



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:41 PM UTC

PDB ID : 8PWU / pdb_00008pwu
Title : PfRH5 bound to monoclonal antibody MAD10-255
Authors : Farrell, B.; Higgins, M.K.
Deposited on : 2023-07-21
Resolution : 3.15 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

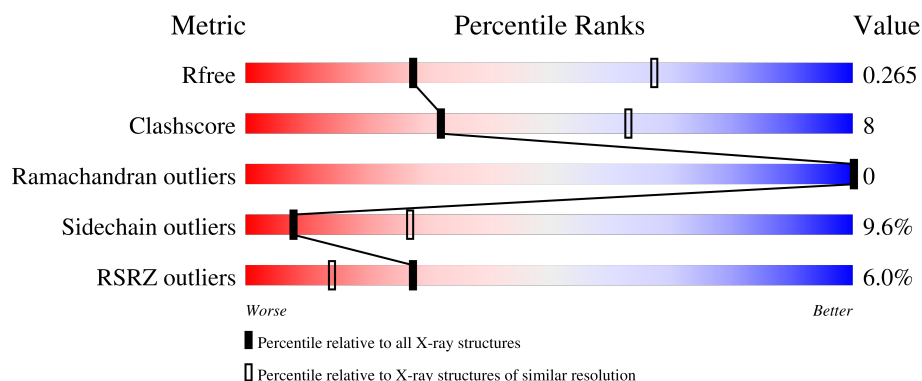
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	338	3% 65% 18% • 15%
1	C	338	5% 61% 22% • 15%
1	E	338	5% 65% 17% • 15%
1	G	338	2% 66% 16% • 15%
1	I	338	7% 64% 18% • 15%

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Mol	Chain	Length	Quality of chain
1	K	338	11% 66% 17% • 15%
2	B	250	3% 59% 26% • • 11%
2	D	250	4% 64% 22% • 10%
2	F	250	2% 62% 25% • 10%
2	H	250	2% 62% 25% • 10%
2	J	250	12% 64% 22% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23363 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 Reticulocyte-binding protein homolog 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2443	1575	411	442	15			
1	C	288	Total	C	N	O	S	0	0	0
			2443	1575	411	442	15			
1	E	287	Total	C	N	O	S	0	0	0
			2435	1571	409	440	15			
1	G	286	Total	C	N	O	S	0	0	0
			2424	1562	408	439	15			
1	I	288	Total	C	N	O	S	0	0	0
			2443	1575	411	442	15			
1	K	288	Total	C	N	O	S	0	0	0
			2443	1575	411	442	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	TYR	CYS	engineered mutation	UNP Q8IFM5
A	216	ALA	THR	engineered mutation	UNP Q8IFM5
A	299	ALA	THR	engineered mutation	UNP Q8IFM5
C	203	TYR	CYS	engineered mutation	UNP Q8IFM5
C	216	ALA	THR	engineered mutation	UNP Q8IFM5
C	299	ALA	THR	engineered mutation	UNP Q8IFM5
E	203	TYR	CYS	engineered mutation	UNP Q8IFM5
E	216	ALA	THR	engineered mutation	UNP Q8IFM5
E	299	ALA	THR	engineered mutation	UNP Q8IFM5
G	203	TYR	CYS	engineered mutation	UNP Q8IFM5
G	216	ALA	THR	engineered mutation	UNP Q8IFM5
G	299	ALA	THR	engineered mutation	UNP Q8IFM5
I	203	TYR	CYS	engineered mutation	UNP Q8IFM5
I	216	ALA	THR	engineered mutation	UNP Q8IFM5
I	299	ALA	THR	engineered mutation	UNP Q8IFM5
K	203	TYR	CYS	engineered mutation	UNP Q8IFM5
K	216	ALA	THR	engineered mutation	UNP Q8IFM5

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Chain	Residue	Modelled	Actual	Comment	Reference
K	299	ALA	THR	engineered mutation	UNP Q8IFM5

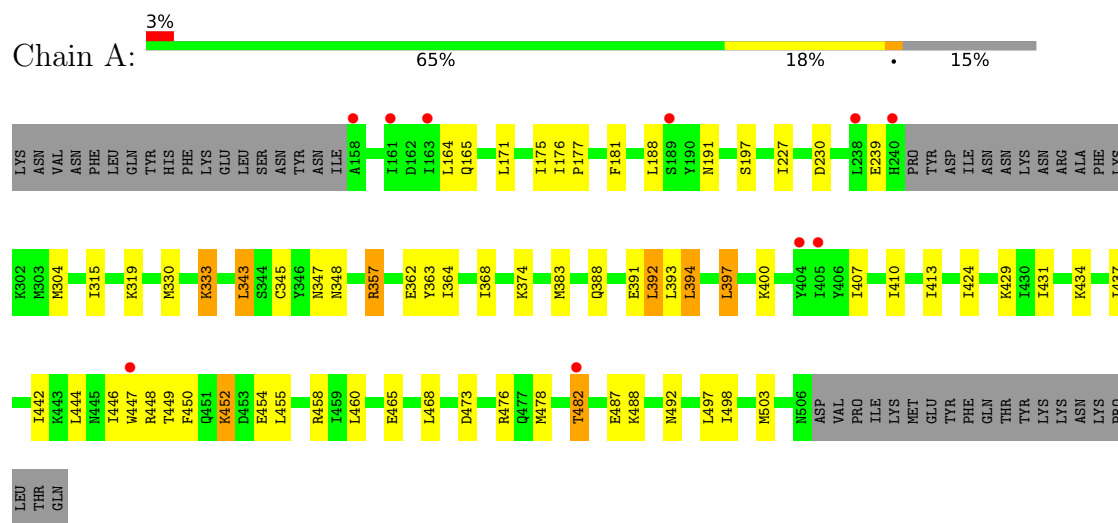
- Molecule 2 is a protein called monoclonal antibody MAD10-255.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	223	Total	C	N	O	S	0	1	0
			1736	1099	288	343	6			
2	D	226	Total	C	N	O	S	0	1	0
			1756	1109	291	350	6			
2	F	226	Total	C	N	O	S	0	1	0
			1756	1109	291	350	6			
2	H	226	Total	C	N	O	S	0	1	0
			1756	1109	291	350	6			
2	J	222	Total	C	N	O	S	0	1	0
			1728	1093	287	342	6			

