



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:12 PM UTC

PDB ID : 1WE0 / pdb_00001we0
Title : Crystal structure of peroxiredoxin (AhpC) from *Amphibacillus xylanus*
Authors : Kitano, K.; Kita, A.; Hakoshima, T.; Niimura, Y.; Miki, K.
Deposited on : 2004-05-21
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

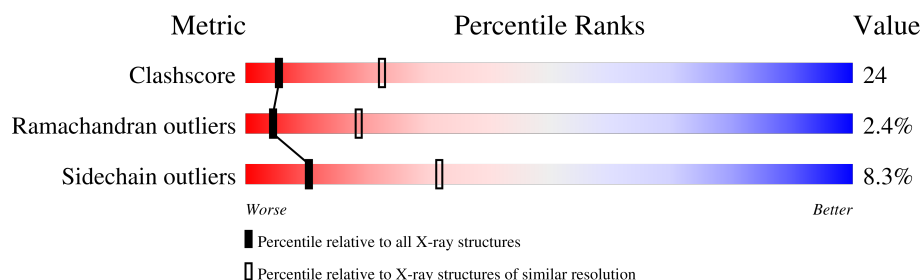
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	187	45% 40% • 11%
1	B	187	47% 37% 5% 11%
1	C	187	52% 27% 9% 11%
1	D	187	44% 39% 6% 11%
1	E	187	45% 41% • 11%
1	F	187	44% 39% 6% 11%
1	G	187	48% 36% 5% 11%
1	H	187	44% 37% 7% 11%

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Mol	Chain	Length	Quality of chain			
1	I	187				
1	J	187				

2 Entry composition

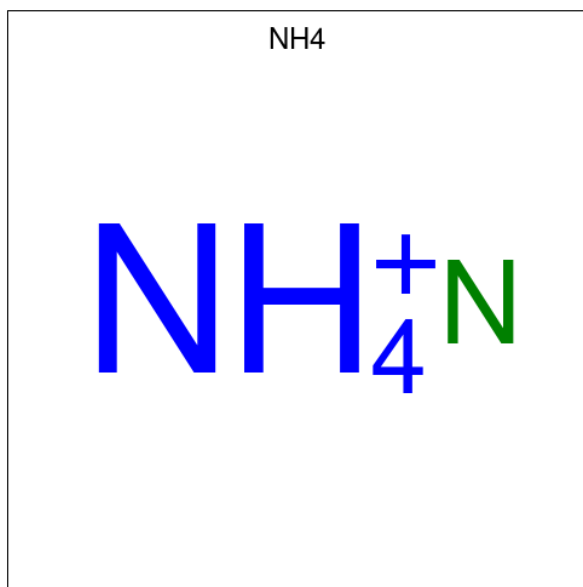
There are 2 unique types of molecules in this entry. The entry contains 12982 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 alkyl hydroperoxide reductase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	B	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	C	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	D	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	E	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	F	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	G	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	H	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	I	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	J	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			

- Molecule 2 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



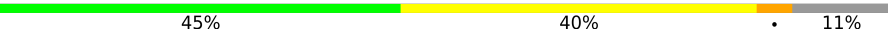
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	1	Total	N	0	0
			1	1		
2	J	1	Total	N	0	0
			1	1		

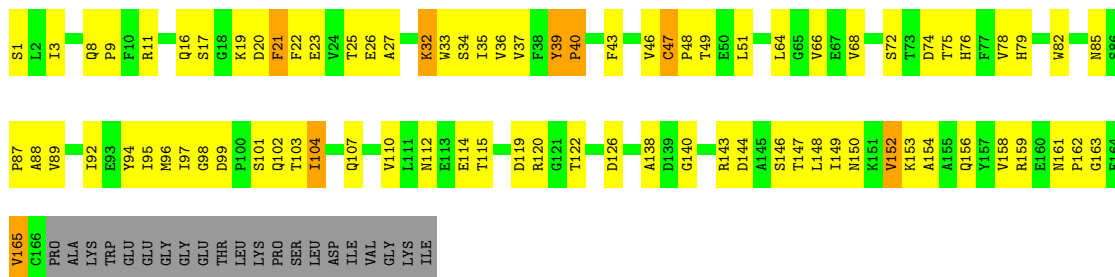
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

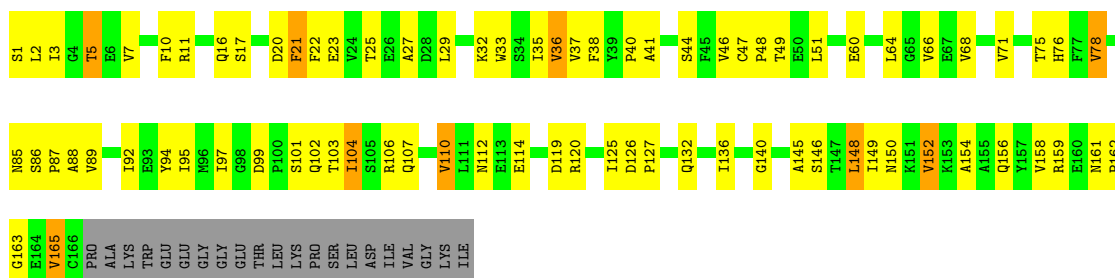
• Molecule 1: alkyl hydroperoxide reductase C

Chain A: 



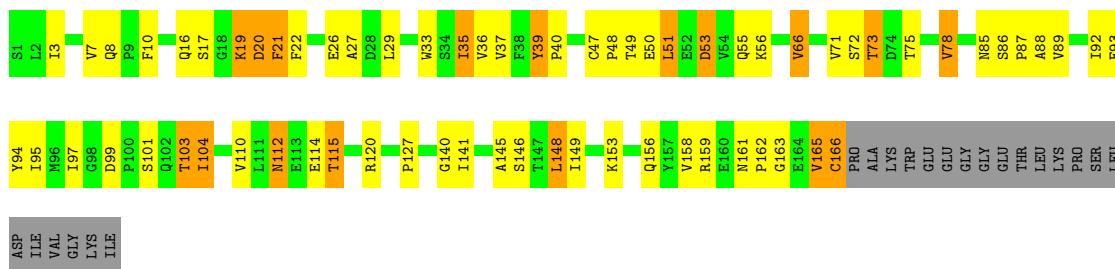
• Molecule 1: alkyl hydroperoxide reductase C

Chain B: 

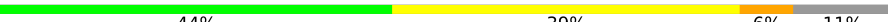


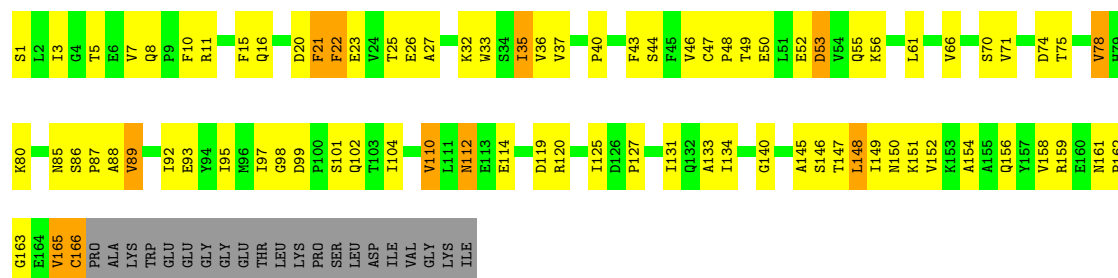
• Molecule 1: alkyl hydroperoxide reductase C

Chain C: 



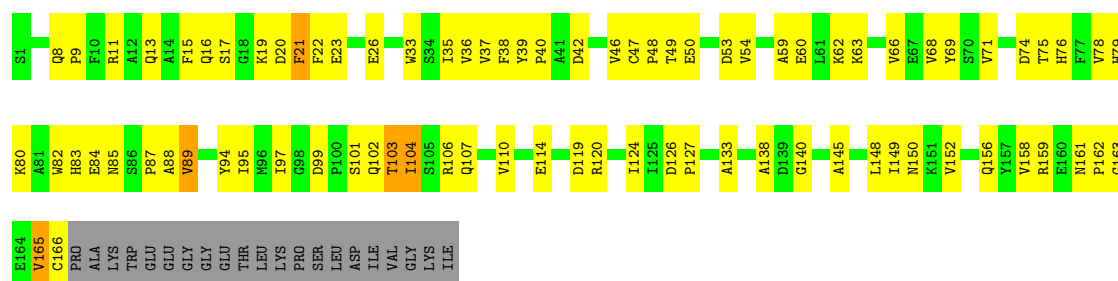
- Molecule 1: alkyl hydroperoxide reductase C

Chain D:  44% 39% 6% 11%

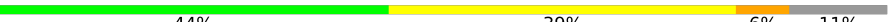


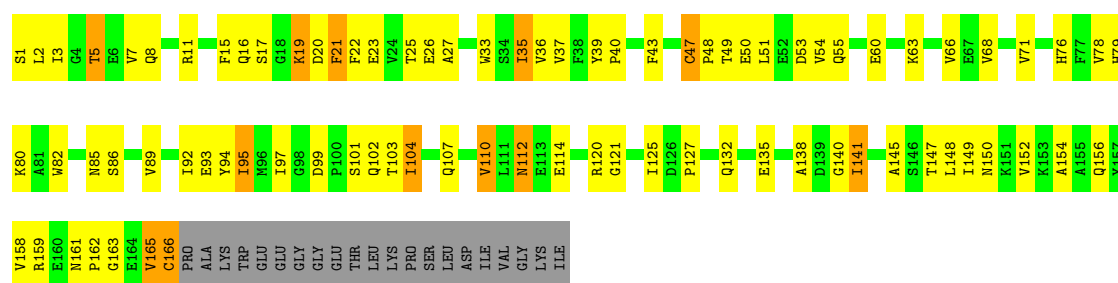
- Molecule 1: alkyl hydroperoxide reductase C

