



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:05 AM UTC

PDB ID : 6CHB / pdb_00006chb
Title : Crystal structure of a natively-glycosylated BG505 SOSIP.664 HIV-1 Envelope Trimer in complex with the broadly-neutralizing antibodies BG18 and IOMA
Authors : Barnes, C.O.; Bjorkman, P.J.
Deposited on : 2018-02-22
Resolution : 6.80 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

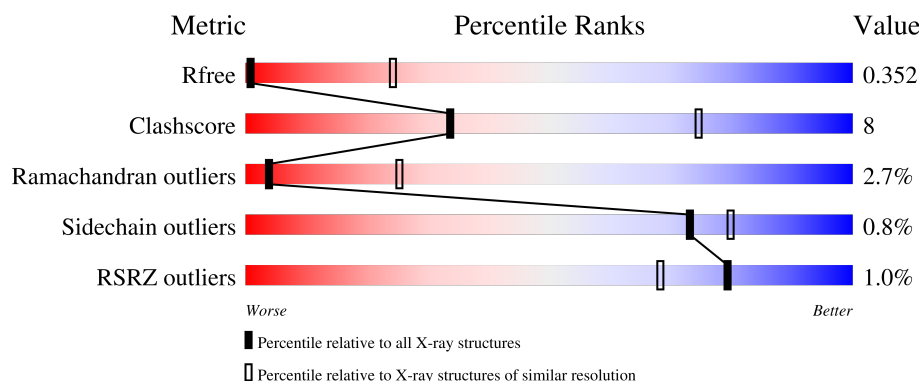
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.80 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	1165 (9.50-4.00)
Clashscore	190562	1006 (9.50-4.04)
Ramachandran outliers	187476	1052 (9.50-4.00)
Sidechain outliers	187428	1015 (9.50-4.00)
RSRZ outliers	180081	1158 (9.50-4.00)

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	153	
1	B	153	
1	C	153	
2	F	479	
2	G	479	

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Mol	Chain	Length	Quality of chain
2	H	479	
3	I	241	
3	J	241	
3	Q	241	
4	K	215	
4	L	215	
4	R	215	
5	D	232	
5	M	232	
5	O	232	
6	E	214	
6	N	214	
6	P	214	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28753 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 Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	126	Total	C	N	O	S	0	0	0
			1001	633	172	190	6			
1	A	126	Total	C	N	O	S	0	0	0
			1001	633	172	190	6			
1	C	126	Total	C	N	O	S	0	0	0
			1001	633	172	190	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	engineered mutation	UNP Q2N0S7
A	605	CYS	THR	engineered mutation	UNP Q2N0S7
C	605	CYS	THR	engineered mutation	UNP Q2N0S7

- Molecule 2 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	450	Total	C	N	O	S	0	0	0
			3538	2221	624	666	27			
2	F	450	Total	C	N	O	S	0	0	0
			3538	2221	624	666	27			
2	H	450	Total	C	N	O	S	0	0	0
			3538	2221	624	666	27			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
F	332	ASN	THR	conflict	UNP Q2N0S6
F	501	CYS	ALA	engineered mutation	UNP Q2N0S6
H	332	ASN	THR	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	501	CYS	ALA	engineered mutation	UNP Q2N0S6

- Molecule 3 is a protein called BG18 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	227	Total	C	N	O	S	0	0	0
			1723	1086	297	332	8			
3	I	227	Total	C	N	O	S	0	0	0
			1723	1086	297	332	8			
3	Q	227	Total	C	N	O	S	0	0	0
			1723	1086	297	332	8			

- Molecule 4 is a protein called BG18 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	205	Total	C	N	O	S	0	0	0
			1540	963	257	314	6			
4	L	205	Total	C	N	O	S	0	0	0
			1540	963	257	314	6			
4	R	205	Total	C	N	O	S	0	0	0
			1540	963	257	314	6			

- Molecule 5 is a protein called IOMA Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	125	Total	C	N	O	S	0	0	0
			992	629	173	181	9			
5	M	125	Total	C	N	O	S	0	0	0
			992	629	173	181	9			
5	O	125	Total	C	N	O	S	0	0	0
			992	629	173	181	9			

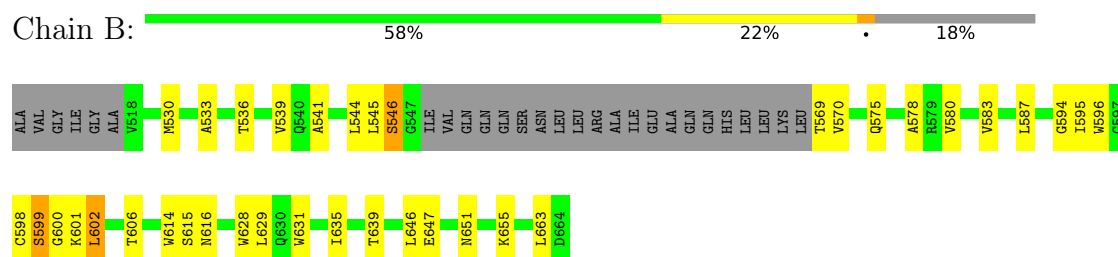
- Molecule 6 is a protein called IOMA Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	107	Total	C	N	O	S	0	0	0
			786	491	133	160	2			
6	N	109	Total	C	N	O	S	0	0	0
			799	498	136	163	2			
6	P	107	Total	C	N	O	S	0	0	0
			786	491	133	160	2			

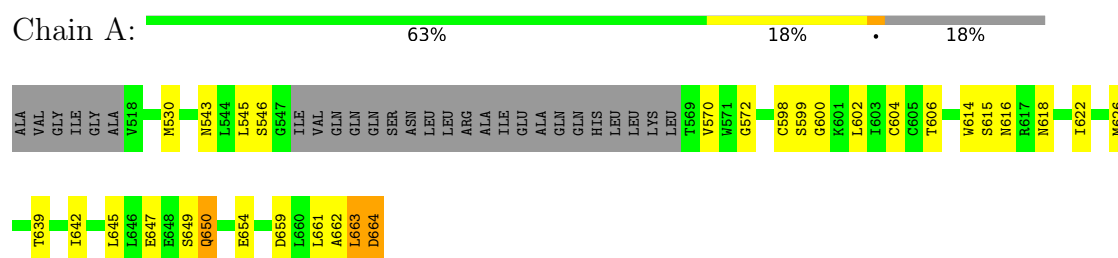
3 Residue-property plots [i](#)

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.

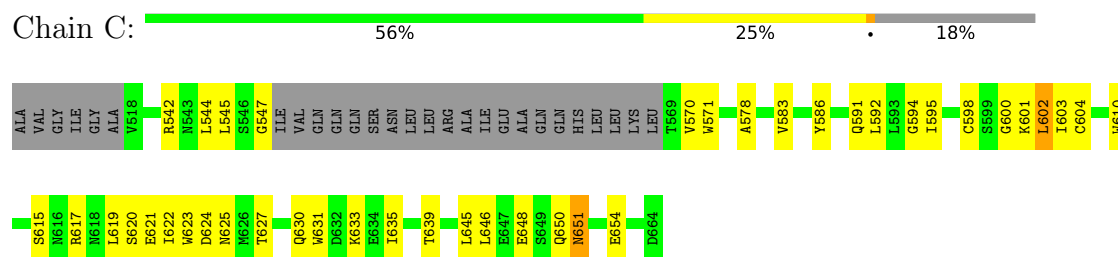
- Molecule 1: Envelope glycoprotein gp41



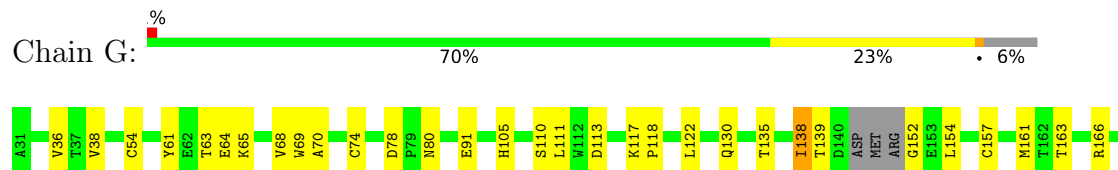
- Molecule 1: Envelope glycoprotein gp41

