



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:25 PM UTC

PDB ID : 9LV3 / pdb_00009lv3
Title : Crystal structure of mutant H1 Haemagglutinin HN/18-HA FPP from Influenza A virus
Authors : Deng, G.; Wei, X.; Sun, H.
Deposited on : 2025-02-11
Resolution : 2.70 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:

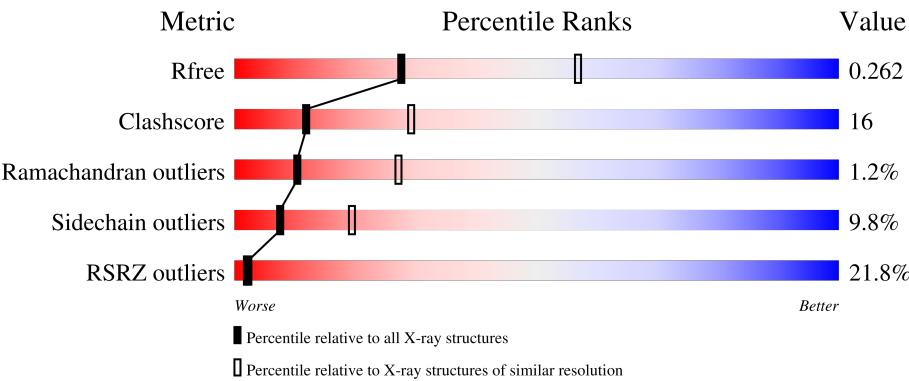
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	321	<div><div>17%</div><div>69%</div><div>27%</div><div>.</div></div>
1	C	321	<div><div>17%</div><div>75%</div><div>20%</div><div>.</div></div>
1	E	321	<div><div>14%</div><div>72%</div><div>26%</div><div>..</div></div>
1	G	321	<div><div>11%</div><div>70%</div><div>25%</div><div>5%.</div></div>
1	I	321	<div><div>11%</div><div>75%</div><div>22%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	K	321	
2	B	156	
2	D	156	
2	F	156	
2	H	156	
2	J	156	
2	L	156	

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
3	NAG	E	402	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22926 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	321	Total	C	N	O	S	0	0	0
			2515	1583	441	480	11			
1	I	321	Total	C	N	O	S	0	0	0
			2515	1583	441	480	11			
1	K	321	Total	C	N	O	S	0	0	0
			2515	1583	441	480	11			
1	A	321	Total	C	N	O	S	0	0	0
			2515	1583	441	480	11			
1	C	321	Total	C	N	O	S	0	0	0
			2515	1583	441	480	11			
1	E	321	Total	C	N	O	S	0	0	0
			2515	1583	441	480	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	5	ILE	VAL	conflict	UNP A0A6G5UYK1
G	321	VAL	ILE	conflict	UNP A0A6G5UYK1
I	5	ILE	VAL	conflict	UNP A0A6G5UYK1
I	321	VAL	ILE	conflict	UNP A0A6G5UYK1
K	5	ILE	VAL	conflict	UNP A0A6G5UYK1
K	321	VAL	ILE	conflict	UNP A0A6G5UYK1
A	5	ILE	VAL	conflict	UNP A0A6G5UYK1
A	321	VAL	ILE	conflict	UNP A0A6G5UYK1
C	5	ILE	VAL	conflict	UNP A0A6G5UYK1
C	321	VAL	ILE	conflict	UNP A0A6G5UYK1
E	5	ILE	VAL	conflict	UNP A0A6G5UYK1
E	321	VAL	ILE	conflict	UNP A0A6G5UYK1

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	156	Total	C	N	O	S	0	0	0
			1250	786	212	245	7			
2	J	156	Total	C	N	O	S	0	0	0
			1250	786	212	245	7			
2	L	156	Total	C	N	O	S	0	0	0
			1250	786	212	245	7			
2	B	156	Total	C	N	O	S	0	0	0
			1250	786	212	245	7			
2	D	156	Total	C	N	O	S	0	0	0
			1250	786	212	245	7			
2	F	156	Total	C	N	O	S	0	0	0
			1250	786	212	245	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	38	LEU	GLN	conflict	UNP A0A6G5UYL6
H	110	TYR	PHE	conflict	UNP A0A6G5UYL6
H	113	SER	LEU	conflict	UNP A0A6G5UYL6
J	38	LEU	GLN	conflict	UNP A0A6G5UYL6
J	110	TYR	PHE	conflict	UNP A0A6G5UYL6
J	113	SER	LEU	conflict	UNP A0A6G5UYL6
L	38	LEU	GLN	conflict	UNP A0A6G5UYL6
L	110	TYR	PHE	conflict	UNP A0A6G5UYL6
L	113	SER	LEU	conflict	UNP A0A6G5UYL6
B	38	LEU	GLN	conflict	UNP A0A6G5UYL6
B	110	TYR	PHE	conflict	UNP A0A6G5UYL6
B	113	SER	LEU	conflict	UNP A0A6G5UYL6
D	38	LEU	GLN	conflict	UNP A0A6G5UYL6
D	110	TYR	PHE	conflict	UNP A0A6G5UYL6
D	113	SER	LEU	conflict	UNP A0A6G5UYL6
F	38	LEU	GLN	conflict	UNP A0A6G5UYL6
F	110	TYR	PHE	conflict	UNP A0A6G5UYL6
F	113	SER	LEU	conflict	UNP A0A6G5UYL6

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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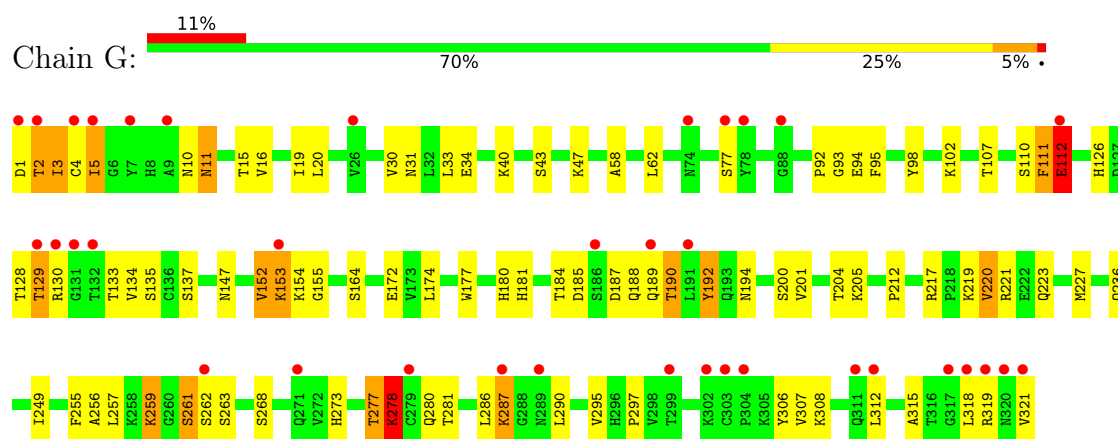
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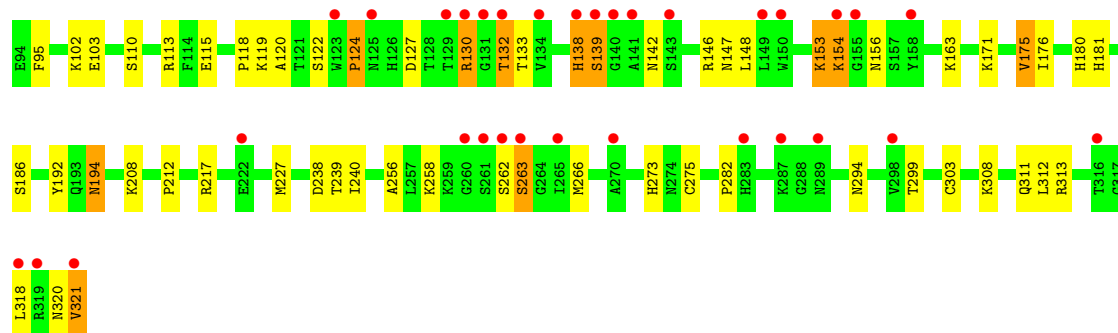
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots [i](#)

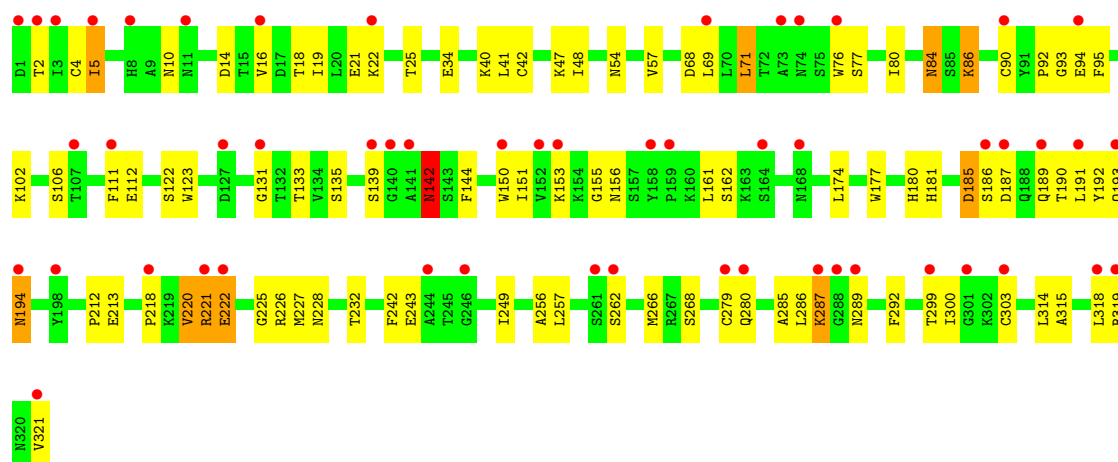
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Hemagglutinin

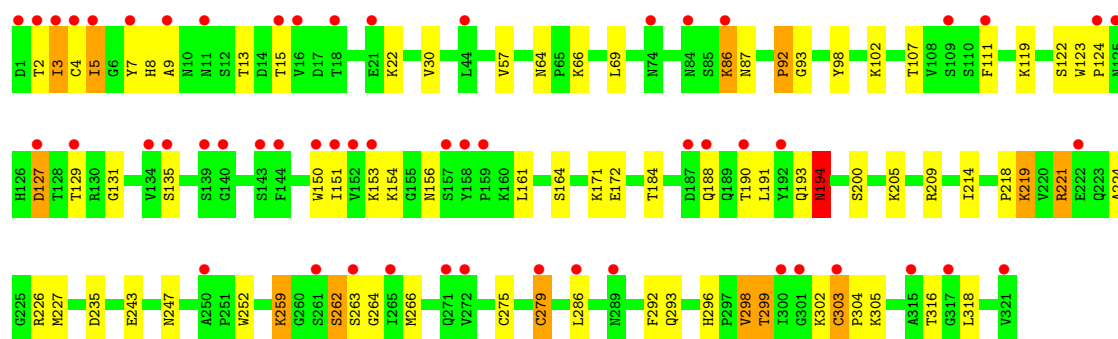
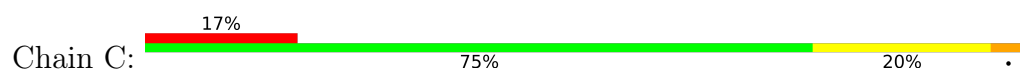




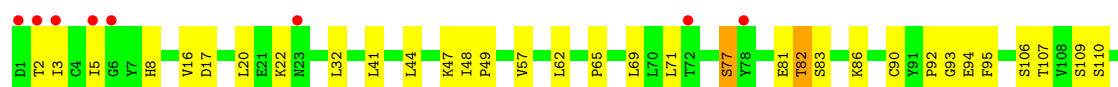
• Molecule 1: Hemagglutinin

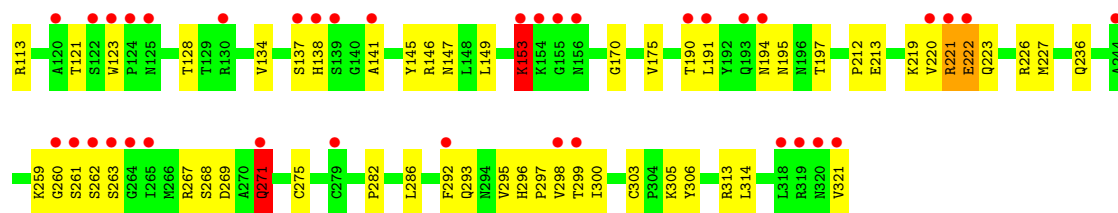


• Molecule 1: Hemagglutinin

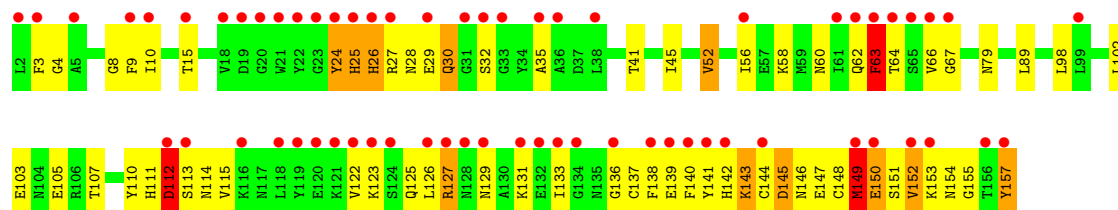
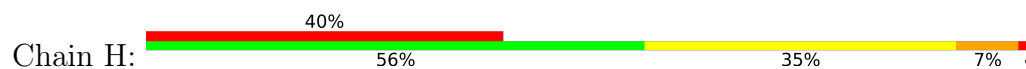


