



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:36 AM UTC

PDB ID : 4J8R / pdb_00004j8r
Title : Structure of an octapeptide repeat of the prion protein bound to the POM2 Fab antibody fragment
Authors : Swayampakula, M.; Baral, P.K.; Kav, N.N.V.; Aguzzi, A.; James, M.N.G.
Deposited on : 2013-02-14
Resolution : 2.30 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

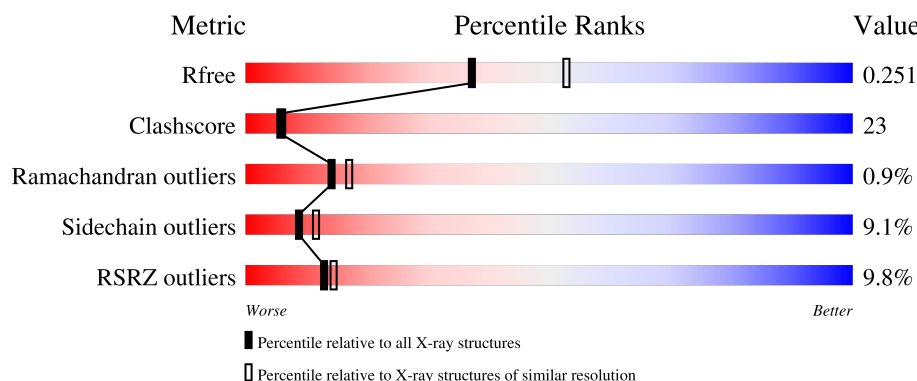
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	210	9% 56% 37% 6%
1	C	210	7% 53% 40% 7%
2	B	220	10% 54% 36% 8% .
2	D	220	9% 56% 35% 9%
3	I	16	50% 6% 19% 19% 12% 44%

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Mol	Chain	Length	Quality of chain
3	J	16	38% 12% 12% 25% 50%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6791 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 Light chain of POM2 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1619	1007	273	332	7			
1	C	210	Total	C	N	O	S	0	0	0
			1624	1010	274	333	7			

- Molecule 2 is a protein called Heavy chain of POM2 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	0	0	0
			1630	1032	268	323	7			
2	D	220	Total	C	N	O	S	0	0	0
			1630	1032	268	323	7			

- Molecule 3 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	9	Total	C	N	O	0	0	0
			65	41	13	11			
3	J	8	Total	C	N	O	0	0	0
			58	36	12	10			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	48	Total	O	0	0
			48	48		
4	I	1	Total	O	0	0
			1	1		
4	C	48	Total	O	0	0
			48	48		

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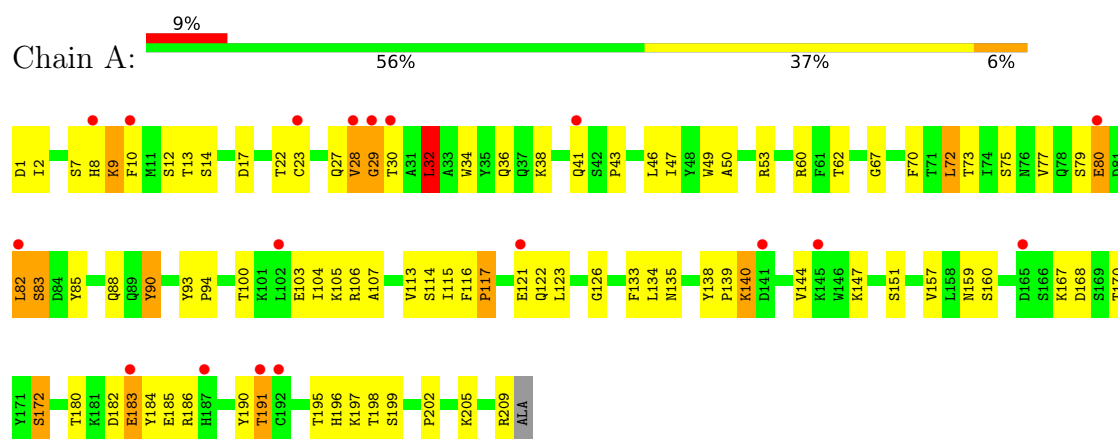
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	36	Total	O	0	0
			36	36		

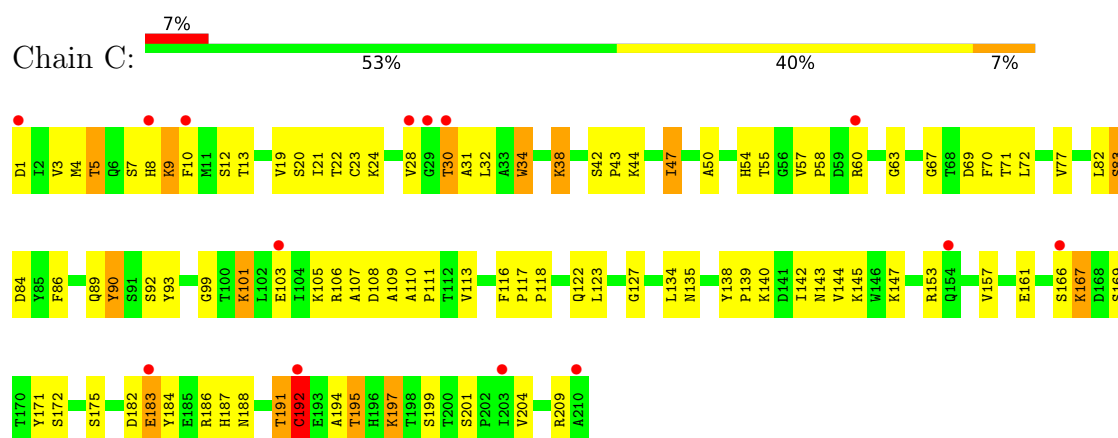
3 Residue-property plots [i](#)

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.

