



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:03 PM UTC

PDB ID : 3KIF / pdb_00003kif
Title : The crystal structures of two fragments truncated from 5-bladed beta-propeller lectin, tachylectin-2 (Lib1-B7-18 and Lib2-D2-15)
Authors : Dym, O.; Tawfik, D.S.; Yadid, I.; Israel Structural Proteomics Center (ISPC)
Deposited on : 2009-11-02
Resolution : 2.50 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

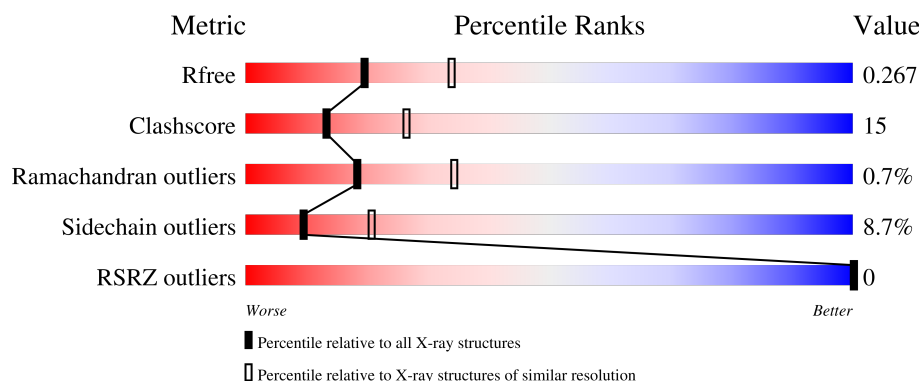
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	106	
1	B	106	
1	C	106	
1	D	106	
1	E	106	

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Mol	Chain	Length	Quality of chain
1	F	106	
1	G	106	
1	H	106	
1	I	106	
1	J	106	

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
2	GDL	J	110	-	-	X	-

2 Entry composition

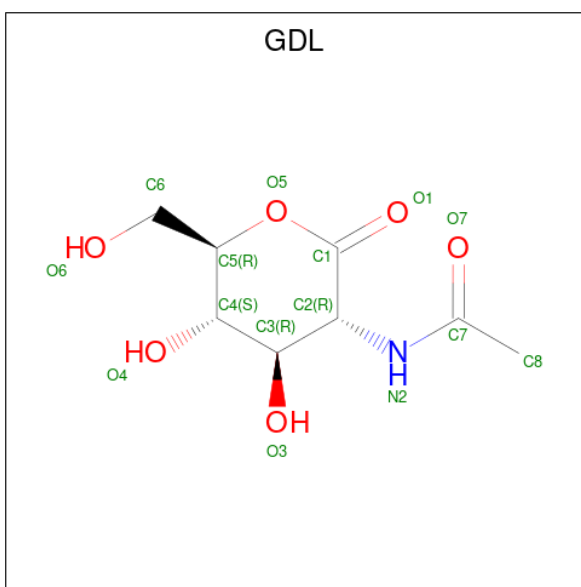
There are 4 unique types of molecules in this entry. The entry contains 7530 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 5-bladed beta-propeller lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	93	Total	C	N	O	S	0	0	0
			756	494	126	135	1			
1	B	88	Total	C	N	O	S	0	0	0
			719	474	120	124	1			
1	C	85	Total	C	N	O		0	0	0
			689	455	112	122				
1	D	91	Total	C	N	O	S	0	0	0
			740	486	124	129	1			
1	E	93	Total	C	N	O	S	0	0	0
			757	495	128	133	1			
1	F	92	Total	C	N	O	S	0	0	0
			748	490	125	132	1			
1	G	88	Total	C	N	O	S	0	0	0
			719	474	120	124	1			
1	H	85	Total	C	N	O		0	0	0
			689	455	112	122				
1	I	94	Total	C	N	O	S	0	0	0
			762	497	127	137	1			
1	J	93	Total	C	N	O	S	0	0	0
			757	495	128	133	1			

- Molecule 2 is 2-(acetylamido)-2-deoxy-D-glucono-1,5-lactone (CCD ID: GDL) (formula: $C_8H_{13}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	D	1	Total	C	N	O	0	0
			15	8	1	6		
2	D	1	Total	C	N	O	0	0
			15	8	1	6		
2	E	1	Total	C	N	O	0	0
			15	8	1	6		
2	F	1	Total	C	N	O	0	0
			15	8	1	6		
2	G	1	Total	C	N	O	0	0
			15	8	1	6		
2	I	1	Total	C	N	O	0	0
			15	8	1	6		
2	J	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		

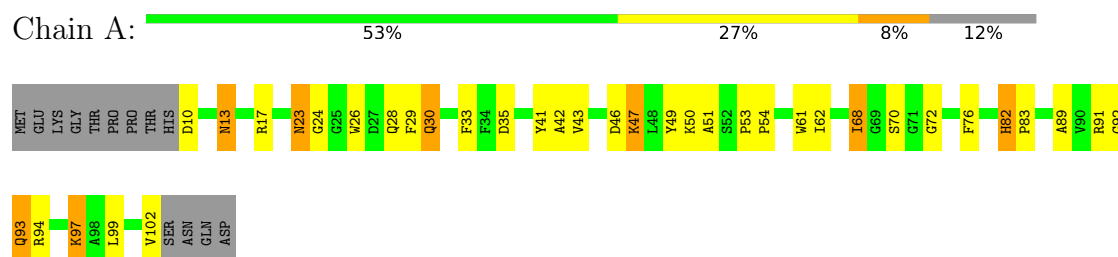
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	3	Total	O	0	0
			3	3		
4	C	2	Total	O	0	0
			2	2		
4	D	7	Total	O	0	0
			7	7		
4	E	3	Total	O	0	0
			3	3		
4	F	3	Total	O	0	0
			3	3		
4	G	6	Total	O	0	0
			6	6		
4	H	3	Total	O	0	0
			3	3		
4	I	5	Total	O	0	0
			5	5		
4	J	15	Total	O	0	0
			15	15		

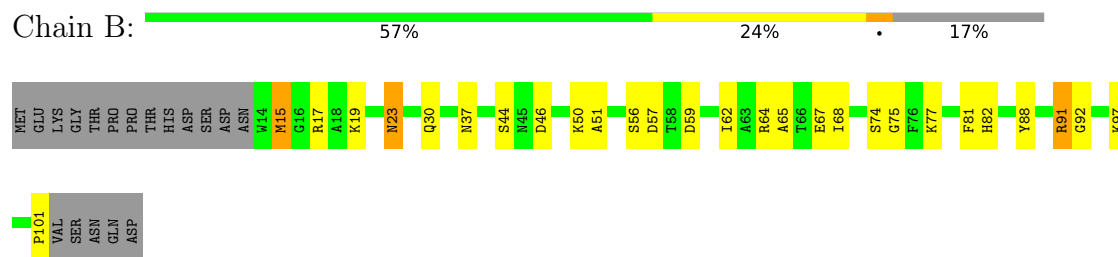
3 Residue-property plots [i](#)

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.