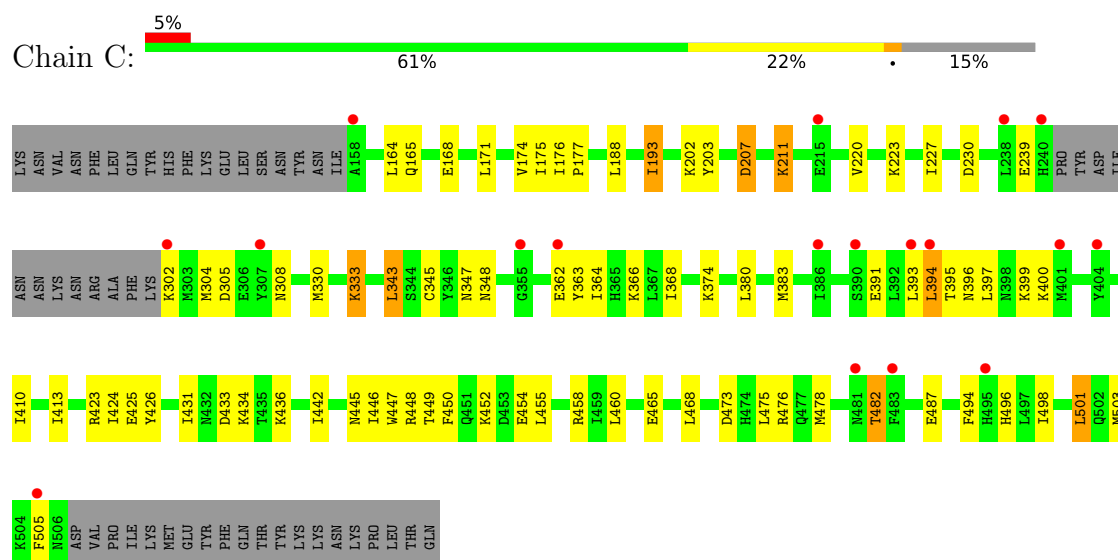
3 Residue-property plots

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

• Molecule 1: Reticulocyte-binding protein homolog 5

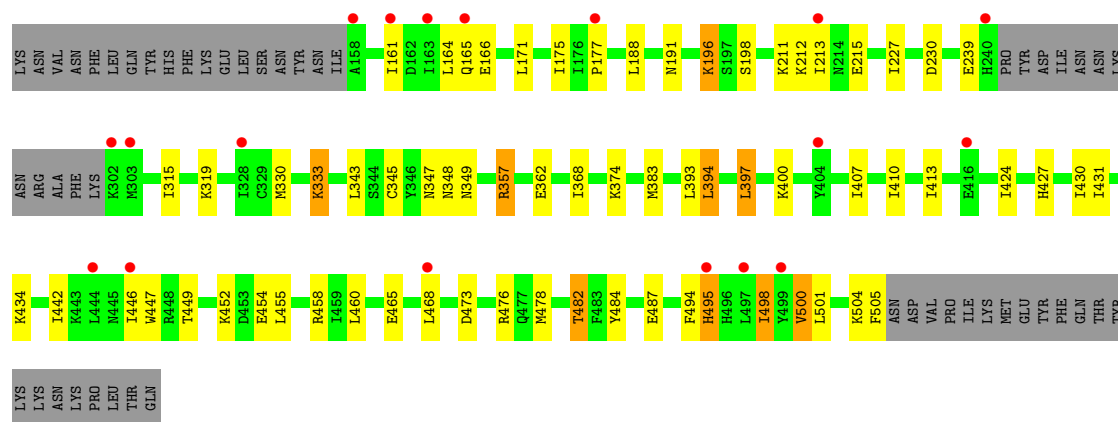


• Molecule 1: Reticulocyte-binding protein homolog 5

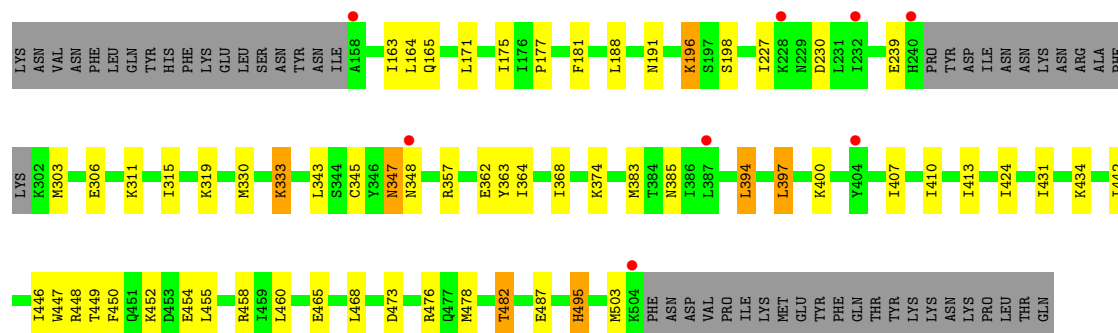


• Molecule 1: Reticulocyte-binding protein homolog 5

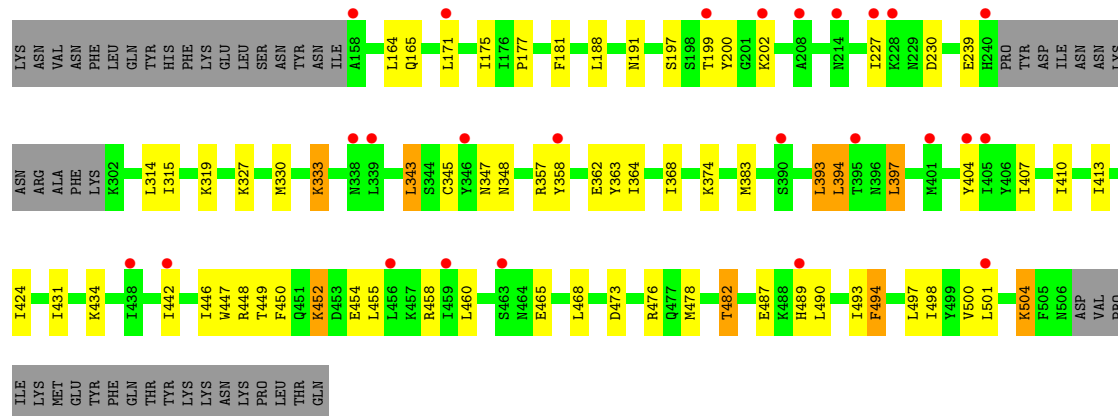




• Molecule 1: Reticulocyte-binding protein homolog 5

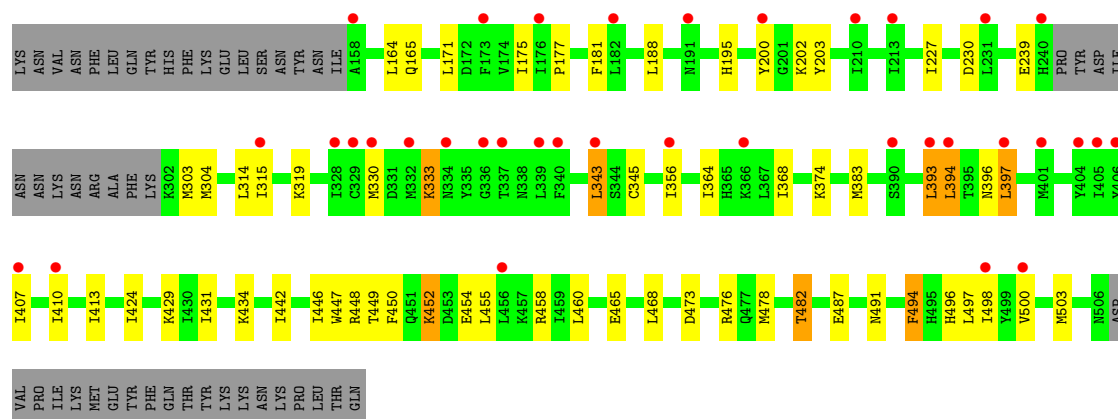


• Molecule 1: Reticulocyte-binding protein homolog 5

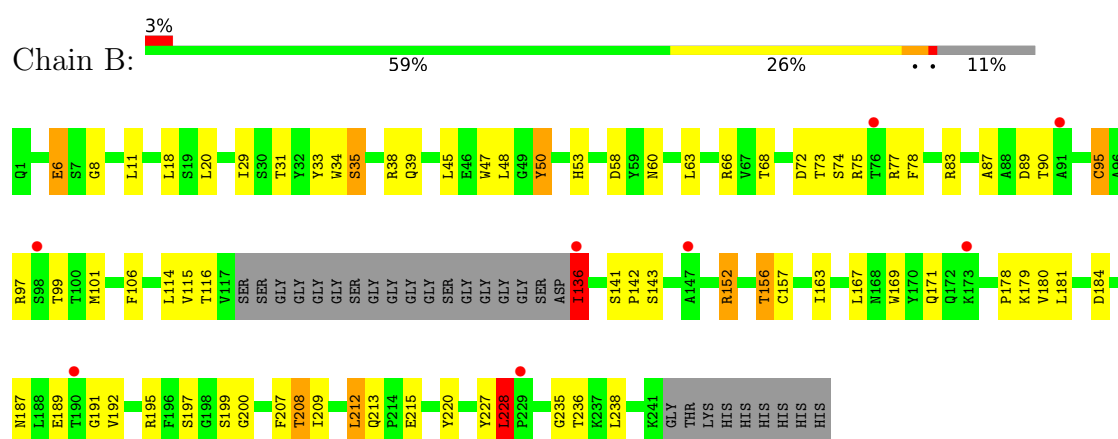


• Molecule 1: Reticulocyte-binding protein homolog 5

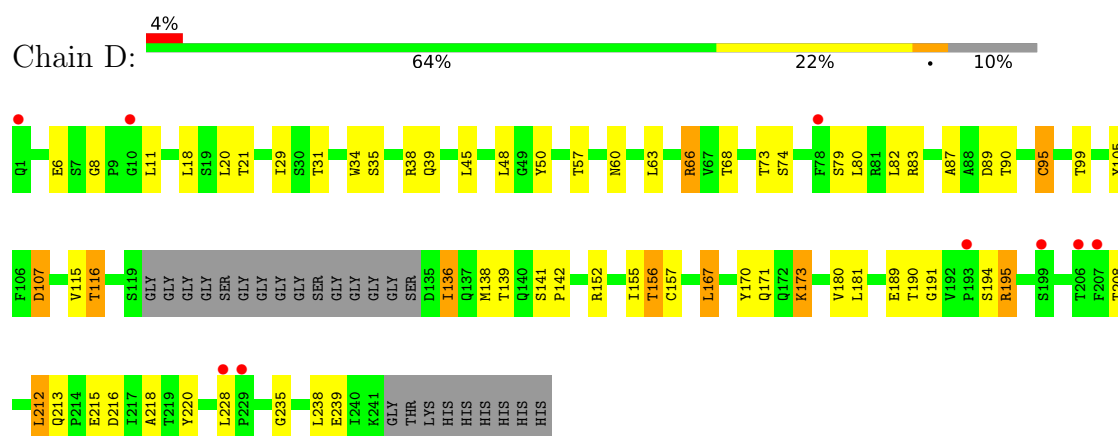




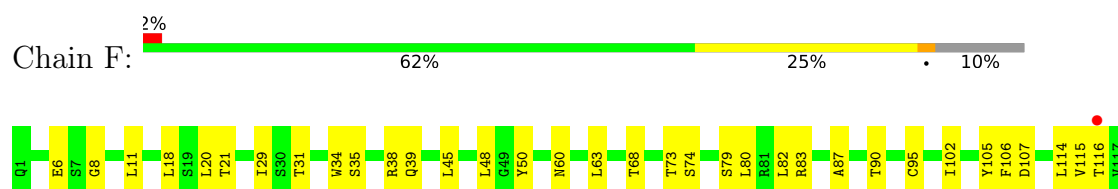
• Molecule 2: monoclonal antibody MAD10-255