• Molecule 1: Hemagglutinin

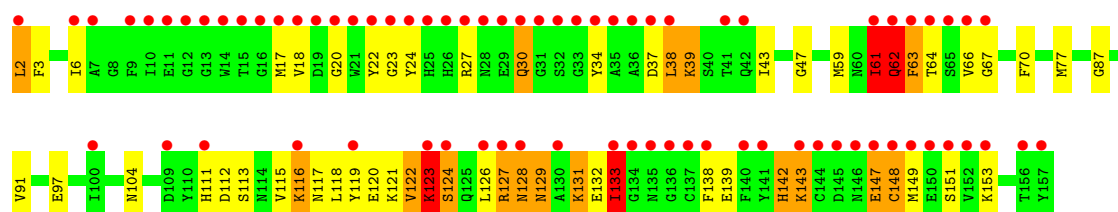




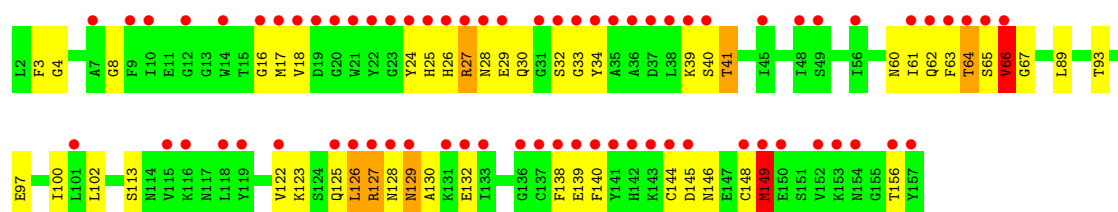
• Molecule 2: Hemagglutinin



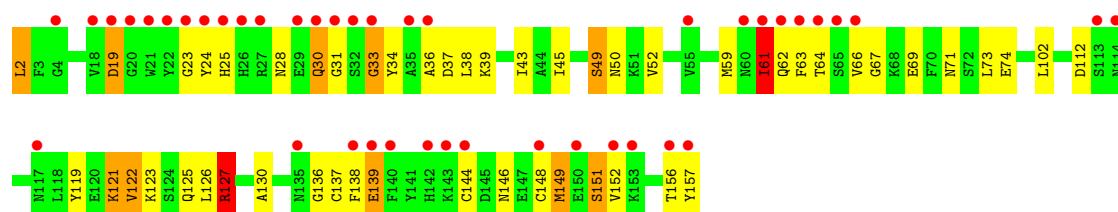
• Molecule 2: Hemagglutinin



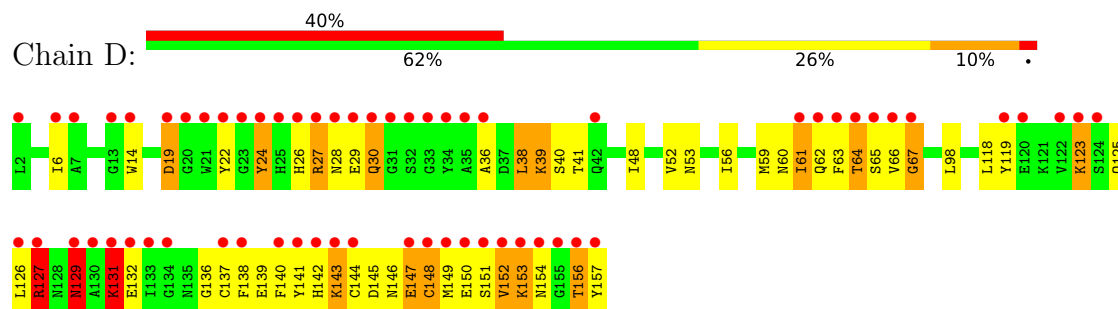
• Molecule 2: Hemagglutinin



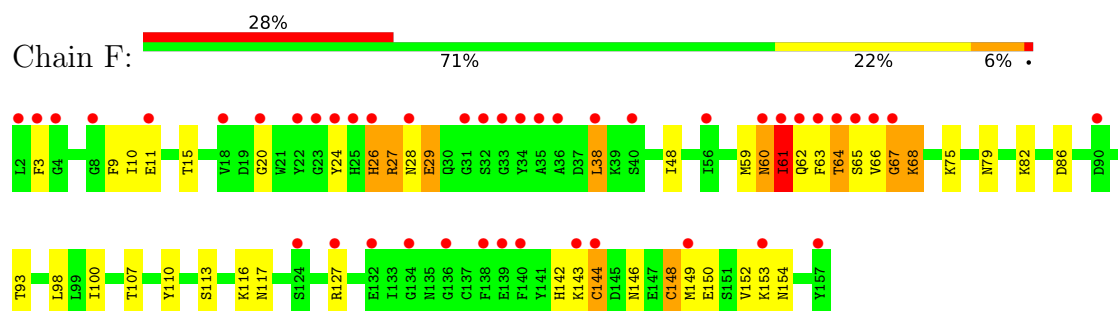
• Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.78Å 251.37Å 113.10Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	43.61 – 2.70 43.61 – 2.70	Depositor EDS
% Data completeness (in resolution range)	86.4 (43.61-2.70) 87.0 (43.61-2.70)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.234 , 0.253 0.244 , 0.262	Depositor DCC
R_{free} test set	4557 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	22926	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5136e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.54	0/2577	0.73	6/3506 (0.2%)
1	C	0.51	2/2577 (0.1%)	0.73	8/3506 (0.2%)
1	E	0.47	0/2577	0.67	4/3506 (0.1%)
1	G	0.58	1/2577 (0.0%)	0.68	6/3506 (0.2%)
1	I	0.46	1/2577 (0.0%)	0.67	3/3506 (0.1%)
1	K	0.45	0/2577	0.64	4/3506 (0.1%)
2	B	0.69	1/1274 (0.1%)	0.88	8/1713 (0.5%)
2	D	0.51	0/1274	0.83	4/1713 (0.2%)
2	F	0.51	0/1274	0.74	2/1713 (0.1%)
2	H	0.63	0/1274	0.86	3/1713 (0.2%)
2	J	0.59	0/1274	0.79	5/1713 (0.3%)
2	L	0.56	0/1274	0.82	3/1713 (0.2%)
All	All	0.53	5/23106 (0.0%)	0.73	56/31314 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	69	GLU	C-O	-5.70	1.16	1.24
1	C	259	LYS	CA-C	-5.67	1.47	1.53
1	I	284	GLY	C-O	-5.50	1.17	1.24
1	C	266	MET	C-O	-5.42	1.17	1.23
1	G	133	THR	C-O	-5.07	1.17	1.23

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	122	VAL	N-CA-C	-9.92	100.19	111.00
2	D	147	GLU	N-CA-C	-9.13	102.65	113.88
1	A	142	ASN	N-CA-C	9.03	121.97	110.24
1	C	86	LYS	N-CA-C	8.84	120.68	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	41	THR	N-CA-C	-8.81	102.66	113.50
1	C	262	SER	N-CA-C	7.99	120.66	109.15
1	C	87	ASN	N-CA-C	7.88	120.50	109.15
1	K	124	PRO	CA-C-N	-7.73	109.83	122.65
1	K	124	PRO	C-N-CA	-7.73	109.83	122.65
1	E	194	ASN	N-CA-C	7.39	120.55	110.35
1	C	129	THR	N-CA-C	7.36	122.55	113.50
2	F	29	GLU	N-CA-C	-7.26	103.43	112.72
1	C	2	THR	N-CA-C	7.19	119.00	108.86
1	G	277	THR	N-CA-C	7.07	117.36	108.45
2	H	129	ASN	N-CA-C	-6.92	104.44	113.17
2	H	147	GLU	N-CA-C	-6.72	105.21	113.41
2	F	26	HIS	N-CA-C	6.72	120.46	109.85
2	L	148	CYS	N-CA-C	-6.71	105.23	113.41
2	B	151	SER	N-CA-C	-6.63	103.31	111.40
2	B	31	GLY	N-CA-C	6.40	119.83	110.80
1	E	153	LYS	N-CA-C	6.32	118.82	108.52
1	I	193	GLN	N-CA-C	6.29	118.14	111.28
2	D	131	LYS	CA-C-N	-6.12	114.03	122.30
2	D	131	LYS	C-N-CA	-6.12	114.03	122.30
1	G	111	PHE	CB-CA-C	-6.01	100.94	112.43
2	B	63	PHE	N-CA-C	5.98	121.87	113.56
1	G	10	ASN	N-CA-C	5.97	115.89	108.19
1	K	275	CYS	N-CA-C	5.89	118.15	110.43
2	H	24	TYR	N-CA-C	5.78	117.39	109.18
1	C	194	ASN	N-CA-C	5.77	117.97	110.53
2	J	128	ASN	N-CA-C	5.73	119.45	112.23
2	B	62	GLN	N-CA-C	5.66	118.01	107.99
2	B	149	MET	N-CA-C	-5.66	105.02	111.07
1	A	222	GLU	N-CA-CB	-5.58	105.44	113.65
2	B	33	GLY	N-CA-C	5.58	119.46	110.87
2	J	133	ILE	N-CA-C	5.56	115.76	110.53
2	D	129	ASN	N-CA-C	5.54	122.61	110.80
1	G	278	LYS	N-CA-C	-5.51	107.81	114.75
2	L	149	MET	N-CA-C	-5.51	105.28	111.28
1	C	275	CYS	N-CA-C	5.51	117.64	110.43
1	I	222	GLU	CA-CB-CG	-5.45	103.21	114.10
2	J	147	GLU	CB-CA-C	-5.41	102.39	110.88
1	K	84	ASN	CB-CG-ND2	-5.34	108.39	116.40
1	A	122	SER	N-CA-C	5.32	119.84	112.45
2	J	123	LYS	N-CA-C	-5.30	105.39	111.07
1	A	10	ASN	N-CA-C	5.23	114.93	108.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ASN	CB-CG-ND2	-5.21	108.58	116.40
1	I	257	LEU	N-CA-C	5.19	118.47	110.42
1	G	129	THR	CB-CA-C	5.17	117.76	109.07
1	C	92	PRO	N-CA-C	5.13	119.25	111.19
1	E	271	GLN	N-CA-CB	5.13	117.56	110.17
1	A	190	THR	N-CA-C	5.13	116.95	111.36
1	E	275	CYS	N-CA-C	5.12	117.14	110.43
2	B	61	ILE	N-CA-C	-5.08	98.77	109.34
1	G	187	ASP	N-CA-C	-5.06	105.46	111.69
2	J	133	ILE	CB-CA-C	-5.01	105.45	112.02

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	2515	0	2454	73	0
1	C	2515	0	2452	65	0
1	E	2515	0	2452	74	0
1	G	2515	0	2452	69	0
1	I	2515	0	2452	54	0
1	K	2515	0	2452	70	0
2	B	1250	0	1188	68	0
2	D	1250	0	1190	64	0
2	F	1250	0	1188	64	0
2	H	1250	0	1190	81	0
2	J	1250	0	1188	77	0
2	L	1250	0	1190	77	0
3	A	56	0	52	4	0
3	C	56	0	52	0	0
3	E	56	0	52	0	0
3	G	56	0	52	0	0
3	I	56	0	52	1	0
3	K	56	0	52	1	0
All	All	22926	0	22160	709	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 16.