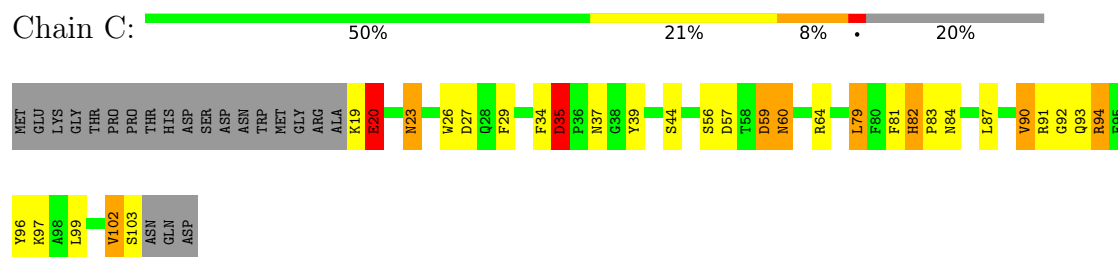
- Molecule 1: 5-bladed beta-propeller lectin



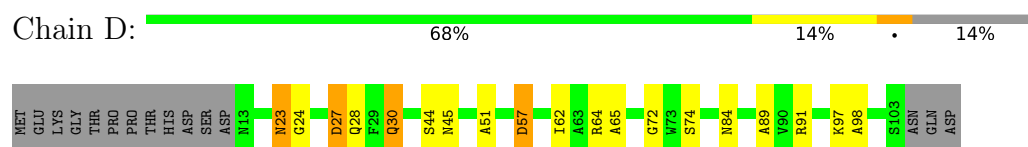
- Molecule 1: 5-bladed beta-propeller lectin



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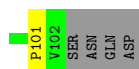
- Molecule 1: 5-bladed beta-propeller lectin

Chain E:  65% 17% 6% 12%



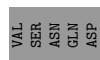
- Molecule 1: 5-bladed beta-propeller lectin

Chain F:  58% 23% 6% 13%

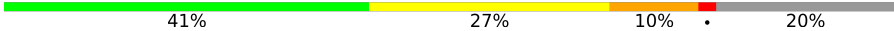


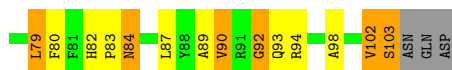
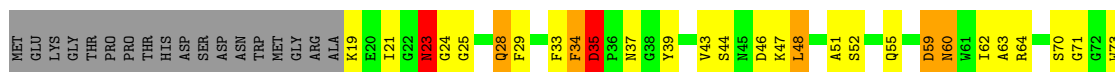
- Molecule 1: 5-bladed beta-propeller lectin

Chain G:  56% 23% 5% 17%



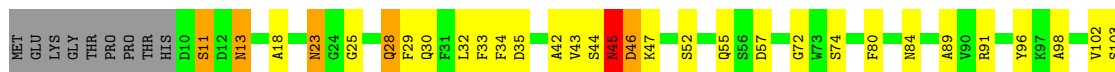
- Molecule 1: 5-bladed beta-propeller lectin

Chain H:  41% 27% 10% 20%



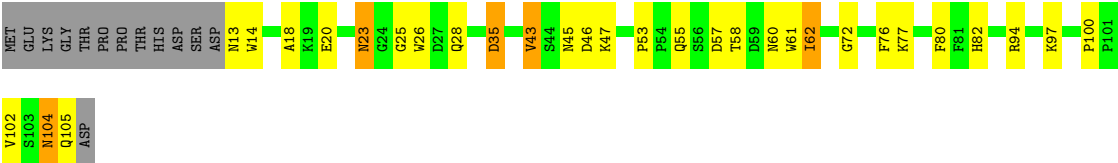
- Molecule 1: 5-bladed beta-propeller lectin

Chain I:  59% 24% 5% 11%



- Molecule 1: 5-bladed beta-propeller lectin

Chain J:  58% 25% 5% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	80.56Å 80.56Å 170.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.50) 99.2 (50.00-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.71 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.213 , 0.276 0.202 , 0.267	Depositor DCC
R_{free} test set	2145 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 7.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l 0.469 for h,-h-k,-l 0.032 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7530	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDL, SO4

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	1.36	3/785 (0.4%)	1.30	7/1065 (0.7%)
1	B	1.37	3/748 (0.4%)	1.35	6/1014 (0.6%)
1	C	1.44	5/716 (0.7%)	1.52	9/971 (0.9%)
1	D	1.36	2/769 (0.3%)	1.29	2/1043 (0.2%)
1	E	1.40	2/786 (0.3%)	1.46	10/1066 (0.9%)
1	F	1.38	6/777 (0.8%)	1.30	3/1054 (0.3%)
1	G	1.37	4/748 (0.5%)	1.32	5/1014 (0.5%)
1	H	1.43	2/716 (0.3%)	1.57	16/971 (1.6%)
1	I	1.38	2/791 (0.3%)	1.39	7/1073 (0.7%)
1	J	1.35	2/786 (0.3%)	1.48	10/1066 (0.9%)
All	All	1.38	31/7622 (0.4%)	1.40	75/10337 (0.7%)

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	C	0	2
1	G	0	1
1	H	0	2
1	I	0	1
All	All	0	6

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	89	ALA	CA-CB	-6.92	1.42	1.53
1	H	60	ASN	CA-C	6.54	1.60	1.53
1	C	35	ASP	CB-CG	-6.54	1.35	1.52
1	C	35	ASP	CA-C	-6.51	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	81	PHE	CA-C	-6.50	1.44	1.52
1	I	89	ALA	CA-CB	-6.46	1.42	1.53
1	H	35	ASP	CB-CG	-6.36	1.36	1.52
1	F	53	PRO	C-O	-6.35	1.19	1.24
1	F	91	ARG	N-CA	6.35	1.53	1.46
1	E	24	GLY	N-CA	6.30	1.51	1.45
1	F	93	GLN	CB-CG	6.12	1.70	1.52
1	A	82	HIS	CA-C	6.04	1.60	1.53
1	A	62	ILE	CA-CB	5.94	1.62	1.54
1	B	67	GLU	N-CA	-5.94	1.39	1.46
1	A	53	PRO	C-O	-5.85	1.20	1.25
1	J	76	PHE	CA-C	-5.82	1.45	1.52
1	F	82	HIS	CA-C	5.61	1.60	1.53
1	G	67	GLU	N-CA	-5.55	1.39	1.46
1	G	24	GLY	N-CA	5.47	1.50	1.44
1	B	77	LYS	C-O	-5.43	1.17	1.24
1	C	102	VAL	CA-CB	5.42	1.62	1.55
1	E	79	LEU	CA-C	-5.40	1.46	1.52
1	G	17	ARG	CA-C	5.32	1.60	1.52
1	C	60	ASN	CA-C	5.28	1.59	1.52
1	B	81	PHE	CA-C	-5.27	1.46	1.52
1	F	62	ILE	CA-CB	5.27	1.61	1.54
1	J	43	VAL	CA-CB	-5.26	1.48	1.54
1	D	30	GLN	CA-C	5.25	1.59	1.52
1	F	93	GLN	CG-CD	5.19	1.65	1.52
1	C	81	PHE	C-O	-5.13	1.17	1.23
1	I	32	LEU	C-O	-5.09	1.18	1.23

