



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:59 AM UTC

PDB ID : 2X7L / pdb_00002x7l
Title : Implications of the HIV-1 Rev dimer structure at 3.2Å resolution for multi-
meric binding to the Rev response element
Authors : DiMattia, M.A.; Watts, N.R.; Stahl, S.J.; Rader, C.; Wingfield, P.T.; Stuart,
D.I.; Steven, A.C.; Grimes, J.M.
Deposited on : 2010-03-01
Resolution : 3.17 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

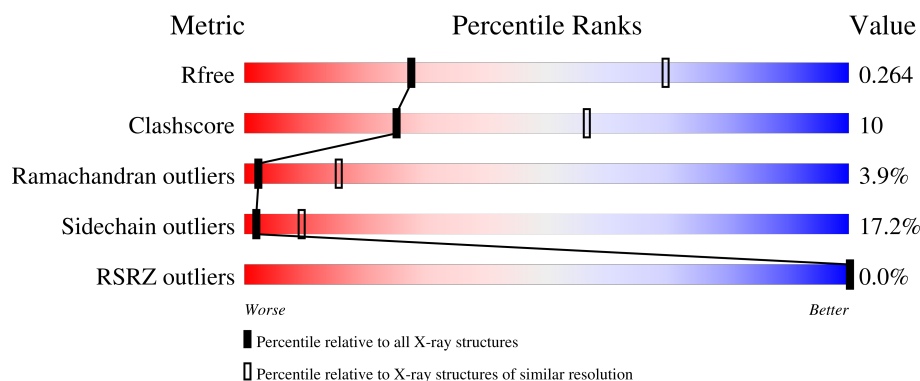
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 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.



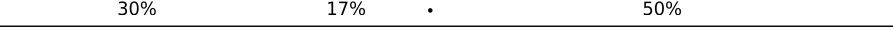
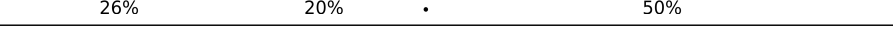
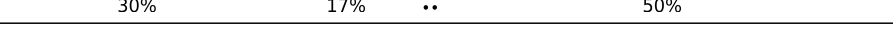
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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	231	
1	C	231	
1	E	231	
1	G	231	
1	H	231	

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Mol	Chain	Length	Quality of chain
1	J	231	 62% 28% 6% .
2	B	217	 62% 29% 8% .
2	D	217	 61% 28% 8% .
2	F	217	 60% 29% 9% .
2	I	217	 61% 29% 8% .
2	K	217	 61% 29% 10% .
2	L	217	 61% 29% 8% .
3	M	115	 31% 17% . 50%
3	N	115	 30% 17% . 50%
3	O	115	 30% 17% . 50%
3	P	115	 30% 17% . 50%
3	Q	115	 26% 20% . 50%
3	R	115	 30% 17% .. 50%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22554 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 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	1
			1628	1033	267	323	5			
1	C	221	Total	C	N	O	S	0	0	1
			1628	1033	267	323	5			
1	E	221	Total	C	N	O	S	0	0	1
			1628	1033	267	323	5			
1	G	221	Total	C	N	O	S	0	0	1
			1628	1033	267	323	5			
1	H	221	Total	C	N	O	S	0	0	1
			1628	1033	267	323	5			
1	J	221	Total	C	N	O	S	0	0	1
			1628	1033	267	323	5			

- Molecule 2 is a protein called FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1639	1026	269	337	7			
2	D	217	Total	C	N	O	S	0	0	0
			1639	1026	269	337	7			
2	F	217	Total	C	N	O	S	0	0	0
			1639	1026	269	337	7			
2	I	217	Total	C	N	O	S	0	0	0
			1639	1026	269	337	7			
2	K	217	Total	C	N	O	S	0	0	0
			1639	1026	269	337	7			
2	L	217	Total	C	N	O	S	0	0	0
			1639	1026	269	337	7			

- Molecule 3 is a protein called PROTEIN REV.

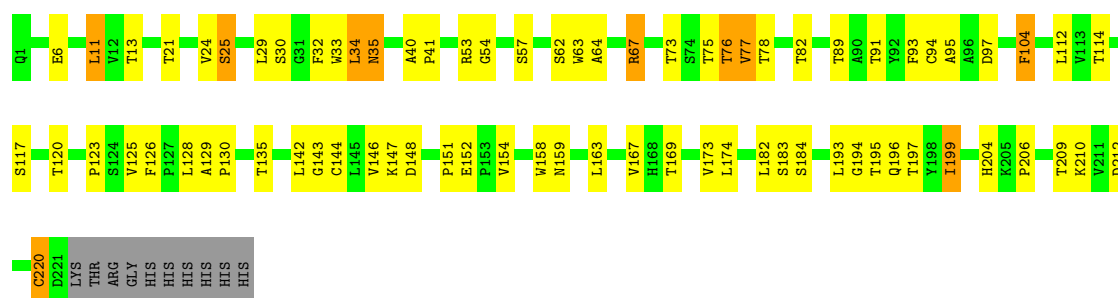
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	57	Total 492	C 303	N 105	O 84	0	0	0
3	N	57	Total 492	C 303	N 105	O 84	0	0	0
3	O	57	Total 492	C 303	N 105	O 84	0	0	0
3	P	57	Total 492	C 303	N 105	O 84	0	0	0
3	Q	57	Total 492	C 303	N 105	O 84	0	0	0
3	R	57	Total 492	C 303	N 105	O 84	0	0	0

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.

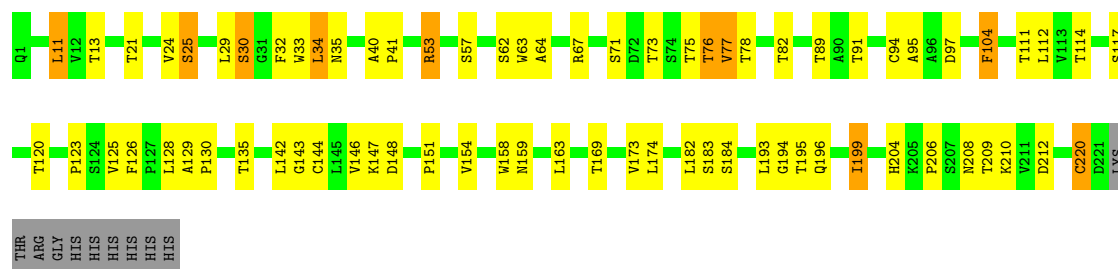
• Molecule 1: FAB HEAVY CHAIN

Chain A: 



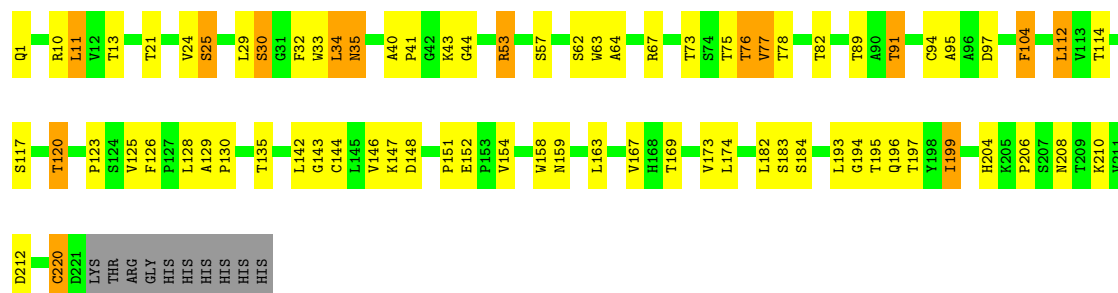
• Molecule 1: FAB HEAVY CHAIN

Chain C: 

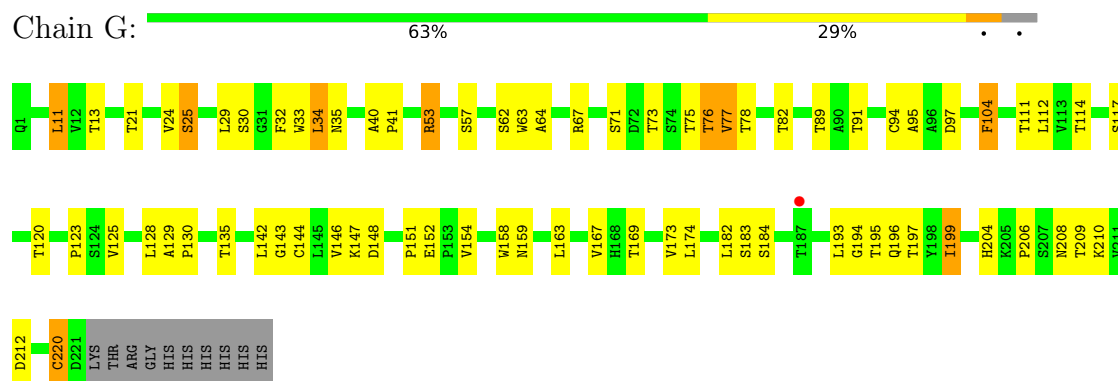


• Molecule 1: FAB HEAVY CHAIN

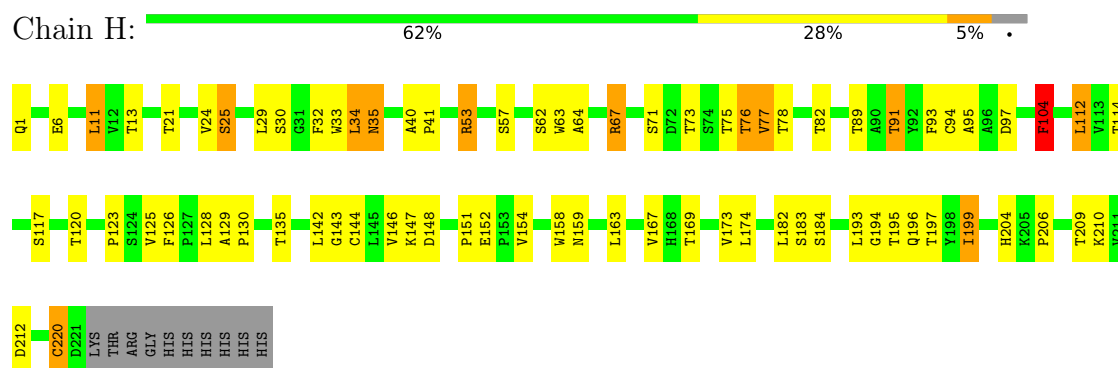
Chain E: 