All (709) 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:C:279:CYS:SG	1:C:286:LEU:HB2	1.63	1.38
2:F:9:PHE:CE1	2:F:10:ILE:CD1	2.14	1.29
2:F:9:PHE:CE1	2:F:10:ILE:HD11	1.68	1.28
2:F:9:PHE:CD1	2:F:10:ILE:HD12	1.70	1.27
1:E:305:LYS:CE	2:F:61:ILE:HD11	1.64	1.25
1:K:2:THR:HG22	2:L:139:GLU:HA	1.25	1.14
1:I:5:ILE:CD1	2:J:119:TYR:HA	1.77	1.14
1:I:5:ILE:HD13	2:J:119:TYR:HA	1.20	1.13
1:E:305:LYS:HE2	2:F:61:ILE:HD11	1.23	1.07
2:D:29:GLU:C	2:D:30:GLN:OE1	1.99	1.05
2:F:9:PHE:CD1	2:F:10:ILE:CD1	2.37	1.05
2:B:144:CYS:SG	2:B:149:MET:CE	2.45	1.04
2:L:132:GLU:HG3	2:L:138:PHE:CE1	1.94	1.03
1:K:2:THR:HG22	2:L:139:GLU:CA	1.89	1.01
1:E:305:LYS:HE3	2:F:61:ILE:HD11	1.40	1.00
1:G:130:ARG:HB2	1:G:152:VAL:HG21	1.42	1.00
1:C:279:CYS:SG	1:C:286:LEU:CB	2.49	0.99
2:B:122:VAL:HG23	2:B:138:PHE:CE2	1.97	0.99
1:E:305:LYS:HE3	2:F:61:ILE:CD1	1.93	0.98
1:E:305:LYS:HE3	2:F:61:ILE:CG1	1.93	0.97
1:A:2:THR:HB	2:B:139:GLU:OE1	1.66	0.96
1:A:5:ILE:HD11	2:B:122:VAL:HG11	1.46	0.96
2:B:122:VAL:CG2	2:B:138:PHE:HE2	1.78	0.95
1:E:2:THR:HG22	2:F:27:ARG:HB2	1.46	0.95
2:H:142:HIS:CE1	2:H:143:LYS:HE3	2.02	0.95
1:E:5:ILE:CD1	2:F:24:TYR:CD2	2.51	0.94
1:E:305:LYS:CE	2:F:61:ILE:CD1	2.47	0.93
2:F:9:PHE:HE1	2:F:10:ILE:HD11	1.25	0.92
2:B:144:CYS:SG	2:B:149:MET:HE2	2.10	0.91
1:K:54:ASN:HA	1:K:84:ASN:O	1.72	0.90
2:H:149:MET:CG	2:H:150:GLU:N	2.35	0.90
1:G:130:ARG:HB2	1:G:152:VAL:CG2	2.02	0.90
1:I:5:ILE:HD13	2:J:119:TYR:CA	2.02	0.90
1:A:2:THR:CB	2:B:139:GLU:OE1	2.20	0.90
1:K:5:ILE:CD1	2:L:24:TYR:CD2	2.55	0.89
2:H:26:HIS:ND1	2:H:26:HIS:O	2.07	0.88
2:B:122:VAL:CG2	2:B:138:PHE:CE2	2.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:HD13	2:D:119:TYR:HA	1.56	0.88
1:C:303:CYS:O	2:D:61:ILE:HG12	1.75	0.87
1:E:153:LYS:HE2	1:E:190:THR:O	1.74	0.87
2:L:27:ARG:HG2	2:L:27:ARG:HH11	1.38	0.87
2:J:122:VAL:HG12	2:J:138:PHE:HE2	1.37	0.86
1:K:2:THR:HG22	2:L:139:GLU:CB	2.05	0.86
2:J:131:LYS:CD	2:J:139:GLU:HB3	2.04	0.86
2:D:30:GLN:OE1	2:D:30:GLN:N	2.08	0.85
1:K:5:ILE:HD13	2:L:24:TYR:CD2	2.12	0.85
2:H:149:MET:HG3	2:H:150:GLU:N	1.91	0.85
2:L:17:MET:O	2:L:18:VAL:HG12	1.77	0.84
1:A:153:LYS:HE2	1:A:155:GLY:O	1.77	0.84
2:H:144:CYS:SG	2:H:148:CYS:HB3	2.17	0.84
2:H:143:LYS:H	2:H:143:LYS:HD2	1.43	0.83
2:D:62:GLN:HG2	2:D:64:THR:HG23	1.60	0.83
2:L:26:HIS:CB	2:L:149:MET:HE3	2.07	0.83
2:D:126:LEU:O	2:D:127:ARG:O	1.97	0.83
1:I:303:CYS:O	2:J:61:ILE:HG12	1.79	0.82
2:L:132:GLU:CG	2:L:138:PHE:CE1	2.63	0.82
2:J:122:VAL:HG12	2:J:138:PHE:CE2	2.14	0.81
1:A:279:CYS:HG	1:A:303:CYS:HG	0.83	0.81
1:G:2:THR:HG22	2:H:139:GLU:HG3	1.61	0.81
1:A:2:THR:HB	2:B:139:GLU:CD	2.05	0.81
1:E:153:LYS:HG3	1:E:191:LEU:O	1.81	0.81
1:E:3:ILE:HB	2:F:149:MET:HE3	1.63	0.81
2:B:139:GLU:OE1	2:B:139:GLU:HA	1.80	0.81
1:E:2:THR:HG22	2:F:27:ARG:CB	2.10	0.80
1:K:153:LYS:HD2	1:K:156:ASN:HA	1.62	0.80
2:H:149:MET:HG2	2:H:150:GLU:HG2	1.64	0.80
1:G:19:ILE:HG23	1:G:20:LEU:HD22	1.64	0.79
2:B:122:VAL:HG21	2:B:138:PHE:HE2	1.46	0.79
2:J:117:ASN:O	2:J:121:LYS:HB2	1.83	0.79
2:D:28:ASN:HB3	2:D:30:GLN:H	1.48	0.78
1:E:221:ARG:O	1:E:222:GLU:HB2	1.80	0.77
1:G:34:GLU:HG3	1:G:290:LEU:HD12	1.67	0.77
1:A:41:LEU:HD13	1:A:80:ILE:HD13	1.67	0.77
1:C:172:GLU:OE2	1:C:259:LYS:HE3	1.85	0.77
2:B:130:ALA:HB1	2:B:139:GLU:O	1.85	0.76
2:H:28:ASN:HD21	2:H:145:ASP:HA	1.50	0.76
1:E:5:ILE:CD1	2:F:24:TYR:HD2	1.95	0.76
2:H:122:VAL:HG23	2:H:152:VAL:HG12	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:143:LYS:HD2	2:H:143:LYS:N	2.01	0.76
2:L:26:HIS:HB2	2:L:149:MET:HE3	1.69	0.75
1:C:127:ASP:OD1	1:C:154:LYS:HD3	1.85	0.75
2:B:127:ARG:NH1	2:B:127:ARG:HB3	2.02	0.75
1:C:188:GLN:HG3	1:C:214:ILE:HD11	1.67	0.75
1:A:94:GLU:OE1	1:A:228:ASN:ND2	2.20	0.75
1:G:135:SER:O	1:G:221:ARG:NH1	2.20	0.75
1:G:130:ARG:CB	1:G:152:VAL:HG21	2.14	0.74
2:H:142:HIS:ND1	2:H:143:LYS:HE3	2.02	0.74
1:E:303:CYS:O	2:F:61:ILE:HG21	1.86	0.74
1:I:172:GLU:OE2	1:I:259:LYS:HE3	1.87	0.74
2:B:119:TYR:O	2:B:122:VAL:HG22	1.87	0.74
1:E:2:THR:CG2	2:F:27:ARG:HB2	2.18	0.74
1:K:5:ILE:HD13	2:L:24:TYR:HD2	1.52	0.74
2:F:60:ASN:O	2:F:61:ILE:HG12	1.88	0.74
2:J:131:LYS:HD2	2:J:139:GLU:HB3	1.69	0.73
2:B:144:CYS:SG	2:B:149:MET:HE1	2.28	0.73
2:D:125:GLN:HE21	2:D:152:VAL:HG12	1.53	0.73
1:A:76:TRP:HH2	1:A:111:PHE:CE1	2.07	0.73
1:C:5:ILE:HD13	2:D:119:TYR:CA	2.20	0.72
2:J:133:ILE:N	2:J:133:ILE:HD12	2.05	0.71
2:H:142:HIS:CE1	2:H:143:LYS:CE	2.72	0.71
2:J:148:CYS:O	2:J:151:SER:HB3	1.89	0.71
2:H:144:CYS:SG	2:H:148:CYS:CB	2.78	0.71
2:H:142:HIS:ND1	2:H:143:LYS:HD2	2.05	0.71
2:L:26:HIS:HB3	2:L:149:MET:HE3	1.71	0.71
2:D:38:LEU:N	2:D:38:LEU:HD12	2.05	0.71
1:I:5:ILE:HD12	2:J:119:TYR:HD1	1.54	0.71
1:E:305:LYS:HE3	2:F:61:ILE:HG12	1.72	0.71
2:F:150:GLU:O	2:F:154:ASN:HB2	1.90	0.71
1:C:194:ASN:OD1	1:C:194:ASN:N	2.24	0.71
1:E:221:ARG:O	1:E:222:GLU:CB	2.36	0.71
2:L:127:ARG:O	2:L:129:ASN:N	2.20	0.70
1:C:293:GLN:CG	1:C:304:PRO:HB2	2.21	0.70
1:K:122:SER:HB3	1:K:163:LYS:HE3	1.74	0.70
2:H:149:MET:CG	2:H:150:GLU:HG2	2.21	0.70
1:K:194:ASN:N	1:K:194:ASN:OD1	2.25	0.70
1:E:5:ILE:HD13	2:F:24:TYR:CD2	2.25	0.69
2:H:142:HIS:CE1	2:H:143:LYS:CD	2.74	0.69
1:K:8:HIS:HE1	1:K:10:ASN:ND2	1.90	0.69
1:A:194:ASN:OD1	1:A:194:ASN:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:2:THR:CG2	2:L:139:GLU:HA	2.14	0.69
1:G:5:ILE:O	2:H:10:ILE:HD13	1.92	0.69
2:L:17:MET:O	2:L:18:VAL:CG1	2.41	0.69
2:B:148:CYS:O	2:B:151:SER:HB3	1.93	0.69
1:G:261:SER:HB3	2:H:63:PHE:HZ	1.57	0.69
1:C:4:CYS:O	2:D:14:TRP:HH2	1.76	0.69
1:A:187:ASP:O	1:A:191:LEU:HD23	1.92	0.69
2:J:131:LYS:CD	2:J:139:GLU:CB	2.70	0.69
1:K:5:ILE:CD1	2:L:24:TYR:CE2	2.77	0.68
2:H:149:MET:CG	2:H:150:GLU:H	2.06	0.68
2:L:17:MET:C	2:L:18:VAL:HG12	2.18	0.68
2:F:142:HIS:HE1	2:F:144:CYS:SG	2.16	0.68
1:G:126:HIS:HA	1:G:154:LYS:HB2	1.74	0.67
2:L:65:SER:C	2:L:66:VAL:HG22	2.19	0.67
2:D:24:TYR:CE1	2:D:153:LYS:HD2	2.29	0.67
2:J:113:SER:O	2:J:117:ASN:ND2	2.27	0.67
2:L:27:ARG:HG2	2:L:27:ARG:NH1	2.04	0.67
1:C:5:ILE:CD1	2:D:119:TYR:N	2.57	0.67
2:H:112:ASP:O	2:H:113:SER:C	2.37	0.67
1:C:127:ASP:OD1	1:C:154:LYS:CD	2.42	0.67
2:H:122:VAL:HG23	2:H:152:VAL:CG1	2.25	0.67
2:D:145:ASP:CG	2:D:146:ASN:H	2.02	0.67
2:L:27:ARG:HG3	2:L:27:ARG:O	1.92	0.67
1:E:86:LYS:HE3	1:E:86:LYS:HA	1.76	0.67
2:F:82:LYS:NZ	2:F:86:ASP:OD2	2.27	0.67
2:J:131:LYS:HD3	2:J:139:GLU:CB	2.25	0.67
1:A:21:GLU:OE2	1:A:319:ARG:NH2	2.28	0.67
2:D:38:LEU:HD12	2:D:38:LEU:H	1.59	0.67
1:G:308:LYS:HE3	2:H:89:LEU:HD21	1.76	0.66
1:K:308:LYS:HD2	2:L:89:LEU:HD21	1.77	0.66
2:J:131:LYS:HD3	2:J:139:GLU:HB3	1.78	0.66
2:B:149:MET:HE2	2:B:149:MET:HA	1.77	0.66
1:E:271:GLN:HA	1:E:271:GLN:OE1	1.96	0.66
1:G:2:THR:CG2	2:H:139:GLU:HG3	2.26	0.66
2:H:24:TYR:CD2	2:H:153:LYS:HE2	2.30	0.66
2:J:123:LYS:HG2	2:J:124:SER:N	2.11	0.65
2:J:123:LYS:HB2	2:J:138:PHE:CZ	2.31	0.65
1:I:108:VAL:HG21	1:I:257:LEU:HD22	1.77	0.65
1:E:303:CYS:O	2:F:61:ILE:CG2	2.44	0.65
2:D:19:ASP:HB3	2:D:36:ALA:HB3	1.79	0.65
1:K:266:MET:HG3	1:K:282:PRO:HG3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:116:LYS:HD2	2:J:120:GLU:HG3	1.79	0.65
2:H:27:ARG:HG3	2:H:32:SER:OG	1.96	0.65
2:H:35:ALA:HB3	2:H:153:LYS:NZ	2.12	0.65
1:A:47:LYS:HB3	1:A:77:SER:HB3	1.79	0.65
1:C:5:ILE:HD11	2:D:119:TYR:HB2	1.77	0.65
1:G:184:THR:HG22	1:G:185:ASP:N	2.12	0.64
1:I:112:GLU:HB3	1:I:256:ALA:HB3	1.80	0.64
1:I:131:GLY:HA3	1:I:150:TRP:HB3	1.79	0.64
1:C:5:ILE:CD1	2:D:119:TYR:CA	2.74	0.64
2:H:52:VAL:O	2:H:56:ILE:HD12	1.97	0.64
2:H:149:MET:HG2	2:H:150:GLU:H	1.63	0.64
2:L:132:GLU:CG	2:L:138:PHE:HE1	2.09	0.64
1:K:5:ILE:CD1	2:L:24:TYR:HD2	2.03	0.64
1:G:204:THR:HG22	1:G:205:LYS:HD2	1.79	0.64
1:I:262:SER:HA	2:J:63:PHE:HZ	1.63	0.64
2:L:28:ASN:HD21	2:L:145:ASP:HA	1.63	0.64
1:A:292:PHE:CZ	2:B:59:MET:HE3	2.33	0.63
2:H:151:SER:OG	2:H:157:TYR:C	2.41	0.63
1:A:279:CYS:HG	1:A:303:CYS:CB	2.10	0.63
2:J:133:ILE:HD12	2:J:133:ILE:H	1.61	0.63
2:B:122:VAL:HG23	2:B:123:LYS:N	2.13	0.63
1:I:107:THR:HG23	1:I:259:LYS:HD2	1.78	0.63
1:C:3:ILE:HD13	2:D:26:HIS:HB3	1.81	0.63
1:I:8:HIS:CE1	2:J:18:VAL:HA	2.33	0.63
1:G:11:ASN:OD1	1:G:11:ASN:N	2.32	0.63
2:D:29:GLU:HB3	2:D:30:GLN:OE1	1.99	0.63
1:E:113:ARG:NH1	1:E:147:ASN:OD1	2.31	0.63
2:L:126:LEU:N	2:L:126:LEU:HD23	2.14	0.63
1:K:238:ASP:OD1	1:K:239:THR:N	2.32	0.62
1:E:5:ILE:HD11	2:F:24:TYR:CD2	2.35	0.62
1:I:27:THR:C	1:I:28:HIS:HD1	2.07	0.62
1:I:262:SER:HA	2:J:63:PHE:CZ	2.34	0.62
2:J:129:ASN:N	2:J:129:ASN:OD1	2.28	0.62
1:C:221:ARG:CG	1:C:221:ARG:HH11	2.13	0.62
1:C:299:THR:O	2:D:65:SER:HB3	2.00	0.62
2:F:148:CYS:O	2:F:152:VAL:HG23	1.99	0.62
2:L:30:GLN:OE1	2:L:146:ASN:N	2.25	0.62
2:J:131:LYS:HD2	2:J:139:GLU:CB	2.29	0.61
1:A:5:ILE:HD11	2:B:122:VAL:CG1	2.26	0.61
1:E:5:ILE:HD13	2:F:24:TYR:HD2	1.61	0.61
2:F:64:THR:O	2:F:64:THR:HG22	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:LYS:O	2:B:121:LYS:HG2	2.01	0.61
2:F:26:HIS:HB2	2:F:149:MET:HE2	1.81	0.61
1:A:133:THR:O	1:A:142:ASN:HB3	2.01	0.61
1:I:261:SER:O	1:I:263:SER:N	2.34	0.61
2:H:123:LYS:HA	2:H:138:PHE:HE2	1.65	0.61
2:J:123:LYS:CB	2:J:138:PHE:HZ	2.13	0.60
1:G:153:LYS:HG3	1:G:153:LYS:O	1.99	0.60
2:B:23:GLY:HA3	2:B:36:ALA:HA	1.83	0.60
1:A:227:MET:HE3	1:A:249:ILE:HG13	1.83	0.60
1:A:292:PHE:HZ	2:B:59:MET:HE3	1.65	0.60
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.36	0.60
2:D:150:GLU:HA	2:D:153:LYS:HE2	1.84	0.60
2:J:62:GLN:C	2:J:64:THR:H	2.09	0.60
2:F:38:LEU:N	2:F:38:LEU:HD12	2.15	0.60
1:A:22:LYS:HB3	3:A:402:NAG:H81	1.83	0.60
2:B:39:LYS:O	2:B:43:ILE:HG13	2.01	0.60
2:B:149:MET:CE	2:B:149:MET:HA	2.30	0.60
2:L:132:GLU:HG3	2:L:138:PHE:CD1	2.36	0.60
2:H:142:HIS:ND1	2:H:143:LYS:CE	2.64	0.60
1:C:293:GLN:HG3	1:C:304:PRO:HB2	1.84	0.60
2:F:75:LYS:O	2:F:79:ASN:ND2	2.34	0.60
2:H:142:HIS:ND1	2:H:143:LYS:CD	2.64	0.60
2:J:17:MET:HE1	2:J:23:GLY:N	2.16	0.60
1:A:2:THR:HB	2:B:139:GLU:OE2	2.02	0.60
2:F:38:LEU:HD12	2:F:38:LEU:H	1.65	0.60
2:B:61:ILE:HG23	2:B:61:ILE:O	2.01	0.60
1:K:48:ILE:HD12	1:K:48:ILE:H	1.67	0.59
1:E:77:SER:O	1:E:263:SER:HA	2.02	0.59
1:K:61:ILE:O	1:K:147:ASN:ND2	2.35	0.59
1:G:92:PRO:HB3	1:G:220:VAL:HG22	1.84	0.59
1:I:292:PHE:HZ	2:J:59:MET:HE3	1.68	0.59
1:A:22:LYS:HD3	3:A:402:NAG:H81	1.83	0.59
1:E:82:THR:HG22	1:E:269:ASP:HA	1.84	0.59
2:H:30:GLN:OE1	2:H:145:ASP:HB2	2.03	0.59
2:J:131:LYS:HB3	2:J:139:GLU:HB3	1.85	0.59
1:A:2:THR:CA	2:B:139:GLU:OE1	2.50	0.59
1:E:5:ILE:CD1	2:F:24:TYR:CE2	2.86	0.59
2:J:61:ILE:HG23	2:J:61:ILE:O	2.03	0.59
1:A:221:ARG:O	1:A:222:GLU:HB2	2.03	0.58
1:I:321:VAL:O	1:I:321:VAL:HG22	2.04	0.58
