD1	1:D:189:ARG:NH2	2.23	0.72
1:B:62:VAL:HA	1:B:65:THR:HG22	1.71	0.71
1:E:149:HIS:CE1	1:H:164:TRP:HZ2	2.08	0.71
1:C:162:PRO:HD2	1:C:165:HIS:CE1	2.26	0.71
1:H:154:ILE:O	1:H:156:THR:N	2.24	0.71
1:B:219:ASN:HB3	1:B:222:ARG:HB3	1.74	0.70
1:D:241:LEU:HB3	1:D:245:MET:HE1	1.73	0.70
1:A:182:LEU:HD23	1:A:254:TYR:HB3	1.74	0.69
1:H:104:GLY:HA3	1:H:189:ARG:HB3	1.75	0.69
1:C:116:ALA:HA	1:C:121:PHE:HB3	1.74	0.69
1:F:149:HIS:H	1:G:165:HIS:CE1	2.10	0.69
1:H:116:ALA:HB1	1:H:123:TRP:CD1	2.27	0.69
1:A:166:SER:HB2	1:A:238:ILE:HD13	1.74	0.69
1:A:188:THR:N	1:A:189:ARG:HA	2.08	0.68
1:B:119:ARG:HB2	1:B:189:ARG:HH12	1.57	0.68
1:C:126:VAL:HG13	1:C:127:PRO:HD3	1.74	0.68
1:G:188:THR:N	1:G:189:ARG:HA	2.08	0.68
1:G:104:GLY:HA2	1:G:189:ARG:HB3	1.73	0.68
1:E:187:ASP:HA	1:E:189:ARG:CZ	2.24	0.68
1:F:214:SER:O	1:F:239:TYR:OH	2.10	0.68
1:C:166:SER:HB2	1:C:238:ILE:HD12	1.75	0.68
1:A:164:TRP:HZ2	1:C:149:HIS:NE2	1.91	0.67
1:E:188:THR:N	1:E:189:ARG:HA	2.08	0.67
1:E:144:LEU:O	1:E:148:ILE:HG12	1.95	0.67
1:A:187:ASP:HA	1:A:189:ARG:NH2	2.09	0.67
1:G:157:THR:HG21	1:G:217:SER:HB2	1.77	0.67
1:D:188:THR:N	1:D:189:ARG:HA	2.10	0.67
1:E:173:VAL:HA	1:G:64:MET:HE1	1.77	0.67
1:B:149:HIS:HD1	1:C:165:HIS:CE1	2.13	0.66
1:D:63:PHE:HA	1:D:144:LEU:HD11	1.76	0.66
1:A:63:PHE:HA	1:A:144:LEU:HD11	1.77	0.66
1:F:54:GLU:HG3	1:F:129:TYR:CE1	2.30	0.66
1:H:188:THR:N	1:H:189:ARG:HA	2.11	0.66
1:E:149:HIS:HE1	1:H:164:TRP:HZ2	1.44	0.66
1:H:233:PHE:HD2	1:H:236:LEU:HD22	1.59	0.66
1:A:140:ALA:O	1:A:144:LEU:HD12	1.96	0.66
1:A:213:ILE:HD11	1:C:148:ILE:HG22	1.76	0.66
1:E:53:SER:HB3	1:E:99:VAL:HB	1.77	0.66
1:F:188:THR:HB	1:F:191:VAL:HG21	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:GLY:HA2	1:E:189:ARG:H	1.61	0.66
1:F:56:VAL:HG11	1:G:253:THR:HG21	1.78	0.65
1:C:187:ASP:HA	1:C:189:ARG:HE	1.61	0.65
1:B:149:HIS:ND1	1:C:165:HIS:NE2	2.45	0.65
1:E:62:VAL:HA	1:E:65:THR:HG22	1.79	0.65
1:B:187:ASP:HA	1:B:189:ARG:HD2	1.79	0.65
1:F:148:ILE:HD11	1:F:154:ILE:HD12	1.77	0.65
1:C:171:VAL:HG11	1:C:245:MET:HE3	1.77	0.65
1:D:206:THR:HG23	1:D:210:ALA:HB3	1.79	0.64
1:H:59:PHE:HD1	1:H:60:LEU:HD12	1.61	0.64
1:D:62:VAL:HA	1:D:65:THR:HG22	1.78	0.64
1:E:101:HIS:CD2	1:E:102:ILE:HG13	2.33	0.64
1:B:187:ASP:OD1	1:B:189:ARG:NH2	2.31	0.64
1:A:62:VAL:HA	1:A:65:THR:HG22	1.78	0.64
1:F:212:ALA:HB2	1:H:79:ILE:HG13	1.80	0.63
1:B:119:ARG:HG3	1:B:182:LEU:HD11	1.80	0.63
1:B:157:THR:HG21	1:B:217:SER:HB2	1.78	0.63
1:F:148:ILE:HG22	1:G:213:ILE:HD11	1.80	0.63
1:H:54:GLU:HG3	1:H:129:TYR:CD1	2.34	0.63
1:H:61:LEU:O	1:H:65:THR:HG22	1.99	0.63
1:D:214:SER:O	1:D:239:TYR:OH	2.13	0.63
1:G:92:VAL:HG21	1:G:203:VAL:HG11	1.80	0.63
1:A:97:TYR:HD2	1:D:198:ALA:HB2	1.62	0.63
1:C:119:ARG:HD3	1:C:187:ASP:OD1	1.98	0.63
1:E:157:THR:HG21	1:E:217:SER:HB2	1.81	0.63
1:F:134:PHE:CE1	1:F:224:LEU:HD12	2.34	0.63
1:F:149:HIS:HD1	1:G:165:HIS:HE2	1.40	0.62
1:F:186:THR:O	1:F:187:ASP:HB2	1.98	0.62
1:D:47:LEU:HA	1:D:50:LYS:HB2	1.81	0.62
1:A:148:ILE:HD11	1:A:154:ILE:HD12	1.79	0.62
1:B:144:LEU:O	1:B:148:ILE:HG12	1.99	0.62
1:F:147:VAL:HG11	1:G:169:VAL:HG23	1.82	0.62
1:B:76:LEU:HD11	1:B:81:GLN:HB2	1.82	0.62
1:A:149:HIS:CB	1:D:165:HIS:HE1	2.02	0.62
1:B:47:LEU:HB3	1:B:125:GLN:HE21	1.64	0.62
1:H:134:PHE:CE1	1:H:224:LEU:HD12	2.34	0.62
1:F:143:VAL:O	1:F:147:VAL:HG23	1.99	0.61
1:B:224:LEU:HD23	1:B:236:LEU:HD11	1.82	0.61
1:D:173:VAL:HG11	1:D:210:ALA:HB2	1.83	0.61
1:E:122:PRO:HB2	1:E:125:GLN:HG3	1.80	0.61
1:H:104:GLY:CA	1:H:189:ARG:HB3	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:O	1:A:147:VAL:HG23	2.00	0.61
1:C:165:HIS:HB3	1:C:213:ILE:HG23	1.82	0.61
1:A:54:GLU:OE2	1:A:107:MET:N	2.30	0.60
1:B:112:THR:OG1	1:B:133:GLN:NE2	2.33	0.60
1:F:79:ILE:HD11	1:G:209:PHE:HA	1.81	0.60
1:D:235:GLY:O	1:D:238:ILE:HG12	2.01	0.60
1:E:101:HIS:HD2	1:E:102:ILE:HG13	1.67	0.60
1:F:101:HIS:O	1:G:260:GLU:HG3	2.02	0.60
1:A:119:ARG:NH1	1:A:185:ALA:HB3	2.16	0.60