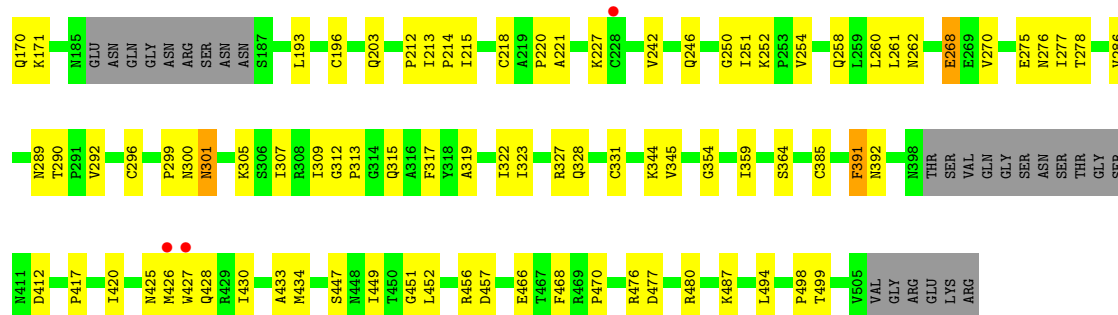


- Molecule 1: Envelope glycoprotein gp41

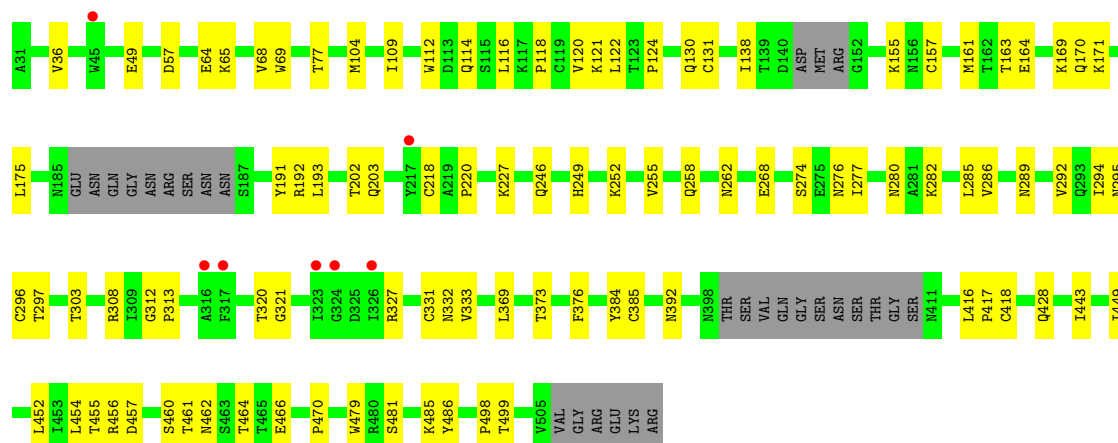
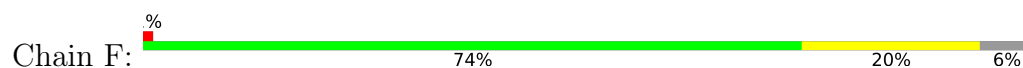


- Molecule 2: Envelope glycoprotein gp120

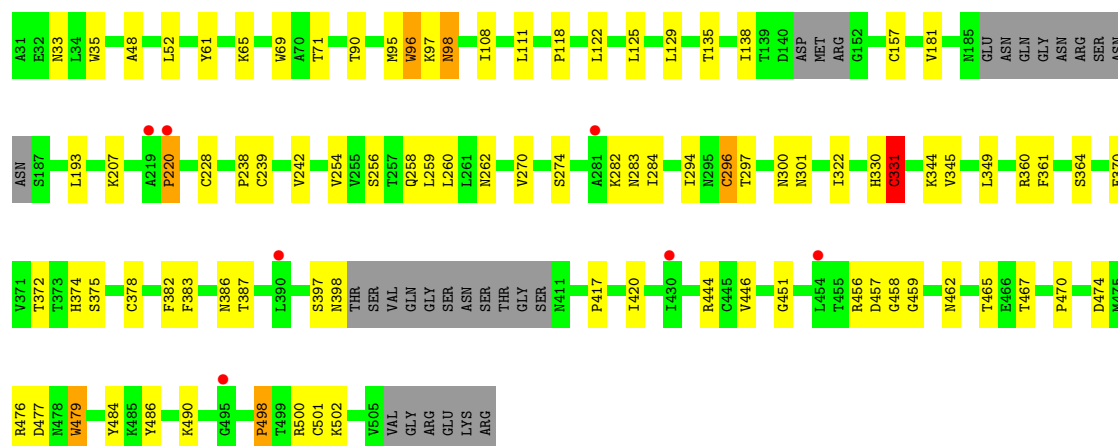
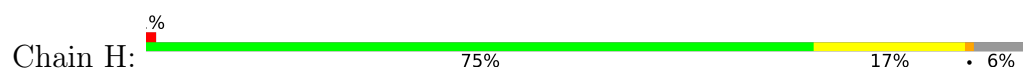




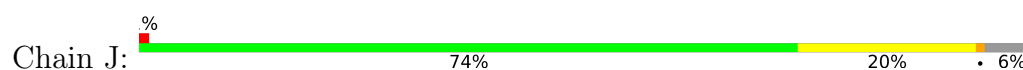
• Molecule 2: Envelope glycoprotein gp120

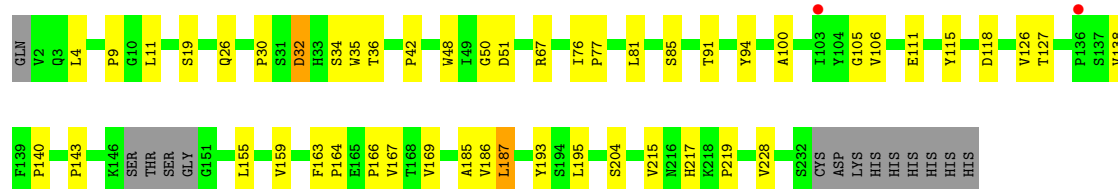


• Molecule 2: Envelope glycoprotein gp120

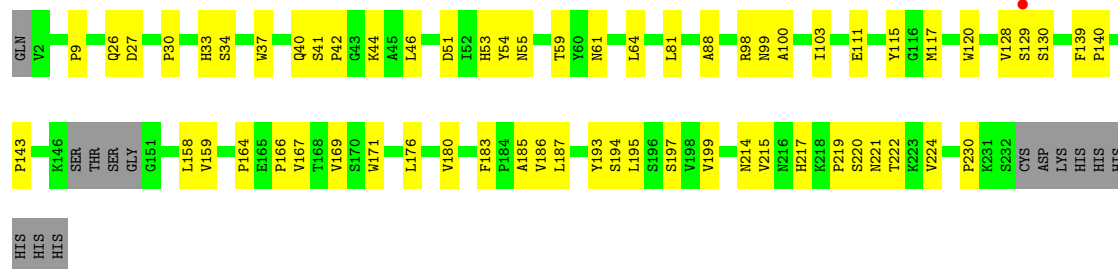


• Molecule 3: BG18 Heavy Chain

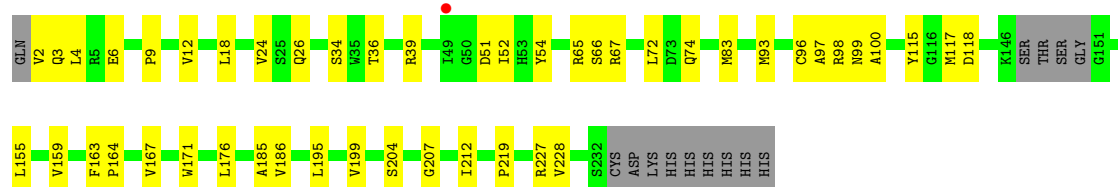




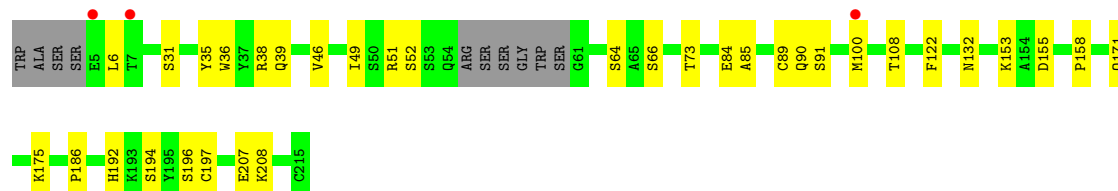
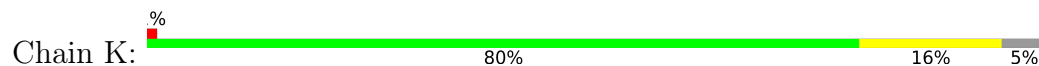
• Molecule 3: BG18 Heavy Chain



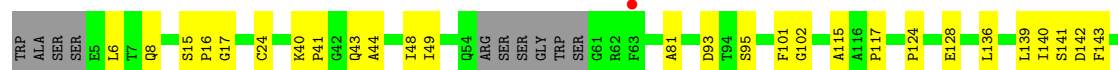
• Molecule 3: BG18 Heavy Chain



• Molecule 4: BG18 Light Chain

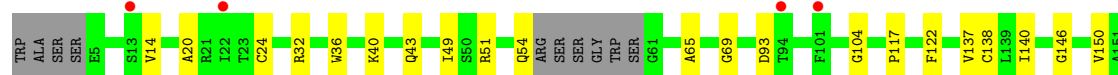
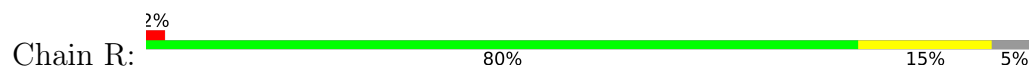


• Molecule 4: BG18 Light Chain

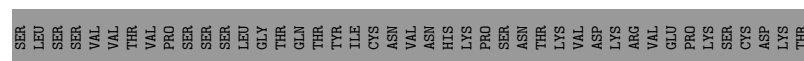
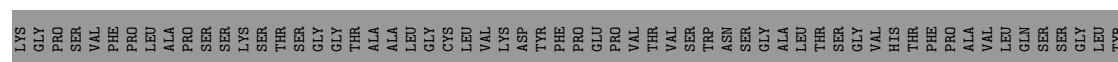
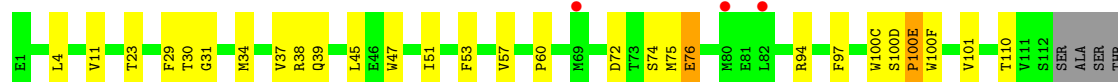