2:L:18:VAL:HG22	2:L:18:VAL:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:139:SER:O	1:K:139:SER:OG	2.17	0.58
2:D:26:HIS:CD2	2:D:149:MET:HG2	2.39	0.58
1:K:154:LYS:O	1:K:154:LYS:HG2	2.01	0.58
2:L:18:VAL:O	2:L:18:VAL:HG13	2.03	0.58
2:D:129:ASN:OD1	2:D:129:ASN:N	2.33	0.58
2:J:143:LYS:O	2:J:143:LYS:HG3	2.03	0.58
2:L:62:GLN:HB3	2:L:64:THR:HG23	1.84	0.58
1:G:130:ARG:HG2	1:G:130:ARG:HH11	1.68	0.58
2:L:125:GLN:C	2:L:126:LEU:HD23	2.29	0.58
2:H:28:ASN:ND2	2:H:30:GLN:HG3	2.19	0.58
2:H:149:MET:O	2:H:151:SER:N	2.36	0.58
1:G:130:ARG:HG2	1:G:130:ARG:NH1	2.17	0.58
1:K:153:LYS:HD2	1:K:156:ASN:CA	2.34	0.57
2:B:123:LYS:HB2	2:B:138:PHE:HZ	1.69	0.57
1:I:321:VAL:O	1:I:321:VAL:HG13	2.03	0.57
2:J:123:LYS:HB2	2:J:138:PHE:HZ	1.67	0.57
1:E:292:PHE:CZ	2:F:59:MET:HE3	2.38	0.57
2:L:26:HIS:HB2	2:L:149:MET:CE	2.34	0.57
1:A:144:PHE:HZ	1:A:227:MET:HE1	1.69	0.57
1:A:5:ILE:CD1	2:B:122:VAL:HG11	2.29	0.57
1:A:34:GLU:OE2	1:A:287:LYS:HB2	2.05	0.57
1:A:92:PRO:HB3	1:A:220:VAL:HG22	1.87	0.57
1:G:43:SER:O	1:G:277:THR:HG22	2.05	0.57
1:I:5:ILE:HD12	2:J:119:TYR:CD1	2.36	0.57
1:E:305:LYS:HE2	2:F:61:ILE:CD1	2.16	0.56
1:K:53:GLY:O	1:K:82:THR:OG1	2.23	0.56
1:C:188:GLN:HE21	1:C:247:ASN:HD21	1.52	0.56
1:G:172:GLU:OE2	1:G:259:LYS:HE2	2.06	0.56
1:A:102:LYS:O	1:A:106:SER:OG	2.20	0.56
2:J:62:GLN:O	2:J:64:THR:N	2.39	0.56
2:B:127:ARG:HB3	2:B:127:ARG:HH11	1.69	0.56
1:C:221:ARG:HH11	1:C:221:ARG:HG3	1.71	0.56
1:E:220:VAL:O	1:E:221:ARG:HB2	2.05	0.56
1:G:93:GLY:HA3	1:G:227:MET:O	2.06	0.56
2:B:122:VAL:HG21	2:B:138:PHE:CE2	2.32	0.56
1:K:54:ASN:OD1	1:K:54:ASN:N	2.38	0.56
2:L:26:HIS:ND1	2:L:149:MET:HG3	2.21	0.56
1:G:261:SER:CB	2:H:63:PHE:HZ	2.19	0.55
1:K:119:LYS:HG3	1:K:120:ALA:N	2.21	0.55
1:K:57:VAL:HG21	1:K:102:LYS:HG2	1.86	0.55
1:K:320:ASN:O	1:K:321:VAL:C	2.50	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:112:ASP:O	2:H:114:ASN:N	2.39	0.55
1:I:262:SER:O	1:I:262:SER:OG	2.23	0.55
1:A:76:TRP:HH2	1:A:111:PHE:CD1	2.24	0.55
1:G:185:ASP:O	1:G:188:GLN:HB3	2.07	0.55
1:C:209:ARG:HD3	1:E:213:GLU:OE1	2.06	0.55
2:D:61:ILE:O	2:D:61:ILE:HG23	2.07	0.55
1:K:148:LEU:HD21	1:K:176:ILE:HD12	1.89	0.55
2:D:140:PHE:CE1	2:D:144:CYS:SG	3.00	0.55
2:J:70:PHE:CE1	2:J:77:MET:HG2	2.42	0.55
2:L:127:ARG:O	2:L:129:ASN:OD1	2.25	0.55
2:D:38:LEU:H	2:D:38:LEU:CD1	2.19	0.55
2:J:62:GLN:HB2	2:J:64:THR:HG22	1.90	0.54
2:F:60:ASN:C	2:F:60:ASN:HD22	2.13	0.54
2:J:123:LYS:CB	2:J:138:PHE:CZ	2.90	0.54
2:J:142:HIS:O	2:J:142:HIS:ND1	2.41	0.54
1:K:2:THR:CG2	2:L:139:GLU:CB	2.84	0.54
2:H:125:GLN:OE1	2:H:155:GLY:HA2	2.06	0.54
2:D:145:ASP:CG	2:D:146:ASN:N	2.63	0.54
1:G:1:ASP:HB3	2:H:140:PHE:HB2	1.89	0.54
1:G:318:LEU:HD12	1:G:319:ARG:O	2.08	0.54
1:A:218:PRO:O	1:A:226:ARG:NH2	2.32	0.54
2:B:25:HIS:HB2	2:B:34:TYR:CD1	2.42	0.54
1:G:134:VAL:O	1:G:137:SER:OG	2.26	0.54
2:H:111:HIS:O	2:H:112:ASP:O	2.26	0.54
1:K:132:THR:OG1	1:K:142:ASN:HB3	2.08	0.54
1:A:2:THR:HA	2:B:139:GLU:OE1	2.08	0.54
2:L:28:ASN:HD21	2:L:145:ASP:C	2.15	0.54
2:J:17:MET:O	2:J:17:MET:HG2	2.06	0.53
1:A:174:LEU:HB2	1:A:257:LEU:HD11	1.90	0.53
1:C:299:THR:O	2:D:65:SER:CB	2.56	0.53
2:J:133:ILE:H	2:J:133:ILE:CD1	2.21	0.53
1:K:113:ARG:NH1	1:K:147:ASN:OD1	2.41	0.53
1:A:303:CYS:O	2:B:61:ILE:HG21	2.08	0.53
2:H:148:CYS:O	2:H:149:MET:C	2.52	0.53
2:L:30:GLN:O	2:L:30:GLN:HG3	2.09	0.53
2:D:126:LEU:O	2:D:127:ARG:C	2.51	0.53
1:E:41:LEU:HD21	1:E:268:SER:OG	2.09	0.53
1:I:7:TYR:CZ	2:J:6:ILE:HG23	2.44	0.53
2:L:16:GLY:O	2:L:34:TYR:CD2	2.62	0.53
2:D:131:LYS:HD3	2:D:139:GLU:HB3	1.91	0.53
1:A:4:CYS:HA	2:B:137:CYS:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:MET:HE2	2:B:149:MET:CA	2.37	0.53
2:H:146:ASN:HA	2:H:149:MET:HB3	1.90	0.53
2:H:148:CYS:O	2:H:149:MET:O	2.26	0.53
2:H:150:GLU:HA	2:H:153:LYS:HG3	1.89	0.53
1:I:301:GLY:H	2:J:63:PHE:HE1	1.56	0.53
1:A:94:GLU:OE1	1:A:94:GLU:N	2.40	0.53
2:F:107:THR:O	2:F:110:TYR:HB3	2.08	0.53
2:B:123:LYS:HB2	2:B:138:PHE:CZ	2.44	0.52
1:C:131:GLY:HA3	1:C:150:TRP:HB3	1.91	0.52
2:D:24:TYR:CD1	2:D:153:LYS:HD2	2.45	0.52
1:E:71:LEU:HD21	1:E:146:ARG:HD2	1.90	0.52
1:G:34:GLU:CD	1:G:287:LYS:HB2	2.35	0.52
1:A:279:CYS:SG	1:A:286:LEU:HD12	2.50	0.52
1:G:184:THR:HG22	1:G:185:ASP:H	1.74	0.52
1:C:107:THR:HG23	1:C:259:LYS:HD3	1.91	0.52
1:K:312:LEU:HD22	2:L:100:ILE:HG13	1.91	0.52
1:C:296:HIS:CE1	1:C:298:VAL:HG13	2.44	0.52
1:G:174:LEU:HB2	1:G:257:LEU:HD11	1.92	0.52
1:I:132:THR:HG23	1:I:142:ASN:HB3	1.92	0.52
1:E:41:LEU:HB2	1:E:271:GLN:O	2.10	0.52
2:F:38:LEU:H	2:F:38:LEU:CD1	2.21	0.52
1:G:1:ASP:O	2:H:140:PHE:HB2	2.09	0.51
1:I:260:GLY:O	1:I:262:SER:N	2.43	0.51
2:F:143:LYS:HD3	2:F:144:CYS:N	2.24	0.51
2:L:65:SER:C	2:L:66:VAL:CG2	2.84	0.51
2:L:127:ARG:C	2:L:129:ASN:H	2.17	0.51
1:A:123:TRP:CE2	1:A:151:ILE:HD11	2.46	0.51
1:C:263:SER:OG	1:C:264:GLY:N	2.36	0.51
1:E:5:ILE:HD11	2:F:24:TYR:HD2	1.73	0.51
1:E:32:LEU:HD12	2:F:100:ILE:HD11	1.92	0.51
1:C:4:CYS:HA	2:D:137:CYS:HA	1.92	0.51
1:G:181:HIS:CE1	1:G:212:PRO:HA	2.46	0.51
2:H:133:ILE:HB	2:H:137:CYS:O	2.11	0.51
1:A:180:HIS:ND1	1:A:192:TYR:OH	2.35	0.51
2:B:28:ASN:ND2	2:B:146:ASN:OD1	2.43	0.51
1:C:5:ILE:HD12	2:D:118:LEU:HB3	1.93	0.51
1:I:281:THR:HG22	1:I:284:GLY:H	1.76	0.51
1:K:2:THR:CG2	2:L:139:GLU:HG3	2.41	0.51
2:L:26:HIS:O	2:L:32:SER:HA	2.11	0.51
1:G:112:GLU:HB3	1:G:256:ALA:HB3	1.92	0.51
2:H:123:LYS:HA	2:H:138:PHE:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:GLN:HE21	1:A:285:ALA:HB2	1.76	0.51
2:F:75:LYS:HG3	2:F:79:ASN:HD21	1.76	0.51
1:G:20:LEU:HD23	2:H:105:GLU:CD	2.36	0.50
1:I:148:LEU:HD21	1:I:176:ILE:HG13	1.93	0.50
1:A:93:GLY:HA3	1:A:227:MET:O	2.11	0.50
2:J:47:GLY:HA2	1:K:20:LEU:O	2.12	0.50
2:J:148:CYS:O	2:J:151:SER:N	2.44	0.50
1:C:221:ARG:CG	1:C:221:ARG:NH1	2.73	0.50
1:E:107:THR:HG23	1:E:259:LYS:HG3	1.91	0.50
1:C:98:TYR:CZ	1:C:102:LYS:HD2	2.46	0.50
1:E:282:PRO:HG2	1:E:296:HIS:CD2	2.45	0.50
1:K:138:HIS:CD2	1:K:138:HIS:C	2.85	0.50
2:H:145:ASP:OD1	2:H:145:ASP:N	2.37	0.50
2:L:28:ASN:HD21	2:L:145:ASP:CA	2.23	0.50
2:B:50:ASN:OD1	1:C:22:LYS:HE3	2.11	0.50
2:B:122:VAL:CG2	2:B:123:LYS:N	2.74	0.50
2:H:52:VAL:HG13	2:H:56:ILE:HD11	1.93	0.50
1:A:76:TRP:CH2	1:A:111:PHE:CD1	2.99	0.50
1:A:68:ASP:HA	1:A:71:LEU:HD22	1.94	0.50
1:G:3:ILE:HD12	2:H:152:VAL:HG21	1.94	0.50
2:J:18:VAL:HG23	2:J:18:VAL:O	2.12	0.50
1:A:185:ASP:OD1	1:A:185:ASP:N	2.29	0.50
2:J:37:ASP:O	2:J:38:LEU:C	2.54	0.50
1:K:299:THR:HB	1:K:303:CYS:SG	2.52	0.50
2:H:111:HIS:O	2:H:112:ASP:C	2.51	0.49
2:L:30:GLN:OE1	2:L:145:ASP:HB3	2.11	0.49
2:B:2:LEU:O	2:F:113:SER:OG	2.29	0.49
1:C:3:ILE:HG22	2:D:138:PHE:HB2	1.93	0.49
2:D:53:ASN:HA	2:D:56:ILE:HG12	1.95	0.49
1:C:123:TRP:CE2	1:C:151:ILE:HD11	2.47	0.49
2:D:38:LEU:O	2:D:41:THR:N	2.45	0.49
1:E:106:SER:O	1:E:263:SER:HB3	2.12	0.49
1:A:84:ASN:HA	1:A:86:LYS:HG2	1.94	0.49
1:I:266:MET:HG3	1:I:282:PRO:HG3	1.94	0.49
2:J:17:MET:HB2	2:J:34:TYR:CD1	2.47	0.49
1:C:303:CYS:SG	1:C:304:PRO:HD2	2.53	0.49
2:B:19:ASP:OD1	2:B:19:ASP:N	2.45	0.49
2:B:122:VAL:HG23	2:B:138:PHE:CZ	2.47	0.49
1:G:34:GLU:CG	1:G:290:LEU:HD12	2.42	0.49
1:C:30:VAL:HG23	1:C:316:THR:HG21	1.95	0.49
1:G:77:SER:O	1:G:263:SER:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1:ASP:HB3	2:L:140:PHE:HB2	1.95	0.49
1:C:172:GLU:OE2	1:C:259:LYS:CE	2.60	0.49
2:D:38:LEU:C	2:D:40:SER:N	2.70	0.49
2:F:149:MET:O	2:F:153:LYS:HG3	2.13	0.49
1:I:1:ASP:C	1:I:2:THR:CG2	2.86	0.49
2:J:127:ARG:CZ	2:J:127:ARG:CB	2.91	0.49
2:J:142:HIS:ND1	2:J:142:HIS:C	2.71	0.49
2:J:131:LYS:HD2	2:J:139:GLU:CG	2.42	0.49
1:K:2:THR:HG22	2:L:139:GLU:HB2	1.93	0.49
2:L:129:ASN:N	2:L:129:ASN:OD1	2.46	0.49
1:E:47:LYS:HB3	1:E:77:SER:OG	2.13	0.49
1:I:296:HIS:CE1	1:I:298:VAL:HG12	2.48	0.48
1:A:156:ASN:O	1:A:193:GLN:NE2	2.46	0.48
1:A:279:CYS:SG	1:A:303:CYS:HB3	2.53	0.48
1:G:280:GLN:HE21	1:G:281:THR:H	1.60	0.48
1:A:112:GLU:HB3	1:A:256:ALA:HB3	1.94	0.48
2:B:119:TYR:HE1	2:B:136:GLY:HA2	1.76	0.48
2:D:131:LYS:CD	2:D:139:GLU:HB3	2.43	0.48
2:L:25:HIS:HB2	2:L:34:TYR:CD1	2.48	0.48
1:C:293:GLN:HG2	1:C:304:PRO:HB2	1.93	0.48
2:H:35:ALA:HB3	2:H:153:LYS:HZ1	1.78	0.48
1:K:65:PRO:HB3	1:K:146:ARG:NH2	2.28	0.48
2:J:61:ILE:O	2:J:63:PHE:N	2.46	0.48
1:K:27:THR:HG23	1:K:318:LEU:O	2.14	0.48
1:A:144:PHE:CZ	1:A:227:MET:HE1	2.48	0.48
1:E:92:PRO:HB2	1:E:226:ARG:HD3	1.95	0.48
1:G:297:PRO:HG3	1:G:306:TYR:CE2	2.49	0.48
2:H:3:PHE:HD2	2:H:112:ASP:HB3	1.78	0.48
1:C:296:HIS:ND1	1:C:298:VAL:HG13	2.29	0.48
2:H:142:HIS:CG	2:H:143:LYS:HD2	2.48	0.48
1:C:156:ASN:ND2	1:C:193:GLN:OE1	2.46	0.48
1:G:33:LEU:HB2	1:G:312:LEU:HB2	1.95	0.48
2:L:27:ARG:HH11	2:L:27:ARG:CG	2.18	0.48
1:C:93:GLY:HA3	1:C:227:MET:O	2.14	0.48
2:D:30:GLN:N	2:D:30:GLN:CD	2.72	0.48
1:G:3:ILE:HB	2:H:140:PHE:HE1	1.78	0.47
1:I:93:GLY:HA3	1:I:227:MET:O	2.14	0.47
1:I:171:LYS:HD2	1:I:256:ALA:HB1	1.95	0.47
2:J:2:LEU:HB3	2:J:112:ASP:OD2	2.13	0.47
2:B:25:HIS:HD2	2:B:33:GLY:C	2.22	0.47
2:D:27:ARG:O	2:D:27:ARG:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:LYS:HA	1:E:86:LYS:CE	2.41	0.47
1:G:47:LYS:HB3	1:G:77:SER:HB3	1.96	0.47
2:H:103:GLU:O	2:H:107:THR:OG1	2.22	0.47
2:H:140:PHE:CE2	2:H:144:CYS:CB	2.98	0.47
2:H:140:PHE:CE2	2:H:144:CYS:SG	3.07	0.47
2:J:61:ILE:O	2:J:61:ILE:HG13	2.14	0.47
2:L:25:HIS:HB2	2:L:34:TYR:HD1	1.79	0.47
1:C:3:ILE:CG2	2:D:138:PHE:HB2	2.44	0.47
2:D:129:ASN:O	2:D:141:TYR:HB2	2.13	0.47
2:B:25:HIS:CD2	2:B:33:GLY:O	2.67	0.47
2:H:140:PHE:CD2	2:H:144:CYS:HB2	2.49	0.47
2:J:62:GLN:C	2:J:64:THR:N	2.73	0.47
1:A:314:LEU:HD23	2:B:52:VAL:HG22	1.97	0.47
2:D:147:GLU:OE1	2:D:147:GLU:HA	2.15	0.47
1:C:316:THR:HB	2:D:48:ILE:HG21	1.96	0.47
2:D:123:LYS:HA	2:D:138:PHE:HE2	1.79	0.47
1:G:189:GLN:HG2	1:G:189:GLN:O	2.13	0.47
2:J:131:LYS:HD3	2:J:139:GLU:HB2	1.95	0.47
2:H:3:PHE:CE2	2:H:113:SER:HB2	2.49	0.47
1:I:18:THR:HG22	2:J:104:ASN:HB3	1.96	0.47
2:B:2:LEU:HG	2:B:112:ASP:OD2	2.15	0.47
1:C:92:PRO:O	1:C:226:ARG:HD3	2.13	0.47
2:D:38:LEU:O	2:D:40:SER:N	2.48	0.47
1:K:122:SER:O	1:K:124:PRO:HD3	2.14	0.47
1:A:287:LYS:HZ2	1:A:287:LYS:HG3	1.67	0.47
1:E:92:PRO:HG2	1:E:223:GLN:HB2	1.95	0.47
1:E:170:GLY:HA2	1:E:236:GLN:HG3	1.97	0.47
2:H:4:GLY:O	2:H:8:GLY:HA3	2.15	0.47
2:H:79:ASN:ND2	1:K:103:GLU:OE2	2.37	0.47
1:A:19:ILE:HB	2:B:102:LEU:HD23	1.97	0.47
2:B:30:GLN:C	2:B:30:GLN:NE2	2.73	0.47
1:I:27:THR:HG23	1:I:318:LEU:O	2.15	0.46
1:A:162:SER:HA	1:A:242:PHE:O	2.15	0.46
1:E:260:GLY:O	1:E:262:SER:N	2.48	0.46
2:H:112:ASP:O	2:H:115:VAL:N	2.48	0.46
1:K:5:ILE:HD12	2:L:24:TYR:CE2	2.49	0.46
