



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:05 AM UTC

PDB ID : 6M3C / pdb_00006m3c
Title : hAPC-h1573 Fab complex
Authors : Wang, X.; Wang, D.; Zhao, X.; Egner, U.
Deposited on : 2020-03-03
Resolution : 3.70 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

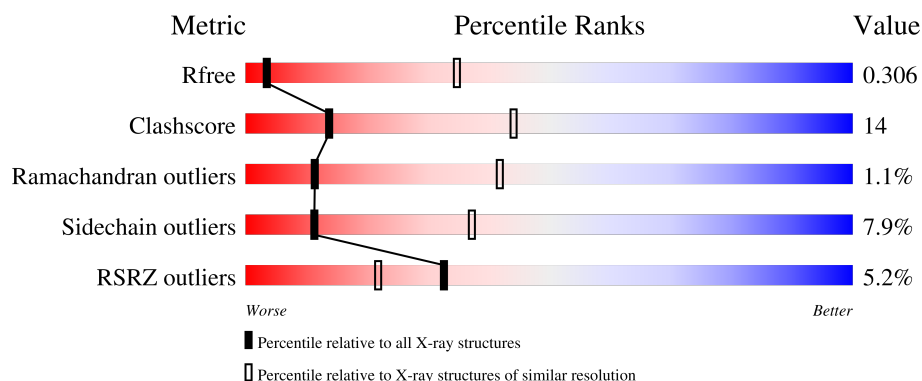
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	250	
1	C	250	
1	G	250	
2	B	155	
2	D	155	

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Mol	Chain	Length	Quality of chain
2	I	155	
3	E	218	
3	J	218	
3	L	218	
4	F	221	
4	H	221	
4	K	221	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16911 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 Vitamin K-dependent protein C heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1883	1193	331	346	13			
1	C	239	Total	C	N	O	S	0	0	0
			1883	1193	331	346	13			
1	G	239	Total	C	N	O	S	0	0	0
			1883	1193	331	346	13			

- Molecule 2 is a protein called Vitamin K-dependent protein C light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	53	Total	C	N	O	S	0	0	0
			412	259	74	72	7			
2	D	53	Total	C	N	O	S	0	0	0
			412	259	74	72	7			
2	I	53	Total	C	N	O	S	0	0	0
			412	259	74	72	7			

- Molecule 3 is a protein called h1573 Fab H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	218	Total	C	N	O	S	0	0	0
			1669	1043	278	342	6			
3	E	218	Total	C	N	O	S	0	0	0
			1669	1043	278	342	6			
3	J	218	Total	C	N	O	S	0	0	0
			1669	1043	278	342	6			

- Molecule 4 is a protein called h1573 Fab L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	221	Total	C	N	O	S	0	0	0
			1673	1055	280	332	6			

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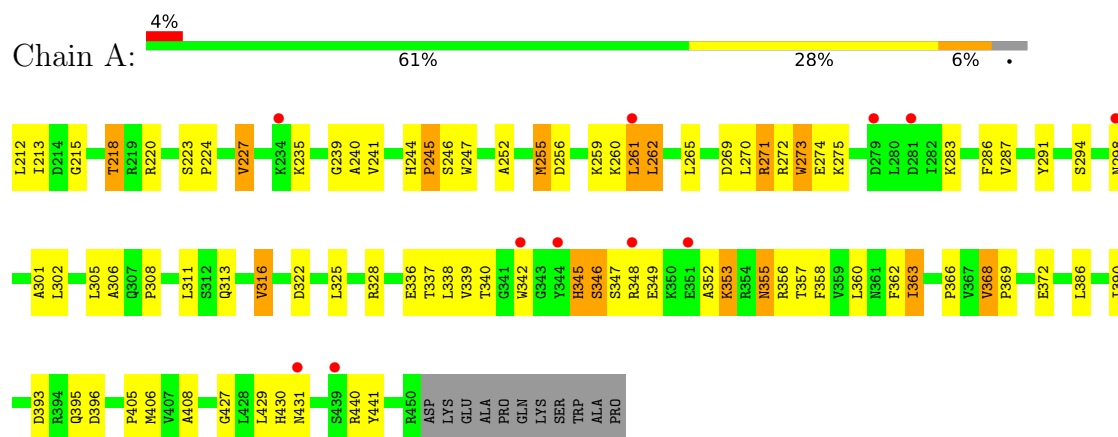
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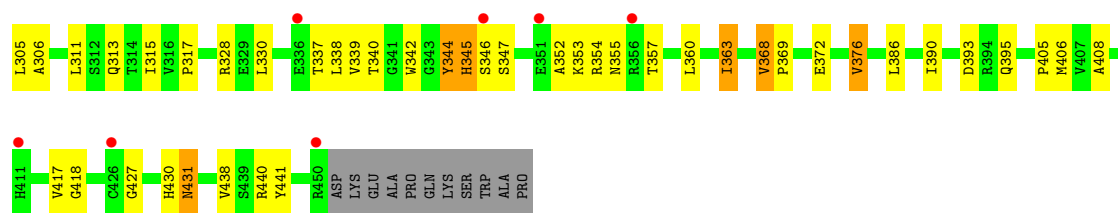
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	221	Total	C	N	O	S	0	0	0
			1673	1055	280	332	6			
4	K	221	Total	C	N	O	S	0	0	0
			1673	1055	280	332	6			

3 Residue-property plots [i](#)

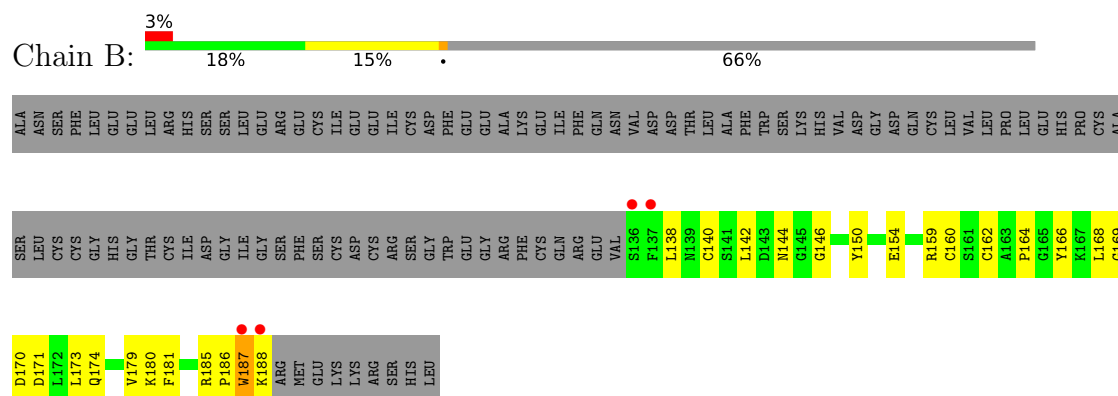
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Vitamin K-dependent protein C heavy chain

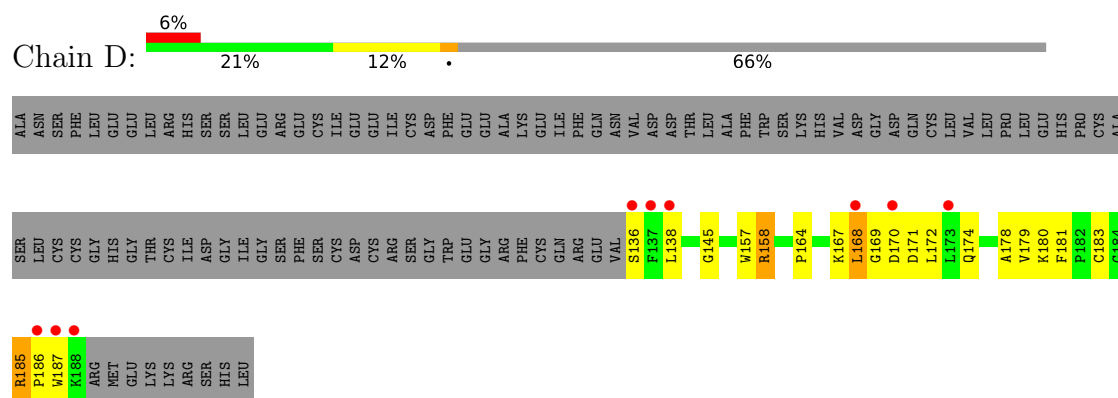




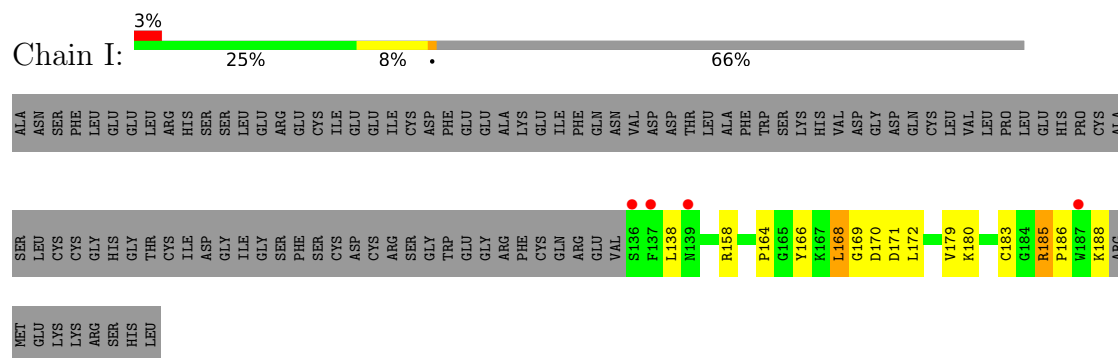
• Molecule 2: Vitamin K-dependent protein C light chain