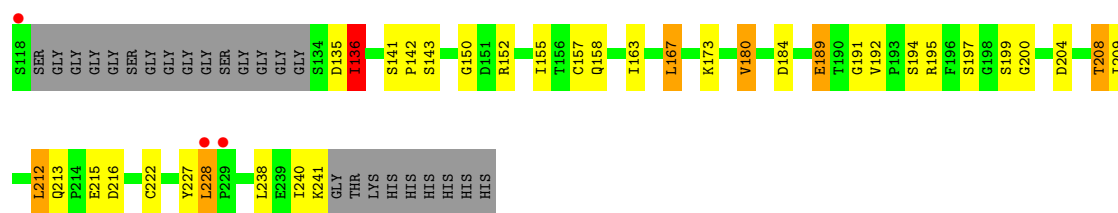


• Molecule 2: monoclonal antibody MAD10-255

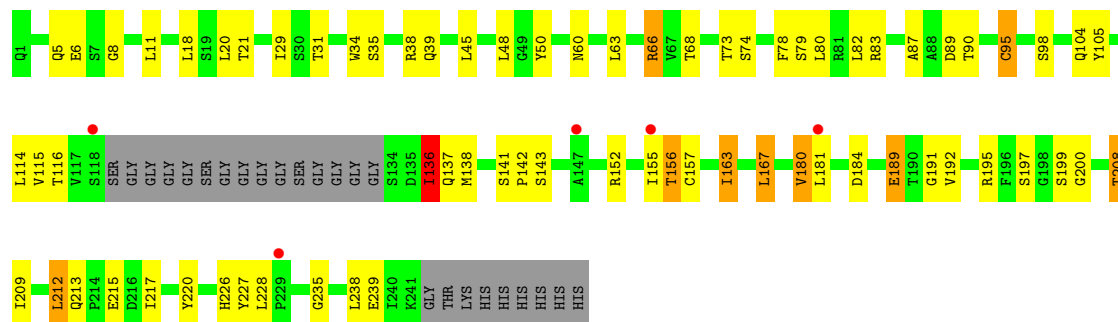


• Molecule 2: monoclonal antibody MAD10-255

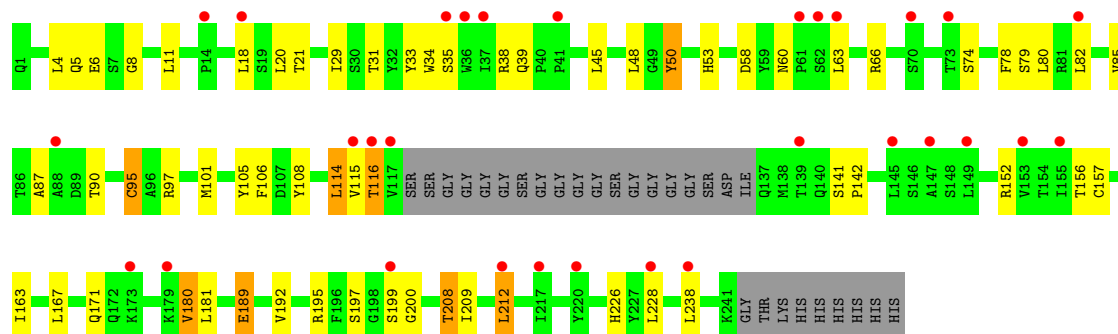




• Molecule 2: monoclonal antibody MAD10-255



• Molecule 2: monoclonal antibody MAD10-255



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.31Å 134.52Å 198.67Å 90.00° 93.56° 90.00°	Depositor
Resolution (Å)	87.45 – 3.15 87.45 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (87.45-3.15) 99.8 (87.45-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.13Å)	Xtriage
Refinement program	BUSTER 2.10.4 (20-OCT-2021)	Depositor
R, R_{free}	0.242 , 0.264 0.245 , 0.265	Depositor DCC
R_{free} test set	5254 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	102.5	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 108.7	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	0.92	EDS
Total number of atoms	23363	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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	0.77	0/2493	1.21	6/3342 (0.2%)
1	C	0.77	1/2493 (0.0%)	1.23	8/3342 (0.2%)
1	E	0.76	0/2485	1.23	6/3331 (0.2%)
1	G	0.75	0/2473	1.21	5/3315 (0.2%)
1	I	0.65	0/2493	1.19	6/3342 (0.2%)
1	K	0.65	0/2493	1.18	4/3342 (0.1%)
2	B	0.85	1/1781 (0.1%)	1.19	12/2426 (0.5%)
2	D	0.85	2/1801 (0.1%)	1.16	6/2453 (0.2%)
2	F	0.83	1/1801 (0.1%)	1.16	10/2453 (0.4%)
2	H	0.82	1/1801 (0.1%)	1.18	9/2453 (0.4%)
2	J	0.67	0/1773	1.08	5/2415 (0.2%)
All	All	0.76	6/23887 (0.0%)	1.19	77/32214 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	190	THR	CA-C	7.87	1.63	1.52
2	H	136	ILE	CG1-CD1	-6.43	1.26	1.51
2	F	136	ILE	CG1-CD1	-6.01	1.28	1.51
2	B	136	ILE	CG1-CD1	-5.65	1.29	1.51
2	D	136	ILE	CG1-CD1	-5.24	1.31	1.51
1	C	343	LEU	CA-C	-5.05	1.47	1.53

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	362	GLU	CB-CG-CD	8.53	127.10	112.60
1	C	362	GLU	CB-CG-CD	7.95	126.11	112.60
1	A	364	ILE	N-CA-C	6.93	117.77	111.81
1	G	362	GLU	CB-CG-CD	6.75	124.07	112.60
1	C	364	ILE	N-CA-C	6.65	117.53	111.81
2	B	200	GLY	N-CA-C	6.57	118.19	111.95
2	F	200	GLY	N-CA-C	6.56	118.19	111.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	200	GLY	N-CA-C	6.55	118.18	111.95
2	B	106	PHE	CA-C-N	6.54	128.94	120.44
2	B	106	PHE	C-N-CA	6.54	128.94	120.44
1	A	362	GLU	CB-CG-CD	6.50	123.66	112.60
1	G	364	ILE	N-CA-C	6.38	117.30	111.81
1	C	168	GLU	CB-CG-CD	6.32	123.35	112.60
1	I	364	ILE	N-CA-C	6.08	117.04	111.81
1	K	364	ILE	N-CA-C	6.04	117.00	111.81
2	J	200	GLY	N-CA-C	6.03	117.68	111.95
1	E	498	ILE	CA-C-N	6.00	128.24	120.44
1	E	498	ILE	C-N-CA	6.00	128.24	120.44
2	H	228	LEU	CA-C-O	-5.93	112.86	118.44
2	F	184	ASP	CA-C-N	5.92	132.84	121.54
2	F	184	ASP	C-N-CA	5.92	132.84	121.54
1	K	374	LYS	N-CA-C	5.82	117.71	111.36
1	A	345	CYS	N-CA-C	-5.81	98.34	107.93
1	I	374	LYS	N-CA-C	5.74	117.62	111.36
1	I	362	GLU	CB-CG-CD	5.71	122.31	112.60
2	B	228	LEU	CA-C-O	-5.71	113.08	118.44
2	D	107	ASP	CA-CB-CG	5.70	118.30	112.60
2	H	87	ALA	CA-C-N	5.69	127.91	120.28
2	H	87	ALA	C-N-CA	5.69	127.91	120.28
1	E	345	CYS	N-CA-C	-5.65	98.41	108.13
2	J	87	ALA	CA-C-N	5.64	127.84	120.28
2	J	87	ALA	C-N-CA	5.64	127.84	120.28
1	C	345	CYS	N-CA-C	-5.63	98.64	107.93
2	D	73	THR	CA-C-N	5.60	127.72	120.44
2	D	73	THR	C-N-CA	5.60	127.72	120.44
2	F	87	ALA	CA-C-N	5.58	127.76	120.28
2	F	87	ALA	C-N-CA	5.58	127.76	120.28
2	F	228	LEU	CA-C-O	-5.55	113.23	118.44
2	B	87	ALA	CA-C-N	5.53	127.69	120.28
2	B	87	ALA	C-N-CA	5.53	127.69	120.28
1	C	363	TYR	N-CA-C	5.52	118.48	111.69
2	H	184	ASP	CA-C-N	5.50	132.04	121.54
2	H	184	ASP	C-N-CA	5.50	132.04	121.54
2	F	106	PHE	CA-C-N	5.50	128.43	120.79
2	F	106	PHE	C-N-CA	5.50	128.43	120.79
2	B	181	LEU	N-CA-C	-5.49	105.63	112.93
1	A	357	ARG	N-CA-CB	5.47	118.01	110.07
1	C	207	ASP	CA-CB-CG	5.47	118.07	112.60
2	J	106	PHE	CA-C-N	5.46	127.91	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	106	PHE	C-N-CA	5.46	127.91	120.54
1	C	445	ASN	CA-CB-CG	5.44	118.04	112.60
1	G	363	TYR	N-CA-C	5.44	118.38	111.69
2	H	73	THR	CA-C-N	5.43	127.50	120.44
2	H	73	THR	C-N-CA	5.43	127.50	120.44
1	I	363	TYR	N-CA-C	5.41	118.35	111.69
2	B	73	THR	CA-C-N	5.40	127.46	120.44
2	B	73	THR	C-N-CA	5.40	127.46	120.44
1	I	504	LYS	CA-C-N	5.38	128.03	120.28
1	I	504	LYS	C-N-CA	5.38	128.03	120.28
1	E	374	LYS	N-CA-C	5.36	117.20	111.36
2	D	95	CYS	N-CA-C	-5.36	100.98	109.76
2	D	87	ALA	CA-C-N	5.33	127.43	120.28
2	D	87	ALA	C-N-CA	5.33	127.43	120.28
1	A	374	LYS	N-CA-C	5.28	117.12	111.36
1	C	374	LYS	N-CA-C	5.21	117.04	111.36
1	A	363	TYR	N-CA-C	5.18	118.06	111.69
2	F	73	THR	CA-C-N	5.18	127.17	120.44
2	F	73	THR	C-N-CA	5.18	127.17	120.44
2	B	184	ASP	CA-C-N	5.17	131.41	121.54
2	B	184	ASP	C-N-CA	5.17	131.41	121.54
1	K	356	ILE	CA-C-N	5.17	127.20	120.28
1	K	356	ILE	C-N-CA	5.17	127.20	120.28
1	G	347	ASN	CA-CB-CG	-5.16	107.44	112.60
2	B	163	ILE	N-CA-CB	-5.10	106.26	112.33
2	H	181	LEU	N-CA-C	-5.07	106.18	112.93
1	E	357	ARG	N-CA-CB	5.05	117.40	110.07
1	G	374	LYS	N-CA-C	5.01	116.82	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2443	0	2465	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2443	0	2465	46	0
1	E	2435	0	2459	41	0
1	G	2424	0	2450	45	0
1	I	2443	0	2465	39	0
1	K	2443	0	2465	32	0
2	B	1736	0	1690	37	0
2	D	1756	0	1704	33	0
2	F	1756	0	1704	31	0
2	H	1756	0	1704	32	0
2	J	1728	0	1679	33	0
All	All	23363	0	23250	375	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 8.