2:L:26:HIS:CG	2:L:149:MET:HG3	2.50	0.46
2:B:45:ILE:O	2:B:49:SER:OG	2.32	0.46
2:B:119:TYR:C	2:B:121:LYS:H	2.23	0.46
1:E:8:HIS:HB2	2:F:20:GLY:O	2.14	0.46
2:J:39:LYS:O	2:J:43:ILE:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:GLN:NE2	2:B:152:VAL:O	2.49	0.46
1:C:219:LYS:HE2	1:C:224:ALA:HB2	1.97	0.46
1:K:57:VAL:O	1:K:61:ILE:HG12	2.16	0.46
2:D:48:ILE:O	2:D:52:VAL:HG23	2.15	0.46
2:F:61:ILE:O	2:F:61:ILE:HG22	2.14	0.46
1:G:40:LYS:HD2	1:G:273:HIS:CD2	2.50	0.46
1:C:64:ASN:ND2	1:C:66:LYS:HB2	2.31	0.46
1:E:16:VAL:HG12	1:E:313:ARG:HG2	1.97	0.46
1:E:65:PRO:HB3	1:E:146:ARG:NH2	2.30	0.46
2:F:63:PHE:O	2:F:63:PHE:CD1	2.68	0.46
1:G:5:ILE:HG23	2:H:136:GLY:O	2.15	0.46
1:I:54:ASN:C	1:I:85:SER:HA	2.40	0.46
1:K:2:THR:HG22	2:L:139:GLU:CG	2.45	0.46
1:C:122:SER:O	1:C:124:PRO:HD3	2.16	0.46
2:D:144:CYS:CB	2:D:148:CYS:SG	3.04	0.46
2:H:58:LYS:HD2	2:J:97:GLU:HB3	1.98	0.46
1:A:42:CYS:H	1:A:280:GLN:NE2	2.13	0.46
2:L:63:PHE:O	2:L:65:SER:N	2.49	0.46
1:E:219:LYS:HA	1:E:223:GLN:O	2.16	0.46
1:K:93:GLY:HA3	1:K:227:MET:O	2.16	0.45
1:K:115:GLU:OE2	1:K:118:PRO:HA	2.16	0.45
1:A:16:VAL:HG21	1:A:315:ALA:HB2	1.97	0.45
1:E:90:CYS:O	1:E:221:ARG:CD	2.64	0.45
1:E:314:LEU:HD13	2:F:100:ILE:HD13	1.97	0.45
1:I:3:ILE:HG23	1:I:3:ILE:O	2.14	0.45
1:I:292:PHE:CZ	2:J:59:MET:HE3	2.50	0.45
1:K:311:GLN:HE21	1:K:313:ARG:HB2	1.81	0.45
1:E:93:GLY:HA3	1:E:227:MET:O	2.16	0.45
2:J:30:GLN:HE21	2:J:30:GLN:HB2	1.57	0.45
1:G:5:ILE:O	1:G:5:ILE:HG13	2.06	0.45
1:I:54:ASN:HB2	1:I:87:ASN:ND2	2.30	0.45
3:A:404:NAG:H83	3:A:404:NAG:O3	2.16	0.45
1:C:4:CYS:SG	2:D:14:TRP:HZ2	2.39	0.45
1:K:2:THR:CG2	2:L:139:GLU:HB2	2.47	0.45
2:L:132:GLU:HG2	2:L:138:PHE:HE1	1.82	0.45
2:H:149:MET:O	2:H:152:VAL:HG23	2.17	0.45
1:K:127:ASP:OD1	1:K:130:ARG:HG3	2.17	0.45
2:J:131:LYS:HD3	2:J:133:ILE:HD11	1.99	0.45
2:D:125:GLN:NE2	2:D:152:VAL:HG12	2.28	0.45
1:K:171:LYS:HE3	1:K:256:ALA:HB1	1.98	0.45
1:A:2:THR:CB	2:B:139:GLU:CD	2.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:8:HIS:ND1	2:J:20:GLY:O	2.47	0.45
2:J:142:HIS:O	2:J:142:HIS:CG	2.69	0.45
1:K:180:HIS:ND1	1:K:192:TYR:OH	2.46	0.45
2:L:30:GLN:OE1	2:L:146:ASN:HB2	2.16	0.45
2:L:123:LYS:HE2	2:L:132:GLU:OE2	2.17	0.45
1:G:4:CYS:N	2:H:25:HIS:O	2.40	0.44
2:L:30:GLN:CD	2:L:146:ASN:HB2	2.42	0.44
1:A:279:CYS:SG	1:A:303:CYS:CB	3.01	0.44
1:G:286:LEU:HD21	1:G:295:VAL:HG21	1.98	0.44
1:I:273:HIS:CD2	3:I:402:NAG:H81	2.53	0.44
1:A:225:GLY:O	1:A:226:ARG:NH1	2.42	0.44
2:B:119:TYR:O	2:B:122:VAL:CG2	2.63	0.44
1:E:123:TRP:CZ3	1:E:149:LEU:HD22	2.52	0.44
2:F:3:PHE:O	2:F:116:LYS:HD2	2.17	0.44
1:I:42:CYS:HB2	1:I:277:THR:HG22	1.99	0.44
2:J:131:LYS:HD2	2:J:139:GLU:HG2	1.97	0.44
2:L:30:GLN:OE1	2:L:146:ASN:CB	2.65	0.44
1:C:262:SER:O	1:C:263:SER:HB2	2.17	0.44
1:G:261:SER:HB3	2:H:63:PHE:CZ	2.45	0.44
2:J:37:ASP:OD2	2:J:118:LEU:HD11	2.18	0.44
2:L:122:VAL:HG12	2:L:138:PHE:CE2	2.52	0.44
1:C:305:LYS:HE2	1:C:305:LYS:HB2	1.84	0.44
2:D:98:LEU:HD23	2:D:98:LEU:HA	1.68	0.44
2:D:142:HIS:O	2:D:143:LYS:C	2.60	0.44
1:G:3:ILE:HG13	2:H:26:HIS:HB3	2.00	0.44
1:K:43:SER:HA	1:K:49:PRO:HD3	1.99	0.44
1:A:90:CYS:HB2	1:A:135:SER:O	2.18	0.44
1:K:5:ILE:HD11	2:L:24:TYR:CD2	2.46	0.44
1:G:181:HIS:ND1	1:G:212:PRO:HA	2.32	0.44
1:I:122:SER:C	1:I:124:PRO:HD3	2.43	0.44
1:I:261:SER:O	1:I:262:SER:C	2.60	0.44
1:K:273:HIS:HD2	3:K:403:NAG:H81	1.82	0.44
2:L:26:HIS:O	2:L:26:HIS:CD2	2.71	0.44
2:D:63:PHE:O	2:D:63:PHE:CD1	2.70	0.44
2:J:3:PHE:HB2	2:J:112:ASP:CG	2.43	0.43
1:K:110:SER:HB3	1:K:258:LYS:HB3	2.00	0.43
2:L:25:HIS:HA	2:L:33:GLY:O	2.18	0.43
1:A:303:CYS:O	2:B:61:ILE:HG12	2.18	0.43
1:E:5:ILE:HD12	2:F:24:TYR:CE2	2.53	0.43
1:G:130:ARG:HH11	1:G:130:ARG:CG	2.30	0.43
2:H:123:LYS:HB2	2:H:138:PHE:HZ	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LYS:HD2	1:A:86:LYS:HA	1.79	0.43
1:G:58:ALA:O	1:G:62:LEU:HB2	2.18	0.43
1:I:118:PRO:O	1:I:122:SER:HB2	2.18	0.43
1:I:299:THR:HB	1:I:303:CYS:SG	2.58	0.43
1:A:68:ASP:HA	1:A:71:LEU:CD2	2.48	0.43
1:E:299:THR:O	2:F:65:SER:OG	2.24	0.43
2:F:48:ILE:HD12	2:F:107:THR:HG23	1.99	0.43
1:G:19:ILE:HB	2:H:102:LEU:HD23	2.00	0.43
1:G:92:PRO:HB3	1:G:220:VAL:CG2	2.48	0.43
1:G:308:LYS:HA	1:G:308:LYS:HD3	1.74	0.43
2:H:127:ARG:HE	2:H:127:ARG:HB3	1.54	0.43
2:L:26:HIS:O	2:L:26:HIS:HD2	2.01	0.43
1:A:299:THR:HB	1:A:303:CYS:SG	2.58	0.43
1:C:3:ILE:HD12	1:C:4:CYS:H	1.84	0.43
1:E:197:THR:O	1:E:212:PRO:HD2	2.18	0.43
2:F:24:TYR:CD1	2:F:153:LYS:HD2	2.54	0.43
2:F:75:LYS:HG3	2:F:79:ASN:ND2	2.34	0.43
1:G:318:LEU:HB3	2:H:111:HIS:CG	2.54	0.43
1:A:48:ILE:HD12	1:A:48:ILE:H	1.83	0.43
1:A:181:HIS:CE1	1:A:212:PRO:HA	2.54	0.43
1:E:137:SER:HB2	1:E:141:ALA:O	2.19	0.43
1:I:169:LYS:O	1:I:171:LYS:HG3	2.19	0.43
2:J:61:ILE:O	2:J:62:GLN:C	2.61	0.43
2:J:127:ARG:HB2	2:J:128:ASN:H	1.57	0.43
2:H:126:LEU:HD23	2:H:126:LEU:HA	1.82	0.43
2:L:28:ASN:HD21	2:L:146:ASN:N	2.16	0.43
1:A:40:LYS:O	1:A:280:GLN:NE2	2.50	0.43
2:B:25:HIS:CD2	2:B:33:GLY:C	2.97	0.43
1:C:279:CYS:SG	1:C:286:LEU:CA	3.07	0.43
1:E:286:LEU:HD21	1:E:295:VAL:HG21	1.99	0.43
1:K:65:PRO:C	1:K:67:CYS:H	2.27	0.42
2:B:2:LEU:HD23	2:F:117:ASN:ND2	2.34	0.42
1:E:299:THR:HB	1:E:303:CYS:SG	2.59	0.42
1:G:98:TYR:CZ	1:G:102:LYS:HD2	2.53	0.42
1:G:219:LYS:HA	1:G:223:GLN:O	2.19	0.42
1:C:156:ASN:C	1:C:156:ASN:HD22	2.26	0.42
1:C:161:LEU:O	1:C:243:GLU:HA	2.19	0.42
1:E:17:ASP:OD2	1:E:22:LYS:HD2	2.19	0.42
1:G:147:ASN:ND2	1:G:255:PHE:HZ	2.18	0.42
1:I:318:LEU:HD12	1:I:319:ARG:O	2.20	0.42
1:A:22:LYS:CD	3:A:402:NAG:H81	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:LYS:HE2	1:C:190:THR:O	2.18	0.42
1:E:221:ARG:C	1:E:222:GLU:CG	2.93	0.42
1:E:293:GLN:OE1	1:E:295:VAL:N	2.45	0.42
1:A:266:MET:HE3	1:A:300:ILE:HD12	2.01	0.42
2:F:66:VAL:HG12	2:F:68:LYS:HE2	2.00	0.42
2:F:146:ASN:OD1	2:F:146:ASN:N	2.53	0.42
1:G:184:THR:CG2	1:G:185:ASP:N	2.82	0.42
2:H:131:LYS:HB2	2:H:141:TYR:CE1	2.54	0.42
2:J:64:THR:HG23	2:J:64:THR:O	2.20	0.42
2:J:148:CYS:HA	2:J:151:SER:HB3	2.01	0.42
1:K:19:ILE:HB	2:L:102:LEU:HD23	2.00	0.42
2:L:4:GLY:O	2:L:8:GLY:HA3	2.20	0.42
1:C:7:TYR:CD1	2:D:6:ILE:HD13	2.55	0.42
2:B:24:TYR:CE1	2:B:37:ASP:HB2	2.55	0.42
2:B:119:TYR:C	2:B:121:LYS:N	2.76	0.42
1:A:161:LEU:O	1:A:243:GLU:HA	2.19	0.42
2:F:142:HIS:CE1	2:F:144:CYS:SG	3.06	0.42
2:J:127:ARG:CZ	2:J:127:ARG:HB3	2.46	0.42
1:K:303:CYS:O	2:L:61:ILE:HB	2.20	0.42
2:B:148:CYS:HA	2:B:151:SER:HB2	2.01	0.42
2:D:119:TYR:CE1	2:D:136:GLY:HA2	2.55	0.42
1:E:17:ASP:OD1	1:E:17:ASP:N	2.53	0.42
1:G:31:ASN:O	1:G:290:LEU:HD22	2.19	0.42
1:K:1:ASP:O	2:L:140:PHE:HB2	2.19	0.42
1:K:175:VAL:HG21	1:K:240:ILE:HD13	2.01	0.42
2:L:130:ALA:HB1	2:L:139:GLU:O	2.20	0.42
1:C:3:ILE:O	1:C:3:ILE:HG23	2.20	0.42
1:K:33:LEU:HD21	1:K:294:ASN:ND2	2.34	0.42
1:K:138:HIS:CD2	1:K:138:HIS:O	2.73	0.42
1:A:177:TRP:HZ3	1:A:232:THR:HG22	1.84	0.42
2:B:25:HIS:CD2	2:B:34:TYR:CD1	3.08	0.42
2:B:127:ARG:HB3	2:B:127:ARG:CZ	2.48	0.42
1:C:299:THR:O	2:D:65:SER:OG	2.38	0.42
1:G:177:TRP:CE2	1:G:201:VAL:HG21	2.55	0.41
2:H:107:THR:O	2:H:110:TYR:HB3	2.20	0.41
1:K:49:PRO:HB3	1:K:78:TYR:CZ	2.55	0.41
1:K:181:HIS:CE1	1:K:212:PRO:HA	2.55	0.41
2:L:93:THR:O	2:L:97:GLU:HG2	2.21	0.41
2:B:130:ALA:CB	2:B:139:GLU:O	2.63	0.41
2:J:87:GLY:O	2:J:91:VAL:HG23	2.19	0.41
1:K:74:ASN:OD1	1:K:75:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:61:ILE:HD12	2:L:62:GLN:N	2.35	0.41
1:C:8:HIS:ND1	1:C:9:ALA:N	2.69	0.41
1:I:81:GLU:O	1:I:267:ARG:HA	2.21	0.41
2:J:111:HIS:O	2:J:115:VAL:HG23	2.21	0.41
1:K:132:THR:OG1	1:K:133:THR:N	2.54	0.41
1:A:131:GLY:HA3	1:A:150:TRP:HB3	2.01	0.41
2:B:73:LEU:HD23	2:B:73:LEU:HA	1.89	0.41
1:I:49:PRO:HB3	1:I:78:TYR:CE1	2.55	0.41
1:I:92:PRO:HG2	1:I:226:ARG:HD2	2.02	0.41
1:E:292:PHE:HZ	2:F:59:MET:HE3	1.84	0.41
1:C:292:PHE:CE1	2:D:59:MET:HE2	2.56	0.41
2:F:61:ILE:HD13	2:F:61:ILE:HA	1.83	0.41
1:C:219:LYS:HE2	1:C:219:LYS:HB2	1.36	0.41
2:D:66:VAL:HG22	2:D:67:GLY:H	1.85	0.41
1:E:297:PRO:HD3	1:E:306:TYR:CZ	2.56	0.41
1:I:298:VAL:HG23	2:J:66:VAL:HG23	2.03	0.41
2:J:148:CYS:O	2:J:149:MET:C	2.63	0.41
1:K:47:LYS:HB3	1:K:77:SER:HB3	2.03	0.41
1:A:54:ASN:OD1	1:A:54:ASN:N	2.47	0.41
1:C:205:LYS:HE3	1:C:235:ASP:OD2	2.20	0.41
1:E:20:LEU:HD23	1:E:20:LEU:HA	1.89	0.41
1:E:44:LEU:HD22	1:E:300:ILE:HG22	2.03	0.41
1:E:109:SER:OG	1:E:260:GLY:N	2.42	0.41
2:F:66:VAL:HB	2:F:67:GLY:H	1.70	0.41
2:H:41:THR:O	2:H:45:ILE:HG12	2.21	0.41
1:I:263:SER:OG	1:I:264:GLY:N	2.53	0.41
1:C:5:ILE:HD11	2:D:119:TYR:CB	2.48	0.41
2:D:38:LEU:N	2:D:38:LEU:CD1	2.72	0.41
1:E:81:GLU:O	1:E:267:ARG:HA	2.21	0.41
1:G:180:HIS:HB2	1:G:249:ILE:HD11	2.03	0.40
1:E:62:LEU:HB3	1:E:145:TYR:CD1	2.56	0.40
1:G:16:VAL:HG21	1:G:315:ALA:HB2	2.02	0.40
1:E:5:ILE:HD11	2:F:24:TYR:CE2	2.55	0.40
1:G:47:LYS:HE2	1:G:47:LYS:HB2	1.66	0.40
1:I:43:SER:HA	1:I:49:PRO:HD3	2.03	0.40
2:J:24:TYR:CE1	2:J:153:LYS:HG2	2.56	0.40
2:B:71:ASN:OD1	2:B:74:GLU:HG3	2.20	0.40
2:F:127:ARG:H	2:F:127:ARG:HG3	1.66	0.40
1:G:189:GLN:HA	1:G:192:TYR:O	2.22	0.40
1:G:277:THR:OG1	1:G:278:LYS:N	2.55	0.40
2:H:98:LEU:O	2:H:102:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:27:THR:C	1:I:28:HIS:ND1	2.78	0.40
1:K:59:GLY:N	1:K:88:GLY:HA2	2.36	0.40
1:K:262:SER:O	1:K:263:SER:OG	2.34	0.40
1:C:191:LEU:HD23	1:C:191:LEU:HA	1.87	0.40
2:D:61:ILE:O	2:D:61:ILE:CG2	2.69	0.40
2:D:148:CYS:HA	2:D:151:SER:HB3	2.04	0.40
1:E:71:LEU:CD2	1:E:146:ARG:HD2	2.50	0.40
1:E:293:GLN:NE2	1:E:306:TYR:HB2	2.36	0.40
1:G:153:LYS:HE3	1:G:190:THR:O	2.21	0.40
2:H:9:PHE:CE1	2:H:10:ILE:HG13	2.56	0.40
1:I:177:TRP:CE2	1:I:201:VAL:HG21	2.57	0.40
2:L:3:PHE:CE2	2:L:113:SER:HB2	2.56	0.40
2:L:65:SER:O	2:L:66:VAL:HG22	2.22	0.40
1:A:14:ASP:O	1:A:25:THR:HA	2.21	0.40
1:C:119:LYS:HB2	1:C:252:TRP:CE2	2.57	0.40
2:D:125:GLN:HE21	2:D:152:VAL:CG1	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/321 (99%)	298 (93%)	21 (7%)	0	100	100
1	C	319/321 (99%)	302 (95%)	16 (5%)	1 (0%)	36	60
1	E	319/321 (99%)	297 (93%)	20 (6%)	2 (1%)	21	44
1	G	319/321 (99%)	303 (95%)	14 (4%)	2 (1%)	21	44
1	I	319/321 (99%)	300 (94%)	16 (5%)	3 (1%)	14	35
1	K	319/321 (99%)	299 (94%)	19 (6%)	1 (0%)	36	60
2	B	154/156 (99%)	146 (95%)	5 (3%)	3 (2%)	6	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	154/156 (99%)	136 (88%)	11 (7%)	7 (4%)	2	4
2	F	154/156 (99%)	137 (89%)	15 (10%)	2 (1%)	9	25
2	H	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	3	7
2	J	154/156 (99%)	137 (89%)	13 (8%)	4 (3%)	4	11
2	L	154/156 (99%)	136 (88%)	14 (9%)	4 (3%)	4	11
All	All	2838/2862 (99%)	2627 (93%)	177 (6%)	34 (1%)	10	27