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	14	TRP	N-CA-C	11.81	123.70	111.07
1	E	100	PRO	CA-C-N	-9.70	110.91	120.52
1	E	100	PRO	C-N-CA	-9.70	110.91	120.52
1	E	102	VAL	N-CA-CB	-9.53	100.99	112.33
1	C	59	ASP	N-CA-C	9.19	121.38	111.36
1	A	23	ASN	N-CA-C	8.45	123.80	112.30
1	H	59	ASP	N-CA-C	8.34	120.45	111.36
1	G	100	PRO	O-C-N	8.03	124.92	121.15
1	C	102	VAL	N-CA-C	7.52	120.85	113.71
1	J	100	PRO	CA-C-N	-7.48	113.12	120.52
1	J	100	PRO	C-N-CA	-7.48	113.12	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	18	ALA	N-CA-C	7.43	121.47	110.48
1	J	53	PRO	CA-C-N	-7.42	110.56	119.84
1	J	53	PRO	C-N-CA	-7.42	110.56	119.84
1	D	23	ASN	N-CA-C	7.30	123.84	114.56
1	C	35	ASP	CB-CA-C	-7.11	96.17	110.17
1	G	24	GLY	N-CA-C	6.98	121.93	111.18
1	H	60	ASN	N-CA-C	6.87	119.60	111.02
1	H	90	VAL	N-CA-C	6.75	117.62	108.17
1	F	23	ASN	N-CA-C	6.74	123.06	113.02
1	H	70	SER	N-CA-C	6.72	124.85	114.64
1	H	35	ASP	CB-CA-C	-6.71	96.95	110.17
1	H	84	ASN	CB-CA-C	-6.45	97.94	110.46
1	B	23	ASN	CA-C-N	-6.44	113.26	120.53
1	B	23	ASN	C-N-CA	-6.44	113.26	120.53
1	A	92	GLY	N-CA-C	-6.39	99.13	111.02
1	H	102	VAL	N-CA-C	6.38	119.79	113.53
1	C	20	GLU	N-CA-C	-6.38	99.62	109.76
1	I	45	ASN	CA-C-N	-6.33	113.09	122.83
1	I	45	ASN	C-N-CA	-6.33	113.09	122.83
1	J	35	ASP	N-CA-C	-6.32	102.73	110.31
1	J	82	HIS	N-CA-C	-6.19	101.20	110.24
1	H	34	PHE	N-CA-C	6.19	120.13	110.17
1	B	56	SER	N-CA-C	6.18	117.54	108.14
1	H	59	ASP	CA-C-N	-6.17	113.40	122.78
1	H	59	ASP	C-N-CA	-6.17	113.40	122.78
1	H	52	SER	CA-C-N	-6.01	114.19	120.38
1	H	52	SER	C-N-CA	-6.01	114.19	120.38
1	F	53	PRO	CA-C-N	-5.93	113.67	119.78
1	F	53	PRO	C-N-CA	-5.93	113.67	119.78
1	C	99	LEU	CA-C-N	-5.89	114.31	120.38
1	C	99	LEU	C-N-CA	-5.89	114.31	120.38
1	I	13	ASN	CB-CA-C	5.87	120.20	110.81
1	E	53	PRO	CA-C-N	-5.86	114.71	120.98
1	E	53	PRO	C-N-CA	-5.86	114.71	120.98
1	H	23	ASN	N-CA-C	5.86	120.07	111.34
1	C	82	HIS	N-CA-C	-5.85	102.21	110.29
1	E	102	VAL	N-CA-C	-5.84	107.57	113.47
1	J	23	ASN	N-CA-C	5.82	123.09	113.89
1	A	99	LEU	CA-C-N	5.77	126.33	120.38
1	A	99	LEU	C-N-CA	5.77	126.33	120.38
1	C	23	ASN	N-CA-C	5.77	120.17	109.56
1	H	23	ASN	CA-C-N	-5.72	114.82	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	23	ASN	C-N-CA	-5.72	114.82	120.60
1	J	94	ARG	N-CA-C	5.62	119.14	110.42
1	E	102	VAL	CA-C-O	5.61	124.03	118.98
1	E	82	HIS	N-CA-C	-5.61	102.06	110.24
1	I	102	VAL	N-CA-C	5.54	120.86	109.34
1	E	102	VAL	CG1-CB-CG2	5.49	122.87	110.80
1	I	23	ASN	N-CA-C	5.46	120.42	113.55
1	A	47	LYS	N-CA-C	5.40	118.51	110.14
1	B	15	MET	N-CA-C	-5.29	105.62	111.71
1	B	17	ARG	N-CA-C	5.27	119.27	113.21
1	E	35	ASP	N-CA-C	-5.24	104.10	110.13
1	A	30	GLN	N-CA-C	-5.23	105.66	111.36
1	G	15	MET	N-CA-C	-5.21	106.02	112.38
1	I	35	ASP	N-CA-C	-5.20	104.08	110.31
1	H	73	TRP	N-CA-C	5.18	117.59	111.33
1	A	24	GLY	N-CA-C	-5.15	100.97	113.18
1	J	58	THR	N-CA-C	-5.08	107.11	113.72
1	I	46	ASP	N-CA-C	-5.07	106.84	112.57
1	D	64	ARG	N-CA-C	5.06	119.44	113.16
1	C	90	VAL	N-CA-C	5.06	115.25	108.17
1	B	30	GLN	N-CA-C	-5.04	105.25	111.40
1	G	17	ARG	N-CA-C	5.03	119.05	113.01

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	34	PHE	Peptide
1	C	35	ASP	Mainchain
1	G	75	GLY	Peptide
1	H	34	PHE	Peptide
1	H	35	ASP	Mainchain
1	I	44	SER	Peptide

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	756	0	695	29	0
1	B	719	0	667	26	0
1	C	689	0	640	28	0
1	D	740	0	687	15	0
1	E	757	0	701	19	0
1	F	748	0	691	30	0
1	G	719	0	667	20	0
1	H	689	0	640	35	0
1	I	762	0	700	21	0
1	J	757	0	701	20	0
2	A	15	0	8	1	0
2	B	15	0	8	1	0
2	D	30	0	16	4	0
2	E	15	0	8	1	0
2	F	15	0	8	0	0
2	G	15	0	8	0	0
2	I	15	0	8	1	0
2	J	15	0	8	9	0
3	E	5	0	0	0	0
3	J	5	0	0	0	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	7	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
4	G	6	0	0	1	0
4	H	3	0	0	0	0
4	I	5	0	0	0	0
4	J	15	0	0	1	0
All	All	7530	0	6861	212	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 15.

