



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:55 PM UTC

PDB ID : 6Z7W / pdb_00006z7w
Title : Human insulin in complex with the analytical antibody HUI-018 Fab
Authors : Johansson, E.
Deposited on : 2020-06-02
Resolution : 2.42 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	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

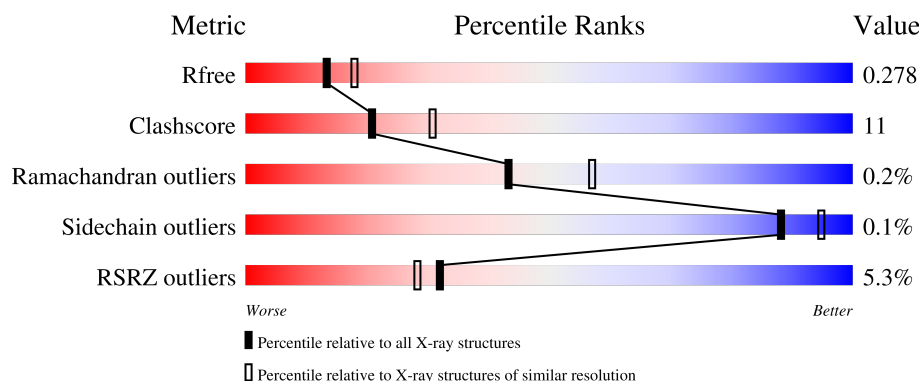
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	214	83% 17%
1	C	214	79% 20%
1	E	214	12% 75% 24%
1	G	214	80% 20%
2	B	224	5% 74% 23%

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Mol	Chain	Length	Quality of chain
2	D	224	
2	F	224	
2	H	224	
3	I	21	
3	K	21	
3	M	21	
3	O	21	
4	J	30	
4	L	30	
4	N	30	
4	P	30	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15292 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 MAb 6H10 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1672	1038	288	338	8			
1	C	213	Total	C	N	O	S	0	0	0
			1665	1035	287	336	7			
1	E	214	Total	C	N	O	S	0	0	0
			1672	1038	288	338	8			
1	G	214	Total	C	N	O	S	0	0	0
			1672	1038	288	338	8			

- Molecule 2 is a protein called HUI-018 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	0	0	0
			1641	1032	274	328	7			
2	D	213	Total	C	N	O	S	0	0	0
			1593	1008	263	316	6			
2	F	216	Total	C	N	O	S	0	0	0
			1618	1021	269	321	7			
2	H	219	Total	C	N	O	S	0	0	0
			1636	1030	273	326	7			

- Molecule 3 is a protein called Insulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	16	Total	C	N	O	S	0	0	0
			126	76	19	27	4			
3	K	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
3	M	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
3	O	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			

- Molecule 4 is a protein called Insulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	24	Total	C	N	O	S	0	0	0
			190	125	31	32	2			
4	L	24	Total	C	N	O	S	0	0	0
			190	125	31	32	2			
4	N	26	Total	C	N	O	S	0	0	0
			207	135	34	36	2			
4	P	26	Total	C	N	O	S	0	0	0
			208	136	35	35	2			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	107	Total	O	0	0
			107	107		
5	B	78	Total	O	0	0
			78	78		
5	C	80	Total	O	0	0
			80	80		
5	D	84	Total	O	0	0
			84	84		
5	E	34	Total	O	0	0
			34	34		
5	F	49	Total	O	0	0
			49	49		
5	G	110	Total	O	0	0
			110	110		
5	H	115	Total	O	0	0
			115	115		
5	I	15	Total	O	0	0
			15	15		
5	J	3	Total	O	0	0
			3	3		
5	K	5	Total	O	0	0
			5	5		
5	L	6	Total	O	0	0
			6	6		
5	M	3	Total	O	0	0
			3	3		
5	N	7	Total	O	0	0
			7	7		
5	O	6	Total	O	0	0
			6	6		

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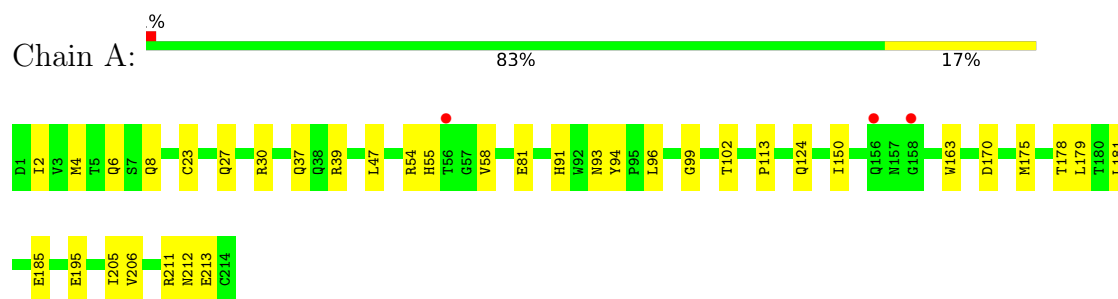
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	11	Total	O	0	0
			11	11		

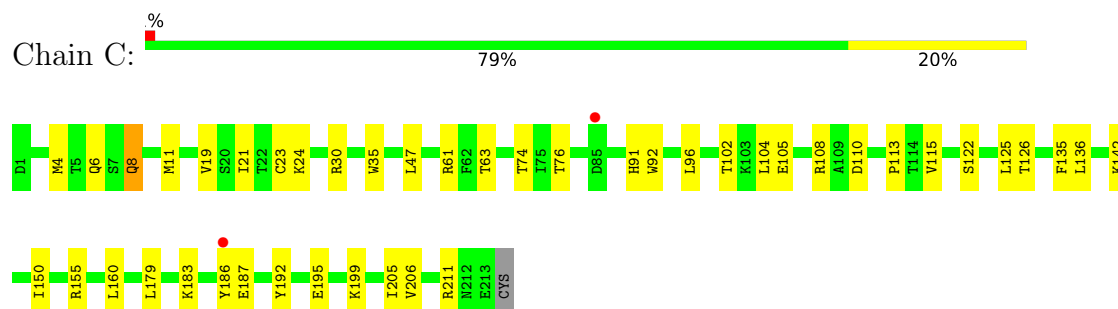
3 Residue-property plots

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.

