



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:32 PM UTC

PDB ID : 2I9L / pdb_00002i9l
Title : Structure of Fab 7D11 from a neutralizing antibody against the poxvirus L1 protein
Authors : Su, H.P.; Golden, J.W.; Gittis, A.G.; Moss, B.; Hooper, J.W.; Garboczi, D.N.
Deposited on : 2006-09-05
Resolution : 3.10 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:

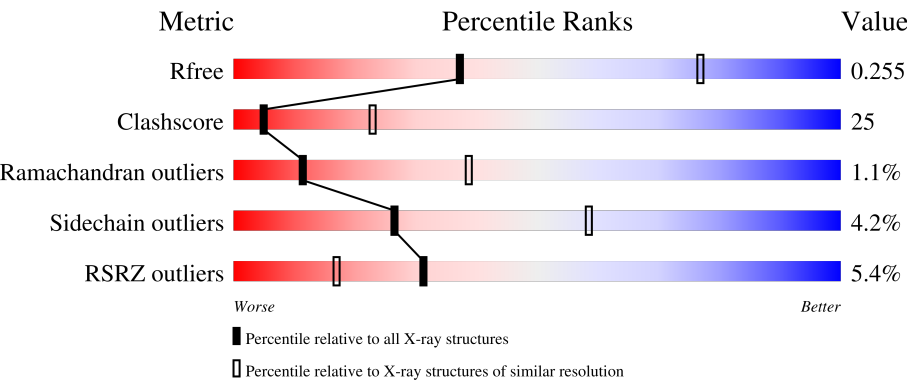
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	219	6% 59%36%5%
1	C	219	% 57%40%.
1	E	219	5% 61%35%.
1	G	219	7% 56%40%.
2	B	219	5% 59%37%.

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Mol	Chain	Length	Quality of chain
2	D	219	
2	F	219	
2	H	219	
3	I	184	
3	J	184	
3	K	184	
3	L	184	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	220	-	-	X	-
4	GOL	E	222	-	-	X	-
4	GOL	J	186	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18674 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 Antibody 7D11 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1696	1056	286	345	9			
1	C	219	Total	C	N	O	S	0	0	0
			1696	1056	286	345	9			
1	E	219	Total	C	N	O	S	0	0	0
			1696	1056	286	345	9			
1	G	219	Total	C	N	O	S	0	0	0
			1696	1056	286	345	9			

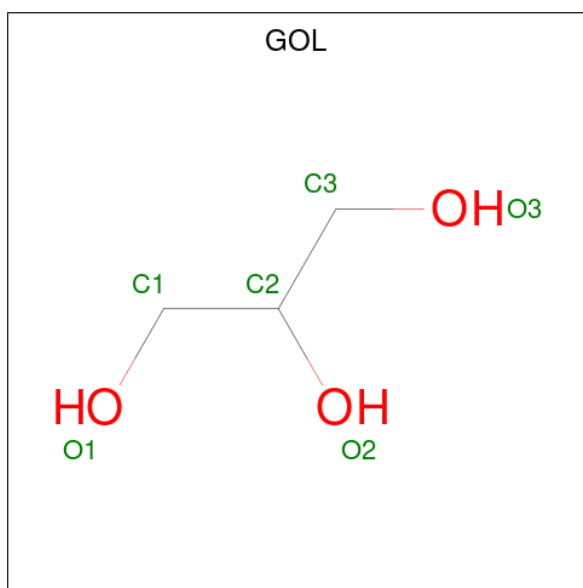
- Molecule 2 is a protein called Antibody 7D11 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1665	1056	272	329	8			
2	D	219	Total	C	N	O	S	0	0	0
			1665	1056	272	329	8			
2	F	219	Total	C	N	O	S	0	0	0
			1665	1056	272	329	8			
2	H	219	Total	C	N	O	S	0	0	0
			1665	1056	272	329	8			

- Molecule 3 is a protein called Virion membrane protein M25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	173	Total	C	N	O	S	0	0	0
			1292	795	220	268	9			
3	J	173	Total	C	N	O	S	0	0	0
			1292	795	220	268	9			
3	K	173	Total	C	N	O	S	0	0	0
			1292	795	220	268	9			
3	L	173	Total	C	N	O	S	0	0	0
			1292	795	220	268	9			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		
4	K	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	C	1	Total	O	0	0
			1	1		
5	D	1	Total	O	0	0
			1	1		

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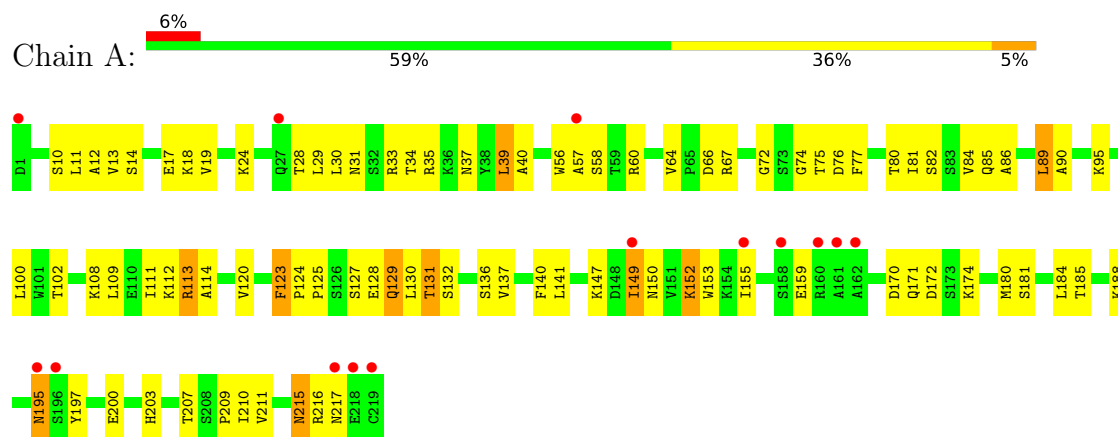
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total 1	O 1	0	0
5	F	4	Total 4	O 4	0	0
5	G	1	Total 1	O 1	0	0
5	H	2	Total 2	O 2	0	0
5	I	1	Total 1	O 1	0	0
5	J	1	Total 1	O 1	0	0

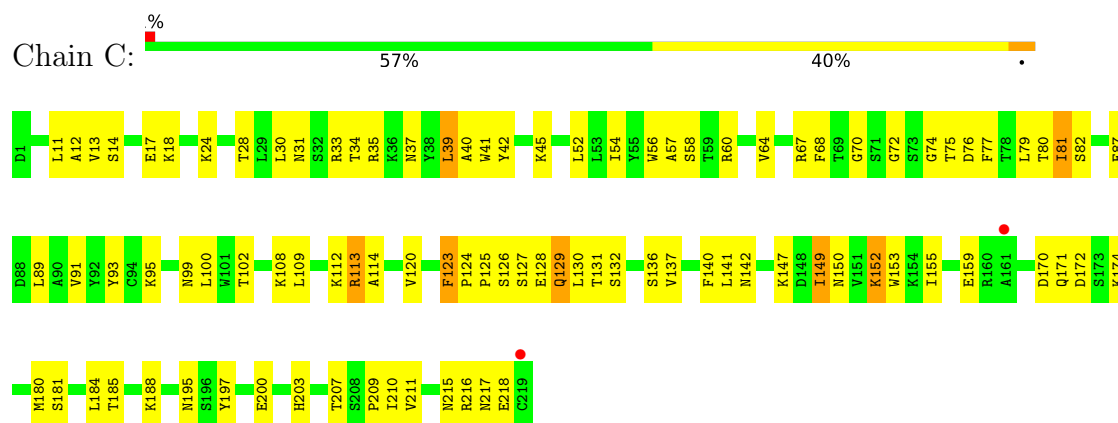
3 Residue-property plots

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 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.