• Molecule 2: Vitamin K-dependent protein C light chain

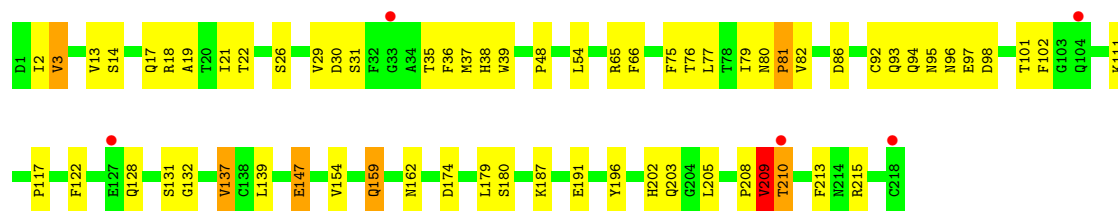


• Molecule 2: Vitamin K-dependent protein C light chain

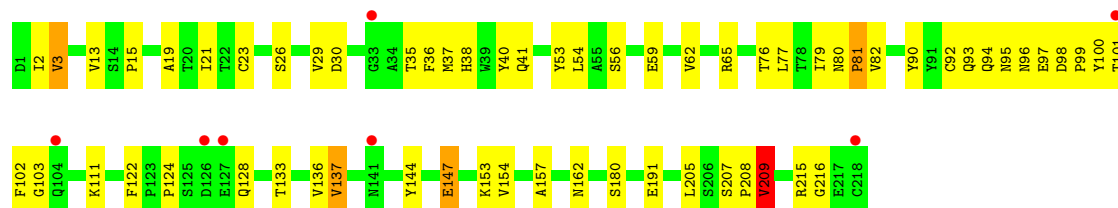


• Molecule 3: h1573 Fab H chain

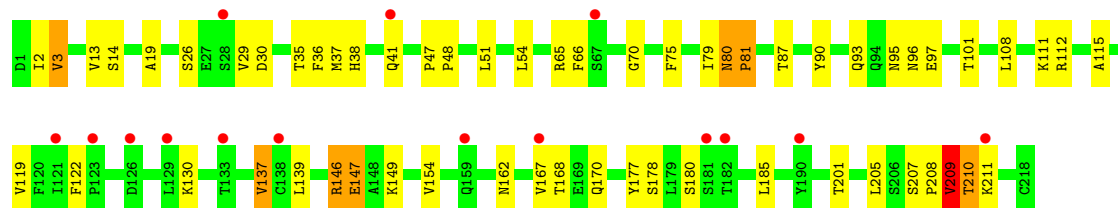
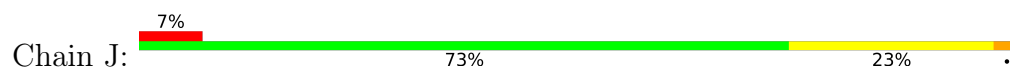




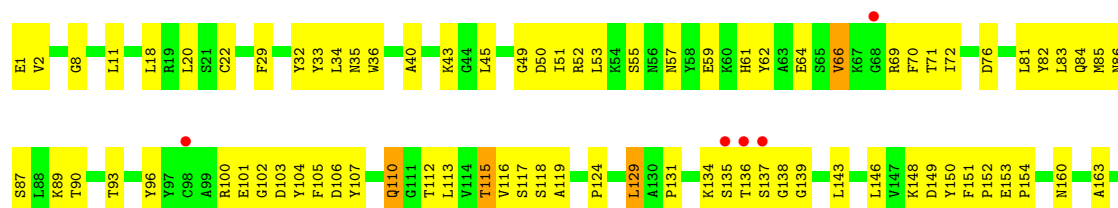
• Molecule 3: h1573 Fab H chain



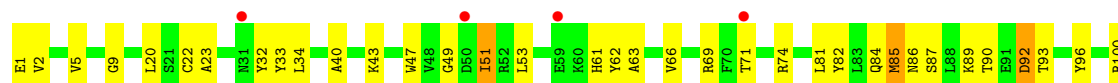
• Molecule 3: h1573 Fab H chain

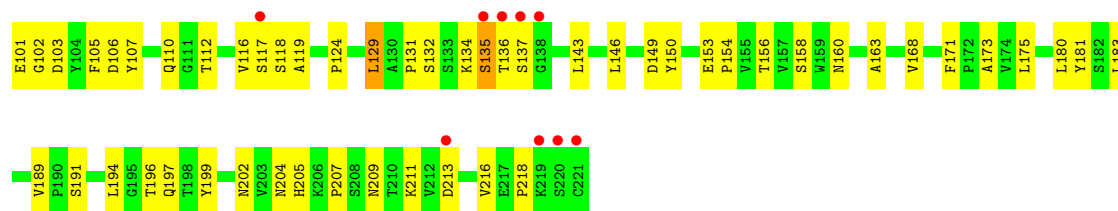


• Molecule 4: h1573 Fab L chain

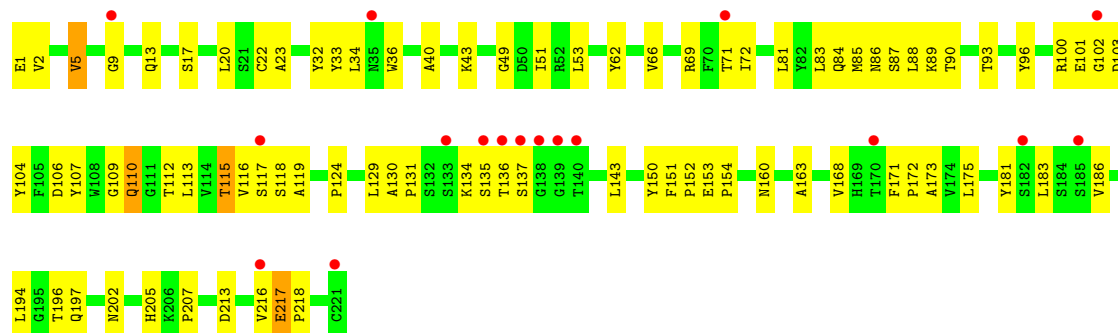


• Molecule 4: h1573 Fab L chain





● Molecule 4: h1573 Fab L chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.34Å 124.34Å 666.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.38 – 3.70 33.38 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (33.38-3.70) 98.2 (33.38-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 3.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.278 , 0.302 0.288 , 0.306	Depositor DCC
R_{free} test set	2855 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	87.4	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.0	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	0.85	EDS
Total number of atoms	16911	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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	0.38	0/1928	1.01	6/2615 (0.2%)
1	C	0.38	0/1928	1.02	6/2615 (0.2%)
1	G	0.38	0/1928	1.03	6/2615 (0.2%)
2	B	0.42	0/425	1.11	2/575 (0.3%)
2	D	0.44	0/425	1.07	1/575 (0.2%)
2	I	0.42	0/425	0.99	0/575
3	E	0.35	0/1706	0.75	0/2321
3	J	0.33	0/1706	0.76	2/2321 (0.1%)
3	L	0.34	0/1706	0.76	0/2321
4	F	0.32	0/1713	0.74	0/2329
4	H	0.32	0/1713	0.79	1/2329 (0.0%)
4	K	0.32	0/1713	0.80	4/2329 (0.2%)
All	All	0.35	0/17316	0.88	28/23520 (0.1%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	223	SER	CA-C-N	9.66	129.91	119.87
1	G	223	SER	C-N-CA	9.66	129.91	119.87
1	A	223	SER	CA-C-N	9.13	128.76	119.82
1	A	223	SER	C-N-CA	9.13	128.76	119.82
1	C	223	SER	CA-C-N	7.52	127.19	119.82
1	C	223	SER	C-N-CA	7.52	127.19	119.82
1	C	274	GLU	N-CA-C	7.22	121.60	110.42
1	C	273	TRP	N-CA-C	-6.55	98.54	108.96
1	G	273	TRP	N-CA-C	-6.32	98.91	108.96
1	A	353	LYS	N-CA-C	-6.29	104.77	112.88
2	D	185	ARG	CB-CA-C	6.05	116.16	110.17
4	K	130	ALA	CA-C-N	6.01	126.32	119.83
4	K	130	ALA	C-N-CA	6.01	126.32	119.83
1	G	431	ASN	N-CA-C	5.82	115.97	108.34
1	C	257	GLU	N-CA-C	-5.74	98.58	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	TRP	N-CA-C	-5.68	99.93	108.96
1	G	328	ARG	N-CA-C	5.43	117.28	111.36
4	H	138	GLY	N-CA-C	-5.42	107.76	115.30
1	A	239	GLY	N-CA-C	-5.42	105.34	112.81
2	B	140	CYS	N-CA-C	-5.32	106.56	112.57
3	J	80	ASN	CA-C-N	-5.29	113.23	119.84
3	J	80	ASN	C-N-CA	-5.29	113.23	119.84
1	A	349	GLU	N-CA-C	5.28	116.89	111.03
1	G	274	GLU	N-CA-C	5.09	118.31	110.42
4	K	217	GLU	CA-C-N	5.07	125.05	120.03
4	K	217	GLU	C-N-CA	5.07	125.05	120.03
1	C	228	VAL	N-CA-C	5.02	115.14	108.11
2	B	146	GLY	N-CA-C	-5.01	108.40	114.92

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1883	0	1853	66	0
1	C	1883	0	1853	45	0
1	G	1883	0	1853	51	1
2	B	412	0	381	17	0
2	D	412	0	381	11	0
2	I	412	0	381	9	0
3	E	1669	0	1605	40	1
3	J	1669	0	1605	45	0
3	L	1669	0	1605	50	0
4	F	1673	0	1629	55	0
4	H	1673	0	1629	75	0
4	K	1673	0	1629	54	0
All	All	16911	0	16404	483	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 14.