Chain E:  45% 41% 11%

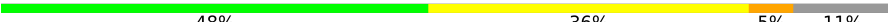


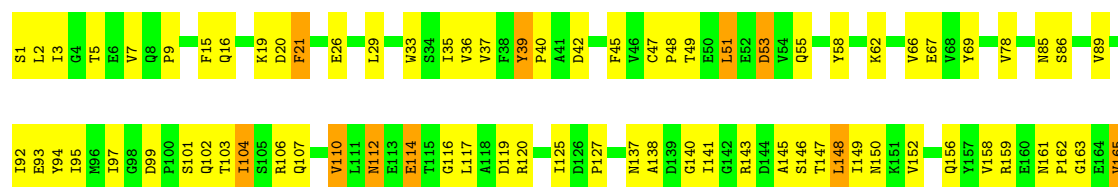
- Molecule 1: alkyl hydroperoxide reductase C

Chain F:  44% 39% 6% 11%



- Molecule 1: alkyl hydroperoxide reductase C

Chain G:  48% 36% 5% 11%



C166
PRO
ALA
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TRP
GLU
GLY
GLY
GLY
THR
LEU
LYS
PRO
SER
LEU
ASP
ILE
VAL
GLY
LYS
ILE

• Molecule 1: alkyl hydroperoxide reductase C

Chain H:  44% 37% 7% 11%

S1	L2	L3	Q8	P9	F10	R11	Q16	K19	D20	F21	E26	K32	V33	S34	I35	V36	V37	F38	Y39	P40	F43	V46	C47	P48	T49	E50	L51	E52	D53	V54	Q55	E57	Y58	L61	K62	V66	E67	V68	Y69	S70	V71	V78	H79	K80	E84	N85	S86
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P87	A88	W89	I92	E93	Y94	I95	P96	I97	S101	Q102	T103	S106	R106	Q107	V110	L111	N112	E113	E114	T115	D119	R120	T124	I125	D126	P127	T131	Q132	A133	G140	A145	S146	T147	L148	V152	K153	A154	A155	Q156	T157	V158	R159	E160	N161	P162	G163	E164	V165	C166
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THR
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LYS
PRO
SER
LEU
ASP
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VAL
GLY
LYS
ILE

• Molecule 1: alkyl hydroperoxide reductase C

Chain I:  52% 31% 6% 11%

S1	L2	L3	Q8	P9	F10	R11	K19	D20	F21	E23	V24	T25	E26	A27	D28	W33	S34	I35	V36	V37	P40	C47	P48	T49	E52	D53	V54	Q55	Y58	K62	V66	V71	D74	T75	H76	F77	V78	N85	S86	P87	A88	V89	I92	E93	Y94
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I95	P96	G98	D99	P100	S101	Q102	T103	I104	Q107	V110	L111	N112	E113	E114	D119	R120	P127	I131	A138	D139	G140	D144	T147	L148	V152	K153	A154	A155	Q156	V158	R159	E160	N161	P162	G163	V165	C166	PRO	ALA	LYS	TRP	GLU	GLY	GLY	E93	Y94
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LEU
LYS
PRO
SER
LEU
ASP
ILE
VAL
GLY
LYS
ILE

• Molecule 1: alkyl hydroperoxide reductase C

Chain J:  48% 34% 7% 11%

S1	L2	L3	T5	Q8	P9	F10	R11	Q16	K19	D20	F21	F22	E23	Y24	T25	E26	A27	W33	S34	I35	V36	V37	F38	P40	F43	S44	F45	V46	C47	P48	T49	E50	L51	E52	D53	Y54	Q55	L64	G65	V66	E67	V68	Y69	S70	V71	D74	T75	H76	F77	V78
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H79	W82	N85	S86	P87	A88	W89	I92	E93	Y94	I95	P96	G98	D99	P100	S101	Q102	T103	I104	S106	R106	Q107	V110	L111	N112	E113	E114	T115	R120	P127	D128	G140	A145	S146	T147	L148	I149	N150	Q156	Y157	V158	R159	E160	N161	P162	G163	E164	V165	C166	PRO
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ALA
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TRP
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THR
LEU
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LYS
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.22Å 79.32Å 104.45Å 77.22° 82.33° 80.08°	Depositor
Resolution (Å)	50.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12982	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NH4

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	0.50	0/1326	0.96	7/1800 (0.4%)
1	B	0.49	0/1326	0.92	1/1800 (0.1%)
1	C	0.50	0/1326	0.94	6/1800 (0.3%)
1	D	0.45	0/1326	0.93	4/1800 (0.2%)
1	E	0.43	0/1326	0.93	4/1800 (0.2%)
1	F	0.48	0/1326	0.97	6/1800 (0.3%)
1	G	0.49	0/1326	0.95	4/1800 (0.2%)
1	H	0.46	0/1326	0.93	7/1800 (0.4%)
1	I	0.49	0/1326	0.95	5/1800 (0.3%)
1	J	0.52	1/1326 (0.1%)	0.95	3/1800 (0.2%)
All	All	0.48	1/13260 (0.0%)	0.94	47/18000 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	110	VAL	CA-CB	5.38	1.61	1.54

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	8	GLN	CA-C-N	6.29	126.63	119.83
1	E	8	GLN	C-N-CA	6.29	126.63	119.83
1	I	114	GLU	N-CA-C	6.18	118.98	111.82
1	G	114	GLU	N-CA-C	5.96	118.74	111.82
1	J	114	GLU	N-CA-C	5.92	118.68	111.82
1	G	39	TYR	CA-C-N	5.91	127.23	119.84
1	G	39	TYR	C-N-CA	5.91	127.23	119.84
1	C	114	GLU	N-CA-C	5.89	119.65	112.23
1	H	8	GLN	CA-C-N	5.88	126.18	119.83
1	H	8	GLN	C-N-CA	5.88	126.18	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	53	ASP	N-CA-C	-5.70	105.06	111.28
1	E	114	GLU	N-CA-C	5.67	118.40	111.82
1	D	114	GLU	N-CA-C	5.61	118.32	111.82
1	D	8	GLN	CA-C-N	5.59	125.87	119.83
1	D	8	GLN	C-N-CA	5.59	125.87	119.83
1	B	114	GLU	N-CA-C	5.57	118.28	111.82
1	I	8	GLN	CA-C-N	5.51	125.78	119.83
1	I	8	GLN	C-N-CA	5.51	125.78	119.83
1	G	53	ASP	N-CA-C	-5.44	105.35	111.28
1	H	114	GLU	N-CA-C	5.41	119.04	112.23
1	A	8	GLN	CA-C-N	5.38	125.64	119.83
1	A	8	GLN	C-N-CA	5.38	125.64	119.83
1	I	28	ASP	N-CA-C	-5.38	106.56	113.01
1	E	53	ASP	N-CA-C	-5.35	105.45	111.28
1	H	47	CYS	CA-C-N	5.29	126.45	119.84
1	H	47	CYS	C-N-CA	5.29	126.45	119.84
1	C	53	ASP	N-CA-C	-5.20	105.61	111.28
1	H	39	TYR	CA-C-N	5.19	126.33	119.84
1	H	39	TYR	C-N-CA	5.19	126.33	119.84
1	A	47	CYS	CA-C-N	5.17	126.31	119.84
1	A	47	CYS	C-N-CA	5.17	126.31	119.84
1	F	114	GLU	N-CA-C	5.17	118.75	112.23
1	A	114	GLU	N-CA-C	5.15	118.72	112.23
1	F	47	CYS	CA-C-N	5.14	126.27	119.84
1	F	47	CYS	C-N-CA	5.14	126.27	119.84
1	D	53	ASP	N-CA-C	-5.08	105.74	111.28
1	I	53	ASP	N-CA-C	-5.07	105.75	111.28
1	J	39	TYR	CA-C-N	5.07	126.17	119.84
1	J	39	TYR	C-N-CA	5.07	126.17	119.84
1	C	39	TYR	CA-C-N	5.06	126.16	119.84
1	C	39	TYR	C-N-CA	5.06	126.16	119.84
1	F	8	GLN	CA-C-N	5.05	125.28	119.83
1	F	8	GLN	C-N-CA	5.05	125.28	119.83
1	C	8	GLN	CA-C-N	5.04	125.28	119.83
1	C	8	GLN	C-N-CA	5.04	125.28	119.83
1	A	39	TYR	CA-C-N	5.04	126.13	119.84
1	A	39	TYR	C-N-CA	5.04	126.13	119.84

There are no chirality outliers.

There are no planarity outliers.

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	A	1298	0	1252	65	0
1	B	1298	0	1252	62	0
1	C	1298	0	1252	58	0
1	D	1298	0	1252	74	0
1	E	1298	0	1252	58	0
1	F	1298	0	1252	68	0
1	G	1298	0	1252	63	0
1	H	1298	0	1252	74	0
1	I	1298	0	1252	59	0
1	J	1298	0	1252	74	0
2	F	1	0	0	0	0
2	J	1	0	0	0	0
All	All	12982	0	12520	606	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 24.