All (212) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ASN:O	1:A:23:ASN:ND2	1.85	1.10
1:H:82:HIS:CD2	1:H:84:ASN:H	1.79	0.99
1:C:82:HIS:CD2	1:C:84:ASN:H	1.81	0.99
1:F:91:ARG:HH11	1:G:15:MET:HE1	1.29	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:30:GLN:HE22	1:I:74:SER:CB	1.79	0.95
1:H:25:GLY:O	1:H:28:GLN:HG3	1.66	0.94
1:G:91:ARG:HG2	1:G:91:ARG:HH11	1.29	0.94
1:I:30:GLN:HE22	1:I:74:SER:HB2	1.33	0.94
2:J:110:GDL:O7	2:J:110:GDL:H3	1.63	0.94
1:H:71:GLY:O	1:I:11:SER:HB3	1.68	0.94
1:D:30:GLN:HE22	1:D:74:SER:HB2	1.34	0.92
1:A:46:ASP:OD2	1:A:72:GLY:N	2.02	0.91
1:C:82:HIS:HD2	1:C:84:ASN:N	1.71	0.87
1:H:82:HIS:HD2	1:H:84:ASN:N	1.72	0.86
1:G:27:ASP:O	1:G:28:GLN:HB2	1.75	0.85
1:E:23:ASN:OD1	1:E:24:GLY:N	2.09	0.85
1:F:23:ASN:O	1:F:23:ASN:ND2	2.10	0.85
1:C:82:HIS:HD2	1:C:84:ASN:H	0.88	0.83
1:C:92:GLY:O	1:D:27:ASP:OD1	1.97	0.83
1:H:82:HIS:HD2	1:H:84:ASN:H	0.88	0.82
1:A:97:LYS:O	1:A:97:LYS:HG3	1.81	0.81
1:B:68:ILE:HG22	1:B:101:PRO:HG2	1.65	0.79
1:H:35:ASP:HB3	1:H:37:ASN:H	1.48	0.78
1:C:35:ASP:HB2	1:C:39:TYR:H	1.52	0.75
1:H:92:GLY:O	1:H:93:GLN:HB2	1.87	0.75
1:H:25:GLY:O	1:H:28:GLN:CG	2.35	0.74
1:D:30:GLN:HE22	1:D:74:SER:CB	1.99	0.74
1:C:35:ASP:HB3	1:C:37:ASN:H	1.52	0.73
1:C:56:SER:HB2	1:E:105:GLN:HG2	1.69	0.73
1:H:79:LEU:HD22	1:H:87:LEU:HD11	1.69	0.73
1:E:20:GLU:HG2	1:E:57:ASP:OD1	1.89	0.72
1:C:82:HIS:CD2	1:C:84:ASN:CG	2.68	0.71
1:E:23:ASN:OD1	1:E:23:ASN:C	2.32	0.71
1:J:62:ILE:H	2:J:110:GDL:H6C2	1.54	0.71
1:A:23:ASN:O	1:A:23:ASN:CG	2.35	0.70
1:G:91:ARG:HG2	1:G:91:ARG:NH1	2.04	0.69
1:B:50:LYS:HD3	1:B:68:ILE:HD11	1.74	0.69
1:C:94:ARG:HG3	1:C:96:TYR:OH	1.94	0.69
1:C:56:SER:CB	1:E:105:GLN:HG2	2.23	0.68
1:D:57:ASP:O	2:D:238:GDL:H6C2	1.93	0.68
1:A:50:LYS:HB2	1:A:68:ILE:HD11	1.76	0.68
1:C:79:LEU:HD22	1:C:87:LEU:HD11	1.75	0.67
1:F:75:GLY:HA3	1:F:91:ARG:HH21	1.60	0.66
1:J:23:ASN:OD1	1:J:23:ASN:O	2.12	0.66
1:B:92:GLY:O	1:C:27:ASP:HB3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:ALA:HB2	1:F:65:ALA:HA	1.77	0.66
1:B:51:ALA:HB2	1:B:65:ALA:HA	1.79	0.65
1:D:57:ASP:O	2:D:238:GDL:C6	2.45	0.65
1:I:30:GLN:HE22	1:I:74:SER:HB3	1.59	0.65
1:F:18:ALA:HA	1:H:51:ALA:HB2	1.79	0.65
1:A:68:ILE:CG2	1:A:102:VAL:HA	2.26	0.65
1:F:23:ASN:O	1:F:23:ASN:CG	2.40	0.64
1:F:29:PHE:CD1	1:F:42:ALA:HB1	2.32	0.64
1:B:75:GLY:HA3	1:B:91:ARG:NH2	2.13	0.63
1:I:30:GLN:NE2	1:I:74:SER:CB	2.59	0.63
1:B:50:LYS:CB	1:B:68:ILE:HD12	2.29	0.63
1:J:61:TRP:HB3	2:J:110:GDL:H6C1	1.81	0.62
1:G:91:ARG:HH11	1:G:91:ARG:CG	2.10	0.61
1:C:35:ASP:HB3	1:C:37:ASN:N	2.15	0.61
1:A:93:GLN:O	1:B:23:ASN:O	2.18	0.61
1:A:29:PHE:CD1	1:A:42:ALA:HB1	2.35	0.61
1:B:50:LYS:CD	1:B:68:ILE:HD11	2.31	0.61
1:B:50:LYS:HB2	1:B:68:ILE:HD12	1.82	0.60
1:B:62:ILE:HG22	2:B:110:GDL:O7	2.02	0.60
1:A:50:LYS:CB	1:A:68:ILE:HD11	2.32	0.60
1:I:46:ASP:CG	1:I:72:GLY:H	2.11	0.58
1:A:91:ARG:NH1	1:B:15:MET:HE1	2.18	0.58
1:E:13:ASN:ND2	1:E:16:GLY:H	2.02	0.58
1:A:68:ILE:HG22	1:A:102:VAL:CA	2.34	0.57
1:F:93:GLN:H	1:F:93:GLN:CD	2.13	0.57
1:C:35:ASP:HB2	1:C:39:TYR:N	2.19	0.57
1:G:51:ALA:HB2	1:G:65:ALA:HA	1.87	0.57
1:F:21:ILE:CD1	1:H:48:LEU:HD13	2.35	0.56
1:A:13:ASN:HD22	1:A:13:ASN:H	1.53	0.56
1:A:23:ASN:ND2	1:A:23:ASN:C	2.61	0.56