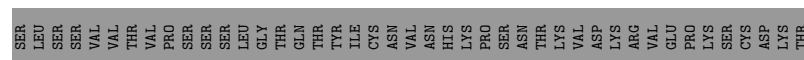
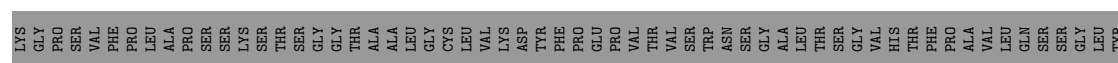
• Molecule 4: BG18 Light Chain



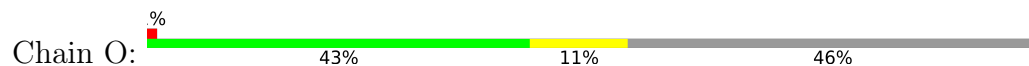
• Molecule 5: IOMA Heavy Chain



• Molecule 5: IOMA Heavy Chain



• Molecule 5: IOMA Heavy Chain



VAL	THR	VAL	PRO	PRO	SER	SER	SER	LEU	GLY	THR	THR	GLN	THR	TYR	ILE	CYS	ASN	VAL	ASN	HIS	LYS	PRO	SER	ASN	THR	LYS	VAL	ASP	LYS	ARG	GLY	GLU	PRO	LYS	SER	CYS	ASP	LYS	THR
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● Molecule 6: IOMA Light Chain



GLN	S2	V33	S34	W35	Y36	Q37	L46	I47	I48	V51	S65	S72	Y86	Y87	C88	A92	D93	G94	L107	GLY	GLN	PRO	LYS	ALA	PRO	ALA	SER	VAL	THR	LEU	PHE	PRO	PRO	SER	SER	GLU	GLU	LEU	GLN	ALA	ASN	LYS	ALA	SER	TYR	THR	LEU	VAL	CYS	LEU	ILE	SER	ASP
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PHE	TYR	PRO	GLY	ALA	VAL	THR	VAL	ALA	ALA	LYS	TRP	LYS	ALA	ASP	SER	SER	PRO	VAL	LYS	ALA	GLY	VAL	GLU	THR	THR	PRO	SER	SER	LYS	ASN	ASN	LYS	TYR	ALA	ALA	SER	SER	SER	TYR	LEU	SER	LEU	PRO	THR	PRO	GLU	GLN	TRP	LYS	LYS	HIS	ARG	LYS	ALA	SER	TYR	THR	CYS	GLN	VAL	THR	HIS	GLU
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GLY	SER	THR	VAL	GLU	LYS	THR	VAL	ALA	ALA	THR	PRO	GLU	THR	CYS	SER
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● Molecule 6: IOMA Light Chain

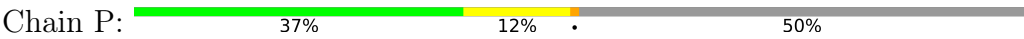


GLN	S2	A3	L4	D31	Q38	R39	P40	L46	I47	I48	Y49	P55	I58	A64	A84	D93	G94	V96	G99	G108	Q109	PRO	LYS	ALA	ASN	LYS	TYR	ALA	ALA	PRO	SER	VAL	SER	THR	THR	LEU	PHE	PRO	PRO	LEU	PRO	SER	SER	GLN	GLU	TRP	LYS	GLN	ALA	SER	HIS	ARG	LYS	SER	ALA	TYR	THR	LEU	VAL	CYS	GLN	VAL	THR	ILE
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SER	ASP	PHE	TYR	PRO	GLY	ALA	VAL	THR	THR	VAL	ALA	ALA	TRP	LYS	ALA	ASP	SER	SER	PRO	VAL	LYS	ALA	GLY	VAL	GLU	THR	THR	THR	PRO	SER	LYS	GLN	SER	ASN	LYS	TYR	ALA	ALA	ALA	SER	SER	THR	LEU	TYR	LEU	SER	LEU	THR	PRO	GLU	GLU	GLN	TRP	LYS	SER	HIS	ARG	LYS	SER	ALA	TYR	THR	CYS	GLN	VAL	THR
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HIS	GLU	GLY	SER	THR	VAL	GLU	LYS	THR	VAL	ALA	ALA	PRO	THR	GLU	CYS	SER
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● Molecule 6: IOMA Light Chain



GLN	S2	A3	L4	D27B	V27C	G28	V33	S34	W35	Y36	H39	P40	G41	L46	E50	V51	N52	K66	M69	T70	A71	L78	G79	E80	E83	Y89	S90	F91	A92	D93	G94	G99	L104	T105	V106	L107	GLY	GLN	PRO	ASN	LYS	ALA	TYR	ALA	PRO	SER	VAL	SER	THR	LEU
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PHE	PRO	PRO	SER	SER	GLU	GLU	LEU	GLN	ALA	ASN	LYS	ARG	ALA	THR	LEU	VAL	CYS	GLN	VAL	ILE	SER	ASP	PHE	TYR	PRO	GLY	ALA	VAL	VAL	ALA	TRP	LYS	ALA	ASP	SER	SER	PRO	VAL	LYS	ALA	GLY	GLU	GLU	THR	THR	THR	PRO	SER	SER	LYS	GLN	SER	ASN	ASN	LYS	ALA	TYR	ALA	ALA	SER	VAL	SER	THR	THR	LEU
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LEU	SER	LEU	THR	PRO	GLU	GLN	TRP	LYS	HIS	HIS	ARG	SER	TYR	SER	CYS	VAL	THR	THR	HIS	GLU	GLY	SER	THR	VAL	GLU	LYS	THR	VAL	VAL	PRO	THR	GLU	CYS	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	176.75Å 176.75Å 458.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.63 – 6.80 39.63 – 6.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.63-6.80) 99.1 (39.63-6.80)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 6.65Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.318 , 0.417 0.333 , 0.352	Depositor DCC
R_{free} test set	670 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	369.1	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 680.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	28753	wwPDB-VP
Average B, all atoms (Å ²)	411.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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	0.14	0/1019	0.43	0/1382
1	B	0.13	0/1019	0.42	1/1382 (0.1%)
1	C	0.15	0/1019	0.49	1/1382 (0.1%)
2	F	0.15	0/3611	0.43	0/4903
2	G	0.16	0/3611	0.44	0/4903
2	H	0.15	0/3611	0.44	0/4903
3	I	0.16	0/1767	0.43	0/2410
3	J	0.14	0/1767	0.43	0/2410
3	Q	0.15	0/1767	0.41	0/2410
4	K	0.13	0/1577	0.39	0/2153
4	L	0.14	0/1577	0.40	0/2153
4	R	0.14	0/1577	0.35	0/2153
5	D	0.17	0/1021	0.46	0/1384
5	M	0.13	0/1021	0.43	0/1384
5	O	0.17	0/1021	0.47	0/1384
6	E	0.15	0/803	0.39	0/1088
6	N	0.14	0/816	0.41	0/1105
6	P	0.13	0/803	0.43	0/1088
All	All	0.15	0/29407	0.43	2/39977 (0.0%)

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	A	0	1
5	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	544	LEU	N-CA-C	-5.37	108.50	114.62
1	B	602	LEU	CB-CA-C	-5.18	110.58	116.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	659	ASP	Peptide
5	D	100(C)	TRP	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	1001	0	978	17	1
1	B	1001	0	979	28	0
1	C	1001	0	979	25	0
2	F	3538	0	3488	54	0
2	G	3538	0	3493	68	0
2	H	3538	0	3491	47	0
3	I	1723	0	1696	36	0
3	J	1723	0	1694	27	0
3	Q	1723	0	1694	30	0
4	K	1540	0	1492	19	0
4	L	1540	0	1492	27	0
4	R	1540	0	1492	16	0
5	D	992	0	949	20	0
5	M	992	0	947	15	0
5	O	992	0	947	17	0
6	E	786	0	758	7	0
6	N	799	0	769	9	0
6	P	786	0	758	16	0
All	All	28753	0	28096	439	1

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 8.