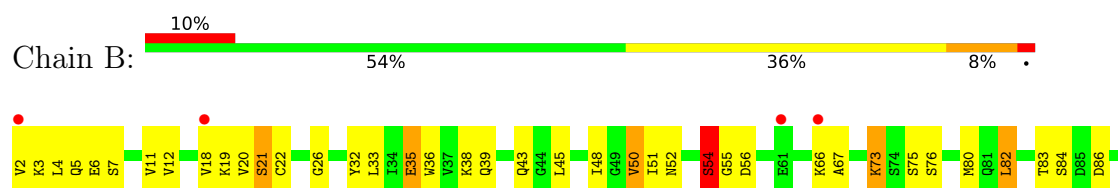
- Molecule 1: Light chain of POM2 Fab

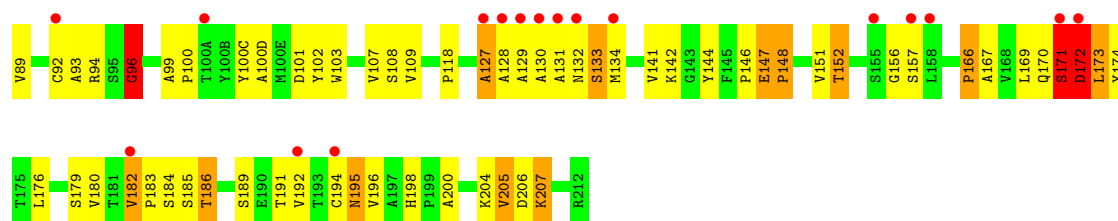


- Molecule 1: Light chain of POM2 Fab

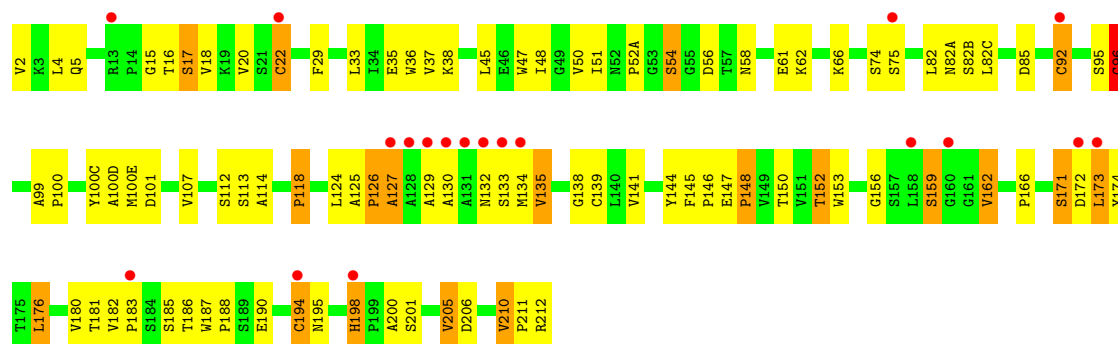


- Molecule 2: Heavy chain of POM2 Fab

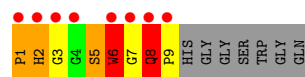




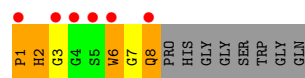
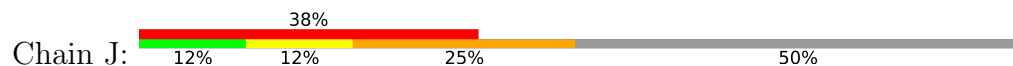
• Molecule 2: Heavy chain of POM2 Fab



• Molecule 3: Major prion protein



• Molecule 3: Major prion protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	65.42Å 71.57Å 207.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.60 – 2.30 39.60 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.60-2.30) 99.8 (39.60-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.247 , 0.257 0.255 , 0.251	Depositor DCC
R_{free} test set	2186 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6791	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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	1.85	16/1655 (1.0%)	1.24	16/2245 (0.7%)
1	C	2.00	26/1660 (1.6%)	1.38	19/2252 (0.8%)
2	B	1.95	22/1672 (1.3%)	1.35	13/2288 (0.6%)
2	D	1.85	13/1672 (0.8%)	1.33	22/2288 (1.0%)
3	I	1.21	0/69	2.40	5/93 (5.4%)
3	J	1.39	0/61	2.06	3/81 (3.7%)
All	All	1.90	77/6789 (1.1%)	1.35	78/9247 (0.8%)

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
2	B	0	1
All	All	0	2

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	191	THR	C-N	13.45	1.51	1.33
1	C	192	CYS	C-N	12.03	1.49	1.33
1	C	201	SER	C-O	-7.33	1.18	1.24
2	B	195	ASN	CG-ND2	-6.59	1.19	1.33
1	C	101	LYS	C-O	-6.47	1.16	1.24
2	D	125	ALA	C-O	-6.37	1.17	1.24
2	D	183	PRO	N-CD	-6.15	1.39	1.47
2	B	198	HIS	C-O	-6.14	1.19	1.24
2	D	36	TRP	C-O	-6.12	1.16	1.24
2	B	180	VAL	C-O	-6.05	1.18	1.24
2	D	171	SER	C-O	-5.99	1.18	1.24
2	B	182	VAL	C-O	-5.99	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	118	PRO	C-O	-5.97	1.17	1.24
1	C	188	ASN	CG-ND2	-5.95	1.20	1.33
1	A	100	THR	C-O	-5.92	1.17	1.24
1	A	115	ILE	C-O	-5.92	1.18	1.24
1	A	93	TYR	C-O	-5.77	1.16	1.24
1	C	8	HIS	C-O	-5.74	1.17	1.23
1	C	20	SER	C-O	-5.73	1.17	1.24
1	C	144	VAL	C-O	-5.69	1.18	1.24
1	C	84	ASP	C-O	-5.68	1.17	1.23
2	B	118	PRO	C-O	-5.67	1.18	1.24
1	C	63	GLY	C-O	-5.67	1.16	1.23
2	B	109	VAL	C-O	-5.66	1.18	1.24
1	C	47	ILE	C-O	-5.61	1.18	1.24
1	A	77	VAL	C-O	-5.60	1.18	1.24
1	C	83	SER	C-O	-5.60	1.18	1.24
2	D	198	HIS	CD2-NE2	-5.55	1.31	1.37
1	C	3	VAL	C-O	-5.54	1.17	1.24
1	A	123	LEU	C-O	-5.53	1.17	1.24
2	B	43	GLN	CD-NE2	-5.52	1.21	1.33
1	C	50	ALA	C-O	-5.49	1.17	1.24
2	D	5	GLN	C-O	-5.46	1.17	1.24
1	A	122	GLN	C-O	-5.44	1.17	1.24
2	B	5	GLN	C-O	-5.43	1.17	1.24
1	A	32	LEU	C-O	-5.41	1.17	1.23
2	B	84	SER	C-O	-5.40	1.17	1.24
1	C	44	LYS	C-O	-5.37	1.17	1.24
1	C	19	VAL	C-O	-5.36	1.18	1.24
2	D	58	ASN	C-O	-5.32	1.18	1.24
2	B	144	TYR	C-O	-5.31	1.17	1.23
1	A	157	VAL	C-O	-5.31	1.18	1.24
2	B	192	VAL	C-O	-5.30	1.18	1.24
1	C	21	ILE	C-O	-5.29	1.18	1.24
2	B	82	LEU	N-CA	-5.27	1.39	1.46
2	B	147	GLU	CA-C	-5.27	1.47	1.53
1	C	71	THR	C-O	-5.26	1.18	1.24
1	A	183	GLU	CA-CB	5.25	1.62	1.53
2	B	35	GLU	C-O	-5.24	1.17	1.23
1	A	190	TYR	C-O	-5.23	1.18	1.24
2	B	102	TYR	C-O	-5.21	1.17	1.23
2	D	166	PRO	C-O	-5.21	1.17	1.23
2	B	205	VAL	C-O	-5.20	1.18	1.24
2	B	50	VAL	C-O	-5.18	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	175	SER	C-O	-5.18	1.18	1.24
1	A	117	PRO	C-O	-5.16	1.18	1.24
1	C	118	PRO	C-O	-5.13	1.17	1.23
2	D	92	CYS	C-O	-5.13	1.17	1.24
2	B	21	SER	C-O	-5.13	1.17	1.24
2	B	51	ILE	C-O	-5.13	1.19	1.24
2	B	141	VAL	C-O	-5.11	1.18	1.24
1	A	47	ILE	C-O	-5.11	1.18	1.24
1	C	142	ILE	C-O	-5.11	1.17	1.23
2	D	85	ASP	C-O	-5.10	1.17	1.24
2	D	138	GLY	C-O	-5.09	1.18	1.23
1	A	172	SER	C-O	-5.08	1.17	1.23
2	D	141	VAL	C-O	-5.08	1.18	1.24
2	B	166	PRO	C-O	-5.07	1.18	1.23
1	A	7	SER	C-O	-5.07	1.18	1.24
1	C	143	ASN	C-O	-5.06	1.18	1.24
2	B	39	GLN	C-O	-5.06	1.18	1.24
1	C	34	TRP	C-O	-5.06	1.17	1.24
1	A	93	TYR	CA-C	-5.05	1.48	1.53
1	A	144	VAL	C-O	-5.04	1.18	1.24
1	C	22	THR	C-O	-5.04	1.17	1.24
1	C	89	GLN	C-O	-5.02	1.17	1.24
1	C	199	SER	C-O	-5.00	1.17	1.23