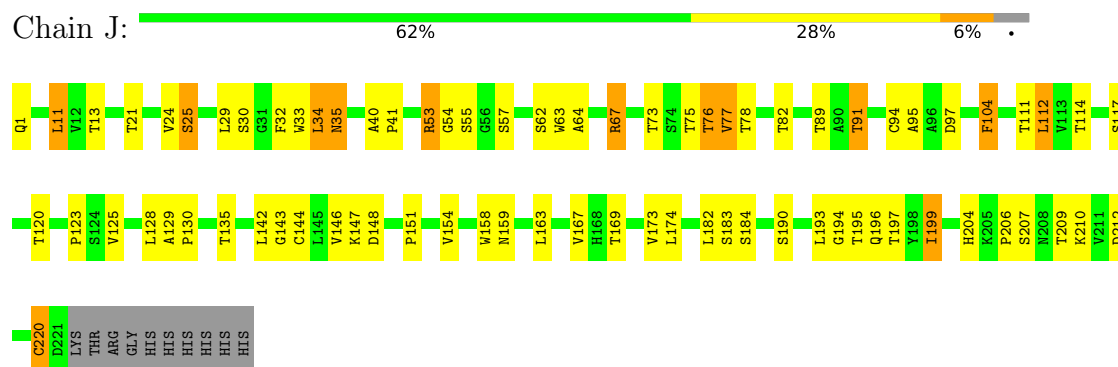
• Molecule 1: FAB HEAVY CHAIN



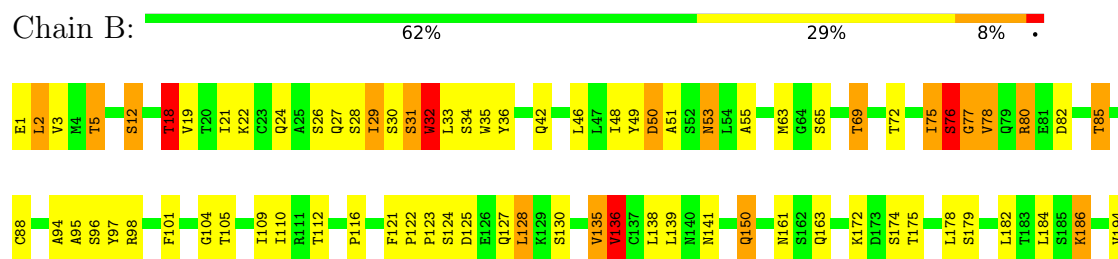
• Molecule 1: FAB HEAVY CHAIN



• Molecule 1: FAB HEAVY CHAIN

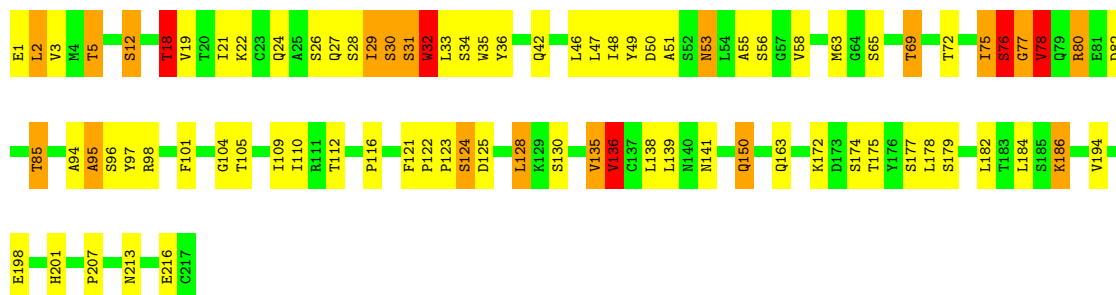


• Molecule 2: FAB LIGHT CHAIN

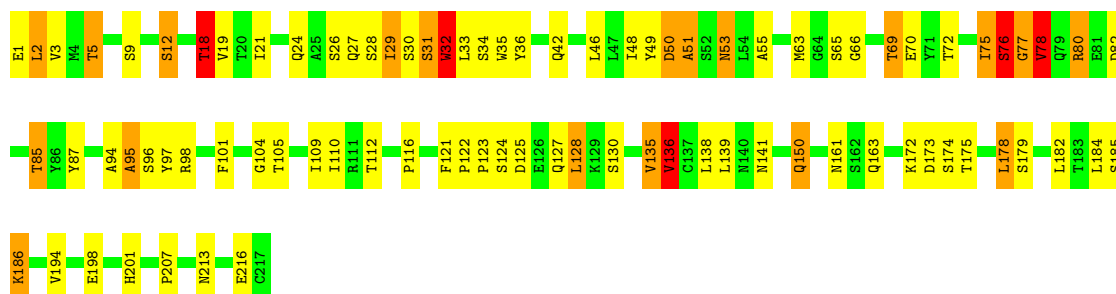




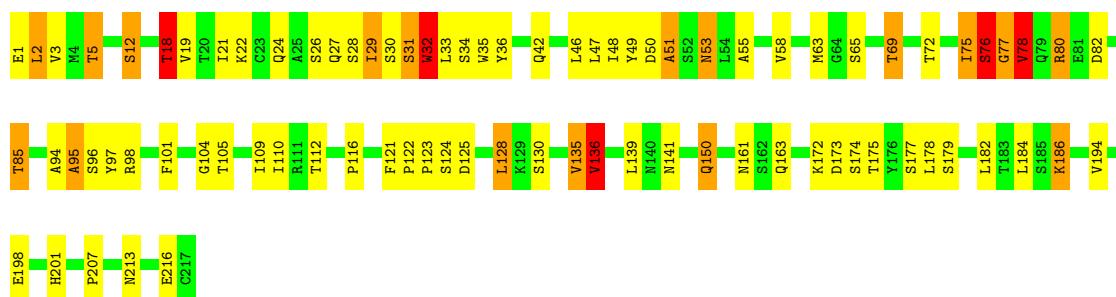
• Molecule 2: FAB LIGHT CHAIN

Chain D: 

• Molecule 2: FAB LIGHT CHAIN

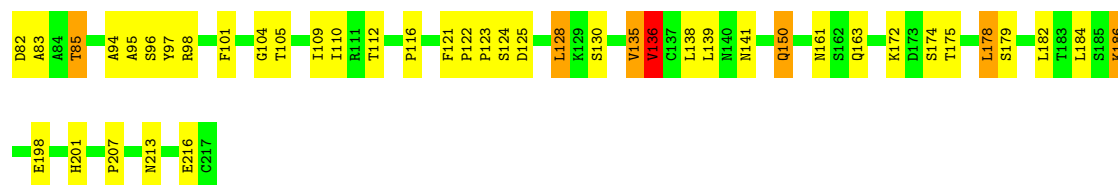
Chain F: 

• Molecule 2: FAB LIGHT CHAIN

Chain I: 

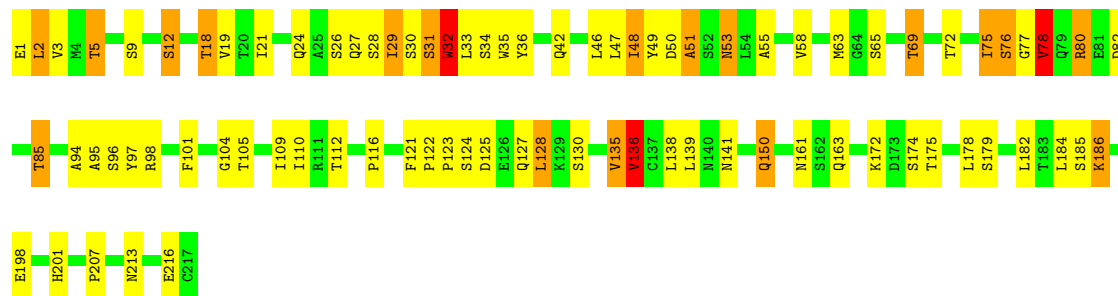
• Molecule 2: FAB LIGHT CHAIN

Chain K: 



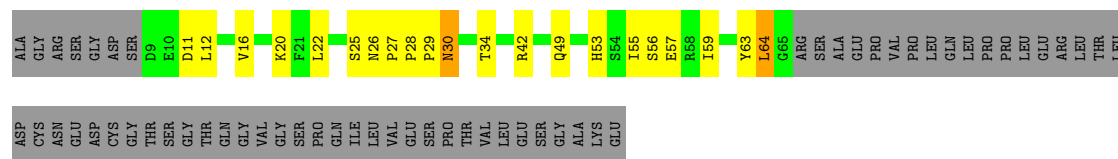
• Molecule 2: FAB LIGHT CHAIN

Chain L: 61% 29% 8% .



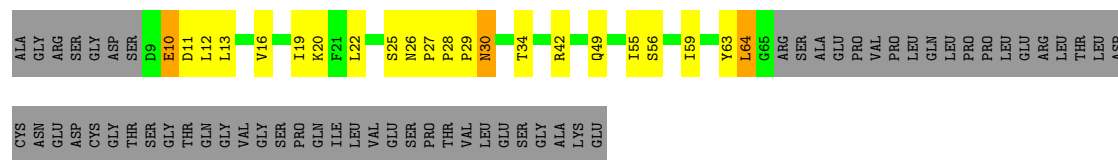
• Molecule 3: PROTEIN REV

Chain M: 31% 17% . 50%



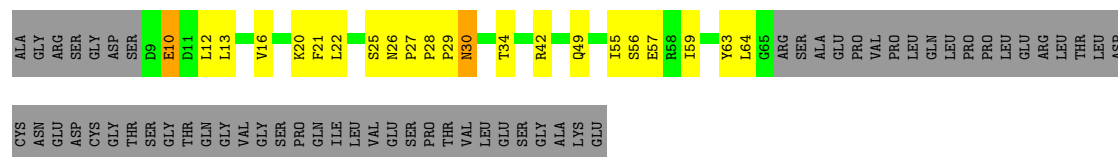
• Molecule 3: PROTEIN REV

Chain N: 30% 17% . 50%



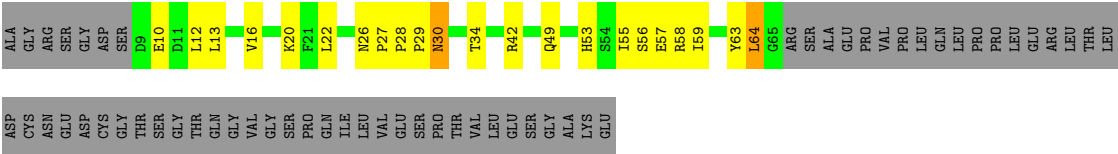
• Molecule 3: PROTEIN REV

Chain O: 30% 17% . 50%

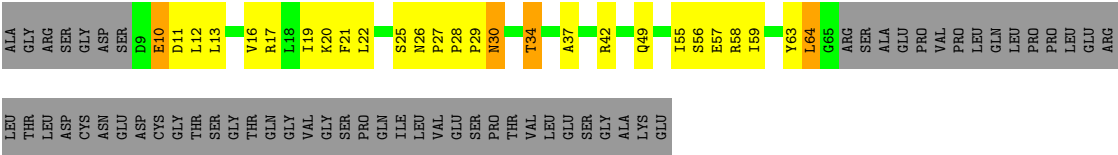
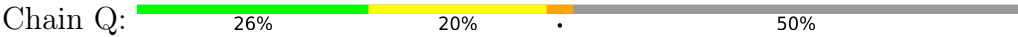