All (606) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASN:ND2	1:J:85:ASN:HD22	1.53	1.06
1:B:85:ASN:HD22	1:C:85:ASN:HD22	1.12	0.96
1:D:85:ASN:HD22	1:E:85:ASN:ND2	1.63	0.96
1:A:85:ASN:HD22	1:J:85:ASN:HD22	1.03	0.94
1:H:85:ASN:HD22	1:I:85:ASN:HD22	1.13	0.92
1:J:106:ARG:HB2	1:J:106:ARG:HH11	1.34	0.92
1:G:112:ASN:C	1:G:112:ASN:HD22	1.80	0.90
1:H:85:ASN:HD22	1:I:85:ASN:ND2	1.69	0.89
1:F:112:ASN:C	1:F:112:ASN:HD22	1.81	0.88
1:E:103:THR:O	1:E:107:GLN:HG3	1.73	0.88
1:F:141:ILE:HD12	1:F:141:ILE:H	1.40	0.86
1:D:85:ASN:HD22	1:E:85:ASN:HD22	1.21	0.86
1:D:71:VAL:HG11	1:D:104:ILE:HD11	1.58	0.85
1:B:103:THR:O	1:B:107:GLN:HG3	1.82	0.80
1:C:140:GLY:HA3	1:D:158:VAL:HG21	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:ARG:HD2	1:E:23:GLU:CD	2.07	0.80
1:J:106:ARG:HB2	1:J:106:ARG:NH1	1.96	0.80
1:E:99:ASP:CG	1:E:104:ILE:HG23	2.08	0.79
1:I:148:LEU:O	1:I:152:VAL:HG12	1.81	0.79
1:I:140:GLY:HA3	1:J:158:VAL:HG21	1.66	0.78
1:F:1:SER:OG	1:F:3:ILE:HG22	1.84	0.78
1:B:85:ASN:ND2	1:C:85:ASN:HD22	1.82	0.77
1:I:158:VAL:HG21	1:J:140:GLY:HA3	1.66	0.77
1:C:112:ASN:C	1:C:112:ASN:HD22	1.93	0.76
1:E:83:HIS:HA	1:E:89:VAL:HG23	1.69	0.74
1:A:110:VAL:HG22	1:A:119:ASP:HB2	1.70	0.74
1:J:99:ASP:CG	1:J:104:ILE:HG23	2.11	0.74
1:F:2:LEU:O	1:F:5:THR:HG23	1.86	0.74
1:H:52:GLU:HG3	1:H:56:LYS:HZ2	1.54	0.73
1:A:11:ARG:HD2	1:A:23:GLU:OE1	1.89	0.73
1:H:85:ASN:ND2	1:I:85:ASN:HD22	1.86	0.73
1:C:158:VAL:HG21	1:D:140:GLY:HA3	1.71	0.72
1:J:103:THR:O	1:J:107:GLN:HG3	1.88	0.72
1:C:99:ASP:CG	1:C:104:ILE:HG23	2.15	0.72
1:H:85:ASN:ND2	1:I:85:ASN:ND2	2.38	0.71
1:H:52:GLU:HG3	1:H:56:LYS:NZ	2.06	0.71
1:A:37:VAL:HG12	1:A:122:THR:HG23	1.73	0.71
1:F:103:THR:O	1:F:107:GLN:HG3	1.90	0.71
1:I:99:ASP:CG	1:I:104:ILE:HG23	2.14	0.71
1:A:74:ASP:HB3	1:A:78:VAL:HG11	1.72	0.70
1:I:156:GLN:O	1:I:159:ARG:HB3	1.91	0.70
1:D:61:LEU:HD22	1:D:66:VAL:HG11	1.73	0.70
1:D:71:VAL:CG1	1:D:104:ILE:HD11	2.21	0.70
1:A:99:ASP:CG	1:A:104:ILE:HG23	2.17	0.69
1:B:110:VAL:HG22	1:B:119:ASP:HB2	1.73	0.69
1:J:147:THR:HA	1:J:150:ASN:HD22	1.58	0.69
1:D:112:ASN:C	1:D:112:ASN:HD22	1.98	0.69
1:H:103:THR:O	1:H:107:GLN:HG3	1.93	0.69
1:A:148:LEU:O	1:A:152:VAL:HG13	1.93	0.68
1:A:85:ASN:HD22	1:J:85:ASN:ND2	1.87	0.68
1:D:85:ASN:ND2	1:E:85:ASN:ND2	2.38	0.68
1:G:66:VAL:HG21	1:G:152:VAL:HG21	1.75	0.68
1:J:106:ARG:HH11	1:J:106:ARG:CB	2.05	0.68
1:B:99:ASP:CG	1:B:104:ILE:HG23	2.19	0.67
1:D:53:ASP:HA	1:D:56:LYS:HE2	1.76	0.67
1:A:74:ASP:HB3	1:A:78:VAL:CG1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LYS:H	1:C:19:LYS:HD2	1.60	0.66
1:H:112:ASN:C	1:H:112:ASN:HD22	2.04	0.66
1:D:85:ASN:ND2	1:E:85:ASN:HD22	1.93	0.66
1:J:87:PRO:HG2	1:J:88:ALA:H	1.61	0.66
1:J:112:ASN:HD21	1:J:114:GLU:HG3	1.60	0.66
1:F:120:ARG:HH11	1:F:120:ARG:HG2	1.60	0.66
1:H:57:GLU:O	1:H:61:LEU:HD12	1.96	0.66
1:B:25:THR:C	1:B:27:ALA:H	2.04	0.65
1:G:112:ASN:HD21	1:G:114:GLU:HG2	1.60	0.65
1:B:11:ARG:HD2	1:B:23:GLU:OE1	1.95	0.65
1:I:87:PRO:HG2	1:I:88:ALA:H	1.61	0.65
1:D:156:GLN:O	1:D:159:ARG:HB3	1.97	0.65
1:F:66:VAL:HG21	1:F:152:VAL:HG21	1.77	0.65
1:G:99:ASP:CG	1:G:104:ILE:HG23	2.22	0.65
1:B:156:GLN:O	1:B:159:ARG:HB3	1.98	0.64
1:A:154:ALA:O	1:A:158:VAL:HG23	1.98	0.64
1:C:165:VAL:O	1:C:166:CYS:HB2	1.98	0.64
1:D:99:ASP:CG	1:D:104:ILE:HG12	2.22	0.64
1:H:112:ASN:OD1	1:H:115:THR:HG23	1.98	0.64
1:F:7:VAL:HG21	1:F:125:ILE:HD13	1.79	0.64
1:F:112:ASN:C	1:F:112:ASN:ND2	2.54	0.63
1:B:154:ALA:O	1:B:158:VAL:HG23	1.98	0.63
1:I:71:VAL:HG22	1:I:97:ILE:HB	1.81	0.63
1:J:156:GLN:O	1:J:159:ARG:HB3	1.99	0.63
1:I:120:ARG:HG2	1:I:120:ARG:HH11	1.62	0.63
1:G:1:SER:OG	1:G:3:ILE:HG22	1.99	0.62
1:H:53:ASP:HA	1:H:56:LYS:HZ3	1.64	0.62
1:H:55:GLN:OE1	1:H:92:ILE:HA	1.99	0.62
1:G:161:ASN:N	1:G:162:PRO:HD3	2.14	0.62
1:I:144:ASP:OD2	1:I:147:THR:HG23	1.99	0.62
1:A:103:THR:O	1:A:107:GLN:HG3	2.00	0.62
1:A:85:ASN:ND2	1:J:85:ASN:ND2	2.37	0.62
1:C:73:THR:HG22	1:C:99:ASP:O	2.00	0.62
1:E:110:VAL:HG22	1:E:119:ASP:HB2	1.82	0.62
1:G:140:GLY:HA3	1:H:158:VAL:HG21	1.80	0.62
1:D:11:ARG:HD2	1:D:23:GLU:CD	2.25	0.62
1:A:1:SER:OG	1:A:3:ILE:HG22	1.98	0.62
1:F:161:ASN:N	1:F:162:PRO:HD3	2.14	0.62
1:B:2:LEU:O	1:B:5:THR:HG23	1.99	0.61
1:E:156:GLN:O	1:E:159:ARG:HB3	2.00	0.61
1:H:52:GLU:C	1:H:56:LYS:HZ2	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:ALA:HB2	1:F:3:ILE:HD11	1.82	0.61
1:G:110:VAL:HG22	1:G:119:ASP:HB2	1.82	0.61
1:E:74:ASP:HB3	1:E:78:VAL:CG1	2.30	0.61
1:H:145:ALA:HA	1:H:148:LEU:HD23	1.81	0.61
1:A:149:ILE:O	1:A:153:LYS:HG3	2.00	0.61
1:D:149:ILE:HG13	1:D:150:ASN:N	2.14	0.61
1:J:26:GLU:HG2	1:J:27:ALA:N	2.16	0.61
1:A:64:LEU:HD22	1:A:156:GLN:HE22	1.65	0.60
1:D:33:TRP:O	1:D:66:VAL:HA	2.01	0.60
1:A:79:HIS:ND1	1:A:96:MET:HB3	2.16	0.60
1:H:112:ASN:CG	1:H:115:THR:HG23	2.26	0.60
1:F:141:ILE:HD12	1:F:141:ILE:N	2.13	0.60
1:J:120:ARG:HG2	1:J:120:ARG:HH11	1.67	0.60
1:F:71:VAL:HG22	1:F:97:ILE:HB	1.84	0.60
1:F:120:ARG:HG2	1:F:120:ARG:NH1	2.16	0.60
1:B:85:ASN:HD22	1:C:85:ASN:ND2	1.92	0.60
1:C:156:GLN:O	1:C:159:ARG:HB3	2.01	0.60
1:H:156:GLN:O	1:H:159:ARG:HB3	2.01	0.60
1:I:33:TRP:O	1:I:66:VAL:HA	2.01	0.60
1:H:33:TRP:O	1:H:66:VAL:HA	2.02	0.60
1:F:2:LEU:C	1:F:5:THR:HG23	2.27	0.59
1:B:33:TRP:O	1:B:66:VAL:HA	2.02	0.59
1:G:145:ALA:O	1:G:148:LEU:HB2	2.01	0.59
1:B:60:GLU:O	1:B:64:LEU:HD12	2.03	0.59
1:A:161:ASN:N	1:A:162:PRO:HD3	2.17	0.59
1:C:112:ASN:C	1:C:112:ASN:ND2	2.60	0.59
1:F:147:THR:HA	1:F:150:ASN:HD22	1.67	0.59
1:G:158:VAL:HG21	1:H:140:GLY:HA3	1.84	0.59
1:C:33:TRP:O	1:C:66:VAL:HA	2.02	0.59
1:E:158:VAL:HG21	1:F:140:GLY:HA3	1.84	0.59
1:H:71:VAL:HG22	1:H:97:ILE:HB	1.85	0.59
1:J:147:THR:HA	1:J:150:ASN:ND2	2.18	0.59
1:F:33:TRP:O	1:F:66:VAL:HA	2.01	0.59
1:I:120:ARG:HG2	1:I:120:ARG:NH1	2.18	0.59
1:E:33:TRP:O	1:E:66:VAL:HA	2.02	0.59
1:J:120:ARG:HG2	1:J:120:ARG:NH1	2.16	0.59
1:J:161:ASN:N	1:J:162:PRO:HD3	2.18	0.59
1:H:58:TYR:CZ	1:H:62:LYS:HE2	2.38	0.58
1:I:22:PHE:HZ	1:I:95:ILE:HD12	1.68	0.58
1:D:1:SER:OG	1:D:3:ILE:HG22	2.03	0.58
1:B:35:ILE:CD1	1:B:148:LEU:HG	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ASP:HB3	1:E:78:VAL:HG11	1.83	0.58
1:E:161:ASN:N	1:E:162:PRO:HD3	2.18	0.58
1:G:33:TRP:O	1:G:66:VAL:HA	2.03	0.58
1:H:33:TRP:CE2	1:H:127:PRO:HD3	2.39	0.58
1:D:161:ASN:N	1:D:162:PRO:HD3	2.18	0.58
1:H:53:ASP:HA	1:H:56:LYS:CD	2.34	0.58
1:H:69:TYR:CE1	1:H:95:ILE:HG13	2.39	0.58
1:F:85:ASN:ND2	1:G:85:ASN:HB3	2.19	0.58
1:J:55:GLN:OE1	1:J:93:GLU:N	2.35	0.58
1:B:161:ASN:N	1:B:162:PRO:HD3	2.18	0.57
1:E:83:HIS:HA	1:E:89:VAL:CG2	2.33	0.57
1:F:51:LEU:HB3	1:F:92:ILE:HD11	1.87	0.57
1:A:22:PHE:HZ	1:A:95:ILE:HD12	1.70	0.57
1:B:1:SER:OG	1:B:3:ILE:HG22	2.05	0.57
1:D:7:VAL:HG21	1:D:125:ILE:HD13	1.85	0.57