1:B:123:TRP:HD1	1:B:126:VAL:HG11	1.66	0.60
1:D:157:THR:HG1	1:D:222:ARG:NH1	2.00	0.60
1:A:166:SER:HB2	1:A:238:ILE:CD1	2.32	0.60
1:B:154:ILE:H	1:B:230:SER:HB3	1.67	0.60
1:E:148:ILE:HG22	1:H:213:ILE:HD11	1.82	0.60
1:C:157:THR:HG23	1:C:222:ARG:NH1	2.17	0.60
1:D:174:THR:HG21	1:D:243:PRO:HA	1.83	0.60
1:F:47:LEU:HD21	1:F:125:GLN:HB3	1.83	0.60
1:F:173:VAL:HA	1:H:64:MET:HE1	1.84	0.60
1:F:142:PHE:CE1	1:F:229:ALA:HA	2.36	0.59
1:H:106:HIS:HD2	1:H:111:VAL:HG12	1.67	0.59
1:B:162:PRO:HB2	1:B:165:HIS:CD2	2.37	0.59
1:G:187:ASP:HA	1:G:189:ARG:HD2	1.85	0.59
1:B:113:LEU:HB2	1:B:130:TRP:HZ2	1.68	0.59
1:F:52:VAL:HG21	1:G:256:PHE:HE2	1.68	0.59
1:A:165:HIS:NE2	1:C:149:HIS:CD2	2.71	0.59
1:D:71:ILE:HG23	1:D:78:ARG:HE	1.68	0.59
1:D:108:ASN:HB3	1:D:111:VAL:HB	1.85	0.59
1:E:187:ASP:HA	1:E:189:ARG:NH2	2.18	0.59
1:G:116:ALA:HB1	1:G:123:TRP:CD1	2.38	0.59
1:B:59:PHE:HD1	1:B:60:LEU:HD12	1.67	0.58
1:D:241:LEU:O	1:D:245:MET:HB3	2.04	0.58
1:E:149:HIS:HE1	1:H:164:TRP:CZ2	2.21	0.58
1:E:231:ASN:OD1	1:E:233:PHE:CE1	2.55	0.58
1:A:92:VAL:HG21	1:A:203:VAL:HG11	1.85	0.58
1:A:122:PRO:HB2	1:A:125:GLN:HB2	1.84	0.58
1:H:157:THR:HG21	1:H:217:SER:HB2	1.85	0.58
1:F:101:HIS:CD2	1:F:102:ILE:HG13	2.38	0.58
1:D:55:VAL:HG12	1:D:132:ALA:O	2.04	0.58
1:H:188:THR:O	1:H:188:THR:HG22	2.04	0.58
1:A:116:ALA:HB1	1:A:123:TRP:CD1	2.39	0.58
1:C:144:LEU:O	1:C:148:ILE:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:ALA:HB1	1:E:123:TRP:CD1	2.39	0.58
1:E:143:VAL:O	1:E:147:VAL:HG23	2.04	0.57
1:H:47:LEU:HA	1:H:50:LYS:HB2	1.86	0.57
1:A:235:GLY:O	1:A:238:ILE:HG22	2.04	0.57
1:E:194:LEU:HB3	1:G:193:GLU:HG3	1.86	0.57
1:G:63:PHE:CD2	1:G:144:LEU:HD11	2.39	0.57
1:B:122:PRO:HB2	1:B:125:GLN:HB2	1.86	0.57
1:H:66:CYS:SG	1:H:222:ARG:NE	2.76	0.57
1:A:81:GLN:O	1:A:84:GLN:HG3	2.04	0.57
1:A:144:LEU:O	1:A:148:ILE:HG12	2.04	0.57
1:C:47:LEU:HD23	1:C:47:LEU:H	1.68	0.57
1:B:147:VAL:HG23	1:B:148:ILE:HG23	1.87	0.57
1:B:121:PHE:CD1	1:B:122:PRO:HD2	2.40	0.57
1:H:116:ALA:HA	1:H:121:PHE:HB3	1.87	0.57
1:B:148:ILE:HD11	1:B:154:ILE:HD12	1.86	0.57
1:F:187:ASP:OD1	1:F:189:ARG:CZ	2.52	0.57
1:B:148:ILE:HD12	1:B:151:VAL:HG13	1.86	0.57
1:B:209:PHE:HA	1:D:79:ILE:HD11	1.87	0.57
1:B:243:PRO:O	1:B:247:THR:HG23	2.04	0.57
1:A:173:VAL:HG11	1:A:210:ALA:HB2	1.86	0.56
1:D:237:TRP:CE3	1:D:241:LEU:HD12	2.40	0.56
1:B:123:TRP:HA	1:B:126:VAL:HG12	1.87	0.56
1:C:104:GLY:CA	1:C:189:ARG:HB3	2.35	0.56
1:C:154:ILE:O	1:C:226:PRO:HB3	2.05	0.56
1:E:55:VAL:HG12	1:E:132:ALA:O	2.05	0.56
1:E:163:HIS:NE2	1:E:234:ASP:OD2	2.29	0.56
1:F:224:LEU:HD23	1:F:236:LEU:HD11	1.87	0.56
1:G:214:SER:O	1:G:239:TYR:OH	2.20	0.56
1:A:148:ILE:HG22	1:D:213:ILE:HD11	1.86	0.56
1:B:235:GLY:O	1:B:238:ILE:HG12	2.06	0.56
1:G:134:PHE:CE1	1:G:224:LEU:HD12	2.40	0.56
1:G:157:THR:HG23	1:G:222:ARG:NH1	2.20	0.56
1:B:75:ASP:HB3	1:B:78:ARG:HB2	1.87	0.55
1:G:140:ALA:O	1:G:143:VAL:N	2.39	0.55
1:C:143:VAL:O	1:C:147:VAL:HG23	2.05	0.55
1:D:238:ILE:O	1:D:242:GLY:N	2.30	0.55
1:G:144:LEU:O	1:G:148:ILE:HG12	2.06	0.55
1:B:212:ALA:O	1:D:78:ARG:HD2	2.06	0.55
1:C:61:LEU:O	1:C:65:THR:HG22	2.06	0.55
1:C:126:VAL:CG1	1:C:127:PRO:HD3	2.36	0.55
1:C:235:GLY:O	1:C:238:ILE:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLY:HA2	1:A:215:GLY:C	2.26	0.55
1:B:66:CYS:SG	1:B:226:PRO:HG3	2.46	0.55
1:B:149:HIS:CE1	1:C:164:TRP:HZ2	2.25	0.55
1:B:47:LEU:H	1:B:47:LEU:HD23	1.72	0.55
1:B:173:VAL:HG11	1:B:210:ALA:HB2	1.89	0.55
1:E:233:PHE:HD2	1:E:236:LEU:HD22	1.72	0.55
1:B:71:ILE:HG23	1:B:78:ARG:HD3	1.89	0.55
1:B:202:ALA:HA	1:B:205:ILE:HD12	1.88	0.55
1:E:52:VAL:O	1:E:56:VAL:HG12	2.07	0.55
1:E:60:LEU:HD12	1:H:176:ASN:HB2	1.88	0.55
1:G:52:VAL:O	1:G:56:VAL:HG12	2.06	0.54
1:H:92:VAL:HG21	1:H:203:VAL:HG21	1.89	0.54
1:B:62:VAL:HG13	1:B:66:CYS:SG	2.47	0.54
1:C:157:THR:HG23	1:C:222:ARG:HH12	1.71	0.54
1:C:165:HIS:HB3	1:C:213:ILE:CG2	2.37	0.54