All (483) 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:C:345:HIS:CD2	1:C:357:THR:OG1	2.02	1.11
1:C:345:HIS:CD2	1:C:357:THR:HG1	1.70	1.08
2:D:145:GLY:O	2:D:158:ARG:NH2	2.08	0.87
1:G:345:HIS:CD2	1:G:357:THR:HG1	1.96	0.84
4:F:71:THR:HB	4:F:84:GLN:HB3	1.60	0.83
1:C:345:HIS:NE2	1:C:357:THR:OG1	2.07	0.83
4:F:51:ILE:HD13	4:F:74:ARG:HD2	1.61	0.82
2:B:154:GLU:OE2	2:B:159:ARG:NH1	2.13	0.81
3:L:3:VAL:HG22	3:L:26:SER:HB3	1.63	0.80
4:H:33:TYR:HB2	4:H:101:GLU:HB3	1.63	0.78
1:C:272:ARG:HG2	1:C:274:GLU:HG3	1.65	0.78
1:G:272:ARG:HG2	1:G:274:GLU:HG3	1.65	0.78
1:C:244:HIS:HB3	1:C:247:TRP:HB2	1.64	0.78
1:A:342:TRP:CZ2	1:A:360:LEU:HG	2.21	0.75
4:K:136:THR:HB	4:K:137:SER:HA	1.67	0.75
4:F:40:ALA:HB3	4:F:43:LYS:HB2	1.68	0.75
1:A:244:HIS:HB3	1:A:247:TRP:HB2	1.69	0.75
4:K:71:THR:HB	4:K:84:GLN:HB3	1.68	0.74
1:G:244:HIS:HB3	1:G:247:TRP:HB2	1.69	0.74
1:G:345:HIS:NE2	1:G:357:THR:OG1	2.17	0.74
3:E:3:VAL:HG22	3:E:26:SER:HB3	1.70	0.73
1:G:344:TYR:H	1:G:344:TYR:HD2	1.36	0.73
1:A:224:PRO:HB2	1:A:316:VAL:H	1.53	0.73
4:H:136:THR:HB	4:H:137:SER:HA	1.69	0.73
1:C:259:LYS:HB3	1:C:260:LYS:HA	1.69	0.73
1:A:227:VAL:HG22	1:A:240:ALA:HB3	1.68	0.72
4:H:191:SER:HA	4:H:194:LEU:HD13	1.71	0.72
1:A:252:ALA:HA	1:A:301:ALA:HB2	1.71	0.72
1:A:272:ARG:HG2	1:A:274:GLU:HG3	1.71	0.72
2:B:166:TYR:OH	2:B:185:ARG:HD3	1.89	0.72
4:H:22:CYS:HB3	4:H:81:LEU:HB3	1.70	0.72
4:K:5:VAL:HG23	4:K:23:ALA:HB3	1.70	0.72
3:L:30:ASP:O	3:L:96:ASN:ND2	2.23	0.71
1:C:252:ALA:HA	1:C:301:ALA:HB2	1.71	0.71
1:A:353:LYS:HD2	1:A:356:ARG:HD3	1.73	0.71
1:C:430:HIS:ND1	1:C:431:ASN:OD1	2.24	0.70
3:L:2:ILE:HD11	3:L:97:GLU:HG3	1.73	0.70
4:H:51:ILE:HD11	4:H:72:ILE:HG12	1.71	0.70
1:A:345:HIS:H	1:A:345:HIS:CD2	2.08	0.69
4:F:136:THR:HB	4:F:137:SER:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:345:HIS:CD2	1:G:357:THR:OG1	2.45	0.69
1:G:430:HIS:ND1	1:G:431:ASN:OD1	2.25	0.68
1:G:259:LYS:HB3	1:G:260:LYS:HA	1.74	0.68
3:L:95:ASN:ND2	4:H:103:ASP:O	2.26	0.68
1:G:252:ALA:HA	1:G:301:ALA:HB2	1.76	0.68
3:L:36:PHE:HB3	3:L:95:ASN:HB3	1.76	0.68
1:A:313:GLN:NE2	2:B:188:LYS:HE3	2.08	0.68
4:H:71:THR:HB	4:H:84:GLN:HB3	1.74	0.67
1:A:213:ILE:HD13	1:A:427:GLY:HA3	1.76	0.67
1:A:430:HIS:ND1	1:A:431:ASN:OD1	2.27	0.67
1:G:227:VAL:HG22	1:G:240:ALA:HB3	1.75	0.67
1:G:213:ILE:HD13	1:G:427:GLY:HA3	1.75	0.67
3:L:22:THR:HG22	3:L:76:THR:HG22	1.76	0.67
3:J:65:ARG:HB3	3:J:81:PRO:HD2	1.76	0.67
4:H:34:LEU:HB3	4:H:81:LEU:HD22	1.76	0.66
4:K:51:ILE:HD11	4:K:72:ILE:HG12	1.78	0.66
4:H:131:PRO:HG3	4:H:143:LEU:HB3	1.76	0.66
4:H:149:ASP:HA	4:H:180:LEU:HB3	1.75	0.66
3:J:95:ASN:ND2	4:K:103:ASP:O	2.29	0.66
1:C:344:TYR:HB3	1:C:352:ALA:HB1	1.77	0.66
1:G:346:SER:HB2	1:G:352:ALA:CB	2.26	0.66
1:C:224:PRO:HB2	1:C:316:VAL:H	1.60	0.66
3:E:65:ARG:HB3	3:E:81:PRO:HD2	1.78	0.66
4:K:33:TYR:HB2	4:K:101:GLU:HB3	1.77	0.66
1:G:227:VAL:HB	1:G:265:LEU:HD23	1.77	0.65
1:C:344:TYR:CD2	1:C:399:GLU:HB3	2.32	0.65
3:J:146:ARG:HD2	3:J:167:VAL:HG21	1.78	0.65
1:C:317:PRO:O	2:D:183:CYS:HB2	1.97	0.64
3:J:149:LYS:HB3	3:J:201:THR:HB	1.79	0.64
1:C:283:LYS:HB2	1:C:306:ALA:HB2	1.80	0.64
1:A:328:ARG:NH2	2:B:144:ASN:OD1	2.25	0.64
3:J:122:PHE:HB2	3:J:137:VAL:HG13	1.79	0.64
1:A:241:VAL:HB	1:A:405:PRO:HB3	1.80	0.64
3:E:2:ILE:HD11	3:E:97:GLU:HG3	1.79	0.64
4:F:92:ASP:OD1	4:F:92:ASP:N	2.29	0.64
4:F:34:LEU:HB3	4:F:81:LEU:HD22	1.80	0.64
4:F:124:PRO:HB3	4:F:150:TYR:HB3	1.78	0.64
1:G:215:GLY:HA2	1:G:363:ILE:HD13	1.80	0.64
1:C:344:TYR:HD2	1:C:399:GLU:HB3	1.63	0.63
4:H:106:ASP:OD1	4:H:107:TYR:N	2.29	0.63
1:G:363:ILE:HD11	1:G:395:GLN:HG2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:30:ASP:O	3:E:96:ASN:ND2	2.29	0.63
4:K:1:GLU:HG3	4:K:2:VAL:HG23	1.81	0.63
4:K:124:PRO:HB3	4:K:150:TYR:HB3	1.80	0.62
3:J:2:ILE:HD11	3:J:97:GLU:HG3	1.82	0.62
1:C:241:VAL:HB	1:C:405:PRO:HB3	1.81	0.62
4:K:22:CYS:HB3	4:K:81:LEU:HB3	1.81	0.62
4:F:33:TYR:HB2	4:F:101:GLU:HB3	1.81	0.61
4:H:1:GLU:HG3	4:H:2:VAL:HG23	1.81	0.61
3:E:122:PHE:HB2	3:E:137:VAL:HG13	1.82	0.61
3:E:36:PHE:HB3	3:E:95:ASN:HB3	1.82	0.61
1:A:227:VAL:HB	1:A:265:LEU:HD23	1.83	0.61
4:K:106:ASP:OD1	4:K:107:TYR:N	2.31	0.61
1:C:368:VAL:HG22	1:C:369:PRO:HD2	1.83	0.60
3:J:3:VAL:HG22	3:J:26:SER:HB3	1.83	0.60
3:L:38:HIS:CE1	3:L:54:LEU:H	2.20	0.60
3:J:30:ASP:O	3:J:96:ASN:ND2	2.35	0.60
4:K:34:LEU:HB3	4:K:81:LEU:HD22	1.83	0.60
1:A:283:LYS:HB2	1:A:306:ALA:HB2	1.84	0.60
2:B:169:GLY:C	2:B:171:ASP:H	2.09	0.60
1:C:342:TRP:CH2	1:C:360:LEU:HG	2.37	0.60
4:H:135:SER:O	4:H:136:THR:OG1	2.19	0.59
1:G:339:VAL:HB	1:G:363:ILE:HG22	1.84	0.59
4:H:124:PRO:HB3	4:H:150:TYR:HB3	1.84	0.59
1:A:368:VAL:HG22	1:A:369:PRO:HD2	1.85	0.59
3:J:13:VAL:HG21	3:J:19:ALA:HB2	1.85	0.59
3:L:98:ASP:OD1	3:L:98:ASP:N	2.33	0.59
1:G:241:VAL:HB	1:G:405:PRO:HB3	1.83	0.59
4:F:1:GLU:HG3	4:F:2:VAL:HG23	1.84	0.59
1:G:317:PRO:O	2:I:183:CYS:HB2	2.03	0.59
3:L:65:ARG:HB3	3:L:81:PRO:HD2	1.85	0.59
3:L:65:ARG:NH1	3:L:86:ASP:OD2	2.25	0.58
1:C:317:PRO:O	2:D:183:CYS:CB	2.51	0.58
4:H:40:ALA:HB3	4:H:43:LYS:HB2	1.86	0.58
3:E:80:ASN:HB3	3:E:81:PRO:HD3	1.85	0.58
3:E:93:GLN:NE2	3:E:94:GLN:O	2.37	0.58
3:J:80:ASN:HB3	3:J:81:PRO:HD3	1.86	0.57
3:L:80:ASN:HB3	3:L:81:PRO:HD3	1.85	0.57
4:K:135:SER:O	4:K:136:THR:OG1	2.16	0.57
3:L:35:THR:HG22	3:L:37:MET:H	1.70	0.57
4:K:131:PRO:HG3	4:K:143:LEU:HB3	1.86	0.57
1:A:336:GLU:HA	1:A:366:PRO:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:169:GLY:C	2:D:171:ASP:H	2.12	0.56
3:J:38:HIS:HB2	3:J:93:GLN:HG3	1.87	0.56
1:A:345:HIS:CD2	1:A:345:HIS:N	2.72	0.56
1:A:366:PRO:HG2	1:A:390:ILE:HD11	1.87	0.56
3:E:93:GLN:HB2	3:E:102:PHE:CD1	2.41	0.56
1:G:368:VAL:HG22	1:G:369:PRO:HD2	1.88	0.56
1:A:215:GLY:HA2	1:A:363:ILE:HD13	1.87	0.56
2:I:169:GLY:C	2:I:171:ASP:H	2.13	0.56
3:E:98:ASP:OD1	3:E:98:ASP:N	2.36	0.56
4:K:101:GLU:HG2	4:K:102:GLY:H	1.69	0.56
3:J:41:GLN:HG3	3:J:90:TYR:HE1	1.71	0.55
1:G:298:ASN:HA	1:G:441:TYR:OH	2.05	0.55
4:H:160:ASN:HB2	4:H:163:ALA:HB3	1.89	0.55
2:I:168:LEU:HD23	2:I:172:LEU:HA	1.88	0.55
4:H:173:ALA:HB2	4:H:183:LEU:HD23	1.87	0.55
4:F:149:ASP:HA	4:F:180:LEU:HB3	1.88	0.55
1:A:342:TRP:CH2	1:A:360:LEU:HG	2.41	0.55
1:G:353:LYS:O	1:G:353:LYS:HG3	2.06	0.55
3:L:48:PRO:HG3	4:H:45:LEU:HD21	1.89	0.55
1:C:212:LEU:HD12	1:C:397:ALA:HA	1.87	0.55
4:K:13:GLN:HE22	4:K:119:ALA:HB2	1.72	0.55
4:K:40:ALA:HB3	4:K:43:LYS:HB2	1.88	0.55
1:C:298:ASN:OD1	1:C:384:ASN:ND2	2.38	0.54
3:L:159:GLN:HG3	3:L:162:ASN:HD21	1.72	0.54
4:H:20:LEU:HD11	4:H:96:TYR:HD2	1.73	0.54
1:A:339:VAL:HB	1:A:363:ILE:HG22	1.88	0.54
3:L:180:SER:HB3	4:H:171:PHE:CZ	2.42	0.54
4:H:101:GLU:HG2	4:H:102:GLY:H	1.72	0.54
4:H:204:ASN:HB3	4:H:211:LYS:HG3	1.89	0.54
4:K:113:LEU:HD21	4:K:115:THR:HG23	1.89	0.54
1:C:316:VAL:HG23	2:D:181:PHE:HB3	1.90	0.54
3:J:210:THR:O	3:J:210:THR:OG1	2.21	0.54
4:F:101:GLU:HG2	4:F:102:GLY:H	1.73	0.54
3:L:38:HIS:NE2	4:H:104:TYR:HB3	2.23	0.53
1:C:339:VAL:HB	1:C:363:ILE:HG22	1.90	0.53
4:F:106:ASP:OD1	4:F:107:TYR:N	2.32	0.53
2:D:168:LEU:HD23	2:D:172:LEU:HA	1.89	0.53
1:C:213:ILE:HG13	1:C:345:HIS:O	2.07	0.53
4:F:129:LEU:HD21	4:F:146:LEU:HB2	1.90	0.53