• Molecule 3: PROTEIN REV

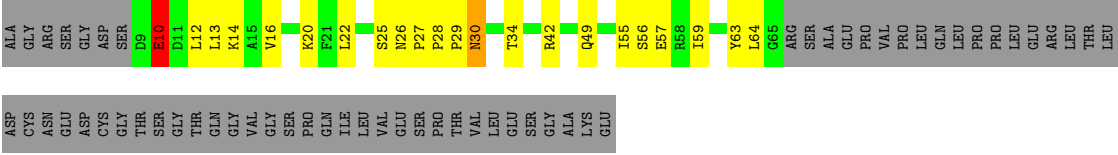
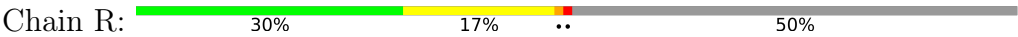
Chain P: 30% 17% . 50%



• Molecule 3: PROTEIN REV



• Molecule 3: PROTEIN REV



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.68Å 87.69Å 176.33Å 94.86° 95.50° 104.60°	Depositor
Resolution (Å)	48.78 – 3.17 48.78 – 3.17	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.78-3.17) 97.6 (48.78-3.17)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.234 , 0.250 0.251 , 0.264	Depositor DCC
R_{free} test set	4187 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	85.2	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 101.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.327 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22554	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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	0.95	1/1671 (0.1%)	1.44	14/2288 (0.6%)
1	C	0.77	1/1671 (0.1%)	1.39	18/2288 (0.8%)
1	E	0.91	1/1671 (0.1%)	1.43	20/2288 (0.9%)
1	G	0.78	1/1671 (0.1%)	1.39	17/2288 (0.7%)
1	H	0.87	1/1671 (0.1%)	1.41	17/2288 (0.7%)
1	J	0.84	1/1671 (0.1%)	1.40	19/2288 (0.8%)
2	B	0.95	1/1675 (0.1%)	1.43	22/2278 (1.0%)
2	D	0.82	0/1675	1.40	23/2278 (1.0%)
2	F	0.94	2/1675 (0.1%)	1.43	27/2278 (1.2%)
2	I	0.81	1/1675 (0.1%)	1.39	25/2278 (1.1%)
2	K	0.89	1/1675 (0.1%)	1.41	19/2278 (0.8%)
2	L	0.92	2/1675 (0.1%)	1.41	22/2278 (1.0%)
3	M	0.83	1/501 (0.2%)	1.51	6/672 (0.9%)
3	N	0.90	3/501 (0.6%)	1.48	4/672 (0.6%)
3	O	0.95	1/501 (0.2%)	1.54	6/672 (0.9%)
3	P	0.85	1/501 (0.2%)	1.51	5/672 (0.7%)
3	Q	0.85	1/501 (0.2%)	1.47	6/672 (0.9%)
3	R	0.91	2/501 (0.4%)	1.51	8/672 (1.2%)
All	All	0.88	22/23082 (0.1%)	1.42	278/31428 (0.9%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	95	ALA	CA-C	5.86	1.61	1.53
3	N	26	ASN	CA-CB	5.72	1.56	1.52
1	E	220	CYS	C-N	-5.67	1.25	1.33
3	N	26	ASN	CG-OD1	5.66	1.34	1.23
2	K	161	ASN	CG-OD1	5.64	1.34	1.23
3	Q	26	ASN	CG-OD1	5.63	1.34	1.23
1	C	220	CYS	C-N	-5.62	1.25	1.33
1	A	220	CYS	C-N	-5.60	1.25	1.33
1	H	220	CYS	C-N	-5.60	1.25	1.33
1	G	220	CYS	C-N	-5.59	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	26	ASN	CA-CB	5.57	1.56	1.52
2	L	161	ASN	CG-OD1	5.55	1.34	1.23
3	O	26	ASN	CG-OD1	5.55	1.34	1.23
3	R	26	ASN	CG-OD1	5.54	1.34	1.23
1	J	220	CYS	C-N	-5.48	1.25	1.33
2	F	161	ASN	CG-OD1	5.21	1.33	1.23
3	M	26	ASN	CG-OD1	5.20	1.33	1.23
2	I	161	ASN	CG-OD1	5.07	1.33	1.23
2	B	161	ASN	CG-OD1	5.06	1.33	1.23
3	P	26	ASN	CG-OD1	5.06	1.33	1.23
3	N	26	ASN	CA-C	5.04	1.57	1.53
2	L	48	ILE	CA-CB	5.01	1.60	1.54