1:D:237:TRP:CZ3	1:D:241:LEU:HD12	2.41	0.54
1:H:122:PRO:HB2	1:H:125:GLN:HG3	1.90	0.54
1:B:209:PHE:HB2	1:D:68:ALA:HB2	1.89	0.54
1:D:99:VAL:HG23	1:D:105:ALA:HB2	1.88	0.54
1:E:175:PHE:CE2	1:E:250:GLY:HA2	2.41	0.54
1:F:54:GLU:HG3	1:F:129:TYR:CD1	2.42	0.54
1:G:139:CYS:O	1:G:143:VAL:HG23	2.08	0.54
1:D:142:PHE:CE1	1:D:229:ALA:HA	2.42	0.54
1:E:219:ASN:HB3	1:E:222:ARG:HB3	1.89	0.54
1:B:175:PHE:CE2	1:B:250:GLY:HA2	2.42	0.54
1:B:220:PRO:HB3	1:B:240:PHE:CE1	2.43	0.54
1:G:61:LEU:O	1:G:65:THR:HG22	2.07	0.54
1:E:102:ILE:HA	1:H:260:GLU:HG3	1.89	0.54
1:C:62:VAL:HA	1:C:65:THR:HG22	1.89	0.54
1:E:163:HIS:HE2	1:E:234:ASP:CG	2.11	0.53
1:H:70:GLY:CA	1:H:155:GLY:H	2.21	0.53
1:A:108:ASN:HB3	1:A:111:VAL:HB	1.90	0.53
1:B:144:LEU:HA	1:B:147:VAL:HG22	1.89	0.53
1:E:49:LYS:NZ	1:H:259:PHE:HB2	2.23	0.53
1:F:188:THR:N	1:F:189:ARG:HA	2.22	0.53
1:A:169:VAL:HG23	1:C:147:VAL:HG11	1.89	0.53
1:C:71:ILE:HG23	1:C:78:ARG:HD3	1.90	0.53
1:B:149:HIS:CE1	1:C:165:HIS:HE2	2.27	0.53
1:E:126:VAL:CG2	1:E:127:PRO:HD3	2.38	0.53
1:F:149:HIS:CE1	1:G:164:TRP:HZ2	2.27	0.53
1:F:81:GLN:O	1:F:84:GLN:HG3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:VAL:HG21	1:F:203:VAL:HG11	1.91	0.52
1:A:224:LEU:HD11	1:A:240:PHE:HZ	1.74	0.52
1:C:230:SER:OG	1:C:231:ASN:N	2.42	0.52
1:E:59:PHE:CE1	1:E:140:ALA:HA	2.44	0.52
1:H:59:PHE:CE2	1:H:140:ALA:HA	2.43	0.52
1:B:47:LEU:HB3	1:B:125:GLN:NE2	2.25	0.52
1:C:138:ILE:HA	1:C:225:GLY:HA2	1.91	0.52
1:E:152:ASP:C	1:E:152:ASP:OD2	2.43	0.52
1:F:97:TYR:OH	1:F:197:LEU:HD12	2.09	0.52
1:C:62:VAL:HG13	1:C:66:CYS:SG	2.50	0.52
1:D:63:PHE:CD2	1:D:144:LEU:HD11	2.44	0.52
1:E:75:ASP:OD2	1:E:78:ARG:HB2	2.10	0.52
1:G:138:ILE:HG12	1:G:225:GLY:HA2	1.91	0.52
1:C:157:THR:HG21	1:C:217:SER:HB2	1.91	0.52
1:C:159:PRO:HG2	1:C:163:HIS:HD2	1.71	0.52
1:A:209:PHE:HB2	1:C:68:ALA:HB2	1.92	0.52
1:B:188:THR:HG22	1:B:188:THR:O	2.09	0.52
1:B:194:LEU:HD23	1:D:193:GLU:HB2	1.92	0.52
1:E:134:PHE:CE1	1:E:224:LEU:HD12	2.45	0.52
1:D:157:THR:HG22	1:D:239:TYR:CZ	2.45	0.51
1:H:58:THR:HA	1:H:61:LEU:HB3	1.92	0.51
1:G:188:THR:HG22	1:G:188:THR:O	2.09	0.51
1:A:112:THR:HG22	1:A:126:VAL:HG23	1.91	0.51
1:F:47:LEU:O	1:F:51:VAL:HG22	2.10	0.51
1:H:219:ASN:HB3	1:H:222:ARG:HB3	1.92	0.51
1:F:108:ASN:HA	1:F:219:ASN:OD1	2.11	0.51
1:H:59:PHE:HA	1:H:140:ALA:HB2	1.92	0.51
1:G:211:GLY:HA2	1:G:215:GLY:C	2.30	0.51
1:B:259:PHE:HB3	1:D:46:HIS:HE1	1.76	0.51
1:C:113:LEU:HD13	1:C:130:TRP:CZ2	2.45	0.51
1:F:165:HIS:NE2	1:H:149:HIS:HB2	2.26	0.51
1:C:88:GLY:O	1:C:92:VAL:HG23	2.11	0.51
1:C:174:THR:HG21	1:C:243:PRO:HA	1.91	0.51
1:G:92:VAL:O	1:G:96:ILE:HG13	2.11	0.51
1:F:53:SER:OG	1:G:257:ILE:HB	2.11	0.51
1:F:228:LEU:HA	1:F:233:PHE:CZ	2.46	0.51
1:G:231:ASN:HA	1:G:233:PHE:CE1	2.46	0.51
1:B:93:THR:OG1	1:B:200:GLY:HA3	2.11	0.51
1:C:97:TYR:OH	1:C:197:LEU:HD12	2.11	0.51
1:B:138:ILE:HA	1:B:225:GLY:HA2	1.93	0.50
1:C:186:THR:O	1:C:187:ASP:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:LEU:HD12	1:F:233:PHE:HZ	1.74	0.50
1:B:155:GLY:O	1:B:226:PRO:HB3	2.11	0.50
1:B:188:THR:N	1:B:189:ARG:CA	2.74	0.50
1:D:72:SER:HB2	1:D:79:ILE:HG22	1.92	0.50
1:D:167:LEU:HD13	1:D:238:ILE:HA	1.93	0.50
1:F:59:PHE:CD1	1:F:60:LEU:HD12	2.40	0.50
1:F:157:THR:HG22	1:F:239:TYR:CZ	2.46	0.50
1:H:186:THR:O	1:H:187:ASP:HB2	2.12	0.50
1:H:188:THR:HB	1:H:191:VAL:HG21	1.94	0.50
1:C:104:GLY:HA2	1:C:189:ARG:HB3	1.93	0.50
1:D:57:ALA:O	1:D:61:LEU:N	2.29	0.50
1:G:219:ASN:HB3	1:G:222:ARG:HB3	1.94	0.50
1:B:54:GLU:HG3	1:B:129:TYR:CD1	2.47	0.50
1:B:171:VAL:HG12	1:B:242:GLY:O	2.10	0.50
1:D:162:PRO:O	1:D:165:HIS:HB2	2.11	0.50
1:H:175:PHE:HD1	1:H:250:GLY:CA	2.24	0.50
1:B:169:VAL:HG23	1:D:147:VAL:HG11	1.94	0.50
1:D:162:PRO:HD2	1:D:165:HIS:ND1	2.26	0.50
1:F:197:LEU:HD23	1:H:197:LEU:HD11	1.94	0.50
1:C:116:ALA:CA	1:C:121:PHE:HB3	2.40	0.49
1:C:188:THR:HG23	1:C:191:VAL:HG11	1.93	0.49
1:B:159:PRO:HD2	1:B:234:ASP:OD2	2.12	0.49