All (439) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:159:VAL:HG11	3:Q:167:VAL:HG11	1.67	0.77
6:P:83:GLU:HG3	6:P:105:THR:HA	1.66	0.77
3:J:140:PRO:HB3	3:J:228:VAL:HG13	1.73	0.71
2:F:295:ASN:HB2	2:F:332:ASN:HB2	1.72	0.70
2:G:212:PRO:HB2	2:G:252:LYS:HB3	1.74	0.69
6:N:46:LEU:HD21	6:N:49:TYR:HB3	1.73	0.69
2:G:301:ASN:HB3	2:G:323:ILE:HB	1.74	0.69
1:C:617:ARG:HB2	1:C:622:ILE:HG13	1.73	0.69
1:B:575:GLN:NE2	2:G:54:CYS:SG	2.66	0.69
3:I:143:PRO:HD2	3:I:230:PRO:HA	1.75	0.68
1:A:663:LEU:HA	2:H:501:CYS:HB2	1.76	0.68
5:D:39:GLN:HB2	5:D:45:LEU:HG	1.75	0.67
2:F:276:ASN:HB3	2:F:282:LYS:HG3	1.77	0.66
2:G:163:THR:O	2:G:166:ARG:NH2	2.29	0.66
2:F:170:GLN:NE2	2:F:171:LYS:O	2.29	0.66
2:F:285:LEU:HD21	2:F:481:SER:HB3	1.76	0.65
4:R:188:GLN:HA	4:R:191:SER:HB3	1.77	0.65
3:Q:2:VAL:HG11	3:Q:98:ARG:HD3	1.79	0.65
2:F:124:PRO:HB2	2:F:161:MET:HE1	1.79	0.65
2:F:456:ARG:NH2	6:N:93:ASP:OD1	2.30	0.64
6:N:4:LEU:HB3	6:N:99:GLY:HA2	1.78	0.63
1:C:592:LEU:HD23	1:C:595:ILE:HD11	1.79	0.63
4:K:38:ARG:O	4:K:46:VAL:N	2.30	0.63
1:C:617:ARG:H	1:C:622:ILE:HD11	1.64	0.63
5:O:51:ILE:HD11	5:O:71:ARG:HD2	1.79	0.63
3:Q:2:VAL:N	3:Q:26:GLN:O	2.32	0.63
3:J:169:VAL:HG12	3:J:215:VAL:HA	1.82	0.62
3:I:40:GLN:HB2	3:I:46:LEU:HD23	1.81	0.62
2:H:270:VAL:HG21	2:H:344:LYS:HB3	1.80	0.62
2:F:131:CYS:HB3	2:F:155:LYS:HB3	1.80	0.62
1:A:650:GLN:O	1:A:654:GLU:N	2.29	0.62
3:J:185:ALA:HB2	3:J:195:LEU:HD23	1.81	0.61
5:O:41:PRO:HD3	5:O:88:ALA:HA	1.82	0.61
3:Q:164:PRO:HD2	3:Q:219:PRO:HG2	1.83	0.61
3:J:67:ARG:NH2	3:J:85:SER:O	2.33	0.61
5:D:4:LEU:HD11	5:D:94:ARG:HB3	1.83	0.61
2:G:292:VAL:HB	2:G:449:ILE:HB	1.82	0.60
3:I:34:SER:HB3	3:I:99:ASN:HB3	1.81	0.60
2:G:290:THR:OG1	2:G:344:LYS:NZ	2.34	0.60
1:B:635:ILE:O	1:B:639:THR:N	2.34	0.60
1:C:651:ASN:HA	1:C:654:GLU:HB3	1.83	0.60
3:I:33:HIS:HB3	3:I:100:ALA:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:274:SER:HB2	2:H:284:ILE:HG23	1.85	0.59
3:J:217:HIS:CD2	3:J:219:PRO:HD2	2.38	0.59
2:H:98:ASN:ND2	2:H:486:TYR:O	2.36	0.59
1:B:606:THR:HB	1:B:646:LEU:HD21	1.83	0.58
1:B:598:CYS:O	1:B:600:GLY:N	2.36	0.58
2:G:91:GLU:HG2	2:G:487:LYS:HD3	1.85	0.58
3:Q:176:LEU:HD13	3:Q:199:VAL:HG21	1.83	0.58
5:M:97:PHE:HB3	5:M:100(E):PRO:HD3	1.84	0.58
3:I:51:ASP:OD1	3:I:59:THR:OG1	2.22	0.58
5:M:49:GLY:HA3	5:M:69:MET:HE1	1.85	0.57
2:G:299:PRO:HG2	2:G:327:ARG:HB2	1.86	0.57
2:G:456:ARG:NH2	2:G:457:ASP:OD1	2.37	0.57
6:E:47:ILE:HG22	6:E:48:ILE:HG13	1.85	0.57
2:H:108:ILE:HD12	2:H:111:LEU:HD21	1.87	0.57
6:N:47:ILE:HG22	6:N:48:ILE:HG12	1.87	0.57
1:B:631:TRP:HE1	2:G:498:PRO:HD3	1.69	0.57
1:A:639:THR:HA	1:A:642:ILE:HB	1.86	0.57
2:F:292:VAL:HB	2:F:449:ILE:HB	1.87	0.57
5:M:69:MET:HE2	5:M:80:MET:HG3	1.87	0.56
3:I:41:SER:HB2	3:I:44:LYS:HB2	1.87	0.56
2:F:161:MET:O	2:F:169:LYS:HB3	2.05	0.56
2:H:294:ILE:HD11	2:H:331:CYS:SG	2.46	0.56
3:Q:186:VAL:HG13	4:R:166:THR:HB	1.88	0.56
2:G:139:THR:OG1	4:K:51:ARG:NH2	2.39	0.55
2:F:455:THR:OG1	2:F:456:ARG:N	2.39	0.55
5:D:75:MET:C	5:D:76:GLU:HG3	2.32	0.55
3:J:100:ALA:HB3	3:J:115:TYR:HB3	1.87	0.55
1:A:606:THR:OG1	2:F:36:VAL:O	2.21	0.55
2:F:175:LEU:H	2:F:320:THR:HB	1.71	0.55
2:H:48:ALA:HB3	2:H:490:LYS:HB2	1.88	0.55
2:G:70:ALA:HB2	2:G:111:LEU:HD21	1.89	0.55
1:A:598:CYS:O	1:A:600:GLY:N	2.40	0.55
3:I:220:SER:O	3:I:222:THR:N	2.40	0.55
3:Q:99:ASN:HA	3:Q:117:MET:HA	1.88	0.55
2:G:63:THR:HG21	2:G:213:ILE:HD12	1.88	0.54
5:M:12:LYS:HG3	5:M:18:VAL:HG22	1.90	0.54
6:P:27(C):VAL:HG13	6:P:66:LYS:HG2	1.88	0.54
2:H:108:ILE:HG21	2:H:479:TRP:HE1	1.72	0.54
1:B:606:THR:OG1	2:G:36:VAL:O	2.18	0.54
4:L:115:ALA:O	4:L:201:HIS:NE2	2.41	0.54
2:H:386:ASN:HB3	2:H:417:PRO:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:215:ILE:O	2:G:250:GLY:HA2	2.07	0.54
2:F:252:LYS:HD2	2:F:262:ASN:HB3	1.90	0.54
4:R:40:LYS:HB2	4:R:43:GLN:HG3	1.90	0.54
3:J:118:ASP:OD1	3:J:118:ASP:N	2.41	0.53
1:C:627:THR:O	1:C:631:TRP:N	2.37	0.53
1:B:578:ALA:HB1	2:G:220:PRO:HG3	1.89	0.53
2:F:280:ASN:ND2	2:F:457:ASP:O	2.41	0.53
6:N:55:PRO:HD2	6:N:58:ILE:HG13	1.91	0.53
2:G:286:VAL:HB	2:G:452:LEU:HB3	1.91	0.53
6:N:2:SER:OG	6:N:3:ALA:N	2.42	0.53
2:G:170:GLN:NE2	2:G:171:LYS:O	2.42	0.53
1:B:594:GLY:HA2	1:B:599:SER:HA	1.90	0.53
3:Q:98:ARG:NH2	3:Q:118:ASP:OD2	2.42	0.53
2:F:268:GLU:O	2:F:289:ASN:ND2	2.42	0.53
1:B:541:ALA:O	1:C:591:GLN:NE2	2.41	0.53
2:G:305:LYS:HB2	2:G:319:ALA:HB3	1.91	0.53
3:I:100:ALA:HB3	3:I:115:TYR:HB3	1.90	0.53
3:Q:212:ILE:HA	3:Q:227:ARG:HA	1.90	0.53
6:P:50:GLU:O	6:P:52:ASN:N	2.42	0.52
3:J:138:VAL:HG12	3:J:159:VAL:HG22	1.91	0.52
3:I:159:VAL:HG11	3:I:167:VAL:HG21	1.92	0.52
5:O:50:TRP:NE1	5:O:58:LYS:HB2	2.24	0.52
5:D:29:PHE:O	5:D:31:GLY:N	2.43	0.52
2:F:121:LYS:HA	2:F:202:THR:HA	1.90	0.52
2:F:454:LEU:HA	2:F:470:PRO:HA	1.91	0.52
2:G:130:GLN:O	2:G:157:CYS:HA	2.10	0.52
3:J:11:LEU:HD13	3:J:164:PRO:HG3	1.92	0.52
5:O:50:TRP:HE1	5:O:58:LYS:HB2	1.75	0.52
3:Q:4:LEU:HB3	3:Q:96:CYS:SG	2.50	0.52
2:F:297:THR:HA	2:F:443:ILE:O	2.10	0.52
2:F:369:LEU:O	2:F:373:THR:OG1	2.26	0.52
6:E:33:VAL:HB	6:E:51:VAL:HA	1.90	0.52
3:J:36:THR:HG22	3:J:51:ASP:HB3	1.91	0.51
5:M:39:GLN:HB2	5:M:45:LEU:HG	1.91	0.51
3:I:169:VAL:HG21	3:I:197:SER:CB	2.40	0.51
2:H:239:CYS:HB2	2:H:242:VAL:HG22	1.92	0.51
5:M:40:ALA:HB3	5:M:43:ARG:HB2	1.91	0.51
6:P:92:ALA:O	6:P:94:GLY:N	2.44	0.51
2:H:283:ASN:ND2	2:H:477:ASP:OD2	2.30	0.51
2:H:476:ARG:HD2	5:O:100(A):ALA:HA	1.91	0.51
2:G:65:LYS:HB2	2:G:68:VAL:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:163:VAL:HG22	4:L:182:LEU:HB2	1.91	0.51
1:C:650:GLN:O	1:C:654:GLU:N	2.40	0.51
2:G:110:SER:HA	2:G:113:ASP:HB2	1.92	0.51
2:G:252:LYS:HD2	2:G:262:ASN:HB3	1.91	0.51
2:G:261:LEU:HB3	2:G:447:SER:OG	2.11	0.51
2:F:161:MET:N	2:F:170:GLN:O	2.38	0.51
1:C:578:ALA:HB1	2:H:220:PRO:HG3	1.93	0.51
4:K:196:SER:HA	4:K:208:LYS:O	2.10	0.51
5:O:52:ASN:HB3	5:O:56:ALA:HB3	1.93	0.51
2:H:96:TRP:HE1	5:O:100(B):ASP:HB3	1.76	0.50
3:I:169:VAL:HA	3:I:214:ASN:O	2.12	0.50
1:B:614:TRP:O	1:B:616:ASN:N	2.43	0.50
3:I:139:PHE:HB2	3:I:158:LEU:HB3	1.94	0.50
3:I:164:PRO:HD2	3:I:219:PRO:HB3	1.94	0.50
2:G:426:MET:HG3	2:G:427:TRP:H	1.77	0.50
2:F:385:CYS:HA	2:F:418:CYS:HA	1.92	0.50
1:C:601:LYS:O	1:C:602:LEU:HB2	2.10	0.50
4:L:154:ALA:O	4:L:156:SER:N	2.44	0.50
5:D:97:PHE:HB2	5:D:100(E):PRO:HG3	1.93	0.50
4:L:189:TRP:O	4:L:195:TYR:OH	2.27	0.50
6:P:4:LEU:HB2	6:P:99:GLY:HA2	1.93	0.50