All (278) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	31	SER	N-CA-C	-8.28	103.28	112.72
2	L	85	THR	CB-CA-C	7.98	123.15	109.51
2	L	31	SER	N-CA-C	-7.88	103.74	112.72
2	K	85	THR	CB-CA-C	7.87	122.97	109.51
2	K	31	SER	N-CA-C	-7.81	103.82	112.72
2	I	31	SER	N-CA-C	-7.81	103.82	112.72
2	D	31	SER	N-CA-C	-7.79	103.84	112.72
2	F	31	SER	N-CA-C	-7.71	103.77	113.02
2	B	85	THR	CB-CA-C	7.60	122.51	109.51
2	F	85	THR	CB-CA-C	7.58	122.47	109.51
2	D	85	THR	CB-CA-C	7.57	122.45	109.51
2	I	85	THR	CB-CA-C	7.49	122.31	109.51
2	B	136	VAL	N-CA-C	7.32	118.35	108.11
2	F	136	VAL	N-CA-C	7.02	117.94	108.11
1	H	53	ARG	N-CA-C	6.89	119.43	111.02
1	J	53	ARG	N-CA-C	6.89	119.43	111.02
2	I	136	VAL	N-CA-C	6.88	117.75	108.11
1	C	53	ARG	N-CA-C	6.86	119.39	111.02
2	D	136	VAL	N-CA-C	6.80	117.64	108.11
1	E	53	ARG	N-CA-C	6.77	119.28	111.02
2	L	136	VAL	N-CA-C	6.67	117.45	108.11
2	K	136	VAL	N-CA-C	6.58	117.32	108.11
1	G	53	ARG	N-CA-C	6.57	119.03	111.02
1	E	25	SER	N-CA-C	6.51	118.68	107.93
1	A	25	SER	N-CA-C	6.50	118.65	107.93
1	A	210	LYS	CA-C-N	6.40	129.32	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	LYS	C-N-CA	6.40	129.32	120.49
1	H	25	SER	N-CA-C	6.35	118.41	107.93
1	J	25	SER	N-CA-C	6.30	118.33	107.93
2	B	80	ARG	CA-C-N	6.27	128.59	120.44
2	B	80	ARG	C-N-CA	6.27	128.59	120.44
2	K	104	GLY	N-CA-C	6.27	120.58	112.68
2	K	75	ILE	N-CA-CB	6.27	118.66	111.39
1	C	25	SER	N-CA-C	6.21	118.18	107.93
2	D	75	ILE	N-CA-CB	6.21	118.59	111.39
1	E	210	LYS	CA-C-N	6.19	129.04	120.49
1	E	210	LYS	C-N-CA	6.19	129.04	120.49
1	A	125	VAL	N-CA-C	6.19	116.53	107.37
2	L	75	ILE	N-CA-CB	6.16	118.53	111.39
2	I	75	ILE	N-CA-CB	6.15	118.52	111.39
2	B	5	THR	CB-CA-C	6.12	121.81	111.41
2	B	104	GLY	CA-C-N	6.12	129.89	121.33
2	B	104	GLY	C-N-CA	6.12	129.89	121.33
1	A	77	VAL	N-CA-C	6.11	117.62	109.37
2	F	104	GLY	N-CA-C	6.07	120.33	112.68
2	F	75	ILE	N-CA-CB	6.07	118.43	111.39
1	G	25	SER	N-CA-C	6.04	117.90	107.93
2	D	104	GLY	N-CA-C	6.04	120.29	112.68
1	E	63	TRP	CA-C-N	6.03	128.36	120.28
1	E	63	TRP	C-N-CA	6.03	128.36	120.28
2	L	104	GLY	N-CA-C	6.03	120.28	112.68
1	C	77	VAL	N-CA-C	6.01	117.48	109.37
1	E	77	VAL	N-CA-C	5.99	117.45	109.37
1	E	112	LEU	N-CA-C	5.97	118.03	108.41
1	H	77	VAL	N-CA-C	5.97	117.43	109.37
1	G	64	ALA	N-CA-C	5.96	117.78	111.28
1	H	125	VAL	N-CA-C	5.94	116.17	107.37
1	J	77	VAL	N-CA-C	5.92	117.36	109.37
2	I	104	GLY	N-CA-C	5.92	120.14	112.68
2	B	75	ILE	N-CA-CB	5.88	118.22	111.39
1	G	77	VAL	N-CA-C	5.86	117.28	109.37
1	C	63	TRP	CA-C-N	5.86	128.13	120.28
1	C	63	TRP	C-N-CA	5.86	128.13	120.28
1	H	35	ASN	CA-CB-CG	5.85	118.45	112.60
1	A	35	ASN	CA-CB-CG	5.85	118.45	112.60
2	F	80	ARG	CA-C-N	5.85	128.43	120.54
2	F	80	ARG	C-N-CA	5.85	128.43	120.54
2	B	72	THR	N-CA-C	5.85	118.64	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	104	GLY	CA-C-N	5.84	129.50	121.33
2	F	104	GLY	C-N-CA	5.84	129.50	121.33
2	D	80	ARG	CA-C-N	5.83	128.02	120.44
2	D	80	ARG	C-N-CA	5.83	128.02	120.44
1	C	64	ALA	N-CA-C	5.82	117.62	111.28
1	J	210	LYS	CA-C-N	5.79	128.47	120.49
1	J	210	LYS	C-N-CA	5.79	128.47	120.49
2	L	5	THR	CB-CA-C	5.78	121.24	111.41
1	H	64	ALA	N-CA-C	5.77	117.57	111.28
2	F	5	THR	CB-CA-C	5.77	121.22	111.41
1	H	210	LYS	CA-C-N	5.72	128.39	120.49
1	H	210	LYS	C-N-CA	5.72	128.39	120.49
1	A	63	TRP	CA-C-N	5.70	127.91	120.28
1	A	63	TRP	C-N-CA	5.70	127.91	120.28
2	L	80	ARG	CA-C-N	5.69	128.22	120.54
2	L	80	ARG	C-N-CA	5.69	128.22	120.54
1	J	64	ALA	N-CA-C	5.69	117.48	111.28
1	G	63	TRP	CA-C-N	5.69	127.90	120.28
1	G	63	TRP	C-N-CA	5.69	127.90	120.28
2	D	72	THR	N-CA-C	5.69	118.37	108.76
2	K	80	ARG	CA-C-N	5.67	128.20	120.54
2	K	80	ARG	C-N-CA	5.67	128.20	120.54
1	J	125	VAL	N-CA-C	5.65	115.73	107.37
1	C	210	LYS	CA-C-N	5.61	128.23	120.49
1	C	210	LYS	C-N-CA	5.61	128.23	120.49
2	F	72	THR	N-CA-C	5.60	118.22	108.76
1	J	35	ASN	CA-CB-CG	5.60	118.20	112.60
2	F	101	PHE	CA-C-N	5.59	126.15	119.94
2	F	101	PHE	C-N-CA	5.59	126.15	119.94
2	K	5	THR	CB-CA-C	5.59	120.92	111.41
2	K	69	THR	CB-CA-C	5.58	119.35	109.75
1	J	63	TRP	CA-C-N	5.56	127.73	120.28
1	J	63	TRP	C-N-CA	5.56	127.73	120.28
2	I	5	THR	CB-CA-C	5.56	120.86	111.41
2	I	104	GLY	CA-C-N	5.56	129.11	121.33
2	I	104	GLY	C-N-CA	5.56	129.11	121.33
2	F	124	SER	CA-C-N	5.54	128.02	120.54
2	F	124	SER	C-N-CA	5.54	128.02	120.54
2	F	18	THR	CB-CA-C	5.54	119.35	109.38
1	H	63	TRP	CA-C-N	5.54	127.70	120.28
1	H	63	TRP	C-N-CA	5.54	127.70	120.28
1	H	135	THR	N-CA-C	5.54	117.77	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	56	SER	CA-C-N	5.54	128.49	120.79
3	P	56	SER	C-N-CA	5.54	128.49	120.79
1	G	210	LYS	CA-C-N	5.54	128.13	120.49
1	G	210	LYS	C-N-CA	5.54	128.13	120.49
2	B	124	SER	CA-C-N	5.53	128.01	120.54
2	B	124	SER	C-N-CA	5.53	128.01	120.54
2	L	124	SER	CA-C-N	5.53	128.01	120.54
2	L	124	SER	C-N-CA	5.53	128.01	120.54
1	E	125	VAL	N-CA-C	5.53	115.55	107.37
2	I	124	SER	CA-C-N	5.52	127.99	120.54
2	I	124	SER	C-N-CA	5.52	127.99	120.54
2	D	124	SER	CA-C-N	5.52	127.99	120.54
2	D	124	SER	C-N-CA	5.52	127.99	120.54
1	J	135	THR	N-CA-C	5.52	117.73	108.96
2	B	101	PHE	CA-C-N	5.51	126.22	119.99
2	B	101	PHE	C-N-CA	5.51	126.22	119.99
2	I	72	THR	N-CA-C	5.49	118.05	108.76
1	J	190	SER	CA-C-N	5.47	127.55	120.44
1	J	190	SER	C-N-CA	5.47	127.55	120.44
2	K	124	SER	CA-C-N	5.47	127.92	120.54
2	K	124	SER	C-N-CA	5.47	127.92	120.54
2	D	101	PHE	CA-C-N	5.46	126.01	119.94
2	D	101	PHE	C-N-CA	5.46	126.01	119.94
2	K	104	GLY	CA-C-N	5.46	128.98	121.33
2	K	104	GLY	C-N-CA	5.46	128.98	121.33
2	I	80	ARG	CA-C-N	5.45	127.90	120.54
2	I	80	ARG	C-N-CA	5.45	127.90	120.54
1	G	125	VAL	N-CA-C	5.44	115.43	107.37
3	N	56	SER	CA-C-N	5.43	128.34	120.79