3:E:38:HIS:CE1	3:E:54:LEU:H	2.27	0.53
4:F:135:SER:O	4:F:136:THR:OG1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:29:VAL:C	3:L:96:ASN:HD22	2.15	0.53
3:L:35:THR:HG21	3:L:75:PHE:CE2	2.43	0.53
4:K:100:ARG:NH1	4:K:106:ASP:OD2	2.42	0.53
4:H:118:SER:OG	4:H:119:ALA:N	2.41	0.53
4:H:93:THR:HG22	4:H:116:VAL:H	1.73	0.53
4:H:129:LEU:HD21	4:H:146:LEU:HB2	1.90	0.53
1:G:317:PRO:O	2:I:183:CYS:CB	2.57	0.53
1:A:283:LYS:HE3	1:A:306:ALA:HA	1.91	0.53
1:G:283:LYS:HB2	1:G:306:ALA:HB2	1.91	0.53
1:A:255:MET:HE1	1:A:261:LEU:HD11	1.90	0.52
1:A:363:ILE:HD11	1:A:395:GLN:HG2	1.91	0.52
4:H:175:LEU:HB3	4:H:181:TYR:CE1	2.44	0.52
1:C:330:LEU:HB3	1:C:417:VAL:HG22	1.91	0.52
3:E:147:GLU:CD	3:E:147:GLU:H	2.15	0.52
4:F:47:TRP:CE3	4:F:63:ALA:HB2	2.44	0.52
4:K:116:VAL:O	4:K:118:SER:N	2.43	0.52
1:A:390:ILE:HB	1:A:393:ASP:HB3	1.92	0.52
4:F:131:PRO:HD2	4:F:218:PRO:HA	1.90	0.52
4:K:134:LYS:HB3	4:K:135:SER:HA	1.92	0.52
3:L:93:GLN:HB2	3:L:102:PHE:CD1	2.44	0.52
3:L:210:THR:O	3:L:210:THR:OG1	2.28	0.52
4:F:93:THR:HG22	4:F:116:VAL:H	1.75	0.52
4:H:64:GLU:OE2	4:H:64:GLU:N	2.43	0.52
1:G:330:LEU:HB3	1:G:417:VAL:HG22	1.92	0.52
4:K:202:ASN:ND2	4:K:213:ASP:OD2	2.44	0.52
1:A:353:LYS:HG3	1:A:353:LYS:O	2.09	0.51
1:G:344:TYR:CD2	1:G:344:TYR:N	2.76	0.51
2:D:138:LEU:HD22	2:D:157:TRP:HA	1.93	0.51
3:J:38:HIS:N	3:J:93:GLN:O	2.39	0.51
3:L:122:PHE:HB2	3:L:137:VAL:HG13	1.92	0.51
3:E:41:GLN:HG3	3:E:90:TYR:HE1	1.75	0.51
3:J:35:THR:HG21	3:J:75:PHE:CE1	2.46	0.51
3:J:41:GLN:HB2	3:J:51:LEU:HD21	1.92	0.51
2:D:167:LYS:HG3	2:D:178:ALA:HB2	1.93	0.51
4:H:153:GLU:CG	4:H:154:PRO:HA	2.41	0.50
1:C:298:ASN:HA	1:C:441:TYR:OH	2.10	0.50
3:E:100:TYR:HD2	4:F:47:TRP:CE2	2.29	0.50
1:A:227:VAL:HG13	1:A:240:ALA:C	2.36	0.50
1:A:322:ASP:HB2	2:B:150:TYR:CD1	2.47	0.50
4:F:9:GLY:HA3	4:F:112:THR:HG21	1.93	0.50
4:H:134:LYS:HB3	4:H:135:SER:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:SER:OG	2:D:145:GLY:O	2.28	0.49
1:G:418:GLY:HA2	1:G:438:VAL:HG23	1.94	0.49
4:K:69:ARG:HD2	4:K:87:SER:O	2.12	0.49
3:L:65:ARG:HD3	1:C:273:TRP:CZ2	2.47	0.49
4:H:11:LEU:HB2	4:H:152:PRO:HG3	1.94	0.49
4:F:131:PRO:HG3	4:F:143:LEU:HB3	1.93	0.49
3:L:93:GLN:NE2	3:L:94:GLN:O	2.45	0.49
1:G:255:MET:HG3	1:G:285:VAL:HG21	1.93	0.49
3:J:29:VAL:C	3:J:96:ASN:HD22	2.20	0.49
3:J:38:HIS:CE1	3:J:54:LEU:H	2.30	0.49
3:L:147:GLU:CD	3:L:147:GLU:H	2.19	0.49
1:G:369:PRO:HG2	1:G:372:GLU:HG3	1.94	0.49
1:A:337:THR:HG22	1:A:408:ALA:HB2	1.94	0.49
4:H:202:ASN:HD22	4:H:213:ASP:HB3	1.78	0.49
3:J:87:THR:HG21	3:J:170:GLN:HB3	1.94	0.49
4:H:173:ALA:HA	4:H:183:LEU:HB3	1.93	0.49
3:L:18:ARG:HB2	1:C:275:LYS:NZ	2.26	0.49
4:H:85:MET:HE1	4:H:96:TYR:CE2	2.48	0.49
1:G:390:ILE:HB	1:G:393:ASP:HB3	1.93	0.49
4:H:189:VAL:HG21	4:H:199:TYR:CE2	2.47	0.49
3:J:211:LYS:HD2	4:K:134:LYS:HD2	1.95	0.49
1:A:218:THR:HG23	1:A:360:LEU:O	2.12	0.49
4:F:32:TYR:CD1	4:F:100:ARG:HD3	2.47	0.49
3:J:35:THR:HG22	3:J:37:MET:H	1.78	0.48
4:H:113:LEU:HD21	4:H:115:THR:HG23	1.96	0.48
1:G:257:GLU:OE1	1:G:258:SER:N	2.35	0.48
3:E:15:PRO:HA	3:E:82:VAL:HG13	1.94	0.48
3:E:128:GLN:HG2	3:E:133:THR:O	2.14	0.48
4:K:205:HIS:CD2	4:K:207:PRO:HD2	2.49	0.48
4:H:8:GLY:O	4:H:112:THR:HG21	2.13	0.48
1:G:337:THR:HG22	1:G:408:ALA:HB2	1.96	0.48
1:G:342:TRP:CH2	1:G:360:LEU:HG	2.48	0.48
1:G:345:HIS:CD2	1:G:345:HIS:N	2.81	0.48
3:J:14:SER:HA	3:J:111:LYS:HB2	1.95	0.48
4:K:36:TRP:HD1	4:K:72:ILE:HD11	1.77	0.48
4:K:118:SER:OG	4:K:119:ALA:N	2.47	0.48
4:F:205:HIS:CD2	4:F:207:PRO:HD2	2.48	0.48
1:G:227:VAL:HG13	1:G:240:ALA:C	2.39	0.48
1:A:269:ASP:OD1	1:A:271:ARG:HB2	2.14	0.48
2:I:138:LEU:HD23	2:I:138:LEU:H	1.77	0.48
3:J:38:HIS:NE2	4:K:104:TYR:HB3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:PHE:HB2	1:A:302:LEU:HB3	1.94	0.48
4:F:132:SER:HB2	4:F:134:LYS:NZ	2.29	0.48
1:A:262:LEU:HD12	1:A:262:LEU:H	1.79	0.47
1:C:363:ILE:HG13	1:C:395:GLN:HB3	1.96	0.47
3:E:29:VAL:C	3:E:96:ASN:HD22	2.22	0.47
4:K:62:TYR:CZ	4:K:72:ILE:HG22	2.49	0.47
1:A:259:LYS:HB3	1:A:260:LYS:HG2	1.95	0.47
1:A:298:ASN:HA	1:A:441:TYR:OH	2.14	0.47
3:L:38:HIS:N	3:L:93:GLN:O	2.41	0.47
4:K:160:ASN:HB2	4:K:163:ALA:HB3	1.96	0.47
4:H:18:LEU:H	4:H:85:MET:HB2	1.79	0.47
4:F:118:SER:OG	4:F:119:ALA:N	2.46	0.47
3:L:191:GLU:HG2	3:L:215:ARG:HH21	1.78	0.47
1:A:259:LYS:HB3	1:A:260:LYS:HA	1.97	0.47
4:F:100:ARG:NH1	4:F:106:ASP:OD2	2.48	0.47
4:F:132:SER:HB2	4:F:134:LYS:HZ2	1.79	0.47
1:C:215:GLY:HA2	1:C:363:ILE:HD13	1.96	0.47
1:C:286:PHE:HB2	1:C:302:LEU:HB3	1.97	0.47
1:G:278:LEU:HD13	1:G:315:ILE:HD12	1.96	0.47
3:E:205:LEU:HB3	3:E:207:SER:O	2.15	0.47
1:A:313:GLN:HG3	2:B:187:TRP:CE3	2.50	0.46
4:F:90:THR:O	4:F:93:THR:HG23	2.14	0.46
1:A:347:SER:HB2	1:A:348:ARG:HH11	1.81	0.46
2:B:138:LEU:HD23	2:B:138:LEU:H	1.79	0.46
4:F:22:CYS:HB3	4:F:81:LEU:HB3	1.97	0.46
1:G:363:ILE:HD12	1:G:363:ILE:HA	1.72	0.46
3:J:180:SER:HB3	4:K:171:PHE:CZ	2.51	0.46
2:B:179:VAL:HG22	2:B:180:LYS:H	1.80	0.46
3:E:21:ILE:HD12	3:E:77:LEU:HD23	1.97	0.46
4:F:116:VAL:O	4:F:118:SER:N	2.48	0.46
4:K:175:LEU:HB3	4:K:181:TYR:CE1	2.50	0.46
1:A:313:GLN:HE22	2:B:188:LYS:HE3	1.77	0.46
2:B:162:CYS:HB3	2:B:166:TYR:HB2	1.97	0.46
1:A:313:GLN:CD	2:B:187:TRP:CE3	2.94	0.46
3:L:21:ILE:HD12	3:L:77:LEU:HD23	1.96	0.46
4:H:85:MET:HE1	4:H:96:TYR:HE2	1.81	0.46
1:G:354:ARG:HD2	1:G:354:ARG:HA	1.71	0.46
4:K:20:LEU:HB2	4:K:83:LEU:HB3	1.98	0.46
4:H:62:TYR:CZ	4:H:72:ILE:HG22	2.50	0.46
2:I:158:ARG:HD2	2:I:158:ARG:C	2.41	0.46
4:H:32:TYR:CD1	4:H:100:ARG:HD3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:38:HIS:O	3:J:93:GLN:N	2.46	0.46
1:A:346:SER:HB2	1:A:352:ALA:CB	2.46	0.45
2:D:187:TRP:CD1	2:D:187:TRP:N	2.85	0.45
4:H:148:LYS:NZ	4:H:149:ASP:OD2	2.48	0.45
4:H:152:PRO:O	4:H:205:HIS:NE2	2.34	0.45
1:C:326:ALA:C	1:C:331:ASN:HD22	2.24	0.45
1:C:345:HIS:HD2	1:C:357:THR:OG1	1.85	0.45
1:G:363:ILE:CG1	1:G:395:GLN:HB3	2.46	0.45
2:B:180:LYS:HD3	2:B:181:PHE:CE2	2.52	0.45
4:H:36:TRP:HD1	4:H:72:ILE:HD11	1.82	0.45
3:E:92:CYS:O	3:E:103:GLY:N	2.49	0.45
3:J:38:HIS:HD1	3:J:54:LEU:H	1.64	0.45
3:L:117:PRO:HD3	3:L:202:HIS:CD2	2.51	0.45
4:H:33:TYR:C	4:H:34:LEU:HD12	2.41	0.45
1:A:346:SER:HB2	1:A:352:ALA:HA	1.98	0.45
4:F:160:ASN:HB2	4:F:163:ALA:HB3	1.97	0.45
4:F:175:LEU:HB3	4:F:181:TYR:CE1	2.51	0.45
4:F:189:VAL:HG11	4:F:199:TYR:CE2	2.50	0.45
3:J:139:LEU:HD22	4:K:186:VAL:HG11	1.96	0.45
4:H:29:PHE:HE2	4:H:76:ASP:HA	1.81	0.45
4:H:32:TYR:CG	4:H:100:ARG:HD3	2.52	0.45
3:E:13:VAL:HG11	3:E:19:ALA:HB2	1.98	0.45
3:E:54:LEU:O	3:E:56:SER:N	2.47	0.45
1:G:313:GLN:NE2	2:I:188:LYS:HD3	2.32	0.45
3:J:47:PRO:HA	3:J:48:PRO:HD2	1.82	0.45
3:J:90:TYR:HE2	3:J:108:LEU:HD22	1.81	0.45
4:K:32:TYR:CD1	4:K:100:ARG:HD3	2.52	0.45
1:A:346:SER:CB	1:A:352:ALA:HB2	2.47	0.45
4:H:102:GLY:HA2	4:H:103:ASP:HA	1.76	0.45
3:L:13:VAL:HG11	3:L:19:ALA:HB2	1.99	0.45
3:E:208:PRO:O	3:E:209:VAL:HG22	2.16	0.45
1:G:345:HIS:CD2	1:G:345:HIS:H	2.35	0.45
4:K:175:LEU:H	4:K:175:LEU:HD23	1.82	0.45
4:F:51:ILE:HD11	4:F:81:LEU:HD13	1.99	0.44
1:G:440:ARG:HE	1:G:440:ARG:HB3	1.63	0.44
1:A:348:ARG:HA	3:L:31:SER:OG	2.18	0.44