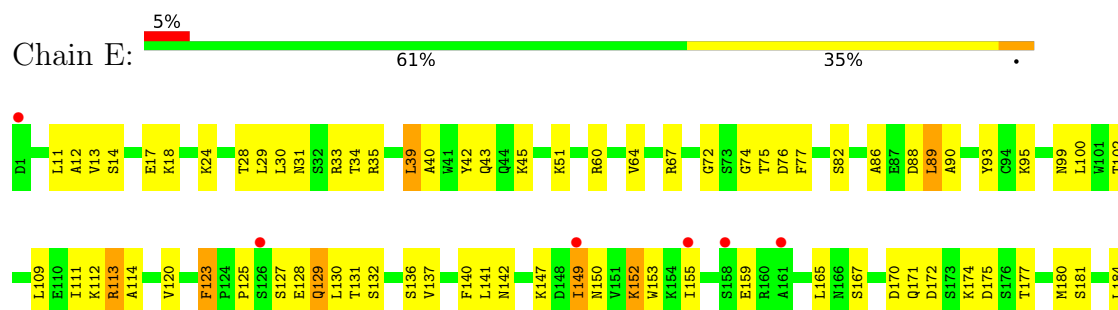
• Molecule 1: Antibody 7D11 light chain



• Molecule 1: Antibody 7D11 light chain

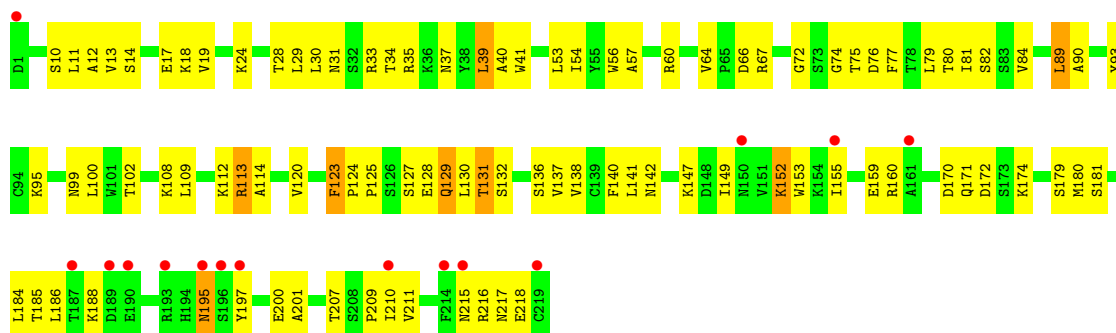


• Molecule 1: Antibody 7D11 light chain

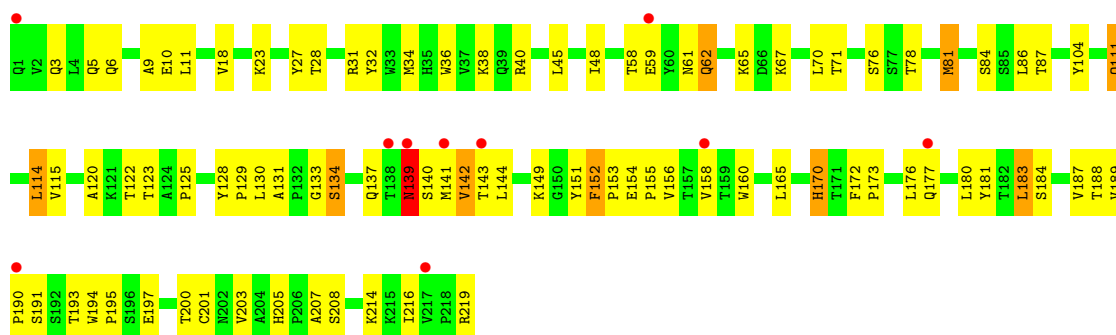




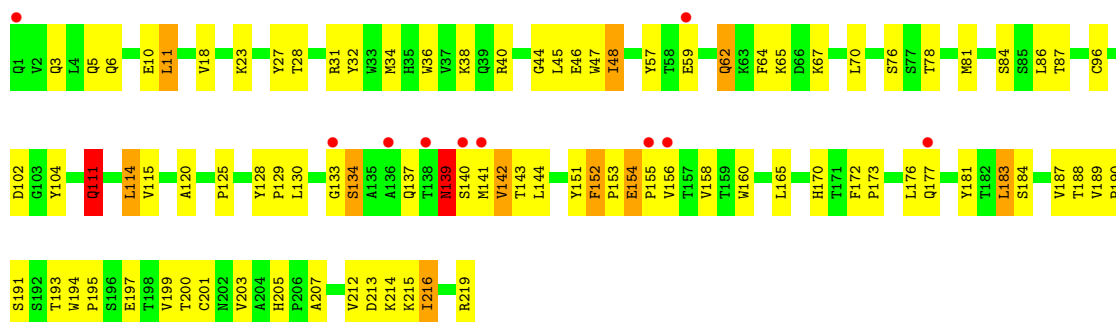
- Molecule 1: Antibody 7D11 light chain



- Molecule 2: Antibody 7D11 heavy chain

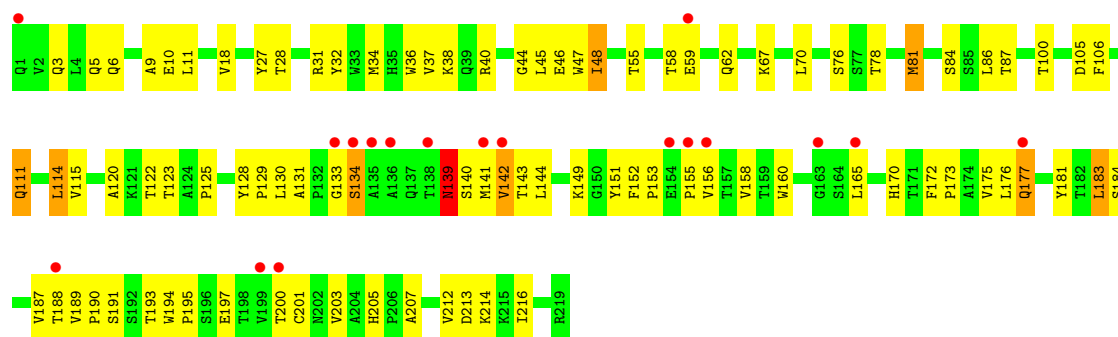


- Molecule 2: Antibody 7D11 heavy chain

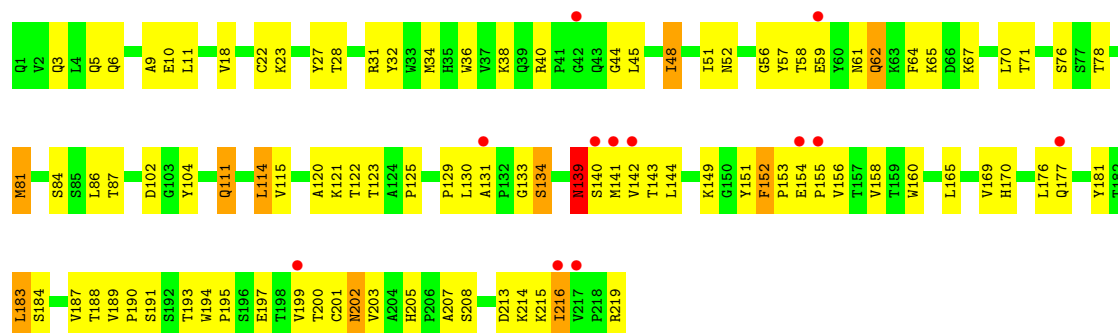


- Molecule 2: Antibody 7D11 heavy chain

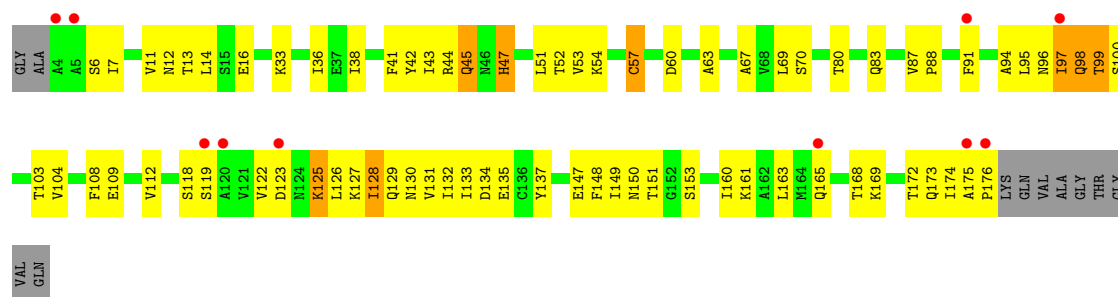




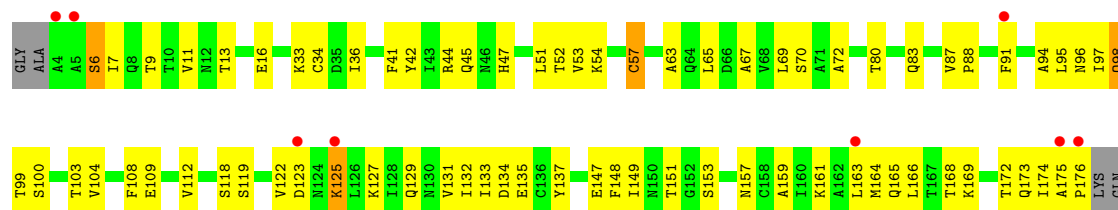
• Molecule 2: Antibody 7D11 heavy chain



• Molecule 3: Virion membrane protein M25

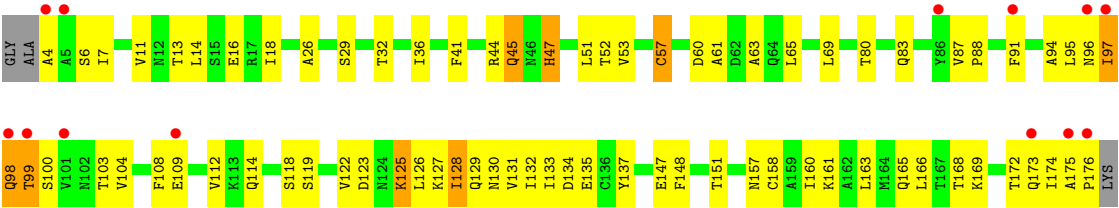


• Molecule 3: Virion membrane protein M25



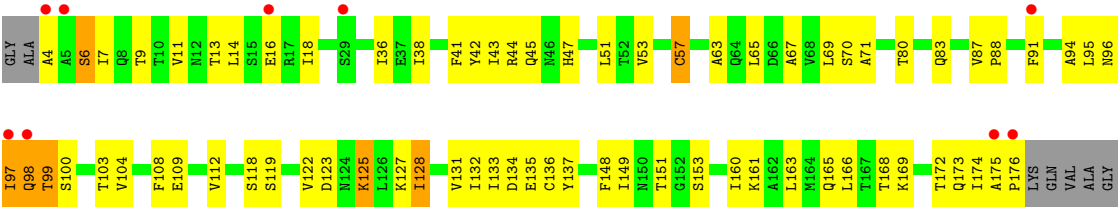
VAL
ALA
GLY
THR
GLY
VAL
GLN

• Molecule 3: Virion membrane protein M25



GLN
VAL
ALA
GLY
THR
GLY
VAL
GLN

• Molecule 3: Virion membrane protein M25



THR
GLY
VAL
GLN

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.77Å 85.56Å 211.84Å 90.00° 119.60° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-3.10) 98.3 (50.00-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.259 0.237 , 0.255	Depositor DCC
R_{free} test set	3111 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	18674	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.51	2/1733 (0.1%)	0.93	5/2348 (0.2%)
1	C	0.51	1/1733 (0.1%)	0.93	5/2348 (0.2%)
1	E	0.51	2/1733 (0.1%)	0.93	5/2348 (0.2%)
1	G	0.52	2/1733 (0.1%)	0.93	6/2348 (0.3%)
2	B	0.65	4/1710 (0.2%)	1.08	10/2337 (0.4%)
2	D	0.66	5/1710 (0.3%)	1.07	9/2337 (0.4%)
2	F	0.68	5/1710 (0.3%)	1.07	9/2337 (0.4%)
2	H	0.64	4/1710 (0.2%)	1.07	8/2337 (0.3%)
3	I	0.64	3/1306 (0.2%)	1.11	12/1775 (0.7%)
3	J	0.57	0/1306	1.10	10/1775 (0.6%)
3	K	0.66	2/1306 (0.2%)	1.12	12/1775 (0.7%)
3	L	0.58	0/1306	1.10	9/1775 (0.5%)
All	All	0.60	30/18996 (0.2%)	1.03	100/25840 (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
2	H	0	1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	139	ASN	CG-OD1	6.69	1.36	1.23
2	D	3	GLN	CD-OE1	5.84	1.34	1.23
2	F	139	ASN	CG-OD1	5.83	1.34	1.23
2	F	3	GLN	CD-OE1	5.78	1.34	1.23
2	B	3	GLN	CD-OE1	5.59	1.34	1.23
2	H	139	ASN	CG-OD1	5.55	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	3	GLN	CD-OE1	5.51	1.34	1.23
1	G	195	ASN	CG-OD1	5.51	1.34	1.23
2	D	139	ASN	CG-OD1	5.44	1.33	1.23
3	I	47	HIS	ND1-CE1	5.42	1.38	1.32
2	F	170	HIS	ND1-CE1	5.37	1.38	1.32
1	E	195	ASN	CG-OD1	5.35	1.33	1.23
1	A	195	ASN	CG-OD1	5.34	1.33	1.23
2	D	170	HIS	ND1-CE1	5.25	1.37	1.32
3	K	47	HIS	ND1-CE1	5.22	1.37	1.32
1	G	215	ASN	CG-OD1	5.21	1.33	1.23
2	B	170	HIS	ND1-CE1	5.15	1.37	1.32
3	I	12	ASN	CG-OD1	5.14	1.33	1.23
1	A	215	ASN	CG-OD1	5.08	1.33	1.23
1	C	195	ASN	CG-OD1	5.08	1.33	1.23
2	B	177	GLN	CD-OE1	5.07	1.33	1.23
2	F	5	GLN	CD-OE1	5.06	1.33	1.23
2	H	5	GLN	CD-OE1	5.06	1.33	1.23
3	K	45	GLN	CD-OE1	5.06	1.33	1.23
2	D	177	GLN	CD-OE1	5.06	1.33	1.23
3	I	45	GLN	CD-OE1	5.05	1.33	1.23
2	H	202	ASN	CG-OD1	5.04	1.33	1.23
2	F	62	GLN	CD-OE1	5.03	1.33	1.23
2	D	111	GLN	CD-OE1	5.01	1.33	1.23
1	E	215	ASN	CG-OD1	5.00	1.33	1.23

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	62	GLN	OE1-CD-NE2	-10.32	112.28	122.60
2	H	5	GLN	OE1-CD-NE2	-9.85	112.75	122.60
3	K	98	GLN	OE1-CD-NE2	-9.83	112.77	122.60
2	B	177	GLN	OE1-CD-NE2	-9.83	112.77	122.60
2	B	5	GLN	OE1-CD-NE2	-9.81	112.79	122.60
2	F	177	GLN	OE1-CD-NE2	-9.81	112.79	122.60
3	I	173	GLN	OE1-CD-NE2	-9.81	112.79	122.60
3	K	45	GLN	OE1-CD-NE2	-9.81	112.79	122.60
2	H	177	GLN	OE1-CD-NE2	-9.80	112.80	122.60
3	J	173	GLN	OE1-CD-NE2	-9.80	112.80	122.60
2	F	5	GLN	OE1-CD-NE2	-9.80	112.80	122.60
3	K	173	GLN	OE1-CD-NE2	-9.80	112.80	122.60
3	L	98	GLN	OE1-CD-NE2	-9.80	112.80	122.60
3	J	45	GLN	OE1-CD-NE2	-9.78	112.82	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	177	GLN	OE1-CD-NE2	-9.77	112.83	122.60
3	I	98	GLN	OE1-CD-NE2	-9.77	112.83	122.60
3	L	45	GLN	OE1-CD-NE2	-9.77	112.83	122.60
3	I	45	GLN	OE1-CD-NE2	-9.77	112.83	122.60
3	L	173	GLN	OE1-CD-NE2	-9.77	112.83	122.60
3	J	98	GLN	OE1-CD-NE2	-9.76	112.84	122.60
2	H	62	GLN	OE1-CD-NE2	-9.75	112.85	122.60
2	D	5	GLN	OE1-CD-NE2	-9.74	112.86	122.60
2	D	62	GLN	OE1-CD-NE2	-9.70	112.91	122.60
2	B	62	GLN	OE1-CD-NE2	-9.53	113.07	122.60
2	D	62	GLN	CG-CD-NE2	7.12	127.08	116.40
2	H	62	GLN	CG-CD-NE2	6.84	126.66	116.40
2	D	170	HIS	CB-CG-CD2	-6.76	122.42	131.20
2	F	170	HIS	CB-CG-CD2	-6.74	122.44	131.20
3	K	47	HIS	CB-CG-CD2	-6.69	122.50	131.20
2	B	5	GLN	CG-CD-NE2	6.69	126.44	116.40
3	K	173	GLN	CG-CD-NE2	6.68	126.42	116.40
3	L	173	GLN	CG-CD-NE2	6.68	126.42	116.40
2	H	177	GLN	CG-CD-NE2	6.67	126.41	116.40
3	I	173	GLN	CG-CD-NE2	6.67	126.41	116.40
3	J	98	GLN	CG-CD-NE2	6.67	126.40	116.40
3	J	173	GLN	CG-CD-NE2	6.66	126.39	116.40
2	F	177	GLN	CG-CD-NE2	6.66	126.39	116.40
3	J	45	GLN	CG-CD-NE2	6.66	126.39	116.40
3	L	45	GLN	CG-CD-NE2	6.66	126.39	116.40
3	I	98	GLN	CG-CD-NE2	6.65	126.38	116.40
2	D	5	GLN	CG-CD-NE2	6.65	126.37	116.40
3	K	98	GLN	CG-CD-NE2	6.65	126.37	116.40
3	L	98	GLN	CG-CD-NE2	6.64	126.36	116.40
2	B	170	HIS	CB-CG-CD2	-6.61	122.61	131.20
3	I	47	HIS	CB-CG-CD2	-6.51	122.73	131.20
2	B	149	LYS	N-CA-C	6.36	119.27	108.90
2	B	62	GLN	CG-CD-NE2	6.33	125.89	116.40
1	A	123	PHE	CA-C-N	6.16	124.09	119.66
1	A	123	PHE	C-N-CA	6.16	124.09	119.66
3	J	127	LYS	N-CA-C	5.92	117.41	111.07
1	G	123	PHE	CA-C-N	5.87	123.89	119.66
1	G	123	PHE	C-N-CA	5.87	123.89	119.66
2	D	170	HIS	CB-CG-ND1	5.75	131.32	122.70
3	K	47	HIS	CB-CG-ND1	5.74	131.30	122.70
2	F	170	HIS	CB-CG-ND1	5.72	131.29	122.70
1	E	123	PHE	CA-C-N	5.72	123.78	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	123	PHE	C-N-CA	5.72	123.78	119.66
1	A	120	VAL	N-CA-C	5.71	116.97	109.21
1	E	120	VAL	N-CA-C	5.69	116.95	109.21
3	I	63	ALA	N-CA-C	-5.67	105.18	111.36
3	L	127	LYS	N-CA-C	5.65	117.13	110.97
2	B	170	HIS	CB-CG-ND1	5.61	131.12	122.70
3	I	47	HIS	CB-CG-ND1	5.60	131.10	122.70
1	C	120	VAL	N-CA-C	5.56	116.77	109.21
3	K	57	CYS	N-CA-C	5.50	118.62	110.48
2	B	131	ALA	CA-C-N	5.47	125.47	119.89
2	B	131	ALA	C-N-CA	5.47	125.47	119.89
1	G	120	VAL	N-CA-C	5.43	116.59	109.21
3	J	57	CYS	N-CA-C	5.42	118.50	110.48
3	J	63	ALA	N-CA-C	-5.42	105.45	111.36
3	K	6	SER	N-CA-C	-5.41	106.18	112.89
1	C	123	PHE	CA-C-N	5.41	123.56	119.66
1	C	123	PHE	C-N-CA	5.41	123.56	119.66
3	I	127	LYS	N-CA-C	5.40	116.85	110.97
1	C	129	GLN	N-CA-C	-5.37	105.47	112.23
3	K	60	ASP	N-CA-C	5.37	118.10	108.17
3	L	6	SER	N-CA-C	-5.35	106.25	112.89
3	L	57	CYS	N-CA-C	5.35	118.40	110.48
1	A	129	GLN	N-CA-C	-5.29	105.56	112.23
2	H	131	ALA	CA-C-N	5.28	125.28	119.89
2	H	131	ALA	C-N-CA	5.28	125.28	119.89
1	C	142	ASN	N-CA-C	5.27	118.41	109.76
1	E	129	GLN	N-CA-C	-5.23	105.64	112.23
3	I	6	SER	N-CA-C	-5.23	106.40	112.89
2	D	96	CYS	N-CA-C	-5.22	101.65	109.95
3	I	57	CYS	N-CA-C	5.21	118.19	110.48
1	A	131	THR	N-CA-C	-5.20	105.73	111.71
1	G	142	ASN	N-CA-C	5.20	118.28	109.76
3	K	127	LYS	N-CA-C	5.17	116.60	111.07
3	J	6	SER	N-CA-C	-5.15	106.51	112.89
2	F	100	THR	N-CA-C	-5.14	103.25	110.35
1	G	131	THR	N-CA-C	-5.14	105.80	111.71
2	H	154	GLU	N-CA-C	5.08	121.03	109.81
1	E	142	ASN	N-CA-C	5.07	118.08	109.76
1	G	129	GLN	N-CA-C	-5.06	105.85	112.23
3	K	63	ALA	N-CA-C	-5.05	105.86	111.36
3	I	60	ASP	N-CA-C	5.05	117.51	108.17
2	D	154	GLU	N-CA-C	5.02	120.91	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	131	ALA	CA-C-N	5.00	124.99	119.89
2	F	131	ALA	C-N-CA	5.00	124.99	119.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	149	LYS	Mainchain

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	1696	0	1638	76	0
1	C	1696	0	1638	77	0
1	E	1696	0	1638	70	0
1	G	1696	0	1638	82	0
2	B	1665	0	1620	80	0
2	D	1665	0	1620	85	0
2	F	1665	0	1620	84	0
2	H	1665	0	1622	103	0
3	I	1292	0	1276	94	0
3	J	1292	0	1276	73	0
3	K	1292	0	1276	84	0
3	L	1292	0	1276	75	0
4	A	6	0	8	4	0
4	E	18	0	24	7	0
4	I	6	0	8	2	0
4	J	6	0	8	4	0
4	K	6	0	8	3	0
4	L	6	0	8	0	0
5	A	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	4	0	0	0	0
5	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	2	0	0	0	0
5	I	1	0	0	1	0
5	J	1	0	0	0	0
All	All	18674	0	18202	924	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 25.