All (375) 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:G:163:ILE:HG23	1:G:171:LEU:HD21	1.22	1.10
2:D:29:ILE:HG23	2:D:34:TRP:NE1	1.83	0.93
1:E:196:LYS:NZ	1:E:198:SER:HB3	1.83	0.93
2:F:29:ILE:HG23	2:F:34:TRP:NE1	1.83	0.92
1:G:196:LYS:HZ2	1:G:198:SER:HB3	1.34	0.91
2:H:29:ILE:HG23	2:H:34:TRP:NE1	1.86	0.91
1:E:196:LYS:HZ2	1:E:198:SER:HB3	1.36	0.91
1:I:446:ILE:HG23	1:I:447:TRP:CD1	2.06	0.91
1:C:503:MET:HA	1:E:400:LYS:NZ	1.86	0.91
1:K:446:ILE:HG23	1:K:447:TRP:CD1	2.06	0.90
1:G:446:ILE:HG23	1:G:447:TRP:CD1	2.07	0.90
1:C:446:ILE:HG23	1:C:447:TRP:CD1	2.07	0.90
1:E:446:ILE:HG23	1:E:447:TRP:CD1	2.07	0.89
1:A:503:MET:HA	1:G:400:LYS:NZ	1.88	0.89
1:A:446:ILE:HG23	1:A:447:TRP:CD1	2.07	0.88
1:G:196:LYS:NZ	1:G:198:SER:HB3	1.88	0.88
1:A:392:LEU:HG	1:I:358:TYR:CD2	2.13	0.83
1:C:207:ASP:O	1:C:211:LYS:HD2	1.79	0.83
1:C:393:LEU:HD12	1:E:495:HIS:CD2	2.14	0.82
2:B:8:GLY:HA3	2:B:20:LEU:HD23	1.62	0.82
2:B:29:ILE:HG23	2:B:34:TRP:NE1	1.95	0.82
1:A:400:LYS:NZ	1:G:503:MET:HG2	1.94	0.82
1:E:330:MET:HE2	2:F:31:THR:HG21	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:ARG:HG2	2:B:77:ARG:HD2	1.63	0.80
1:A:392:LEU:HG	1:I:358:TYR:CE2	2.18	0.79
1:A:400:LYS:HZ3	1:G:503:MET:HG2	1.45	0.78
1:I:330:MET:HE2	2:J:31:THR:HG21	1.65	0.78
2:B:191:GLY:HA3	1:C:347:ASN:HB2	1.66	0.77
1:C:503:MET:HA	1:E:400:LYS:HZ3	1.48	0.76
1:A:503:MET:HA	1:G:400:LYS:HZ3	1.51	0.76
1:G:330:MET:HE2	2:H:31:THR:HG21	1.69	0.73
1:A:393:LEU:HD12	1:G:495:HIS:HD2	1.54	0.72
1:G:163:ILE:CG2	1:G:171:LEU:HD21	2.13	0.72
1:K:500:VAL:HA	1:K:503:MET:HG3	1.74	0.69
1:E:165:GLN:HG3	1:E:171:LEU:HD23	1.75	0.69
1:I:500:VAL:O	1:I:504:LYS:HG2	1.94	0.68
2:H:8:GLY:HA3	2:H:20:LEU:HD23	1.77	0.67
2:B:212:LEU:HD21	2:B:238:LEU:HD21	1.76	0.67
2:D:212:LEU:HD21	2:D:238:LEU:HD21	1.78	0.66
1:A:330:MET:HE3	1:A:333:LYS:HD2	1.77	0.66
2:D:171:GLN:HB2	2:D:181:LEU:HD11	1.78	0.66
2:H:212:LEU:HD21	2:H:238:LEU:HD21	1.77	0.65
2:F:8:GLY:HA3	2:F:20:LEU:HD23	1.77	0.65
1:C:330:MET:HE3	1:C:333:LYS:HD2	1.78	0.65
2:D:60:ASN:HB3	2:D:63:LEU:HD23	1.78	0.65
2:F:191:GLY:HA3	1:G:347:ASN:HB2	1.79	0.65
1:C:498:ILE:HG12	1:E:498:ILE:HG12	1.80	0.64
2:F:212:LEU:HD21	2:F:238:LEU:HD21	1.78	0.64
2:J:212:LEU:HD21	2:J:238:LEU:HD21	1.79	0.64
2:D:90:THR:HG23	2:D:116:THR:HG22	1.78	0.64
1:G:239:GLU:HG2	1:G:413:ILE:HD11	1.80	0.64
1:I:330:MET:HE3	1:I:333:LYS:HD2	1.80	0.63
1:C:501:LEU:HB3	1:E:501:LEU:HD23	1.80	0.63
1:E:330:MET:HE3	1:E:333:LYS:HD2	1.80	0.63
2:D:8:GLY:HA3	2:D:20:LEU:HD23	1.80	0.63
1:I:165:GLN:HG3	1:I:171:LEU:HD23	1.81	0.63
2:J:29:ILE:HG23	2:J:34:TRP:NE1	2.14	0.62
1:A:347:ASN:HB2	2:D:191:GLY:HA3	1.81	0.62
2:J:90:THR:HG23	2:J:116:THR:HG22	1.82	0.62
1:A:165:GLN:HG3	1:A:171:LEU:HD23	1.81	0.62
1:A:393:LEU:HD12	1:G:495:HIS:CD2	2.33	0.62
1:A:388:GLN:HG2	1:I:197:SER:HB2	1.82	0.62
1:C:175:ILE:HG22	1:C:177:PRO:HD2	1.81	0.62
1:C:393:LEU:HD12	1:E:495:HIS:HD2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:8:GLY:HA3	2:J:20:LEU:HD23	1.81	0.62
1:C:330:MET:HE2	2:D:31:THR:HG21	1.82	0.62
1:E:347:ASN:HB2	2:H:191:GLY:HA3	1.81	0.62
1:K:165:GLN:HG3	1:K:171:LEU:HD23	1.81	0.62
1:K:330:MET:HE3	1:K:333:LYS:HD2	1.82	0.61
2:B:189:GLU:O	2:B:192:VAL:HG12	2.00	0.61
1:C:220:VAL:HA	1:C:223:LYS:HE3	1.83	0.61
1:E:196:LYS:HZ3	1:E:198:SER:HB3	1.65	0.61
1:G:330:MET:HE3	1:G:333:LYS:HD2	1.83	0.61
1:E:239:GLU:HG2	1:E:413:ILE:HD11	1.84	0.60
1:A:239:GLU:HG2	1:A:413:ILE:HD11	1.83	0.60
1:I:239:GLU:HG2	1:I:413:ILE:HD11	1.83	0.60
1:K:239:GLU:HG2	1:K:413:ILE:HD11	1.84	0.60
1:A:454:GLU:O	1:A:458:ARG:HG2	2.02	0.60
1:G:165:GLN:HG3	1:G:171:LEU:HD23	1.83	0.59
2:H:197:SER:HB2	2:H:208:THR:HG23	1.84	0.59
1:A:503:MET:HA	1:G:400:LYS:HZ2	1.66	0.59
1:A:330:MET:HE2	2:B:31:THR:HG21	1.84	0.59
2:F:141:SER:HB2	2:F:142:PRO:HD3	1.84	0.58
2:J:141:SER:HB2	2:J:142:PRO:HD3	1.85	0.58
1:C:239:GLU:HG2	1:C:413:ILE:HD11	1.85	0.58
2:H:217:ILE:HG23	2:H:239:GLU:HA	1.85	0.58
2:J:197:SER:HB2	2:J:208:THR:HG23	1.86	0.58
1:E:213:ILE:HD13	2:F:102:ILE:HG13	1.86	0.57
2:B:197:SER:HB2	2:B:208:THR:HG23	1.85	0.57
2:B:72:ASP:OD2	2:B:75:ARG:HB2	2.03	0.57
2:B:58:ASP:HB3	2:B:228:LEU:HD11	1.87	0.56
2:H:189:GLU:O	2:H:192:VAL:HG12	2.05	0.56
2:F:197:SER:HB2	2:F:208:THR:HG23	1.87	0.56
1:G:397:LEU:HD23	1:G:407:ILE:HG22	1.87	0.56
1:A:397:LEU:HD23	1:A:407:ILE:HG22	1.87	0.56
2:J:97:ARG:NH1	2:J:108:TYR:HE2	2.04	0.55
1:E:427:HIS:HA	1:E:430:ILE:HD12	1.88	0.55
2:J:163:ILE:HG23	2:J:226:HIS:HB2	1.87	0.55
2:B:29:ILE:HG23	2:B:34:TRP:CD1	2.42	0.55
2:F:158:GLN:NE2	2:F:204:ASP:OD1	2.32	0.54
2:B:60:ASN:HB3	2:B:63:LEU:HD23	1.90	0.54
2:H:66:ARG:NH2	2:H:89:ASP:OD2	2.42	0.53
1:I:315:ILE:HG22	1:I:319:LYS:HE2	1.90	0.53
1:A:315:ILE:HG22	1:A:319:LYS:HE2	1.89	0.53
2:F:60:ASN:HB3	2:F:63:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:393:LEU:HD22	1:I:494:PHE:CE1	2.44	0.53
1:C:395:THR:HG21	1:K:200:TYR:HB3	1.91	0.53
1:E:397:LEU:HD23	1:E:407:ILE:HG22	1.90	0.53
2:F:105:TYR:HD1	2:F:180:VAL:HG21	1.74	0.53
2:F:189:GLU:O	2:F:192:VAL:HG12	2.09	0.53
1:A:448:ARG:NH1	1:A:450:PHE:CD1	2.77	0.52
1:E:211:LYS:O	1:E:215:GLU:HG3	2.09	0.52
2:H:60:ASN:HB3	2:H:63:LEU:HD23	1.90	0.52
2:D:90:THR:CG2	2:D:116:THR:HG22	2.39	0.52
1:K:315:ILE:HG22	1:K:319:LYS:HE2	1.91	0.52
1:I:397:LEU:HD23	1:I:407:ILE:HG22	1.92	0.52
2:J:189:GLU:O	2:J:192:VAL:HG12	2.10	0.52
1:A:164:LEU:HD22	1:A:478:MET:HB3	1.93	0.51
1:C:505:PHE:HZ	1:E:504:LYS:HB2	1.73	0.51
2:D:29:ILE:HG23	2:D:34:TRP:CD1	2.46	0.51
1:E:315:ILE:HG22	1:E:319:LYS:HE2	1.92	0.51
1:E:164:LEU:HD22	1:E:478:MET:HB3	1.93	0.51
2:F:20:LEU:HD12	2:F:80:LEU:HD23	1.93	0.51
2:B:169:TRP:CE2	2:B:207:PHE:HB2	2.46	0.51
2:B:35:SER:HB3	2:B:50:TYR:HB3	1.92	0.51
1:K:397:LEU:HD23	1:K:407:ILE:HG22	1.93	0.51
1:K:491:ASN:HA	1:K:494:PHE:HB2	1.93	0.51
1:I:199:THR:HG23	1:I:202:LYS:HB3	1.92	0.51
1:G:315:ILE:HG22	1:G:319:LYS:HE2	1.91	0.51
1:C:380:LEU:HD13	1:C:425:GLU:HG3	1.93	0.50
1:E:394:LEU:HD23	1:E:410:ILE:HG22	1.93	0.50
1:K:164:LEU:HD22	1:K:478:MET:HB3	1.93	0.50
2:H:163:ILE:HD13	2:H:226:HIS:HB3	1.93	0.50
1:I:404:TYR:HE1	1:I:504:LYS:HE3	1.76	0.50
1:A:400:LYS:HZ3	1:G:503:MET:CG	2.22	0.50
1:G:164:LEU:HD22	1:G:478:MET:HB3	1.92	0.50
1:K:394:LEU:HD23	1:K:410:ILE:HG22	1.93	0.50
2:B:152:ARG:NH1	2:F:150:GLY:O	2.43	0.50
1:C:498:ILE:HG21	1:E:393:LEU:HD11	1.92	0.50
2:D:39:GLN:HB2	2:D:45:LEU:HD23	1.93	0.50
1:C:176:ILE:HD12	1:C:475:LEU:HD13	1.94	0.50
2:H:66:ARG:HH22	2:H:89:ASP:CG	2.19	0.50
1:I:394:LEU:HD23	1:I:410:ILE:HG22	1.93	0.50
2:J:97:ARG:NH1	2:J:108:TYR:CE2	2.79	0.50
2:B:63:LEU:O	2:B:66:ARG:HG2	2.11	0.49
1:A:347:ASN:O	1:A:348:ASN:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:448:ARG:NH1	1:G:450:PHE:CD1	2.80	0.49
2:H:142:PRO:HD2	2:H:155:ILE:HG23	1.94	0.49
1:I:494:PHE:O	1:I:498:ILE:HG13	2.12	0.49
2:J:90:THR:CG2	2:J:116:THR:HG22	2.42	0.49
1:I:164:LEU:HD22	1:I:478:MET:HB3	1.93	0.49
1:G:196:LYS:HZ3	1:G:198:SER:HB3	1.76	0.49
1:E:347:ASN:O	1:E:348:ASN:HB2	2.12	0.49
1:I:227:ILE:HD12	1:I:227:ILE:H	1.77	0.49
2:J:20:LEU:HD12	2:J:80:LEU:HD23	1.94	0.49
1:E:227:ILE:HD12	1:E:227:ILE:H	1.77	0.49
2:D:141:SER:HB2	2:D:156:THR:OG1	2.11	0.49
1:I:448:ARG:NH1	1:I:450:PHE:CD1	2.81	0.49
2:B:39:GLN:HB2	2:B:45:LEU:HD23	1.95	0.49
2:H:20:LEU:HD12	2:H:80:LEU:HD23	1.93	0.49
2:H:29:ILE:HG23	2:H:34:TRP:CD1	2.46	0.49
2:J:60:ASN:HB3	2:J:63:LEU:HD23	1.94	0.49
1:C:227:ILE:HD12	1:C:227:ILE:H	1.78	0.49
1:C:494:PHE:O	1:C:498:ILE:HG13	2.13	0.49
1:C:448:ARG:NH1	1:C:450:PHE:CD1	2.81	0.48
1:G:227:ILE:HD12	1:G:227:ILE:H	1.78	0.48
1:G:347:ASN:O	1:G:348:ASN:HB2	2.13	0.48
1:K:494:PHE:O	1:K:498:ILE:HG13	2.13	0.48
1:C:394:LEU:HD23	1:C:410:ILE:HG22	1.95	0.48
2:F:29:ILE:HG23	2:F:34:TRP:CD1	2.47	0.48
2:F:142:PRO:HD2	2:F:155:ILE:HG23	1.94	0.48
1:A:388:GLN:HG2	1:I:197:SER:CB	2.42	0.48
1:C:347:ASN:O	1:C:348:ASN:HB2	2.14	0.48
1:K:448:ARG:NH1	1:K:450:PHE:CD1	2.81	0.48
1:E:330:MET:CE	2:F:31:THR:HG21	2.39	0.48
1:E:383:MET:HE1	1:E:424:ILE:HD13	1.94	0.48
1:I:410:ILE:HD11	1:I:493:ILE:HB	1.95	0.48
1:A:227:ILE:H	1:A:227:ILE:HD12	1.79	0.48
1:C:383:MET:HE1	1:C:424:ILE:HD13	1.96	0.48
2:F:39:GLN:HB2	2:F:45:LEU:HD23	1.95	0.48
1:G:188:LEU:HD11	1:G:460:LEU:HD23	1.96	0.48
1:K:195:HIS:CD2	1:K:343:LEU:CD1	2.97	0.48
1:A:394:LEU:HD23	1:A:410:ILE:HG22	1.96	0.48
2:B:136:ILE:HD13	2:B:227:TYR:HB2	1.95	0.48
1:C:448:ARG:HH11	1:C:448:ARG:HB3	1.79	0.48
1:G:163:ILE:HD13	1:G:311:LYS:HE3	1.96	0.48
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:78:PHE:CZ	2:J:95:CYS:SG	3.06	0.48
2:D:66:ARG:NH2	2:D:89:ASP:OD2	2.47	0.48
1:G:434:LYS:HE2	1:G:468:LEU:HD12	1.96	0.48
2:J:39:GLN:HB2	2:J:45:LEU:HD23	1.96	0.48
1:A:400:LYS:NZ	1:G:503:MET:CG	2.71	0.47
2:D:105:TYR:HD1	2:D:180:VAL:HG21	1.78	0.47
1:G:442:ILE:HG13	1:G:446:ILE:HD12	1.96	0.47
1:K:227:ILE:H	1:K:227:ILE:HD12	1.78	0.47
2:B:78:PHE:CZ	2:B:95:CYS:SG	3.08	0.47
2:D:20:LEU:HD12	2:D:80:LEU:HD23	1.95	0.47
2:B:33:TYR:CE2	2:B:101:MET:HG2	2.49	0.47
2:D:63:LEU:O	2:D:66:ARG:HG2	2.14	0.47
1:K:383:MET:HE1	1:K:424:ILE:HD13	1.96	0.47
1:A:488:LYS:HE2	1:A:492:ASN:HD21	1.80	0.47