4:H:66:VAL:HG13	4:H:70:PHE:HB2	1.99	0.44
4:H:116:VAL:O	4:H:118:SER:N	2.50	0.44
3:E:35:THR:HG22	3:E:37:MET:H	1.82	0.44
2:I:179:VAL:HG22	2:I:180:LYS:H	1.83	0.44
1:A:355:ASN:CB	1:A:356:ARG:HA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:59:GLU:O	3:E:62:VAL:HG12	2.17	0.44
3:E:93:GLN:HB2	3:E:102:PHE:HD1	1.83	0.44
3:J:147:GLU:CD	3:J:147:GLU:H	2.25	0.44
4:K:90:THR:O	4:K:93:THR:HG23	2.17	0.44
4:H:64:GLU:C	4:H:66:VAL:H	2.25	0.44
4:H:69:ARG:HD2	4:H:87:SER:O	2.17	0.44
3:E:23:CYS:SG	3:E:37:MET:HE1	2.57	0.44
4:H:100:ARG:O	4:H:105:PHE:HA	2.17	0.44
4:H:153:GLU:HG3	4:H:154:PRO:HA	2.00	0.44
4:F:156:THR:OG1	4:F:204:ASN:OD1	2.35	0.44
4:K:85:MET:HE1	4:K:96:TYR:HE2	1.83	0.44
4:H:110:GLN:CD	4:H:110:GLN:H	2.26	0.44
3:J:36:PHE:HB3	3:J:95:ASN:HB3	1.99	0.44
3:L:174:ASP:HA	1:C:307:GLN:HB2	2.00	0.44
3:L:202:HIS:CG	3:L:203:GLN:N	2.86	0.44
3:L:208:PRO:O	3:L:209:VAL:HG22	2.18	0.44
1:C:288:HIS:HA	1:C:289:PRO:HD3	1.88	0.44
4:F:153:GLU:CG	4:F:154:PRO:HA	2.48	0.44
4:F:202:ASN:HD22	4:F:213:ASP:HB3	1.82	0.44
3:L:66:PHE:CE1	3:L:79:ILE:HG12	2.53	0.44
4:H:20:LEU:HB2	4:H:83:LEU:HB3	2.00	0.44
1:C:242:LEU:HD22	1:C:265:LEU:HD23	1.98	0.44
3:E:124:PRO:HD3	3:E:136:VAL:HG22	2.00	0.44
1:A:313:GLN:HG3	2:B:187:TRP:CD2	2.53	0.44
1:A:346:SER:HB2	1:A:352:ALA:HB2	2.00	0.44
4:F:175:LEU:H	4:F:175:LEU:HD23	1.83	0.44
1:G:363:ILE:HG13	1:G:395:GLN:HB3	1.99	0.44
3:L:139:LEU:HD22	4:H:186:VAL:HG11	2.00	0.43
4:H:20:LEU:O	4:H:82:TYR:HA	2.18	0.43
1:C:269:ASP:OD1	1:C:271:ARG:HB2	2.17	0.43
3:E:53:TYR:HD1	3:E:54:LEU:HD13	1.82	0.43
4:F:69:ARG:HD2	4:F:87:SER:O	2.19	0.43
4:K:153:GLU:CG	4:K:154:PRO:HA	2.48	0.43
1:A:218:THR:HG22	1:A:362:PHE:HB3	2.00	0.43
3:J:112:ARG:NH1	3:J:115:ALA:HB2	2.33	0.43
4:K:173:ALA:HB2	4:K:183:LEU:HD23	2.01	0.43
4:H:35:ASN:OD1	4:H:50:ASP:HB3	2.18	0.43
4:F:102:GLY:HA2	4:F:103:ASP:HA	1.84	0.43
4:K:151:PHE:HA	4:K:152:PRO:HA	1.86	0.43
1:A:369:PRO:HG2	1:A:372:GLU:HG3	1.99	0.43
3:L:196:TYR:HB2	3:L:213:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:36:TRP:CE2	4:H:83:LEU:HB2	2.54	0.43
3:E:38:HIS:HD1	3:E:54:LEU:H	1.66	0.43
2:B:160:CYS:SG	2:B:173:LEU:HA	2.58	0.43
3:E:54:LEU:C	3:E:56:SER:H	2.27	0.43
3:E:98:ASP:HA	3:E:99:PRO:C	2.42	0.43
4:F:33:TYR:C	4:F:34:LEU:HD12	2.44	0.43
4:F:175:LEU:HB3	4:F:181:TYR:CD1	2.54	0.43
3:L:17:GLN:O	3:L:82:VAL:HG12	2.18	0.43
3:L:179:LEU:HD23	3:L:180:SER:N	2.34	0.43
3:J:66:PHE:CE1	3:J:79:ILE:HG12	2.54	0.43
4:K:9:GLY:HA3	4:K:112:THR:HG21	2.01	0.43
4:K:32:TYR:CG	4:K:100:ARG:HD3	2.53	0.43
4:F:173:ALA:HB2	4:F:183:LEU:HD23	2.01	0.43
3:J:47:PRO:HB3	4:K:109:GLY:O	2.19	0.43
4:K:49:GLY:HA3	4:K:62:TYR:HA	2.00	0.43
4:F:49:GLY:HA3	4:F:62:TYR:HA	2.00	0.43
4:H:139:GLY:O	4:H:191:SER:N	2.30	0.43
1:C:363:ILE:CG1	1:C:395:GLN:HB3	2.49	0.43
4:F:204:ASN:HB3	4:F:211:LYS:HG3	2.01	0.43
3:J:208:PRO:O	3:J:209:VAL:HG22	2.18	0.43
3:L:2:ILE:HD12	3:L:2:ILE:N	2.34	0.42
3:E:40:TYR:OH	4:F:105:PHE:HB2	2.18	0.42
4:F:194:LEU:HD23	4:F:194:LEU:HA	1.86	0.42
4:F:196:THR:OG1	4:F:197:GLN:N	2.51	0.42
1:A:218:THR:HG23	1:A:360:LEU:C	2.44	0.42
2:B:185:ARG:HA	2:B:186:PRO:HD2	1.93	0.42
3:E:180:SER:HB3	4:F:171:PHE:CZ	2.54	0.42
4:K:196:THR:OG1	4:K:197:GLN:N	2.52	0.42
3:J:70:GLY:HA3	3:J:75:PHE:CD1	2.54	0.42
1:A:218:THR:HG23	1:A:360:LEU:HB3	2.01	0.42
4:F:158:SER:OG	4:F:202:ASN:HB2	2.19	0.42
3:E:41:GLN:HG3	3:E:90:TYR:CE1	2.54	0.42
3:E:191:GLU:HG2	3:E:215:ARG:HH21	1.84	0.42
4:K:33:TYR:C	4:K:34:LEU:HD12	2.44	0.42
1:A:246:SER:HB3	1:A:308:PRO:HA	2.01	0.42
3:L:38:HIS:O	3:L:93:GLN:N	2.46	0.42
4:H:175:LEU:HB3	4:H:181:TYR:HE1	1.85	0.42
2:I:166:TYR:OH	2:I:185:ARG:HD2	2.19	0.42
3:J:2:ILE:N	3:J:2:ILE:HD12	2.35	0.42
4:K:102:GLY:HA2	4:K:103:ASP:HA	1.82	0.42
4:H:35:ASN:CG	4:H:105:PHE:HE1	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:85:MET:HE1	4:F:96:TYR:CE2	2.55	0.42
1:G:223:SER:HA	1:G:224:PRO:HD2	1.85	0.42
3:J:205:LEU:HB3	3:J:207:SER:O	2.20	0.42
4:H:151:PHE:HA	4:H:152:PRO:HA	1.82	0.42
3:E:153:LYS:HA	3:E:157:ALA:O	2.19	0.42
4:F:5:VAL:O	4:F:23:ALA:N	2.53	0.42
4:F:20:LEU:O	4:F:82:TYR:HA	2.20	0.42
3:L:14:SER:HA	3:L:111:LYS:HB2	2.02	0.42
1:C:390:ILE:HB	1:C:393:ASP:HB3	2.02	0.42
1:G:342:TRP:CZ2	1:G:360:LEU:HG	2.55	0.42
3:L:13:VAL:HG13	3:L:82:VAL:HG11	2.02	0.41
3:L:180:SER:O	3:L:180:SER:OG	2.35	0.41
4:H:52:ARG:HG2	4:H:59:GLU:O	2.19	0.41
1:G:219:ARG:HE	1:G:220:ARG:HG2	1.85	0.41
1:G:230:LEU:HD23	1:G:236:LEU:HA	2.02	0.41
1:A:275:LYS:HE3	3:J:80:ASN:OD1	2.20	0.41
2:D:179:VAL:HG22	2:D:180:LYS:H	1.85	0.41
1:A:271:ARG:HH11	1:A:358:PHE:HD2	1.68	0.41
3:L:39:TRP:CD2	3:L:77:LEU:HB2	2.55	0.41
4:F:191:SER:O	4:F:194:LEU:HB2	2.20	0.41
1:A:291:TYR:HA	1:A:298:ASN:HB2	2.01	0.41
1:A:440:ARG:HE	1:A:440:ARG:HB3	1.59	0.41
4:H:34:LEU:CD2	4:H:81:LEU:HB2	2.51	0.41
3:J:180:SER:O	3:J:180:SER:OG	2.36	0.41
1:G:376:VAL:HG11	1:G:431:ASN:HA	2.01	0.41
4:K:217:GLU:HA	4:K:218:PRO:HD3	1.76	0.41
1:A:244:HIS:CG	1:A:245:PRO:HD2	2.56	0.41
1:C:363:ILE:HD12	1:C:363:ILE:HA	1.73	0.41
1:G:269:ASP:HB3	1:G:272:ARG:HB3	2.02	0.41
4:K:85:MET:HE1	4:K:96:TYR:CE2	2.55	0.41
1:A:269:ASP:HB3	1:A:272:ARG:HB3	2.03	0.41
1:A:271:ARG:HG3	1:A:358:PHE:CG	2.56	0.41
1:A:363:ILE:HD12	1:A:363:ILE:HA	1.71	0.41
3:L:18:ARG:HB2	1:C:275:LYS:HZ1	1.83	0.41
4:H:49:GLY:HA3	4:H:62:TYR:HA	2.02	0.41
4:H:175:LEU:HD23	4:H:175:LEU:H	1.85	0.41
1:G:430:HIS:NE2	3:J:54:LEU:HD22	2.35	0.41
3:J:177:TYR:C	3:J:178:SER:HG	2.25	0.41
1:A:252:ALA:O	1:A:255:MET:HB2	2.20	0.41
1:A:345:HIS:H	1:A:345:HIS:HD2	1.66	0.41
1:A:363:ILE:CG1	1:A:395:GLN:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:132:GLY:HA2	3:L:187:LYS:HD2	2.02	0.41
4:H:55:SER:C	4:H:57:ASN:H	2.29	0.41
4:H:90:THR:O	4:H:93:THR:HG23	2.21	0.41
4:H:205:HIS:CD2	4:H:207:PRO:HD2	2.56	0.41
1:C:244:HIS:ND1	1:C:247:TRP:HD1	2.19	0.41
4:K:5:VAL:HG12	4:K:110:GLN:NE2	2.35	0.41
1:A:355:ASN:HB2	1:A:356:ARG:HA	2.02	0.41
1:C:363:ILE:HD11	1:C:395:GLN:HG2	2.04	0.41
4:F:100:ARG:O	4:F:105:PHE:HA	2.20	0.41
3:J:41:GLN:HG3	3:J:90:TYR:CE1	2.52	0.41
1:C:218:THR:HG23	1:C:219:ARG:N	2.35	0.40
3:E:19:ALA:HB3	3:E:79:ILE:HB	2.03	0.40
3:J:168:THR:HG22	4:K:172:PRO:HD3	2.04	0.40
1:A:213:ILE:HG22	1:A:396:ASP:O	2.21	0.40
2:B:169:GLY:C	2:B:171:ASP:N	2.76	0.40
3:L:39:TRP:CZ3	3:L:92:CYS:HB3	2.55	0.40
3:L:128:GLN:O	3:L:131:SER:OG	2.38	0.40
4:H:175:LEU:HB3	4:H:181:TYR:CD1	2.57	0.40
4:H:196:THR:OG1	4:H:197:GLN:N	2.54	0.40
3:E:2:ILE:HD12	3:E:2:ILE:N	2.37	0.40
4:H:72:ILE:HG13	4:H:83:LEU:HD23	2.03	0.40
4:H:206:LYS:HB2	4:H:207:PRO:HD3	2.03	0.40
1:C:257:GLU:OE1	1:C:261:LEU:HD11	2.21	0.40
4:K:17:SER:HA	4:K:85:MET:HB2	2.03	0.40
4:K:194:LEU:HD23	4:K:194:LEU:HA	1.92	0.40
3:L:117:PRO:HD2	3:L:205:LEU:HD13	2.04	0.40
1:C:212:LEU:N	1:C:401:ASP:OD2	2.55	0.40
3:E:111:LYS:HA	3:E:144:TYR:OH	2.22	0.40
4:F:81:LEU:HD12	4:F:82:TYR:H	1.87	0.40
1:G:244:HIS:CG	1:G:245:PRO:HD2	2.57	0.40
1:G:244:HIS:ND1	1:G:247:TRP:HD1	2.19	0.40
3:J:130:LYS:HE3	3:J:130:LYS:HB3	1.95	0.40
4:K:88:LEU:HA	4:K:88:LEU:HD12	1.81	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)
3:E:216:GLY:O	1:G:216:LYS:NZ[7_655]	2.17	0.03