1:F:141:ILE:H	1:F:141:ILE:CD1	2.16	0.57
1:H:148:LEU:O	1:H:152:VAL:HG13	2.05	0.57
1:G:120:ARG:HG2	1:G:120:ARG:HH11	1.69	0.57
1:C:161:ASN:N	1:C:162:PRO:HD3	2.18	0.57
1:A:33:TRP:O	1:A:66:VAL:HA	2.05	0.57
1:C:22:PHE:HZ	1:C:95:ILE:HD12	1.70	0.57
1:H:26:GLU:H	1:H:26:GLU:CD	2.13	0.57
1:F:55:GLN:OE1	1:F:92:ILE:HA	2.04	0.56
1:F:55:GLN:OE1	1:F:93:GLU:N	2.35	0.56
1:E:22:PHE:HZ	1:E:95:ILE:HD12	1.70	0.56
1:I:33:TRP:CE2	1:I:127:PRO:HD3	2.40	0.56
1:C:33:TRP:CE2	1:C:127:PRO:HD3	2.41	0.56
1:H:154:ALA:O	1:H:158:VAL:HG23	2.06	0.56
1:G:2:LEU:O	1:G:5:THR:HG23	2.06	0.56
1:H:69:TYR:CD1	1:H:95:ILE:HB	2.40	0.56
1:J:89:VAL:HG23	1:J:92:ILE:HD12	1.87	0.56
1:I:35:ILE:O	1:I:35:ILE:HG12	2.06	0.56
1:J:99:ASP:OD1	1:J:104:ILE:HG23	2.06	0.56
1:B:75:THR:O	1:B:78:VAL:HG13	2.05	0.56
1:B:25:THR:C	1:B:27:ALA:N	2.63	0.56
1:C:141:ILE:H	1:C:141:ILE:HD12	1.71	0.56
1:H:46:VAL:HG21	1:H:120:ARG:NH2	2.20	0.56
1:I:103:THR:O	1:I:107:GLN:HG3	2.06	0.56
1:H:57:GLU:C	1:H:61:LEU:HD12	2.31	0.55
1:C:101:SER:OG	1:C:103:THR:HG23	2.07	0.55
1:D:89:VAL:HG23	1:D:92:ILE:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:GLU:O	1:E:54:VAL:HG23	2.06	0.55
1:F:99:ASP:CG	1:F:104:ILE:HG23	2.31	0.55
1:H:52:GLU:O	1:H:56:LYS:HD2	2.06	0.55
1:B:51:LEU:HB3	1:B:92:ILE:HD11	1.89	0.55
1:C:120:ARG:NH1	1:C:120:ARG:HG2	2.22	0.55
1:B:2:LEU:C	1:B:5:THR:HG23	2.32	0.55
1:B:87:PRO:HG2	1:B:88:ALA:H	1.72	0.55
1:C:10:PHE:CD1	1:C:10:PHE:C	2.85	0.55
1:G:9:PRO:HA	1:G:26:GLU:OE1	2.06	0.55
1:H:55:GLN:OE1	1:H:93:GLU:N	2.39	0.55
1:H:112:ASN:OD1	1:H:115:THR:CG2	2.55	0.55
1:F:85:ASN:ND2	1:G:85:ASN:HD22	2.05	0.54
1:E:75:THR:O	1:E:78:VAL:HG12	2.07	0.54
1:F:101:SER:O	1:F:102:GLN:HB2	2.07	0.54
1:J:86:SER:HB3	1:J:89:VAL:CG1	2.38	0.54
1:J:86:SER:OG	1:J:89:VAL:HG12	2.08	0.54
1:B:99:ASP:OD1	1:B:104:ILE:HG23	2.07	0.54
1:D:33:TRP:CD2	1:D:127:PRO:HD3	2.43	0.54
1:F:148:LEU:O	1:F:152:VAL:HG12	2.07	0.54
1:J:33:TRP:O	1:J:66:VAL:HA	2.07	0.54
1:C:87:PRO:HG2	1:C:88:ALA:H	1.72	0.54
1:H:124:ILE:HB	1:H:133:ALA:HB3	1.90	0.54
1:B:71:VAL:HG22	1:B:97:ILE:HB	1.89	0.54
1:E:26:GLU:CD	1:E:26:GLU:H	2.16	0.53
1:F:85:ASN:HB3	1:G:85:ASN:ND2	2.23	0.53
1:F:86:SER:HB3	1:F:89:VAL:HG12	1.90	0.53
1:G:55:GLN:OE1	1:G:93:GLU:N	2.28	0.53
1:I:74:ASP:HB3	1:I:78:VAL:CG1	2.38	0.53
1:I:87:PRO:HG2	1:I:88:ALA:N	2.23	0.53
1:G:103:THR:O	1:G:107:GLN:HG3	2.08	0.53
1:G:156:GLN:O	1:G:159:ARG:HB3	2.08	0.53
1:H:9:PRO:HA	1:H:26:GLU:OE1	2.07	0.53
1:D:49:THR:HG22	1:D:53:ASP:OD2	2.08	0.53
1:F:85:ASN:HD22	1:G:85:ASN:ND2	2.06	0.53
1:H:87:PRO:HG2	1:H:88:ALA:H	1.74	0.53
1:H:161:ASN:N	1:H:162:PRO:HD3	2.24	0.53
1:C:35:ILE:HG12	1:C:35:ILE:O	2.07	0.53
1:D:87:PRO:HG2	1:D:88:ALA:H	1.74	0.53
1:G:51:LEU:HB3	1:G:92:ILE:HD11	1.90	0.53
1:J:145:ALA:O	1:J:148:LEU:HB2	2.08	0.53
1:D:165:VAL:O	1:D:166:CYS:HB2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ASN:ND2	1:C:85:ASN:ND2	2.52	0.53
1:C:86:SER:HB3	1:C:89:VAL:CG1	2.39	0.53
1:D:43:PHE:CE2	1:D:78:VAL:HG23	2.44	0.53
1:E:124:ILE:HB	1:E:133:ALA:HB3	1.91	0.53
1:F:15:PHE:CE1	1:F:80:LYS:HD2	2.44	0.53
1:J:101:SER:O	1:J:102:GLN:HB2	2.07	0.53
1:J:165:VAL:O	1:J:166:CYS:HB2	2.09	0.53
1:E:42:ASP:OD2	1:E:79:HIS:ND1	2.40	0.52
1:G:33:TRP:CE2	1:G:156:GLN:HG2	2.45	0.52
1:C:89:VAL:HG23	1:C:92:ILE:HD12	1.90	0.52
1:D:35:ILE:HG12	1:D:35:ILE:O	2.08	0.52
1:D:110:VAL:HG13	1:D:110:VAL:O	2.09	0.52
1:D:112:ASN:C	1:D:112:ASN:ND2	2.60	0.52
1:E:87:PRO:HG2	1:E:88:ALA:H	1.74	0.52
1:E:140:GLY:HA2	1:F:165:VAL:HG11	1.92	0.52
1:D:11:ARG:HD2	1:D:23:GLU:OE1	2.08	0.52
1:I:131:ILE:N	1:I:131:ILE:HD12	2.24	0.52
1:B:21:PHE:CD1	1:B:76:HIS:HD2	2.27	0.52
1:E:59:ALA:HA	1:E:62:LYS:HE2	1.92	0.52
1:E:46:VAL:HG21	1:E:120:ARG:NH2	2.25	0.52
1:F:156:GLN:O	1:F:159:ARG:HB3	2.09	0.52
1:H:50:GLU:O	1:H:54:VAL:HG23	2.09	0.52
1:J:33:TRP:CE2	1:J:127:PRO:HD3	2.45	0.52
1:B:46:VAL:HG21	1:B:120:ARG:HH22	1.74	0.52
1:A:138:ALA:HB2	1:B:3:ILE:HD11	1.92	0.52
1:G:7:VAL:HG21	1:G:125:ILE:HD13	1.91	0.52
1:H:16:GLN:OE1	1:H:19:LYS:HE3	2.09	0.52
1:I:110:VAL:HG22	1:I:119:ASP:HB2	1.90	0.52
1:G:112:ASN:C	1:G:112:ASN:ND2	2.53	0.52
1:G:137:ASN:ND2	1:G:143:ARG:HG2	2.25	0.52
1:D:22:PHE:N	1:D:22:PHE:CD2	2.78	0.52
1:A:51:LEU:HB3	1:A:92:ILE:HD11	1.92	0.51
1:E:71:VAL:HG22	1:E:97:ILE:HB	1.92	0.51
1:H:33:TRP:CZ3	1:H:126:ASP:HA	2.46	0.51
1:D:33:TRP:CB	1:D:66:VAL:HG22	2.40	0.51
1:J:128:ASP:OD2	1:J:159:ARG:NH1	2.43	0.51
1:F:11:ARG:HD2	1:F:23:GLU:CD	2.35	0.51
1:H:53:ASP:HA	1:H:56:LYS:HD2	1.91	0.51
1:J:67:GLU:OE1	1:J:67:GLU:HA	2.10	0.51
1:A:165:VAL:HG21	1:B:140:GLY:HA2	1.93	0.51
1:I:89:VAL:HG23	1:I:92:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:THR:C	1:A:27:ALA:N	2.68	0.51
1:F:54:VAL:HG12	1:F:94:TYR:CE2	2.46	0.51
1:G:112:ASN:HD21	1:G:114:GLU:CG	2.23	0.51
1:H:101:SER:O	1:H:102:GLN:HB2	2.11	0.51
1:H:33:TRP:CE3	1:H:126:ASP:HA	2.45	0.51
1:I:161:ASN:N	1:I:162:PRO:HD3	2.26	0.51
1:C:86:SER:HB3	1:C:89:VAL:HG12	1.94	0.51
1:E:148:LEU:O	1:E:152:VAL:HG13	2.11	0.51
1:F:154:ALA:O	1:F:158:VAL:HG23	2.11	0.51
1:H:3:ILE:HD11	1:H:132:GLN:C	2.36	0.51
1:A:85:ASN:HB3	1:J:85:ASN:ND2	2.26	0.50
1:A:87:PRO:HG2	1:A:88:ALA:H	1.76	0.50
1:D:154:ALA:O	1:D:158:VAL:HG23	2.11	0.50
1:E:60:GLU:HG2	1:E:63:LYS:NZ	2.25	0.50
1:C:71:VAL:HG22	1:C:97:ILE:HB	1.94	0.50
1:G:69:TYR:CD1	1:G:97:ILE:HD11	2.45	0.50
1:C:120:ARG:HG2	1:C:120:ARG:HH11	1.74	0.50
1:D:75:THR:O	1:D:78:VAL:HG13	2.12	0.50
1:G:116:GLY:C	1:G:117:LEU:HD23	2.36	0.50
1:I:66:VAL:HG21	1:I:152:VAL:HG21	1.93	0.50
1:E:69:TYR:CD1	1:E:95:ILE:HB	2.47	0.50
1:F:132:GLN:NE2	1:F:132:GLN:HA	2.26	0.50
1:D:86:SER:HB3	1:D:89:VAL:CG1	2.42	0.50
1:D:145:ALA:O	1:D:148:LEU:HB2	2.11	0.50
1:I:49:THR:HG22	1:I:53:ASP:OD2	2.11	0.50
1:G:3:ILE:HG23	1:G:3:ILE:O	2.11	0.50
1:H:16:GLN:CD	1:H:95:ILE:HD13	2.37	0.50
1:I:47:CYS:C	1:I:49:THR:H	2.20	0.50
1:B:25:THR:OG1	1:B:27:ALA:HB3	2.11	0.50
1:E:16:GLN:CD	1:E:95:ILE:HD13	2.37	0.50
1:A:25:THR:OG1	1:A:27:ALA:HB3	2.12	0.50
1:A:75:THR:O	1:A:78:VAL:HG12	2.11	0.49
1:D:47:CYS:C	1:D:49:THR:H	2.19	0.49
1:E:33:TRP:CD2	1:E:127:PRO:HD3	2.47	0.49
1:G:120:ARG:HG2	1:G:120:ARG:NH1	2.27	0.49
1:B:35:ILE:HD11	1:B:148:LEU:HG	1.93	0.49
1:G:2:LEU:C	1:G:5:THR:HG23	2.38	0.49
1:G:165:VAL:HG11	1:H:140:GLY:HA2	1.94	0.49
1:J:2:LEU:O	1:J:5:THR:HG23	2.12	0.49
1:J:67:GLU:HG3	1:J:69:TYR:CE2	2.47	0.49
1:E:60:GLU:HA	1:E:63:LYS:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:76:HIS:HA	1:J:79:HIS:HD2	1.76	0.49
1:D:33:TRP:CE2	1:D:127:PRO:HD3	2.47	0.49
1:D:43:PHE:HE2	1:D:78:VAL:HG23	1.77	0.49
1:I:101:SER:O	1:I:102:GLN:HB2	2.11	0.49
1:A:25:THR:C	1:A:27:ALA:H	2.20	0.49
1:A:97:ILE:HG22	1:A:98:GLY:N	2.27	0.49
1:C:39:TYR:CZ	1:C:72:SER:HB3	2.48	0.49