3	N	56	SER	C-N-CA	5.43	128.34	120.79
1	E	35	ASN	CA-CB-CG	5.43	118.03	112.60
1	A	135	THR	N-CA-C	5.43	117.59	108.96
1	E	135	THR	N-CA-C	5.41	117.56	108.96
2	B	104	GLY	N-CA-C	5.41	119.49	112.68
3	Q	56	SER	CA-C-N	5.40	128.30	120.79
3	Q	56	SER	C-N-CA	5.40	128.30	120.79
2	F	69	THR	CB-CA-C	5.39	119.02	109.75
1	G	111	THR	CB-CA-C	5.39	119.00	109.89
2	D	5	THR	CB-CA-C	5.39	120.57	111.41
1	G	135	THR	N-CA-C	5.38	117.51	108.96
1	A	167	VAL	N-CA-CB	5.38	116.39	110.53
2	L	72	THR	N-CA-C	5.37	117.84	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	72	THR	N-CA-C	5.37	117.83	108.76
1	A	64	ALA	N-CA-C	5.37	117.13	111.28
2	F	185	SER	CA-C-N	5.36	127.46	120.28
2	F	185	SER	C-N-CA	5.36	127.46	120.28
1	C	125	VAL	N-CA-C	5.34	115.28	107.37
3	Q	25	SER	N-CA-C	-5.34	103.33	110.55
2	D	104	GLY	CA-C-N	5.34	128.81	121.33
2	D	104	GLY	C-N-CA	5.34	128.81	121.33
1	A	112	LEU	N-CA-C	5.34	117.45	108.96
3	R	25	SER	N-CA-C	-5.33	103.36	110.55
1	C	111	THR	CB-CA-C	5.32	118.84	109.80
1	E	120	THR	CB-CA-C	5.31	118.54	109.72
3	O	25	SER	N-CA-C	-5.31	103.52	110.53
3	R	42	ARG	N-CA-C	-5.31	105.39	111.07
1	E	64	ALA	N-CA-C	5.31	117.06	111.28
3	N	25	SER	N-CA-C	-5.31	103.38	110.55
3	N	42	ARG	N-CA-C	-5.31	105.39	111.07
3	M	56	SER	CA-C-N	5.30	128.16	120.79
3	M	56	SER	C-N-CA	5.30	128.16	120.79
2	L	104	GLY	CA-C-N	5.29	128.74	121.33
2	L	104	GLY	C-N-CA	5.29	128.74	121.33
1	C	135	THR	N-CA-C	5.28	117.36	108.96
2	L	78	VAL	N-CA-CB	5.27	118.63	110.14
3	O	42	ARG	N-CA-C	-5.27	105.43	111.07
1	J	112	LEU	N-CA-C	5.26	117.33	108.96
3	O	57	GLU	CA-C-N	5.26	127.28	120.44
3	O	57	GLU	C-N-CA	5.26	127.28	120.44
2	B	50	ASP	CA-C-N	5.26	131.59	121.54
2	B	50	ASP	C-N-CA	5.26	131.59	121.54
2	L	101	PHE	CA-C-N	5.26	125.78	119.94
2	L	101	PHE	C-N-CA	5.26	125.78	119.94
1	C	112	LEU	N-CA-C	5.25	117.31	108.96
3	M	42	ARG	N-CA-C	-5.25	105.45	111.07
1	G	194	GLY	CA-C-N	5.24	127.30	120.28
1	G	194	GLY	C-N-CA	5.24	127.30	120.28
2	L	69	THR	CB-CA-C	5.23	118.75	109.75
3	P	42	ARG	N-CA-C	-5.23	105.47	111.07
3	Q	57	GLU	CA-C-N	5.22	127.23	120.44
3	Q	57	GLU	C-N-CA	5.22	127.23	120.44
2	I	95	ALA	CA-C-N	5.22	131.10	121.70
2	I	95	ALA	C-N-CA	5.22	131.10	121.70
1	E	208	ASN	CA-C-N	5.22	128.51	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	208	ASN	C-N-CA	5.22	128.51	121.05
2	I	101	PHE	CA-C-N	5.21	125.72	119.94
2	I	101	PHE	C-N-CA	5.21	125.72	119.94
1	H	194	GLY	CA-C-N	5.20	127.25	120.28
1	H	194	GLY	C-N-CA	5.20	127.25	120.28
1	C	194	GLY	CA-C-N	5.19	127.24	120.28
1	C	194	GLY	C-N-CA	5.19	127.24	120.28
2	F	173	ASP	CA-CB-CG	5.19	117.79	112.60
3	R	57	GLU	CA-C-N	5.19	127.19	120.44
3	R	57	GLU	C-N-CA	5.19	127.19	120.44
1	E	30	SER	CA-C-N	5.19	125.76	122.18
1	E	30	SER	C-N-CA	5.19	125.76	122.18
1	G	112	LEU	N-CA-C	5.19	117.21	108.96
3	M	57	GLU	CA-C-N	5.18	127.18	120.44
3	M	57	GLU	C-N-CA	5.18	127.18	120.44
1	C	30	SER	CA-C-N	5.18	125.75	122.18
1	C	30	SER	C-N-CA	5.18	125.75	122.18
3	R	56	SER	CA-C-N	5.18	127.99	120.79
3	R	56	SER	C-N-CA	5.18	127.99	120.79
2	F	78	VAL	N-CA-CB	5.17	118.82	110.13
2	B	186	LYS	CA-C-N	5.17	127.47	120.65
2	B	186	LYS	C-N-CA	5.17	127.47	120.65
2	K	186	LYS	CA-C-N	5.17	127.47	120.65
2	K	186	LYS	C-N-CA	5.17	127.47	120.65
2	D	69	THR	CB-CA-C	5.17	118.64	109.75
3	O	56	SER	CA-C-N	5.16	127.96	120.79
3	O	56	SER	C-N-CA	5.16	127.96	120.79
2	K	51	ALA	N-CA-C	5.15	121.78	110.80
2	B	69	THR	CB-CA-C	5.15	118.61	109.75
1	C	208	ASN	CA-C-N	5.15	128.16	120.90
1	C	208	ASN	C-N-CA	5.15	128.16	120.90
1	J	194	GLY	CA-C-N	5.15	127.18	120.28
1	J	194	GLY	C-N-CA	5.15	127.18	120.28
2	D	18	THR	CB-CA-C	5.14	118.64	109.38
2	F	186	LYS	CA-C-N	5.14	127.44	120.65
2	F	186	LYS	C-N-CA	5.14	127.44	120.65
1	G	208	ASN	CA-C-N	5.13	128.14	120.90
1	G	208	ASN	C-N-CA	5.13	128.14	120.90
3	R	10	GLU	CA-C-N	5.13	127.47	120.54
3	R	10	GLU	C-N-CA	5.13	127.47	120.54
2	I	18	THR	CB-CA-C	5.13	118.61	109.38
1	H	112	LEU	N-CA-C	5.12	117.10	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	42	ARG	N-CA-C	-5.12	105.59	111.07
2	F	50	ASP	CA-C-N	5.11	131.31	121.54
2	F	50	ASP	C-N-CA	5.11	131.31	121.54
2	L	186	LYS	CA-C-N	5.11	127.40	120.65
2	L	186	LYS	C-N-CA	5.11	127.40	120.65
1	G	167	VAL	N-CA-CB	5.09	116.08	110.53
2	D	95	ALA	CA-C-N	5.09	130.86	121.70
2	D	95	ALA	C-N-CA	5.09	130.86	121.70
1	E	194	GLY	CA-C-N	5.09	127.09	120.28
1	E	194	GLY	C-N-CA	5.09	127.09	120.28
3	P	57	GLU	CA-C-N	5.08	127.05	120.44
3	P	57	GLU	C-N-CA	5.08	127.05	120.44
2	D	194	VAL	N-CA-C	5.08	114.89	107.37
1	E	167	VAL	N-CA-CB	5.07	116.06	110.53
2	B	194	VAL	N-CA-C	5.07	114.87	107.37
2	I	51	ALA	N-CA-C	5.06	121.58	110.80
2	D	186	LYS	CA-C-N	5.06	127.33	120.65
2	D	186	LYS	C-N-CA	5.06	127.33	120.65
2	F	194	VAL	N-CA-C	5.05	114.85	107.37
1	A	194	GLY	CA-C-N	5.05	127.05	120.28
1	A	194	GLY	C-N-CA	5.05	127.05	120.28
2	L	185	SER	CA-C-N	5.05	127.56	120.28
2	L	185	SER	C-N-CA	5.05	127.56	120.28
2	I	78	VAL	N-CA-CB	5.04	118.26	110.14
1	J	111	THR	CB-CA-C	5.04	118.37	109.80
2	I	194	VAL	N-CA-C	5.04	114.83	107.37
2	K	101	PHE	CA-C-N	5.04	125.53	119.94
2	K	101	PHE	C-N-CA	5.04	125.53	119.94
3	M	25	SER	N-CA-C	-5.04	103.75	110.55
2	I	186	LYS	CA-C-N	5.03	127.29	120.65
2	I	186	LYS	C-N-CA	5.03	127.29	120.65
1	J	55	SER	CB-CA-C	-5.03	108.12	114.40
2	B	18	THR	CB-CA-C	5.02	118.42	109.38
2	D	78	VAL	N-CA-CB	5.02	118.22	110.14
2	I	69	THR	CB-CA-C	5.02	118.38	109.75
2	I	173	ASP	CA-CB-CG	5.01	117.61	112.60
2	F	51	ALA	N-CA-C	5.01	121.48	110.80
1	H	167	VAL	N-CA-CB	5.01	115.99	110.53
1	J	167	VAL	N-CA-CB	5.01	115.99	110.53
1	H	104	PHE	CA-C-N	5.01	127.25	120.44
1	H	104	PHE	C-N-CA	5.01	127.25	120.44
2	L	51	ALA	N-CA-C	5.00	121.46	110.80