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	237/250 (95%)	219 (92%)	16 (7%)	2 (1%)	16	48
1	C	237/250 (95%)	220 (93%)	14 (6%)	3 (1%)	9	38
1	G	237/250 (95%)	217 (92%)	19 (8%)	1 (0%)	30	60
2	B	51/155 (33%)	44 (86%)	7 (14%)	0	100	100
2	D	51/155 (33%)	42 (82%)	9 (18%)	0	100	100
2	I	51/155 (33%)	43 (84%)	7 (14%)	1 (2%)	6	32
3	E	216/218 (99%)	194 (90%)	19 (9%)	3 (1%)	9	37
3	J	216/218 (99%)	192 (89%)	21 (10%)	3 (1%)	9	37
3	L	216/218 (99%)	193 (89%)	20 (9%)	3 (1%)	9	37
4	F	219/221 (99%)	186 (85%)	30 (14%)	3 (1%)	9	37
4	H	219/221 (99%)	187 (85%)	30 (14%)	2 (1%)	14	45
4	K	219/221 (99%)	186 (85%)	31 (14%)	2 (1%)	14	45
All	All	2169/2532 (86%)	1923 (89%)	223 (10%)	23 (1%)	11	42

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	ASN
4	H	117	SER
1	C	257	GLU
4	F	117	SER
4	K	117	SER
1	A	256	ASP
3	L	81	PRO
3	L	209	VAL
1	C	355	ASN
3	E	81	PRO
3	E	209	VAL
3	J	81	PRO