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	172	ASP	N-CA-C	-14.75	94.75	111.71
1	C	9	LYS	N-CA-C	12.68	127.84	112.38
1	C	191	THR	O-C-N	11.77	137.71	123.24
1	C	192	CYS	O-C-N	11.56	137.06	123.30
1	C	191	THR	CA-C-N	-11.14	107.29	122.99
1	C	191	THR	C-N-CA	-11.14	107.29	122.99
3	I	5	SER	N-CA-C	11.04	123.29	108.38
2	B	101	ASP	N-CA-C	10.77	123.10	111.36
3	J	3	GLY	CA-C-O	-9.95	115.37	122.23
2	B	127	ALA	N-CA-C	9.70	121.61	111.14
1	A	8	HIS	N-CA-C	-9.70	95.93	110.28
1	C	192	CYS	CA-C-N	-9.54	106.30	122.33
1	C	192	CYS	C-N-CA	-9.54	106.30	122.33
2	B	54	SER	N-CA-C	9.40	121.29	111.14
1	C	182	ASP	N-CA-C	8.92	120.62	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	30	THR	N-CA-C	8.64	123.55	112.92
2	D	99	ALA	N-CA-C	-8.23	100.81	108.22
2	D	101	ASP	N-CA-C	8.19	121.32	111.82
1	A	182	ASP	N-CA-C	8.02	119.65	111.07
2	D	159	SER	N-CA-C	-7.80	97.14	109.23
2	B	173	LEU	N-CA-C	7.55	120.89	109.41
2	D	66	LYS	N-CA-C	7.53	119.57	111.36
3	I	2	HIS	N-CA-C	7.43	120.43	107.49
1	C	183	GLU	N-CA-CB	7.36	121.68	110.28
2	B	66	LYS	N-CA-C	7.27	119.29	111.36
3	J	2	HIS	N-CA-C	7.22	120.06	107.49
1	C	167	LYS	N-CA-C	7.18	118.75	111.07
2	D	54	SER	N-CA-C	7.15	119.16	111.36
1	A	167	LYS	N-CA-C	6.87	118.85	111.36
2	D	22	CYS	N-CA-C	-6.73	97.44	108.41
2	D	210	VAL	N-CA-C	6.70	115.19	107.89
1	C	7	SER	N-CA-C	6.67	118.35	111.14
3	I	3	GLY	CA-C-O	-6.57	115.02	121.86
2	D	198	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	A	199	SER	N-CA-C	6.55	120.19	109.06
2	D	173	LEU	N-CA-C	6.54	119.34	109.41
2	B	99	ALA	N-CA-C	-6.48	102.30	108.13
1	A	28	VAL	N-CA-C	6.48	117.53	110.21
2	B	133	SER	N-CA-C	6.40	118.05	111.14
1	A	183	GLU	N-CA-CB	6.26	120.78	110.39
2	D	96	GLY	N-CA-C	6.24	127.97	113.18
2	B	3	LYS	N-CA-C	6.21	118.21	108.96
1	A	9	LYS	N-CA-C	6.19	123.37	114.39
1	A	183	GLU	CB-CG-CD	6.19	123.12	112.60
2	D	126	PRO	N-CA-C	6.19	122.32	113.47
2	B	96	GLY	N-CA-C	6.13	127.72	113.18
1	A	8	HIS	CB-CA-C	6.12	120.12	109.65
2	B	191	THR	N-CA-C	6.07	119.79	110.20
2	D	132	ASN	N-CA-C	6.04	117.87	111.28
1	A	191	THR	N-CA-C	5.92	119.12	109.06
1	A	10	PHE	N-CA-C	-5.88	100.21	109.50
2	D	15	GLY	N-CA-C	-5.85	107.58	115.36
2	D	134	MET	N-CA-C	-5.81	100.72	109.79
1	C	8	HIS	CA-C-N	5.80	129.88	120.60
1	C	8	HIS	C-N-CA	5.80	129.88	120.60
2	D	198	HIS	CB-CG-ND1	5.70	131.25	122.70
2	D	174	TYR	N-CA-C	5.65	118.84	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	8	GLN	N-CA-C	5.59	122.18	109.81
1	A	126	GLY	N-CA-C	5.59	123.68	115.08
3	J	3	GLY	N-CA-C	-5.58	106.04	112.29
2	D	183	PRO	CA-N-CD	-5.53	104.25	112.00
1	C	194	ALA	N-CA-C	5.52	117.90	108.90
1	A	104	ILE	CB-CA-C	-5.51	104.08	110.91
2	D	171	SER	CB-CA-C	-5.50	110.25	116.63
1	C	192	CYS	N-CA-C	-5.50	99.94	108.90
1	C	157	VAL	N-CA-C	5.29	115.93	108.36
2	B	82	LEU	CB-CA-C	5.27	119.24	109.70
2	D	162	VAL	N-CA-C	5.22	115.42	108.11
1	A	135	ASN	N-CA-C	5.16	117.66	109.50
2	B	93	ALA	N-CA-C	5.13	117.19	109.23
1	C	22	THR	N-CA-C	5.12	117.74	109.40
3	I	6	TRP	CA-CB-CG	5.11	123.31	113.60
2	D	2	VAL	CB-CA-C	-5.10	101.70	111.40
1	C	204	VAL	N-CA-C	5.09	115.44	108.12
1	A	140	LYS	N-CA-C	5.07	116.81	111.28
2	D	186	THR	N-CA-C	5.02	116.75	111.28
1	A	159	ASN	N-CA-C	5.01	117.07	108.90
2	D	133	SER	N-CA-C	5.00	116.73	108.48