1:E:38:PHE:CD1	1:E:71:VAL:HB	2.47	0.49
1:H:112:ASN:C	1:H:112:ASN:ND2	2.65	0.49
1:I:58:TYR:CZ	1:I:62:LYS:HE2	2.47	0.49
1:F:47:CYS:C	1:F:49:THR:H	2.20	0.49
1:G:15:PHE:HB2	1:G:21:PHE:CE1	2.48	0.49
1:D:22:PHE:HZ	1:D:95:ILE:HD12	1.78	0.49
1:C:47:CYS:H	1:D:166:CYS:HB3	1.77	0.49
1:F:50:GLU:OE1	1:F:120:ARG:NH1	2.46	0.49
1:D:110:VAL:HG22	1:D:119:ASP:HB2	1.95	0.49
1:I:131:ILE:HD12	1:I:131:ILE:H	1.78	0.49
1:B:152:VAL:O	1:B:156:GLN:HG3	2.13	0.48
1:E:80:LYS:O	1:E:84:GLU:HG3	2.13	0.48
1:I:140:GLY:HA2	1:J:165:VAL:HG11	1.95	0.48
1:I:165:VAL:O	1:I:166:CYS:HB2	2.13	0.48
1:J:112:ASN:HD21	1:J:114:GLU:CG	2.25	0.48
1:E:145:ALA:HA	1:E:148:LEU:HD13	1.95	0.48
1:A:147:THR:HA	1:A:150:ASN:HD22	1.78	0.48
1:C:47:CYS:C	1:C:49:THR:H	2.22	0.48
1:E:9:PRO:HA	1:E:26:GLU:OE1	2.14	0.48
1:I:11:ARG:HD2	1:I:23:GLU:CD	2.38	0.48
1:C:26:GLU:O	1:C:29:LEU:HB2	2.14	0.48
1:D:55:GLN:OE1	1:D:93:GLU:N	2.41	0.48
1:J:9:PRO:HA	1:J:26:GLU:OE1	2.13	0.48
1:A:32:LYS:NZ	1:A:34:SER:HB3	2.29	0.48
1:A:101:SER:O	1:A:102:GLN:HB2	2.13	0.48
1:A:110:VAL:CG2	1:A:119:ASP:HB2	2.41	0.48
1:A:156:GLN:O	1:A:159:ARG:HB3	2.13	0.48
1:B:146:SER:O	1:B:149:ILE:HG12	2.14	0.48
1:G:141:ILE:HD12	1:G:141:ILE:H	1.79	0.48
1:B:33:TRP:CE2	1:B:127:PRO:HD3	2.49	0.48
1:D:22:PHE:N	1:D:22:PHE:HD2	2.12	0.48
1:D:74:ASP:HB3	1:D:78:VAL:CG1	2.44	0.48
1:H:47:CYS:C	1:H:49:THR:H	2.22	0.48
1:J:11:ARG:HD2	1:J:23:GLU:CD	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:TYR:CE1	1:E:95:ILE:HG13	2.49	0.48
1:H:125:ILE:HD12	1:H:125:ILE:N	2.28	0.47
1:C:141:ILE:HD12	1:C:141:ILE:N	2.29	0.47
1:D:5:THR:O	1:D:131:ILE:HD12	2.14	0.47
1:G:102:GLN:HE21	1:G:106:ARG:NH2	2.12	0.47
1:J:47:CYS:C	1:J:49:THR:H	2.22	0.47
1:F:85:ASN:HD22	1:G:85:ASN:CB	2.27	0.47
1:J:35:ILE:HG12	1:J:35:ILE:O	2.13	0.47
1:J:49:THR:HG22	1:J:53:ASP:OD2	2.14	0.47
1:B:47:CYS:C	1:B:49:THR:H	2.22	0.47
1:F:85:ASN:HD22	1:G:85:ASN:HB3	1.77	0.47
1:H:53:ASP:N	1:H:56:LYS:HZ2	2.13	0.47
1:H:71:VAL:HG11	1:H:104:ILE:HD11	1.96	0.47
1:J:71:VAL:HG22	1:J:97:ILE:HB	1.94	0.47
1:A:140:GLY:HA2	1:B:165:VAL:HG11	1.97	0.47
1:B:85:ASN:HB3	1:C:85:ASN:ND2	2.30	0.47
1:D:74:ASP:HB3	1:D:78:VAL:HG11	1.97	0.47
1:H:86:SER:HB3	1:H:89:VAL:CG1	2.44	0.47
1:J:87:PRO:HG2	1:J:88:ALA:N	2.26	0.47
1:C:145:ALA:O	1:C:148:LEU:HB2	2.14	0.47
1:D:120:ARG:NH1	1:D:120:ARG:HG2	2.29	0.47
1:D:52:GLU:O	1:D:56:LYS:HG3	2.14	0.47
1:E:11:ARG:HD2	1:E:23:GLU:OE1	2.14	0.47
1:F:33:TRP:CE2	1:F:127:PRO:HD3	2.50	0.47
1:C:16:GLN:CD	1:C:95:ILE:HD13	2.40	0.47
1:D:25:THR:C	1:D:27:ALA:N	2.71	0.47
1:E:47:CYS:C	1:E:49:THR:H	2.23	0.47
1:C:51:LEU:HD12	1:C:94:TYR:OH	2.15	0.47
1:A:163:GLY:C	1:A:165:VAL:H	2.23	0.47
1:B:112:ASN:C	1:B:112:ASN:ND2	2.72	0.47
1:G:7:VAL:HG11	1:G:29:LEU:HD12	1.96	0.47
1:G:33:TRP:CE2	1:G:127:PRO:HD3	2.50	0.47
1:G:86:SER:HB3	1:G:89:VAL:HG12	1.97	0.47
1:A:47:CYS:C	1:A:49:THR:H	2.21	0.46
1:B:33:TRP:HB3	1:B:66:VAL:HG22	1.96	0.46
1:B:38:PHE:CD1	1:B:71:VAL:HB	2.50	0.46
1:F:163:GLY:C	1:F:165:VAL:H	2.21	0.46
1:I:10:PHE:CE2	1:I:26:GLU:HA	2.51	0.46
1:J:101:SER:OG	1:J:103:THR:HG23	2.16	0.46
1:J:163:GLY:C	1:J:165:VAL:H	2.24	0.46
1:B:20:ASP:O	1:B:21:PHE:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:VAL:HG13	1:F:110:VAL:O	2.15	0.46
1:H:2:LEU:HB3	1:H:131:ILE:HD12	1.98	0.46
1:J:10:PHE:CD1	1:J:10:PHE:C	2.93	0.46
1:E:33:TRP:CE2	1:E:127:PRO:HD3	2.51	0.46
1:F:7:VAL:CG2	1:F:125:ILE:HD13	2.44	0.46
1:G:58:TYR:CE1	1:G:62:LYS:HE2	2.50	0.46
1:H:26:GLU:CD	1:H:26:GLU:N	2.72	0.46
1:C:53:ASP:HA	1:C:56:LYS:HD2	1.97	0.46
1:D:33:TRP:HB3	1:D:66:VAL:HG22	1.98	0.46
1:G:67:GLU:OE1	1:G:67:GLU:HA	2.15	0.46
1:B:51:LEU:O	1:B:94:TYR:OH	2.32	0.46
1:F:35:ILE:HG23	1:F:68:VAL:HG22	1.97	0.46
1:H:33:TRP:CD2	1:H:127:PRO:HD3	2.51	0.46
1:J:69:TYR:N	1:J:69:TYR:CD2	2.84	0.46
1:D:20:ASP:O	1:D:21:PHE:C	2.58	0.46
1:H:92:ILE:HG23	1:H:94:TYR:CZ	2.50	0.46
1:H:163:GLY:C	1:H:165:VAL:H	2.24	0.46
1:B:22:PHE:HZ	1:B:95:ILE:HD12	1.80	0.46
1:H:35:ILE:HG22	1:H:66:VAL:CG1	2.45	0.46
1:H:80:LYS:O	1:H:84:GLU:HG3	2.16	0.46
1:H:53:ASP:HA	1:H:56:LYS:NZ	2.31	0.46
1:I:19:LYS:H	1:I:19:LYS:HD2	1.81	0.46
1:E:163:GLY:C	1:E:165:VAL:H	2.24	0.46
1:I:138:ALA:HB2	1:J:3:ILE:HD11	1.98	0.46
1:E:20:ASP:O	1:E:21:PHE:C	2.59	0.45
1:G:102:GLN:NE2	1:G:106:ARG:NH2	2.64	0.45
1:A:146:SER:O	1:A:149:ILE:HG12	2.16	0.45
1:D:44:SER:OG	1:D:46:VAL:HG22	2.17	0.45
1:G:47:CYS:C	1:G:49:THR:H	2.24	0.45
1:C:163:GLY:C	1:C:165:VAL:H	2.23	0.45
1:F:16:GLN:CD	1:F:95:ILE:HD13	2.41	0.45
1:F:26:GLU:OE1	1:F:26:GLU:N	2.40	0.45
1:H:53:ASP:CA	1:H:56:LYS:HD2	2.46	0.45
1:I:20:ASP:O	1:I:21:PHE:C	2.59	0.45
1:I:154:ALA:O	1:I:158:VAL:HG23	2.16	0.45
1:B:148:LEU:O	1:B:152:VAL:HG13	2.16	0.45
1:E:15:PHE:CD1	1:E:16:GLN:N	2.84	0.45
1:G:152:VAL:O	1:G:156:GLN:HG3	2.17	0.45
1:J:64:LEU:HD22	1:J:156:GLN:HE22	1.81	0.45
1:A:43:PHE:CZ	1:A:82:TRP:HA	2.51	0.45
1:D:163:GLY:C	1:D:165:VAL:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:163:GLY:C	1:I:165:VAL:H	2.24	0.45
1:J:43:PHE:CZ	1:J:82:TRP:HA	2.51	0.45
1:A:122:THR:OG1	1:A:143:ARG:HD2	2.16	0.45
1:B:126:ASP:OD1	1:B:126:ASP:C	2.59	0.45
1:H:20:ASP:O	1:H:21:PHE:C	2.59	0.45
1:A:3:ILE:HG23	1:A:3:ILE:O	2.16	0.45
1:B:101:SER:O	1:B:102:GLN:HB2	2.17	0.45
1:G:163:GLY:C	1:G:165:VAL:H	2.25	0.45
1:H:89:VAL:HG23	1:H:92:ILE:HD12	1.97	0.45
1:A:89:VAL:HG23	1:A:92:ILE:HD12	1.98	0.45
1:A:126:ASP:OD1	1:A:126:ASP:C	2.60	0.45
1:C:55:GLN:NE2	1:C:93:GLU:HG3	2.32	0.45
1:A:32:LYS:HZ1	1:A:34:SER:HB3	1.81	0.45
1:B:36:VAL:HG12	1:B:125:ILE:HD11	1.98	0.45
1:E:101:SER:O	1:E:102:GLN:HB2	2.16	0.45
1:E:126:ASP:C	1:E:126:ASP:OD1	2.60	0.45
1:G:20:ASP:O	1:G:21:PHE:C	2.59	0.45
1:F:39:TYR:OH	1:F:79:HIS:CE1	2.70	0.44
1:A:20:ASP:O	1:A:21:PHE:C	2.60	0.44
1:B:35:ILE:HG23	1:B:68:VAL:HG22	2.00	0.44
1:D:152:VAL:O	1:D:156:GLN:HG3	2.17	0.44
1:E:165:VAL:HG12	1:E:165:VAL:O	2.17	0.44
1:B:87:PRO:HG2	1:B:88:ALA:N	2.32	0.44
1:H:110:VAL:HG22	1:H:119:ASP:HB2	1.99	0.44
1:D:101:SER:O	1:D:102:GLN:HB2	2.18	0.44
1:A:39:TYR:CZ	1:A:72:SER:HB3	2.53	0.44
1:A:140:GLY:HA2	1:B:165:VAL:HG21	2.00	0.44
1:B:163:GLY:C	1:B:165:VAL:H	2.24	0.44
1:C:112:ASN:OD1	1:C:115:THR:HG23	2.17	0.44
1:F:21:PHE:CD1	1:F:76:HIS:HD2	2.35	0.44
1:F:138:ALA:HB3	1:F:141:ILE:HD13	1.99	0.44
1:F:165:VAL:O	1:F:166:CYS:CB	2.63	0.44
1:I:21:PHE:CD1	1:I:76:HIS:HD2	2.36	0.44
1:C:20:ASP:O	1:C:21:PHE:C	2.60	0.44
1:G:15:PHE:HB2	1:G:21:PHE:HE1	1.81	0.44
1:H:53:ASP:N	1:H:56:LYS:NZ	2.66	0.44
1:E:33:TRP:CE3	1:E:126:ASP:HA	2.52	0.44
1:H:50:GLU:OE1	1:H:120:ARG:NH1	2.51	0.44
1:D:16:GLN:CD	1:D:95:ILE:HD13	2.42	0.44
1:H:51:LEU:H	1:H:51:LEU:HD22	1.83	0.44
1:A:37:VAL:HG23	1:A:37:VAL:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ALA:O	1:B:44:SER:HB2	2.18	0.44