All (924) 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)
3:I:91:PHE:CE2	3:I:97:ILE:HB	1.16	1.60
3:I:91:PHE:HE2	3:I:97:ILE:CB	1.16	1.57
3:I:91:PHE:CE2	3:I:97:ILE:CB	1.83	1.50
3:I:91:PHE:CE2	3:I:97:ILE:CG2	2.06	1.38
3:I:91:PHE:HE2	3:I:97:ILE:CG2	1.38	1.33
1:C:100:LEU:HD21	2:D:59:GLU:OE2	1.28	1.31
3:K:91:PHE:CE2	3:K:104:VAL:HG13	1.80	1.16
2:F:140:SER:O	2:F:141:MET:HG2	1.43	1.15
3:I:38:ILE:HD11	3:I:150:ASN:HB2	1.16	1.14
3:K:14:LEU:HD21	3:K:163:LEU:HD21	1.30	1.13
3:I:43:ILE:HD12	3:I:133:ILE:HB	1.25	1.09
2:H:199:VAL:O	2:H:216:ILE:HD13	1.53	1.08
1:G:100:LEU:HD21	2:H:59:GLU:OE2	1.51	1.08
3:L:14:LEU:HD21	3:L:163:LEU:HD21	1.36	1.08
3:I:14:LEU:HD21	3:I:163:LEU:HD21	1.34	1.08
2:D:199:VAL:O	2:D:216:ILE:HD13	1.54	1.06
1:E:100:LEU:HD21	2:F:59:GLU:OE2	1.57	1.04
1:E:43:GLN:HE22	4:E:222:GOL:H31	1.18	1.04
1:A:100:LEU:HD21	2:B:59:GLU:OE2	1.57	1.03
3:L:91:PHE:CE2	3:L:104:VAL:HG13	1.93	1.02
3:J:91:PHE:CE2	3:J:104:VAL:HG13	1.97	0.99
3:I:91:PHE:CZ	3:I:97:ILE:HG21	1.97	0.99
2:F:140:SER:O	2:F:141:MET:CG	2.12	0.98
2:H:51:ILE:HD13	2:H:58:THR:HG23	1.45	0.97
3:K:87:VAL:CG1	3:K:91:PHE:CZ	2.47	0.97
2:H:51:ILE:HD13	2:H:58:THR:CG2	1.95	0.97
3:I:118:SER:HB3	5:I:187:HOH:O	1.61	0.97
3:K:91:PHE:CE2	3:K:104:VAL:CG1	2.48	0.96
3:I:38:ILE:HD11	3:I:150:ASN:CB	1.94	0.96
3:J:44:ARG:NE	3:L:44:ARG:HH21	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:91:PHE:CZ	3:I:97:ILE:HB	2.00	0.96
2:B:141:MET:HG2	2:B:142:VAL:H	1.28	0.96
3:I:91:PHE:CE2	3:I:97:ILE:HG22	2.01	0.96
3:K:87:VAL:HG12	3:K:91:PHE:CE2	2.01	0.95
2:B:141:MET:SD	2:B:188:THR:HG21	2.07	0.95
3:I:91:PHE:CZ	3:I:97:ILE:CG2	2.49	0.95
3:J:44:ARG:HE	3:L:44:ARG:HH21	1.15	0.94
3:K:87:VAL:HG12	3:K:91:PHE:CZ	2.01	0.94
2:D:23:LYS:HD3	2:D:78:THR:CG2	1.98	0.93
2:D:48:ILE:HD12	2:D:64:PHE:CE2	2.04	0.92
3:L:38:ILE:HD12	3:L:53:VAL:CG1	1.99	0.91
2:H:202:ASN:ND2	2:H:213:ASP:OD2	2.03	0.91
3:I:91:PHE:CZ	3:I:97:ILE:CB	2.53	0.90
3:I:91:PHE:CD2	3:I:97:ILE:HB	2.07	0.89
2:H:22:CYS:O	2:H:78:THR:HG23	1.72	0.89
2:B:141:MET:SD	2:B:188:THR:CG2	2.61	0.89
3:L:38:ILE:HD12	3:L:53:VAL:HG13	1.55	0.87
3:J:44:ARG:HE	3:L:44:ARG:NH2	1.73	0.86
1:C:100:LEU:CD2	2:D:59:GLU:OE2	2.20	0.86
3:K:91:PHE:CZ	3:K:104:VAL:HG13	2.11	0.86
3:J:94:ALA:HB2	3:J:169:LYS:HG3	1.59	0.85
1:A:149:ILE:HD12	1:A:203:HIS:HB2	1.59	0.85
1:E:51:LYS:NZ	4:E:222:GOL:O1	2.09	0.84
2:D:23:LYS:CD	2:D:78:THR:CG2	2.55	0.84
1:G:124:PRO:HD2	2:H:219:ARG:HH12	1.42	0.84
2:D:151:TYR:CE2	2:D:156:VAL:HG11	2.13	0.84
3:I:94:ALA:HB2	3:I:169:LYS:HG3	1.60	0.84
3:I:44:ARG:HG3	3:I:44:ARG:HH11	1.42	0.83
2:B:141:MET:HG2	2:B:142:VAL:N	1.92	0.83
3:K:94:ALA:HB2	3:K:169:LYS:HG3	1.58	0.83
3:L:94:ALA:HB2	3:L:169:LYS:HG3	1.60	0.83
3:K:91:PHE:CZ	3:K:104:VAL:CG1	2.62	0.83
1:C:149:ILE:HD12	1:C:203:HIS:HB2	1.59	0.83
2:D:23:LYS:CD	2:D:78:THR:HG22	2.08	0.83
2:D:11:LEU:HG	2:D:153:PRO:CG	2.09	0.83
3:K:44:ARG:HG3	3:K:44:ARG:HH11	1.43	0.83
3:J:129:GLN:OE1	4:J:186:GOL:H12	1.77	0.83
2:D:11:LEU:HG	2:D:153:PRO:HG3	1.58	0.82
2:H:51:ILE:HD12	2:H:57:TYR:O	1.80	0.82
3:J:133:ILE:HG22	3:J:134:ASP:H	1.44	0.82
2:F:37:VAL:HA	2:F:48:ILE:HD13	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:91:PHE:CD2	3:I:97:ILE:O	2.33	0.81
3:I:91:PHE:HD2	3:I:97:ILE:O	1.63	0.81
3:K:96:ASN:O	3:K:97:ILE:HG13	1.82	0.80
3:L:44:ARG:HG3	3:L:44:ARG:HH11	1.47	0.80
3:I:38:ILE:CD1	3:I:150:ASN:HB2	2.06	0.79
3:J:159:ALA:O	3:J:163:LEU:HD13	1.83	0.79
1:E:43:GLN:NE2	4:E:222:GOL:H31	1.97	0.79
3:L:91:PHE:CZ	3:L:104:VAL:HG13	2.18	0.79
3:K:133:ILE:HG22	3:K:134:ASP:H	1.47	0.78
1:E:149:ILE:HD13	1:E:150:ASN:N	1.99	0.78
3:J:108:PHE:HZ	3:J:163:LEU:HD12	1.47	0.78
3:I:133:ILE:HG22	3:I:134:ASP:H	1.48	0.78
3:J:69:LEU:HD21	3:J:112:VAL:HG21	1.65	0.78
3:J:96:ASN:O	3:J:97:ILE:HG13	1.85	0.77
2:F:38:LYS:N	2:F:48:ILE:HD11	2.00	0.77
1:G:53:LEU:HB3	1:G:54:ILE:HD12	1.66	0.76
3:J:44:ARG:HG3	3:J:44:ARG:HH11	1.48	0.76
2:F:151:TYR:CE2	2:F:156:VAL:HG11	2.21	0.76
3:J:54:LYS:HD3	3:J:149:ILE:HD12	1.66	0.76
2:F:76:SER:OG	2:F:78:THR:HG22	1.86	0.76
3:K:69:LEU:HD21	3:K:112:VAL:HG21	1.68	0.75
2:D:23:LYS:HA	2:D:78:THR:HG22	1.67	0.75
2:B:76:SER:OG	2:B:78:THR:HG22	1.86	0.75
2:D:23:LYS:HD2	2:D:78:THR:HG22	1.67	0.75
3:I:54:LYS:HD3	3:I:149:ILE:HD12	1.69	0.74
3:I:69:LEU:HD21	3:I:112:VAL:HG21	1.68	0.74
3:L:69:LEU:HD21	3:L:112:VAL:HG21	1.69	0.74
3:K:14:LEU:HD21	3:K:163:LEU:CD2	2.15	0.74
3:I:91:PHE:HZ	3:I:97:ILE:HG21	1.52	0.74
3:L:100:SER:O	3:L:104:VAL:HG23	1.88	0.74
1:A:124:PRO:HD2	2:B:219:ARG:HH12	1.50	0.74
2:H:143:THR:HG22	2:H:188:THR:OG1	1.86	0.74
2:F:143:THR:HG22	2:F:188:THR:OG1	1.87	0.74
2:H:165:LEU:HD21	2:H:187:VAL:HG21	1.70	0.74
3:L:133:ILE:HG22	3:L:134:ASP:H	1.51	0.74
2:B:141:MET:CG	2:B:142:VAL:H	2.01	0.73
2:B:125:PRO:HB3	2:B:151:TYR:HB3	1.70	0.73
2:H:67:LYS:HE2	2:H:84:SER:O	1.89	0.73
1:A:170:ASP:O	4:A:220:GOL:H11	1.87	0.73
2:D:67:LYS:HE2	2:D:84:SER:O	1.89	0.73
3:K:29:SER:HG	3:K:32:THR:HG1	1.29	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:91:PHE:CZ	3:J:104:VAL:HG13	2.24	0.73
2:F:140:SER:C	2:F:141:MET:HG2	2.13	0.72
2:F:67:LYS:HE2	2:F:84:SER:O	1.90	0.72
2:D:143:THR:HG22	2:D:188:THR:OG1	1.89	0.72
2:F:10:GLU:HG2	2:F:18:VAL:HG21	1.71	0.72
2:B:129:PRO:HG3	2:B:214:LYS:HG2	1.72	0.72
2:F:129:PRO:HG3	2:F:214:LYS:HG2	1.71	0.72
3:I:100:SER:O	3:I:104:VAL:HG23	1.90	0.71
3:K:100:SER:O	3:K:104:VAL:HG23	1.89	0.71
1:A:86:ALA:HA	1:A:111:ILE:HD13	1.71	0.71
3:I:43:ILE:CD1	3:I:133:ILE:HB	2.14	0.71
2:B:143:THR:HG22	2:B:188:THR:OG1	1.90	0.71
3:I:38:ILE:HD13	3:I:53:VAL:HG11	1.71	0.71
2:H:40:ARG:HG2	2:H:40:ARG:HH11	1.56	0.71
2:H:141:MET:HE2	2:H:188:THR:CG2	2.21	0.71
3:I:96:ASN:O	3:I:97:ILE:HG12	1.91	0.70
2:B:153:PRO:HD2	2:B:207:ALA:HB1	1.73	0.70
2:H:153:PRO:HD2	2:H:207:ALA:HB1	1.73	0.70
2:H:151:TYR:CE2	2:H:156:VAL:HG11	2.27	0.70
2:D:129:PRO:HG3	2:D:214:LYS:HG2	1.73	0.70
1:E:86:ALA:HA	1:E:111:ILE:HD13	1.74	0.70
2:F:37:VAL:CA	2:F:48:ILE:HD13	2.22	0.70
3:J:100:SER:O	3:J:104:VAL:HG23	1.90	0.70
2:F:40:ARG:HG2	2:F:40:ARG:HH11	1.57	0.70
1:A:14:SER:HB2	1:A:17:GLU:OE2	1.91	0.69
1:A:149:ILE:HG13	1:A:150:ASN:H	1.57	0.69
2:H:129:PRO:HG3	2:H:214:LYS:HG2	1.72	0.69
3:K:87:VAL:HG11	3:K:91:PHE:CZ	2.28	0.69
1:E:100:LEU:HD21	2:F:59:GLU:CD	2.17	0.69
1:G:124:PRO:CD	2:H:219:ARG:HH12	2.05	0.69
2:H:125:PRO:HB3	2:H:151:TYR:HB3	1.73	0.69
2:B:67:LYS:HE2	2:B:84:SER:O	1.92	0.69
3:I:14:LEU:HD21	3:I:163:LEU:CD2	2.19	0.69
3:K:91:PHE:HE2	3:K:104:VAL:CG1	2.04	0.69
1:C:149:ILE:HG13	1:C:150:ASN:H	1.58	0.69
3:K:14:LEU:CD2	3:K:163:LEU:HD21	2.17	0.69
1:C:127:SER:O	1:C:131:THR:HG23	1.93	0.68
2:F:153:PRO:HD2	2:F:207:ALA:HB1	1.75	0.68
2:H:51:ILE:HD12	2:H:52:ASN:H	1.58	0.68
1:C:14:SER:HB2	1:C:17:GLU:OE2	1.93	0.68
1:E:127:SER:O	1:E:131:THR:HG23	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:14:LEU:CD2	3:I:163:LEU:HD21	2.20	0.68
3:L:14:LEU:HD21	3:L:163:LEU:CD2	2.20	0.68
3:L:38:ILE:HD12	3:L:53:VAL:HG11	1.73	0.68
3:L:14:LEU:CD2	3:L:163:LEU:HD21	2.21	0.68
1:A:127:SER:O	1:A:131:THR:HG23	1.94	0.68
2:H:141:MET:HE2	2:H:188:THR:HG21	1.76	0.68
2:B:10:GLU:HG2	2:B:18:VAL:HG21	1.75	0.68
2:F:165:LEU:HD21	2:F:187:VAL:HG21	1.75	0.68
1:E:14:SER:HB2	1:E:17:GLU:OE2	1.93	0.68
3:L:18:ILE:HD13	3:L:71:ALA:HB3	1.75	0.68
2:D:23:LYS:HD3	2:D:78:THR:HG21	1.76	0.67
2:D:10:GLU:HG2	2:D:18:VAL:HG21	1.75	0.67
2:D:40:ARG:HH11	2:D:40:ARG:HG2	1.60	0.67
3:K:129:GLN:OE1	4:K:186:GOL:H12	1.94	0.67
2:F:58:THR:H	3:K:125:LYS:HD2	1.60	0.67
1:C:124:PRO:HD2	2:D:219:ARG:HH12	1.59	0.67
3:K:96:ASN:C	3:K:97:ILE:HG13	2.20	0.67
3:I:174:ILE:HG13	3:I:175:ALA:N	2.10	0.67
3:J:157:ASN:HB2	4:J:186:GOL:H11	1.77	0.67
1:A:172:ASP:HB2	4:A:220:GOL:H2	1.77	0.66
1:G:127:SER:O	1:G:131:THR:HG23	1.96	0.66
2:H:10:GLU:HG2	2:H:18:VAL:HG21	1.78	0.66
3:K:174:ILE:HG13	3:K:175:ALA:N	2.11	0.66
3:I:133:ILE:HG22	3:I:134:ASP:N	2.11	0.66
3:K:161:LYS:O	3:K:165:GLN:HG3	1.96	0.66
1:G:14:SER:HB2	1:G:17:GLU:OE2	1.96	0.65
3:J:133:ILE:HG22	3:J:134:ASP:N	2.11	0.65
2:F:48:ILE:HD12	2:F:48:ILE:N	2.11	0.65
2:B:40:ARG:HG2	2:B:40:ARG:HH11	1.61	0.65
2:F:37:VAL:HA	2:F:48:ILE:CD1	2.26	0.65
2:F:125:PRO:HB3	2:F:151:TYR:HB3	1.77	0.65
2:H:158:VAL:HG22	2:H:203:VAL:HG22	1.78	0.65
1:C:68:PHE:CD2	1:C:81:ILE:HD12	2.31	0.65
2:H:51:ILE:HD11	2:H:56:GLY:HA2	1.79	0.65
3:J:108:PHE:HZ	3:J:163:LEU:CD1	2.08	0.65
1:A:180:MET:HG2	1:A:181:SER:N	2.12	0.65
3:L:96:ASN:O	3:L:97:ILE:HG12	1.96	0.65
1:E:28:THR:HA	1:E:75:THR:HG22	1.79	0.64
1:G:28:THR:HA	1:G:75:THR:HG22	1.80	0.64
3:J:57:CYS:HA	3:J:151:THR:O	1.98	0.64
1:A:149:ILE:HG13	1:A:150:ASN:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:180:MET:HG2	1:G:181:SER:N	2.13	0.64
2:D:125:PRO:HB3	2:D:151:TYR:HB3	1.78	0.64
2:H:48:ILE:HD13	2:H:64:PHE:CE2	2.32	0.64
3:L:128:ILE:HD12	3:L:128:ILE:H	1.62	0.63
1:C:180:MET:HG2	1:C:181:SER:N	2.12	0.63
2:B:151:TYR:CE2	2:B:156:VAL:HG11	2.33	0.63
2:D:151:TYR:CE2	2:D:156:VAL:CG1	2.80	0.63
3:I:57:CYS:HA	3:I:151:THR:O	1.99	0.63
3:J:54:LYS:HD3	3:J:149:ILE:CD1	2.28	0.63
2:H:216:ILE:N	2:H:216:ILE:HD12	2.14	0.63
3:I:38:ILE:HD12	3:I:38:ILE:H	1.63	0.63
2:D:46:GLU:O	2:D:48:ILE:HD13	1.99	0.63
1:C:149:ILE:HG13	1:C:150:ASN:N	2.14	0.63
3:I:38:ILE:HD13	3:I:53:VAL:CG1	2.28	0.63
2:D:23:LYS:HD2	2:D:78:THR:CG2	2.27	0.63
2:F:10:GLU:HG2	2:F:18:VAL:CG2	2.28	0.63
2:H:151:TYR:CE2	2:H:156:VAL:CG1	2.82	0.63
3:L:57:CYS:HA	3:L:151:THR:O	1.98	0.63
3:J:100:SER:OG	3:J:103:THR:HG23	1.99	0.62
1:A:149:ILE:CD1	1:A:203:HIS:HB2	2.29	0.62
2:D:216:ILE:N	2:D:216:ILE:HD12	2.14	0.62
3:L:100:SER:OG	3:L:103:THR:HG23	1.99	0.62
1:E:180:MET:HG2	1:E:181:SER:N	2.12	0.62
2:H:165:LEU:HD21	2:H:187:VAL:CG2	2.29	0.62
1:C:28:THR:HA	1:C:75:THR:HG22	1.81	0.62
3:K:133:ILE:HG22	3:K:134:ASP:N	2.15	0.62
2:B:28:THR:HB	2:B:31:ARG:CG	2.30	0.62
2:H:28:THR:HB	2:H:31:ARG:CG	2.29	0.62
1:C:80:THR:C	1:C:81:ILE:HD13	2.25	0.62
2:D:11:LEU:HB2	2:D:153:PRO:HG2	1.82	0.62
2:B:10:GLU:HG2	2:B:18:VAL:CG2	2.30	0.62
2:H:129:PRO:HG3	2:H:214:LYS:CG	2.30	0.62
3:I:91:PHE:HE2	3:I:97:ILE:HG22	1.38	0.62
2:D:129:PRO:HG3	2:D:214:LYS:CG	2.30	0.61
3:J:42:TYR:CD1	3:J:132:ILE:HD12	2.35	0.61
2:B:129:PRO:HG3	2:B:214:LYS:CG	2.30	0.61
3:I:42:TYR:O	3:I:43:ILE:HD13	1.99	0.61
3:I:134:ASP:OD1	3:K:44:ARG:NH1	2.33	0.61
2:B:158:VAL:HG22	2:B:203:VAL:HG22	1.81	0.61
1:C:45:LYS:HE2	1:C:87:GLU:O	2.00	0.61
2:D:10:GLU:HG2	2:D:18:VAL:CG2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:128:ILE:HD12	3:K:128:ILE:H	1.64	0.61
1:A:28:THR:HA	1:A:75:THR:HG22	1.81	0.61
3:I:54:LYS:HB3	3:I:149:ILE:HD13	1.83	0.61
2:D:70:LEU:CD1	2:D:81:MET:HG2	2.31	0.61
3:I:54:LYS:HD3	3:I:149:ILE:CD1	2.30	0.61
3:J:96:ASN:C	3:J:97:ILE:HG13	2.25	0.61
1:A:19:VAL:HG23	1:A:81:ILE:HD13	1.83	0.61
3:I:42:TYR:C	3:I:43:ILE:HD13	2.26	0.61
3:K:45:GLN:OE1	3:K:137:TYR:OH	2.16	0.61
3:L:42:TYR:CD1	3:L:132:ILE:HD12	2.35	0.61
3:I:161:LYS:O	3:I:165:GLN:HG3	2.00	0.61
2:B:123:THR:HG21	2:B:180:LEU:HD21	1.81	0.61
2:H:31:ARG:HH12	3:L:63:ALA:CB	2.14	0.61
3:L:161:LYS:O	3:L:165:GLN:HG3	2.00	0.61
2:D:183:LEU:C	2:D:183:LEU:HD23	2.26	0.60
2:F:114:LEU:HD13	2:F:155:PRO:HG3	1.82	0.60
2:H:153:PRO:HD2	2:H:207:ALA:CB	2.30	0.60
3:I:100:SER:OG	3:I:103:THR:HG23	2.01	0.60
3:I:128:ILE:H	3:I:128:ILE:HD12	1.66	0.60
2:D:38:LYS:HB3	2:D:48:ILE:HD11	1.82	0.60
1:A:12:ALA:HB1	1:A:112:LYS:HG3	1.83	0.60
2:H:122:THR:O	2:H:123:THR:CG2	2.50	0.60
3:J:54:LYS:HB3	3:J:149:ILE:HD13	1.83	0.60
2:B:70:LEU:CD1	2:B:81:MET:HG2	2.32	0.60
1:C:129:GLN:O	1:C:132:SER:HB3	2.01	0.60
2:F:129:PRO:HG3	2:F:214:LYS:CG	2.31	0.60
3:K:87:VAL:CG1	3:K:91:PHE:CE2	2.80	0.60
1:G:19:VAL:HG23	1:G:81:ILE:HD13	1.83	0.60
3:K:91:PHE:CZ	3:K:104:VAL:HG11	2.37	0.60
2:H:23:LYS:HD3	2:H:78:THR:OG1	2.01	0.60
1:E:149:ILE:HD13	1:E:150:ASN:C	2.27	0.59
1:A:18:LYS:HE3	1:A:82:SER:HA	1.85	0.59
1:C:100:LEU:HD21	2:D:59:GLU:CD	2.21	0.59
2:D:70:LEU:HD12	2:D:81:MET:HG2	1.83	0.59
1:C:34:THR:O	1:C:35:ARG:HB2	2.01	0.59
2:D:28:THR:HB	2:D:31:ARG:CG	2.33	0.59
1:G:129:GLN:O	1:G:132:SER:HB3	2.02	0.59
2:H:122:THR:O	2:H:123:THR:HG23	2.03	0.59
3:I:131:VAL:C	3:I:132:ILE:HD12	2.27	0.59
3:L:91:PHE:CZ	3:L:104:VAL:CG1	2.83	0.59
3:J:161:LYS:O	3:J:165:GLN:HG3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:133:ILE:HG22	3:L:134:ASP:N	2.17	0.59
1:C:42:TYR:CE1	1:C:52:LEU:HD13	2.38	0.59
1:E:34:THR:O	1:E:35:ARG:HB2	2.02	0.59
1:G:113:ARG:HG2	1:G:114:ALA:H	1.68	0.59
2:D:114:LEU:HD13	2:D:155:PRO:HG3	1.84	0.59
1:G:53:LEU:CB	1:G:54:ILE:HD12	2.32	0.59
2:H:10:GLU:HG2	2:H:18:VAL:CG2	2.33	0.59
1:C:81:ILE:HD13	1:C:81:ILE:N	2.17	0.59
2:D:158:VAL:HG22	2:D:203:VAL:HG22	1.85	0.59
3:L:131:VAL:O	3:L:132:ILE:HD13	2.03	0.58
2:F:183:LEU:C	2:F:183:LEU:HD23	2.28	0.58
2:B:70:LEU:HD12	2:B:81:MET:HG2	1.85	0.58
2:B:114:LEU:HD13	2:B:155:PRO:HG3	1.84	0.58
4:A:220:GOL:O2	2:B:170:HIS:CE1	2.56	0.58
3:K:57:CYS:HA	3:K:151:THR:O	2.02	0.58
1:A:129:GLN:O	1:A:132:SER:HB3	2.02	0.58
1:A:34:THR:O	1:A:35:ARG:HB2	2.01	0.58
1:C:149:ILE:CD1	1:C:203:HIS:HB2	2.31	0.58
1:E:123:PHE:CD2	2:F:130:LEU:HB3	2.39	0.58
2:B:123:THR:HG21	2:B:180:LEU:CD2	2.33	0.58
2:B:153:PRO:HD2	2:B:207:ALA:CB	2.33	0.58
1:C:18:LYS:HE3	1:C:82:SER:HA	1.85	0.58
1:G:34:THR:O	1:G:35:ARG:HB2	2.03	0.58
3:I:96:ASN:C	3:I:97:ILE:HG12	2.27	0.58
3:I:126:LEU:HD23	3:K:96:ASN:HB3	1.85	0.58
1:E:18:LYS:HE3	1:E:82:SER:HA	1.86	0.58
2:H:22:CYS:C	2:H:78:THR:HG23	2.29	0.58
3:K:131:VAL:C	3:K:132:ILE:HD12	2.29	0.58
2:F:46:GLU:O	2:F:48:ILE:HD12	2.03	0.57
2:H:70:LEU:CD1	2:H:81:MET:HG2	2.34	0.57
2:H:28:THR:CG2	2:H:31:ARG:HG2	2.34	0.57
3:J:131:VAL:O	3:J:132:ILE:HD13	2.04	0.57
1:E:129:GLN:O	1:E:132:SER:HB3	2.04	0.57
3:J:157:ASN:CB	4:J:186:GOL:H11	2.34	0.57