1:F:63:PHE:HA	1:F:144:LEU:HD11	1.94	0.49
1:F:56:VAL:HG21	1:G:253:THR:HG21	1.93	0.49
1:H:170:GLU:OE1	1:H:218:MET:N	2.43	0.49
1:E:64:MET:HE1	1:H:173:VAL:HA	1.95	0.49
1:F:115:PHE:CD1	1:F:189:ARG:NH1	2.81	0.49
1:F:146:ALA:HB1	1:G:164:TRP:HH2	1.78	0.49
1:G:62:VAL:HG21	1:G:137:ALA:HB1	1.94	0.49
1:D:92:VAL:O	1:D:96:ILE:HG13	2.13	0.49
1:D:167:LEU:HD22	1:D:237:TRP:CZ3	2.48	0.49
1:F:114:ALA:HA	1:F:248:LEU:HD23	1.95	0.49
1:F:157:THR:HG22	1:F:239:TYR:CE1	2.47	0.49
1:F:169:VAL:HG21	1:F:213:ILE:HD12	1.95	0.49
1:G:157:THR:HG23	1:G:222:ARG:HH12	1.76	0.49
1:H:69:ALA:HB3	1:H:155:GLY:HA2	1.94	0.49
1:H:223:THR:HG21	1:H:239:TYR:CD2	2.48	0.49
1:D:253:THR:O	1:D:257:ILE:HG12	2.12	0.49
1:E:222:ARG:NH2	1:E:226:PRO:HG2	2.28	0.49
1:A:173:VAL:HG12	1:C:64:MET:HE2	1.95	0.49
1:D:238:ILE:HD11	1:D:239:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:157:THR:HG1	1:H:222:ARG:NH1	2.06	0.49
1:A:259:PHE:CE2	1:F:259:PHE:HE1	2.31	0.48
1:C:55:VAL:HG12	1:C:132:ALA:O	2.13	0.48
1:F:67:GLY:HA3	1:F:144:LEU:HD22	1.95	0.48
1:F:116:ALA:HA	1:F:121:PHE:HB3	1.95	0.48
1:G:187:ASP:OD1	1:G:189:ARG:CZ	2.60	0.48
1:D:143:VAL:O	1:D:147:VAL:HG23	2.13	0.48
1:E:129:TYR:O	1:E:132:ALA:N	2.46	0.48
1:E:189:ARG:HA	1:E:189:ARG:HD2	1.68	0.48
1:B:176:ASN:OD1	1:D:60:LEU:HD23	2.13	0.48
1:E:123:TRP:O	1:E:126:VAL:HG22	2.12	0.48
1:B:212:ALA:HB2	1:D:79:ILE:HG13	1.95	0.48
1:F:55:VAL:HG12	1:F:132:ALA:O	2.13	0.48
1:H:62:VAL:HA	1:H:65:THR:HG22	1.94	0.48
1:H:119:ARG:HB3	1:H:189:ARG:HH12	1.79	0.48
1:H:144:LEU:O	1:H:148:ILE:HG12	2.14	0.48
1:A:116:ALA:HB1	1:A:123:TRP:NE1	2.29	0.48
1:E:49:LYS:HZ2	1:H:259:PHE:HB2	1.77	0.48
1:A:106:HIS:CE1	1:A:189:ARG:HG2	2.48	0.48
1:D:62:VAL:HA	1:D:65:THR:CG2	2.44	0.48
1:G:148:ILE:HD11	1:G:154:ILE:HD12	1.95	0.48
1:A:87:ALA:HB2	1:D:208:ILE:HG21	1.95	0.48
1:C:231:ASN:OD1	1:C:232:LYS:N	2.47	0.48
1:D:175:PHE:CE2	1:D:250:GLY:HA2	2.48	0.48
1:G:121:PHE:CD1	1:G:122:PRO:HD2	2.49	0.48
1:C:145:LYS:HA	1:C:154:ILE:CD1	2.44	0.48
1:F:119:ARG:NH2	1:F:182:LEU:O	2.47	0.48
1:A:79:ILE:HG13	1:D:212:ALA:HB2	1.95	0.48
1:E:159:PRO:HB2	1:E:163:HIS:CD2	2.49	0.48
1:A:55:VAL:HG12	1:A:132:ALA:O	2.13	0.48
1:F:228:LEU:HD12	1:F:233:PHE:CZ	2.49	0.48
1:A:167:LEU:H	1:A:238:ILE:HD11	1.78	0.47
1:C:152:ASP:O	1:C:230:SER:HB3	2.13	0.47
1:D:148:ILE:HD11	1:D:154:ILE:HD12	1.95	0.47
1:G:153:VAL:HG13	1:G:156:THR:HG23	1.96	0.47
1:H:210:ALA:O	1:H:214:SER:N	2.45	0.47
1:C:139:CYS:O	1:C:143:VAL:HG23	2.14	0.47
1:G:113:LEU:HD21	1:G:248:LEU:HD11	1.96	0.47
1:A:59:PHE:HD2	1:A:60:LEU:HD12	1.78	0.47
1:H:92:VAL:O	1:H:96:ILE:HG13	2.15	0.47
1:F:48:LEU:O	1:F:52:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:PRO:O	1:G:165:HIS:HB2	2.15	0.47
1:C:81:GLN:O	1:C:84:GLN:HG3	2.14	0.47
1:G:81:GLN:O	1:G:84:GLN:HG3	2.14	0.47
1:H:47:LEU:O	1:H:51:VAL:HG22	2.14	0.47
1:H:108:ASN:ND2	1:H:219:ASN:HA	2.30	0.47
1:H:255:THR:HA	1:H:258:ARG:HB2	1.96	0.47
1:C:175:PHE:CE2	1:C:250:GLY:HA2	2.50	0.47
1:D:61:LEU:O	1:D:65:THR:HG22	2.14	0.47
1:E:187:ASP:OD1	1:E:189:ARG:NH1	2.48	0.47
1:G:243:PRO:O	1:G:247:THR:HG23	2.15	0.47
1:H:222:ARG:O	1:H:226:PRO:HD2	2.14	0.47
1:A:126:VAL:CG1	1:A:127:PRO:HD3	2.45	0.47
1:E:194:LEU:HD23	1:G:193:GLU:HB2	1.97	0.47
1:F:241:LEU:HA	1:F:241:LEU:HD23	1.51	0.47
1:A:97:TYR:CD1	1:A:97:TYR:N	2.79	0.47
1:B:75:ASP:HB3	1:B:78:ARG:CB	2.44	0.47
1:C:222:ARG:O	1:C:222:ARG:HD3	2.15	0.47
1:E:115:PHE:HB3	1:E:121:PHE:HB2	1.97	0.47
1:F:186:THR:O	1:F:187:ASP:CB	2.63	0.47
1:A:108:ASN:HA	1:A:219:ASN:OD1	2.15	0.47
1:B:241:LEU:HA	1:B:241:LEU:HD23	1.54	0.47
1:C:159:PRO:HG3	1:C:238:ILE:HD11	1.96	0.47
1:E:223:THR:HG21	1:E:239:TYR:CG	2.50	0.47
1:H:223:THR:HG21	1:H:239:TYR:CG	2.50	0.47
1:A:102:ILE:HG12	1:D:259:PHE:O	2.14	0.46
1:F:245:MET:HE2	1:F:245:MET:HB3	1.69	0.46
1:E:224:LEU:HD11	1:E:240:PHE:HZ	1.80	0.46
1:E:54:GLU:OE1	1:E:106:HIS:HB2	2.16	0.46
1:E:147:VAL:CG1	1:H:169:VAL:HG23	2.45	0.46