1:I:55:GLN:NE2	1:I:93:GLU:HG3	2.33	0.44
1:A:138:ALA:CB	1:B:132:GLN:NE2	2.81	0.43
1:J:20:ASP:O	1:J:21:PHE:C	2.60	0.43
1:J:112:ASN:ND2	1:J:114:GLU:HG3	2.31	0.43
1:B:7:VAL:HG11	1:B:29:LEU:HD12	1.99	0.43
1:E:35:ILE:HG23	1:E:35:ILE:O	2.18	0.43
1:A:120:ARG:HH11	1:A:120:ARG:HG2	1.83	0.43
1:B:20:ASP:OD1	1:B:21:PHE:N	2.51	0.43
1:F:85:ASN:ND2	1:G:85:ASN:ND2	2.65	0.43
1:J:158:VAL:HG22	1:J:165:VAL:HG22	2.01	0.43
1:C:55:GLN:CD	1:C:93:GLU:HG3	2.43	0.43
1:D:146:SER:C	1:D:148:LEU:H	2.27	0.43
1:F:35:ILE:HG22	1:F:66:VAL:CG1	2.48	0.43
1:I:74:ASP:HB3	1:I:78:VAL:HG13	1.99	0.43
1:J:55:GLN:OE1	1:J:92:ILE:HA	2.19	0.43
1:J:86:SER:CB	1:J:89:VAL:HG12	2.49	0.43
1:F:20:ASP:O	1:F:21:PHE:C	2.61	0.43
1:J:87:PRO:CG	1:J:88:ALA:H	2.31	0.43
1:J:112:ASN:HD22	1:J:112:ASN:C	2.26	0.43
1:D:131:ILE:HD12	1:D:131:ILE:H	1.83	0.43
1:I:25:THR:C	1:I:27:ALA:N	2.75	0.43
1:J:26:GLU:HG2	1:J:27:ALA:H	1.82	0.43
1:C:146:SER:C	1:C:148:LEU:H	2.27	0.43
1:C:149:ILE:O	1:C:153:LYS:HG3	2.18	0.43
1:E:102:GLN:NE2	1:E:106:ARG:HH22	2.17	0.43
1:G:147:THR:HA	1:G:150:ASN:HD22	1.84	0.43
1:I:87:PRO:CG	1:I:88:ALA:H	2.30	0.43
1:J:106:ARG:NH1	1:J:111:LEU:HD22	2.34	0.43
1:D:33:TRP:HB2	1:D:66:VAL:HG22	2.01	0.43
1:G:101:SER:O	1:G:102:GLN:HB2	2.19	0.43
1:J:2:LEU:C	1:J:5:THR:HG23	2.44	0.43
1:D:120:ARG:HG2	1:D:120:ARG:HH11	1.84	0.42
1:E:39:TYR:HE2	1:E:42:ASP:OD1	2.02	0.42
1:I:71:VAL:HG21	1:I:104:ILE:HD11	2.01	0.42
1:C:3:ILE:HG23	1:C:3:ILE:O	2.17	0.42
1:E:13:GLN:HB2	1:E:76:HIS:ND1	2.34	0.42
1:H:165:VAL:HG12	1:H:165:VAL:O	2.19	0.42
1:A:9:PRO:HA	1:A:26:GLU:OE1	2.19	0.42
1:C:165:VAL:HG11	1:D:140:GLY:HA2	2.02	0.42
1:D:22:PHE:CZ	1:D:95:ILE:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:GLN:HE21	1:B:106:ARG:NH2	2.17	0.42
1:A:21:PHE:CD1	1:A:76:HIS:HD2	2.37	0.42
1:E:149:ILE:HG13	1:E:150:ASN:N	2.33	0.42
1:C:22:PHE:CZ	1:C:95:ILE:HD12	2.52	0.42
1:C:75:THR:OG1	1:C:78:VAL:HG13	2.20	0.42
1:F:16:GLN:O	1:F:17:SER:C	2.63	0.42
1:G:7:VAL:CG2	1:G:125:ILE:HD13	2.50	0.42
1:J:112:ASN:HD22	1:J:115:THR:H	1.66	0.42
1:F:145:ALA:O	1:F:148:LEU:HB2	2.19	0.42
1:I:49:THR:O	1:I:52:GLU:HG2	2.20	0.42
1:I:74:ASP:HB3	1:I:78:VAL:HG11	2.02	0.42
1:A:147:THR:HA	1:A:150:ASN:ND2	2.34	0.42
1:D:7:VAL:CG2	1:D:125:ILE:HD13	2.49	0.42
1:D:3:ILE:O	1:D:3:ILE:HG23	2.20	0.42
1:G:39:TYR:CE2	1:G:42:ASP:OD1	2.73	0.42
1:G:49:THR:HG22	1:G:53:ASP:OD2	2.20	0.42
1:I:86:SER:HB3	1:I:89:VAL:CG1	2.50	0.42
1:B:33:TRP:CE3	1:B:126:ASP:HA	2.55	0.41
1:C:19:LYS:H	1:C:19:LYS:CD	2.30	0.41
1:C:29:LEU:HD23	1:C:29:LEU:HA	1.86	0.41
1:F:25:THR:OG1	1:F:27:ALA:HB3	2.19	0.41
1:F:43:PHE:CZ	1:F:82:TRP:HA	2.55	0.41
1:F:161:ASN:N	1:F:162:PRO:CD	2.82	0.41
1:H:146:SER:C	1:H:148:LEU:H	2.28	0.41
1:I:87:PRO:CG	1:I:88:ALA:N	2.83	0.41
1:J:146:SER:C	1:J:148:LEU:H	2.28	0.41
1:C:140:GLY:CA	1:D:158:VAL:HG21	2.41	0.41
1:D:147:THR:O	1:D:151:LYS:HG3	2.20	0.41
1:F:22:PHE:HZ	1:F:95:ILE:HD12	1.85	0.41
1:G:146:SER:C	1:G:148:LEU:H	2.28	0.41
1:C:51:LEU:HB3	1:C:92:ILE:HD11	2.03	0.41
1:D:15:PHE:CE2	1:D:80:LYS:HA	2.55	0.41
1:G:161:ASN:N	1:G:162:PRO:CD	2.81	0.41
1:J:16:GLN:CD	1:J:95:ILE:HD13	2.45	0.41
1:E:82:TRP:CE2	1:E:89:VAL:HG11	2.56	0.41
1:G:66:VAL:CG2	1:G:152:VAL:HG21	2.46	0.41
1:I:99:ASP:OD1	1:I:104:ILE:HG23	2.19	0.41
1:A:120:ARG:HG2	1:A:120:ARG:NH1	2.35	0.41
1:B:145:ALA:O	1:B:148:LEU:HB2	2.19	0.41
1:D:75:THR:O	1:D:78:VAL:CG1	2.68	0.41
1:E:16:GLN:O	1:E:17:SER:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:ALA:CB	1:H:132:GLN:HE21	2.33	0.41
1:I:92:ILE:HG23	1:I:94:TYR:CE2	2.54	0.41
1:A:46:VAL:HG21	1:A:120:ARG:HH22	1.86	0.41
1:A:68:VAL:O	1:A:94:TYR:HB2	2.20	0.41
1:C:16:GLN:O	1:C:17:SER:C	2.63	0.41
1:D:10:PHE:O	1:D:25:THR:HA	2.21	0.41
1:F:165:VAL:O	1:F:166:CYS:HB2	2.21	0.41
1:J:74:ASP:HB3	1:J:78:VAL:HG13	2.03	0.41
1:C:33:TRP:HB3	1:C:66:VAL:HG22	2.01	0.41
1:F:19:LYS:HD2	1:F:19:LYS:H	1.86	0.41
1:A:16:GLN:O	1:A:17:SER:C	2.64	0.41
1:B:3:ILE:O	1:B:3:ILE:HG23	2.21	0.41
1:D:75:THR:OG1	1:D:78:VAL:HG12	2.20	0.41
1:G:69:TYR:HD1	1:G:97:ILE:HD11	1.83	0.41
1:I:112:ASN:C	1:I:112:ASN:ND2	2.77	0.41
1:I:140:GLY:HA2	1:J:165:VAL:CG1	2.50	0.41
1:A:87:PRO:HG2	1:A:88:ALA:N	2.35	0.41
1:A:112:ASN:OD1	1:A:115:THR:HG23	2.21	0.41
1:B:86:SER:HB3	1:B:89:VAL:HG12	2.02	0.41
1:C:26:GLU:HG2	1:C:27:ALA:N	2.36	0.41
1:D:25:THR:C	1:D:27:ALA:H	2.28	0.41
1:F:15:PHE:CD1	1:F:80:LYS:HD2	2.55	0.41
1:F:21:PHE:HE2	1:G:45:PHE:CZ	2.39	0.41
1:H:102:GLN:HE21	1:H:106:ARG:HH22	1.68	0.41
1:I:166:CYS:HB3	1:J:47:CYS:H	1.86	0.41
1:J:51:LEU:HB3	1:J:92:ILE:HD11	2.03	0.41
1:A:19:LYS:H	1:A:19:LYS:HG3	1.56	0.41
1:B:16:GLN:O	1:B:17:SER:C	2.63	0.41
1:E:22:PHE:CZ	1:E:95:ILE:HD12	2.53	0.41
1:H:52:GLU:O	1:H:55:GLN:HB3	2.21	0.41
1:I:33:TRP:CD2	1:I:127:PRO:HD3	2.56	0.41
1:A:33:TRP:CE3	1:A:126:ASP:HA	2.56	0.40
1:B:10:PHE:CD1	1:B:10:PHE:C	2.99	0.40
1:E:68:VAL:O	1:E:94:TYR:HB2	2.21	0.40
1:G:16:GLN:CD	1:G:95:ILE:HD13	2.46	0.40
1:H:43:PHE:CE2	1:H:78:VAL:HG23	2.56	0.40
1:A:20:ASP:OD1	1:A:21:PHE:N	2.54	0.40
1:B:149:ILE:HG13	1:B:150:ASN:N	2.36	0.40
1:G:58:TYR:CE2	1:G:94:TYR:HB3	2.56	0.40
1:H:68:VAL:O	1:H:94:TYR:HB2	2.21	0.40
1:I:3:ILE:O	1:I:3:ILE:CG2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:25:THR:O	1:J:26:GLU:C	2.65	0.40
1:A:165:VAL:O	1:A:165:VAL:HG12	2.22	0.40
1:C:112:ASN:CG	1:C:115:THR:HG23	2.46	0.40
1:D:133:ALA:C	1:D:134:ILE:HG13	2.45	0.40
1:F:60:GLU:OE2	1:F:63:LYS:HD2	2.22	0.40
1:I:33:TRP:HB3	1:I:66:VAL:HG22	2.03	0.40
1:I:35:ILE:HG22	1:I:66:VAL:HG13	2.03	0.40
1:J:102:GLN:HB2	1:J:102:GLN:HE21	1.63	0.40
1:A:144:ASP:OD1	1:A:144:ASP:C	2.64	0.40
1:C:49:THR:HG22	1:C:50:GLU:N	2.37	0.40
1:D:50:GLU:OE1	1:D:120:ARG:NH1	2.54	0.40
1:D:97:ILE:HG22	1:D:98:GLY:N	2.36	0.40
1:F:95:ILE:H	1:F:95:ILE:HG12	1.68	0.40
1:F:121:GLY:HA2	1:F:135:GLU:O	2.21	0.40
1:J:8:GLN:HA	1:J:9:PRO:HD3	1.95	0.40
1:J:45:PHE:HD1	1:J:45:PHE:HA	1.78	0.40
1:J:112:ASN:ND2	1:J:112:ASN:C	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	164/187 (88%)	144 (88%)	16 (10%)	4 (2%)	4	18
1	B	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	4	18
1	C	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	4	18
1	D	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	4	18
1	E	164/187 (88%)	144 (88%)	16 (10%)	4 (2%)	4	18
1	F	164/187 (88%)	145 (88%)	15 (9%)	4 (2%)	4	18
1	G	164/187 (88%)	145 (88%)	15 (9%)	4 (2%)	4	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	164/187 (88%)	144 (88%)	16 (10%)	4 (2%)	4	18
1	I	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	4	18
1	J	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	4	18
All	All	1640/1870 (88%)	1437 (88%)	163 (10%)	40 (2%)	4	18