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	1628	0	1594	29	0
1	C	1628	0	1594	25	0
1	E	1628	0	1594	28	0
1	G	1628	0	1594	24	0
1	H	1628	0	1594	29	0
1	J	1628	0	1594	28	0
2	B	1639	0	1581	40	0
2	D	1639	0	1581	43	0
2	F	1639	0	1581	41	0
2	I	1639	0	1581	40	0
2	K	1639	0	1581	42	0
2	L	1639	0	1581	39	0
3	M	492	0	504	7	0
3	N	492	0	504	9	0
3	O	492	0	504	7	0
3	P	492	0	504	11	0
3	Q	492	0	504	13	0
3	R	492	0	504	7	0
All	All	22554	0	22074	434	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 10.

All (434) 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)
2:I:21:ILE:HG21	2:I:105:THR:HG21	1.26	1.14
2:L:21:ILE:HG21	2:L:105:THR:HG21	1.28	1.12
2:D:21:ILE:HG21	2:D:105:THR:HG21	1.24	1.11
2:K:21:ILE:HG21	2:K:105:THR:HG21	1.28	1.10
2:B:21:ILE:HG21	2:B:105:THR:HG21	1.27	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:21:ILE:HG21	2:F:105:THR:HG21	1.25	1.08
1:A:75:THR:HA	1:A:76:THR:HG23	1.43	1.00
1:C:75:THR:HA	1:C:76:THR:HG23	1.45	0.97
1:G:75:THR:HA	1:G:76:THR:HG23	1.45	0.96
1:J:75:THR:HA	1:J:76:THR:HG23	1.44	0.96
1:E:75:THR:HA	1:E:76:THR:HG23	1.46	0.96
1:H:75:THR:HA	1:H:76:THR:HG23	1.45	0.95
2:F:46:LEU:HD23	2:F:55:ALA:HB2	1.62	0.81
2:B:46:LEU:HD23	2:B:55:ALA:HB2	1.62	0.80
2:I:128:LEU:HD12	2:I:186:LYS:HG3	1.64	0.79
2:B:21:ILE:CG2	2:B:105:THR:HG21	2.12	0.79
2:F:95:ALA:HA	2:F:98:ARG:H	1.48	0.79
2:B:95:ALA:HA	2:B:98:ARG:H	1.47	0.79
2:D:21:ILE:CG2	2:D:105:THR:HG21	2.12	0.79
2:K:95:ALA:HA	2:K:98:ARG:H	1.48	0.79
2:I:95:ALA:HA	2:I:98:ARG:H	1.48	0.78
2:L:128:LEU:HD12	2:L:186:LYS:HG3	1.63	0.78
2:D:128:LEU:HD12	2:D:186:LYS:HG3	1.66	0.77
2:D:95:ALA:HA	2:D:98:ARG:H	1.48	0.77
2:K:128:LEU:HD12	2:K:186:LYS:HG3	1.64	0.77
2:L:95:ALA:HA	2:L:98:ARG:H	1.49	0.77
2:I:21:ILE:CG2	2:I:105:THR:HG21	2.12	0.76
2:F:21:ILE:CG2	2:F:105:THR:HG21	2.11	0.76
2:I:46:LEU:HD23	2:I:55:ALA:HB2	1.67	0.75
2:B:128:LEU:HD12	2:B:186:LYS:HG3	1.67	0.75
2:D:46:LEU:HD23	2:D:55:ALA:HB2	1.68	0.75
2:L:95:ALA:HB1	2:L:96:SER:HA	1.69	0.74
1:E:40:ALA:HB1	1:E:41:PRO:HD2	1.69	0.74
2:L:46:LEU:HD23	2:L:55:ALA:HB2	1.68	0.74
2:B:95:ALA:HB1	2:B:96:SER:HA	1.69	0.74
2:D:95:ALA:HB1	2:D:96:SER:HA	1.69	0.73
2:K:46:LEU:HD23	2:K:55:ALA:HB2	1.70	0.73
2:F:128:LEU:HD12	2:F:186:LYS:HG3	1.68	0.73
2:K:95:ALA:HB1	2:K:96:SER:HA	1.71	0.72
2:F:95:ALA:HB1	2:F:96:SER:HA	1.70	0.72
2:I:95:ALA:HB1	2:I:96:SER:HA	1.70	0.72
1:A:40:ALA:HB1	1:A:41:PRO:HD2	1.73	0.69
3:N:27:PRO:HB2	3:N:28:PRO:HD2	1.75	0.69
2:B:150:GLN:HB2	2:B:198:GLU:HB3	1.75	0.69
1:A:24:VAL:HB	1:A:76:THR:HG21	1.75	0.69
2:L:21:ILE:CG2	2:L:105:THR:HG21	2.16	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ALA:HB1	2:B:96:SER:CA	2.23	0.69
2:K:150:GLN:HB2	2:K:198:GLU:HB3	1.75	0.69
2:D:150:GLN:HB2	2:D:198:GLU:HB3	1.75	0.68
1:J:89:THR:HG23	1:J:114:THR:HA	1.75	0.68
1:J:75:THR:HA	1:J:76:THR:CG2	2.22	0.68
3:P:27:PRO:HB2	3:P:28:PRO:HD2	1.75	0.68
2:L:95:ALA:HB1	2:L:96:SER:CA	2.22	0.68
2:L:150:GLN:HB2	2:L:198:GLU:HB3	1.76	0.68
1:G:24:VAL:HB	1:G:76:THR:HG21	1.74	0.68
2:I:95:ALA:HB1	2:I:96:SER:CA	2.23	0.68
1:J:24:VAL:HB	1:J:76:THR:HG21	1.74	0.68
1:H:24:VAL:HB	1:H:76:THR:HG21	1.74	0.68
2:I:150:GLN:HB2	2:I:198:GLU:HB3	1.76	0.67
3:M:27:PRO:HB2	3:M:28:PRO:HD2	1.76	0.67
3:O:27:PRO:HB2	3:O:28:PRO:HD2	1.76	0.67
2:D:95:ALA:HB1	2:D:96:SER:CA	2.23	0.67
1:C:89:THR:HG23	1:C:114:THR:HA	1.77	0.67
3:R:27:PRO:HB2	3:R:28:PRO:HD2	1.76	0.67
1:H:75:THR:HA	1:H:76:THR:CG2	2.24	0.67
1:H:89:THR:HG23	1:H:114:THR:HA	1.76	0.66
2:K:95:ALA:HB1	2:K:96:SER:CA	2.24	0.66
1:E:24:VAL:HB	1:E:76:THR:HG21	1.77	0.66
1:E:89:THR:HG23	1:E:114:THR:HA	1.77	0.66
1:G:75:THR:HA	1:G:76:THR:CG2	2.24	0.66
3:Q:27:PRO:HB2	3:Q:28:PRO:HD2	1.76	0.66
1:C:24:VAL:HB	1:C:76:THR:HG21	1.76	0.66
1:G:89:THR:HG23	1:G:114:THR:HA	1.78	0.66
2:L:116:PRO:HD3	2:L:201:HIS:CD2	2.30	0.66
2:F:150:GLN:HB2	2:F:198:GLU:HB3	1.76	0.66
1:A:75:THR:HA	1:A:76:THR:CG2	2.22	0.66
1:E:129:ALA:HB3	2:F:122:PRO:HD2	1.78	0.66
1:C:75:THR:HA	1:C:76:THR:CG2	2.24	0.65
2:F:95:ALA:HB1	2:F:96:SER:CA	2.24	0.65
2:K:21:ILE:CG2	2:K:105:THR:HG21	2.17	0.65
2:B:95:ALA:HB3	3:O:63:TYR:OH	1.96	0.65
1:A:89:THR:HG23	1:A:114:THR:HA	1.77	0.65
2:K:116:PRO:HD3	2:K:201:HIS:CD2	2.32	0.65
2:D:116:PRO:HD3	2:D:201:HIS:CD2	2.34	0.63
2:B:116:PRO:HD3	2:B:201:HIS:CD2	2.34	0.63
1:G:40:ALA:HB1	1:G:41:PRO:HD2	1.82	0.62
2:I:116:PRO:HD3	2:I:201:HIS:CD2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:135:VAL:HG23	2:D:182:LEU:HB3	1.81	0.61
3:N:55:ILE:HG22	3:N:59:ILE:HD11	1.82	0.61
3:R:55:ILE:HG22	3:R:59:ILE:HD11	1.82	0.61
2:K:135:VAL:HG23	2:K:182:LEU:HB3	1.81	0.61
1:E:75:THR:HA	1:E:76:THR:CG2	2.24	0.61
2:L:135:VAL:HG23	2:L:182:LEU:HB3	1.81	0.61
2:F:116:PRO:HD3	2:F:201:HIS:CD2	2.35	0.61
2:B:135:VAL:HG23	2:B:182:LEU:HB3	1.83	0.60
2:L:95:ALA:HB3	3:N:63:TYR:OH	2.00	0.60
1:E:123:PRO:HD3	1:E:204:HIS:HD2	1.66	0.60
2:I:135:VAL:HG23	2:I:182:LEU:HB3	1.82	0.60
2:F:135:VAL:HG23	2:F:182:LEU:HB3	1.84	0.59
2:I:76:SER:OG	2:I:77:GLY:N	2.32	0.59
1:C:40:ALA:HB1	1:C:41:PRO:HD2	1.84	0.58
1:A:123:PRO:HD3	1:A:204:HIS:HD2	1.67	0.58
2:I:95:ALA:HB3	3:M:63:TYR:OH	2.04	0.58
2:D:76:SER:OG	2:D:77:GLY:N	2.30	0.58
1:C:104:PHE:N	1:C:104:PHE:CD1	2.71	0.58
1:G:104:PHE:CD1	1:G:104:PHE:N	2.70	0.58
1:A:104:PHE:CD1	1:A:104:PHE:N	2.70	0.58
1:A:33:TRP:HB2	1:A:97:ASP:HB3	1.86	0.58
2:K:95:ALA:HB3	3:Q:63:TYR:OH	2.03	0.58
2:B:95:ALA:CB	2:B:96:SER:HA	2.35	0.57
2:D:95:ALA:HB3	3:P:63:TYR:OH	2.04	0.57
1:J:123:PRO:HD3	1:J:204:HIS:HD2	1.69	0.57
1:E:104:PHE:N	1:E:104:PHE:CD1	2.71	0.57
2:F:36:TYR:CE2	2:F:46:LEU:HD12	2.39	0.57
2:F:3:VAL:H	2:F:26:SER:HB3	1.69	0.57
3:Q:55:ILE:HG22	3:Q:59:ILE:HD11	1.85	0.57
1:G:123:PRO:HD3	1:G:204:HIS:HD2	1.68	0.57
1:H:104:PHE:CD1	1:H:104:PHE:N	2.71	0.57
1:H:123:PRO:HD3	1:H:204:HIS:HD2	1.69	0.57
3:O:55:ILE:HG22	3:O:59:ILE:HD11	1.87	0.57
1:C:33:TRP:HB2	1:C:97:ASP:HB3	1.87	0.57
1:A:123:PRO:HD3	1:A:204:HIS:CD2	2.40	0.57
2:L:95:ALA:CB	2:L:96:SER:HA	2.34	0.57
1:E:123:PRO:HD3	1:E:204:HIS:CD2	2.40	0.56
2:F:95:ALA:CB	2:F:96:SER:HA	2.34	0.56
1:E:33:TRP:HB2	1:E:97:ASP:HB3	1.85	0.56
1:A:158:TRP:HB3	1:A:163:LEU:HD23	1.88	0.56
2:B:36:TYR:CE2	2:B:46:LEU:HD12	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:53:HIS:CE1	3:N:64:LEU:HB2	2.39	0.56
1:J:40:ALA:HB1	1:J:41:PRO:HD2	1.87	0.56
1:J:104:PHE:N	1:J:104:PHE:CD1	2.71	0.56
1:C:123:PRO:HD3	1:C:204:HIS:HD2	1.69	0.56