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	GLY	Peptide
2	B	172	ASP	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	1619	0	1550	75	0
1	C	1624	0	1555	72	0
2	B	1630	0	1596	72	0
2	D	1630	0	1596	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	65	0	55	19	0
3	J	58	0	48	18	0
4	A	32	0	0	4	0
4	B	48	0	0	1	0
4	C	48	0	0	3	0
4	D	36	0	0	3	0
4	I	1	0	0	0	0
All	All	6791	0	6400	304	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 23.

All (304) 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:J:6:TRP:CE3	3:J:7:GLY:HA3	1.33	1.58
3:I:6:TRP:CG	3:I:7:GLY:HA2	1.38	1.58
1:C:183:GLU:CG	1:C:186:ARG:HH21	1.19	1.52
1:C:183:GLU:CG	1:C:186:ARG:NH2	1.74	1.49
3:I:6:TRP:CD1	3:I:7:GLY:HA2	1.53	1.42
1:A:183:GLU:CG	1:A:186:ARG:HH21	1.46	1.25
1:C:183:GLU:HG2	1:C:186:ARG:NH2	1.42	1.21
1:C:183:GLU:HG3	1:C:186:ARG:NH2	1.40	1.20
1:A:183:GLU:HG3	1:A:186:ARG:NH2	1.55	1.19
3:J:6:TRP:CE3	3:J:7:GLY:CA	2.29	1.16
2:D:145:PHE:HB2	2:D:173:LEU:CD2	1.76	1.15
3:I:6:TRP:CG	3:I:7:GLY:CA	2.28	1.14
2:D:129:ALA:HB1	2:D:130:ALA:HB2	1.29	1.12
1:A:82:LEU:C	1:A:82:LEU:HD23	1.72	1.12
3:I:6:TRP:CD1	3:I:7:GLY:CA	2.35	1.09
1:A:121:GLU:HG3	4:A:327:HOH:O	1.54	1.07
2:D:147:GLU:HG3	2:D:148:PRO:HA	1.39	1.04
2:D:147:GLU:HG3	2:D:148:PRO:CA	1.88	1.03
2:D:145:PHE:CB	2:D:173:LEU:CD2	2.36	1.03
3:I:6:TRP:CB	3:I:7:GLY:HA2	1.91	1.00
1:A:9:LYS:O	1:A:9:LYS:HG2	1.64	0.97
1:A:183:GLU:HG2	1:A:186:ARG:HE	1.30	0.94
2:D:96:GLY:HA2	3:J:8:GLN:HE22	1.33	0.94
2:D:145:PHE:HB2	2:D:173:LEU:HD23	1.49	0.93
1:A:82:LEU:HD23	1:A:82:LEU:O	1.68	0.92
1:C:183:GLU:HG2	1:C:186:ARG:HH21	0.76	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:5:SER:O	3:I:6:TRP:HE3	1.53	0.90
1:A:30:THR:HG22	1:A:30:THR:O	1.69	0.89
1:A:183:GLU:HG3	1:A:186:ARG:HH21	0.72	0.89
2:D:135:VAL:HG12	2:D:182:VAL:HG22	1.54	0.88
1:C:183:GLU:HG3	1:C:186:ARG:HH22	1.29	0.87
1:A:82:LEU:C	1:A:82:LEU:CD2	2.47	0.87
2:D:126:PRO:O	2:D:127:ALA:HB3	1.74	0.87
2:D:145:PHE:HB2	2:D:173:LEU:HD22	1.54	0.86
3:J:6:TRP:HE3	3:J:7:GLY:HA3	1.05	0.86
3:J:1:PRO:O	3:J:2:HIS:CD2	2.29	0.86
1:A:28:VAL:HG23	1:A:67:GLY:HA2	1.58	0.85
3:I:1:PRO:O	3:I:2:HIS:CG	2.30	0.85
1:C:12:SER:HB3	1:C:105:LYS:HE3	1.58	0.85
1:A:113:VAL:HG22	1:A:134:LEU:HD22	1.59	0.84
3:I:1:PRO:O	3:I:2:HIS:CD2	2.30	0.84
1:C:31:ALA:HB1	1:C:90:TYR:CD1	2.13	0.84
2:D:16:THR:HG22	2:D:17:SER:N	1.93	0.83
2:D:100(D):ALA:H	3:J:6:TRP:CD1	2.00	0.80
2:D:145:PHE:CB	2:D:173:LEU:HD22	2.09	0.80
3:J:6:TRP:CD2	3:J:7:GLY:HA3	2.12	0.79
1:A:30:THR:O	1:A:30:THR:CG2	2.29	0.79
1:A:82:LEU:O	1:A:82:LEU:CD2	2.30	0.79
1:C:30:THR:CG2	1:C:30:THR:O	2.29	0.79
3:J:1:PRO:O	3:J:2:HIS:CG	2.36	0.79
1:C:183:GLU:HG2	1:C:186:ARG:CZ	2.13	0.79
2:D:126:PRO:O	2:D:127:ALA:CB	2.31	0.79
1:C:30:THR:O	1:C:30:THR:HG22	1.83	0.78
2:D:145:PHE:HB3	2:D:173:LEU:CD2	2.15	0.77
1:C:9:LYS:O	1:C:9:LYS:CG	2.29	0.77
2:D:4:LEU:HB3	2:D:22:CYS:SG	2.25	0.77
1:A:183:GLU:CG	1:A:186:ARG:NH2	2.28	0.76
1:C:32:LEU:HD13	1:C:70:PHE:CG	2.20	0.76
1:C:9:LYS:O	1:C:9:LYS:HG3	1.86	0.75
1:A:12:SER:HB2	1:A:105:LYS:HE3	1.68	0.75
1:A:183:GLU:HG2	1:A:186:ARG:NE	2.02	0.75
2:D:16:THR:CG2	2:D:17:SER:N	2.50	0.74
1:A:113:VAL:HG22	1:A:134:LEU:CD2	2.18	0.73
2:D:147:GLU:CG	2:D:148:PRO:HA	2.19	0.72
1:A:196:HIS:CE1	1:A:198:THR:HG23	2.24	0.72
2:B:96:GLY:HA3	2:B:100(C):TYR:CD2	2.26	0.70
2:D:135:VAL:CG1	2:D:182:VAL:HG22	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LEU:HD13	1:C:70:PHE:CD2	2.27	0.70
2:D:147:GLU:HG3	2:D:148:PRO:CB	2.23	0.69
2:D:100(D):ALA:H	3:J:6:TRP:HD1	1.39	0.68
2:B:52:ASN:O	2:B:55:GLY:HA2	1.93	0.68
1:A:82:LEU:O	1:A:83:SER:HB3	1.94	0.68
2:B:169:LEU:HD13	2:B:174:TYR:CE1	2.29	0.68
2:D:135:VAL:CG1	2:D:135:VAL:O	2.40	0.68
1:A:12:SER:CB	1:A:105:LYS:HE3	2.23	0.68
2:B:52:ASN:O	2:B:55:GLY:CA	2.41	0.67
1:C:183:GLU:CD	1:C:186:ARG:HH21	2.02	0.67
1:A:138:TYR:CD1	1:A:139:PRO:HA	2.29	0.67
1:C:1:ASP:H1	1:C:93:TYR:HE2	1.41	0.67
1:C:113:VAL:CG1	1:C:192:CYS:SG	2.83	0.67
1:C:24:LYS:HD3	1:C:69:ASP:OD1	1.95	0.66
2:B:127:ALA:N	2:B:128:ALA:HA	2.10	0.66
2:B:96:GLY:HA3	2:B:100(C):TYR:CE2	2.31	0.66
1:C:31:ALA:HB1	1:C:90:TYR:CG	2.30	0.66
2:D:16:THR:CG2	2:D:17:SER:H	2.09	0.66
3:J:8:GLN:CD	3:J:8:GLN:H	1.99	0.66
3:I:6:TRP:CB	3:I:7:GLY:CA	2.62	0.65
2:D:114:ALA:HB2	2:D:172:ASP:OD1	1.96	0.65
1:C:106:ARG:NH1	1:C:107:ALA:O	2.30	0.65
2:D:145:PHE:HB3	2:D:173:LEU:HD21	1.78	0.64
1:A:106:ARG:NH1	1:A:107:ALA:O	2.29	0.64
1:A:32:LEU:HD13	1:A:70:PHE:CD2	2.33	0.64
3:J:8:GLN:OE1	3:J:8:GLN:N	2.30	0.64
2:B:172:ASP:HB2	2:B:173:LEU:HG	1.79	0.64
1:A:180:THR:HG23	4:A:332:HOH:O	1.99	0.63
3:J:6:TRP:HE3	3:J:7:GLY:CA	1.88	0.63
2:D:37:VAL:HG22	2:D:47:TRP:HA	1.81	0.63
2:B:189:SER:HA	4:B:331:HOH:O	1.97	0.63