1:C:123:PHE:CD2	2:D:130:LEU:HB3	2.39	0.57
2:D:11:LEU:HG	2:D:153:PRO:HG2	1.84	0.57
3:I:130:ASN:HB3	3:I:132:ILE:HD11	1.86	0.57
2:F:153:PRO:HD2	2:F:207:ALA:CB	2.34	0.57
1:A:210:ILE:H	1:A:210:ILE:HD12	1.70	0.57
2:D:28:THR:CG2	2:D:31:ARG:HG2	2.35	0.57
1:G:18:LYS:HE3	1:G:82:SER:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:ILE:HD13	2:H:58:THR:HG22	1.82	0.57
3:K:100:SER:OG	3:K:103:THR:HG23	2.04	0.57
1:E:113:ARG:HG2	1:E:114:ALA:N	2.19	0.57
2:F:28:THR:CG2	2:F:31:ARG:HG2	2.34	0.57
1:A:113:ARG:HG2	1:A:114:ALA:H	1.70	0.57
2:F:70:LEU:CD1	2:F:81:MET:HG2	2.34	0.57
3:L:42:TYR:CE1	3:L:132:ILE:HD12	2.40	0.57
1:G:141:LEU:HD23	1:G:149:ILE:HD13	1.86	0.57
2:H:70:LEU:HD12	2:H:81:MET:HG2	1.86	0.57
3:I:119:SER:HB3	3:K:114:GLN:OE1	2.05	0.57
3:J:44:ARG:HH21	3:L:44:ARG:HH22	1.53	0.57
1:E:113:ARG:HG2	1:E:114:ALA:H	1.70	0.56
2:F:158:VAL:HG22	2:F:203:VAL:HG22	1.86	0.56
1:C:210:ILE:H	1:C:210:ILE:HD12	1.70	0.56
1:G:113:ARG:HG2	1:G:114:ALA:N	2.20	0.56
3:K:4:ALA:O	3:K:7:ILE:HD13	2.05	0.56
2:B:58:THR:H	3:I:125:LYS:HD2	1.71	0.56
2:F:38:LYS:H	2:F:48:ILE:HD11	1.66	0.56
3:J:137:TYR:CE2	3:J:172:THR:HG22	2.41	0.56
1:E:136:SER:OG	2:F:149:LYS:HE3	2.06	0.56
3:J:13:THR:O	3:J:16:GLU:HG3	2.06	0.56
3:K:130:ASN:HB3	3:K:132:ILE:HD11	1.88	0.56
1:E:12:ALA:HB1	1:E:112:LYS:HG3	1.88	0.56
2:H:114:LEU:HD23	2:H:115:VAL:N	2.21	0.56
2:H:194:TRP:CG	2:H:195:PRO:HA	2.41	0.56
3:L:4:ALA:O	3:L:7:ILE:HD13	2.05	0.56
3:L:96:ASN:C	3:L:97:ILE:HG12	2.30	0.56
2:F:151:TYR:CE2	2:F:156:VAL:CG1	2.88	0.56
1:G:124:PRO:CG	2:H:219:ARG:HH12	2.18	0.56
1:G:210:ILE:HD12	1:G:210:ILE:H	1.70	0.56
2:D:27:TYR:OH	2:D:34:MET:HE1	2.05	0.56
3:I:38:ILE:HD11	3:I:150:ASN:CG	2.30	0.56
2:B:194:TRP:CG	2:B:195:PRO:HA	2.41	0.56
1:C:200:GLU:HG3	1:C:211:VAL:CG1	2.36	0.56
2:F:120:ALA:HB3	2:F:152:PHE:CE2	2.41	0.56
2:F:55:THR:CG2	3:K:61:ALA:HB2	2.35	0.56
3:J:44:ARG:HG3	3:J:44:ARG:NH1	2.21	0.56
3:J:133:ILE:HD11	3:J:164:MET:SD	2.45	0.56
1:G:124:PRO:O	2:H:219:ARG:NH2	2.38	0.55
2:H:122:THR:C	2:H:123:THR:HG23	2.31	0.55
2:B:183:LEU:HD23	2:B:183:LEU:C	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:ALA:HB1	1:G:112:LYS:HG3	1.87	0.55
2:H:140:SER:HA	2:H:191:SER:OG	2.06	0.55
2:D:199:VAL:O	2:D:216:ILE:CD1	2.42	0.55
3:J:44:ARG:NE	3:L:44:ARG:NH2	2.39	0.55
2:F:165:LEU:HD21	2:F:187:VAL:CG2	2.34	0.55
1:A:113:ARG:HG2	1:A:114:ALA:N	2.21	0.55
3:J:91:PHE:CZ	3:J:104:VAL:CG1	2.89	0.55
1:A:12:ALA:HB3	1:A:112:LYS:HE3	1.88	0.55
2:D:47:TRP:C	2:D:48:ILE:HD13	2.32	0.55
3:K:13:THR:O	3:K:16:GLU:HG3	2.06	0.55
1:C:60:ARG:HG2	1:C:60:ARG:HH21	1.72	0.55
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.89	0.55
1:C:12:ALA:HB1	1:C:112:LYS:HG3	1.88	0.55
3:I:137:TYR:CE2	3:I:172:THR:HG22	2.42	0.55
3:J:161:LYS:HD3	4:J:186:GOL:O3	2.07	0.55
3:J:42:TYR:CE1	3:J:132:ILE:HD12	2.42	0.55
2:B:141:MET:HG3	2:B:189:VAL:O	2.07	0.54
2:F:70:LEU:HD12	2:F:81:MET:HG2	1.88	0.54
1:C:113:ARG:HG2	1:C:114:ALA:H	1.72	0.54
1:E:12:ALA:HB3	1:E:112:LYS:HE3	1.89	0.54
2:H:143:THR:C	2:H:144:LEU:HD12	2.31	0.54
3:K:52:THR:HG23	3:K:147:GLU:HG3	1.88	0.54
3:K:174:ILE:HG13	3:K:175:ALA:H	1.72	0.54
3:I:36:ILE:HD13	3:I:153:SER:HA	1.88	0.54
3:J:44:ARG:CZ	3:L:44:ARG:HH21	2.21	0.54
1:C:217:ASN:O	1:C:218:GLU:HG2	2.07	0.54
1:G:81:ILE:N	1:G:81:ILE:HD12	2.21	0.54
3:J:36:ILE:HD13	3:J:153:SER:HA	1.89	0.54
3:J:174:ILE:HD12	3:J:175:ALA:N	2.21	0.54
2:B:140:SER:HA	2:B:191:SER:OG	2.07	0.54
1:G:200:GLU:HG3	1:G:211:VAL:CG1	2.37	0.54
2:H:114:LEU:HD13	2:H:155:PRO:HG3	1.88	0.54
1:A:81:ILE:HD12	1:A:81:ILE:N	2.22	0.54
2:H:28:THR:HB	2:H:31:ARG:HG3	1.89	0.54
1:A:123:PHE:CD2	2:B:130:LEU:HB3	2.43	0.54
2:F:160:TRP:CZ3	2:F:201:CYS:HB2	2.43	0.54
2:H:51:ILE:HD11	2:H:56:GLY:CA	2.38	0.54
2:H:183:LEU:C	2:H:183:LEU:HD23	2.32	0.54
3:I:128:ILE:HD12	3:I:128:ILE:N	2.23	0.54
2:D:18:VAL:HG12	2:D:86:LEU:HD11	1.90	0.54
2:H:51:ILE:HD11	2:H:56:GLY:C	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:13:THR:O	3:I:16:GLU:HG3	2.08	0.54
3:I:174:ILE:HG13	3:I:175:ALA:H	1.72	0.54
3:L:174:ILE:HD12	3:L:175:ALA:N	2.22	0.54
2:B:18:VAL:HG12	2:B:86:LEU:HD11	1.90	0.54
3:J:44:ARG:HH21	3:L:44:ARG:NH2	2.06	0.54
1:C:113:ARG:HG2	1:C:114:ALA:N	2.22	0.54
2:F:28:THR:HB	2:F:31:ARG:CG	2.37	0.54
3:I:44:ARG:NH1	3:K:134:ASP:HB2	2.23	0.54
3:J:137:TYR:CD2	3:J:172:THR:HG22	2.43	0.54
3:K:128:ILE:HD12	3:K:128:ILE:N	2.23	0.54
3:L:36:ILE:HD13	3:L:153:SER:HA	1.89	0.53
3:L:137:TYR:CE2	3:L:172:THR:HG22	2.43	0.53
1:A:67:ARG:HB2	1:A:82:SER:OG	2.07	0.53
2:F:18:VAL:HG12	2:F:86:LEU:HD11	1.90	0.53
2:B:28:THR:CG2	2:B:31:ARG:HG2	2.38	0.53
1:G:141:LEU:HD12	1:G:141:LEU:N	2.23	0.53
1:G:172:ASP:OD2	1:G:174:LYS:HB3	2.08	0.53
1:A:30:LEU:HD12	1:A:31:ASN:H	1.72	0.53
1:A:172:ASP:OD2	1:A:174:LYS:HB3	2.08	0.53
1:E:200:GLU:HG3	1:E:211:VAL:CG1	2.39	0.53
1:G:217:ASN:O	1:G:218:GLU:HG2	2.09	0.53
3:I:44:ARG:HG3	3:I:44:ARG:NH1	2.16	0.53
3:I:137:TYR:CD2	3:I:172:THR:HG22	2.44	0.53
3:K:96:ASN:O	3:K:97:ILE:CG1	2.56	0.53
3:L:128:ILE:HD12	3:L:128:ILE:N	2.23	0.53
1:E:45:LYS:NZ	4:E:222:GOL:H32	2.24	0.53
2:F:40:ARG:HG2	2:F:40:ARG:NH1	2.23	0.53
2:H:48:ILE:HD13	2:H:64:PHE:CD2	2.43	0.53
2:H:51:ILE:HD12	2:H:52:ASN:N	2.24	0.53
3:K:41:PHE:CE2	3:K:51:LEU:HB3	2.44	0.53
2:F:27:TYR:OH	2:F:34:MET:HE1	2.09	0.53
3:K:137:TYR:CE2	3:K:172:THR:HG22	2.44	0.53
3:K:157:ASN:HB2	4:K:186:GOL:H11	1.91	0.53
3:L:118:SER:O	3:L:122:VAL:HG22	2.09	0.53
1:A:200:GLU:HG3	1:A:211:VAL:CG1	2.38	0.53
1:G:136:SER:OG	1:G:185:THR:HG23	2.09	0.53
3:J:119:SER:O	3:J:123:ASP:HB2	2.08	0.53
2:H:27:TYR:OH	2:H:34:MET:HE1	2.08	0.53
3:K:91:PHE:CE2	3:K:104:VAL:HG11	2.41	0.53
3:L:13:THR:O	3:L:16:GLU:HG3	2.09	0.53
3:L:137:TYR:CD2	3:L:172:THR:HG22	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ASP:CB	4:A:220:GOL:H2	2.38	0.53
2:H:160:TRP:CZ3	2:H:201:CYS:HB2	2.44	0.53
2:B:143:THR:C	2:B:144:LEU:HD12	2.34	0.52
2:B:151:TYR:CE2	2:B:156:VAL:CG1	2.92	0.52
1:G:30:LEU:HD12	1:G:31:ASN:H	1.74	0.52
2:B:27:TYR:OH	2:B:34:MET:HE1	2.09	0.52
2:H:40:ARG:HG2	2:H:40:ARG:NH1	2.23	0.52
2:D:194:TRP:CG	2:D:195:PRO:HA	2.44	0.52
2:H:202:ASN:CG	2:H:213:ASP:OD2	2.51	0.52
1:A:100:LEU:HD21	2:B:59:GLU:CD	2.32	0.52
1:A:210:ILE:HD12	1:A:210:ILE:N	2.25	0.52
1:G:141:LEU:HD22	1:G:180:MET:HE2	1.92	0.52
2:H:18:VAL:HG12	2:H:86:LEU:HD11	1.90	0.52
3:K:137:TYR:CD2	3:K:172:THR:HG22	2.45	0.52
2:B:28:THR:HB	2:B:31:ARG:HG3	1.92	0.52
2:F:194:TRP:CG	2:F:195:PRO:HA	2.44	0.52
2:H:151:TYR:CZ	2:H:156:VAL:HG11	2.44	0.52
3:L:18:ILE:CD1	3:L:71:ALA:HB3	2.39	0.52
1:E:141:LEU:N	1:E:141:LEU:HD12	2.25	0.52
1:G:210:ILE:HD12	1:G:210:ILE:N	2.25	0.52
1:C:39:LEU:HG	1:C:40:ALA:N	2.25	0.52
2:D:140:SER:HA	2:D:191:SER:OG	2.10	0.52
3:I:161:LYS:HD3	4:I:186:GOL:O1	2.10	0.51
1:A:140:PHE:C	1:A:141:LEU:HD12	2.35	0.51
2:D:160:TRP:CZ3	2:D:201:CYS:HB2	2.46	0.51
1:C:172:ASP:OD2	1:C:174:LYS:HB3	2.09	0.51
1:G:12:ALA:HB3	1:G:112:LYS:HE3	1.92	0.51
1:G:124:PRO:HD2	2:H:219:ARG:NH1	2.18	0.51
3:I:44:ARG:HH11	3:I:44:ARG:CG	2.17	0.51
3:K:91:PHE:HE2	3:K:104:VAL:CG2	2.23	0.51
2:F:36:TRP:CD2	2:F:81:MET:HG3	2.46	0.51
1:G:60:ARG:HG2	1:G:60:ARG:HH21	1.74	0.51
1:G:140:PHE:C	1:G:141:LEU:HD12	2.36	0.51
2:H:216:ILE:N	2:H:216:ILE:CD1	2.73	0.51
1:C:140:PHE:C	1:C:141:LEU:HD12	2.35	0.51
2:D:40:ARG:HG2	2:D:40:ARG:NH1	2.26	0.51
2:D:143:THR:C	2:D:144:LEU:HD12	2.34	0.51
1:E:30:LEU:HD12	1:E:31:ASN:H	1.75	0.51
2:F:38:LYS:N	2:F:48:ILE:CD1	2.72	0.51
1:G:67:ARG:HB2	1:G:82:SER:OG	2.10	0.51
3:I:38:ILE:HD12	3:I:38:ILE:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:91:PHE:HD2	3:K:99:THR:HG21	1.76	0.51
1:E:172:ASP:OD2	1:E:174:LYS:HB3	2.11	0.51
3:I:96:ASN:O	3:I:97:ILE:CG1	2.58	0.51
3:J:52:THR:HG23	3:J:147:GLU:HG3	1.92	0.51
1:C:136:SER:OG	1:C:185:THR:HG23	2.11	0.51
1:C:210:ILE:HD12	1:C:210:ILE:N	2.25	0.51
2:F:143:THR:C	2:F:144:LEU:HD12	2.36	0.51
1:A:60:ARG:HG2	1:A:60:ARG:HH21	1.76	0.51
2:D:28:THR:HB	2:D:31:ARG:HG3	1.92	0.51
2:D:216:ILE:N	2:D:216:ILE:CD1	2.74	0.51
1:G:141:LEU:HD23	1:G:149:ILE:CD1	2.41	0.51
3:L:44:ARG:HH11	3:L:44:ARG:CG	2.23	0.51
1:C:12:ALA:HB3	1:C:112:LYS:HE3	1.92	0.50
2:H:165:LEU:CD2	2:H:187:VAL:HG21	2.39	0.50
3:J:108:PHE:CZ	3:J:163:LEU:CD1	2.92	0.50
3:K:95:LEU:O	3:K:96:ASN:HB2	2.11	0.50
1:E:60:ARG:HG2	1:E:60:ARG:HH21	1.77	0.50
2:H:199:VAL:O	2:H:216:ILE:CD1	2.42	0.50
3:I:118:SER:O	3:I:122:VAL:HG22	2.11	0.50
3:I:119:SER:O	3:I:123:ASP:HB2	2.12	0.50
1:A:152:LYS:NZ	1:A:152:LYS:HB2	2.27	0.50
2:F:114:LEU:HD23	2:F:115:VAL:N	2.26	0.50
3:L:47:HIS:HB2	3:L:137:TYR:CD1	2.46	0.50
1:A:141:LEU:HD12	1:A:141:LEU:N	2.26	0.50
1:E:140:PHE:C	1:E:141:LEU:HD12	2.37	0.50
1:A:56:TRP:O	1:A:57:ALA:HB3	2.11	0.50
3:K:44:ARG:HH11	3:K:44:ARG:CG	2.18	0.50
1:C:30:LEU:HD12	1:C:31:ASN:H	1.75	0.50
3:K:47:HIS:HB2	3:K:137:TYR:CD1	2.47	0.50
1:C:141:LEU:HD12	1:C:141:LEU:N	2.26	0.50
1:E:152:LYS:HB2	1:E:152:LYS:NZ	2.27	0.50
3:I:45:GLN:OE1	3:I:137:TYR:OH	2.20	0.50
2:B:114:LEU:HD23	2:B:115:VAL:N	2.26	0.49
2:B:154:GLU:O	2:B:154:GLU:CD	2.55	0.49
1:C:56:TRP:O	1:C:57:ALA:HB3	2.11	0.49
2:H:23:LYS:CD	2:H:78:THR:OG1	2.59	0.49
3:I:41:PHE:CE2	3:I:51:LEU:HB3	2.47	0.49
3:J:118:SER:O	3:J:122:VAL:HG22	2.13	0.49
3:K:69:LEU:HD13	3:K:109:GLU:HG2	1.93	0.49
1:E:39:LEU:HG	1:E:40:ALA:N	2.25	0.49
3:K:119:SER:O	3:K:123:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:ALA:HB3	2:D:152:PHE:CE2	2.47	0.49
3:I:174:ILE:O	3:I:176:PRO:HD3	2.12	0.49
2:B:160:TRP:CZ3	2:B:201:CYS:HB2	2.47	0.49
2:D:205:HIS:NE2	2:D:207:ALA:HB3	2.27	0.49
2:F:140:SER:HA	2:F:191:SER:OG	2.13	0.49
2:F:205:HIS:NE2	2:F:207:ALA:HB3	2.28	0.49
1:G:147:LYS:O	1:G:147:LYS:HG2	2.12	0.49
1:A:39:LEU:HG	1:A:40:ALA:N	2.26	0.49
1:E:60:ARG:HG3	1:E:64:VAL:HB	1.95	0.49
2:H:36:TRP:CD2	2:H:81:MET:HG3	2.48	0.49
1:A:141:LEU:HD22	1:A:180:MET:HE2	1.95	0.49
2:D:48:ILE:HD13	2:D:48:ILE:N	2.28	0.49
3:K:118:SER:O	3:K:122:VAL:HG22	2.12	0.49
1:A:60:ARG:HG3	1:A:64:VAL:HB	1.95	0.49
2:H:48:ILE:HD13	2:H:64:PHE:CZ	2.48	0.49
3:J:47:HIS:HB2	3:J:137:TYR:CD1	2.47	0.49
2:F:46:GLU:O	2:F:48:ILE:CD1	2.61	0.49
3:I:91:PHE:CE2	3:I:97:ILE:O	2.66	0.49
3:K:36:ILE:HD12	3:K:126:LEU:O	2.13	0.49
2:B:40:ARG:HG2	2:B:40:ARG:NH1	2.26	0.48
3:I:47:HIS:HB2	3:I:137:TYR:CD1	2.47	0.48
1:E:67:ARG:HB2	1:E:82:SER:OG	2.14	0.48
1:E:141:LEU:HD22	1:E:180:MET:HE2	1.93	0.48
1:E:147:LYS:O	1:E:147:LYS:HG2	2.12	0.48
2:F:165:LEU:CD2	2:F:187:VAL:HG21	2.43	0.48
1:G:60:ARG:HG3	1:G:64:VAL:HB	1.95	0.48
2:H:31:ARG:NH1	3:L:63:ALA:CB	2.76	0.48
3:I:7:ILE:O	3:I:11:VAL:HG13	2.13	0.48
1:A:147:LYS:O	1:A:147:LYS:HG2	2.14	0.48
2:D:76:SER:O	2:D:78:THR:HG23	2.14	0.48
3:L:174:ILE:O	3:L:176:PRO:HD3	2.14	0.48
1:G:152:LYS:HB2	1:G:152:LYS:NZ	2.28	0.48
1:A:155:ILE:HD12	1:A:197:TYR:CD1	2.49	0.48
2:B:205:HIS:NE2	2:B:207:ALA:HB3	2.27	0.48
3:J:95:LEU:O	3:J:96:ASN:HB2	2.13	0.48
1:C:37:ASN:CB	1:C:57:ALA:HB2	2.43	0.48
1:E:45:LYS:CE	4:E:222:GOL:H32	2.44	0.48
2:F:141:MET:HA	2:F:190:PRO:HA	1.96	0.48
1:G:155:ILE:HD12	1:G:197:TYR:CD1	2.48	0.48
2:H:120:ALA:HB3	2:H:152:PHE:CE2	2.47	0.48
3:I:43:ILE:HD12	3:I:133:ILE:CB	2.18	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:41:PHE:CE2	3:L:51:LEU:HB3	2.48	0.48
1:C:54:ILE:HD13	1:C:70:GLY:HA3	1.96	0.48
2:B:139:ASN:OD1	2:B:139:ASN:N	2.46	0.48
1:C:152:LYS:HB2	1:C:152:LYS:NZ	2.29	0.47
1:G:216:ARG:NH2	1:G:216:ARG:HB3	2.29	0.47
3:J:41:PHE:CE2	3:J:51:LEU:HB3	2.49	0.47
3:K:91:PHE:CD2	3:K:99:THR:HG21	2.49	0.47
1:C:60:ARG:HG3	1:C:64:VAL:HB	1.96	0.47
1:E:136:SER:OG	1:E:185:THR:HG23	2.14	0.47
2:F:47:TRP:C	2:F:48:ILE:HD12	2.39	0.47
2:B:165:LEU:HD21	2:B:187:VAL:HG21	1.95	0.47
2:D:114:LEU:HD23	2:D:115:VAL:N	2.29	0.47
2:F:48:ILE:N	2:F:48:ILE:CD1	2.77	0.47
1:G:39:LEU:HG	1:G:40:ALA:N	2.29	0.47
2:H:141:MET:HA	2:H:190:PRO:HA	1.96	0.47
1:C:147:LYS:HG2	1:C:147:LYS:O	2.13	0.47
3:K:108:PHE:O	3:K:112:VAL:HG23	2.14	0.47
3:L:44:ARG:HG3	3:L:44:ARG:NH1	2.20	0.47
3:L:96:ASN:O	3:L:97:ILE:CG1	2.61	0.47
3:L:149:ILE:HD12	3:L:149:ILE:N	2.29	0.47
1:A:37:ASN:CB	1:A:57:ALA:HB2	2.45	0.47
2:B:141:MET:HA	2:B:190:PRO:HA	1.96	0.47
2:D:36:TRP:CD2	2:D:81:MET:HG3	2.50	0.47
1:E:155:ILE:HD12	1:E:197:TYR:CD1	2.49	0.47
3:I:98:GLN:O	3:I:99:THR:HB	2.15	0.47
2:B:28:THR:HB	2:B:31:ARG:HG2	1.96	0.47
2:H:139:ASN:N	2:H:139:ASN:OD1	2.47	0.47
1:A:136:SER:OG	1:A:185:THR:HG23	2.14	0.47
2:B:36:TRP:CD2	2:B:81:MET:HG3	2.49	0.47
1:C:128:GLU:O	1:C:132:SER:HB2	2.14	0.47
1:C:155:ILE:HD12	1:C:197:TYR:CD1	2.50	0.47
1:C:200:GLU:HG3	1:C:211:VAL:HG12	1.96	0.47
2:D:165:LEU:HD21	2:D:187:VAL:HG21	1.97	0.47
2:F:139:ASN:OD1	2:F:139:ASN:N	2.47	0.47
1:G:19:VAL:CG2	1:G:81:ILE:HD13	2.45	0.47
3:L:95:LEU:O	3:L:96:ASN:HB2	2.14	0.47
2:B:104:TYR:CE1	3:I:33:LYS:HD3	2.50	0.47
1:E:13:VAL:CG2	1:E:17:GLU:HB2	2.45	0.47
2:H:176:LEU:HD13	2:H:181:TYR:CZ	2.49	0.47
3:L:119:SER:O	3:L:123:ASP:HB2	2.15	0.47
2:D:6:GLN:HB2	2:D:111:GLN:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:183:LEU:HD23	2:D:184:SER:N	2.30	0.47
2:F:28:THR:HB	2:F:31:ARG:HG3	1.97	0.47
2:H:51:ILE:CD1	2:H:56:GLY:C	2.88	0.47
2:H:141:MET:CE	2:H:188:THR:HG21	2.44	0.47
3:I:44:ARG:NH1	3:I:44:ARG:CG	2.76	0.47
3:L:38:ILE:HD11	3:L:148:PHE:HD2	1.80	0.47
1:E:95:LYS:NZ	2:F:105:ASP:HA	2.30	0.47
2:H:51:ILE:CD1	2:H:57:TYR:O	2.58	0.47
3:J:44:ARG:HH11	3:J:44:ARG:CG	2.23	0.47
3:K:91:PHE:HE1	3:K:166:LEU:HD13	1.80	0.47
1:A:89:LEU:O	1:A:90:ALA:HB2	2.15	0.46
1:C:67:ARG:HB2	1:C:82:SER:OG	2.15	0.46
2:D:139:ASN:OD1	2:D:139:ASN:N	2.48	0.46
3:J:174:ILE:O	3:J:176:PRO:HD3	2.15	0.46
1:A:13:VAL:HG22	1:A:17:GLU:HB2	1.97	0.46
2:B:6:GLN:HB2	2:B:111:GLN:OE1	2.15	0.46
3:I:95:LEU:O	3:I:96:ASN:HB2	2.15	0.46
1:C:95:LYS:HA	1:C:102:THR:O	2.16	0.46
1:G:200:GLU:HG3	1:G:211:VAL:HG12	1.98	0.46
2:H:31:ARG:C	2:H:32:TYR:CD1	2.93	0.46