2:I:32:TRP:HA	2:I:32:TRP:CE3	2.41	0.56
1:H:40:ALA:HB1	1:H:41:PRO:HD2	1.87	0.56
2:K:32:TRP:HE3	2:K:32:TRP:HA	1.71	0.56
2:D:32:TRP:HA	2:D:32:TRP:HE3	1.71	0.56
1:H:129:ALA:HB3	2:L:122:PRO:HD2	1.87	0.56
2:I:32:TRP:HA	2:I:32:TRP:HE3	1.71	0.56
2:K:36:TYR:CE2	2:K:46:LEU:HD12	2.41	0.56
2:L:19:VAL:HG23	2:L:78:VAL:HG11	1.87	0.56
2:B:3:VAL:H	2:B:26:SER:HB3	1.71	0.55
1:E:158:TRP:HB3	1:E:163:LEU:HD23	1.88	0.55
1:A:129:ALA:HB3	2:B:122:PRO:HD2	1.89	0.55
1:H:33:TRP:HB2	1:H:97:ASP:HB3	1.89	0.55
1:J:33:TRP:HB2	1:J:97:ASP:HB3	1.89	0.55
2:K:32:TRP:HA	2:K:32:TRP:CE3	2.42	0.55
2:D:3:VAL:H	2:D:26:SER:HB3	1.72	0.55
1:G:33:TRP:HB2	1:G:97:ASP:HB3	1.88	0.55
2:K:3:VAL:H	2:K:26:SER:HB3	1.71	0.55
2:L:32:TRP:HE3	2:L:32:TRP:HA	1.71	0.55
3:N:12:LEU:O	3:N:16:VAL:HG23	2.07	0.55
2:B:49:TYR:O	2:B:53:ASN:ND2	2.40	0.55
2:L:36:TYR:CE2	2:L:46:LEU:HD12	2.41	0.55
2:B:32:TRP:HE3	2:B:32:TRP:HA	1.72	0.55
2:L:32:TRP:HA	2:L:32:TRP:CE3	2.42	0.55
3:O:55:ILE:O	3:O:59:ILE:HG13	2.07	0.55
1:A:11:LEU:HB2	1:A:151:PRO:HG3	1.89	0.54
1:G:123:PRO:HD3	1:G:204:HIS:CD2	2.42	0.54
2:L:3:VAL:H	2:L:26:SER:HB3	1.72	0.54
1:G:129:ALA:HB3	2:I:122:PRO:HD2	1.89	0.54
2:F:19:VAL:HG23	2:F:78:VAL:HG11	1.90	0.54
1:H:158:TRP:HB3	1:H:163:LEU:HD23	1.89	0.54
2:F:32:TRP:CE3	2:F:32:TRP:HA	2.43	0.54
2:I:3:VAL:H	2:I:26:SER:HB3	1.73	0.54
2:I:95:ALA:CB	2:I:96:SER:HA	2.37	0.54
3:R:12:LEU:O	3:R:16:VAL:HG23	2.07	0.54
2:D:32:TRP:HA	2:D:32:TRP:CE3	2.42	0.54
2:F:32:TRP:HA	2:F:32:TRP:HE3	1.72	0.54
1:J:158:TRP:HB3	1:J:163:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:TRP:HA	2:B:32:TRP:CE3	2.42	0.54
1:H:34:LEU:HD21	1:H:94:CYS:HB2	1.90	0.54
3:P:55:ILE:HG22	3:P:59:ILE:HD11	1.90	0.54
2:K:49:TYR:O	2:K:53:ASN:ND2	2.41	0.54
2:D:95:ALA:CB	2:D:96:SER:HA	2.37	0.53
1:E:11:LEU:HB2	1:E:151:PRO:HG3	1.90	0.53
1:C:123:PRO:HD3	1:C:204:HIS:CD2	2.43	0.53
2:K:19:VAL:HG23	2:K:78:VAL:HG11	1.89	0.53
1:E:32:PHE:H	1:E:53:ARG:HB2	1.74	0.53
3:M:55:ILE:O	3:M:59:ILE:HG13	2.09	0.53
3:R:55:ILE:O	3:R:59:ILE:HG13	2.08	0.53
1:A:32:PHE:H	1:A:53:ARG:HB2	1.74	0.52
1:H:123:PRO:HD3	1:H:204:HIS:CD2	2.44	0.52
1:C:158:TRP:HB3	1:C:163:LEU:HD23	1.90	0.52
1:J:123:PRO:HD3	1:J:204:HIS:CD2	2.44	0.52
2:K:95:ALA:CB	2:K:96:SER:HA	2.37	0.52
3:P:64:LEU:HD22	3:Q:19:ILE:HG22	1.92	0.52
1:A:34:LEU:HD21	1:A:94:CYS:HB2	1.91	0.52
2:I:36:TYR:CE2	2:I:46:LEU:HD12	2.45	0.52
2:D:12:SER:CB	2:D:110:ILE:HD11	2.40	0.52
2:L:12:SER:CB	2:L:110:ILE:HD11	2.40	0.52
3:P:12:LEU:O	3:P:16:VAL:HG23	2.10	0.52
2:D:36:TYR:CE2	2:D:46:LEU:HD12	2.44	0.52
2:F:123:PRO:HD3	2:F:135:VAL:HG13	1.92	0.52
2:L:49:TYR:O	2:L:53:ASN:ND2	2.43	0.52
2:B:95:ALA:HB1	2:B:96:SER:C	2.36	0.52
2:K:12:SER:CB	2:K:110:ILE:HD11	2.40	0.52
2:B:123:PRO:HD3	2:B:135:VAL:HG13	1.92	0.51
1:H:32:PHE:H	1:H:53:ARG:HB2	1.76	0.51
1:G:95:ALA:HB1	1:G:104:PHE:HB3	1.92	0.51
1:G:158:TRP:HB3	1:G:163:LEU:HD23	1.90	0.51
1:J:32:PHE:H	1:J:53:ARG:HB2	1.76	0.51
3:M:12:LEU:O	3:M:16:VAL:HG23	2.10	0.51
3:M:55:ILE:HG22	3:M:59:ILE:HD11	1.91	0.51
1:E:34:LEU:HD21	1:E:94:CYS:HB2	1.92	0.51
2:F:49:TYR:O	2:F:53:ASN:ND2	2.43	0.51
2:I:12:SER:CB	2:I:110:ILE:HD11	2.41	0.51
2:L:76:SER:OG	2:L:77:GLY:N	2.35	0.51
1:J:34:LEU:HD21	1:J:94:CYS:HB2	1.92	0.51
3:P:55:ILE:O	3:P:59:ILE:HG13	2.11	0.51
2:F:12:SER:CB	2:F:110:ILE:HD11	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:55:ILE:O	3:N:59:ILE:HG13	2.10	0.51
3:Q:12:LEU:O	3:Q:16:VAL:HG23	2.10	0.51
2:L:95:ALA:HB1	2:L:96:SER:C	2.36	0.50
1:C:32:PHE:H	1:C:53:ARG:HB2	1.76	0.50
2:F:95:ALA:HB1	2:F:96:SER:C	2.36	0.50
3:M:64:LEU:HD22	3:N:19:ILE:HG22	1.93	0.50
2:F:76:SER:OG	2:F:77:GLY:N	2.37	0.50
2:K:76:SER:OG	2:K:77:GLY:N	2.34	0.50
1:G:34:LEU:HD21	1:G:94:CYS:HB2	1.93	0.50
3:O:12:LEU:O	3:O:16:VAL:HG23	2.12	0.50
2:B:19:VAL:HG23	2:B:78:VAL:HG11	1.93	0.50
2:D:49:TYR:O	2:D:53:ASN:ND2	2.43	0.50
2:L:12:SER:HB3	2:L:110:ILE:HD11	1.94	0.50
1:C:34:LEU:HD21	1:C:94:CYS:HB2	1.94	0.50
2:I:2:LEU:HB2	2:I:97:TYR:HB2	1.94	0.50
2:K:123:PRO:HD3	2:K:135:VAL:HG13	1.94	0.50
1:A:95:ALA:HB1	1:A:104:PHE:HB3	1.94	0.50
2:L:123:PRO:HD3	2:L:135:VAL:HG13	1.93	0.50
2:B:12:SER:CB	2:B:110:ILE:HD11	2.42	0.50
1:J:11:LEU:HB2	1:J:151:PRO:HG3	1.93	0.50
1:H:128:LEU:HD12	1:H:143:GLY:HA3	1.94	0.50
1:J:128:LEU:HD12	1:J:143:GLY:HA3	1.93	0.50
1:E:95:ALA:HB1	1:E:104:PHE:HB3	1.94	0.49
2:K:95:ALA:HB1	2:K:96:SER:C	2.37	0.49
1:G:32:PHE:H	1:G:53:ARG:HB2	1.76	0.49
1:A:146:VAL:HG11	1:A:154:VAL:HG11	1.94	0.49
1:C:95:ALA:HB1	1:C:104:PHE:HB3	1.94	0.49
1:H:11:LEU:HB2	1:H:151:PRO:HG3	1.94	0.49
1:G:11:LEU:HB2	1:G:151:PRO:HG3	1.95	0.49
3:Q:55:ILE:O	3:Q:59:ILE:HG13	2.12	0.49
2:F:95:ALA:HA	2:F:98:ARG:N	2.24	0.49
2:I:49:TYR:O	2:I:53:ASN:ND2	2.44	0.49
2:B:213:ASN:HB2	2:B:216:GLU:HB2	1.94	0.49
1:H:146:VAL:HG12	1:H:146:VAL:O	2.12	0.49
2:L:213:ASN:HB2	2:L:216:GLU:HB2	1.95	0.49
2:F:95:ALA:HB3	3:R:63:TYR:OH	2.12	0.48
1:A:146:VAL:HG12	1:A:146:VAL:O	2.14	0.48
2:I:19:VAL:HG23	2:I:78:VAL:HG11	1.95	0.48
1:G:128:LEU:HD12	1:G:143:GLY:HA3	1.96	0.48
2:D:2:LEU:HB2	2:D:97:TYR:HB2	1.95	0.48
1:J:95:ALA:HB1	1:J:104:PHE:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LEU:HD12	1:C:143:GLY:HA3	1.95	0.48
2:D:18:THR:HB	2:D:76:SER:HA	1.94	0.48
2:L:95:ALA:CB	2:L:96:SER:CA	2.91	0.48
2:B:121:PHE:HD2	2:B:136:VAL:HG12	1.78	0.48
1:C:11:LEU:HB2	1:C:151:PRO:HG3	1.96	0.48
1:G:146:VAL:HG11	1:G:154:VAL:HG11	1.96	0.48
2:I:5:THR:HB	2:I:24:GLN:HB3	1.94	0.48
1:A:54:GLY:HA3	3:O:21:PHE:HZ	1.79	0.48
2:D:123:PRO:HD3	2:D:135:VAL:HG13	1.95	0.47
2:D:19:VAL:HG23	2:D:78:VAL:HG11	1.95	0.47
1:E:126:PHE:CE2	2:F:127:GLN:HG3	2.49	0.47
1:E:146:VAL:HG11	1:E:154:VAL:HG11	1.96	0.47
1:G:159:ASN:HA	1:G:199:ILE:HD12	1.96	0.47
2:I:95:ALA:HB1	2:I:96:SER:C	2.40	0.47
2:I:123:PRO:HD3	2:I:135:VAL:HG13	1.94	0.47
2:K:12:SER:HB3	2:K:110:ILE:HD11	1.96	0.47
2:B:95:ALA:CB	2:B:96:SER:CA	2.92	0.47
1:C:159:ASN:HA	1:C:199:ILE:HD12	1.97	0.47
2:F:2:LEU:HD11	2:F:29:ILE:HD11	1.97	0.47
1:J:146:VAL:HG11	1:J:154:VAL:HG11	1.95	0.47
2:D:5:THR:HB	2:D:24:GLN:HB3	1.95	0.47
2:D:95:ALA:HB1	2:D:96:SER:C	2.40	0.47
1:E:128:LEU:HD12	1:E:143:GLY:HA3	1.97	0.47
2:I:213:ASN:HB2	2:I:216:GLU:HB2	1.96	0.47
1:J:151:PRO:HD2	1:J:206:PRO:HB2	1.97	0.47
3:P:53:HIS:CE1	3:Q:64:LEU:HB2	2.49	0.47
2:K:121:PHE:HD2	2:K:136:VAL:HG12	1.80	0.47
2:L:2:LEU:HD11	2:L:29:ILE:HD11	1.96	0.47
2:I:18:THR:HB	2:I:76:SER:HA	1.97	0.47
2:L:121:PHE:HD2	2:L:136:VAL:HG12	1.80	0.46