1:F:174:THR:OG1	1:F:218:MET:HG2	2.15	0.46
1:B:149:HIS:CE1	1:C:164:TRP:CZ2	3.04	0.46
1:C:111:VAL:HG22	1:C:178:MET:SD	2.56	0.46
1:D:144:LEU:O	1:D:148:ILE:HG12	2.14	0.46
1:D:187:ASP:HA	1:D:189:ARG:NH2	2.31	0.46
1:F:222:ARG:O	1:F:226:PRO:HD2	2.16	0.46
1:D:47:LEU:HD21	1:D:125:GLN:CG	2.46	0.46
1:E:203:VAL:HA	1:E:218:MET:HE1	1.97	0.46
1:F:104:GLY:HA2	1:F:189:ARG:H	1.81	0.46
1:A:194:LEU:HD12	1:A:194:LEU:C	2.36	0.46
1:D:175:PHE:CD2	1:D:250:GLY:HA2	2.51	0.46
1:G:122:PRO:HB2	1:G:125:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:PHE:CE1	1:C:224:LEU:HD12	2.51	0.46
1:B:126:VAL:CG1	1:B:127:PRO:HD3	2.46	0.46
1:B:241:LEU:O	1:B:245:MET:HB3	2.16	0.46
1:D:187:ASP:HA	1:D:189:ARG:HH21	1.81	0.46
1:F:188:THR:O	1:F:188:THR:HG22	2.15	0.46
1:H:143:VAL:O	1:H:147:VAL:HG23	2.15	0.46
1:A:187:ASP:OD1	1:A:189:ARG:NH2	2.49	0.46
1:A:189:ARG:HA	1:A:189:ARG:HD2	1.69	0.46
1:D:167:LEU:HD22	1:D:237:TRP:CH2	2.50	0.46
1:H:224:LEU:HD11	1:H:240:PHE:HZ	1.80	0.46
1:B:104:GLY:HA2	1:B:189:ARG:HB3	1.97	0.46
1:E:49:LYS:CD	1:H:257:ILE:HA	2.45	0.46
1:G:111:VAL:O	1:G:114:ALA:N	2.48	0.46
1:H:54:GLU:HG3	1:H:129:TYR:CE1	2.50	0.46
1:H:119:ARG:HB3	1:H:189:ARG:NH1	2.30	0.46
1:A:97:TYR:CE1	1:A:196:GLY:HA3	2.52	0.45
1:C:206:THR:HG23	1:C:210:ALA:HB3	1.98	0.45
1:D:170:GLU:HG2	1:D:214:SER:OG	2.15	0.45
1:F:62:VAL:HG13	1:F:66:CYS:SG	2.55	0.45
1:F:159:PRO:HG2	1:F:163:HIS:ND1	2.31	0.45
1:G:157:THR:CG2	1:G:222:ARG:NH1	2.79	0.45
1:A:174:THR:HG21	1:A:243:PRO:HA	1.98	0.45
1:B:197:LEU:HD11	1:C:197:LEU:HD23	1.98	0.45
1:D:148:ILE:HD11	1:D:154:ILE:CD1	2.47	0.45
1:E:159:PRO:HG2	1:E:163:HIS:HD2	1.80	0.45
1:F:101:HIS:HD2	1:F:102:ILE:HG13	1.81	0.45
1:F:165:HIS:HA	1:H:147:VAL:HG13	1.99	0.45
1:A:138:ILE:HG12	1:A:225:GLY:HA2	1.98	0.45
1:A:241:LEU:HD23	1:A:241:LEU:HA	1.54	0.45
1:E:92:VAL:HG21	1:E:203:VAL:HG11	1.98	0.45
1:E:189:ARG:CA	1:E:189:ARG:HH21	2.28	0.45
1:F:222:ARG:O	1:F:222:ARG:HD3	2.16	0.45
1:G:116:ALA:HA	1:G:121:PHE:HB3	1.97	0.45
1:A:123:TRP:O	1:A:126:VAL:HG12	2.17	0.45
1:H:157:THR:HG22	1:H:239:TYR:CE1	2.52	0.45
1:C:228:LEU:HD23	1:C:233:PHE:HZ	1.81	0.45
1:F:79:ILE:HG13	1:G:212:ALA:HB2	1.99	0.45
1:F:173:VAL:HG12	1:H:64:MET:HE2	1.98	0.45
1:D:166:SER:HB3	1:D:238:ILE:CD1	2.47	0.45
1:F:52:VAL:HG21	1:G:256:PHE:CE2	2.50	0.45
1:F:164:TRP:HH2	1:H:146:ALA:HB1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:PHE:HA	1:G:144:LEU:HD11	1.99	0.45
1:G:169:VAL:O	1:G:173:VAL:HG22	2.17	0.45
1:A:188:THR:O	1:A:188:THR:OG1	2.33	0.45
1:C:169:VAL:O	1:C:173:VAL:HG22	2.16	0.45
1:E:49:LYS:HD3	1:H:257:ILE:HA	1.98	0.45
1:A:173:VAL:HG23	1:A:218:MET:HG2	1.98	0.45
1:B:54:GLU:HG3	1:B:129:TYR:CE1	2.51	0.45
1:B:63:PHE:HA	1:B:144:LEU:HD11	1.99	0.45
1:B:197:LEU:HD23	1:D:197:LEU:HD11	1.98	0.45
1:D:47:LEU:HD11	1:D:125:GLN:HG2	1.99	0.45
1:E:47:LEU:HD21	1:E:125:GLN:CD	2.37	0.45
1:E:95:MET:HB3	1:E:107:MET:SD	2.56	0.45
1:H:144:LEU:HD13	1:H:154:ILE:HG21	1.99	0.45
1:A:183:ALA:HA	1:A:254:TYR:CZ	2.51	0.45
1:B:91:ILE:HD12	1:B:94:VAL:CG2	2.46	0.45
1:B:182:LEU:HD23	1:B:254:TYR:HB3	1.99	0.45
1:C:111:VAL:O	1:C:114:ALA:N	2.50	0.45
1:H:62:VAL:HG13	1:H:66:CYS:SG	2.56	0.45
1:A:193:GLU:HB2	1:D:194:LEU:HD23	1.99	0.45
1:E:147:VAL:HG11	1:H:169:VAL:HG23	1.98	0.45
1:F:116:ALA:CA	1:F:121:PHE:HB3	2.47	0.45
1:F:212:ALA:HB1	1:H:78:ARG:HG2	1.99	0.45
1:E:92:VAL:O	1:E:96:ILE:HG13	2.17	0.44
1:E:173:VAL:HG11	1:E:210:ALA:HB2	1.99	0.44
1:E:194:LEU:C	1:E:194:LEU:HD12	2.38	0.44
1:A:171:VAL:HG12	1:A:242:GLY:O	2.18	0.44
1:B:113:LEU:HB2	1:B:130:TRP:CZ2	2.49	0.44
1:D:47:LEU:HD21	1:D:125:GLN:HG2	1.99	0.44
1:E:149:HIS:CE1	1:H:164:TRP:CZ2	2.96	0.44
1:H:75:ASP:HB3	1:H:78:ARG:CB	2.47	0.44
1:E:101:HIS:NE2	1:H:254:TYR:OH	2.39	0.44
1:H:92:VAL:HG21	1:H:203:VAL:HG11	1.99	0.44
1:H:108:ASN:HA	1:H:219:ASN:OD1	2.18	0.44
1:A:167:LEU:HD13	1:A:237:TRP:CZ3	2.52	0.44
1:B:108:ASN:HB3	1:B:111:VAL:HB	2.00	0.44
1:C:142:PHE:CE1	1:C:229:ALA:HA	2.53	0.44