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Mol	Chain	Res	Type
3	J	209	VAL
3	L	101	THR
3	E	101	THR
3	J	101	THR
4	H	86	ASN
1	C	351	GLU
4	F	85	MET
4	F	86	ASN
1	G	355	ASN
2	I	186	PRO
4	K	86	ASN

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	206/215 (96%)	178 (86%)	28 (14%)	3	19
1	C	206/215 (96%)	182 (88%)	24 (12%)	5	24
1	G	206/215 (96%)	181 (88%)	25 (12%)	5	22
2	B	45/136 (33%)	39 (87%)	6 (13%)	4	20
2	D	45/136 (33%)	38 (84%)	7 (16%)	2	15
2	I	45/136 (33%)	41 (91%)	4 (9%)	9	33
3	E	189/189 (100%)	182 (96%)	7 (4%)	30	54
3	J	189/189 (100%)	179 (95%)	10 (5%)	20	46
3	L	189/189 (100%)	182 (96%)	7 (4%)	30	54
4	F	188/188 (100%)	176 (94%)	12 (6%)	16	43
4	H	188/188 (100%)	179 (95%)	9 (5%)	23	48
4	K	188/188 (100%)	179 (95%)	9 (5%)	23	48
All	All	1884/2184 (86%)	1736 (92%)	148 (8%)	11	37