1:C:442:ILE:HG13	1:C:446:ILE:HD12	1.96	0.47
1:E:442:ILE:HG13	1:E:446:ILE:HD12	1.97	0.47
1:A:442:ILE:HG13	1:A:446:ILE:HD12	1.96	0.47
1:C:448:ARG:HD3	1:C:450:PHE:CZ	2.50	0.47
2:D:195:ARG:NH1	2:D:216:ASP:OD1	2.43	0.47
1:I:347:ASN:O	1:I:348:ASN:HB2	2.14	0.47
2:J:34:TRP:CZ3	2:J:97:ARG:HB2	2.50	0.47
2:J:82:LEU:HD12	2:J:85:VAL:HG12	1.97	0.47
2:H:195:ARG:HG3	2:H:209:ILE:HG23	1.97	0.47
1:I:343:LEU:O	1:I:452:LYS:HE3	2.14	0.47
1:A:188:LEU:HD11	1:A:460:LEU:HD23	1.95	0.47
1:C:431:ILE:HD11	1:C:473:ASP:HA	1.97	0.47
1:I:442:ILE:HG13	1:I:446:ILE:HD12	1.96	0.47
2:J:29:ILE:HG23	2:J:34:TRP:CD1	2.50	0.47
1:C:188:LEU:HD11	1:C:460:LEU:HD23	1.97	0.46
1:E:431:ILE:HD11	1:E:473:ASP:HA	1.97	0.46
1:G:196:LYS:HZ2	1:G:198:SER:CB	2.17	0.46
1:A:448:ARG:HD3	1:A:450:PHE:CZ	2.50	0.46
1:C:165:GLN:HG3	1:C:171:LEU:HD23	1.96	0.46
1:C:434:LYS:HE2	1:C:468:LEU:HD12	1.98	0.46
1:E:494:PHE:O	1:E:498:ILE:HG13	2.15	0.46
2:J:4:LEU:HD21	2:J:34:TRP:HZ3	1.80	0.46
1:G:383:MET:HE1	1:G:424:ILE:HD13	1.98	0.46
1:I:383:MET:HE1	1:I:424:ILE:HD13	1.97	0.46
1:K:343:LEU:O	1:K:452:LYS:HE3	2.16	0.46
1:A:383:MET:HE1	1:A:424:ILE:HD13	1.97	0.46
2:D:18:LEU:HD13	2:D:115:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:394:LEU:HD23	1:G:410:ILE:HG22	1.97	0.46
1:G:454:GLU:O	1:G:458:ARG:HG2	2.16	0.46
1:C:304:MET:HE3	1:C:308:ASN:HD21	1.81	0.46
2:D:141:SER:HB2	2:D:142:PRO:HD3	1.97	0.46
1:I:404:TYR:CE1	1:I:504:LYS:HE3	2.50	0.46
1:E:434:LYS:HE2	1:E:468:LEU:HD12	1.98	0.45
2:F:90:THR:HG23	2:F:116:THR:HA	1.99	0.45
1:G:448:ARG:HD3	1:G:450:PHE:CZ	2.51	0.45
1:K:442:ILE:HG13	1:K:446:ILE:HD12	1.97	0.45
1:G:175:ILE:HG22	1:G:177:PRO:HD2	1.98	0.45
2:B:171:GLN:HG3	2:B:220:TYR:CE2	2.51	0.45
1:C:399:LYS:HG3	1:C:400:LYS:HG3	1.98	0.45
1:G:448:ARG:HH11	1:G:448:ARG:HB3	1.81	0.45
2:H:63:LEU:HD12	2:H:82:LEU:HD11	1.98	0.45
1:I:454:GLU:O	1:I:458:ARG:HG2	2.17	0.45
1:K:188:LEU:HD11	1:K:460:LEU:HD23	1.98	0.45
1:K:454:GLU:O	1:K:458:ARG:HG2	2.16	0.45
1:I:175:ILE:HG22	1:I:177:PRO:HD2	1.97	0.45
1:I:448:ARG:HH11	1:I:448:ARG:HB3	1.82	0.45
1:A:400:LYS:HZ1	1:G:503:MET:HG2	1.81	0.45
1:I:188:LEU:HD11	1:I:460:LEU:HD23	1.98	0.45
2:J:18:LEU:HD13	2:J:115:VAL:HG11	1.99	0.45
1:A:175:ILE:HG22	1:A:177:PRO:HD2	1.99	0.45
2:B:18:LEU:HD13	2:B:115:VAL:HG11	1.97	0.45
2:B:195:ARG:HG3	2:B:209:ILE:HG23	1.99	0.45
1:C:478:MET:O	1:C:482:THR:HG23	2.17	0.45
2:D:66:ARG:HH22	2:D:89:ASP:CG	2.25	0.45
2:D:195:ARG:NH1	2:D:216:ASP:OD2	2.50	0.45
1:E:175:ILE:HG22	1:E:177:PRO:HD2	1.99	0.45
1:A:431:ILE:HD11	1:A:473:ASP:HA	1.99	0.45
2:J:195:ARG:HG3	2:J:209:ILE:HG23	1.99	0.45
2:B:6:GLU:OE1	2:B:95:CYS:HB3	2.17	0.44
2:H:141:SER:HB2	2:H:142:PRO:HD3	1.98	0.44
1:A:478:MET:O	1:A:482:THR:HG23	2.17	0.44
2:B:68:THR:OG1	2:B:83:ARG:NH2	2.50	0.44
1:E:454:GLU:O	1:E:458:ARG:HG2	2.17	0.44
2:F:38:ARG:HG2	2:F:48:LEU:HD21	1.99	0.44
1:G:303:MET:HE3	1:G:306:GLU:HB2	2.00	0.44
1:I:489:HIS:O	1:I:493:ILE:HG13	2.17	0.44
1:K:175:ILE:HG22	1:K:177:PRO:HD2	1.99	0.44
1:E:500:VAL:O	1:E:504:LYS:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:ARG:HG2	2:H:48:LEU:HD21	1.98	0.44
1:I:431:ILE:HD11	1:I:473:ASP:HA	1.98	0.44
1:E:188:LEU:HD11	1:E:460:LEU:HD23	1.99	0.44
1:G:163:ILE:HG23	1:G:171:LEU:CD2	2.16	0.44
1:K:202:LYS:HG3	1:K:202:LYS:O	2.18	0.44
1:C:433:ASP:HA	1:C:436:LYS:HD2	1.99	0.44
2:F:18:LEU:HD13	2:F:115:VAL:HG11	2.00	0.44
2:J:114:LEU:HD11	2:J:116:THR:HG23	1.98	0.44
1:K:448:ARG:HD3	1:K:450:PHE:CZ	2.52	0.44
1:E:478:MET:O	1:E:482:THR:HG23	2.18	0.44
2:F:63:LEU:HD12	2:F:82:LEU:HD11	2.00	0.44
1:A:393:LEU:CD1	1:G:495:HIS:CD2	2.99	0.44
1:C:203:TYR:CD1	1:C:203:TYR:C	2.95	0.44
2:D:68:THR:OG1	2:D:83:ARG:NH2	2.50	0.44
2:F:29:ILE:HG23	2:F:34:TRP:HE1	1.74	0.44
2:F:195:ARG:NH1	2:F:216:ASP:OD2	2.47	0.44
2:J:33:TYR:CE2	2:J:101:MET:HG2	2.52	0.44
1:K:431:ILE:HD11	1:K:473:ASP:HA	1.98	0.44
2:B:142:PRO:O	2:B:236:THR:HG23	2.18	0.44
2:B:90:THR:HG23	2:B:116:THR:HA	1.99	0.44
2:H:220:TYR:O	2:H:235:GLY:HA2	2.18	0.44
1:K:448:ARG:HH11	1:K:448:ARG:HB3	1.82	0.44
1:A:448:ARG:HB3	1:A:448:ARG:HH11	1.82	0.43
1:A:434:LYS:HE2	1:A:468:LEU:HD12	1.99	0.43
2:D:29:ILE:HG23	2:D:34:TRP:HE1	1.74	0.43
2:J:105:TYR:HD1	2:J:180:VAL:HG21	1.83	0.43
2:J:38:ARG:HG2	2:J:48:LEU:HD21	2.00	0.43
1:I:448:ARG:HD3	1:I:450:PHE:CZ	2.53	0.43
1:K:195:HIS:CD2	1:K:343:LEU:HD11	2.53	0.43
2:B:35:SER:HB3	2:B:47:TRP:HE1	1.83	0.43
1:G:431:ILE:HD11	1:G:473:ASP:HA	1.98	0.43
1:I:327:LYS:HG2	2:J:53:HIS:HE1	1.83	0.43
2:F:195:ARG:HG3	2:F:209:ILE:HG23	2.01	0.43
2:H:18:LEU:HD13	2:H:115:VAL:HG11	2.00	0.43
2:D:63:LEU:HD12	2:D:82:LEU:HD11	2.00	0.43
2:H:29:ILE:HG23	2:H:34:TRP:HE1	1.76	0.43
1:I:478:MET:O	1:I:482:THR:HG23	2.18	0.43
2:D:38:ARG:HG2	2:D:48:LEU:HD21	2.00	0.43
2:H:78:PHE:CZ	2:H:95:CYS:SG	3.11	0.43
2:J:50:TYR:CE1	2:J:58:ASP:HB2	2.54	0.43
1:K:478:MET:O	1:K:482:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:LEU:HD22	1:C:478:MET:HB3	1.99	0.43
2:D:170:TYR:CE2	2:D:180:VAL:HG22	2.54	0.43
1:G:478:MET:O	1:G:482:THR:HG23	2.19	0.43
1:K:181:PHE:CZ	1:K:333:LYS:HB2	2.54	0.43
1:A:343:LEU:O	1:A:452:LYS:HE3	2.18	0.42
2:B:141:SER:HB2	2:B:156:THR:OG1	2.19	0.42
1:I:434:LYS:HE2	1:I:468:LEU:HD12	2.01	0.42
1:K:393:LEU:HD22	1:K:494:PHE:CE1	2.54	0.42
2:D:90:THR:HG23	2:D:116:THR:HA	2.01	0.42
2:B:29:ILE:HA	2:B:34:TRP:CZ2	2.55	0.42
1:C:396:ASN:HA	1:C:399:LYS:HG2	2.02	0.42
2:H:90:THR:HG23	2:H:116:THR:HA	2.01	0.42
2:B:38:ARG:HG2	2:B:48:LEU:HD21	2.01	0.42
2:H:138:MET:HE2	2:H:167:LEU:HD21	2.01	0.42
2:F:142:PRO:HG2	2:F:155:ILE:HA	2.01	0.42
2:H:98:SER:HB3	2:H:104:GLN:HE21	1.84	0.42
1:K:496:HIS:ND1	1:K:497:LEU:HD23	2.34	0.42
1:E:347:ASN:HD22	1:E:349:ASN:HB2	1.84	0.42
2:D:142:PRO:HD2	2:D:155:ILE:HG23	2.02	0.42
2:F:29:ILE:HG23	2:F:34:TRP:CE2	2.52	0.42
1:G:181:PHE:CZ	1:G:333:LYS:HB2	2.55	0.42
2:J:97:ARG:HD2	2:J:108:TYR:HD2	1.85	0.42
2:B:212:LEU:HD22	2:B:212:LEU:HA	1.96	0.41
1:I:181:PHE:CZ	1:I:333:LYS:HB2	2.54	0.41
2:J:171:GLN:HB2	2:J:181:LEU:HD11	2.01	0.41
1:C:174:VAL:HG11	1:C:475:LEU:HD21	2.03	0.41
1:E:166:GLU:HG2	1:E:482:THR:HG22	2.01	0.41
1:C:393:LEU:CD1	1:E:495:HIS:CD2	2.96	0.41
1:E:383:MET:HE3	1:E:484:TYR:HE2	1.85	0.41
2:F:136:ILE:HD13	2:F:227:TYR:HB2	2.01	0.41
2:H:63:LEU:O	2:H:66:ARG:HG2	2.20	0.41
2:H:136:ILE:HD13	2:H:227:TYR:HB2	2.01	0.41
1:A:181:PHE:CZ	1:A:333:LYS:HB2	2.56	0.41
2:B:66:ARG:HH22	2:B:89:ASP:CG	2.29	0.41
2:B:220:TYR:O	2:B:235:GLY:HA2	2.20	0.41
1:C:193:ILE:HG22	1:C:202:LYS:HD3	2.01	0.41
1:A:330:MET:HB3	2:B:53:HIS:CE1	2.56	0.41
1:A:434:LYS:HD3	1:A:437:ILE:HD12	2.02	0.41
2:H:68:THR:OG1	2:H:83:ARG:NH2	2.54	0.41
2:B:178:PRO:O	2:B:179:LYS:HD3	2.21	0.41
1:C:176:ILE:HD12	1:C:475:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:LYS:HD3	1:A:434:LYS:HA	1.92	0.41
2:B:191:GLY:HA3	1:C:347:ASN:CB	2.46	0.41
2:D:195:ARG:NH1	2:D:216:ASP:CG	2.79	0.41
2:D:220:TYR:O	2:D:235:GLY:HA2	2.21	0.41
2:H:141:SER:HB2	2:H:156:THR:OG1	2.21	0.41
2:J:63:LEU:HD12	2:J:82:LEU:HD21	2.03	0.41
2:J:90:THR:HG23	2:J:116:THR:HA	2.03	0.41
1:A:176:ILE:HB	1:A:177:PRO:HD3	2.03	0.40
1:C:423:ARG:NH1	1:C:426:TYR:CD2	2.89	0.40
2:D:173:LYS:HE2	2:D:218:ALA:HB2	2.03	0.40
2:F:29:ILE:HA	2:F:34:TRP:CZ2	2.56	0.40
2:F:167:LEU:HD11	2:F:222:CYS:HB2	2.02	0.40
2:J:90:THR:HG23	2:J:116:THR:CG2	2.51	0.40
1:K:434:LYS:HE2	1:K:468:LEU:HD12	2.02	0.40
1:C:454:GLU:O	1:C:458:ARG:HG2	2.22	0.40
1:A:503:MET:SD	1:G:400:LYS:NZ	2.88	0.40
2:D:29:ILE:HA	2:D:34:TRP:CZ2	2.55	0.40
1:A:429:LYS:HE2	1:A:429:LYS:HB3	1.88	0.40
2:D:138:MET:HE2	2:D:167:LEU:HD21	2.03	0.40
2:F:68:THR:OG1	2:F:83:ARG:NH2	2.54	0.40
2:H:105:TYR:CD1	2:H:180:VAL:HG21	2.56	0.40
1:I:404:TYR:OH	1:I:501:LEU:HA	2.22	0.40
1:I:410:ILE:HG21	1:I:494:PHE:HE1	1.85	0.40
1:K:429:LYS:HE2	1:K:429:LYS:HB3	1.86	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	284/338 (84%)	269 (95%)	15 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	284/338 (84%)	268 (94%)	16 (6%)	0	100	100
1	E	283/338 (84%)	271 (96%)	12 (4%)	0	100	100
1	G	282/338 (83%)	265 (94%)	17 (6%)	0	100	100
1	I	284/338 (84%)	264 (93%)	20 (7%)	0	100	100
1	K	284/338 (84%)	267 (94%)	17 (6%)	0	100	100
2	B	220/250 (88%)	201 (91%)	19 (9%)	0	100	100
2	D	223/250 (89%)	206 (92%)	17 (8%)	0	100	100
2	F	223/250 (89%)	202 (91%)	21 (9%)	0	100	100
2	H	223/250 (89%)	203 (91%)	20 (9%)	0	100	100
2	J	219/250 (88%)	202 (92%)	17 (8%)	0	100	100
All	All	2809/3278 (86%)	2618 (93%)	191 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	278/327 (85%)	256 (92%)	22 (8%)	11	34
1	C	278/327 (85%)	257 (92%)	21 (8%)	12	35
1	E	277/327 (85%)	256 (92%)	21 (8%)	12	35
1	G	276/327 (84%)	257 (93%)	19 (7%)	14	38
1	I	278/327 (85%)	256 (92%)	22 (8%)	11	34
1	K	278/327 (85%)	257 (92%)	21 (8%)	12	35
2	B	195/208 (94%)	172 (88%)	23 (12%)	5	19
2	D	198/208 (95%)	169 (85%)	29 (15%)	3	12
2	F	198/208 (95%)	169 (85%)	29 (15%)	3	12
2	H	198/208 (95%)	172 (87%)	26 (13%)	4	16
2	J	194/208 (93%)	172 (89%)	22 (11%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2648/3002 (88%)	2393 (90%)	255 (10%)	8 27