3:I:69:LEU:HD13	3:I:109:GLU:HG2	1.96	0.46
3:J:44:ARG:NH2	3:L:44:ARG:NH2	2.63	0.46
1:C:13:VAL:CG2	1:C:17:GLU:HB2	2.46	0.46
1:C:141:LEU:HD22	1:C:180:MET:HE2	1.96	0.46
1:E:88:ASP:OD1	4:E:222:GOL:O3	2.30	0.46
1:A:33:ARG:CZ	1:A:33:ARG:HB3	2.46	0.46
2:D:141:MET:HA	2:D:190:PRO:HA	1.97	0.46
1:G:216:ARG:HB3	1:G:216:ARG:HH21	1.81	0.46
2:H:205:HIS:NE2	2:H:207:ALA:HB3	2.30	0.46
3:K:98:GLN:O	3:K:99:THR:HB	2.15	0.46
1:C:37:ASN:HB2	1:C:57:ALA:HB2	1.98	0.46
1:E:216:ARG:NH2	1:E:216:ARG:HB3	2.31	0.46
3:I:91:PHE:HE2	3:I:97:ILE:CA	2.13	0.46
3:L:38:ILE:CD1	3:L:148:PHE:HD2	2.28	0.46
3:L:98:GLN:O	3:L:99:THR:HB	2.16	0.46
2:B:31:ARG:C	2:B:32:TYR:CD1	2.94	0.46
1:C:33:ARG:HB3	1:C:33:ARG:CZ	2.45	0.46
1:E:43:GLN:OE1	4:E:222:GOL:H11	2.16	0.46
1:E:93:TYR:OH	2:F:44:GLY:HA2	2.16	0.46
3:K:174:ILE:O	3:K:176:PRO:HD3	2.16	0.46
3:L:125:LYS:HB2	3:L:125:LYS:NZ	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:THR:HG23	2:B:151:TYR:HA	1.97	0.46
3:J:65:LEU:O	3:J:65:LEU:HD23	2.16	0.46
1:A:37:ASN:HB2	1:A:57:ALA:HB2	1.97	0.46
1:E:167:SER:HB2	2:F:175:VAL:CG2	2.46	0.46
3:I:119:SER:HB2	3:K:114:GLN:HB3	1.97	0.46
1:A:19:VAL:CG2	1:A:81:ILE:HD13	2.45	0.45
1:A:124:PRO:CD	2:B:219:ARG:HH12	2.25	0.45
1:A:216:ARG:HB3	1:A:216:ARG:NH2	2.31	0.45
1:C:54:ILE:HD13	1:C:70:GLY:CA	2.45	0.45
1:E:33:ARG:CZ	1:E:33:ARG:HB3	2.44	0.45
3:J:125:LYS:HB2	3:J:125:LYS:NZ	2.32	0.45
3:K:44:ARG:HG3	3:K:44:ARG:NH1	2.17	0.45
2:B:154:GLU:O	2:B:154:GLU:CG	2.64	0.45
1:G:13:VAL:CG2	1:G:17:GLU:HB2	2.45	0.45
3:L:7:ILE:O	3:L:11:VAL:HG13	2.16	0.45
1:A:95:LYS:HA	1:A:102:THR:O	2.15	0.45
1:A:128:GLU:O	1:A:132:SER:HB2	2.16	0.45
3:J:87:VAL:HB	3:J:88:PRO:HD3	1.98	0.45
3:L:69:LEU:HD13	3:L:109:GLU:HG2	1.97	0.45
1:A:86:ALA:HA	1:A:111:ILE:CD1	2.44	0.45
1:C:149:ILE:HD12	1:C:203:HIS:CB	2.39	0.45
1:G:24:LYS:HE2	1:G:76:ASP:OD2	2.16	0.45
1:G:100:LEU:HD21	2:H:59:GLU:CD	2.33	0.45
1:G:128:GLU:O	1:G:132:SER:HB2	2.15	0.45
1:G:170:ASP:O	1:G:171:GLN:C	2.59	0.45
2:H:28:THR:HB	2:H:31:ARG:HG2	1.98	0.45
3:K:87:VAL:HB	3:K:88:PRO:HD3	1.98	0.45
1:A:37:ASN:HB2	1:A:57:ALA:CB	2.47	0.45
2:B:141:MET:CG	2:B:188:THR:CG2	2.94	0.45
1:C:217:ASN:C	1:C:218:GLU:HG2	2.41	0.45
1:E:13:VAL:HG22	1:E:17:GLU:HB2	1.97	0.45
2:F:31:ARG:HH12	3:K:26:ALA:HA	1.81	0.45
2:F:31:ARG:C	2:F:32:TYR:CD1	2.95	0.45
1:G:13:VAL:HG22	1:G:17:GLU:HB2	1.97	0.45
3:J:108:PHE:O	3:J:112:VAL:HG23	2.17	0.45
2:D:62:GLN:HE22	2:D:65:LYS:HD2	1.82	0.45
1:E:128:GLU:O	1:E:132:SER:HB2	2.16	0.45
1:G:33:ARG:CZ	1:G:33:ARG:HB3	2.45	0.45
3:J:53:VAL:HG22	3:J:148:PHE:HB3	1.99	0.45
1:A:13:VAL:CG2	1:A:17:GLU:HB2	2.47	0.45
1:A:95:LYS:HE2	1:A:95:LYS:HB3	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:VAL:HG22	1:C:17:GLU:HB2	1.98	0.45
2:D:154:GLU:OE1	2:D:181:TYR:CD2	2.70	0.45
1:G:138:VAL:HG21	2:H:130:LEU:HD11	1.99	0.45
3:K:94:ALA:HB2	3:K:169:LYS:CG	2.40	0.45
1:C:170:ASP:O	1:C:171:GLN:C	2.60	0.45
2:D:214:LYS:O	2:D:216:ILE:HD12	2.17	0.45
1:G:217:ASN:C	1:G:218:GLU:HG2	2.41	0.45
3:J:98:GLN:O	3:J:99:THR:HB	2.17	0.45
1:C:37:ASN:HB2	1:C:57:ALA:CB	2.47	0.44
3:I:43:ILE:HG12	3:I:51:LEU:HD11	1.99	0.44
2:D:31:ARG:C	2:D:32:TYR:CD1	2.95	0.44
2:H:193:THR:O	2:H:197:GLU:HB2	2.17	0.44
1:A:30:LEU:HD12	1:A:31:ASN:N	2.32	0.44
2:D:128:TYR:HA	2:D:129:PRO:HD3	1.83	0.44
2:D:141:MET:O	2:D:142:VAL:HB	2.17	0.44
3:J:44:ARG:NH1	3:J:44:ARG:CG	2.81	0.44
3:J:54:LYS:HB3	3:J:149:ILE:CD1	2.47	0.44
3:K:132:ILE:HD12	3:K:132:ILE:N	2.32	0.44
1:A:60:ARG:NH2	1:A:66:ASP:HA	2.32	0.44
2:D:193:THR:O	2:D:197:GLU:HB2	2.17	0.44
1:E:24:LYS:HE2	1:E:76:ASP:OD2	2.17	0.44
2:F:129:PRO:HB3	2:F:216:ILE:HD13	1.99	0.44
3:I:148:PHE:CE1	3:I:160:ILE:HG22	2.52	0.44
3:L:148:PHE:CE1	3:L:160:ILE:HG22	2.52	0.44
1:A:149:ILE:HD12	1:A:203:HIS:CB	2.39	0.44
2:B:193:THR:O	2:B:197:GLU:HB2	2.17	0.44
1:G:95:LYS:HA	1:G:102:THR:O	2.17	0.44
2:B:183:LEU:HD23	2:B:184:SER:N	2.33	0.44
1:C:93:TYR:OH	2:D:44:GLY:HA2	2.18	0.44
2:D:212:VAL:HG22	2:D:213:ASP:N	2.33	0.44
2:H:6:GLN:HB2	2:H:111:GLN:OE1	2.18	0.44
1:A:200:GLU:HG3	1:A:211:VAL:HG12	1.99	0.44
1:A:216:ARG:HB3	1:A:216:ARG:HH21	1.83	0.44
1:E:95:LYS:HA	1:E:102:THR:O	2.18	0.44
1:G:130:LEU:HD22	1:G:188:LYS:HG3	1.99	0.44
2:H:62:GLN:HE22	2:H:65:LYS:HD2	1.83	0.44
3:K:53:VAL:HG22	3:K:148:PHE:HB3	1.98	0.44
3:K:158:CYS:HA	4:K:186:GOL:O3	2.18	0.44
2:B:128:TYR:HA	2:B:129:PRO:HD3	1.83	0.44
1:C:207:THR:O	1:C:209:PRO:HD3	2.18	0.44
2:D:140:SER:O	2:D:141:MET:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:THR:O	1:E:209:PRO:HD3	2.18	0.44
1:E:216:ARG:HB3	1:E:216:ARG:HH21	1.83	0.44
3:L:87:VAL:HB	3:L:88:PRO:HD3	1.98	0.44
2:B:176:LEU:HD13	2:B:181:TYR:CZ	2.52	0.44
2:B:194:TRP:CD1	2:B:195:PRO:HA	2.53	0.44
1:C:39:LEU:HD22	1:C:77:PHE:CG	2.53	0.44
1:E:200:GLU:HG3	1:E:211:VAL:HG12	1.99	0.43
3:L:80:THR:HG23	3:L:83:GLN:OE1	2.17	0.43
1:G:179:SER:OG	2:H:170:HIS:CE1	2.71	0.43
2:H:121:LYS:O	2:H:123:THR:HG23	2.18	0.43
2:H:214:LYS:O	2:H:216:ILE:HD12	2.18	0.43
3:J:69:LEU:HD13	3:J:109:GLU:HG2	1.99	0.43
2:F:111:GLN:H	2:F:111:GLN:NE2	2.16	0.43
2:F:193:THR:O	2:F:197:GLU:HB2	2.18	0.43
2:F:212:VAL:HG22	2:F:213:ASP:N	2.32	0.43
1:G:29:LEU:HD12	1:G:77:PHE:CE2	2.53	0.43
3:K:65:LEU:HD23	3:K:65:LEU:O	2.18	0.43
3:L:65:LEU:O	3:L:65:LEU:HD23	2.17	0.43
2:B:141:MET:HA	2:B:189:VAL:O	2.19	0.43
2:D:111:GLN:H	2:D:111:GLN:NE2	2.15	0.43
2:F:128:TYR:HA	2:F:129:PRO:HD3	1.85	0.43
3:K:7:ILE:O	3:K:11:VAL:HG13	2.18	0.43
3:K:125:LYS:HB2	3:K:125:LYS:NZ	2.32	0.43
1:C:72:GLY:HA3	1:C:77:PHE:HA	2.00	0.43
1:E:99:ASN:O	1:E:100:LEU:HB2	2.19	0.43
1:E:170:ASP:O	1:E:171:GLN:C	2.61	0.43
1:G:207:THR:O	1:G:209:PRO:HD3	2.18	0.43
1:A:39:LEU:HD22	1:A:77:PHE:CG	2.54	0.43
1:C:24:LYS:HE2	1:C:76:ASP:OD2	2.18	0.43
1:G:149:ILE:HD11	1:G:201:ALA:HB1	1.99	0.43
1:A:19:VAL:O	1:A:80:THR:HG23	2.19	0.43
1:A:170:ASP:O	1:A:171:GLN:C	2.61	0.43
2:B:129:PRO:HB3	2:B:216:ILE:HD13	2.00	0.43
2:B:141:MET:O	2:B:142:VAL:HB	2.19	0.43
1:C:216:ARG:HH21	1:C:216:ARG:HB3	1.84	0.43
2:D:57:TYR:HA	3:J:125:LYS:HD3	2.00	0.43
1:E:72:GLY:HA3	1:E:77:PHE:HA	2.01	0.43
3:J:67:ALA:O	3:J:70:SER:HB3	2.19	0.43
1:E:30:LEU:HD12	1:E:31:ASN:N	2.33	0.43
1:G:30:LEU:HD12	1:G:31:ASN:N	2.33	0.43
1:G:60:ARG:NH2	1:G:66:ASP:HA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LYS:HE2	1:A:76:ASP:OD2	2.18	0.43
1:A:72:GLY:HA3	1:A:77:PHE:HA	2.00	0.43
2:B:120:ALA:HB3	2:B:152:PHE:CE2	2.54	0.43
1:C:99:ASN:O	1:C:100:LEU:HB2	2.17	0.43
2:D:143:THR:HG22	2:D:188:THR:HG1	1.80	0.43
2:D:176:LEU:HD13	2:D:181:TYR:CZ	2.54	0.43
1:E:42:TYR:HH	2:F:106:PHE:H	1.67	0.43
3:I:132:ILE:HD12	3:I:132:ILE:N	2.34	0.43
2:F:6:GLN:HB2	2:F:111:GLN:OE1	2.19	0.42
2:H:61:ASN:O	2:H:62:GLN:C	2.59	0.42
3:I:108:PHE:O	3:I:112:VAL:HG23	2.18	0.42
3:J:135:GLU:O	3:J:168:THR:HB	2.19	0.42
1:C:216:ARG:HB3	1:C:216:ARG:NH2	2.33	0.42
1:E:39:LEU:HD22	1:E:77:PHE:CG	2.54	0.42
1:G:56:TRP:O	1:G:57:ALA:HB3	2.19	0.42
3:I:67:ALA:O	3:I:70:SER:HB3	2.19	0.42
3:K:18:ILE:HD11	3:K:163:LEU:CD2	2.50	0.42
2:B:23:LYS:HE3	2:B:76:SER:O	2.19	0.42
1:C:130:LEU:HD22	1:C:188:LYS:HG3	2.00	0.42
1:E:175:ASP:OD1	1:E:177:THR:HG23	2.19	0.42
2:F:58:THR:H	3:K:125:LYS:CD	2.29	0.42
2:F:141:MET:HA	2:F:189:VAL:O	2.19	0.42
3:I:133:ILE:CG2	3:I:134:ASP:N	2.82	0.42
3:L:53:VAL:HG22	3:L:148:PHE:HB3	2.01	0.42
2:B:62:GLN:HE22	2:B:65:LYS:HD2	1.84	0.42
2:B:70:LEU:HD11	2:B:81:MET:HG2	2.01	0.42
2:B:140:SER:O	2:B:141:MET:HB3	2.19	0.42
2:D:172:PHE:HA	2:D:173:PRO:HD3	1.87	0.42
1:G:72:GLY:HA3	1:G:77:PHE:HA	2.00	0.42
1:E:153:TRP:O	1:E:159:GLU:HA	2.20	0.42
1:G:41:TRP:CE2	1:G:79:LEU:HB2	2.55	0.42
2:H:215:LYS:C	2:H:216:ILE:HD12	2.44	0.42
3:I:87:VAL:HB	3:I:88:PRO:HD3	2.01	0.42
1:E:29:LEU:HD12	1:E:77:PHE:CE2	2.54	0.42
1:G:125:PRO:HD3	1:G:137:VAL:HG22	2.00	0.42
3:K:44:ARG:NH1	3:K:44:ARG:CG	2.77	0.42
1:A:130:LEU:HD22	1:A:188:LYS:HG3	2.01	0.42
2:F:141:MET:O	2:F:142:VAL:HB	2.20	0.42
2:F:183:LEU:HD23	2:F:184:SER:N	2.34	0.42
1:G:19:VAL:O	1:G:80:THR:HG23	2.20	0.42
2:H:23:LYS:HE3	2:H:76:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:141:MET:HA	2:H:189:VAL:O	2.19	0.42
3:I:129:GLN:HB3	4:I:186:GOL:H32	2.01	0.42
1:C:42:TYR:CZ	1:C:52:LEU:HD13	2.54	0.42
1:G:37:ASN:HB2	1:G:57:ALA:CB	2.50	0.42
3:K:80:THR:HG23	3:K:83:GLN:OE1	2.20	0.42
1:G:10:SER:HA	1:G:108:LYS:O	2.20	0.42
1:G:17:GLU:O	1:G:84:VAL:HG12	2.20	0.42
1:G:153:TRP:O	1:G:159:GLU:HA	2.20	0.42
3:K:135:GLU:O	3:K:168:THR:HB	2.19	0.42
2:B:219:ARG:HG3	2:B:219:ARG:HH11	1.85	0.42
2:D:102:ASP:OD1	2:D:104:TYR:HB2	2.20	0.42
1:E:86:ALA:HA	1:E:111:ILE:CD1	2.47	0.42
1:G:93:TYR:OH	2:H:44:GLY:HA2	2.19	0.42
3:I:135:GLU:O	3:I:168:THR:HB	2.19	0.42
3:J:91:PHE:CE1	3:J:166:LEU:HD13	2.55	0.42
3:L:67:ALA:O	3:L:70:SER:HB3	2.19	0.42
1:C:153:TRP:O	1:C:159:GLU:HA	2.20	0.41
3:J:6:SER:O	3:J:9:THR:HB	2.20	0.41
3:J:80:THR:HG23	3:J:83:GLN:OE1	2.20	0.41
1:C:81:ILE:N	1:C:81:ILE:CD1	2.82	0.41
2:F:55:THR:HG22	3:K:61:ALA:CB	2.50	0.41
2:F:190:PRO:O	2:F:191:SER:C	2.64	0.41
3:J:133:ILE:CG2	3:J:134:ASP:N	2.83	0.41
2:B:137:GLN:HG2	2:B:137:GLN:O	2.20	0.41
2:B:172:PHE:HA	2:B:173:PRO:HD3	1.86	0.41
1:C:30:LEU:HD12	1:C:31:ASN:N	2.34	0.41
1:E:33:ARG:CZ	1:E:33:ARG:CB	2.98	0.41
1:E:130:LEU:HD22	1:E:188:LYS:HG3	2.02	0.41
2:F:141:MET:H	2:F:191:SER:H	1.68	0.41
1:G:33:ARG:CZ	1:G:33:ARG:CB	2.99	0.41
1:G:99:ASN:O	1:G:100:LEU:HB2	2.19	0.41
2:H:122:THR:C	2:H:123:THR:CG2	2.92	0.41
1:A:29:LEU:HD12	1:A:77:PHE:CE2	2.54	0.41
3:L:38:ILE:CD1	3:L:148:PHE:CD2	3.03	0.41
1:G:39:LEU:HD22	1:G:77:PHE:CG	2.55	0.41
1:G:53:LEU:HB3	1:G:54:ILE:CD1	2.43	0.41
1:G:81:ILE:HD12	1:G:81:ILE:H	1.85	0.41
2:H:169:VAL:O	2:H:170:HIS:HD2	2.02	0.41
2:H:194:TRP:CD1	2:H:195:PRO:HA	2.55	0.41
3:L:133:ILE:HG21	3:L:168:THR:HG21	2.02	0.41
1:A:207:THR:O	1:A:209:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:55:THR:HG22	3:K:61:ALA:HB2	2.03	0.41
2:F:151:TYR:O	2:F:152:PHE:HB2	2.19	0.41
1:A:10:SER:HA	1:A:108:LYS:O	2.21	0.41
2:H:140:SER:O	2:H:141:MET:HB2	2.21	0.41
2:H:151:TYR:CE2	2:H:156:VAL:HG13	2.54	0.41
2:H:183:LEU:HD23	2:H:184:SER:N	2.34	0.41
3:L:94:ALA:O	3:L:95:LEU:HD23	2.21	0.41
2:D:194:TRP:CD1	2:D:195:PRO:HA	2.56	0.41
1:G:89:LEU:O	1:G:90:ALA:HB2	2.20	0.41
1:G:155:ILE:HD12	1:G:197:TYR:CE1	2.56	0.41
2:H:31:ARG:HH12	3:L:63:ALA:HB1	1.86	0.41
3:I:52:THR:O	3:I:147:GLU:HA	2.20	0.41
3:J:94:ALA:O	3:J:95:LEU:HD23	2.21	0.41
1:A:153:TRP:O	1:A:159:GLU:HA	2.21	0.41
2:B:111:GLN:H	2:B:111:GLN:NE2	2.18	0.41
2:D:137:GLN:O	2:D:137:GLN:HG2	2.21	0.41
2:D:141:MET:HA	2:D:189:VAL:O	2.19	0.41
2:D:153:PRO:HD2	2:D:207:ALA:HB1	2.03	0.41
1:E:89:LEU:O	1:E:90:ALA:HB2	2.21	0.41
1:E:95:LYS:HZ1	2:F:105:ASP:HA	1.86	0.41
1:E:165:LEU:HD21	2:F:177:GLN:OE1	2.20	0.41
1:G:37:ASN:CB	1:G:57:ALA:HB2	2.51	0.41
3:J:7:ILE:O	3:J:11:VAL:HG13	2.21	0.41
3:J:72:ALA:HB2	3:J:163:LEU:HD21	2.02	0.41
3:K:29:SER:OG	3:K:32:THR:OG1	2.12	0.41
3:L:135:GLU:O	3:L:168:THR:HB	2.21	0.41
1:A:33:ARG:CZ	1:A:33:ARG:CB	2.99	0.41
1:A:195:ASN:ND2	1:A:217:ASN:OD1	2.40	0.41
2:B:141:MET:H	2:B:191:SER:H	1.69	0.41
2:D:141:MET:H	2:D:191:SER:H	1.68	0.41
1:E:195:ASN:O	1:E:215:ASN:HA	2.21	0.41
2:H:9:ALA:CB	2:H:155:PRO:HG2	2.51	0.41
2:H:102:ASP:OD1	2:H:104:TYR:HB2	2.20	0.41
3:J:33:LYS:HG3	3:J:34:CYS:N	2.35	0.41
3:L:6:SER:O	3:L:9:THR:HB	2.20	0.41
3:L:91:PHE:CE1	3:L:166:LEU:HD13	2.56	0.41
1:A:125:PRO:HD3	1:A:137:VAL:HG22	2.03	0.40
1:C:41:TRP:CE2	1:C:79:LEU:HB2	2.56	0.40
1:C:124:PRO:CD	2:D:219:ARG:HH12	2.29	0.40
2:D:70:LEU:HD11	2:D:81:MET:HG2	2.02	0.40
3:I:80:THR:HG23	3:I:83:GLN:OE1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:ALA:CB	2:B:155:PRO:HG2	2.51	0.40
2:B:61:ASN:O	2:B:62:GLN:C	2.64	0.40
1:C:33:ARG:CZ	1:C:33:ARG:CB	2.99	0.40
1:C:91:VAL:HG22	1:C:108:LYS:HA	2.02	0.40
1:E:125:PRO:HD3	1:E:137:VAL:HG22	2.03	0.40
1:G:195:ASN:ND2	1:G:217:ASN:OD1	2.42	0.40
2:H:38:LYS:HB2	2:H:48:ILE:HD11	2.02	0.40
2:H:111:GLN:NE2	2:H:111:GLN:H	2.19	0.40
3:L:108:PHE:O	3:L:112:VAL:HG23	2.21	0.40
1:A:86:ALA:O	1:A:111:ILE:HD11	2.20	0.40
2:D:215:LYS:C	2:D:216:ILE:HD12	2.46	0.40
1:E:172:ASP:C	1:E:174:LYS:H	2.29	0.40
2:F:9:ALA:CB	2:F:155:PRO:HG2	2.51	0.40
2:F:176:LEU:HD13	2:F:181:TYR:CZ	2.56	0.40
1:G:160:ARG:HH12	1:G:186:LEU:HD21	1.86	0.40
3:L:18:ILE:HD13	3:L:71:ALA:CB	2.47	0.40
3:L:43:ILE:HD13	3:L:136:CYS:CB	2.51	0.40
1:A:84:VAL:CG2	1:A:85:GLN:N	2.85	0.40
2:B:141:MET:N	2:B:191:SER:OG	2.55	0.40
1:C:125:PRO:HD3	1:C:137:VAL:HG22	2.02	0.40
1:C:126:SER:CB	2:D:128:TYR:HB3	2.52	0.40
1:C:136:SER:HG	1:C:185:THR:HG23	1.86	0.40
2:F:122:THR:HG22	2:F:123:THR:N	2.36	0.40
3:J:96:ASN:O	3:J:97:ILE:CG1	2.62	0.40
3:K:148:PHE:CE1	3:K:160:ILE:HG22	2.56	0.40
2:B:122:THR:CG2	2:B:208:SER:HB3	2.52	0.40
2:F:172:PHE:HA	2:F:173:PRO:HD3	1.87	0.40
1:G:123:PHE:HA	1:G:124:PRO:HD3	1.89	0.40
2:H:122:THR:CG2	2:H:208:SER:HB3	2.51	0.40
3:I:44:ARG:HH12	3:K:134:ASP:HB2	1.85	0.40
3:I:53:VAL:HG22	3:I:148:PHE:HB3	2.02	0.40
3:I:91:PHE:CE2	3:I:97:ILE:C	3.00	0.40
3:J:94:ALA:HB2	3:J:169:LYS:CG	2.41	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	217/219 (99%)	193 (89%)	22 (10%)	2 (1%)	14	44
1	C	217/219 (99%)	193 (89%)	22 (10%)	2 (1%)	14	44
1	E	217/219 (99%)	193 (89%)	23 (11%)	1 (0%)	24	57
1	G	217/219 (99%)	194 (89%)	22 (10%)	1 (0%)	24	57
2	B	217/219 (99%)	198 (91%)	15 (7%)	4 (2%)	6	28
2	D	217/219 (99%)	198 (91%)	15 (7%)	4 (2%)	6	28
2	F	217/219 (99%)	197 (91%)	17 (8%)	3 (1%)	9	34
2	H	217/219 (99%)	198 (91%)	15 (7%)	4 (2%)	6	28
3	I	171/184 (93%)	147 (86%)	22 (13%)	2 (1%)	10	37
3	J	171/184 (93%)	146 (85%)	25 (15%)	0	100	100
3	K	171/184 (93%)	147 (86%)	22 (13%)	2 (1%)	10	37
3	L	171/184 (93%)	147 (86%)	22 (13%)	2 (1%)	10	37
All	All	2420/2488 (97%)	2151 (89%)	242 (10%)	27 (1%)	11	39