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	150	GLU
1	I	261	SER
2	J	63	PHE
2	L	128	ASN
2	D	127	ARG
2	D	154	ASN
2	F	61	ILE
2	H	63	PHE
1	I	262	SER
2	L	64	THR
2	B	67	GLY
2	B	127	ARG
2	D	39	LYS
2	D	129	ASN
2	D	143	LYS
1	E	261	SER
2	J	62	GLN
2	B	61	ILE
2	D	156	THR
1	G	112	GLU
2	H	149	MET
1	K	71	LEU
2	L	66	VAL
2	F	67	GLY
1	E	49	PRO
2	H	112	ASP
2	J	61	ILE
1	C	218	PRO
1	I	218	PRO
2	L	67	GLY

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Mol	Chain	Res	Type
2	H	67	GLY
2	J	67	GLY
2	D	67	GLY
1	G	155	GLY

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	282/282 (100%)	260 (92%)	22 (8%)	11	29
1	C	282/282 (100%)	259 (92%)	23 (8%)	10	27
1	E	282/282 (100%)	261 (93%)	21 (7%)	13	32
1	G	282/282 (100%)	250 (89%)	32 (11%)	5	14
1	I	282/282 (100%)	258 (92%)	24 (8%)	10	25
1	K	282/282 (100%)	262 (93%)	20 (7%)	13	33
2	B	134/134 (100%)	120 (90%)	14 (10%)	7	17
2	D	134/134 (100%)	114 (85%)	20 (15%)	3	8
2	F	134/134 (100%)	119 (89%)	15 (11%)	6	15
2	H	134/134 (100%)	115 (86%)	19 (14%)	3	8
2	J	134/134 (100%)	112 (84%)	22 (16%)	2	6
2	L	134/134 (100%)	121 (90%)	13 (10%)	8	20
All	All	2496/2496 (100%)	2251 (90%)	245 (10%)	7	19

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	2	THR
1	G	3	ILE
1	G	5	ILE
1	G	11	ASN
1	G	15	THR
1	G	30	VAL

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Mol	Chain	Res	Type
1	G	94	GLU
1	G	95	PHE
1	G	107	THR
1	G	110	SER
1	G	111	PHE
1	G	112	GLU
1	G	128	THR
1	G	129	THR
1	G	152	VAL
1	G	153	LYS
1	G	164	SER
1	G	190	THR
1	G	192	TYR
1	G	194	ASN
1	G	200	SER
1	G	217	ARG
1	G	220	VAL
1	G	236	GLN
1	G	259	LYS
1	G	261	SER
1	G	262	SER
1	G	268	SER
1	G	278	LYS
1	G	287	LYS
1	G	307	VAL
1	G	321	VAL
2	H	15	THR
2	H	25	HIS
2	H	26	HIS
2	H	29	GLU
2	H	30	GLN
2	H	52	VAL
2	H	60	ASN
2	H	62	GLN
2	H	63	PHE
2	H	64	THR
2	H	66	VAL
2	H	112	ASP
2	H	127	ARG
2	H	143	LYS
2	H	145	ASP
2	H	149	MET

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Mol	Chain	Res	Type
2	H	152	VAL
2	H	154	ASN
2	H	157	TYR
1	I	2	THR
1	I	15	THR
1	I	26	VAL
1	I	27	THR
1	I	57	VAL
1	I	111	PHE
1	I	121	THR
1	I	122	SER
1	I	129	THR
1	I	132	THR
1	I	135	SER
1	I	153	LYS
1	I	154	LYS
1	I	157	SER
1	I	171	LYS
1	I	192	TYR
1	I	195	ASN
1	I	200	SER
1	I	257	LEU
1	I	258	LYS
1	I	265	ILE
1	I	281	THR
1	I	300	ILE
1	I	318	LEU
2	J	2	LEU
2	J	22	TYR
2	J	27	ARG
2	J	30	GLN
2	J	38	LEU
2	J	39	LYS
2	J	61	ILE
2	J	62	GLN
2	J	116	LYS
2	J	122	VAL
2	J	123	LYS
2	J	124	SER
2	J	126	LEU
2	J	127	ARG
2	J	129	ASN

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Mol	Chain	Res	Type
2	J	131	LYS
2	J	132	GLU
2	J	133	ILE
2	J	142	HIS
2	J	143	LYS
2	J	147	GLU
2	J	148	CYS
1	K	1	ASP
1	K	43	SER
1	K	54	ASN
1	K	57	VAL
1	K	72	THR
1	K	84	ASN
1	K	95	PHE
1	K	130	ARG
1	K	132	THR
1	K	138	HIS
1	K	139	SER
1	K	153	LYS
1	K	154	LYS
1	K	175	VAL
1	K	186	SER
1	K	194	ASN
1	K	208	LYS
1	K	217	ARG
1	K	263	SER
1	K	321	VAL
2	L	27	ARG
2	L	29	GLU
2	L	39	LYS
2	L	40	SER
2	L	41	THR
2	L	60	ASN
2	L	66	VAL
2	L	126	LEU
2	L	127	ARG
2	L	129	ASN
2	L	144	CYS
2	L	149	MET
2	L	156	THR
1	A	5	ILE
1	A	18	THR

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Mol	Chain	Res	Type
1	A	57	VAL
1	A	69	LEU
1	A	71	LEU
1	A	86	LYS
1	A	95	PHE
1	A	139	SER
1	A	142	ASN
1	A	185	ASP
1	A	186	SER
1	A	189	GLN
1	A	194	ASN
1	A	213	GLU
1	A	220	VAL
1	A	221	ARG
1	A	262	SER
1	A	268	SER
1	A	287	LYS
1	A	289	ASN
1	A	318	LEU
1	A	321	VAL
2	B	2	LEU
2	B	19	ASP
2	B	30	GLN
2	B	38	LEU
2	B	49	SER
2	B	61	ILE
2	B	64	THR
2	B	66	VAL
2	B	121	LYS
2	B	126	LEU
2	B	127	ARG
2	B	139	GLU
2	B	156	THR
2	B	157	TYR
1	C	3	ILE
1	C	5	ILE
1	C	13	THR
1	C	15	THR
1	C	57	VAL
1	C	69	LEU
1	C	86	LYS
1	C	111	PHE

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Mol	Chain	Res	Type
1	C	127	ASP
1	C	135	SER
1	C	164	SER
1	C	171	LYS
1	C	184	THR
1	C	194	ASN
1	C	200	SER
1	C	219	LYS
1	C	221	ARG
1	C	279	CYS
1	C	298	VAL
1	C	299	THR
1	C	302	LYS
1	C	303	CYS
1	C	318	LEU
2	D	19	ASP
2	D	22	TYR
2	D	24	TYR
2	D	27	ARG
2	D	30	GLN
2	D	38	LEU
2	D	39	LYS
2	D	60	ASN
2	D	61	ILE
2	D	64	THR
2	D	123	LYS
2	D	127	ARG
2	D	129	ASN
2	D	131	LYS
2	D	132	GLU
2	D	148	CYS
2	D	152	VAL
2	D	153	LYS
2	D	156	THR
2	D	157	TYR
1	E	48	ILE
1	E	57	VAL
1	E	69	LEU
1	E	77	SER
1	E	82	THR
1	E	83	SER
1	E	94	GLU

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Mol	Chain	Res	Type
1	E	95	PHE
1	E	110	SER
1	E	121	THR
1	E	128	THR
1	E	134	VAL
1	E	138	HIS
1	E	153	LYS
1	E	175	VAL
1	E	195	ASN
1	E	221	ARG
1	E	222	GLU
1	E	271	GLN
1	E	298	VAL
1	E	321	VAL
2	F	11	GLU
2	F	15	THR
2	F	27	ARG
2	F	28	ASN
2	F	29	GLU
2	F	38	LEU
2	F	60	ASN
2	F	61	ILE
2	F	62	GLN
2	F	64	THR
2	F	68	LYS
2	F	93	THR
2	F	98	LEU
2	F	144	CYS
2	F	148	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	31	ASN
1	G	194	ASN
1	G	228	ASN
1	G	271	GLN
1	G	289	ASN
2	H	28	ASN
1	I	87	ASN
1	I	126	HIS
1	I	167	ASN