1:B:50:LYS:HB3	1:B:68:ILE:CD1	2.34	0.56
1:J:80:PHE:CD1	1:J:80:PHE:N	2.74	0.56
1:F:54:PRO:HD3	1:F:61:TRP:CD1	2.41	0.56
1:C:23:ASN:C	1:C:23:ASN:HD22	2.14	0.55
1:G:86:TYR:CE2	4:J:120:HOH:O	2.53	0.55
1:I:84:ASN:OD1	1:I:84:ASN:C	2.50	0.55
1:H:60:ASN:ND2	1:H:63:ALA:HB2	2.22	0.55
1:C:56:SER:OG	1:E:105:GLN:HG2	2.07	0.54
1:J:62:ILE:O	1:J:62:ILE:HG13	2.06	0.54
1:H:29:PHE:CD2	1:H:44:SER:HB2	2.43	0.54
1:G:30:GLN:HE22	1:G:74:SER:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:ASP:HB3	1:H:37:ASN:N	2.21	0.54
1:D:44:SER:O	1:D:45:ASN:C	2.50	0.54
1:H:35:ASP:HB2	1:H:39:TYR:H	1.73	0.54
1:F:13:ASN:HD22	1:F:13:ASN:H	1.56	0.53
1:G:29:PHE:CD1	1:G:44:SER:HB3	2.43	0.53
1:I:30:GLN:NE2	1:I:74:SER:HB2	2.15	0.53
1:G:82:HIS:CG	1:G:83:PRO:HD2	2.43	0.53
1:A:23:ASN:C	1:A:23:ASN:HD22	2.16	0.53
1:A:68:ILE:HG22	1:A:102:VAL:HA	1.90	0.52
1:F:101:PRO:HA	1:G:17:ARG:HH21	1.73	0.52
1:H:60:ASN:HD21	1:H:63:ALA:HB2	1.74	0.52
1:H:79:LEU:HD23	1:H:89:ALA:HB2	1.90	0.52
1:F:84:ASN:C	1:F:84:ASN:OD1	2.52	0.52
1:I:25:GLY:O	1:I:28:GLN:HG2	2.09	0.52
1:J:25:GLY:O	1:J:28:GLN:HG2	2.10	0.52
1:F:91:ARG:HH11	1:G:15:MET:CE	2.13	0.52
1:J:46:ASP:CG	1:J:72:GLY:H	2.17	0.52
1:I:72:GLY:O	1:I:91:ARG:NH2	2.42	0.52
1:H:102:VAL:O	1:H:103:SER:CB	2.58	0.51
1:D:97:LYS:O	1:D:98:ALA:HB2	2.10	0.51
1:I:30:GLN:NE2	1:I:74:SER:HB3	2.25	0.51
1:I:43:VAL:HA	1:I:47:LYS:O	2.11	0.51
1:J:104:ASN:HD22	1:J:105:GLN:N	2.08	0.51
1:F:33:PHE:CD1	1:F:33:PHE:N	2.79	0.51
1:F:97:LYS:O	1:F:97:LYS:HG3	2.09	0.50
1:C:57:ASP:O	1:E:105:GLN:HG3	2.12	0.50
1:C:29:PHE:CD2	1:C:44:SER:HB2	2.47	0.49
1:C:56:SER:HB2	1:E:105:GLN:CG	2.40	0.49
1:B:37:ASN:ND2	1:E:86:TYR:OH	2.44	0.49
1:D:51:ALA:HB2	1:D:65:ALA:HA	1.95	0.49
1:B:46:ASP:OD1	1:B:74:SER:HB2	2.13	0.49
1:A:41:TYR:N	1:A:41:TYR:CD1	2.80	0.49
1:F:91:ARG:NH1	1:G:15:MET:HE1	2.12	0.49
1:H:80:PHE:HE2	1:I:34:PHE:CE2	2.30	0.49
1:J:23:ASN:N	2:J:110:GDL:O3	2.45	0.49
1:F:21:ILE:HD11	1:H:48:LEU:HD13	1.95	0.49
1:E:60:ASN:OD1	1:E:60:ASN:C	2.54	0.49
1:B:50:LYS:CD	1:B:68:ILE:CD1	2.91	0.49
1:C:94:ARG:HG3	1:C:96:TYR:CZ	2.48	0.49
1:C:26:TRP:CE3	1:C:29:PHE:HE1	2.32	0.48
1:F:101:PRO:HA	1:G:17:ARG:NH2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASP:CG	1:B:64:ARG:HE	2.21	0.48
1:B:50:LYS:CB	1:B:68:ILE:CD1	2.90	0.48
1:B:50:LYS:HD2	1:B:68:ILE:CD1	2.44	0.47
1:F:11:SER:HB3	1:H:24:GLY:O	2.14	0.47
1:I:96:TYR:CE2	1:J:20:GLU:HG3	2.48	0.47
1:J:35:ASP:OD1	1:J:35:ASP:C	2.57	0.47
1:F:11:SER:CB	1:H:24:GLY:O	2.62	0.47
1:J:104:ASN:HD22	1:J:104:ASN:C	2.22	0.47
2:J:110:GDL:O7	2:J:110:GDL:C3	2.44	0.47
1:G:94:ARG:HG2	1:H:23:ASN:HD22	1.80	0.46
1:J:45:ASN:O	1:J:46:ASP:CB	2.63	0.46
1:B:75:GLY:CA	1:B:91:ARG:NH2	2.78	0.46
1:C:23:ASN:C	1:C:23:ASN:ND2	2.74	0.46
1:F:25:GLY:H	1:H:46:ASP:CG	2.24	0.46
1:C:59:ASP:O	1:C:60:ASN:C	2.57	0.46
1:G:86:TYR:N	1:G:86:TYR:CD2	2.83	0.46
1:H:80:PHE:CE2	1:I:34:PHE:CE2	3.04	0.46
1:J:23:ASN:O	1:J:23:ASN:CG	2.59	0.45
1:G:75:GLY:HA3	1:G:91:ARG:HE	1.82	0.45
1:I:33:PHE:CD1	1:I:33:PHE:N	2.84	0.45
1:D:72:GLY:O	1:D:91:ARG:NH2	2.49	0.45
1:F:25:GLY:O	1:F:28:GLN:NE2	2.50	0.45
1:A:94:ARG:NH2	1:B:23:ASN:HD21	2.14	0.45
1:H:82:HIS:CD2	1:H:84:ASN:CG	2.94	0.45
1:D:91:ARG:HD2	1:E:15:MET:HE2	1.98	0.45