1:C:188:THR:CG2	1:C:191:VAL:HG11	2.47	0.44
1:D:222:ARG:O	1:D:226:PRO:HD2	2.18	0.44
1:F:52:VAL:HB	1:G:257:ILE:HG22	1.99	0.44
1:H:116:ALA:HB1	1:H:123:TRP:HD1	1.78	0.44
1:E:57:ALA:HB1	1:E:107:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:ILE:HG21	1:G:83:GLY:O	2.18	0.44
1:H:112:THR:HG22	1:H:126:VAL:HG23	2.00	0.44
1:C:46:HIS:NE2	1:C:49:LYS:HD2	2.31	0.44
1:G:171:VAL:HG12	1:G:242:GLY:O	2.18	0.44
1:H:93:THR:OG1	1:H:200:GLY:HA3	2.18	0.44
1:D:67:GLY:CA	1:D:144:LEU:HD22	2.48	0.44
1:F:189:ARG:HA	1:F:189:ARG:HD2	1.31	0.44
1:A:53:SER:HB3	1:A:99:VAL:HB	2.00	0.44
1:A:101:HIS:ND1	1:A:102:ILE:HG13	2.33	0.44
1:B:213:ILE:HD11	1:D:148:ILE:HG22	2.00	0.44
1:D:104:GLY:HA3	1:D:189:ARG:CB	2.31	0.44
1:E:75:ASP:HB3	1:E:78:ARG:CB	2.47	0.44
1:E:256:PHE:HZ	1:G:48:LEU:HD21	1.83	0.44
1:D:59:PHE:CD1	1:D:60:LEU:HD12	2.44	0.44
1:E:148:ILE:HD11	1:E:154:ILE:CD1	2.48	0.44
1:F:209:PHE:HA	1:H:79:ILE:HD11	1.99	0.44
1:G:59:PHE:CD2	1:G:140:ALA:HB2	2.52	0.44
1:G:245:MET:HE2	1:G:245:MET:HB3	1.80	0.44
1:B:183:ALA:HA	1:B:254:TYR:CZ	2.53	0.43
1:B:231:ASN:OD1	1:B:233:PHE:HE1	2.00	0.43
1:C:57:ALA:HB1	1:C:107:MET:SD	2.58	0.43
1:C:224:LEU:HD11	1:C:240:PHE:HZ	1.83	0.43
1:H:113:LEU:HD21	1:H:248:LEU:HD11	2.00	0.43
1:H:187:ASP:HA	1:H:189:ARG:CZ	2.47	0.43
1:C:228:LEU:HD23	1:C:228:LEU:HA	1.79	0.43
1:A:153:VAL:HG23	1:A:153:VAL:O	2.19	0.43
1:A:202:ALA:HA	1:A:205:ILE:HD12	2.00	0.43
1:B:228:LEU:HD12	1:B:233:PHE:HE2	1.82	0.43
1:C:113:LEU:HD13	1:C:130:TRP:HZ2	1.84	0.43
1:D:238:ILE:HG13	1:D:239:TYR:N	2.33	0.43
1:F:56:VAL:HG21	1:G:253:THR:CG2	2.48	0.43
1:G:188:THR:N	1:G:189:ARG:CA	2.80	0.43
1:H:63:PHE:CD2	1:H:144:LEU:HG	2.53	0.43
1:A:134:PHE:CE1	1:A:224:LEU:HD12	2.53	0.43
1:E:54:GLU:HG3	1:E:129:TYR:CE1	2.53	0.43
1:E:224:LEU:HD23	1:E:236:LEU:HD11	2.00	0.43
1:H:54:GLU:OE1	1:H:106:HIS:HB2	2.18	0.43
1:A:175:PHE:CE1	1:C:60:LEU:HD11	2.54	0.43
1:A:186:THR:O	1:A:187:ASP:HB2	2.18	0.43
1:A:228:LEU:HD12	1:A:233:PHE:HE2	1.83	0.43
1:C:189:ARG:HA	1:C:189:ARG:HD2	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:LEU:HD11	1:H:197:LEU:HD23	2.00	0.43
1:D:101:HIS:ND1	1:D:102:ILE:HG13	2.34	0.43
1:D:188:THR:N	1:D:189:ARG:CA	2.80	0.43
1:E:113:LEU:CD2	1:E:244:VAL:HG13	2.48	0.43
1:F:67:GLY:CA	1:F:144:LEU:HD22	2.49	0.43
1:G:238:ILE:O	1:G:242:GLY:N	2.44	0.43
1:A:238:ILE:HD13	1:A:238:ILE:HG21	1.76	0.43
1:B:259:PHE:O	1:B:260:GLU:HB3	2.19	0.43
1:F:107:MET:O	1:F:219:ASN:ND2	2.50	0.43
1:F:138:ILE:HG12	1:F:225:GLY:HA2	2.01	0.43
1:A:122:PRO:O	1:A:125:GLN:HB2	2.19	0.43
1:B:238:ILE:O	1:B:242:GLY:N	2.45	0.43
1:E:241:LEU:HA	1:E:241:LEU:HD23	1.67	0.43
1:H:116:ALA:CA	1:H:121:PHE:HB3	2.47	0.43
1:A:157:THR:HG21	1:A:222:ARG:NH1	2.33	0.43
1:A:242:GLY:O	1:A:246:GLY:N	2.51	0.43
1:C:104:GLY:HA3	1:C:189:ARG:HB3	1.99	0.43
1:C:182:LEU:HA	1:C:182:LEU:HD12	1.83	0.43
1:E:71:ILE:HG23	1:E:78:ARG:HD3	2.00	0.43
1:E:188:THR:H	1:E:189:ARG:HA	1.83	0.43
1:A:165:HIS:NE2	1:C:149:HIS:HD2	2.14	0.43
1:D:222:ARG:O	1:D:222:ARG:HD3	2.18	0.43
1:F:162:PRO:HD2	1:F:165:HIS:CD2	2.53	0.43
1:A:176:ASN:HB2	1:C:60:LEU:HD22	2.00	0.42
1:B:141:SER:HB3	1:B:226:PRO:HD3	2.01	0.42
1:D:123:TRP:HA	1:D:126:VAL:HG23	2.00	0.42
1:E:116:ALA:HB1	1:E:123:TRP:NE1	2.34	0.42
1:G:62:VAL:HG21	1:G:137:ALA:CB	2.49	0.42
1:G:99:VAL:HG23	1:G:105:ALA:HB2	2.01	0.42
1:B:211:GLY:HA2	1:B:215:GLY:C	2.40	0.42
1:B:237:TRP:CZ3	1:B:238:ILE:HG22	2.54	0.42
1:E:126:VAL:HG23	1:E:127:PRO:HD3	2.01	0.42
1:H:55:VAL:HG12	1:H:132:ALA:O	2.19	0.42
1:F:49:LYS:HG2	1:G:257:ILE:HA	2.00	0.42
1:F:210:ALA:O	1:F:215:GLY:N	2.52	0.42
1:A:72:SER:HB2	1:A:79:ILE:HG22	2.02	0.42
1:A:79:ILE:HD11	1:D:209:PHE:HA	2.00	0.42
1:A:167:LEU:HD12	1:A:238:ILE:HG13	2.01	0.42
1:C:109:PRO:HB3	1:C:130:TRP:CD1	2.54	0.42
1:C:187:ASP:HA	1:C:189:ARG:NE	2.30	0.42
1:F:217:SER:O	1:F:218:MET:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:157:THR:HG21	1:H:217:SER:CB	2.49	0.42