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	LEU
1	A	218	THR
1	A	220	ARG
1	A	227	VAL
1	A	235	LYS
1	A	245	PRO
1	A	255	MET
1	A	261	LEU
1	A	262	LEU
1	A	270	LEU
1	A	271	ARG
1	A	273	TRP
1	A	287	VAL
1	A	294	SER
1	A	305	LEU
1	A	311	LEU
1	A	316	VAL
1	A	325	LEU
1	A	338	LEU
1	A	340	THR
1	A	345	HIS
1	A	346	SER
1	A	357	THR
1	A	363	ILE
1	A	368	VAL
1	A	386	LEU
1	A	406	MET
1	A	429	LEU
2	B	142	LEU
2	B	164	PRO
2	B	168	LEU
2	B	170	ASP
2	B	174	GLN
2	B	187	TRP
3	L	3	VAL
3	L	137	VAL
3	L	147	GLU
3	L	154	VAL
3	L	159	GLN
3	L	209	VAL
3	L	210	THR
4	H	53	LEU
4	H	61	HIS

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Mol	Chain	Res	Type
4	H	66	VAL
4	H	89	LYS
4	H	110	GLN
4	H	115	THR
4	H	129	LEU
4	H	209	ASN
4	H	216	VAL
1	C	212	LEU
1	C	218	THR
1	C	220	ARG
1	C	235	LYS
1	C	245	PRO
1	C	255	MET
1	C	265	LEU
1	C	270	LEU
1	C	271	ARG
1	C	280	LEU
1	C	287	VAL
1	C	294	SER
1	C	305	LEU
1	C	311	LEU
1	C	316	VAL
1	C	325	LEU
1	C	338	LEU
1	C	340	THR
1	C	346	SER
1	C	360	LEU
1	C	363	ILE
1	C	368	VAL
1	C	386	LEU
1	C	406	MET
2	D	158	ARG
2	D	164	PRO
2	D	168	LEU
2	D	170	ASP
2	D	174	GLN
2	D	185	ARG
2	D	186	PRO
3	E	3	VAL
3	E	76	THR
3	E	137	VAL
3	E	147	GLU

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Mol	Chain	Res	Type
3	E	154	VAL
3	E	162	ASN
3	E	209	VAL
4	F	51	ILE
4	F	53	LEU
4	F	61	HIS
4	F	66	VAL
4	F	89	LYS
4	F	92	ASP
4	F	110	GLN
4	F	129	LEU
4	F	135	SER
4	F	168	VAL
4	F	209	ASN
4	F	216	VAL
1	G	212	LEU
1	G	218	THR
1	G	220	ARG
1	G	227	VAL
1	G	235	LYS
1	G	245	PRO
1	G	255	MET
1	G	257	GLU
1	G	270	LEU
1	G	271	ARG
1	G	273	TRP
1	G	287	VAL
1	G	294	SER
1	G	305	LEU
1	G	311	LEU
1	G	338	LEU
1	G	340	THR
1	G	344	TYR
1	G	345	HIS
1	G	347	SER
1	G	363	ILE
1	G	368	VAL
1	G	376	VAL
1	G	386	LEU
1	G	406	MET
2	I	164	PRO
2	I	168	LEU

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Mol	Chain	Res	Type
2	I	170	ASP
2	I	185	ARG
3	J	3	VAL
3	J	119	VAL
3	J	137	VAL
3	J	146	ARG
3	J	147	GLU
3	J	154	VAL
3	J	162	ASN
3	J	185	LEU
3	J	209	VAL
3	J	210	THR
4	K	5	VAL
4	K	53	LEU
4	K	66	VAL
4	K	89	LYS
4	K	110	GLN
4	K	115	THR
4	K	129	LEU
4	K	168	VAL
4	K	216	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	GLN
1	A	345	HIS
1	A	395	GLN
3	L	93	GLN
3	L	96	ASN
4	H	110	GLN
1	C	307	GLN
3	E	41	GLN
3	E	80	ASN
3	E	96	ASN
4	F	56	ASN
4	F	169	HIS
4	F	176	GLN
1	G	313	GLN
1	G	331	ASN
1	G	384	ASN
1	G	395	GLN

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Mol	Chain	Res	Type
3	J	93	GLN
3	J	96	ASN
3	J	214	ASN
4	K	13	GLN

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	239/250 (95%)	0.62	11 (4%) 37 24	51, 88, 109, 127	0
1	C	239/250 (95%)	0.70	13 (5%) 31 21	53, 97, 122, 134	0
1	G	239/250 (95%)	0.73	8 (3%) 49 31	51, 93, 113, 125	0
2	B	53/155 (34%)	0.66	4 (7%) 20 15	30, 103, 126, 133	0
2	D	53/155 (34%)	0.97	9 (16%) 4 5	30, 149, 185, 193	0
2	I	53/155 (34%)	0.75	4 (7%) 20 15	30, 122, 156, 166	0
3	E	218/218 (100%)	0.59	7 (3%) 50 31	86, 96, 113, 118	0
3	J	218/218 (100%)	0.83	15 (6%) 23 17	90, 114, 199, 225	0
3	L	218/218 (100%)	0.41	5 (2%) 61 38	72, 87, 131, 153	0
4	F	221/221 (100%)	0.64	13 (5%) 28 19	92, 114, 137, 143	0
4	H	221/221 (100%)	0.53	7 (3%) 50 31	78, 101, 129, 147	0
4	K	221/221 (100%)	0.95	17 (7%) 19 15	99, 147, 172, 189	0
All	All	2193/2532 (86%)	0.68	113 (5%) 33 22	30, 101, 163, 225	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	218	CYS	8.1
4	K	138	GLY	6.0
1	A	281	ASP	4.1
3	L	33	GLY	3.9
4	F	117	SER	3.8
4	H	136	THR	3.7
4	H	221	CYS	3.6
3	J	121	ILE	3.5
4	K	137	SER	3.5
4	F	138	GLY	3.5
4	F	137	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	136	SER	3.2
3	E	127	GLU	3.2
1	G	273	TRP	3.1
4	K	102	GLY	3.1
4	F	136	THR	3.1
1	C	344	TYR	3.0
3	E	33	GLY	3.0
3	J	129	LEU	3.0
4	K	185	SER	3.0
1	G	351	GLU	3.0
4	K	140	THR	3.0
4	K	136	THR	3.0
1	C	234	LYS	2.9
2	D	187	TRP	2.9
3	J	28	SER	2.9
1	C	278	LEU	2.9
4	K	35	ASN	2.9
1	A	431	ASN	2.8
2	I	187	TRP	2.8
1	C	333	ALA	2.8
1	G	336	GLU	2.8
4	K	170	THR	2.8
3	E	126	ASP	2.7
3	E	141	ASN	2.7
3	J	182	THR	2.7
1	A	344	TYR	2.6
1	A	351	GLU	2.6
2	D	138	LEU	2.6
4	K	71	THR	2.6
3	J	138	CYS	2.5
2	D	137	PHE	2.5
1	G	346	SER	2.5
2	D	168	LEU	2.5
4	F	59	GLU	2.5
1	C	431	ASN	2.5
1	A	279	ASP	2.5
1	A	234	LYS	2.5
4	K	139	GLY	2.5
2	D	188	LYS	2.5
1	C	273	TRP	2.5
1	C	272	ARG	2.5
1	G	356	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
3	J	167	VAL	2.5
3	J	159	GLN	2.4
2	B	188	LYS	2.4
4	H	68	GLY	2.4
1	C	426	CYS	2.4
4	F	135	SER	2.4
1	A	348	ARG	2.4
2	I	139	ASN	2.3
4	F	220	SER	2.3
3	L	104	GLN	2.3
4	K	9	GLY	2.3
3	L	218	CYS	2.3
4	F	50	ASP	2.3
3	J	190	TYR	2.3
4	F	31	ASN	2.3
2	I	136	SER	2.3
1	C	399	GLU	2.3
2	B	136	SER	2.3
4	H	137	SER	2.3
2	B	187	TRP	2.2
3	J	67	SER	2.2
4	F	219	LYS	2.2
4	H	98	CYS	2.2
3	E	104	GLN	2.2
4	K	133	SER	2.2
1	G	450	ARG	2.2
2	I	137	PHE	2.2
1	A	439	SER	2.2
3	J	211	LYS	2.2
4	H	219	LYS	2.2
4	F	213	ASP	2.2
3	J	123	PRO	2.2
1	A	261	LEU	2.2
4	K	221	CYS	2.1
1	C	385	MET	2.1
3	J	41	GLN	2.1
4	K	117	SER	2.1
1	G	411	HIS	2.1
1	G	426	CYS	2.1
4	F	221	CYS	2.1
2	B	137	PHE	2.1
4	K	216	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	345	HIS	2.1
1	A	342	TRP	2.1
2	D	170	ASP	2.1
1	C	357	THR	2.1
3	E	101	THR	2.1
3	J	133	THR	2.1
4	F	71	THR	2.1
3	J	181	SER	2.1
4	K	135	SER	2.1
1	A	298	ASN	2.1
1	C	275	LYS	2.0
3	L	127	GLU	2.0
4	H	135	SER	2.0
3	J	126	ASP	2.0
2	D	186	PRO	2.0
3	L	210	THR	2.0
2	D	173	LEU	2.0
4	K	182	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.