1:H:94:ARG:H	1:H:94:ARG:HG2	1.73	0.45
1:H:43:VAL:HA	1:H:47:LYS:O	2.17	0.44
1:E:79:LEU:HD12	1:E:79:LEU:HA	1.81	0.44
1:A:82:HIS:ND1	1:A:83:PRO:HD2	2.33	0.44
1:H:19:LYS:HB2	1:H:19:LYS:HE3	1.83	0.44
1:B:68:ILE:HG22	1:B:68:ILE:O	2.18	0.44
1:H:92:GLY:O	1:H:93:GLN:CB	2.57	0.44
1:A:41:TYR:HA	1:A:49:TYR:O	2.17	0.44
1:B:82:HIS:HB2	1:B:88:TYR:CE1	2.53	0.44
1:E:57:ASP:O	2:E:110:GDL:H6C1	2.17	0.43
1:G:16:GLY:N	4:G:107:HOH:O	2.40	0.43
1:A:33:PHE:CD1	1:A:33:PHE:N	2.85	0.43
1:E:44:SER:O	1:E:45:ASN:C	2.62	0.43
1:H:59:ASP:O	1:H:60:ASN:C	2.61	0.43
1:A:72:GLY:O	1:A:91:ARG:NH2	2.51	0.43
1:B:50:LYS:HB3	1:B:68:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:43:VAL:HA	1:J:47:LYS:O	2.19	0.43
1:I:23:ASN:HB2	2:I:110:GDL:O4	2.18	0.43
1:A:29:PHE:CE1	1:A:42:ALA:HB1	2.53	0.43
1:A:54:PRO:HD3	1:A:61:TRP:CD1	2.54	0.42
1:F:41:TYR:N	1:F:41:TYR:CD1	2.86	0.42
1:G:48:LEU:HD22	1:G:73:TRP:CZ3	2.54	0.42
1:A:91:ARG:HH11	1:B:15:MET:HE1	1.85	0.42
1:H:33:PHE:CD1	1:H:33:PHE:N	2.88	0.42
1:H:82:HIS:CD2	1:H:83:PRO:HD2	2.54	0.42
1:E:69:GLY:HA3	1:E:73:TRP:NE1	2.35	0.42
1:C:29:PHE:HD2	1:C:44:SER:HB2	1.84	0.42
1:C:91:ARG:O	1:C:94:ARG:HG2	2.20	0.42
1:F:35:ASP:C	1:F:35:ASP:OD1	2.63	0.42
1:D:84:ASN:OD1	1:D:84:ASN:C	2.63	0.42
1:D:23:ASN:O	1:D:23:ASN:CG	2.63	0.42
1:A:76:PHE:CD1	1:A:89:ALA:HB1	2.54	0.42
1:F:13:ASN:HD22	1:F:13:ASN:N	2.17	0.42
1:J:61:TRP:H	2:J:110:GDL:H5	1.85	0.42
1:A:43:VAL:HA	1:A:47:LYS:O	2.20	0.42
1:C:93:GLN:HA	1:D:27:ASP:OD1	2.20	0.42
1:I:98:ALA:HB2	1:J:18:ALA:HA	2.02	0.42
1:C:19:LYS:HG2	1:C:20:GLU:N	2.35	0.41
1:D:24:GLY:H	2:D:238:GDL:H3	1.84	0.41
1:E:13:ASN:HD22	1:E:16:GLY:H	1.65	0.41
1:A:35:ASP:OD1	1:A:35:ASP:C	2.64	0.41
1:B:68:ILE:CG2	1:B:101:PRO:HG2	2.44	0.41
1:E:82:HIS:HB2	1:E:88:TYR:CE1	2.55	0.41
1:J:26:TRP:CZ2	2:J:110:GDL:H6C1	2.55	0.41
1:B:64:ARG:O	1:B:65:ALA:C	2.64	0.41
1:D:57:ASP:O	2:D:238:GDL:H6C1	2.17	0.41
1:J:57:ASP:O	2:J:110:GDL:O7	2.38	0.41
1:F:35:ASP:HB2	1:F:36:PRO:CD	2.51	0.41
1:A:10:ASP:HB3	1:A:13:ASN:ND2	2.35	0.41
1:F:76:PHE:CD1	1:F:89:ALA:HB1	2.55	0.41
1:I:29:PHE:CD1	1:I:42:ALA:HB1	2.56	0.41
1:C:83:PRO:HA	1:E:83:PRO:HG3	2.03	0.41
1:I:45:ASN:HB3	1:I:46:ASP:H	1.68	0.41
1:F:23:ASN:ND2	1:F:23:ASN:C	2.77	0.41
1:H:21:ILE:HG22	1:H:55:GLN:HB2	2.03	0.41
1:H:98:ALA:HB2	1:I:18:ALA:HA	2.04	0.40
1:A:26:TRP:NE1	2:A:110:GDL:O3	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:62:ILE:N	2:J:110:GDL:H6C2	2.29	0.40
1:F:19:LYS:HG3	1:F:21:ILE:HG23	2.03	0.40
1:G:23:ASN:HB2	1:G:57:ASP:OD1	2.21	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	91/106 (86%)	88 (97%)	2 (2%)	1 (1%)	11	22
1	B	86/106 (81%)	80 (93%)	6 (7%)	0	100	100
1	C	83/106 (78%)	78 (94%)	5 (6%)	0	100	100
1	D	89/106 (84%)	83 (93%)	6 (7%)	0	100	100
1	E	91/106 (86%)	86 (94%)	4 (4%)	1 (1%)	11	22
1	F	90/106 (85%)	87 (97%)	3 (3%)	0	100	100
1	G	86/106 (81%)	82 (95%)	3 (4%)	1 (1%)	10	20
1	H	83/106 (78%)	75 (90%)	7 (8%)	1 (1%)	10	20
1	I	92/106 (87%)	88 (96%)	3 (3%)	1 (1%)	11	22
1	J	91/106 (86%)	87 (96%)	3 (3%)	1 (1%)	11	22
All	All	882/1060 (83%)	834 (95%)	42 (5%)	6 (1%)	18	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	92	GLY
1	I	45	ASN
1	J	60	ASN
1	A	51	ALA