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	PHE
1	B	21	PHE
1	C	21	PHE
1	D	21	PHE
1	E	21	PHE
1	F	21	PHE
1	G	21	PHE
1	H	21	PHE
1	I	21	PHE
1	J	21	PHE
1	A	40	PRO
1	B	40	PRO
1	C	40	PRO
1	D	40	PRO
1	E	40	PRO
1	F	40	PRO
1	G	40	PRO
1	H	40	PRO
1	I	40	PRO
1	J	40	PRO
1	A	48	PRO
1	B	48	PRO
1	F	48	PRO
1	G	48	PRO
1	B	165	VAL
1	H	48	PRO
1	A	165	VAL
1	E	48	PRO
1	E	165	VAL
1	F	165	VAL
1	I	48	PRO
1	J	48	PRO
1	C	48	PRO

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Mol	Chain	Res	Type
1	C	165	VAL
1	D	48	PRO
1	H	165	VAL
1	G	165	VAL
1	I	165	VAL
1	J	165	VAL
1	D	165	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	141/158 (89%)	135 (96%)	6 (4%)	26	60
1	B	141/158 (89%)	131 (93%)	10 (7%)	13	40
1	C	141/158 (89%)	124 (88%)	17 (12%)	5	16
1	D	141/158 (89%)	128 (91%)	13 (9%)	8	27
1	E	141/158 (89%)	134 (95%)	7 (5%)	22	53
1	F	141/158 (89%)	128 (91%)	13 (9%)	8	27
1	G	141/158 (89%)	129 (92%)	12 (8%)	10	31
1	H	141/158 (89%)	126 (89%)	15 (11%)	6	22
1	I	141/158 (89%)	131 (93%)	10 (7%)	13	40
1	J	141/158 (89%)	127 (90%)	14 (10%)	7	24
All	All	1410/1580 (89%)	1293 (92%)	117 (8%)	10	32