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	133	GLY
2	B	142	VAL
2	D	133	GLY
2	D	142	VAL
2	F	133	GLY
2	F	142	VAL
2	H	133	GLY
2	H	142	VAL
1	A	58	SER
2	B	134	SER
2	D	134	SER
2	F	134	SER

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Mol	Chain	Res	Type
2	H	134	SER
1	C	58	SER
1	G	74	GLY
3	K	99	THR
1	A	74	GLY
3	I	99	THR
3	L	99	THR
1	C	74	GLY
1	E	74	GLY
2	D	152	PHE
2	H	152	PHE
3	I	97	ILE
2	B	152	PHE
3	K	97	ILE
3	L	97	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/193 (100%)	184 (95%)	9 (5%)	23	55
1	C	193/193 (100%)	183 (95%)	10 (5%)	21	51
1	E	193/193 (100%)	184 (95%)	9 (5%)	23	55
1	G	193/193 (100%)	186 (96%)	7 (4%)	31	62
2	B	186/186 (100%)	175 (94%)	11 (6%)	18	48
2	D	186/186 (100%)	175 (94%)	11 (6%)	18	48
2	F	186/186 (100%)	175 (94%)	11 (6%)	18	48
2	H	186/186 (100%)	173 (93%)	13 (7%)	14	41
3	I	145/151 (96%)	143 (99%)	2 (1%)	59	76
3	J	145/151 (96%)	144 (99%)	1 (1%)	76	82
3	K	145/151 (96%)	143 (99%)	2 (1%)	59	76
3	L	145/151 (96%)	143 (99%)	2 (1%)	59	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2096/2120 (99%)	2008 (96%)	88 (4%)	26 58