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	A	197	SER
1	A	230	ASP
1	A	304	MET
1	A	333	LYS
1	A	343	LEU
1	A	357	ARG
1	A	368	ILE
1	A	391	GLU
1	A	392	LEU
1	A	394	LEU
1	A	397	LEU
1	A	444	LEU
1	A	449	THR
1	A	452	LYS
1	A	455	LEU
1	A	465	GLU
1	A	476	ARG
1	A	482	THR
1	A	487	GLU
1	A	497	LEU
1	A	498	ILE
2	B	6	GLU
2	B	11	LEU
2	B	35	SER
2	B	50	TYR
2	B	74	SER
2	B	95	CYS
2	B	97	ARG
2	B	99	THR
2	B	114	LEU
2	B	136	ILE
2	B	143	SER
2	B	152	ARG
2	B	156	THR
2	B	157	CYS
2	B	167	LEU

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Mol	Chain	Res	Type
2	B	180	VAL
2	B	187	ASN
2	B	199	SER
2	B	208	THR
2	B	212	LEU
2	B	213	GLN
2	B	215	GLU
2	B	228	LEU
1	C	193	ILE
1	C	211	LYS
1	C	230	ASP
1	C	302	LYS
1	C	305	ASP
1	C	333	LYS
1	C	343	LEU
1	C	366	LYS
1	C	368	ILE
1	C	391	GLU
1	C	394	LEU
1	C	397	LEU
1	C	449	THR
1	C	452	LYS
1	C	455	LEU
1	C	465	GLU
1	C	476	ARG
1	C	482	THR
1	C	487	GLU
1	C	496	HIS
1	C	501	LEU
2	D	6	GLU
2	D	11	LEU
2	D	21	THR
2	D	35	SER
2	D	50	TYR
2	D	57	THR
2	D	66	ARG
2	D	74	SER
2	D	79	SER
2	D	95	CYS
2	D	99	THR
2	D	107	ASP
2	D	116	THR