2:G:122:LEU:HD11	2:G:203:GLN:HB2	1.94	0.50
3:J:143:PRO:HB3	3:J:155:LEU:HB3	1.94	0.50
2:G:254:VAL:HG21	2:G:262:ASN:HB2	1.93	0.49
2:H:297:THR:OG1	2:H:330:HIS:NE2	2.44	0.49
2:F:312:GLY:HA3	2:F:313:PRO:C	2.36	0.49
2:G:312:GLY:HA2	2:G:315:GLN:HB2	1.94	0.49
2:H:61:TYR:CD1	2:H:71:THR:HB	2.48	0.49
2:F:462:ASN:O	2:F:464:THR:N	2.39	0.49
3:Q:52:ILE:HD11	3:Q:72:LEU:HB2	1.94	0.49
2:G:327:ARG:HG2	3:J:111:GLU:HG2	1.95	0.49
2:F:120:VAL:O	2:F:203:GLN:N	2.45	0.49
5:M:100(E):PRO:HG2	5:M:100(G):ARG:HG2	1.95	0.49
2:H:372:THR:O	2:H:387:THR:OG1	2.21	0.49
1:B:601:LYS:HG2	1:C:594:GLY:HA3	1.94	0.49
5:D:100(F):TRP:CD1	5:D:100(F):TRP:N	2.77	0.49
1:B:596:TRP:HA	1:B:651:ASN:ND2	2.28	0.48
1:B:546:SER:HB2	2:G:221:ALA:HB2	1.95	0.48
3:J:91:THR:HG23	3:J:127:THR:HA	1.94	0.48
1:A:645:LEU:O	1:A:649:SER:N	2.41	0.48
3:Q:36:THR:HB	3:Q:51:ASP:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:120:TRP:HB2	4:L:44:ALA:HB1	1.96	0.48
4:R:117:PRO:HD3	4:R:201:HIS:HB3	1.95	0.48
2:G:214:PRO:HA	2:G:251:ILE:O	2.12	0.48
3:J:167:VAL:HG22	3:J:217:HIS:HA	1.94	0.48
4:L:201:HIS:N	4:L:204:SER:O	2.45	0.48
2:H:129:LEU:HB3	2:H:157:CYS:HB3	1.95	0.48
4:L:6:LEU:HB2	4:L:102:GLY:HA2	1.95	0.48
2:H:364:SER:HB2	2:H:470:PRO:HG2	1.95	0.48
4:L:140:ILE:HG12	4:L:199:VAL:HG21	1.95	0.48
3:I:186:VAL:HG12	3:I:194:SER:O	2.14	0.48
2:H:459:GLY:HA3	6:P:93:ASP:HB3	1.96	0.48
4:L:93:ASP:OD2	4:L:95:SER:OG	2.25	0.48
2:H:296:CYS:O	2:H:444:ARG:HG3	2.13	0.48
4:L:141:SER:OG	4:L:142:ASP:OD2	2.28	0.48
1:B:602:LEU:HG	1:C:595:ILE:HA	1.96	0.47
3:I:176:LEU:HD13	3:I:199:VAL:HG21	1.97	0.47
5:O:23:THR:HA	5:O:77:ILE:HG13	1.96	0.47
3:Q:65:ARG:O	3:Q:67:ARG:N	2.47	0.47
2:F:64:GLU:O	2:F:68:VAL:HG23	2.14	0.47
1:C:617:ARG:HB3	1:C:621:GLU:HB2	1.96	0.47
2:H:370:GLU:OE1	2:H:370:GLU:N	2.46	0.47
2:G:412:ASP:OD1	2:G:412:ASP:N	2.48	0.47
3:Q:155:LEU:HD13	3:Q:228:VAL:HG11	1.96	0.47
2:G:152:GLY:C	2:G:154:LEU:H	2.22	0.47
2:G:218:CYS:HA	2:G:246:GLN:O	2.14	0.47
2:G:138:ILE:HG21	4:K:31:SER:HA	1.97	0.47
2:H:254:VAL:HG21	2:H:262:ASN:HB2	1.96	0.47
6:P:27(C):VAL:HG11	6:P:71:ALA:H	1.80	0.47
4:R:51:ARG:NH2	4:R:54:GLN:OE1	2.48	0.47
1:B:536:THR:HB	1:B:539:VAL:HG22	1.97	0.47
2:G:193:LEU:HB2	2:G:196:CYS:SG	2.55	0.47
2:H:378:CYS:HB3	2:H:383:PHE:CD1	2.50	0.47
4:R:24:CYS:HB2	4:R:36:TRP:CH2	2.50	0.47
1:A:614:TRP:O	1:A:616:ASN:N	2.48	0.47
4:L:195:TYR:N	4:L:210:VAL:O	2.48	0.47
3:I:180:VAL:HG12	3:I:199:VAL:HG23	1.97	0.47
1:C:592:LEU:HA	1:C:595:ILE:HG12	1.97	0.47
2:H:360:ARG:HG2	2:H:361:PHE:N	2.30	0.47
5:D:38:ARG:O	5:D:45:LEU:HA	2.14	0.46
2:F:161:MET:O	2:F:170:GLN:N	2.43	0.46
4:L:117:PRO:HD3	4:L:201:HIS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:598:CYS:O	1:C:600:GLY:N	2.42	0.46
3:Q:36:THR:HA	3:Q:51:ASP:HA	1.96	0.46
2:G:428:GLN:HG3	5:D:53:PHE:CZ	2.51	0.46
1:C:620:SER:HA	1:C:624:ASP:HB2	1.97	0.46
1:B:596:TRP:HE1	1:B:647:GLU:HB2	1.80	0.46
6:E:65:SER:OG	6:E:72:SER:OG	2.33	0.46
1:B:646:LEU:HD23	1:B:646:LEU:HA	1.68	0.46
2:F:65:LYS:HB2	2:F:68:VAL:HG22	1.97	0.46
4:L:201:HIS:CD2	4:L:202:GLU:HG3	2.51	0.46
6:P:33:VAL:HG12	6:P:90:SER:HB2	1.97	0.46
2:G:307:ILE:HB	2:G:317:PHE:HB3	1.97	0.46
2:F:130:GLN:O	2:F:157:CYS:HA	2.16	0.46
2:H:296:CYS:HA	2:H:331:CYS:HA	1.98	0.46
3:Q:171:TRP:HB2	3:Q:176:LEU:HB2	1.97	0.46
2:G:260:LEU:HB3	2:G:451:GLY:HA3	1.98	0.46
5:D:37:VAL:CG1	5:D:45:LEU:HB3	2.45	0.46
3:I:183:PHE:CD1	4:L:139:LEU:HD13	2.51	0.46
1:B:663:LEU:HD21	2:F:499:THR:HB	1.97	0.46
2:H:35:TRP:O	2:H:498:PRO:HA	2.15	0.46
6:E:92:ALA:O	6:E:94:GLY:N	2.49	0.46
2:F:457:ASP:HA	5:M:58:LYS:HD2	1.98	0.46
3:Q:100:ALA:HB3	3:Q:115:TYR:HB3	1.98	0.46
2:F:296:CYS:HA	2:F:331:CYS:HA	1.98	0.45
3:Q:185:ALA:HA	3:Q:195:LEU:HB3	1.97	0.45
3:Q:54:TYR:OH	3:Q:74:GLN:O	2.31	0.45
3:J:34:SER:HB3	3:J:51:ASP:HB2	1.97	0.45
4:K:132:ASN:HA	4:K:186:PRO:HG3	1.97	0.45
2:F:57:ASP:HA	2:F:77:THR:H	1.82	0.45
2:F:218:CYS:HA	2:F:246:GLN:O	2.17	0.45
5:M:96:MET:HB2	5:M:100(H):GLY:HA3	1.99	0.45
3:I:98:ARG:O	3:I:117:MET:HA	2.17	0.45
2:H:95:MET:HB3	2:H:484:TYR:HA	1.98	0.45
3:J:4:LEU:HD21	3:J:35:TRP:HZ3	1.80	0.45
3:J:106:VAL:HB	3:J:111:GLU:OE1	2.17	0.45
3:J:155:LEU:HA	4:K:122:PHE:CZ	2.52	0.45
2:F:460:SER:OG	2:F:461:THR:N	2.46	0.45
3:Q:12:VAL:HG21	3:Q:18:LEU:HB2	1.98	0.45
3:J:94:TYR:CE1	3:J:126:VAL:HB	2.52	0.45
2:G:391:PHE:CZ	2:G:470:PRO:HB3	2.52	0.45
2:F:104:MET:HE2	2:F:479:TRP:CE3	2.52	0.45
3:I:171:TRP:HB2	3:I:176:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:176:LEU:HB3	3:I:199:VAL:HG21	1.97	0.45
2:G:161:MET:O	2:G:170:GLN:N	2.50	0.45
2:G:227:LYS:O	2:G:242:VAL:HA	2.17	0.45
3:J:155:LEU:HA	4:K:122:PHE:HZ	1.81	0.45
1:A:543:ASN:HA	1:A:546:SER:HB2	1.99	0.45
1:A:663:LEU:HD23	1:A:664:ASP:HB2	1.97	0.45
2:F:131:CYS:HB3	2:F:155:LYS:CB	2.45	0.45
1:B:595:ILE:HG21	1:B:647:GLU:HG3	1.98	0.45
2:G:78:ASP:O	2:G:80:ASN:N	2.50	0.45
2:G:425:ASN:HB2	2:G:433:ALA:HB2	1.98	0.45
3:I:129:SER:OG	3:I:130:SER:N	2.49	0.45
3:Q:36:THR:HG23	3:Q:97:ALA:HB3	1.98	0.45
2:F:227:LYS:HA	2:F:485:LYS:O	2.17	0.45
5:M:6:GLU:HG2	5:M:22:CYS:HB2	1.98	0.45
3:I:139:PHE:CZ	4:L:128:GLU:HG3	2.52	0.45
4:L:48:ILE:HG13	4:L:49:ILE:HG12	1.98	0.45
1:B:530:MET:HA	1:B:533:ALA:HB3	1.99	0.44
4:L:40:LYS:HB2	4:L:43:GLN:HG3	1.98	0.44
4:L:124:PRO:HD3	4:L:136:LEU:HD23	1.99	0.44
5:O:51:ILE:CD1	5:O:71:ARG:HD2	2.47	0.44
1:C:630:GLN:O	1:C:633:LYS:HG2	2.17	0.44
2:H:386:ASN:N	2:H:417:PRO:O	2.40	0.44
3:I:37:TRP:CG	3:I:81:LEU:HD22	2.52	0.44
3:I:217:HIS:CE1	3:I:219:PRO:HB2	2.52	0.44
6:P:36:TYR:CZ	6:P:46:LEU:HD13	2.53	0.44
4:R:138:CYS:HB2	4:R:152:TRP:CH2	2.52	0.44
6:P:34:SER:O	6:P:89:TYR:N	2.43	0.44
4:R:122:PHE:HB2	4:R:137:VAL:HB	2.00	0.44
3:I:53:HIS:O	3:I:55:ASN:N	2.51	0.44
3:I:169:VAL:HG21	3:I:197:SER:HB3	1.99	0.44
6:P:78:LEU:HD21	6:P:104:LEU:HD11	1.98	0.44
2:F:131:CYS:HB2	2:F:191:TYR:CD1	2.53	0.44
4:L:152:TRP:HB2	4:L:159:VAL:HB	1.98	0.44
2:G:300:ASN:HB3	2:G:322:ILE:HG23	1.99	0.44
2:F:249:HIS:ND1	2:F:486:TYR:OH	2.43	0.44
2:F:416:LEU:HA	2:F:417:PRO:HD3	1.88	0.44
3:I:46:LEU:O	4:L:101:PHE:HB2	2.17	0.44
2:F:286:VAL:HB	2:F:452:LEU:HB3	1.99	0.44
1:C:545:LEU:O	1:C:547:GLY:N	2.50	0.44
2:G:276:ASN:O	2:G:278:THR:N	2.49	0.44
5:D:100(E):PRO:HB2	5:D:100(F):TRP:H	1.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:327:ARG:HD2	3:I:111:GLU:HG2	1.99	0.44
3:I:185:ALA:HA	3:I:195:LEU:HB3	2.00	0.44
5:O:47:TRP:CZ3	5:O:60:PRO:HD3	2.53	0.44