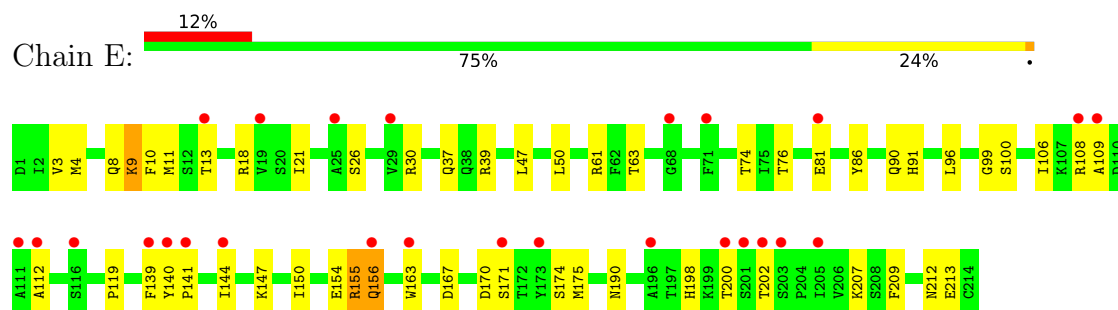
- Molecule 1: MAb 6H10 light chain



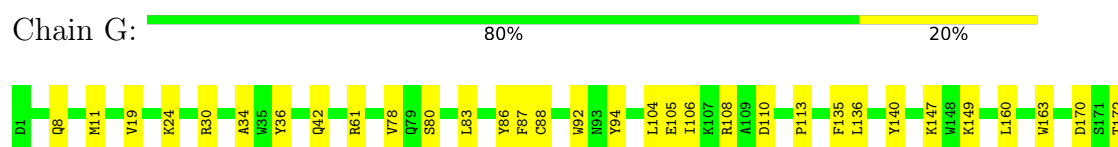
- Molecule 1: MAb 6H10 light chain



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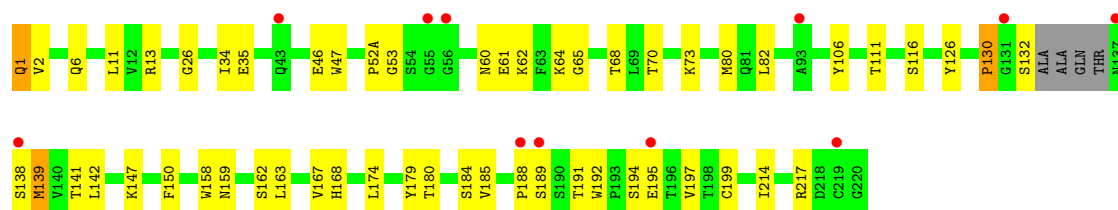
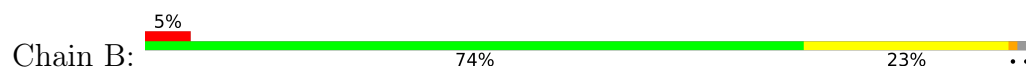


- Molecule 1: MAb 6H10 light chain

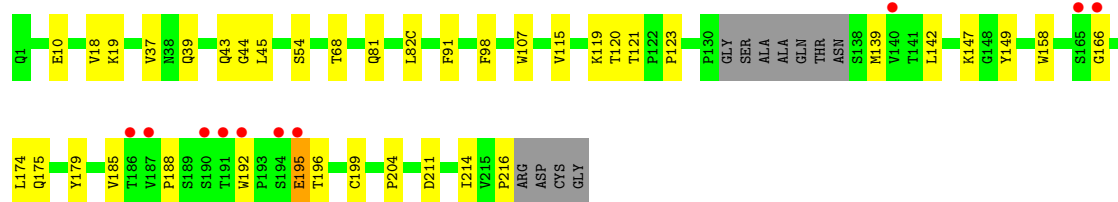
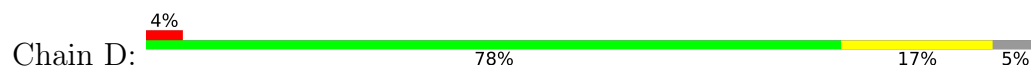




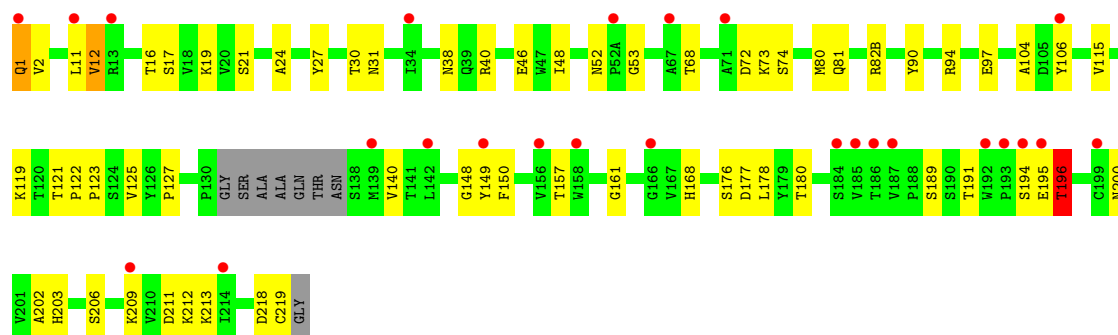
• Molecule 2: HUI-018 Fab Heavy Chain



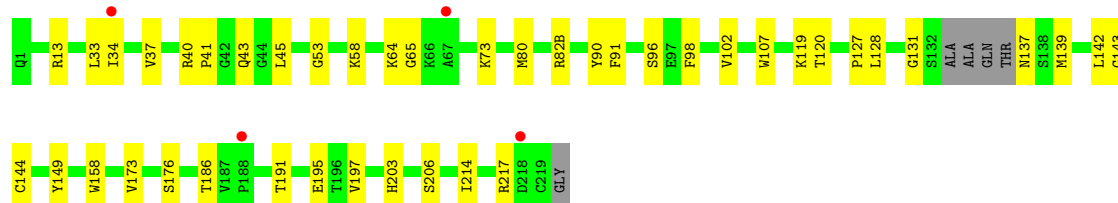
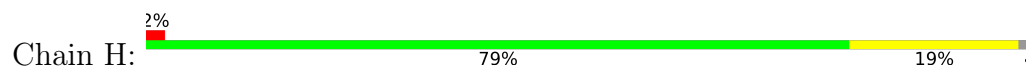
• Molecule 2: HUI-018 Fab Heavy Chain



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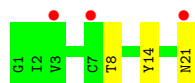
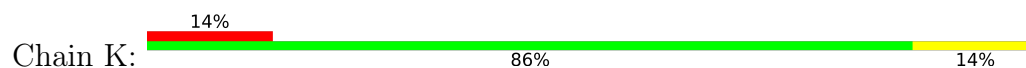
• Molecule 2: HUI-018 Fab Heavy Chain