1:B:54:GLU:OE1	1:B:106:HIS:HB2	2.20	0.42
1:B:110:ALA:HB1	1:B:247:THR:HG21	2.01	0.42
1:B:121:PHE:CZ	1:B:129:TYR:CD2	3.07	0.42
1:F:134:PHE:CE1	1:F:221:ALA:HA	2.54	0.42
1:B:224:LEU:CD2	1:B:236:LEU:HD11	2.48	0.42
1:C:75:ASP:HB3	1:C:78:ARG:HB2	2.01	0.42
1:F:119:ARG:NH1	1:F:187:ASP:OD2	2.44	0.42
1:A:245:MET:HE3	1:A:245:MET:HB3	1.89	0.42
1:B:224:LEU:HD23	1:B:224:LEU:HA	1.73	0.42
1:C:171:VAL:HG12	1:C:242:GLY:O	2.19	0.42
1:D:67:GLY:HA2	1:D:144:LEU:HD22	2.02	0.42
1:D:134:PHE:CE1	1:D:224:LEU:HD12	2.54	0.42
1:E:49:LYS:HD3	1:H:256:PHE:O	2.20	0.42
1:H:72:SER:O	1:H:74:SER:N	2.47	0.42
1:A:175:PHE:CE2	1:A:250:GLY:HA2	2.55	0.42
1:C:158:THR:HG21	1:C:232:LYS:CD	2.50	0.42
1:D:157:THR:HG21	1:D:217:SER:HB2	2.01	0.42
1:F:46:HIS:NE2	1:F:49:LYS:HD2	2.35	0.42
1:F:48:LEU:HD21	1:G:256:PHE:CZ	2.55	0.42
1:F:169:VAL:HG23	1:H:147:VAL:CG1	2.49	0.42
1:A:101:HIS:HA	1:A:191:VAL:HG22	2.02	0.42
1:B:212:ALA:HB1	1:D:78:ARG:HG2	2.02	0.42
1:A:220:PRO:HB3	1:A:240:PHE:CE2	2.54	0.42
1:F:183:ALA:CB	1:H:98:ALA:HA	2.50	0.42
1:G:116:ALA:CA	1:G:121:PHE:HB3	2.49	0.42
1:A:60:LEU:HD21	1:D:175:PHE:HD1	1.85	0.41
1:B:97:TYR:CE1	1:B:196:GLY:HA3	2.55	0.41
1:C:231:ASN:OD1	1:C:233:PHE:CE1	2.73	0.41
1:C:241:LEU:HD23	1:C:241:LEU:HA	1.87	0.41
1:F:56:VAL:O	1:F:60:LEU:HD13	2.20	0.41
1:C:166:SER:HB2	1:C:238:ILE:CD1	2.46	0.41
1:D:63:PHE:CD2	1:D:144:LEU:CD1	3.03	0.41
1:D:145:LYS:HA	1:D:154:ILE:CD1	2.49	0.41
1:D:245:MET:HB3	1:D:245:MET:HE2	1.76	0.41
1:E:75:ASP:HB3	1:E:78:ARG:HB2	2.00	0.41
1:G:60:LEU:HD23	1:G:60:LEU:HA	1.79	0.41
1:B:256:PHE:O	1:D:49:LYS:HD3	2.21	0.41
1:C:175:PHE:HZ	1:C:253:THR:HG1	1.63	0.41
1:F:162:PRO:HB2	1:F:165:HIS:CD2	2.55	0.41
1:G:157:THR:CG2	1:G:222:ARG:HH12	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:O	1:A:145:LYS:C	2.58	0.41
1:B:90:LEU:HA	1:B:90:LEU:HD23	1.88	0.41
1:B:240:PHE:O	1:B:244:VAL:HB	2.20	0.41
1:E:47:LEU:HD21	1:E:125:GLN:OE1	2.20	0.41
1:F:116:ALA:N	1:F:121:PHE:HB3	2.36	0.41
1:G:92:VAL:HG11	1:G:203:VAL:HG21	2.01	0.41
1:G:220:PRO:HB3	1:G:240:PHE:CE1	2.56	0.41
1:H:63:PHE:HA	1:H:144:LEU:HD11	2.03	0.41
1:A:170:GLU:OE2	1:A:214:SER:OG	2.31	0.41
1:E:126:VAL:HG22	1:E:127:PRO:HD3	2.01	0.41
1:F:173:VAL:HG12	1:H:64:MET:CE	2.51	0.41
1:C:156:THR:HG22	1:C:157:THR:N	2.35	0.41
1:H:121:PHE:HZ	1:H:129:TYR:HE2	1.68	0.41
1:A:175:PHE:CD1	1:A:175:PHE:C	2.94	0.41
1:G:162:PRO:HD2	1:G:165:HIS:CE1	2.55	0.41
1:H:126:VAL:CG1	1:H:127:PRO:HD3	2.50	0.41
1:D:71:ILE:HB	1:D:79:ILE:HD12	2.02	0.41
1:D:211:GLY:HA2	1:D:215:GLY:C	2.41	0.41
1:E:48:LEU:O	1:E:52:VAL:HG23	2.21	0.41
1:F:149:HIS:CE1	1:G:164:TRP:CZ2	3.08	0.41
1:B:109:PRO:HA	1:B:130:TRP:CD1	2.56	0.41
1:B:121:PHE:CZ	1:B:129:TYR:CE2	3.09	0.41
1:D:123:TRP:HD1	1:D:126:VAL:HG21	1.86	0.41
1:E:111:VAL:O	1:E:114:ALA:N	2.54	0.41
1:E:175:PHE:CD2	1:E:250:GLY:HA2	2.55	0.41
1:F:148:ILE:HD13	1:F:148:ILE:HG21	1.83	0.41
1:G:101:HIS:ND1	1:G:102:ILE:HG13	2.35	0.41
1:G:143:VAL:O	1:G:147:VAL:HG23	2.20	0.41
1:E:61:LEU:O	1:E:65:THR:HG22	2.21	0.41
1:H:136:GLY:O	1:H:140:ALA:HB2	2.21	0.41
1:B:59:PHE:CD1	1:B:60:LEU:HD12	2.53	0.40
1:C:158:THR:HG21	1:C:232:LYS:HG2	2.03	0.40
1:H:66:CYS:SG	1:H:226:PRO:CG	3.10	0.40
1:A:188:THR:N	1:A:189:ARG:CA	2.80	0.40
1:C:52:VAL:O	1:C:56:VAL:HG12	2.21	0.40
1:C:119:ARG:NH2	1:C:182:LEU:O	2.54	0.40
1:D:187:ASP:O	1:D:188:THR:HG23	2.20	0.40
1:E:183:ALA:CB	1:G:98:ALA:HA	2.52	0.40
1:H:189:ARG:HA	1:H:189:ARG:HD2	1.60	0.40
1:A:96:ILE:HD13	1:A:96:ILE:HG21	1.90	0.40
1:B:148:ILE:HD12	1:B:151:VAL:CG1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:LYS:HA	1:D:154:ILE:HD11	2.03	0.40
1:E:182:LEU:HD23	1:E:254:TYR:HB3	2.03	0.40
1:H:256:PHE:HD2	1:H:257:ILE:HG23	1.87	0.40
1:B:134:PHE:CE1	1:B:224:LEU:HD12	2.57	0.40
1:D:62:VAL:HG13	1:D:66:CYS:SG	2.61	0.40
1:H:193:GLU:O	1:H:197:LEU:HD13	2.22	0.40
1:A:148:ILE:CG2	1:D:213:ILE:HD11	2.52	0.40
1:D:144:LEU:O	1:D:145:LYS:C	2.59	0.40