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Mol	Chain	Res	Type
1	E	60	ASN
1	G	16	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	75/87 (86%)	67 (89%)	8 (11%)	6	13
1	B	70/87 (80%)	65 (93%)	5 (7%)	13	29
1	C	68/87 (78%)	60 (88%)	8 (12%)	5	11
1	D	73/87 (84%)	69 (94%)	4 (6%)	19	40
1	E	75/87 (86%)	71 (95%)	4 (5%)	20	42
1	F	74/87 (85%)	67 (90%)	7 (10%)	8	17
1	G	70/87 (80%)	66 (94%)	4 (6%)	18	39
1	H	68/87 (78%)	60 (88%)	8 (12%)	5	11
1	I	76/87 (87%)	68 (90%)	8 (10%)	6	14
1	J	75/87 (86%)	68 (91%)	7 (9%)	8	18
All	All	724/870 (83%)	661 (91%)	63 (9%)	9	21

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	17	ARG
1	A	28	GLN
1	A	30	GLN
1	A	68	ILE
1	A	70	SER
1	A	93	GLN
1	A	97	LYS
1	B	19	LYS
1	B	44	SER
1	B	57	ASP

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Mol	Chain	Res	Type
1	B	91	ARG
1	B	97	LYS
1	C	20	GLU
1	C	64	ARG
1	C	79	LEU
1	C	90	VAL
1	C	94	ARG
1	C	97	LYS
1	C	102	VAL
1	C	103	SER
1	D	27	ASP
1	D	28	GLN
1	D	57	ASP
1	D	62	ILE
1	E	19	LYS
1	E	55	GLN
1	E	102	VAL
1	E	105	GLN
1	F	13	ASN
1	F	17	ARG
1	F	28	GLN
1	F	62	ILE
1	F	64	ARG
1	F	93	GLN
1	F	97	LYS
1	G	55	GLN
1	G	58	THR
1	G	91	ARG
1	G	97	LYS
1	H	23	ASN
1	H	28	GLN
1	H	48	LEU
1	H	62	ILE
1	H	64	ARG
1	H	79	LEU
1	H	90	VAL
1	H	103	SER
1	I	11	SER
1	I	13	ASN
1	I	28	GLN
1	I	52	SER
1	I	55	GLN

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Mol	Chain	Res	Type
1	I	57	ASP
1	I	80	PHE
1	I	103	SER
1	J	13	ASN
1	J	55	GLN
1	J	62	ILE
1	J	77	LYS
1	J	97	LYS
1	J	102	VAL
1	J	104	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	23	ASN
1	A	28	GLN
1	A	37	ASN
1	A	45	ASN
1	B	23	ASN
1	B	37	ASN
1	C	37	ASN
1	C	82	HIS
1	D	23	ASN
1	D	30	GLN
1	E	13	ASN
1	E	30	GLN
1	E	37	ASN
1	E	45	ASN
1	E	105	GLN
1	F	13	ASN
1	F	23	ASN
1	F	28	GLN
1	F	37	ASN
1	F	55	GLN
1	G	28	GLN
1	G	30	GLN
1	H	23	ASN
1	H	60	ASN
1	H	82	HIS
1	H	93	GLN
1	I	30	GLN

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Mol	Chain	Res	Type
1	J	13	ASN
1	J	30	GLN
1	J	37	ASN
1	J	104	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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
2	GDL	G	110	-	15,15,15	2.93	4 (26%)	17,21,21	2.60	7 (41%)
3	SO4	E	107	-	4,4,4	0.31	0	6,6,6	0.19	0
2	GDL	J	110	-	15,15,15	2.72	5 (33%)	17,21,21	5.01	12 (70%)
2	GDL	E	110	-	15,15,15	1.66	1 (6%)	17,21,21	3.02	6 (35%)
3	SO4	J	107	-	4,4,4	0.33	0	6,6,6	0.44	0
2	GDL	B	110	-	15,15,15	2.82	2 (13%)	17,21,21	2.58	6 (35%)
2	GDL	I	110	-	15,15,15	1.92	1 (6%)	17,21,21	1.72	4 (23%)
2	GDL	D	238	-	15,15,15	2.03	1 (6%)	17,21,21	2.60	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GDL	A	110	-	15,15,15	1.86	1 (6%)	17,21,21	1.97	6 (35%)
2	GDL	F	110	-	15,15,15	1.82	1 (6%)	17,21,21	1.66	3 (17%)
2	GDL	D	241	-	15,15,15	2.51	3 (20%)	17,21,21	4.13	7 (41%)

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
2	GDL	G	110	-	-	1/6/26/26	0/1/1/1
2	GDL	J	110	-	-	3/6/26/26	0/1/1/1
2	GDL	E	110	-	-	3/6/26/26	0/1/1/1
2	GDL	B	110	-	-	3/6/26/26	0/1/1/1
2	GDL	I	110	-	-	1/6/26/26	0/1/1/1
2	GDL	D	238	-	-	1/6/26/26	0/1/1/1
2	GDL	A	110	-	-	2/6/26/26	0/1/1/1
2	GDL	F	110	-	-	2/6/26/26	0/1/1/1
2	GDL	D	241	-	-	2/6/26/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	110	GDL	O5-C1	9.98	1.49	1.34
2	G	110	GDL	O5-C1	9.59	1.48	1.34
2	D	241	GDL	O5-C1	8.49	1.47	1.34
2	D	238	GDL	O5-C1	7.21	1.45	1.34
2	J	110	GDL	O5-C1	6.86	1.44	1.34
2	I	110	GDL	O5-C1	6.73	1.44	1.34
2	A	110	GDL	O5-C1	6.69	1.44	1.34
2	F	110	GDL	O5-C1	6.52	1.44	1.34
2	E	110	GDL	O5-C1	5.68	1.43	1.34
2	J	110	GDL	C2-C1	-4.99	1.44	1.51
2	J	110	GDL	O5-C5	-4.32	1.40	1.46
2	G	110	GDL	C2-C1	3.81	1.57	1.51
2	J	110	GDL	O4-C4	3.06	1.50	1.43
2	J	110	GDL	C4-C5	2.37	1.58	1.53
2	D	241	GDL	C3-C2	-2.34	1.49	1.52
2	B	110	GDL	C2-C1	2.29	1.54	1.51
2	D	241	GDL	C4-C3	2.28	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	110	GDL	O7-C7	2.11	1.28	1.23
2	G	110	GDL	O5-C5	-2.00	1.43	1.46