● Molecule 3: Insulin



● Molecule 3: Insulin



● Molecule 3: Insulin



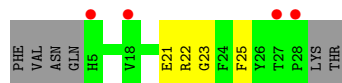
● Molecule 3: Insulin



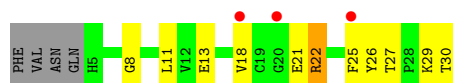
● Molecule 4: Insulin



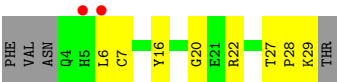
● Molecule 4: Insulin



● Molecule 4: Insulin



● Molecule 4: Insulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.23Å 216.61Å 101.09Å 90.00° 103.84° 90.00°	Depositor
Resolution (Å)	29.87 – 2.42 29.87 – 2.42	Depositor EDS
% Data completeness (in resolution range)	89.8 (29.87-2.42) 89.4 (29.87-2.42)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.209 , 0.275 0.213 , 0.278	Depositor DCC
R_{free} test set	1929 reflections (1.28%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15292	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.93% 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

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	0.44	0/1709	0.66	0/2320
1	C	0.44	0/1702	0.72	3/2312 (0.1%)
1	E	0.42	0/1709	0.82	9/2320 (0.4%)
1	G	0.47	0/1709	0.65	0/2320
2	B	0.42	0/1680	0.79	7/2293 (0.3%)
2	D	0.53	1/1632 (0.1%)	0.74	3/2231 (0.1%)
2	F	0.45	1/1657 (0.1%)	0.78	4/2264 (0.2%)
2	H	0.54	0/1675	0.68	0/2288
3	I	0.43	0/127	0.67	0/170
3	K	0.47	0/164	0.61	0/220
3	M	0.43	0/164	0.69	0/220
3	O	0.50	0/164	1.02	1/220 (0.5%)
4	J	0.38	0/196	0.82	0/265
4	L	0.70	1/196 (0.5%)	1.58	6/265 (2.3%)
4	N	0.56	0/213	1.30	5/286 (1.7%)
4	P	0.42	0/214	0.67	0/288
All	All	0.47	3/14911 (0.0%)	0.76	38/20282 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
4	N	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	12	VAL	C-N	-5.68	1.21	1.33
2	D	68	THR	C-O	-5.34	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	21	GLU	CB-CG	-5.09	1.37	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	21	GLU	CB-CA-C	-10.61	96.92	111.88
2	D	195	GLU	CA-CB-CG	10.61	135.31	114.10
2	B	1	GLN	N-CA-C	-10.05	82.86	111.00
4	L	21	GLU	CA-C-N	-9.19	106.83	121.44
4	L	21	GLU	C-N-CA	-9.19	106.83	121.44
4	N	22	ARG	CG-CD-NE	-8.83	92.56	112.00
4	L	21	GLU	CA-CB-CG	8.21	130.51	114.10
2	D	195	GLU	N-CA-CB	7.75	123.58	110.49
4	L	21	GLU	CB-CG-CD	-7.65	99.60	112.60
1	E	156	GLN	CA-CB-CG	7.59	129.27	114.10
1	E	156	GLN	CB-CG-CD	-7.09	100.55	112.60
1	E	155	ARG	CA-C-N	-7.01	110.44	122.14
1	E	155	ARG	C-N-CA	-7.01	110.44	122.14
2	D	195	GLU	CB-CA-C	-6.91	96.66	110.42
1	C	8	GLN	CA-CB-CG	6.86	127.81	114.10
2	B	139	MET	CG-SD-CE	-6.65	86.27	100.90
4	N	22	ARG	NE-CZ-NH2	6.56	125.11	119.20
4	N	22	ARG	CA-CB-CG	6.50	127.11	114.10
4	L	22	ARG	N-CA-C	-6.42	104.13	114.09
3	O	4	GLU	N-CA-CB	-6.24	96.11	110.83
1	C	24	LYS	CB-CG-CD	6.21	125.59	111.30
1	E	8	GLN	CA-C-N	-6.18	110.77	121.66
1	E	8	GLN	C-N-CA	-6.18	110.77	121.66
2	F	194	SER	CB-CA-C	-6.15	100.52	110.74
2	F	1	GLN	N-CA-C	6.11	128.11	111.00
2	B	194	SER	CA-C-N	-6.08	113.21	121.84
2	B	194	SER	C-N-CA	-6.08	113.21	121.84
1	E	9	LYS	CD-CE-NZ	-5.88	93.08	111.90
1	E	202	THR	CA-C-N	-5.71	113.49	124.01
1	E	202	THR	C-N-CA	-5.71	113.49	124.01
4	N	21	GLU	CB-CG-CD	5.71	122.31	112.60
1	C	8	GLN	CB-CG-CD	5.69	122.27	112.60
2	B	1	GLN	CA-C-N	-5.57	115.19	122.37
2	B	1	GLN	C-N-CA	-5.57	115.19	122.37
2	F	196	THR	N-CA-C	5.49	122.50	110.80
2	B	1	GLN	CA-CB-CG	-5.35	103.40	114.10
2	F	1	GLN	CB-CG-CD	5.22	121.48	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	22	ARG	NE-CZ-NH1	-5.07	116.43	121.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	213	GLU	Peptide
4	N	22	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1672	0	1601	24	0
1	C	1665	0	1597	33	0
1	E	1672	0	1602	45	0
1	G	1672	0	1602	35	0
2	B	1641	0	1609	38	0
2	D	1593	0	1571	30	0
2	F	1618	0	1592	47	0
2	H	1636	0	1607	36	0
3	I	126	0	109	5	0
3	K	163	0	149	4	0
3	M	163	0	149	8	0
3	O	163	0	149	7	0
4	J	190	0	177	12	0
4	L	190	0	177	2	0
4	N	207	0	197	9	0
4	P	208	0	198	9	0
5	A	107	0	0	2	0
5	B	78	0	0	10	0
5	C	80	0	0	4	1
5	D	84	0	0	7	0
5	E	34	0	0	4	1
5	F	49	0	0	6	0
5	G	110	0	0	9	1
5	H	115	0	0	11	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	15	0	0	2	0
5	J	3	0	0	0	0
5	K	5	0	0	0	0
5	L	6	0	0	0	0
5	M	3	0	0	0	0
5	N	7	0	0	2	0
5	O	6	0	0	0	0
5	P	11	0	0	2	0
All	All	15292	0	14086	319	2

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 11.