1:C:134:LEU:HD12	1:C:134:LEU:N	2.13	0.62
2:D:135:VAL:HG12	2:D:182:VAL:CG2	2.25	0.62
2:D:114:ALA:HB1	2:D:172:ASP:OD2	2.00	0.61
2:D:195:ASN:ND2	2:D:206:ASP:OD1	2.29	0.61
1:C:191:THR:CG2	1:C:192:CYS:N	2.63	0.61
1:C:103:GLU:CD	1:C:171:TYR:OH	2.44	0.61
2:D:29:PHE:CE2	2:D:52(A):PRO:HB3	2.35	0.61
2:B:100:PRO:HB2	3:I:1:PRO:HB2	1.82	0.61
2:B:142:LYS:HZ1	2:B:170:GLN:NE2	1.98	0.61
1:A:32:LEU:HD13	1:A:70:PHE:CE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100(C):TYR:HD1	3:I:6:TRP:CE3	2.20	0.60
1:A:12:SER:HB3	1:A:105:LYS:HG3	1.83	0.60
2:B:7:SER:O	2:B:107:VAL:HG22	2.01	0.60
2:B:130:ALA:HB1	2:B:131:ALA:HB2	1.84	0.60
2:B:195:ASN:ND2	2:B:206:ASP:OD1	2.34	0.60
1:A:138:TYR:CG	1:A:139:PRO:HA	2.36	0.60
1:C:184:TYR:CZ	1:C:209:ARG:HD2	2.37	0.59
1:A:133:PHE:CZ	2:B:179:SER:HB3	2.37	0.59
1:A:106:ARG:HG3	1:A:107:ALA:N	2.17	0.59
1:A:185:GLU:O	1:A:209:ARG:NH2	2.36	0.59
1:A:121:GLU:CG	4:A:327:HOH:O	2.31	0.58
2:B:147:GLU:HG3	2:B:148:PRO:HB3	1.86	0.58
1:A:106:ARG:HG3	1:A:107:ALA:O	2.04	0.57
2:D:95:SER:HB2	2:D:100(C):TYR:HB2	1.86	0.57
2:B:12:VAL:HG11	2:B:18:VAL:CG2	2.34	0.57
2:B:129:ALA:C	2:B:130:ALA:O	2.44	0.57
2:D:100:PRO:HA	3:J:1:PRO:HD2	1.87	0.57
1:A:1:ASP:CG	1:A:1:ASP:O	2.47	0.57
1:C:184:TYR:CE2	1:C:209:ARG:HD2	2.40	0.56
2:D:114:ALA:CB	2:D:172:ASP:OD1	2.52	0.56
1:C:1:ASP:N	1:C:93:TYR:CE2	2.74	0.56
1:C:145:LYS:HE3	1:C:147:LYS:HE3	1.88	0.56
2:D:171:SER:OG	2:D:172:ASP:N	2.30	0.56
2:D:38:LYS:HB2	2:D:48:ILE:HD11	1.87	0.55
1:C:138:TYR:CG	1:C:139:PRO:HA	2.41	0.55
2:D:147:GLU:HG3	2:D:148:PRO:HB3	1.88	0.55
2:B:4:LEU:HD22	2:B:22:CYS:SG	2.46	0.55
1:A:53:ARG:HH12	1:A:62:THR:HG22	1.71	0.55
1:A:195:THR:HG22	1:A:202:PRO:HB3	1.88	0.55
2:D:187:TRP:CG	2:D:188:PRO:HA	2.42	0.55
1:A:160:SER:OG	2:B:166:PRO:HD2	2.06	0.55
3:I:5:SER:O	3:I:6:TRP:CE3	2.46	0.55
1:A:80:GLU:HG3	1:C:167:LYS:HD3	1.88	0.54
2:D:62:LYS:HE3	4:D:320:HOH:O	2.06	0.54
1:C:108:ASP:OD2	1:C:197:LYS:HE3	2.08	0.54
1:A:36:GLN:HG3	1:A:85:TYR:CE1	2.43	0.54
2:B:12:VAL:HG11	2:B:18:VAL:HG22	1.90	0.54
1:C:24:LYS:CD	1:C:69:ASP:OD1	2.56	0.54
2:D:153:TRP:CH2	2:D:194:CYS:SG	3.01	0.53
2:D:129:ALA:HB1	2:D:130:ALA:CB	2.19	0.53
2:B:152:THR:HG22	2:B:195:ASN:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:ASP:N	1:C:1:ASP:OD2	2.30	0.53
2:B:11:VAL:HG21	2:B:146:PRO:HG3	1.91	0.52
2:D:145:PHE:CD1	2:D:146:PRO:HA	2.45	0.52
1:A:133:PHE:CE1	2:B:179:SER:HB3	2.44	0.52
1:C:90:TYR:HE1	3:J:6:TRP:HB2	1.73	0.52
2:B:52:ASN:O	2:B:55:GLY:HA3	2.09	0.52
2:B:100(D):ALA:HB3	3:I:6:TRP:CH2	2.44	0.52
2:B:32:TYR:CG	2:B:94:ARG:HD2	2.45	0.52
1:C:5:THR:HG23	4:C:305:HOH:O	2.08	0.52
2:B:142:LYS:NZ	2:B:170:GLN:NE2	2.58	0.52
2:D:35:GLU:HG3	2:D:100(E):MET:HG2	1.91	0.52
1:C:54:HIS:CG	1:C:55:THR:N	2.77	0.52
2:B:171:SER:C	2:B:173:LEU:H	2.16	0.51
2:D:62:LYS:CE	4:D:320:HOH:O	2.58	0.51
3:I:1:PRO:C	3:I:2:HIS:CD2	2.87	0.51
1:A:184:TYR:CZ	1:A:209:ARG:HD3	2.46	0.51
1:C:28:VAL:HG13	1:C:67:GLY:HA2	1.92	0.51
1:C:92:SER:OG	1:C:93:TYR:N	2.43	0.51
2:B:100:PRO:CB	3:I:1:PRO:HB2	2.41	0.51
1:C:32:LEU:HD13	1:C:70:PHE:CD1	2.46	0.51
1:C:113:VAL:HG11	1:C:192:CYS:SG	2.50	0.51
2:B:35:GLU:HG2	2:B:50:VAL:HG23	1.92	0.51
1:A:168:ASP:CG	1:A:170:THR:HG23	2.36	0.50
1:C:54:HIS:CG	1:C:55:THR:H	2.30	0.50
2:B:100(D):ALA:HB3	3:I:6:TRP:HH2	1.76	0.50
1:A:2:ILE:CD1	1:A:27:GLN:HB2	2.41	0.50
1:C:31:ALA:HB1	1:C:90:TYR:CE1	2.47	0.50
1:A:43:PRO:HG2	2:B:103:TRP:CE3	2.46	0.50
2:D:100(D):ALA:N	3:J:6:TRP:CD1	2.77	0.50
1:A:88:GLN:HE21	1:A:94:PRO:HB3	1.77	0.50
2:D:129:ALA:CB	2:D:130:ALA:HB2	2.21	0.50
2:B:96:GLY:HA3	2:B:100(C):TYR:CG	2.46	0.49
1:A:90:TYR:CE2	2:B:100(D):ALA:HB2	2.47	0.49
1:A:60:ARG:HD2	1:A:75:SER:O	2.12	0.49
2:D:135:VAL:HG12	2:D:135:VAL:O	2.13	0.49
1:A:28:VAL:HG22	1:A:29:GLY:N	2.27	0.49
1:A:72:LEU:HD13	1:A:73:THR:N	2.28	0.49
2:D:176:LEU:C	2:D:176:LEU:HD12	2.38	0.49
2:B:6:GLU:HA	2:B:21:SER:O	2.11	0.49
2:D:205:VAL:HG23	2:D:206:ASP:N	2.26	0.49
2:B:129:ALA:O	2:B:130:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:GLN:NE2	1:A:94:PRO:HB3	2.28	0.48
1:C:4:MET:HE3	1:C:23:CYS:SG	2.52	0.48
1:C:191:THR:HG22	1:C:192:CYS:N	2.27	0.48
2:B:171:SER:HB3	2:B:172:ASP:H	1.37	0.48
1:C:106:ARG:HD2	1:C:169:SER:HB2	1.95	0.48
1:A:168:ASP:OD1	1:A:168:ASP:C	2.51	0.48
1:A:183:GLU:HA	1:A:186:ARG:HB2	1.96	0.48
1:C:23:CYS:HB2	1:C:34:TRP:CH2	2.49	0.47
2:B:73:LYS:H	2:B:73:LYS:HG2	1.43	0.47
2:B:151:VAL:HG12	2:B:152:THR:N	2.27	0.47
2:B:6:GLU:HB3	2:B:107:VAL:CG2	2.44	0.47
2:B:96:GLY:HA3	2:B:100(C):TYR:CZ	2.50	0.47
1:A:36:GLN:HB2	1:A:46:LEU:HD11	1.95	0.47
1:C:90:TYR:CE1	3:J:6:TRP:HB2	2.50	0.47
1:A:113:VAL:HG12	1:A:205:LYS:HG3	1.96	0.47
2:D:118:PRO:HG3	2:D:201:SER:HB2	1.96	0.46
2:D:198:HIS:CE1	2:D:200:ALA:HB3	2.50	0.46