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Mol	Chain	Res	Type
2	D	136	ILE
2	D	139	THR
2	D	152	ARG
2	D	156	THR
2	D	157	CYS
2	D	167	LEU
2	D	173	LYS
2	D	189	GLU
2	D	194	SER
2	D	195	ARG
2	D	208	THR
2	D	212	LEU
2	D	213	GLN
2	D	215	GLU
2	D	228	LEU
2	D	239	GLU
1	E	161	ILE
1	E	191	ASN
1	E	196	LYS
1	E	212	LYS
1	E	230	ASP
1	E	333	LYS
1	E	343	LEU
1	E	357	ARG
1	E	368	ILE
1	E	394	LEU
1	E	397	LEU
1	E	449	THR
1	E	452	LYS
1	E	455	LEU
1	E	465	GLU
1	E	476	ARG
1	E	482	THR
1	E	487	GLU
1	E	495	HIS
1	E	500	VAL
1	E	505	PHE
2	F	6	GLU
2	F	11	LEU
2	F	21	THR
2	F	35	SER
2	F	50	TYR

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Mol	Chain	Res	Type
2	F	74	SER
2	F	79	SER
2	F	95	CYS
2	F	107	ASP
2	F	114	LEU
2	F	135	ASP
2	F	136	ILE
2	F	143	SER
2	F	152	ARG
2	F	157	CYS
2	F	163	ILE
2	F	167	LEU
2	F	173	LYS
2	F	180	VAL
2	F	189	GLU
2	F	194	SER
2	F	199	SER
2	F	208	THR
2	F	212	LEU
2	F	213	GLN
2	F	215	GLU
2	F	228	LEU
2	F	240	ILE
2	F	241	LYS
1	G	191	ASN
1	G	196	LYS
1	G	230	ASP
1	G	333	LYS
1	G	343	LEU
1	G	345	CYS
1	G	357	ARG
1	G	368	ILE
1	G	385	ASN
1	G	394	LEU
1	G	397	LEU
1	G	449	THR
1	G	452	LYS
1	G	455	LEU
1	G	465	GLU
1	G	476	ARG
1	G	482	THR
1	G	487	GLU