All (319) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:82(B):ARG:NH2	5:F:301:HOH:O	1.83	1.08
1:G:195:GLU:OE1	5:G:301:HOH:O	1.82	0.97
1:A:54:ARG:HD2	1:A:58:VAL:HG23	1.49	0.94
3:I:6:CYS:N	5:I:101:HOH:O	2.02	0.91
1:C:115:VAL:O	5:C:601:HOH:O	1.90	0.90
2:D:139:MET:O	5:D:301:HOH:O	1.87	0.89
1:E:30:ARG:NH1	5:E:301:HOH:O	2.04	0.89
2:F:191:THR:O	5:F:302:HOH:O	1.91	0.89
1:A:211:ARG:NH2	5:A:302:HOH:O	2.09	0.86
2:B:1:GLN:O	2:B:1:GLN:HG2	1.73	0.86
1:C:6:GLN:O	5:C:602:HOH:O	1.94	0.86
2:D:119:LYS:HE3	2:D:120:THR:H	1.42	0.84
4:P:16:TYR:O	5:P:701:HOH:O	1.94	0.84
4:J:5:HIS:CE1	4:J:9:SER:H	1.98	0.82
2:B:163:LEU:O	5:B:301:HOH:O	1.97	0.81
2:B:138:SER:O	2:B:189:SER:HB2	1.81	0.80
2:F:1:GLN:HG3	2:F:2:VAL:O	1.82	0.80
2:B:191:THR:HA	2:B:195:GLU:OE1	1.82	0.79
4:N:13:GLU:OE1	5:N:101:HOH:O	2.01	0.79
2:H:96:SER:HB3	2:H:102:VAL:HG12	1.65	0.78
2:H:176:SER:OG	5:H:301:HOH:O	2.00	0.78
1:C:195:GLU:HG3	1:C:206:VAL:HG22	1.64	0.77
2:B:35:GLU:OE2	2:B:47:TRP:NE1	2.18	0.77
1:A:54:ARG:NH1	5:A:304:HOH:O	2.17	0.76
1:C:11:MET:HE3	1:C:102:THR:HG21	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:41:PRO:O	5:H:302:HOH:O	2.05	0.75
1:E:91:HIS:O	5:E:302:HOH:O	2.05	0.74
2:F:148:GLY:H	2:F:180:THR:HG22	1.53	0.74
2:B:46:GLU:OE1	5:B:302:HOH:O	2.07	0.72
1:E:30:ARG:NH2	3:M:17:GLU:OE2	2.22	0.72
2:F:200:ASN:ND2	2:F:211:ASP:OD2	2.21	0.72
1:G:185:GLU:OE1	5:G:303:HOH:O	2.07	0.72
2:B:61:GLU:OE2	2:B:64:LYS:NZ	2.19	0.72
1:E:37:GLN:HB2	1:E:47:LEU:HD11	1.71	0.71
1:G:195:GLU:HG2	1:G:206:VAL:HG22	1.69	0.71
2:D:98:PHE:O	5:D:302:HOH:O	2.08	0.71
2:B:159:ASN:HB3	2:B:162:SER:HB2	1.72	0.71
2:F:46:GLU:OE2	5:F:303:HOH:O	2.09	0.70
4:P:20:GLY:N	5:P:701:HOH:O	2.23	0.70
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.73	0.70
2:B:132:SER:O	5:B:303:HOH:O	2.10	0.70
4:J:6:LEU:HD23	4:J:7:CYS:H	1.57	0.69
2:F:16:THR:HG22	2:F:17:SER:H	1.58	0.69
2:H:40:ARG:HH11	2:H:40:ARG:HG3	1.58	0.69
1:E:9:LYS:HE3	1:E:10:PHE:CZ	2.29	0.68
1:C:150:ILE:HD12	1:C:155:ARG:HD3	1.75	0.68
1:C:11:MET:HE1	1:C:21:ILE:HA	1.74	0.68
2:D:19:LYS:NZ	5:D:309:HOH:O	2.27	0.68
1:E:3:VAL:H	1:E:26:SER:HB3	1.56	0.67
2:F:203:HIS:ND1	2:F:206:SER:HB3	2.08	0.67
1:C:122:SER:HA	1:C:125:LEU:HD12	1.76	0.67
1:G:108:ARG:O	5:G:304:HOH:O	2.11	0.67
1:C:110:ASP:OD2	1:C:199:LYS:HE3	1.93	0.67
2:H:119:LYS:HE3	2:H:120:THR:H	1.60	0.67
1:E:108:ARG:NH2	1:E:170:ASP:O	2.29	0.66
2:B:191:THR:HG23	2:B:195:GLU:OE1	1.95	0.66
3:M:3:VAL:O	3:M:7:CYS:HB2	1.95	0.66
1:C:115:VAL:HG22	1:C:136:LEU:HD22	1.79	0.65
2:B:147:LYS:HA	2:B:180:THR:HG23	1.79	0.64
2:H:203:HIS:ND1	2:H:206:SER:HB3	2.12	0.64
2:F:53:GLY:HA2	2:F:73:LYS:HE3	1.79	0.64
1:E:11:MET:HE1	1:E:21:ILE:HA	1.80	0.64
1:E:156:GLN:HG3	5:E:307:HOH:O	1.98	0.63
1:C:108:ARG:O	5:C:604:HOH:O	2.15	0.63
1:A:55:HIS:O	1:A:58:VAL:HG22	1.99	0.63
2:B:34:ILE:HD12	2:B:52(A):PRO:HG3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:ALA:HA	1:E:200:THR:HG21	1.80	0.63
1:G:92:TRP:CE2	3:O:14:TYR:HB2	2.34	0.62
1:C:19:VAL:HG21	1:C:104:LEU:HD11	1.82	0.62
2:B:142:LEU:HD12	2:B:214:ILE:HG21	1.81	0.62
2:B:147:LYS:NZ	5:B:304:HOH:O	2.11	0.62
2:B:139:MET:HE3	2:B:188:PRO:HA	1.79	0.62
2:D:37:VAL:HG22	2:D:91:PHE:HB2	1.80	0.62
2:F:2:VAL:HG23	2:F:27:TYR:CD1	2.34	0.62
2:D:204:PRO:HB2	5:D:368:HOH:O	2.00	0.61
1:C:63:THR:HG23	1:C:74:THR:HB	1.82	0.61
1:E:108:ARG:HD3	1:E:109:ALA:O	2.00	0.61
2:H:137:ASN:O	2:H:139:MET:N	2.33	0.60
4:N:29:LYS:HB3	5:N:102:HOH:O	2.01	0.60
1:A:93:ASN:OD1	1:A:94:TYR:N	2.33	0.60
2:F:80:MET:HE1	2:F:90:TYR:CD2	2.37	0.59
1:C:92:TRP:CE2	3:K:14:TYR:HB2	2.36	0.59
2:D:18:VAL:HG22	2:D:82(C):LEU:HD11	1.84	0.59
2:B:168:HIS:HB2	2:B:184:SER:OG	2.01	0.59
3:O:3:VAL:HG21	4:P:28:PRO:HB3	1.85	0.59
2:D:166:GLY:O	2:D:185:VAL:HA	2.03	0.59
2:F:72:ASP:OD1	2:F:74:SER:OG	2.20	0.58
1:A:163:TRP:CD1	1:A:175:MET:HG3	2.39	0.58
1:C:4:MET:HE3	1:C:23:CYS:SG	2.44	0.58
1:A:181:LEU:HD22	1:A:185:GLU:HG2	1.85	0.58
2:F:1:GLN:CG	2:F:2:VAL:O	2.50	0.58
1:G:8:GLN:HG3	1:G:11:MET:HE3	1.85	0.58
2:D:119:LYS:O	2:D:121:THR:HG23	2.04	0.57
1:E:63:THR:HG23	1:E:74:THR:HB	1.86	0.57
1:E:108:ARG:HH12	1:E:171:SER:C	2.11	0.57
1:E:18:ARG:HD2	1:E:76:THR:HG22	1.85	0.57
3:O:3:VAL:O	3:O:7:CYS:HB3	2.05	0.57
2:F:1:GLN:HG3	2:F:2:VAL:N	2.19	0.57
2:F:1:GLN:HG3	2:F:2:VAL:C	2.30	0.57
2:F:140:VAL:HG12	2:F:189:SER:HA	1.85	0.57
2:D:39:GLN:HB2	2:D:45:LEU:HD23	1.86	0.57
2:H:119:LYS:NZ	5:H:314:HOH:O	2.37	0.56
1:C:35:TRP:O	1:C:47:LEU:HB2	2.05	0.56
1:C:92:TRP:NE1	3:K:14:TYR:HB2	2.20	0.56
2:B:158:TRP:CZ3	2:B:199:CYS:HB3	2.40	0.56
2:D:119:LYS:HE3	2:D:120:THR:N	2.18	0.56