1:A:28:VAL:CG2	1:A:29:GLY:N	2.78	0.46
2:B:146:PRO:HD2	2:B:200:ALA:CB	2.45	0.46
2:D:124:LEU:HG	2:D:139:CYS:HA	1.98	0.46
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.97	0.46
1:C:153:ARG:HD3	4:C:347:HOH:O	2.15	0.46
3:I:1:PRO:C	3:I:2:HIS:CG	2.91	0.46
2:B:75:SER:O	2:B:76:SER:HB2	2.14	0.46
2:B:152:THR:CG2	2:B:195:ASN:HB2	2.46	0.46
1:A:183:GLU:HG2	1:A:186:ARG:NH2	2.24	0.45
1:A:183:GLU:HG2	1:A:186:ARG:CZ	2.45	0.45
2:B:129:ALA:O	2:B:130:ALA:O	2.35	0.45
2:B:167:ALA:HB2	2:B:176:LEU:HD23	1.99	0.45
1:C:183:GLU:HA	1:C:186:ARG:HB2	1.99	0.45
1:C:30:THR:O	1:C:30:THR:HG23	2.14	0.45
2:B:194:CYS:SG	2:B:196:VAL:HG23	2.57	0.45
2:B:207:LYS:HZ3	2:B:207:LYS:HG3	1.40	0.45
2:B:83:THR:O	2:B:86:ASP:HB2	2.16	0.45
1:C:195:THR:HG23	4:C:336:HOH:O	2.17	0.45
1:A:147:LYS:HB2	1:A:191:THR:CG2	2.46	0.45
2:B:80:MET:HE3	2:B:82:LEU:HD11	1.99	0.45
2:B:142:LYS:NZ	2:B:170:GLN:HE22	2.14	0.45
1:C:38:LYS:HG3	1:C:83:SER:HB3	1.99	0.45
1:C:138:TYR:CD1	1:C:139:PRO:HA	2.52	0.45
2:D:100:PRO:HA	3:J:1:PRO:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:TYR:C	2:D:173:LEU:HD22	2.41	0.45
1:A:72:LEU:HD13	1:A:72:LEU:C	2.42	0.44
2:D:152:THR:HG22	2:D:156:GLY:HA2	1.98	0.44
1:A:14:SER:O	1:A:17:ASP:HB2	2.17	0.44
2:D:33:LEU:HB2	2:D:95:SER:OG	2.18	0.44
1:A:116:PHE:HA	1:A:117:PRO:HD3	1.88	0.44
2:D:107:VAL:HA	4:D:331:HOH:O	2.17	0.44
2:D:145:PHE:CG	2:D:146:PRO:HA	2.52	0.44
1:C:123:LEU:HD23	1:C:123:LEU:HA	1.75	0.44
2:B:171:SER:C	2:B:173:LEU:N	2.67	0.44
1:A:82:LEU:O	1:A:83:SER:CB	2.61	0.44
2:B:2:VAL:HA	2:B:26:GLY:HA3	1.99	0.44
2:D:210:VAL:HG13	2:D:211:PRO:HD2	1.99	0.44
1:C:110:ALA:HA	1:C:111:PRO:HD3	1.88	0.43
2:B:147:GLU:HG3	2:B:148:PRO:CB	2.48	0.43
1:C:183:GLU:HG2	1:C:186:ARG:NE	2.33	0.43
2:D:16:THR:HG23	2:D:17:SER:H	1.81	0.43
2:D:162:VAL:HG23	2:D:180:VAL:HG23	2.00	0.43
1:A:113:VAL:HA	1:A:133:PHE:O	2.18	0.43
2:D:114:ALA:CB	2:D:172:ASP:CG	2.91	0.43
2:D:187:TRP:CD1	2:D:188:PRO:HA	2.53	0.43
2:B:100(D):ALA:H	3:I:6:TRP:HZ3	1.67	0.43
2:D:50:VAL:HG22	2:D:51:ILE:N	2.33	0.43
1:A:23:CYS:HB2	1:A:34:TRP:CH2	2.54	0.43
1:A:38:LYS:HB2	1:A:41:GLN:CD	2.44	0.43
2:D:107:VAL:O	2:D:107:VAL:HG13	2.17	0.43
2:D:135:VAL:O	2:D:135:VAL:HG13	2.07	0.43
1:A:49:TRP:O	1:A:50:ALA:HB3	2.18	0.43
2:B:6:GLU:HB3	2:B:107:VAL:HG23	2.01	0.43
1:A:60:ARG:N	4:A:321:HOH:O	2.49	0.43
2:B:182:VAL:HB	2:B:186:THR:HG21	1.99	0.43
1:C:116:PHE:HA	1:C:117:PRO:HD2	1.78	0.43
2:B:147:GLU:HG3	2:B:148:PRO:CA	2.49	0.42
1:C:47:ILE:HD12	1:C:72:LEU:CD1	2.49	0.42
2:B:33:LEU:HD13	2:B:50:VAL:HG21	2.01	0.42
1:C:42:SER:HA	1:C:43:PRO:HD3	1.89	0.42
2:B:133:SER:O	2:B:184:SER:HB3	2.19	0.42
2:B:183:PRO:O	2:B:186:THR:HB	2.19	0.42
2:D:187:TRP:CZ2	2:D:211:PRO:HD3	2.54	0.42
1:A:196:HIS:HE1	1:A:198:THR:HG23	1.80	0.42
2:B:54:SER:HB2	2:B:56:ASP:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:ASN:CG	2:B:133:SER:H	2.27	0.42
3:I:8:GLN:O	3:I:9:PRO:C	2.59	0.42
2:D:180:VAL:O	2:D:180:VAL:HG13	2.18	0.42
1:C:58:PRO:HG2	1:C:60:ARG:NH1	2.33	0.42
1:A:12:SER:HA	1:A:103:GLU:O	2.20	0.42
2:B:36:TRP:CZ3	2:B:92:CYS:HB3	2.55	0.42
2:B:67:ALA:HA	2:B:82:LEU:HD23	2.01	0.42
1:A:2:ILE:HD12	1:A:27:GLN:HB2	2.02	0.41
1:C:106:ARG:NH1	1:C:109:ALA:HB2	2.35	0.41
2:D:100:PRO:C	3:J:1:PRO:H2	2.28	0.41
2:D:194:CYS:O	2:D:206:ASP:HA	2.19	0.41
1:C:13:THR:HG21	1:C:77:VAL:HG21	2.02	0.41
2:D:54:SER:OG	2:D:56:ASP:HB2	2.21	0.41
2:B:89:VAL:HG22	2:B:108:SER:HA	2.03	0.41
2:B:146:PRO:HD2	2:B:200:ALA:HB1	2.02	0.41
2:B:151:VAL:CG1	2:B:152:THR:N	2.83	0.41
1:A:82:LEU:HD23	1:A:83:SER:N	2.26	0.41
1:C:187:HIS:O	1:C:209:ARG:NH1	2.53	0.41
1:C:57:VAL:HA	1:C:58:PRO:HD3	1.85	0.41
1:A:9:LYS:O	1:A:9:LYS:CG	2.49	0.41
1:C:58:PRO:HB2	1:C:60:ARG:HG2	2.02	0.41
1:C:58:PRO:CG	1:C:60:ARG:NH1	2.84	0.41
1:A:12:SER:HB3	1:A:105:LYS:HE3	2.01	0.41
1:C:10:PHE:CE1	1:C:140:LYS:HE3	2.56	0.41
1:C:86:PHE:HB3	1:C:99:GLY:HA2	2.02	0.41
1:C:122:GLN:HG2	1:C:127:GLY:O	2.20	0.41
1:C:9:LYS:HB2	1:C:9:LYS:HE3	1.70	0.41
1:C:135:ASN:HA	1:C:172:SER:OG	2.22	0.40
1:C:134:LEU:N	1:C:134:LEU:CD1	2.79	0.40
1:A:43:PRO:HG2	2:B:103:TRP:CZ3	2.56	0.40
1:A:82:LEU:O	1:A:82:LEU:HD22	2.19	0.40
2:B:152:THR:HG23	2:B:156:GLY:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	207/210 (99%)	203 (98%)	3 (1%)	1 (0%)	24	31
1	C	208/210 (99%)	206 (99%)	2 (1%)	0	100	100
2	B	218/220 (99%)	212 (97%)	3 (1%)	3 (1%)	9	9
2	D	218/220 (99%)	210 (96%)	5 (2%)	3 (1%)	9	9
3	I	7/16 (44%)	5 (71%)	1 (14%)	1 (14%)	0	0
3	J	6/16 (38%)	4 (67%)	2 (33%)	0	100	100
All	All	864/892 (97%)	840 (97%)	16 (2%)	8 (1%)	14	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	148	PRO
2	B	171	SER
2	B	96	GLY
2	D	127	ALA
1	A	83	SER
2	D	96	GLY
2	D	148	PRO
3	I	8	GLN