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	35	ILE
1	A	36	VAL
1	A	40	PRO
1	A	104	ILE
1	A	152	VAL

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Mol	Chain	Res	Type
1	B	5	THR
1	B	32	LYS
1	B	36	VAL
1	B	37	VAL
1	B	78	VAL
1	B	104	ILE
1	B	110	VAL
1	B	136	ILE
1	B	148	LEU
1	B	152	VAL
1	C	7	VAL
1	C	19	LYS
1	C	20	ASP
1	C	35	ILE
1	C	36	VAL
1	C	37	VAL
1	C	51	LEU
1	C	66	VAL
1	C	73	THR
1	C	78	VAL
1	C	103	THR
1	C	104	ILE
1	C	110	VAL
1	C	112	ASN
1	C	115	THR
1	C	148	LEU
1	C	166	CYS
1	D	22	PHE
1	D	26	GLU
1	D	32	LYS
1	D	35	ILE
1	D	36	VAL
1	D	37	VAL
1	D	70	SER
1	D	78	VAL
1	D	89	VAL
1	D	110	VAL
1	D	112	ASN
1	D	148	LEU
1	D	166	CYS
1	E	19	LYS
1	E	36	VAL

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Mol	Chain	Res	Type
1	E	37	VAL
1	E	89	VAL
1	E	103	THR
1	E	104	ILE
1	E	166	CYS
1	F	5	THR
1	F	19	LYS
1	F	35	ILE
1	F	36	VAL
1	F	37	VAL
1	F	78	VAL
1	F	95	ILE
1	F	104	ILE
1	F	110	VAL
1	F	112	ASN
1	F	141	ILE
1	F	149	ILE
1	F	166	CYS
1	G	19	LYS
1	G	35	ILE
1	G	36	VAL
1	G	37	VAL
1	G	51	LEU
1	G	78	VAL
1	G	104	ILE
1	G	110	VAL
1	G	112	ASN
1	G	148	LEU
1	G	149	ILE
1	G	166	CYS
1	H	11	ARG
1	H	19	LYS
1	H	26	GLU
1	H	32	LYS
1	H	35	ILE
1	H	36	VAL
1	H	37	VAL
1	H	78	VAL
1	H	89	VAL
1	H	104	ILE
1	H	110	VAL
1	H	112	ASN

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Mol	Chain	Res	Type
1	H	115	THR
1	H	152	VAL
1	H	166	CYS
1	I	19	LYS
1	I	20	ASP
1	I	35	ILE
1	I	36	VAL
1	I	37	VAL
1	I	78	VAL
1	I	89	VAL
1	I	104	ILE
1	I	152	VAL
1	I	166	CYS
1	J	19	LYS
1	J	35	ILE
1	J	36	VAL
1	J	37	VAL
1	J	51	LEU
1	J	69	TYR
1	J	78	VAL
1	J	103	THR
1	J	104	ILE
1	J	106	ARG
1	J	110	VAL
1	J	112	ASN
1	J	148	LEU
1	J	166	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	102	GLN
1	A	107	GLN
1	A	132	GLN
1	A	150	ASN
1	A	156	GLN
1	A	161	ASN
1	B	85	ASN
1	B	102	GLN
1	B	107	GLN
1	B	132	GLN

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Mol	Chain	Res	Type
1	B	156	GLN
1	C	112	ASN
1	C	156	GLN
1	D	8	GLN
1	D	79	HIS
1	D	102	GLN
1	D	112	ASN
1	D	132	GLN
1	D	156	GLN
1	E	85	ASN
1	E	102	GLN
1	E	107	GLN
1	E	132	GLN
1	E	150	ASN
1	E	156	GLN
1	F	79	HIS
1	F	85	ASN
1	F	102	GLN
1	F	112	ASN
1	F	132	GLN
1	F	150	ASN
1	F	156	GLN
1	G	16	GLN
1	G	79	HIS
1	G	85	ASN
1	G	102	GLN
1	G	112	ASN
1	G	132	GLN
1	G	137	ASN
1	G	150	ASN
1	G	156	GLN
1	G	161	ASN
1	H	102	GLN
1	H	107	GLN
1	H	132	GLN
1	H	156	GLN
1	I	85	ASN
1	I	102	GLN
1	I	107	GLN
1	I	132	GLN
1	I	137	ASN
1	I	156	GLN

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Mol	Chain	Res	Type
1	J	79	HIS
1	J	102	GLN
1	J	107	GLN
1	J	112	ASN
1	J	132	GLN
1	J	150	ASN
1	J	156	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.