2:F:97:GLU:HG3	5:F:332:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:ASN:OD1	5:B:306:HOH:O	2.18	0.56
2:F:2:VAL:HG23	2:F:27:TYR:HD1	1.69	0.56
1:E:190:ASN:ND2	1:E:212:ASN:OD1	2.29	0.56
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.89	0.55
1:G:19:VAL:HG23	1:G:78:VAL:HG21	1.88	0.55
1:G:61:ARG:HG2	1:G:61:ARG:HH11	1.72	0.55
1:C:160:LEU:HD11	2:D:175:GLN:HB3	1.89	0.55
2:F:19:LYS:HA	2:F:80:MET:O	2.06	0.55
1:G:30:ARG:HG3	1:G:92:TRP:CZ3	2.41	0.54
2:F:157:THR:HG22	2:F:161:GLY:H	1.72	0.54
1:E:91:HIS:HA	1:E:96:LEU:HD22	1.88	0.54
2:H:131:GLY:N	5:H:303:HOH:O	2.10	0.54
1:G:170:ASP:OD1	1:G:172:THR:HG22	2.08	0.54
1:E:39:ARG:NH1	1:E:81:GLU:O	2.40	0.54
2:H:137:ASN:N	5:H:317:HOH:O	2.40	0.54
2:F:195:GLU:O	5:F:302:HOH:O	2.18	0.54
2:H:43:GLN:HB3	5:H:304:HOH:O	2.08	0.53
2:B:217:ARG:NE	5:B:312:HOH:O	2.39	0.53
1:E:139:PHE:CE2	1:E:141:PRO:O	2.61	0.53
2:F:157:THR:HB	2:F:200:ASN:HB2	1.90	0.53
1:E:150:ILE:HD12	1:E:155:ARG:HD2	1.90	0.53
1:E:108:ARG:NH1	1:E:170:ASP:O	2.42	0.53
1:E:198:HIS:CE1	1:E:200:THR:HG23	2.43	0.53
1:E:147:LYS:HD2	1:E:154:GLU:CD	2.34	0.53
2:F:125:VAL:O	2:F:212:LYS:HE3	2.09	0.52
2:H:139:MET:HE3	2:H:186:THR:HG22	1.91	0.52
1:G:110:ASP:OD2	1:G:199:LYS:HD2	2.09	0.52
1:G:170:ASP:HA	5:G:320:HOH:O	2.10	0.52
1:G:189:HIS:O	1:G:211:ARG:NH1	2.42	0.52
3:M:7:CYS:SG	4:N:11:LEU:HD11	2.49	0.52
1:C:19:VAL:HG11	1:C:104:LEU:HD21	1.92	0.52
2:D:54:SER:OG	3:K:8:THR:O	2.22	0.52
1:E:144:ILE:HG13	1:E:198:HIS:HB2	1.90	0.51
4:N:27:THR:HG22	4:N:30:THR:HB	1.93	0.51
1:A:195:GLU:HG2	1:A:206:VAL:HG22	1.91	0.51
2:H:131:GLY:HA2	2:H:217:ARG:HD2	1.91	0.51
2:F:16:THR:HG22	2:F:17:SER:N	2.25	0.51
2:B:62:LYS:HD3	5:B:360:HOH:O	2.09	0.51
4:J:5:HIS:CG	4:J:9:SER:HB3	2.45	0.51
2:F:127:PRO:HD3	2:F:212:LYS:HD2	1.93	0.50
2:F:202:ALA:HB2	2:F:209:LYS:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:GLN:NE2	5:D:304:HOH:O	2.19	0.50
2:D:142:LEU:HD22	2:D:214:ILE:HG21	1.94	0.50
2:H:128:LEU:HB2	2:H:143:GLY:C	2.37	0.50
1:C:122:SER:O	1:C:126:THR:HG23	2.12	0.50
1:E:100:SER:HB2	5:E:325:HOH:O	2.11	0.50
1:G:105:GLU:OE2	5:G:305:HOH:O	2.19	0.50
2:D:211:ASP:OD1	5:D:305:HOH:O	2.20	0.50
1:G:197:THR:HG22	1:G:204:PRO:HG3	1.94	0.50
1:G:135:PHE:C	1:G:136:LEU:HD12	2.37	0.50
3:M:12:SER:OG	3:M:15:GLN:HG3	2.12	0.49
2:H:98:PHE:CE1	4:P:7:CYS:HB2	2.47	0.49
1:A:30:ARG:NH2	3:I:17:GLU:OE2	2.45	0.49
1:C:135:PHE:O	1:C:136:LEU:HD23	2.12	0.49
1:E:9:LYS:HE3	1:E:10:PHE:CE2	2.47	0.49
2:F:176:SER:O	2:F:177:ASP:HB2	2.13	0.49
2:H:40:ARG:HG3	2:H:40:ARG:NH1	2.26	0.49
2:D:174:LEU:HG	2:D:179:TYR:CE1	2.47	0.49
2:H:37:VAL:HG22	2:H:91:PHE:HB2	1.95	0.49
1:A:39:ARG:NH2	1:A:81:GLU:O	2.45	0.49
2:D:123:PRO:HB3	2:D:149:TYR:HB3	1.93	0.48
1:E:163:TRP:CZ2	1:E:175:MET:HE3	2.47	0.48
2:F:122:PRO:HB3	2:F:206:SER:OG	2.12	0.48
1:G:136:LEU:HD12	1:G:136:LEU:N	2.28	0.48
2:H:119:LYS:HE3	2:H:120:THR:N	2.27	0.48
2:D:195:GLU:HB2	2:D:196:THR:H	1.33	0.48
3:M:19:TYR:HA	4:N:25:PHE:HE1	1.79	0.48
1:C:183:LYS:O	1:C:187:GLU:HG3	2.14	0.48
3:O:3:VAL:CG2	4:P:28:PRO:HB3	2.44	0.48
1:E:167:ASP:HB3	1:E:171:SER:N	2.29	0.48
3:I:6:CYS:N	5:I:104:HOH:O	2.46	0.48
4:J:5:HIS:ND1	4:J:6:LEU:N	2.61	0.48
2:F:40:ARG:HG3	2:F:40:ARG:HH11	1.79	0.47
2:B:6:GLN:NE2	2:B:111:THR:OG1	2.46	0.47
2:H:191:THR:O	2:H:195:GLU:N	2.37	0.47
4:J:5:HIS:CG	4:J:6:LEU:N	2.82	0.47
1:E:61:ARG:HB3	1:E:76:THR:O	2.14	0.47
2:B:130:PRO:HG3	2:B:141:THR:O	2.14	0.47
1:C:8:GLN:CB	1:C:11:MET:HE2	2.44	0.47
1:G:92:TRP:NE1	3:O:14:TYR:HB2	2.30	0.47
2:D:82(C):LEU:HB3	2:D:115:VAL:HG21	1.96	0.47
1:G:42:GLN:HB2	5:G:318:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:5:HIS:ND1	4:J:6:LEU:C	2.73	0.47
2:D:147:LYS:NZ	2:D:175:GLN:OE1	2.47	0.47
3:O:21:ASN:HB2	4:P:22:ARG:O	2.14	0.47
2:B:174:LEU:HG	2:B:179:TYR:CE1	2.50	0.47
2:F:12:VAL:O	2:F:115:VAL:HA	2.15	0.47
2:D:43:GLN:HB3	5:D:303:HOH:O	2.14	0.46
2:F:24:ALA:HB1	2:F:27:TYR:CE1	2.50	0.46
2:H:53:GLY:HA2	2:H:73:LYS:HD3	1.96	0.46
2:F:206:SER:OG	2:F:206:SER:O	2.34	0.46
1:E:108:ARG:HD3	1:E:109:ALA:N	2.31	0.46
1:G:24:LYS:NZ	5:G:302:HOH:O	1.89	0.46
1:C:61:ARG:HB3	1:C:76:THR:O	2.16	0.46
4:J:5:HIS:HD1	4:J:6:LEU:C	2.22	0.46
1:A:170:ASP:OD1	1:A:170:ASP:C	2.59	0.45
4:J:6:LEU:CD2	4:J:7:CYS:H	2.24	0.45
1:A:91:HIS:HA	1:A:96:LEU:HD22	1.98	0.45
2:D:37:VAL:HG21	2:D:107:TRP:CZ3	2.51	0.45
4:P:27:THR:O	4:P:27:THR:OG1	2.34	0.45
1:A:2:ILE:HG12	1:A:27:GLN:HG2	1.97	0.45
2:B:53:GLY:HA2	2:B:73:LYS:HE3	1.97	0.45
1:G:163:TRP:HB3	5:G:382:HOH:O	2.15	0.45
1:A:4:MET:O	1:A:99:GLY:HA2	2.16	0.45
2:H:144:CYS:HB2	2:H:158:TRP:CH2	2.51	0.45
3:M:16:LEU:HB2	4:N:18:VAL:HG11	1.98	0.45
1:E:108:ARG:NH1	1:E:171:SER:C	2.74	0.45
2:F:30:THR:HG23	2:F:31:ASN:CG	2.42	0.45