4:K:171:GLN:N	4:K:175:LYS:O	2.37	0.43
1:C:635:ILE:O	1:C:639:THR:HG23	2.18	0.43
2:G:64:GLU:O	2:G:68:VAL:HG23	2.18	0.43
3:J:187:LEU:HD13	3:J:193:TYR:CE1	2.53	0.43
1:A:570:VAL:HG21	2:F:114:GLN:HG3	1.99	0.43
2:F:303:THR:HB	2:F:321:GLY:HA3	1.99	0.43
5:O:49:GLY:HA3	5:O:69:MET:HE1	2.00	0.43
1:B:587:LEU:HB3	1:A:545:LEU:HD21	2.01	0.43
2:G:105:HIS:CG	2:G:476:ARG:HG2	2.54	0.43
2:F:294:ILE:HG13	2:F:333:VAL:HG22	2.01	0.43
2:G:61:TYR:OH	2:G:74:CYS:O	2.35	0.43
4:K:35:TYR:O	4:K:90:GLN:N	2.52	0.43
5:D:37:VAL:HG12	5:D:45:LEU:HB3	1.99	0.43
1:A:662:ALA:HB1	2:H:501:CYS:SG	2.58	0.43
4:K:36:TRP:HB2	4:K:49:ILE:HB	2.00	0.43
5:D:97:PHE:O	5:D:100(E):PRO:HD3	2.18	0.43
3:I:103:ILE:HG13	3:I:111:GLU:O	2.18	0.43
2:H:35:TRP:CZ2	2:H:502:LYS:HD3	2.53	0.43
4:R:150:VAL:HG22	4:R:199:VAL:HG13	2.00	0.43
4:R:165:THR:HA	4:R:180:SER:HA	2.01	0.43
3:J:48:TRP:CZ2	3:J:50:GLY:HA2	2.53	0.43
5:D:47:TRP:CZ3	5:D:60:PRO:HG3	2.54	0.43
6:E:37:GLN:HG3	6:E:86:TYR:CE2	2.54	0.43
3:Q:2:VAL:HG21	3:Q:98:ARG:HH11	1.83	0.43
3:Q:67:ARG:O	3:Q:83:MET:HA	2.19	0.43
2:G:38:VAL:HG13	2:G:494:LEU:HD11	1.99	0.43
2:G:268:GLU:O	2:G:289:ASN:ND2	2.52	0.43
3:J:11:LEU:HD12	3:J:127:THR:O	2.18	0.43
1:A:647:GLU:OE2	1:C:542:ARG:HB3	2.18	0.43
2:H:294:ILE:O	2:H:446:VAL:HA	2.18	0.43
2:F:109:ILE:O	2:F:112:TRP:HB3	2.19	0.43
1:C:619:LEU:O	1:C:623:TRP:HB3	2.19	0.43
2:H:97:LYS:NZ	5:O:100(B):ASP:OD2	2.38	0.43
5:O:11:VAL:HG13	5:O:110:THR:HB	2.01	0.43
2:G:307:ILE:HG22	2:G:309:ILE:HG23	2.01	0.43
3:Q:39:ARG:HA	3:Q:93:MET:O	2.19	0.43
6:P:27(C):VAL:HG11	6:P:71:ALA:N	2.34	0.43
2:G:276:ASN:C	2:G:278:THR:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:300:ASN:HB3	2:G:322:ILE:HD12	2.01	0.42
5:M:18:VAL:HG23	5:M:82(C):LEU:HD11	2.00	0.42
3:I:61:ASN:HB3	3:I:64:LEU:HD12	2.01	0.42
4:L:151:ALA:HB3	4:L:198:GLN:HB3	2.01	0.42
5:D:4:LEU:HD13	5:D:34:MET:HE2	2.00	0.42
6:N:48:ILE:HG21	6:N:64:ALA:HB3	2.00	0.42
2:H:65:LYS:HD2	2:H:207:LYS:O	2.19	0.42
2:G:359:ILE:HG23	2:G:468:PHE:CE1	2.54	0.42
2:G:456:ARG:HE	2:G:466:GLU:CD	2.27	0.42
3:J:163:PHE:HA	3:J:164:PRO:HA	1.90	0.42
6:E:35:TRP:CE3	6:E:88:CYS:HB2	2.54	0.42
2:F:164:GLU:CD	2:F:308:ARG:HE	2.27	0.42
4:L:143:PHE:HB2	4:L:201:HIS:CE1	2.55	0.42
4:K:153:LYS:HA	4:K:158:PRO:HA	2.00	0.42
1:A:530:MET:N	1:A:626:MET:O	2.49	0.42
1:A:618:ASN:O	1:A:622:ILE:HG13	2.20	0.42
2:G:385:CYS:HA	2:G:417:PRO:O	2.19	0.42
4:K:6:LEU:HD11	4:K:91:SER:HB3	2.01	0.42
5:D:100(F):TRP:CD1	5:D:100(F):TRP:H	2.37	0.42
6:N:2:SER:HG	6:N:3:ALA:H	1.67	0.42
4:L:81:ALA:O	4:L:174:ASN:ND2	2.42	0.42
3:Q:163:PHE:HA	3:Q:164:PRO:HA	1.87	0.42
2:G:270:VAL:HG11	2:G:345:VAL:HG22	2.02	0.42
2:G:296:CYS:HA	2:G:331:CYS:HA	2.01	0.42
2:F:65:LYS:HB2	2:F:68:VAL:CG2	2.50	0.42
2:F:255:VAL:O	2:F:376:PHE:HA	2.19	0.42
1:C:583:VAL:HA	1:C:586:TYR:HB3	2.00	0.42
6:P:78:LEU:HD13	6:P:104:LEU:HD21	2.01	0.42
6:P:80:GLU:HG2	6:P:106:VAL:HG21	2.02	0.42
3:Q:98:ARG:O	3:Q:118:ASP:N	2.53	0.42
4:R:14:VAL:HG21	4:R:20:ALA:HB2	2.02	0.42
5:O:4:LEU:HD13	5:O:92:CYS:HB2	2.01	0.42
5:O:70:THR:OG1	5:O:71:ARG:N	2.49	0.42
4:R:186:PRO:O	4:R:189:TRP:HB3	2.20	0.42
1:B:533:ALA:HB1	1:B:628:TRP:CD1	2.55	0.42
1:B:655:LYS:HG3	1:A:602:LEU:HD12	2.01	0.42
2:G:214:PRO:HG3	2:G:252:LYS:HE2	2.02	0.42
3:I:27:ASP:OD1	3:I:27:ASP:N	2.51	0.42
2:H:259:LEU:HB2	2:H:374:HIS:CE1	2.55	0.42
4:R:166:THR:HG22	4:R:179:SER:H	1.84	0.42
1:B:545:LEU:HD21	1:B:583:VAL:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:51:ILE:HD11	5:M:71:ARG:HD2	2.01	0.42
3:Q:3:GLN:O	3:Q:24:VAL:HA	2.20	0.42
3:Q:65:ARG:C	3:Q:67:ARG:H	2.27	0.42
4:R:150:VAL:HG22	4:R:199:VAL:HG22	2.00	0.42
4:L:143:PHE:CE1	4:L:146:GLY:HA2	2.55	0.41
2:H:181:VAL:HG12	2:H:193:LEU:HD23	2.02	0.41
3:J:32:ASP:OD1	3:J:32:ASP:N	2.53	0.41
5:D:11:VAL:HG13	5:D:110:THR:O	2.20	0.41
3:I:187:LEU:HB2	3:I:193:TYR:CE2	2.56	0.41
2:H:260:LEU:HB3	2:H:451:GLY:N	2.36	0.41
2:H:397:SER:OG	2:H:398:ASN:N	2.52	0.41
1:B:546:SER:CB	2:G:221:ALA:HB2	2.49	0.41
6:N:38:GLN:C	6:N:84:ALA:HB1	2.46	0.41
6:P:28:GLY:CA	6:P:69:ASN:HA	2.50	0.41
4:K:36:TRP:CH2	4:K:89:CYS:HB3	2.55	0.41
4:K:90:GLN:HG2	4:K:100:MET:O	2.20	0.41
2:H:256:SER:HA	2:H:375:SER:O	2.19	0.41
2:H:457:ASP:OD2	2:H:467:THR:OG1	2.36	0.41
1:B:544:LEU:C	2:G:221:ALA:HB1	2.45	0.41
2:G:328:GLN:HE22	2:G:420:ILE:HG13	1.85	0.41
2:G:477:ASP:HA	2:G:480:ARG:HD2	2.02	0.41
2:F:163:THR:OG1	2:F:164:GLU:N	2.52	0.41
1:C:646:LEU:HD23	1:C:646:LEU:HA	1.94	0.41
3:Q:34:SER:O	3:Q:99:ASN:N	2.53	0.41
4:K:155:ASP:HA	4:K:194:SER:OG	2.20	0.41
3:I:88:ALA:HA	3:I:128:VAL:HB	2.03	0.41
1:B:569:THR:OG1	1:B:570:VAL:N	2.49	0.41
4:K:197:CYS:O	4:K:207:GLU:HA	2.20	0.41
5:D:23:THR:OG1	5:D:76:GLU:O	2.36	0.41
2:F:122:LEU:HD11	2:F:203:GLN:HB2	2.03	0.41
2:F:369:LEU:HB3	2:F:384:TYR:CD2	2.56	0.41
1:C:570:VAL:O	1:C:571:TRP:HB2	2.21	0.41
2:H:122:LEU:HB3	2:H:125:LEU:HD23	2.02	0.41
2:H:456:ARG:NH2	2:H:458:GLY:O	2.54	0.41
2:G:312:GLY:HA3	2:G:313:PRO:C	2.46	0.41
2:G:364:SER:HB2	2:G:470:PRO:HG2	2.03	0.41
3:J:19:SER:HA	3:J:81:LEU:O	2.20	0.41
3:J:76:ILE:H	3:J:77:PRO:HA	1.86	0.41
4:K:39:GLN:O	4:K:85:ALA:HB1	2.20	0.41
4:K:66:SER:N	4:K:73:THR:O	2.46	0.41
2:F:192:ARG:HD2	2:F:193:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:215:VAL:O	3:I:224:VAL:N	2.52	0.41
4:L:8:GLN:HG2	4:L:24:CYS:HB2	2.02	0.41
4:L:155:ASP:HB2	4:L:192:HIS:HB3	2.01	0.41
1:C:619:LEU:HD22	2:H:500:ARG:HD2	2.02	0.41
5:O:5:VAL:HB	5:O:23:THR:HB	2.02	0.41
3:Q:6:GLU:HG3	3:Q:96:CYS:SG	2.61	0.41
4:R:32:ARG:HG3	4:R:93:ASP:O	2.21	0.41
2:H:345:VAL:O	2:H:349:LEU:HG	2.21	0.41
2:H:382:PHE:O	2:H:420:ILE:HA	2.21	0.41
4:K:84:GLU:HG3	4:K:108:THR:HA	2.03	0.40
1:A:650:GLN:HG2	1:A:654:GLU:HB2	2.03	0.40
2:F:274:SER:HB3	2:F:277:ILE:HG22	2.03	0.40
2:H:90:THR:HB	2:H:238:PRO:HB2	2.03	0.40
5:O:100(E):PRO:HB2	5:O:100(F):TRP:H	1.64	0.40
6:P:39:HIS:O	6:P:41:GLY:N	2.54	0.40
4:R:49:ILE:HD13	4:R:65:ALA:HB2	2.04	0.40
2:G:262:ASN:N	2:G:447:SER:OG	2.55	0.40
2:G:434:MET:HE2	2:G:434:MET:HB2	1.83	0.40
5:D:34:MET:HE3	5:D:34:MET:HB2	1.96	0.40
5:D:51:ILE:HA	5:D:57:VAL:HG12	2.03	0.40
4:L:15:SER:O	4:L:17:GLY:N	2.54	0.40
5:M:17:SER:HB3	5:M:82(A):SER:HA	2.03	0.40
1:B:545:LEU:HD23	1:B:545:LEU:HA	1.72	0.40
5:D:101:VAL:HG13	6:E:46:LEU:HD22	2.03	0.40
5:M:23:THR:HA	5:M:77:ILE:HA	2.03	0.40
5:M:87:THR:HG23	5:M:109:VAL:O	2.21	0.40
1:C:620:SER:O	1:C:625:ASN:HB2	2.22	0.40
2:H:300:ASN:HB3	2:H:322:ILE:HD13	2.03	0.40