1:D:173:VAL:HG23	1:D:218:MET:HG2	2.02	0.40
1:D:241:LEU:O	1:D:245:MET:HE2	2.22	0.40
1:E:222:ARG:O	1:E:226:PRO:HD2	2.20	0.40
1:F:169:VAL:O	1:F:173:VAL:HG22	2.21	0.40
1:G:148:ILE:HD11	1:G:154:ILE:CD1	2.51	0.40
1:H:114:ALA:O	1:H:118:PHE:HD2	2.04	0.40
1:H:241:LEU:HD23	1:H:241:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/227 (94%)	192 (90%)	21 (10%)	1 (0%)	29	68
1	B	214/227 (94%)	191 (89%)	20 (9%)	3 (1%)	11	43
1	C	212/227 (93%)	187 (88%)	24 (11%)	1 (0%)	29	68
1	D	214/227 (94%)	187 (87%)	25 (12%)	2 (1%)	17	55
1	E	214/227 (94%)	186 (87%)	26 (12%)	2 (1%)	17	55
1	F	214/227 (94%)	189 (88%)	23 (11%)	2 (1%)	17	55
1	G	214/227 (94%)	190 (89%)	23 (11%)	1 (0%)	29	68
1	H	214/227 (94%)	184 (86%)	26 (12%)	4 (2%)	8	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1710/1816 (94%)	1506 (88%)	188 (11%)	16 (1%)	17 55

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	187	ASP
1	H	155	GLY
1	B	155	GLY
1	B	259	PHE
1	E	232	LYS
1	E	258	ARG
1	F	155	GLY
1	C	187	ASP
1	G	259	PHE
1	H	74	SER
1	B	258	ARG
1	D	243	PRO
1	D	257	ILE
1	A	122	PRO
1	H	122	PRO
1	H	243	PRO

5.3.2 Protein sidechains (i)

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	168/177 (95%)	168 (100%)	0	100 100
1	B	168/177 (95%)	168 (100%)	0	100 100
1	C	166/177 (94%)	166 (100%)	0	100 100
1	D	168/177 (95%)	168 (100%)	0	100 100
1	E	168/177 (95%)	167 (99%)	1 (1%)	86 95
1	F	168/177 (95%)	168 (100%)	0	100 100
1	G	168/177 (95%)	168 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	168/177 (95%)	168 (100%)	0	100 100
All	All	1342/1416 (95%)	1341 (100%)	1 (0%)	93 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	222	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	B	165	HIS
1	C	149	HIS
1	C	163	HIS
1	D	165	HIS
1	F	81	GLN
1	G	81	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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, 95^{th} 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	216/227 (95%)	-0.11	14 (6%) 18 5	28, 70, 110, 168	0
1	B	216/227 (95%)	-0.27	3 (1%) 75 49	35, 73, 103, 146	0
1	C	214/227 (94%)	-0.33	2 (0%) 84 63	25, 58, 84, 133	0
1	D	216/227 (95%)	-0.13	5 (2%) 60 31	40, 76, 106, 146	0
1	E	216/227 (95%)	-0.34	2 (0%) 84 63	24, 57, 96, 135	0
1	F	216/227 (95%)	-0.03	10 (4%) 32 12	43, 78, 116, 153	0
1	G	216/227 (95%)	-0.26	5 (2%) 60 31	35, 74, 108, 155	0
1	H	216/227 (95%)	-0.00	7 (3%) 47 20	39, 78, 118, 133	0
All	All	1726/1816 (95%)	-0.18	48 (2%) 53 25	24, 71, 107, 168	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	HIS	8.0
1	H	230	SER	7.2
1	F	260	GLU	6.3
1	D	231	ASN	5.4
1	H	231	ASN	4.8
1	H	125	GLN	4.7
1	F	75	ASP	4.7
1	F	231	ASN	4.6
1	F	230	SER	4.3
1	A	63	PHE	4.2
1	A	153	VAL	4.1
1	A	154	ILE	3.8
1	H	122	PRO	3.5
1	E	153	VAL	3.5
1	D	119	ARG	3.4
1	F	154	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	152	ASP	3.2
1	G	234	ASP	3.2
1	F	153	VAL	3.2
1	A	148	ILE	3.1
1	G	160	VAL	3.0
1	F	234	ASP	3.0
1	C	149	HIS	3.0
1	A	64	MET	2.9
1	F	226	PRO	2.9
1	B	162	PRO	2.9
1	A	68	ALA	2.7
1	F	156	THR	2.7
1	H	160	VAL	2.7
1	A	229	ALA	2.7
1	A	230	SER	2.5
1	D	230	SER	2.5
1	C	122	PRO	2.4
1	A	65	THR	2.3
1	F	169	VAL	2.3
1	H	245	MET	2.3
1	G	125	GLN	2.2
1	B	158	THR	2.2
1	A	70	GLY	2.2
1	G	235	GLY	2.2
1	B	47	LEU	2.2
1	G	161	GLY	2.1
1	A	145	LYS	2.1
1	A	151	VAL	2.1
1	D	160	VAL	2.1
1	D	232	LYS	2.1
1	H	153	VAL	2.1
1	A	226	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CD	C	301	1/1	0.92	0.20	110,110,110,110	0
2	CD	D	302	1/1	0.95	0.24	113,113,113,113	0
2	CD	D	303	1/1	0.95	0.16	111,111,111,111	0
2	CD	F	301	1/1	0.95	0.23	103,103,103,103	0
2	CD	A	301	1/1	0.96	0.17	117,117,117,117	0
2	CD	B	301	1/1	0.96	0.21	115,115,115,115	0
2	CD	D	301	1/1	0.97	0.25	98,98,98,98	0
2	CD	G	301	1/1	0.97	0.19	109,109,109,109	0
2	CD	H	301	1/1	0.99	0.18	112,112,112,112	0

6.5 Other polymers (i)

There are no such residues in this entry.