2:B:167:VAL:HG22	2:B:185:VAL:HG23	1.99	0.45
2:B:1:GLN:O	2:B:26:GLY:HA3	2.16	0.45
2:B:65:GLY:HA3	5:B:317:HOH:O	2.16	0.45
1:A:178:THR:HG21	5:B:344:HOH:O	2.16	0.45
2:B:2:VAL:HG21	2:B:106:TYR:CE2	2.52	0.45
2:B:11:LEU:HD11	2:B:150:PHE:HZ	1.80	0.45
1:E:9:LYS:CE	1:E:10:PHE:CZ	2.99	0.45
2:F:68:THR:OG1	2:F:81:GLN:HB3	2.17	0.45
1:E:119:PRO:HG3	1:E:209:PHE:CD2	2.52	0.44
1:G:94:TYR:CD2	2:H:58:LYS:HD3	2.53	0.44
2:F:123:PRO:HB3	2:F:149:TYR:HB3	1.97	0.44
1:G:80:SER:O	1:G:83:LEU:HD12	2.17	0.44
2:H:119:LYS:HD2	2:H:119:LYS:HA	1.76	0.44
2:D:119:LYS:HD2	2:D:119:LYS:HA	1.77	0.44
2:H:142:LEU:HD12	2:H:197:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:624:HOH:O	2:D:44:GLY:HA3	2.17	0.44
2:F:38:ASN:HB3	2:F:48:ILE:HD11	2.00	0.44
2:B:73:LYS:H	2:B:73:LYS:HG3	1.61	0.44
1:C:30:ARG:HG3	1:C:92:TRP:CZ3	2.53	0.44
1:E:50:LEU:HD23	1:E:50:LEU:HA	1.84	0.44
2:B:192:TRP:CD1	2:B:197:VAL:HG23	2.53	0.44
1:E:4:MET:O	1:E:99:GLY:HA2	2.17	0.44
2:F:94:ARG:O	2:F:104:ALA:HA	2.17	0.44
2:B:192:TRP:HD1	2:B:197:VAL:HG23	1.82	0.44
1:E:37:GLN:HG3	1:E:86:TYR:CE2	2.53	0.44
2:H:37:VAL:HG21	2:H:107:TRP:CZ3	2.53	0.43
1:E:11:MET:CE	1:E:21:ILE:HA	2.47	0.43
2:D:139:MET:SD	2:D:188:PRO:HA	2.58	0.43
1:E:140:TYR:CD1	1:E:141:PRO:HA	2.53	0.43
1:G:113:PRO:HG2	1:G:205:ILE:HD12	2.00	0.43
1:G:186:TYR:CE2	1:G:211:ARG:HD2	2.53	0.43
4:J:5:HIS:CD2	4:J:9:SER:HB3	2.53	0.43
1:E:9:LYS:CE	1:E:10:PHE:CE2	3.02	0.43
2:H:13:ARG:N	5:H:310:HOH:O	2.29	0.43
4:N:27:THR:CG2	4:N:30:THR:HB	2.49	0.43
1:E:167:ASP:HB3	1:E:171:SER:H	1.82	0.43
2:F:177:ASP:O	2:F:178:LEU:HD23	2.18	0.43
1:C:105:GLU:OE2	1:C:142:LYS:NZ	2.51	0.43
1:G:87:PHE:CD2	2:H:45:LEU:HD12	2.54	0.43
4:J:5:HIS:CE1	4:J:9:SER:HB3	2.54	0.43
1:G:83:LEU:HD13	1:G:106:ILE:HD11	2.01	0.43
2:D:10:GLU:HG2	2:D:18:VAL:HG11	2.01	0.43
2:H:131:GLY:CA	5:H:303:HOH:O	2.63	0.43
2:F:21:SER:OG	5:F:304:HOH:O	2.22	0.43
1:G:147:LYS:HE3	1:G:149:LYS:HE3	2.00	0.43
2:H:65:GLY:O	2:H:82(B):ARG:NH1	2.52	0.43
4:L:23:GLY:HA3	4:N:26:TYR:O	2.19	0.43
4:P:27:THR:C	4:P:29:LYS:H	2.27	0.43
1:E:39:ARG:NH1	1:E:81:GLU:HB2	2.34	0.43
1:G:30:ARG:NH1	5:G:306:HOH:O	2.28	0.43
2:B:70:THR:OG1	5:B:307:HOH:O	2.20	0.42
2:F:11:LEU:HD11	2:F:150:PHE:HZ	1.84	0.42
2:F:196:THR:HG23	2:F:213:LYS:HD2	1.99	0.42
1:E:108:ARG:CZ	1:E:170:ASP:O	2.67	0.42
2:F:52:ASN:N	3:M:10:ILE:HD11	2.35	0.42
2:F:218:ASP:OD1	2:F:219:CYS:N	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:TYR:CD1	1:G:140:TYR:C	2.98	0.42
2:F:195:GLU:OE1	2:F:195:GLU:HA	2.19	0.42
2:F:119:LYS:O	2:F:121:THR:HG23	2.20	0.42
1:G:160:LEU:HD13	2:H:173:VAL:HG21	2.01	0.42
1:C:187:GLU:HA	1:C:211:ARG:CZ	2.50	0.42
3:K:21:ASN:OD1	4:L:25:PHE:CD2	2.73	0.42
3:I:13:LEU:HB3	4:J:18:VAL:CG2	2.50	0.41
4:J:6:LEU:CG	4:J:7:CYS:H	2.33	0.41
3:M:5:GLN:HG2	3:M:11:CYS:SG	2.60	0.41
1:A:4:MET:HE3	1:A:23:CYS:SG	2.59	0.41
1:A:6:GLN:NE2	1:A:102:THR:OG1	2.48	0.41
1:E:207:LYS:HD3	1:E:207:LYS:HA	1.88	0.41
2:H:64:LYS:HA	5:H:306:HOH:O	2.20	0.41
1:A:113:PRO:HG2	1:A:205:ILE:HD12	2.02	0.41
2:H:80:MET:HE1	2:H:90:TYR:CD2	2.56	0.41
1:C:150:ILE:HG12	1:C:192:TYR:CD2	2.56	0.41
1:E:174:SER:OG	2:F:168:HIS:CD2	2.74	0.41
1:C:8:GLN:HG3	1:C:11:MET:HE2	2.02	0.41
2:D:192:TRP:CZ2	2:D:216:PRO:HD3	2.56	0.41
1:A:93:ASN:ND2	3:I:14:TYR:CD2	2.89	0.41
1:A:124:GLN:HG3	2:B:126:TYR:CE2	2.56	0.41
1:E:13:THR:O	1:E:106:ILE:HA	2.20	0.41
3:O:13:LEU:O	3:O:16:LEU:HB2	2.21	0.41
1:A:212:ASN:OD1	1:A:213:GLU:HG3	2.20	0.41
2:B:159:ASN:CB	2:B:162:SER:HB2	2.46	0.41
2:D:158:TRP:CZ3	2:D:199:CYS:HB3	2.55	0.41
2:H:127:PRO:CB	2:H:214:ILE:HD12	2.50	0.41
4:P:6:LEU:HD23	4:P:6:LEU:HA	1.61	0.41
2:B:13:ARG:HA	2:B:116:SER:O	2.20	0.41
4:N:8:GLY:HA2	4:N:11:LEU:HD12	2.03	0.41
1:A:8:GLN:O	1:A:102:THR:HG23	2.21	0.40
2:B:80:MET:HE3	2:B:82:LEU:CD1	2.51	0.40
2:D:19:LYS:HD2	2:D:81:GLN:HB2	2.03	0.40
1:E:4:MET:HE2	1:E:90:GLN:HB3	2.03	0.40
2:H:64:LYS:HE3	5:H:306:HOH:O	2.22	0.40
1:C:113:PRO:HG2	1:C:205:ILE:HD12	2.03	0.40
1:G:30:ARG:HG3	1:G:92:TRP:CH2	2.56	0.40
1:G:34:ALA:O	1:G:88:CYS:HA	2.22	0.40
2:H:33:LEU:O	2:H:34:ILE:HD13	2.21	0.40
2:H:149:TYR:OH	5:H:305:HOH:O	2.22	0.40
1:C:8:GLN:CG	1:C:11:MET:HE2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:LEU:HD23	2:B:174:LEU:HA	1.76	0.40
1:C:91:HIS:HA	1:C:96:LEU:HD22	2.02	0.40
1:C:150:ILE:HD11	1:C:179:LEU:HD21	2.04	0.40
2:F:2:VAL:HG11	2:F:106:TYR:CE2	2.56	0.40
1:G:19:VAL:HG11	1:G:104:LEU:HD11	2.04	0.40
1:C:186:TYR:CE2	1:C:211:ARG:HD2	2.57	0.40
1:G:36:TYR:O	1:G:86:TYR:HA	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:333:HOH:O	5:G:408:HOH:O[1_556]	1.86	0.34
5:C:674:HOH:O	5:H:401:HOH:O[2_344]	2.15	0.05