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	39	LEU
1	A	89	LEU
1	A	109	LEU
1	A	113	ARG
1	A	149	ILE
1	A	152	LYS
1	A	184	LEU
1	A	215	ASN
2	B	11	LEU
2	B	45	LEU
2	B	71	THR
2	B	81	MET
2	B	87	THR
2	B	111	GLN
2	B	114	LEU
2	B	134	SER
2	B	139	ASN
2	B	183	LEU
2	B	200	THR
1	C	11	LEU
1	C	39	LEU
1	C	81	ILE
1	C	89	LEU
1	C	109	LEU
1	C	113	ARG
1	C	149	ILE
1	C	152	LYS
1	C	184	LEU
1	C	215	ASN
2	D	11	LEU
2	D	45	LEU
2	D	48	ILE
2	D	87	THR
2	D	111	GLN
2	D	114	LEU
2	D	134	SER

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Mol	Chain	Res	Type
2	D	139	ASN
2	D	183	LEU
2	D	200	THR
2	D	216	ILE
1	E	11	LEU
1	E	39	LEU
1	E	89	LEU
1	E	109	LEU
1	E	113	ARG
1	E	149	ILE
1	E	152	LYS
1	E	184	LEU
1	E	215	ASN
2	F	11	LEU
2	F	45	LEU
2	F	48	ILE
2	F	81	MET
2	F	87	THR
2	F	111	GLN
2	F	114	LEU
2	F	134	SER
2	F	139	ASN
2	F	183	LEU
2	F	200	THR
1	G	11	LEU
1	G	39	LEU
1	G	89	LEU
1	G	109	LEU
1	G	113	ARG
1	G	152	LYS
1	G	184	LEU
2	H	11	LEU
2	H	45	LEU
2	H	48	ILE
2	H	71	THR
2	H	81	MET
2	H	87	THR
2	H	111	GLN
2	H	114	LEU
2	H	134	SER
2	H	139	ASN
2	H	183	LEU