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Mol	Chain	Res	Type
1	I	193	GLN
1	I	194	ASN
1	I	273	HIS
1	I	320	ASN
2	J	30	GLN
2	J	50	ASN
1	K	8	HIS
1	K	10	ASN
1	K	138	HIS
1	K	283	HIS
1	K	294	ASN
1	K	311	GLN
2	L	26	HIS
1	A	31	ASN
1	A	45	ASN
1	A	236	GLN
1	A	273	HIS
1	A	280	GLN
2	B	25	HIS
1	C	156	ASN
1	C	188	GLN
1	C	273	HIS
1	C	283	HIS
2	D	50	ASN
1	E	28	HIS
1	E	45	ASN
1	E	125	ASN
1	E	194	ASN
1	E	236	GLN
1	E	253	HIS
2	F	26	HIS
2	F	28	ASN
2	F	30	GLN
2	F	60	ASN
2	F	79	ASN
2	F	142	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
3	NAG	E	402	1	14,14,15	0.41	0	17,19,21	0.75	0
3	NAG	G	403	1	14,14,15	0.27	0	17,19,21	0.70	0
3	NAG	I	402	1	14,14,15	0.32	0	17,19,21	0.86	0
3	NAG	C	404	1	14,14,15	0.28	0	17,19,21	0.71	0
3	NAG	K	403	1	14,14,15	0.31	0	17,19,21	0.78	0
3	NAG	C	401	1	14,14,15	0.26	0	17,19,21	0.73	0
3	NAG	A	401	1	14,14,15	0.29	0	17,19,21	0.73	0
3	NAG	E	403	1	14,14,15	0.31	0	17,19,21	0.71	0
3	NAG	I	403	1	14,14,15	0.29	0	17,19,21	0.69	0
3	NAG	G	401	1	14,14,15	0.32	0	17,19,21	0.76	0
3	NAG	E	401	1	14,14,15	0.32	0	17,19,21	0.75	0
3	NAG	K	402	1	14,14,15	0.32	0	17,19,21	0.70	0
3	NAG	A	404	1	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	K	404	1	14,14,15	0.28	0	17,19,21	0.63	0
3	NAG	A	403	1	14,14,15	0.28	0	17,19,21	0.68	0
3	NAG	K	401	1	14,14,15	0.27	0	17,19,21	0.95	0
3	NAG	G	402	1	14,14,15	0.26	0	17,19,21	0.49	0
3	NAG	I	401	1	14,14,15	0.29	0	17,19,21	0.68	0
3	NAG	C	402	1	14,14,15	0.28	0	17,19,21	0.83	0
3	NAG	G	404	1	14,14,15	0.28	0	17,19,21	0.58	0
3	NAG	C	403	1	14,14,15	0.26	0	17,19,21	0.83	0
3	NAG	E	404	1	14,14,15	0.29	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	I	404	1	14,14,15	0.29	0	17,19,21	0.92	1 (5%)
3	NAG	A	402	1	14,14,15	0.35	0	17,19,21	1.10	1 (5%)

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
3	NAG	E	402	1	-	1/6/23/26	0/1/1/1
3	NAG	G	403	1	-	4/6/23/26	0/1/1/1
3	NAG	I	402	1	-	0/6/23/26	0/1/1/1
3	NAG	C	404	1	-	0/6/23/26	0/1/1/1
3	NAG	K	403	1	-	4/6/23/26	0/1/1/1
3	NAG	C	401	1	-	0/6/23/26	0/1/1/1
3	NAG	A	401	1	-	0/6/23/26	0/1/1/1
3	NAG	E	403	1	-	2/6/23/26	0/1/1/1
3	NAG	I	403	1	-	2/6/23/26	0/1/1/1
3	NAG	G	401	1	-	2/6/23/26	0/1/1/1
3	NAG	E	401	1	-	2/6/23/26	0/1/1/1
3	NAG	K	402	1	-	2/6/23/26	0/1/1/1
3	NAG	A	404	1	-	2/6/23/26	0/1/1/1
3	NAG	K	404	1	-	2/6/23/26	0/1/1/1
3	NAG	A	403	1	-	2/6/23/26	0/1/1/1
3	NAG	K	401	1	-	2/6/23/26	0/1/1/1
3	NAG	G	402	1	-	4/6/23/26	0/1/1/1
3	NAG	I	401	1	-	4/6/23/26	0/1/1/1
3	NAG	C	402	1	-	0/6/23/26	0/1/1/1
3	NAG	G	404	1	-	2/6/23/26	0/1/1/1
3	NAG	C	403	1	-	0/6/23/26	0/1/1/1
3	NAG	E	404	1	-	2/6/23/26	0/1/1/1
3	NAG	I	404	1	-	2/6/23/26	0/1/1/1
3	NAG	A	402	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NAG	C2-N2-C7	-2.65	119.35	122.90
3	I	404	NAG	O5-C1-C2	-2.02	108.17	111.29

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	401	NAG	C8-C7-N2-C2
3	G	401	NAG	O7-C7-N2-C2
3	G	402	NAG	C8-C7-N2-C2
3	G	402	NAG	O7-C7-N2-C2
3	G	404	NAG	C8-C7-N2-C2
3	G	404	NAG	O7-C7-N2-C2
3	K	403	NAG	O7-C7-N2-C2
3	A	404	NAG	C8-C7-N2-C2
3	A	404	NAG	O7-C7-N2-C2
3	K	403	NAG	C8-C7-N2-C2
3	G	403	NAG	O7-C7-N2-C2
3	E	403	NAG	O5-C5-C6-O6
3	G	403	NAG	C8-C7-N2-C2
3	I	401	NAG	C8-C7-N2-C2
3	I	401	NAG	O7-C7-N2-C2
3	K	403	NAG	C4-C5-C6-O6
3	E	401	NAG	C8-C7-N2-C2
3	E	401	NAG	O7-C7-N2-C2
3	G	403	NAG	C4-C5-C6-O6
3	K	403	NAG	O5-C5-C6-O6
3	A	402	NAG	C8-C7-N2-C2
3	G	403	NAG	O5-C5-C6-O6
3	K	401	NAG	C8-C7-N2-C2
3	I	404	NAG	C4-C5-C6-O6
3	E	404	NAG	C4-C5-C6-O6
3	E	403	NAG	C4-C5-C6-O6
3	K	404	NAG	C4-C5-C6-O6
3	I	404	NAG	O5-C5-C6-O6
3	E	404	NAG	O5-C5-C6-O6
3	I	403	NAG	C4-C5-C6-O6
3	A	402	NAG	O7-C7-N2-C2
3	K	401	NAG	O7-C7-N2-C2
3	A	402	NAG	C4-C5-C6-O6
3	G	402	NAG	C4-C5-C6-O6
3	I	401	NAG	C4-C5-C6-O6
3	K	404	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	403	NAG	C4-C5-C6-O6
3	I	403	NAG	O5-C5-C6-O6
3	A	402	NAG	O5-C5-C6-O6
3	I	401	NAG	O5-C5-C6-O6
3	A	403	NAG	O5-C5-C6-O6
3	G	402	NAG	O5-C5-C6-O6
3	E	402	NAG	C1-C2-N2-C7
3	K	402	NAG	C4-C5-C6-O6
3	K	402	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	402	NAG	1	0
3	K	403	NAG	1	0
3	A	404	NAG	1	0
3	A	402	NAG	3	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	321/321 (100%)	1.21	53 (16%) 4 4	18, 46, 70, 104	0
1	C	321/321 (100%)	1.16	55 (17%) 4 3	14, 48, 76, 105	0
1	E	321/321 (100%)	1.12	45 (14%) 6 5	16, 48, 69, 88	0
1	G	321/321 (100%)	0.87	36 (11%) 10 8	15, 38, 69, 112	0
1	I	321/321 (100%)	0.94	35 (10%) 10 9	14, 45, 70, 110	0
1	K	321/321 (100%)	1.05	43 (13%) 7 6	15, 45, 73, 102	0
2	B	156/156 (100%)	1.51	42 (26%) 1 1	15, 60, 98, 130	0
2	D	156/156 (100%)	1.86	62 (39%) 1 0	16, 66, 128, 140	0
2	F	156/156 (100%)	1.45	44 (28%) 1 1	17, 60, 94, 115	0
2	H	156/156 (100%)	1.73	63 (40%) 0 0	16, 73, 111, 130	0
2	J	156/156 (100%)	1.90	74 (47%) 0 0	17, 73, 118, 135	0
2	L	156/156 (100%)	1.86	71 (45%) 0 0	13, 69, 111, 120	0
All	All	2862/2862 (100%)	1.27	623 (21%) 2 2	13, 50, 97, 140	0