All (1) 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)
1:A:661:LEU:O	1:A:663:LEU:N[8_554]	2.16	0.04

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	122/153 (80%)	93 (76%)	24 (20%)	5 (4%)	2	18
1	B	122/153 (80%)	104 (85%)	15 (12%)	3 (2%)	4	26
1	C	122/153 (80%)	97 (80%)	20 (16%)	5 (4%)	2	18
2	F	442/479 (92%)	363 (82%)	71 (16%)	8 (2%)	6	34
2	G	442/479 (92%)	377 (85%)	51 (12%)	14 (3%)	3	21
2	H	442/479 (92%)	370 (84%)	57 (13%)	15 (3%)	3	21
3	I	223/241 (92%)	195 (87%)	21 (9%)	7 (3%)	3	22
3	J	223/241 (92%)	188 (84%)	27 (12%)	8 (4%)	2	20
3	Q	223/241 (92%)	195 (87%)	24 (11%)	4 (2%)	6	34
4	K	201/215 (94%)	175 (87%)	24 (12%)	2 (1%)	12	48
4	L	201/215 (94%)	174 (87%)	24 (12%)	3 (2%)	8	40
4	R	201/215 (94%)	175 (87%)	22 (11%)	4 (2%)	6	31
5	D	123/232 (53%)	103 (84%)	16 (13%)	4 (3%)	3	21
5	M	123/232 (53%)	106 (86%)	12 (10%)	5 (4%)	2	18
5	O	123/232 (53%)	98 (80%)	22 (18%)	3 (2%)	4	27
6	E	105/214 (49%)	88 (84%)	16 (15%)	1 (1%)	12	48
6	N	107/214 (50%)	91 (85%)	13 (12%)	3 (3%)	4	24
6	P	105/214 (49%)	81 (77%)	20 (19%)	4 (4%)	2	19
All	All	3650/4602 (79%)	3073 (84%)	479 (13%)	98 (3%)	4	25