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Mol	Chain	Res	Type
2	H	200	THR
2	H	216	ILE
3	I	125	LYS
3	I	128	ILE
3	J	125	LYS
3	K	125	LYS
3	K	128	ILE
3	L	125	LYS
3	L	128	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	150	ASN
1	A	194	HIS
1	A	215	ASN
2	B	39	GLN
2	B	62	GLN
2	B	170	HIS
1	C	44	GLN
1	C	85	GLN
1	C	150	ASN
1	C	194	HIS
1	C	215	ASN
2	D	5	GLN
2	D	39	GLN
2	D	62	GLN
1	E	44	GLN
1	E	85	GLN
1	E	150	ASN
1	E	194	HIS
1	E	215	ASN
2	F	39	GLN
1	G	44	GLN
1	G	85	GLN
1	G	150	ASN
1	G	194	HIS
1	G	215	ASN
2	H	39	GLN
2	H	62	GLN
2	H	170	HIS

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Mol	Chain	Res	Type
3	I	165	GLN
3	J	165	GLN
3	K	31	GLN
3	K	165	GLN
3	L	165	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	E	222	-	5,5,5	0.62	0	5,5,5	0.53	0
4	GOL	L	186	-	5,5,5	0.23	0	5,5,5	0.48	0
4	GOL	K	186	-	5,5,5	0.69	0	5,5,5	0.53	0
4	GOL	J	186	-	5,5,5	0.13	0	5,5,5	0.54	0
4	GOL	I	186	-	5,5,5	0.26	0	5,5,5	0.60	0
4	GOL	E	221	-	5,5,5	0.68	0	5,5,5	0.30	0
4	GOL	E	220	-	5,5,5	0.74	0	5,5,5	0.49	0
4	GOL	A	220	-	5,5,5	0.99	0	5,5,5	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	E	222	-	-	0/4/4/4	-
4	GOL	L	186	-	-	0/4/4/4	-
4	GOL	K	186	-	-	0/4/4/4	-
4	GOL	J	186	-	-	0/4/4/4	-
4	GOL	I	186	-	-	0/4/4/4	-
4	GOL	E	221	-	-	0/4/4/4	-
4	GOL	E	220	-	-	0/4/4/4	-
4	GOL	A	220	-	-	0/4/4/4	-

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.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	222	GOL	7	0
4	K	186	GOL	3	0
4	J	186	GOL	4	0
4	I	186	GOL	2	0
4	A	220	GOL	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	219/219 (100%)	0.29	14 (6%) 25 14	13, 39, 68, 100	0
1	C	219/219 (100%)	0.25	2 (0%) 81 63	12, 39, 68, 99	0
1	E	219/219 (100%)	0.34	10 (4%) 37 20	11, 39, 68, 100	0
1	G	219/219 (100%)	0.44	15 (6%) 23 12	14, 40, 69, 99	0
2	B	219/219 (100%)	0.24	10 (4%) 37 20	11, 34, 72, 101	0
2	D	219/219 (100%)	0.19	10 (4%) 37 20	11, 33, 72, 102	0
2	F	219/219 (100%)	0.46	18 (8%) 17 10	11, 34, 72, 102	0
2	H	219/219 (100%)	0.32	12 (5%) 30 16	11, 33, 73, 102	0
3	I	173/184 (94%)	0.37	10 (5%) 29 16	14, 37, 63, 97	0
3	J	173/184 (94%)	0.41	8 (4%) 37 20	13, 36, 62, 97	0
3	K	173/184 (94%)	0.52	13 (7%) 20 11	13, 36, 62, 97	0
3	L	173/184 (94%)	0.34	9 (5%) 33 17	15, 37, 63, 97	0
All	All	2444/2488 (98%)	0.34	131 (5%) 31 17	11, 37, 69, 102	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	91	PHE	7.9
3	J	175	ALA	5.7
3	L	5	ALA	5.5
3	J	176	PRO	4.9
1	E	1	ASP	4.2
2	F	135	ALA	4.1
3	J	91	PHE	4.1
3	K	96	ASN	4.1
3	I	5	ALA	4.0
3	I	175	ALA	4.0
3	K	175	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	141	MET	3.9
3	K	97	ILE	3.9
3	I	120	ALA	3.8
3	L	176	PRO	3.7
3	I	4	ALA	3.7
3	L	91	PHE	3.6
3	K	98	GLN	3.5
3	I	123	ASP	3.4
2	H	155	PRO	3.3
2	F	141	MET	3.3
3	J	4	ALA	3.3
2	F	142	VAL	3.2
2	H	59	GLU	3.2
2	F	133	GLY	3.2
3	L	97	ILE	3.2
3	L	175	ALA	3.2
3	K	4	ALA	3.1
2	B	143	THR	3.1
2	H	140	SER	3.1
1	G	214	PHE	3.0
1	A	196	SER	3.0
1	E	158	SER	3.0
2	D	136	ALA	3.0
1	E	161	ALA	2.9
1	E	155	ILE	2.9
3	K	176	PRO	2.9
1	A	1	ASP	2.9
1	G	210	ILE	2.9
3	I	97	ILE	2.9
1	G	187	THR	2.9
2	B	139	ASN	2.9
2	F	156	VAL	2.8
2	H	141	MET	2.8
1	G	189	ASP	2.8
2	F	177	GLN	2.8
1	C	219	CYS	2.7
2	D	138	THR	2.7
1	A	57	ALA	2.7
2	B	138	THR	2.7
1	A	195	ASN	2.7
1	A	219	CYS	2.7
2	F	154	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
3	L	4	ALA	2.6
2	B	59	GLU	2.6
2	D	141	MET	2.6
3	I	91	PHE	2.6
3	I	176	PRO	2.6
2	D	59	GLU	2.6
3	I	119	SER	2.5
2	H	217	VAL	2.5
3	K	5	ALA	2.5
1	A	158	SER	2.5
2	H	131	ALA	2.5
3	J	125	LYS	2.5
1	A	161	ALA	2.5
1	E	149	ILE	2.4
2	D	133	GLY	2.4
1	G	161	ALA	2.4
2	B	1	GLN	2.4
3	K	109	GLU	2.4
3	J	5	ALA	2.4
1	E	126	SER	2.4
1	E	187	THR	2.4
1	G	193	ARG	2.4
2	F	134	SER	2.4
2	D	156	VAL	2.4
2	F	1	GLN	2.3
2	B	158	VAL	2.3
2	D	177	GLN	2.3
3	L	98	GLN	2.3
2	H	154	GLU	2.3
1	G	196	SER	2.3
1	C	161	ALA	2.3
3	K	86	TYR	2.3
2	F	136	ALA	2.3
3	K	99	THR	2.3
1	A	160	ARG	2.3
2	F	138	THR	2.2
1	A	217	ASN	2.2
2	F	59	GLU	2.2
1	G	155	ILE	2.2
3	I	165	GLN	2.2
1	G	215	ASN	2.2
1	G	190	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	155	PRO	2.2
2	D	140	SER	2.2
1	A	149	ILE	2.2
2	F	165	LEU	2.2
2	F	199	VAL	2.2
2	B	177	GLN	2.2
1	A	155	ILE	2.1
1	E	189	ASP	2.1
2	H	199	VAL	2.1
2	D	1	GLN	2.1
1	E	190	GLU	2.1
2	H	42	GLY	2.1
2	F	200	THR	2.1
3	K	173	GLN	2.1
1	E	218	GLU	2.1
3	L	29	SER	2.1
2	B	217	VAL	2.1
2	F	188	THR	2.1
2	H	142	VAL	2.1
1	G	195	ASN	2.1
3	J	163	LEU	2.1
1	G	1	ASP	2.1
1	A	162	ALA	2.1
2	F	163	GLY	2.1
2	F	155	PRO	2.1
2	H	216	ILE	2.0
1	G	197	TYR	2.0
1	G	219	CYS	2.0
1	A	27	GLN	2.0
2	B	190	PRO	2.0
3	K	101	VAL	2.0
1	G	150	ASN	2.0
3	J	123	ASP	2.0
2	H	177	GLN	2.0
1	A	218	GLU	2.0
3	L	16	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
4	GOL	A	220	6/6	0.76	0.23	49,54,55,56	0
4	GOL	E	222	6/6	0.80	0.16	57,58,58,58	0
4	GOL	K	186	6/6	0.81	0.20	41,45,47,48	0
4	GOL	L	186	6/6	0.83	0.20	40,43,45,46	0
4	GOL	E	221	6/6	0.88	0.18	52,53,54,54	0
4	GOL	I	186	6/6	0.88	0.17	31,34,36,38	0
4	GOL	E	220	6/6	0.89	0.18	49,50,51,52	0
4	GOL	J	186	6/6	0.91	0.14	39,41,42,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.