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	186/186 (100%)	173 (93%)	13 (7%)	14	19
1	C	186/186 (100%)	176 (95%)	10 (5%)	20	29
2	B	181/181 (100%)	167 (92%)	14 (8%)	12	16
2	D	181/181 (100%)	156 (86%)	25 (14%)	3	4
3	I	6/10 (60%)	3 (50%)	3 (50%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	5/10 (50%)	2 (40%)	3 (60%)	0	0
All	All	745/754 (99%)	677 (91%)	68 (9%)	9	11

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	22	THR
1	A	32	LEU
1	A	72	LEU
1	A	79	SER
1	A	80	GLU
1	A	82	LEU
1	A	90	TYR
1	A	114	SER
1	A	140	LYS
1	A	151	SER
1	A	172	SER
1	A	197	LYS
2	B	19	LYS
2	B	20	VAL
2	B	45	LEU
2	B	54	SER
2	B	73	LYS
2	B	134	MET
2	B	152	THR
2	B	157	SER
2	B	171	SER
2	B	185	SER
2	B	186	THR
2	B	204	LYS
2	B	205	VAL
2	B	207	LYS
3	I	1	PRO
3	I	6	TRP
3	I	8	GLN
1	C	5	THR
1	C	38	LYS
1	C	82	LEU
1	C	90	TYR
1	C	101	LYS
1	C	161	GLU