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	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
1	C	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
1	E	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
1	G	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
2	B	216/224 (96%)	206 (95%)	9 (4%)	1 (0%)	24	35
2	D	209/224 (93%)	200 (96%)	9 (4%)	0	100	100
2	F	212/224 (95%)	204 (96%)	7 (3%)	1 (0%)	24	35
2	H	215/224 (96%)	208 (97%)	7 (3%)	0	100	100
3	I	14/21 (67%)	12 (86%)	1 (7%)	1 (7%)	1	0
3	K	19/21 (90%)	17 (90%)	2 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
3	O	19/21 (90%)	16 (84%)	3 (16%)	0	100	100
4	J	22/30 (73%)	20 (91%)	1 (4%)	1 (4%)	2	1
4	L	22/30 (73%)	21 (96%)	1 (4%)	0	100	100
4	N	24/30 (80%)	22 (92%)	2 (8%)	0	100	100
4	P	24/30 (80%)	23 (96%)	1 (4%)	0	100	100
All	All	1862/1956 (95%)	1781 (96%)	77 (4%)	4 (0%)	43	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	J	6	LEU
2	F	196	THR
2	B	130	PRO
3	I	20	CYS

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	191/191 (100%)	191 (100%)	0	100	100
1	C	190/191 (100%)	190 (100%)	0	100	100
1	E	191/191 (100%)	191 (100%)	0	100	100
1	G	191/191 (100%)	191 (100%)	0	100	100
2	B	187/189 (99%)	186 (100%)	1 (0%)	81	90
2	D	182/189 (96%)	182 (100%)	0	100	100
2	F	185/189 (98%)	185 (100%)	0	100	100
2	H	187/189 (99%)	187 (100%)	0	100	100
3	I	16/20 (80%)	16 (100%)	0	100	100
3	K	20/20 (100%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	20/20 (100%)	20 (100%)	0	100	100
3	O	20/20 (100%)	20 (100%)	0	100	100
4	J	20/26 (77%)	20 (100%)	0	100	100
4	L	20/26 (77%)	20 (100%)	0	100	100
4	N	22/26 (85%)	22 (100%)	0	100	100
4	P	22/26 (85%)	22 (100%)	0	100	100
All	All	1664/1704 (98%)	1663 (100%)	1 (0%)	88	95