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	74	SER
5	D	100(E)	PRO
5	M	100(E)	PRO
3	I	30	PRO

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Mol	Chain	Res	Type
3	I	166	PRO
3	I	221	ASN
1	C	602	LEU
1	C	615	SER
2	H	331	CYS
5	O	100(E)	PRO
3	Q	204	SER
1	B	599	SER
2	G	135	THR
2	G	268	GLU
2	G	301	ASN
2	G	392	ASN
3	J	9	PRO
3	J	30	PRO
3	J	204	SER
1	A	599	SER
1	A	615	SER
5	M	100(H)	GLY
3	I	54	TYR
2	H	33	ASN
2	H	98	ASN
6	P	93	ASP
4	R	69	GLY
4	R	104	GLY
4	R	146	GLY
1	B	546	SER
1	B	615	SER
2	G	69	TRP
2	G	117	LYS
2	G	258	GLN
2	G	277	ILE
2	G	391	PHE
5	D	30	THR
6	E	33	VAL
1	A	663	LEU
2	F	118	PRO
2	F	138	ILE
2	F	392	ASN
2	F	428	GLN
3	I	9	PRO
4	L	155	ASP
1	C	645	LEU

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Mol	Chain	Res	Type
2	H	69	TRP
2	H	96	TRP
2	H	135	THR
2	H	301	ASN
2	H	474	ASP
6	P	27(B)	ASP
3	Q	66	SER
3	Q	207	GLY
2	G	354	GLY
2	G	499	THR
3	J	187	LEU
2	F	69	TRP
2	F	258	GLN
1	C	610	TRP
2	H	138	ILE
2	H	258	GLN
2	H	462	ASN
2	H	465	THR
2	H	498	PRO
6	P	51	VAL
4	R	156	SER
2	G	138	ILE
3	J	105	GLY
4	K	52	SER
4	K	192	HIS
1	A	650	GLN
2	F	220	PRO
5	M	29	PHE
6	N	31	ASP
6	N	40	PRO
6	N	93	ASP
2	H	118	PRO
2	H	220	PRO
5	O	53	PHE
6	P	50	GLU
3	Q	9	PRO
3	J	26	GLN
5	M	60	PRO
4	L	16	PRO
1	C	648	GLU
2	G	118	PRO
2	G	430	ILE

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Mol	Chain	Res	Type
3	J	42	PRO
1	A	572	GLY
2	F	498	PRO
3	I	42	PRO
3	I	140	PRO
4	L	41	PRO
5	M	100(D)	SER
5	O	26	GLY
5	D	100(D)	SER
3	J	166	PRO

5.3.2 Protein sidechains [i](#)

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	108/129 (84%)	106 (98%)	2 (2%)	50	67
1	B	108/129 (84%)	106 (98%)	2 (2%)	50	67
1	C	108/129 (84%)	105 (97%)	3 (3%)	38	60
2	F	401/426 (94%)	398 (99%)	3 (1%)	76	81
2	G	401/426 (94%)	400 (100%)	1 (0%)	87	87
2	H	401/426 (94%)	395 (98%)	6 (2%)	57	72
3	I	195/208 (94%)	194 (100%)	1 (0%)	81	83
3	J	195/208 (94%)	193 (99%)	2 (1%)	68	78
3	Q	195/208 (94%)	195 (100%)	0	100	100
4	K	174/182 (96%)	173 (99%)	1 (1%)	78	83
4	L	174/182 (96%)	174 (100%)	0	100	100
4	R	174/182 (96%)	173 (99%)	1 (1%)	78	83
5	D	104/197 (53%)	102 (98%)	2 (2%)	50	67
5	M	104/197 (53%)	103 (99%)	1 (1%)	68	78
5	O	104/197 (53%)	104 (100%)	0	100	100
6	E	85/177 (48%)	84 (99%)	1 (1%)	63	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	N	86/177 (49%)	85 (99%)	1 (1%)	63	75
6	P	85/177 (48%)	85 (100%)	0	100	100
All	All	3202/3957 (81%)	3175 (99%)	27 (1%)	73	80

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	580	VAL
1	B	629	LEU
2	G	275	GLU
3	J	32	ASP
3	J	186	VAL
4	K	64	SER
5	D	72	ASP
5	D	76	GLU
6	E	88	CYS
1	A	604	CYS
1	A	664	ASP
2	F	49	GLU
2	F	116	LEU
2	F	466	GLU
5	M	59	TYR
6	N	96	VAL
3	I	26	GLN
1	C	603	ILE
1	C	604	CYS
1	C	651	ASN
2	H	52	LEU
2	H	228	CYS
2	H	282	LYS
2	H	296	CYS
2	H	331	CYS
2	H	479	TRP
4	R	140	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	651	ASN
2	G	72	HIS

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Mol	Chain	Res	Type
2	G	287	GLN
2	G	289	ASN
2	G	300	ASN
2	G	432	GLN
3	J	40	GLN
3	J	181	HIS
4	K	39	GLN
4	K	54	GLN
2	F	99	ASN
2	F	103	GLN
2	F	170	GLN
2	F	315	GLN
2	F	422	GLN
6	N	39	HIS
6	N	85	HIS
3	I	172	ASN
2	H	82	GLN
2	H	195	ASN
2	H	203	GLN
2	H	287	GLN
2	H	339	ASN
2	H	374	HIS
3	Q	181	HIS
3	Q	188	GLN
3	Q	216	ASN
4	R	188	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	126/153 (82%)	-0.22	0  	365, 471, 570, 691	0
1	B	126/153 (82%)	-0.13	0  	309, 438, 494, 548	0
1	C	126/153 (82%)	-0.07	0  	329, 445, 536, 592	0
2	F	450/479 (93%)	-0.13	7 (1%)  	209, 400, 510, 597	0
2	G	450/479 (93%)	-0.10	3 (0%)  	212, 372, 474, 595	0
2	H	450/479 (93%)	-0.10	7 (1%)  	241, 392, 532, 589	0
3	I	227/241 (94%)	-0.21	1 (0%)  	277, 411, 505, 576	0
3	J	227/241 (94%)	-0.20	2 (0%)  	270, 380, 474, 594	0
3	Q	227/241 (94%)	-0.17	1 (0%)  	341, 442, 578, 700	0
4	K	205/215 (95%)	-0.13	3 (1%)  	297, 386, 473, 543	0
4	L	205/215 (95%)	-0.20	1 (0%)  	324, 407, 503, 613	0
4	R	205/215 (95%)	-0.03	4 (1%)  	354, 521, 620, 698	0
5	D	125/232 (53%)	-0.11	3 (2%)  	237, 362, 466, 541	0
5	M	125/232 (53%)	-0.23	2 (1%)  	303, 386, 510, 581	0
5	O	125/232 (53%)	-0.02	2 (1%)  	223, 325, 420, 472	0
6	E	107/214 (50%)	-0.16	1 (0%)  	319, 436, 537, 605	0
6	N	109/214 (50%)	-0.08	2 (1%)  	351, 457, 555, 582	0
6	P	107/214 (50%)	-0.24	0  	290, 406, 493, 559	0
All	All	3722/4602 (80%)	-0.14	39 (1%)  	209, 409, 546, 700	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	22	ILE	5.7
2	G	427	TRP	5.2
3	Q	49	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
2	H	281	ALA	4.6
6	N	3	ALA	4.0
2	F	323	ILE	3.4
2	G	228	CYS	3.4
4	R	13	SER	3.3
5	O	74	SER	3.2
4	L	63	PHE	3.1
2	H	219	ALA	3.0
2	F	45	TRP	2.8
4	K	7	THR	2.8
4	K	100	MET	2.7
3	J	136	PRO	2.7
5	O	29	PHE	2.7
5	D	82	LEU	2.6
4	K	5	GLU	2.6
2	H	220	PRO	2.6
2	H	430	ILE	2.6
2	F	316	ALA	2.6
3	J	103	ILE	2.5
3	I	129	SER	2.5
6	N	108	GLY	2.5
5	M	108	LEU	2.5
2	F	317	PHE	2.4
4	R	101	PHE	2.3
2	F	326	ILE	2.3
2	F	324	GLY	2.3
2	G	426	MET	2.3
5	D	80	MET	2.3
2	F	217	TYR	2.2
5	D	69	MET	2.2
4	R	94	THR	2.1
2	H	454	LEU	2.1
6	E	35	TRP	2.1
5	M	109	VAL	2.1
2	H	495	GLY	2.0
2	H	390	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.