All (623) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	157	TYR	6.4
2	H	63	PHE	6.3
2	F	64	THR	6.3
1	C	4	CYS	6.1
2	L	35	ALA	5.9
2	D	157	TYR	5.8
2	D	61	ILE	5.7
2	L	18	VAL	5.7
2	D	156	THR	5.7
2	J	61	ILE	5.6
2	D	63	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
1	I	3	ILE	5.5
1	C	279	CYS	5.4
2	D	33	GLY	5.3
1	C	140	GLY	5.3
2	D	19	ASP	5.3
2	F	61	ILE	5.3
2	H	62	GLN	5.3
2	L	149	MET	5.1
2	D	138	PHE	5.1
2	D	27	ARG	5.1
1	A	3	ILE	5.0
2	L	64	THR	5.0
2	F	35	ALA	4.9
1	K	138	HIS	4.8
2	J	35	ALA	4.8
2	F	66	VAL	4.8
1	G	287	LYS	4.7
2	H	24	TYR	4.7
2	J	63	PHE	4.7
2	B	63	PHE	4.7
2	J	62	GLN	4.7
2	J	23	GLY	4.7
2	H	140	PHE	4.7
1	K	143	SER	4.7
1	C	303	CYS	4.7
2	J	33	GLY	4.6
2	L	33	GLY	4.6
2	L	65	SER	4.6
2	D	152	VAL	4.6
1	K	3	ILE	4.6
2	H	35	ALA	4.6
2	H	23	GLY	4.6
2	L	140	PHE	4.6
2	J	22	TYR	4.5
2	J	138	PHE	4.5
2	L	138	PHE	4.5
1	K	139	SER	4.5
1	G	262	SER	4.5
2	D	154	ASN	4.5
2	J	30	GLN	4.5
2	B	24	TYR	4.5
1	E	138	HIS	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	144	CYS	4.5
2	J	19	ASP	4.5
1	A	153	LYS	4.4
1	E	262	SER	4.4
1	A	189	GLN	4.4
2	H	21	TRP	4.4
2	H	150	GLU	4.3
1	G	5	ILE	4.3
2	J	17	MET	4.3
2	B	23	GLY	4.3
2	D	62	GLN	4.3
1	A	222	GLU	4.3
1	I	5	ILE	4.2
2	L	63	PHE	4.2
2	D	66	VAL	4.2
1	A	1	ASP	4.2
1	I	140	GLY	4.2
1	E	139	SER	4.2
2	D	134	GLY	4.2
2	H	138	PHE	4.2
2	F	138	PHE	4.2
2	J	24	TYR	4.2
2	F	65	SER	4.2
2	F	63	PHE	4.2
2	L	38	LEU	4.2
2	H	149	MET	4.1
2	L	150	GLU	4.1
1	A	111	PHE	4.1
1	E	153	LYS	4.1
2	D	25	HIS	4.1
2	H	64	THR	4.1
1	K	4	CYS	4.0
1	A	287	LYS	4.0
1	G	130	ARG	4.0
2	B	33	GLY	4.0
2	F	24	TYR	4.0
1	A	2	THR	4.0
1	E	264	GLY	4.0
1	A	186	SER	3.9
2	J	36	ALA	3.9
2	H	26	HIS	3.9
2	B	62	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
2	L	127	ARG	3.9
2	L	157	TYR	3.9
2	H	142	HIS	3.9
2	J	16	GLY	3.8
2	J	25	HIS	3.8
2	D	130	ALA	3.8
2	H	144	CYS	3.8
2	F	144	CYS	3.8
2	L	24	TYR	3.8
1	I	4	CYS	3.8
2	D	119	TYR	3.8
1	C	1	ASP	3.7
2	D	64	THR	3.7
1	E	5	ILE	3.7
1	C	317	GLY	3.7
2	H	134	GLY	3.7
2	J	140	PHE	3.7
2	J	152	VAL	3.7
2	F	18	VAL	3.7
2	B	30	GLN	3.7
2	H	141	TYR	3.7
2	J	34	TYR	3.7
2	J	31	GLY	3.7
2	B	35	ALA	3.7
1	E	193	GLN	3.7
2	B	26	HIS	3.7
1	G	1	ASP	3.7
1	E	3	ILE	3.7
2	D	140	PHE	3.7
2	D	153	LYS	3.6
2	H	22	TYR	3.6
2	L	23	GLY	3.6
2	D	142	HIS	3.6
2	L	19	ASP	3.6
1	E	321	VAL	3.6
1	E	154	LYS	3.6
2	J	130	ALA	3.6
2	D	141	TYR	3.6
1	A	318	LEU	3.5
1	E	137	SER	3.5
2	D	32	SER	3.5
1	K	5	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	6	GLY	3.5
1	E	141	ALA	3.5
2	J	136	GLY	3.5
2	F	62	GLN	3.5
1	A	152	VAL	3.5
2	J	157	TYR	3.5
2	D	124	SER	3.5
2	B	144	CYS	3.5
2	D	149	MET	3.5
2	D	143	LYS	3.5
2	D	155	GLY	3.5
1	K	16	VAL	3.5
2	D	126	LEU	3.5
1	E	72	THR	3.5
2	B	64	THR	3.5
1	K	125	ASN	3.5
2	L	7	ALA	3.5
2	B	138	PHE	3.5
2	L	31	GLY	3.4
1	E	191	LEU	3.4
2	H	2	LEU	3.4
1	G	321	VAL	3.4
1	K	26	VAL	3.4
1	K	23	ASN	3.4
2	D	20	GLY	3.4
2	L	145	ASP	3.4
2	L	125	GLN	3.4
1	K	262	SER	3.4
2	D	34	TYR	3.4
2	J	64	THR	3.4
2	F	67	GLY	3.4
1	I	16	VAL	3.4
2	L	66	VAL	3.4
2	L	136	GLY	3.4
2	J	32	SER	3.3
1	C	301	GLY	3.3
1	E	320	ASN	3.3
2	D	137	CYS	3.3
1	G	9	ALA	3.3
2	H	61	ILE	3.3
1	G	318	LEU	3.3
2	B	20	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	187	ASP	3.3
2	H	126	LEU	3.3
2	H	123	LYS	3.3
2	L	142	HIS	3.2
2	B	32	SER	3.2
1	K	140	GLY	3.2
2	L	22	TYR	3.2
2	J	66	VAL	3.2
2	L	144	CYS	3.2
2	L	21	TRP	3.2
2	H	133	ILE	3.2
2	F	140	PHE	3.2
1	C	289	ASN	3.2
1	G	302	LYS	3.2
2	H	124	SER	3.2
2	J	6	ILE	3.2
1	G	112	GLU	3.2
1	A	301	GLY	3.2
1	I	74	ASN	3.1
2	J	148	CYS	3.1
2	J	28	ASN	3.1
1	G	131	GLY	3.1
2	J	124	SER	3.1
2	D	151	SER	3.1
1	C	153	LYS	3.1
2	B	27	ARG	3.1
1	C	158	TYR	3.1
2	L	26	HIS	3.1
2	B	36	ALA	3.1
2	H	116	LYS	3.1
1	A	164	SER	3.1
2	J	141	TYR	3.1
1	K	132	THR	3.1
2	L	20	GLY	3.1
1	E	120	ALA	3.1
2	D	6	ILE	3.1
2	J	127	ARG	3.1
2	L	118	LEU	3.0
1	C	2	THR	3.0
2	L	131	LYS	3.0
2	B	31	GLY	3.0
2	J	14	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	150	GLU	3.0
1	A	11	ASN	3.0
1	C	11	ASN	3.0
1	E	1	ASP	3.0
1	E	299	THR	3.0
1	I	321	VAL	3.0
1	K	298	VAL	3.0
2	J	2	LEU	3.0
2	J	65	SER	3.0
2	J	26	HIS	3.0
1	E	125	ASN	3.0
2	D	129	ASN	3.0
1	I	1	ASP	3.0
2	L	61	ILE	3.0
2	L	62	GLN	3.0
2	L	153	LYS	3.0
2	L	152	VAL	3.0
1	K	318	LEU	2.9
2	H	25	HIS	2.9
2	B	65	SER	2.9
1	A	279	CYS	2.9
2	L	27	ARG	2.9
1	A	288	GLY	2.9
2	D	122	VAL	2.9
1	G	77	SER	2.9
1	G	317	GLY	2.9
1	I	9	ALA	2.9
2	B	29	GLU	2.9
2	B	153	LYS	2.9
1	C	150	TRP	2.9
1	A	193	GLN	2.9
1	C	157	SER	2.9
2	J	27	ARG	2.9
1	C	3	ILE	2.9
2	J	119	TYR	2.9
2	H	36	ALA	2.9
1	C	151	ILE	2.9
2	B	61	ILE	2.9
2	J	37	ASP	2.9
2	L	141	TYR	2.9
1	G	129	THR	2.9
2	J	7	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	152	VAL	2.9
1	E	194	ASN	2.8
2	H	136	GLY	2.8
2	F	136	GLY	2.8
2	J	156	THR	2.8
1	A	321	VAL	2.8
2	F	11	GLU	2.8
1	G	311	GLN	2.8
1	E	271	GLN	2.8
1	C	300	ILE	2.8
2	F	32	SER	2.8
1	K	287	LYS	2.8
2	H	153	LYS	2.8
2	F	2	LEU	2.8
1	I	24	VAL	2.8
1	C	111	PHE	2.8
2	H	139	GLU	2.8
2	H	27	ARG	2.8
1	G	189	GLN	2.8
1	C	139	SER	2.8
2	D	123	LYS	2.8
2	L	12	GLY	2.8
2	F	33	GLY	2.8
1	G	299	THR	2.8
1	A	16	VAL	2.8
2	H	3	PHE	2.8
2	D	22	TYR	2.8
1	E	124	PRO	2.8
2	J	133	ILE	2.8
1	A	131	GLY	2.8
1	C	44	LEU	2.8
2	J	126	LEU	2.8
2	L	148	CYS	2.7
2	D	131	LYS	2.7
1	K	150	TRP	2.7
1	A	168	ASN	2.7
2	J	111	HIS	2.7
2	H	132	GLU	2.7
2	B	19	ASP	2.7
1	I	158	TYR	2.7
2	L	119	TYR	2.7
1	G	303	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	158	TYR	2.7
2	L	133	ILE	2.7
2	D	2	LEU	2.7
1	I	36	SER	2.7
1	A	139	SER	2.7
1	A	261	SER	2.7
2	D	31	GLY	2.7
2	D	65	SER	2.7
2	J	147	GLU	2.7
2	J	143	LYS	2.7
2	D	30	GLN	2.7
1	C	74	ASN	2.7
2	L	132	GLU	2.7
1	E	298	VAL	2.7
2	H	18	VAL	2.7
1	I	15	THR	2.7
2	H	119	TYR	2.6
2	H	157	TYR	2.6
1	I	265	ILE	2.6
1	G	279	CYS	2.6
1	K	155	GLY	2.6
1	I	10	ASN	2.6
2	H	129	ASN	2.6
2	J	21	TRP	2.6
2	B	152	VAL	2.6
2	D	36	ALA	2.6
1	C	222	GLU	2.6
2	J	116	LYS	2.6
1	C	143	SER	2.6
2	H	122	VAL	2.6
2	L	32	SER	2.6
2	J	41	THR	2.6
2	H	19	ASP	2.6
1	C	7	TYR	2.6
1	E	221	ARG	2.6
2	F	25	HIS	2.6
1	A	262	SER	2.6
1	C	135	SER	2.6
1	C	127	ASP	2.6
1	I	191	LEU	2.6
2	F	4	GLY	2.6
1	G	4	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	9	ALA	2.6
1	E	23	ASN	2.6
2	J	135	ASN	2.6
2	B	140	PHE	2.6
1	K	123	TRP	2.5
1	K	1	ASP	2.5
1	A	5	ILE	2.5
1	K	283	HIS	2.5
2	B	22	TYR	2.5
1	K	6	GLY	2.5
2	H	33	GLY	2.5
2	J	67	GLY	2.5
1	C	315	ALA	2.5
2	D	28	ASN	2.5
2	L	48	ILE	2.5
2	L	39	LYS	2.5
2	B	139	GLU	2.5
2	F	22	TYR	2.5
2	D	23	GLY	2.5
2	H	66	VAL	2.5
1	K	141	ALA	2.5
1	G	74	ASN	2.5
1	K	129	THR	2.5
2	D	21	TRP	2.5
1	A	221	ARG	2.5
2	F	127	ARG	2.5
1	A	8	HIS	2.5
2	F	139	GLU	2.5
1	K	260	GLY	2.5
2	L	17	MET	2.5
2	F	3	PHE	2.5
1	A	22	LYS	2.5
1	A	289	ASN	2.5
1	C	5	ILE	2.5
1	C	263	SER	2.5
2	H	65	SER	2.5
2	B	21	TRP	2.5
2	F	38	LEU	2.5
2	J	29	GLU	2.5
1	E	155	GLY	2.5
1	C	124	PRO	2.5
2	H	131	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	J	153	LYS	2.4
1	I	281	THR	2.4
2	L	156	THR	2.4
1	I	156	ASN	2.4
1	I	139	SER	2.4
1	E	263	SER	2.4
2	D	26	HIS	2.4
2	F	149	MET	2.4
1	G	78	TYR	2.4
1	A	141	ALA	2.4
2	D	35	ALA	2.4
1	G	2	THR	2.4
2	H	38	LEU	2.4
1	G	186	SER	2.4
2	B	25	HIS	2.4
1	I	279	CYS	2.4
2	L	14	TRP	2.4
2	H	29	GLU	2.4
1	K	131	GLY	2.4
2	J	123	LYS	2.4
2	L	34	TYR	2.4
2	H	15	THR	2.4
2	L	56	ILE	2.4
2	B	156	THR	2.4
1	G	320	ASN	2.4
2	F	124	SER	2.4
2	J	11	GLU	2.4
2	L	137	CYS	2.4
2	D	120	GLU	2.4
2	J	13	GLY	2.4
2	F	8	GLY	2.4
2	F	23	GLY	2.4
2	F	31	GLY	2.4
1	G	271	GLN	2.4
1	C	129	THR	2.4
1	C	265	ILE	2.4
2	L	10	ILE	2.4
2	H	128	ASN	2.4
1	K	261	SER	2.4
1	E	261	SER	2.4
2	H	32	SER	2.4
2	H	113	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	120	GLU	2.4
2	F	132	GLU	2.4
1	C	271	GLN	2.4
1	C	192	TYR	2.3
2	D	24	TYR	2.3
1	I	316	THR	2.3
1	K	84	ASN	2.3
1	C	21	GLU	2.3
2	J	150	GLU	2.3
2	J	151	SER	2.3
2	L	116	LYS	2.3
1	I	291	PRO	2.3
1	K	319	ARG	2.3
2	H	127	ARG	2.3
2	J	42	GLN	2.3
1	I	26	VAL	2.3
2	B	55	VAL	2.3
1	C	144	PHE	2.3
2	H	5	ALA	2.3
2	L	9	PHE	2.3
2	J	15	THR	2.3
1	A	159	PRO	2.3
2	D	14	TRP	2.3
1	I	155	GLY	2.3
2	J	137	CYS	2.3
1	G	26	VAL	2.3
2	L	115	VAL	2.3
2	B	66	VAL	2.3
1	A	69	LEU	2.3
1	A	198	TYR	2.3
1	C	18	THR	2.3
1	A	74	ASN	2.3
2	L	28	ASN	2.3
2	B	117	ASN	2.3
2	J	109	ASP	2.3
1	E	130	ARG	2.3
1	A	246	GLY	2.3
2	D	13	GLY	2.3
2	F	134	GLY	2.3
1	K	321	VAL	2.3
1	A	303	CYS	2.3
1	C	321	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	122	VAL	2.3
1	G	191	LEU	2.3
2	H	118	LEU	2.3
2	D	133	ILE	2.3
2	L	25	HIS	2.3
2	L	154	ASN	2.3
2	J	20	GLY	2.3
2	B	18	VAL	2.3
1	K	265	ILE	2.2
1	A	73	ALA	2.2
2	B	148	CYS	2.2
2	F	36	ALA	2.2
2	F	26	HIS	2.2
1	G	132	THR	2.2
1	K	222	GLU	2.2
2	L	139	GLU	2.2
2	D	29	GLU	2.2
2	J	146	ASN	2.2
2	H	112	ASP	2.2
1	E	260	GLY	2.2
2	H	20	GLY	2.2
2	B	4	GLY	2.2
2	F	20	GLY	2.2
2	J	38	LEU	2.2
1	I	8	HIS	2.2
1	K	270	ALA	2.2
1	E	244	ALA	2.2
2	L	45	ILE	2.2
2	B	143	LYS	2.2
2	B	135	ASN	2.2
1	A	127	ASP	2.2
2	J	134	GLY	2.2
2	F	40	SER	2.2
1	C	286	LEU	2.2
2	H	99	LEU	2.2
1	K	134	VAL	2.2
2	H	121	LYS	2.2
2	F	153	LYS	2.2
1	E	292	PHE	2.2
2	J	100	ILE	2.2
2	B	142	HIS	2.2
1	C	250	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	150	GLU	2.2
2	D	132	GLU	2.2
2	D	127	ARG	2.2
1	G	7	TYR	2.2
1	G	289	ASN	2.2
1	K	289	ASN	2.2
1	A	194	ASN	2.2
1	C	84	ASN	2.2
2	F	157	TYR	2.2
2	D	42	GLN	2.2
1	A	140	GLY	2.2
1	A	191	LEU	2.2
2	L	126	LEU	2.2
2	J	18	VAL	2.2
2	L	29	GLU	2.2
1	K	2	THR	2.2
1	I	136	CYS	2.2
2	J	144	CYS	2.2
1	I	218	PRO	2.2
2	B	60	ASN	2.2
2	F	34	TYR	2.2
1	G	153	LYS	2.2
1	K	40	LYS	2.2
1	K	149	LEU	2.2
1	C	272	VAL	2.2
2	L	40	SER	2.2
2	B	113	SER	2.2
2	D	7	ALA	2.1
1	G	319	ARG	2.1
1	K	130	ARG	2.1
1	A	299	THR	2.1
1	E	2	THR	2.1
1	A	90	CYS	2.1
1	A	218	PRO	2.1
1	C	188	GLN	2.1
2	L	129	ASN	2.1
2	F	28	ASN	2.1
2	L	16	GLY	2.1
1	C	16	VAL	2.1
2	H	152	VAL	2.1
1	A	76	TRP	2.1
1	A	94	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	319	ARG	2.1
1	A	107	THR	2.1
1	C	15	THR	2.1
2	H	156	THR	2.1
1	I	271	GLN	2.1
1	A	158	TYR	2.1
1	E	318	LEU	2.1
2	L	128	ASN	2.1
2	H	31	GLY	2.1
1	C	134	VAL	2.1
2	F	56	ILE	2.1
2	L	36	ALA	2.1
1	E	123	TRP	2.1
1	K	316	THR	2.1
1	E	190	THR	2.1
2	L	143	LYS	2.1
2	F	143	LYS	2.1
1	G	304	PRO	2.1
1	C	159	PRO	2.1
1	I	189	GLN	2.1
2	J	149	MET	2.1
2	L	101	LEU	2.1
2	D	148	CYS	2.1
1	I	6	GLY	2.1
1	I	28	HIS	2.1
1	I	192	TYR	2.1
2	J	9	PHE	2.1
2	J	145	ASP	2.1
1	C	261	SER	2.1
2	L	49	SER	2.1
1	E	222	GLU	2.1
1	C	86	LYS	2.1
1	A	280	GLN	2.1
1	I	44	LEU	2.1
2	J	128	ASN	2.1
2	B	114	ASN	2.1
1	E	279	CYS	2.1
2	J	12	GLY	2.1
1	E	78	TYR	2.1
1	E	265	ILE	2.1
1	C	187	ASP	2.0
2	H	9	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	37	ASP	2.0
2	D	147	GLU	2.0
1	K	263	SER	2.0
1	E	122	SER	2.0
1	K	154	LYS	2.0
1	A	150	TRP	2.0
1	C	190	THR	2.0
1	E	156	ASN	2.0
2	H	10	ILE	2.0
2	H	56	ILE	2.0
2	J	10	ILE	2.0
2	D	67	GLY	2.0
1	E	220	VAL	2.0
1	A	244	ALA	2.0
2	F	90	ASP	2.0
1	C	109	SER	2.0
1	G	312	LEU	2.0
1	I	51	GLN	2.0
1	G	88	GLY	2.0
1	C	125	ASN	2.0
2	H	67	GLY	2.0
2	F	60	ASN	2.0
1	I	319	ARG	2.0
1	E	319	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
3	NAG	E	402	14/15	0.05	0.51	30,30,30,30	0
3	NAG	G	404	14/15	0.34	0.31	30,30,30,30	0
3	NAG	A	404	14/15	0.35	0.27	30,30,30,30	0
3	NAG	G	401	14/15	0.39	0.38	30,30,30,30	0
3	NAG	G	402	14/15	0.46	0.30	30,30,30,30	0
3	NAG	K	402	14/15	0.52	0.33	30,30,30,30	0
3	NAG	K	403	14/15	0.52	0.33	30,30,30,30	0
3	NAG	C	401	14/15	0.53	0.32	30,30,30,30	0
3	NAG	K	401	14/15	0.53	0.23	30,30,30,30	0
3	NAG	C	402	14/15	0.55	0.23	30,30,30,30	0
3	NAG	A	402	14/15	0.56	0.37	30,30,30,30	0
3	NAG	C	403	14/15	0.57	0.23	30,30,30,30	0
3	NAG	I	401	14/15	0.57	0.26	30,30,30,30	0
3	NAG	E	401	14/15	0.59	0.24	30,30,30,30	0
3	NAG	A	401	14/15	0.59	0.28	30,30,30,30	0
3	NAG	E	403	14/15	0.61	0.23	30,30,30,30	0
3	NAG	K	404	14/15	0.63	0.23	30,30,30,30	0
3	NAG	I	404	14/15	0.63	0.26	30,30,30,30	0
3	NAG	E	404	14/15	0.63	0.31	30,30,30,30	0
3	NAG	I	402	14/15	0.66	0.28	30,30,30,30	0
3	NAG	C	404	14/15	0.66	0.28	30,30,30,30	0
3	NAG	I	403	14/15	0.68	0.25	30,30,30,30	0
3	NAG	G	403	14/15	0.71	0.21	30,30,30,30	0
3	NAG	A	403	14/15	0.72	0.27	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.