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Mol	Chain	Res	Type
1	C	166	SER
1	C	192	CYS
1	C	195	THR
1	C	197	LYS
2	D	17	SER
2	D	18	VAL
2	D	20	VAL
2	D	45	LEU
2	D	61	GLU
2	D	74	SER
2	D	75	SER
2	D	82	LEU
2	D	82(A)	ASN
2	D	82(B)	SER
2	D	82(C)	LEU
2	D	92	CYS
2	D	112	SER
2	D	113	SER
2	D	135	VAL
2	D	150	THR
2	D	152	THR
2	D	159	SER
2	D	176	LEU
2	D	181	THR
2	D	185	SER
2	D	190	GLU
2	D	194	CYS
2	D	205	VAL
2	D	212	ARG
3	J	1	PRO
3	J	6	TRP
3	J	8	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	187	HIS
2	B	39	GLN
2	B	81	GLN
3	I	2	HIS
1	C	136	ASN

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Mol	Chain	Res	Type
1	C	188	ASN
1	C	208	ASN
2	D	163	HIS
3	J	2	HIS

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](#)

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	209/210 (99%)	0.75	18 (8%)	16 17	37, 54, 76, 129	0
1	C	210/210 (100%)	0.74	14 (6%)	24 26	34, 50, 73, 116	0
2	B	220/220 (100%)	0.77	21 (9%)	14 15	36, 53, 84, 115	0
2	D	220/220 (100%)	0.88	19 (8%)	16 17	36, 55, 103, 139	0
3	I	9/16 (56%)	3.16	8 (88%)	0 0	50, 66, 96, 98	0
3	J	8/16 (50%)	3.43	6 (75%)	0 0	49, 58, 69, 84	0
All	All	876/892 (98%)	0.83	86 (9%)	13 14	34, 53, 84, 139	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	172	ASP	8.5
1	C	192	CYS	7.1
1	A	183	GLU	6.4
1	C	183	GLU	5.8
2	D	131	ALA	5.1
1	C	8	HIS	5.1
3	J	4	GLY	5.0
2	B	100(A)	THR	4.9
3	J	6	TRP	4.8
3	I	6	TRP	4.7
1	C	30	THR	4.4
1	C	103	GLU	4.4
3	I	1	PRO	4.3
3	J	8	GLN	4.2
3	I	3	GLY	4.0
2	D	130	ALA	4.0
1	A	29	GLY	3.9
2	B	131	ALA	3.8
2	B	128	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	210	ALA	3.7
2	D	129	ALA	3.6
1	C	29	GLY	3.6
2	D	128	ALA	3.6
1	A	30	THR	3.5
3	I	7	GLY	3.5
1	A	192	CYS	3.4
1	A	10	PHE	3.4
2	D	194	CYS	3.4
1	A	8	HIS	3.4
3	J	1	PRO	3.3
2	D	92	CYS	3.3
2	B	127	ALA	3.3
3	I	9	PRO	3.3
1	A	187	HIS	3.2
1	C	10	PHE	3.2
1	A	165	ASP	3.2
1	C	154	GLN	3.2
3	J	3	GLY	3.2
3	J	5	SER	3.1
2	B	172	ASP	3.1
2	D	75	SER	3.1
2	D	183	PRO	3.1
1	C	60	ARG	3.1
2	D	127	ALA	3.0
1	A	145	LYS	3.0
1	A	28	VAL	3.0
1	A	82	LEU	2.9
2	B	194	CYS	2.9
2	D	158	LEU	2.8
2	B	2	VAL	2.8
2	B	66	LYS	2.8
1	C	28	VAL	2.8
2	B	130	ALA	2.7
2	D	160	GLY	2.7
2	D	133	SER	2.7
2	D	173	LEU	2.7
3	I	2	HIS	2.7
1	A	23	CYS	2.6
1	A	41	GLN	2.6
2	D	132	ASN	2.6
2	D	22	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	I	4	GLY	2.5
1	C	166	SER	2.5
1	A	121	GLU	2.5
1	A	191	THR	2.4
2	D	134	MET	2.4
2	B	134	MET	2.4
2	B	155	SER	2.4
1	C	203	ILE	2.3
2	B	158	LEU	2.3
2	B	132	ASN	2.2
2	D	13	ARG	2.2
2	B	157	SER	2.2
1	C	1	ASP	2.2
2	B	92	CYS	2.2
2	B	61	GLU	2.2
2	B	129	ALA	2.2
2	B	182	VAL	2.1
1	A	80	GLU	2.1
1	A	102	LEU	2.1
2	B	192	VAL	2.1
3	I	8	GLN	2.1
1	A	141	ASP	2.1
2	D	198	HIS	2.1
2	B	18	VAL	2.1
2	B	171	SER	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.