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

Mol	Chain	Res	Type
2	B	68	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	79	GLN
1	A	91	HIS
1	A	210	ASN
1	C	8	GLN
1	C	42	GLN
2	D	32	HIS
1	E	53	ASN
1	E	189	HIS
2	F	43	GLN
2	F	200	ASN
1	G	37	GLN
1	G	53	ASN
4	J	10	HIS
4	L	10	HIS
3	M	18	ASN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	214/214 (100%)	0.17	3 (1%) 73 70	19, 33, 49, 65	0
1	C	213/214 (99%)	0.42	2 (0%) 81 79	22, 43, 57, 70	0
1	E	214/214 (100%)	0.91	26 (12%) 8 6	28, 52, 78, 85	0
1	G	214/214 (100%)	0.06	1 (0%) 87 86	16, 29, 48, 59	0
2	B	220/224 (98%)	0.51	11 (5%) 34 30	25, 41, 65, 85	0
2	D	213/224 (95%)	0.32	10 (4%) 36 32	18, 34, 72, 86	0
2	F	216/224 (96%)	0.93	25 (11%) 9 7	34, 50, 81, 94	0
2	H	219/224 (97%)	0.14	4 (1%) 67 64	16, 30, 47, 67	0
3	I	16/21 (76%)	0.89	1 (6%) 26 22	36, 44, 55, 60	0
3	K	21/21 (100%)	1.15	3 (14%) 6 4	32, 51, 74, 79	0
3	M	21/21 (100%)	1.10	1 (4%) 35 32	45, 59, 69, 72	0
3	O	21/21 (100%)	0.62	1 (4%) 35 32	29, 45, 58, 74	0
4	J	24/30 (80%)	1.24	4 (16%) 4 3	33, 47, 63, 84	0
4	L	24/30 (80%)	1.08	4 (16%) 4 3	40, 48, 75, 81	0
4	N	26/30 (86%)	1.04	3 (11%) 9 7	43, 55, 75, 88	0
4	P	26/30 (86%)	0.50	2 (7%) 19 16	34, 45, 67, 75	0
All	All	1902/1956 (97%)	0.48	101 (5%) 32 28	16, 40, 70, 94	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	J	5	HIS	4.6
2	F	158	TRP	4.6
1	E	200	THR	4.4
1	E	163	TRP	3.8
1	E	139	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
2	F	34	ILE	3.7
2	B	56	GLY	3.7
3	M	3	VAL	3.6
1	E	140	TYR	3.6
2	D	195	GLU	3.5
3	O	3	VAL	3.5
2	F	71	ALA	3.3
3	K	3	VAL	3.2
4	N	25	PHE	3.1
4	J	6	LEU	3.1
2	B	138	SER	3.1
2	D	140	VAL	3.1
1	E	112	ALA	3.0
1	E	71	PHE	3.0
2	D	190	SER	2.9
1	E	109	ALA	2.9
2	B	188	PRO	2.9
2	B	137	ASN	2.8
4	L	5	HIS	2.8
1	E	111	ALA	2.8
1	E	205	ILE	2.8
2	F	187	VAL	2.8
2	D	187	VAL	2.8
2	F	186	THR	2.7
4	J	7	CYS	2.7
4	N	20	GLY	2.7
2	B	131	GLY	2.6
2	F	156	VAL	2.6
2	B	43	GLN	2.6
2	B	219	CYS	2.6
2	F	195	GLU	2.6
1	E	171	SER	2.6
1	E	141	PRO	2.6
1	E	156	GLN	2.6
2	D	165	SER	2.6
1	E	173	TYR	2.6
2	B	55	GLY	2.5
2	F	214	ILE	2.5
1	E	13	THR	2.5
1	E	203	SER	2.5
2	F	184	SER	2.5
4	L	18	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	194	SER	2.5
1	E	25	ALA	2.4
1	E	144	ILE	2.4
1	E	29	VAL	2.4
2	F	185	VAL	2.4
1	E	201	SER	2.4
3	I	7	CYS	2.4
2	D	191	THR	2.4
1	E	116	SER	2.4
1	A	156	GLN	2.4
3	K	21	ASN	2.4
2	H	34	ILE	2.3
2	B	93	ALA	2.3
4	L	28	PRO	2.3
2	F	13	ARG	2.3
2	F	166	GLY	2.3
1	E	19	VAL	2.3
1	E	108	ARG	2.3
2	F	199	CYS	2.3
1	E	202	THR	2.2
2	D	194	SER	2.2
2	F	52(A)	PRO	2.2
2	F	193	PRO	2.2
1	A	158	GLY	2.2
2	D	186	THR	2.2
2	H	218	ASP	2.2
4	N	18	VAL	2.2
2	F	142	LEU	2.2
1	E	81	GLU	2.2
2	D	192	TRP	2.2
2	H	188	PRO	2.2
1	E	68	GLY	2.1
4	P	6	LEU	2.1
1	C	85	ASP	2.1
2	F	149	TYR	2.1
3	K	7	CYS	2.1
2	F	1	GLN	2.1
2	F	11	LEU	2.1
2	B	195	GLU	2.1
2	F	106	TYR	2.1
4	P	5	HIS	2.1
2	F	67	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
4	J	17	LEU	2.1
2	D	166	GLY	2.1
4	L	27	THR	2.1
2	F	209	LYS	2.1
2	B	189	SER	2.1
1	G	214	CYS	2.1
1	E	196	ALA	2.0
2	H	67	ALA	2.0
2	F	139	MET	2.0
1	A	56	THR	2.0
2	F	192	TRP	2.0
1	C	186	TYR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.