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Mol	Chain	Res	Type
1	G	495	HIS
2	H	5	GLN
2	H	6	GLU
2	H	11	LEU
2	H	21	THR
2	H	35	SER
2	H	50	TYR
2	H	66	ARG
2	H	74	SER
2	H	79	SER
2	H	95	CYS
2	H	114	LEU
2	H	136	ILE
2	H	137	GLN
2	H	143	SER
2	H	152	ARG
2	H	156	THR
2	H	157	CYS
2	H	163	ILE
2	H	167	LEU
2	H	180	VAL
2	H	189	GLU
2	H	199	SER
2	H	208	THR
2	H	212	LEU
2	H	213	GLN
2	H	215	GLU
1	I	191	ASN
1	I	200	TYR
1	I	230	ASP
1	I	314	LEU
1	I	333	LYS
1	I	343	LEU
1	I	345	CYS
1	I	357	ARG
1	I	368	ILE
1	I	393	LEU
1	I	394	LEU
1	I	397	LEU
1	I	449	THR
1	I	452	LYS
1	I	455	LEU

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Mol	Chain	Res	Type
1	I	465	GLU
1	I	476	ARG
1	I	482	THR
1	I	487	GLU
1	I	490	LEU
1	I	494	PHE
1	I	497	LEU
2	J	5	GLN
2	J	6	GLU
2	J	11	LEU
2	J	21	THR
2	J	35	SER
2	J	50	TYR
2	J	66	ARG
2	J	74	SER
2	J	79	SER
2	J	95	CYS
2	J	114	LEU
2	J	116	THR
2	J	152	ARG
2	J	156	THR
2	J	157	CYS
2	J	167	LEU
2	J	180	VAL
2	J	189	GLU
2	J	199	SER
2	J	208	THR
2	J	212	LEU
2	J	228	LEU
1	K	203	TYR
1	K	230	ASP
1	K	303	MET
1	K	304	MET
1	K	314	LEU
1	K	333	LYS
1	K	343	LEU
1	K	345	CYS
1	K	368	ILE
1	K	393	LEU
1	K	394	LEU
1	K	396	ASN
1	K	397	LEU

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Mol	Chain	Res	Type
1	K	449	THR
1	K	452	LYS
1	K	455	LEU
1	K	465	GLU
1	K	476	ARG
1	K	482	THR
1	K	487	GLU
1	K	494	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	320	ASN
1	A	427	HIS
1	A	464	ASN
1	A	492	ASN
1	A	496	HIS
1	C	214	ASN
1	C	308	ASN
1	C	389	GLN
1	C	464	ASN
1	C	495	HIS
1	C	506	ASN
2	D	171	GLN
1	E	159	ASN
1	E	214	ASN
1	E	308	ASN
1	E	464	ASN
1	E	502	GLN
1	G	165	GLN
1	G	359	HIS
1	G	388	GLN
1	G	389	GLN
1	G	427	HIS
2	H	1	GLN
2	H	171	GLN
1	I	165	GLN
1	I	214	ASN
1	I	347	ASN
1	I	427	HIS
2	J	103	GLN

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Mol	Chain	Res	Type
2	J	140	GLN
2	J	171	GLN
1	K	159	ASN
1	K	165	GLN
1	K	214	ASN
1	K	427	HIS
1	K	464	ASN

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	288/338 (85%)	0.53	10 (3%)	47	26	73, 111, 167, 193	0
1	C	288/338 (85%)	0.57	18 (6%)	26	13	78, 119, 171, 190	0
1	E	287/338 (84%)	0.62	18 (6%)	26	13	79, 123, 185, 212	0
1	G	286/338 (84%)	0.51	8 (2%)	55	33	72, 110, 184, 218	0
1	I	288/338 (85%)	0.75	25 (8%)	16	8	149, 177, 208, 225	0
1	K	288/338 (85%)	1.01	36 (12%)	8	4	173, 202, 226, 235	0
2	B	223/250 (89%)	0.31	8 (3%)	46	26	64, 103, 135, 149	1 (0%)
2	D	226/250 (90%)	0.33	9 (3%)	42	22	67, 103, 125, 136	1 (0%)
2	F	226/250 (90%)	0.25	4 (1%)	67	46	64, 103, 126, 138	1 (0%)
2	H	226/250 (90%)	0.36	5 (2%)	62	41	65, 104, 133, 145	1 (0%)
2	J	222/250 (88%)	0.95	30 (13%)	7	3	139, 207, 223, 227	1 (0%)
All	All	2848/3278 (86%)	0.58	171 (6%)	27	14	64, 124, 214, 235	5 (0%)

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	158	ALA	6.0
1	K	336	GLY	6.0
2	J	41	PRO	5.7
2	F	118	SER	5.7
1	E	158	ALA	5.3
1	I	438	ILE	5.1
1	A	404	TYR	4.8
1	I	158	ALA	4.7
1	K	390	SER	4.6
1	I	405	ILE	4.2
1	G	404	TYR	4.2
2	J	149	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	158	ALA	4.0
2	F	229	PRO	4.0
1	K	158	ALA	4.0
1	K	404	TYR	4.0
2	H	118	SER	4.0
2	J	145	LEU	3.9
1	C	390	SER	3.8
1	E	163	ILE	3.8
1	I	338	ASN	3.7
1	K	328	ILE	3.7
1	A	158	ALA	3.7
1	I	202	LYS	3.7
1	K	405	ILE	3.7
1	C	238	LEU	3.7
1	K	394	LEU	3.6
1	K	332	MET	3.6
1	K	339	LEU	3.6
1	C	404	TYR	3.6
1	K	456	LEU	3.6
1	I	463	SER	3.6
2	J	238	LEU	3.5
1	K	210	ILE	3.3
1	K	315	ILE	3.2
2	D	229	PRO	3.2
2	J	62	SER	3.2
1	K	191	ASN	3.1
1	I	404	TYR	3.1
2	B	190	THR	3.1
2	H	229	PRO	3.1
1	A	482	THR	3.1
1	K	356	ILE	3.1
2	J	153	VAL	3.1
2	J	155	ILE	3.1
1	E	495	HIS	3.0
2	D	10	GLY	3.0
2	J	115	VAL	3.0
2	J	35	SER	3.0
1	I	456	LEU	3.0
1	E	302	LYS	3.0
2	J	217	ILE	3.0
1	K	182	LEU	2.9
1	A	405	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	500	VAL	2.9
1	I	358	TYR	2.9
1	K	200	TYR	2.9
1	E	468	LEU	2.9
2	B	136	ILE	2.9
1	A	163	ILE	2.9
2	D	228	LEU	2.9
2	J	70	SER	2.8
2	B	147	ALA	2.8
2	J	117	VAL	2.8
1	E	177	PRO	2.8
1	E	499	TYR	2.8
2	J	147	ALA	2.8
1	I	339	LEU	2.8
1	K	329	CYS	2.8
1	A	189	SER	2.8
2	J	116	THR	2.8
1	E	404	TYR	2.7
2	J	212	LEU	2.7
1	I	214	ASN	2.7
1	K	393	LEU	2.7
1	K	397	LEU	2.7
1	I	442	ILE	2.7
1	I	459	ILE	2.7
2	B	98	SER	2.7
1	G	228	LYS	2.7
2	J	37	ILE	2.7
1	I	395	THR	2.7
2	F	116	THR	2.7
1	I	501	LEU	2.7
1	K	334	ASN	2.7
2	D	193	PRO	2.7
2	B	91	ALA	2.7
1	I	390	SER	2.6
1	I	401	MET	2.6
2	D	78	PHE	2.6
2	J	139	THR	2.6
1	E	446	ILE	2.6
1	A	240	HIS	2.6
2	J	199	SER	2.6
1	C	401	MET	2.6
2	D	1	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	416	GLU	2.6
2	J	228	LEU	2.6
1	E	213	ILE	2.6
2	D	207	PHE	2.6
2	J	220	TYR	2.6
2	B	229	PRO	2.6
2	J	88	ALA	2.6
1	C	505	PHE	2.5
1	E	240	HIS	2.5
2	J	179	LYS	2.5
2	D	206	THR	2.5
1	C	386	ILE	2.5
1	K	343	LEU	2.5
2	D	199	SER	2.5
2	F	228	LEU	2.5
2	J	63	LEU	2.5
1	K	401	MET	2.4
2	J	14	PRO	2.4
1	C	307	TYR	2.4
1	G	504	LYS	2.4
1	I	171	LEU	2.4
1	C	495	HIS	2.4
1	A	161	ILE	2.4
1	E	303	MET	2.4
1	C	362	GLU	2.4
1	K	231	LEU	2.4
1	K	407	ILE	2.4
1	E	444	LEU	2.4
1	G	348	ASN	2.4
1	E	328	ILE	2.4
1	A	447	TRP	2.4
1	C	481	ASN	2.3
1	K	176	ILE	2.3
1	C	215	GLU	2.3
2	J	36	TRP	2.3
1	K	213	ILE	2.3
1	C	393	LEU	2.3
2	B	173	LYS	2.3
1	I	199	THR	2.3
1	C	240	HIS	2.3
2	J	18	LEU	2.3
1	I	228	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	366	LYS	2.3
1	I	208	ALA	2.3
2	H	147	ALA	2.3
2	J	73	THR	2.3
1	C	302	LYS	2.3
2	H	155	ILE	2.2
1	C	483	PHE	2.2
1	I	240	HIS	2.2
1	K	337	THR	2.2
2	H	181	LEU	2.2
1	K	410	ILE	2.2
1	I	489	HIS	2.2
1	C	355	GLY	2.2
2	J	61	PRO	2.2
2	B	76	THR	2.1
1	I	346	TYR	2.1
1	I	227	ILE	2.1
1	C	394	LEU	2.1
1	A	238	LEU	2.1
1	E	165	GLN	2.1
1	G	232	ILE	2.1
2	J	82	LEU	2.1
1	G	387	LEU	2.1
1	K	330	MET	2.1
1	K	406	TYR	2.1
1	E	497	LEU	2.1
1	K	498	ILE	2.1
1	K	240	HIS	2.1
1	K	173	PHE	2.1
1	K	340	PHE	2.1
1	G	240	HIS	2.0
2	J	173	LYS	2.0
1	E	161	ILE	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.