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	110	GDL	C1-C2-N2	-10.25	94.24	109.33
2	D	241	GDL	O5-C5-C6	10.06	116.14	106.05
2	J	110	GDL	O5-C5-C6	-10.00	96.02	106.05
2	D	241	GDL	C1-C2-N2	7.65	120.60	109.33
2	E	110	GDL	C3-C2-N2	-7.11	100.82	112.26
2	J	110	GDL	O3-C3-C4	-7.00	93.87	110.38
2	D	241	GDL	O3-C3-C2	-6.62	95.60	108.98
2	D	241	GDL	C3-C2-N2	-6.48	101.84	112.26
2	G	110	GDL	C1-C2-N2	6.13	118.36	109.33
2	J	110	GDL	O4-C4-C5	5.85	123.74	109.32
2	B	110	GDL	C1-C2-N2	5.83	117.92	109.33
2	E	110	GDL	O5-C5-C6	5.57	111.64	106.05
2	B	110	GDL	C3-C2-N2	-5.47	103.47	112.26
2	J	110	GDL	O5-C1-O1	5.40	126.35	118.52
2	J	110	GDL	C6-C5-C4	5.33	126.10	113.02
2	A	110	GDL	C3-C2-N2	-4.96	104.29	112.26
2	E	110	GDL	C5-O5-C1	-4.91	104.58	119.69
2	J	110	GDL	O7-C7-C8	4.89	130.75	122.05
2	D	238	GDL	C1-C2-N2	4.86	116.49	109.33
2	D	238	GDL	C3-C2-N2	-4.64	104.81	112.26
2	J	110	GDL	C5-O5-C1	-4.62	105.46	119.69
2	E	110	GDL	C8-C7-N2	-4.35	108.91	116.12
2	I	110	GDL	C5-O5-C1	-4.30	106.44	119.69
2	D	238	GDL	C5-O5-C1	-4.25	106.59	119.69
2	G	110	GDL	C3-C2-N2	-4.05	105.75	112.26
2	D	238	GDL	C2-N2-C7	4.04	128.76	121.82
2	D	241	GDL	O4-C4-C5	-3.88	99.77	109.32
2	B	110	GDL	C2-N2-C7	3.71	128.19	121.82
2	F	110	GDL	C3-C2-N2	-3.65	106.39	112.26
2	G	110	GDL	C5-O5-C1	-3.58	108.66	119.69
2	D	241	GDL	C3-C4-C5	3.50	116.57	110.23
2	G	110	GDL	O7-C7-N2	3.47	128.11	121.98
2	B	110	GDL	C5-O5-C1	-3.42	109.17	119.69
2	J	110	GDL	O7-C7-N2	-3.36	116.05	121.98
2	F	110	GDL	C5-O5-C1	-3.21	109.80	119.69
2	D	238	GDL	O6-C6-C5	-3.10	100.76	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	110	GDL	C2-N2-C7	3.04	127.04	121.82
2	A	110	GDL	O5-C5-C6	-3.00	103.05	106.05
2	F	110	GDL	C1-C2-N2	2.99	113.73	109.33
2	B	110	GDL	O3-C3-C4	2.96	117.35	110.38
2	D	238	GDL	C3-C4-C5	2.95	115.58	110.23
2	E	110	GDL	C2-N2-C7	2.90	126.79	121.82
2	D	241	GDL	O3-C3-C4	2.79	116.96	110.38
2	E	110	GDL	O7-C7-C8	2.71	126.88	122.05
2	J	110	GDL	C3-C2-N2	2.48	116.24	112.26
2	A	110	GDL	C8-C7-N2	-2.47	112.02	116.12
2	G	110	GDL	C6-C5-C4	2.46	119.07	113.02
2	A	110	GDL	O6-C6-C5	-2.36	103.30	111.33
2	G	110	GDL	O3-C3-C4	2.28	115.76	110.38
2	A	110	GDL	O4-C4-C3	-2.22	105.14	110.38
2	I	110	GDL	O5-C5-C6	2.21	108.27	106.05
2	B	110	GDL	C6-C5-C4	2.18	118.38	113.02
2	A	110	GDL	C2-N2-C7	2.13	125.48	121.82
2	D	238	GDL	O7-C7-N2	2.11	125.70	121.98
2	I	110	GDL	O3-C3-C2	2.06	113.14	108.98
2	I	110	GDL	O5-C1-O1	-2.05	115.55	118.52
2	J	110	GDL	O4-C4-C3	-2.04	105.57	110.38
2	J	110	GDL	O1-C1-C2	-2.03	117.27	123.63

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	110	GDL	C3-C2-N2-C7
2	D	238	GDL	C3-C2-N2-C7
2	G	110	GDL	C3-C2-N2-C7
2	J	110	GDL	C3-C2-N2-C7
2	F	110	GDL	O5-C5-C6-O6
2	A	110	GDL	O5-C5-C6-O6
2	E	110	GDL	O5-C5-C6-O6
2	F	110	GDL	C4-C5-C6-O6
2	D	241	GDL	O5-C5-C6-O6
2	J	110	GDL	O5-C5-C6-O6
2	E	110	GDL	C4-C5-C6-O6
2	A	110	GDL	C4-C5-C6-O6
2	D	241	GDL	C4-C5-C6-O6
2	J	110	GDL	C4-C5-C6-O6
2	B	110	GDL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	I	110	GDL	C3-C2-N2-C7
2	B	110	GDL	C1-C2-N2-C7
2	E	110	GDL	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	110	GDL	9	0
2	E	110	GDL	1	0
2	B	110	GDL	1	0
2	I	110	GDL	1	0
2	D	238	GDL	4	0
2	A	110	GDL	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	93/106 (87%)	-1.27	0 100 100	21, 40, 52, 56	0
1	B	88/106 (83%)	-1.28	0 100 100	23, 40, 54, 63	0
1	C	85/106 (80%)	-1.33	0 100 100	20, 34, 46, 52	0
1	D	91/106 (85%)	-1.31	0 100 100	20, 36, 50, 59	0
1	E	93/106 (87%)	-1.42	0 100 100	19, 29, 43, 53	0
1	F	92/106 (86%)	-1.32	0 100 100	21, 40, 51, 56	0
1	G	88/106 (83%)	-1.27	0 100 100	22, 40, 56, 65	0
1	H	85/106 (80%)	-1.34	0 100 100	22, 34, 46, 52	0
1	I	94/106 (88%)	-1.30	0 100 100	18, 37, 54, 60	0
1	J	93/106 (87%)	-1.38	0 100 100	20, 29, 43, 56	0
All	All	902/1060 (85%)	-1.32	0 100 100	18, 36, 52, 65	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	GDL	D	238	15/15	0.97	0.05	46,56,59,62	0
3	SO4	E	107	5/5	0.97	0.08	92,93,93,94	0
3	SO4	J	107	5/5	0.97	0.06	79,79,81,82	0
2	GDL	I	110	15/15	0.98	0.04	46,54,57,58	0
2	GDL	D	241	15/15	0.98	0.06	37,54,60,61	0
2	GDL	G	110	15/15	0.98	0.04	35,43,52,56	0
2	GDL	A	110	15/15	0.99	0.04	35,47,50,52	0
2	GDL	B	110	15/15	0.99	0.04	32,40,49,50	0
2	GDL	J	110	15/15	0.99	0.04	46,52,55,55	0
2	GDL	E	110	15/15	0.99	0.04	20,37,40,47	0
2	GDL	F	110	15/15	0.99	0.04	42,50,53,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.