2:F:213:ASN:HB2	2:F:216:GLU:HB2	1.97	0.46
2:K:139:LEU:HD13	2:K:178:LEU:HB3	1.97	0.46
1:C:146:VAL:HG11	1:C:154:VAL:HG11	1.96	0.46
2:D:139:LEU:HD13	2:D:178:LEU:HB3	1.96	0.46
1:G:53:ARG:HH12	1:G:76:THR:HG22	1.80	0.46
1:H:151:PRO:HD2	1:H:206:PRO:HB2	1.98	0.46
2:K:213:ASN:HB2	2:K:216:GLU:HB2	1.96	0.46
1:H:95:ALA:HB1	1:H:104:PHE:HB3	1.98	0.46
2:I:139:LEU:HD13	2:I:178:LEU:HB3	1.97	0.46
2:D:213:ASN:HB2	2:D:216:GLU:HB2	1.95	0.46
2:I:95:ALA:HA	2:I:98:ARG:N	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:121:PHE:HD2	2:F:136:VAL:HG12	1.80	0.46
1:H:146:VAL:HG11	1:H:154:VAL:HG11	1.97	0.46
1:J:159:ASN:HA	1:J:199:ILE:HD12	1.98	0.46
1:A:53:ARG:HH12	1:A:76:THR:HG22	1.81	0.46
1:A:128:LEU:HD12	1:A:143:GLY:HA3	1.98	0.46
1:A:169:THR:HG23	1:A:184:SER:HB2	1.98	0.46
1:E:146:VAL:HG12	1:E:146:VAL:O	2.16	0.46
1:G:204:HIS:ND1	1:G:206:PRO:HD2	2.31	0.46
1:J:204:HIS:ND1	1:J:206:PRO:HD2	2.30	0.46
2:L:139:LEU:HD13	2:L:178:LEU:HB3	1.97	0.46
2:D:95:ALA:CB	2:D:96:SER:CA	2.94	0.46
2:D:121:PHE:HD2	2:D:136:VAL:HG12	1.81	0.46
1:H:159:ASN:HA	1:H:199:ILE:HD12	1.98	0.46
1:J:146:VAL:HG12	1:J:146:VAL:O	2.16	0.46
2:K:2:LEU:HD11	2:K:29:ILE:HD11	1.97	0.46
2:L:31:SER:O	2:L:50:ASP:HA	2.16	0.46
2:B:35:TRP:HB2	2:B:48:ILE:HB	1.97	0.46
2:B:76:SER:OG	2:B:77:GLY:N	2.34	0.46
2:B:2:LEU:HD11	2:B:29:ILE:HD11	1.97	0.45
1:C:151:PRO:HD2	1:C:206:PRO:HB2	1.98	0.45
1:C:204:HIS:ND1	1:C:206:PRO:HD2	2.31	0.45
2:D:12:SER:HB3	2:D:110:ILE:HD11	1.98	0.45
2:K:18:THR:HB	2:K:76:SER:HA	1.99	0.45
1:C:53:ARG:HH12	1:C:76:THR:HG22	1.80	0.45
2:B:5:THR:HB	2:B:24:GLN:HB3	1.97	0.45
2:K:5:THR:HB	2:K:24:GLN:HB3	1.98	0.45
2:K:30:SER:HB2	3:Q:58:ARG:HH21	1.82	0.45
2:B:2:LEU:HB2	2:B:97:TYR:HB2	1.99	0.45
1:C:146:VAL:HG12	1:C:146:VAL:O	2.17	0.45
1:E:159:ASN:HA	1:E:199:ILE:HD12	1.97	0.45
1:E:204:HIS:ND1	1:E:206:PRO:HD2	2.32	0.45
1:E:169:THR:HG23	1:E:184:SER:HB2	1.99	0.45
2:F:2:LEU:HB2	2:F:97:TYR:HB2	1.99	0.45
2:F:35:TRP:HB2	2:F:48:ILE:HB	1.98	0.45
1:J:169:THR:HG23	1:J:184:SER:HB2	1.97	0.45
2:L:5:THR:HB	2:L:24:GLN:HB3	1.98	0.45
2:D:35:TRP:HB2	2:D:48:ILE:HB	1.99	0.45
1:G:146:VAL:HG12	1:G:146:VAL:O	2.16	0.45
1:H:204:HIS:ND1	1:H:206:PRO:HD2	2.32	0.45
1:J:67:ARG:H	1:J:67:ARG:HG2	1.64	0.45
1:A:159:ASN:HA	1:A:199:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:LEU:HD11	2:D:29:ILE:HD11	1.98	0.45
1:H:123:PRO:HD2	1:H:209:THR:HG21	1.99	0.45
2:B:95:ALA:HA	2:B:98:ARG:N	2.24	0.45
1:G:151:PRO:HD2	1:G:206:PRO:HB2	1.98	0.45
2:K:2:LEU:HB2	2:K:97:TYR:HB2	1.99	0.45
2:L:2:LEU:HB2	2:L:97:TYR:HB2	1.99	0.44
1:E:91:THR:HG22	1:E:112:LEU:HD13	1.99	0.44
2:B:121:PHE:HA	2:B:122:PRO:HD3	1.86	0.44
2:D:30:SER:HB2	3:P:58:ARG:HH21	1.82	0.44
1:A:204:HIS:ND1	1:A:206:PRO:HD2	2.32	0.44
1:H:126:PHE:CE2	2:L:127:GLN:HG3	2.53	0.44
2:I:121:PHE:HD2	2:I:136:VAL:HG12	1.81	0.44
2:K:31:SER:O	2:K:50:ASP:HA	2.17	0.44
2:F:5:THR:HB	2:F:24:GLN:HB3	1.99	0.44
2:I:2:LEU:HD11	2:I:29:ILE:HD11	1.99	0.44
2:I:35:TRP:HB2	2:I:48:ILE:HB	1.99	0.44
1:J:129:ALA:HB3	2:K:122:PRO:HD2	1.99	0.44
3:O:10:GLU:HA	3:O:13:LEU:HD12	2.00	0.44
2:B:12:SER:HB3	2:B:110:ILE:HD11	1.99	0.43
2:L:95:ALA:HA	2:L:98:ARG:N	2.25	0.43
1:C:129:ALA:HB3	2:D:122:PRO:HD2	1.99	0.43
2:D:128:LEU:HD13	2:D:128:LEU:HA	1.89	0.43
3:P:13:LEU:HD21	3:Q:17:ARG:HH21	1.83	0.43
1:A:67:ARG:H	1:A:67:ARG:HG2	1.65	0.43
2:K:95:ALA:CB	2:K:96:SER:CA	2.93	0.43
1:A:151:PRO:HD2	1:A:206:PRO:HB2	2.00	0.43
2:F:95:ALA:CB	2:F:96:SER:CA	2.93	0.43
1:J:91:THR:HG22	1:J:112:LEU:HD13	2.01	0.43
2:B:18:THR:HB	2:B:76:SER:HA	1.99	0.43
2:B:139:LEU:HD13	2:B:178:LEU:HB3	1.99	0.43
2:F:12:SER:HB3	2:F:110:ILE:HD11	2.00	0.43
2:F:31:SER:O	2:F:50:ASP:HA	2.19	0.43
1:J:53:ARG:HH12	1:J:76:THR:HG22	1.84	0.43
1:A:126:PHE:CE2	2:B:127:GLN:HG3	2.54	0.43
2:F:139:LEU:HD13	2:F:178:LEU:HB3	2.00	0.43
2:L:18:THR:HB	2:L:76:SER:HA	2.01	0.43
2:L:35:TRP:HB2	2:L:48:ILE:HB	2.00	0.43
2:D:31:SER:O	2:D:50:ASP:HA	2.19	0.42
2:F:18:THR:HB	2:F:76:SER:HA	2.00	0.42
1:J:54:GLY:HA3	3:Q:21:PHE:HZ	1.84	0.42
3:N:55:ILE:HG22	3:N:59:ILE:CD1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:10:GLU:HA	3:Q:13:LEU:HD12	2.01	0.42
3:R:10:GLU:HA	3:R:13:LEU:HD12	2.00	0.42
1:E:53:ARG:HH12	1:E:76:THR:HG22	1.84	0.42
1:H:53:ARG:HH12	1:H:76:THR:HG22	1.84	0.42
2:L:47:LEU:HA	2:L:58:VAL:HG21	2.02	0.42
1:A:6:GLU:OE1	1:A:93:PHE:HA	2.19	0.42
1:E:151:PRO:HD2	1:E:206:PRO:HB2	2.00	0.42
2:D:31:SER:H	3:P:58:ARG:HH21	1.67	0.42
1:H:67:ARG:H	1:H:67:ARG:HG2	1.65	0.42
2:I:12:SER:HB3	2:I:110:ILE:HD11	2.00	0.42
2:K:9:SER:O	2:K:105:THR:HA	2.20	0.42
2:K:35:TRP:HB2	2:K:48:ILE:HB	2.01	0.42
2:D:95:ALA:HA	2:D:98:ARG:N	2.25	0.42
2:I:121:PHE:HA	2:I:122:PRO:HD3	1.87	0.42
2:B:31:SER:O	2:B:50:ASP:HA	2.20	0.42
1:G:123:PRO:HD2	1:G:209:THR:HG21	2.02	0.42
3:P:10:GLU:HA	3:P:13:LEU:HD12	2.02	0.42
2:B:22:LYS:HE2	2:B:24:GLN:HB2	2.02	0.42
2:D:139:LEU:O	2:D:177:SER:HA	2.20	0.42
1:G:169:THR:HG23	1:G:184:SER:HB2	2.01	0.42
1:H:169:THR:HG23	1:H:184:SER:HB2	2.01	0.42
1:A:75:THR:HA	1:A:76:THR:CB	2.50	0.42
2:I:31:SER:O	2:I:50:ASP:HA	2.20	0.42
2:D:47:LEU:HA	2:D:58:VAL:HG21	2.02	0.41
1:J:123:PRO:HD2	1:J:209:THR:HG21	2.00	0.41
1:A:123:PRO:HD2	1:A:209:THR:HG21	2.02	0.41
2:I:12:SER:HB2	2:I:110:ILE:HD11	2.01	0.41
1:C:123:PRO:HD2	1:C:209:THR:HG21	2.03	0.41
1:C:126:PHE:HB3	2:D:124:SER:OG	2.20	0.41
2:D:12:SER:HB2	2:D:110:ILE:HD11	2.02	0.41
2:F:121:PHE:HA	2:F:122:PRO:HD3	1.83	0.41
1:E:10:ARG:HD3	1:J:207:SER:HA	2.02	0.41
2:I:139:LEU:O	2:I:177:SER:HA	2.20	0.41
2:B:128:LEU:HD13	2:B:128:LEU:HA	1.90	0.41
2:I:47:LEU:HA	2:I:58:VAL:HG21	2.02	0.41
3:N:10:GLU:HA	3:N:13:LEU:HD12	2.02	0.41
3:Q:55:ILE:HG22	3:Q:59:ILE:CD1	2.50	0.41
1:C:169:THR:HG23	1:C:184:SER:HB2	2.00	0.41
2:I:22:LYS:HE2	2:I:24:GLN:HB2	2.01	0.41
2:I:128:LEU:HD13	2:I:128:LEU:HA	1.89	0.41
2:K:66:GLY:HA2	2:K:70:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:128:LEU:HD13	2:K:128:LEU:HA	1.93	0.41
2:L:9:SER:O	2:L:105:THR:HA	2.21	0.41
2:B:35:TRP:CZ3	2:B:88:CYS:HB3	2.56	0.41
2:K:22:LYS:HE2	2:K:24:GLN:HB2	2.02	0.41
3:Q:34:THR:HB	3:Q:37:ALA:HB3	2.03	0.41
2:F:128:LEU:HD13	2:F:128:LEU:HA	1.91	0.41
1:H:6:GLU:OE1	1:H:93:PHE:HA	2.20	0.41
1:H:75:THR:HA	1:H:76:THR:CB	2.51	0.41
2:K:12:SER:HB2	2:K:110:ILE:HD11	2.03	0.41
2:K:95:ALA:HA	2:K:98:ARG:N	2.24	0.41
2:D:22:LYS:HE2	2:D:24:GLN:HB2	2.02	0.40
2:L:121:PHE:HA	2:L:122:PRO:HD3	1.87	0.40
1:E:44:GLY:HA2	2:F:87:TYR:OH	2.22	0.40
1:E:75:THR:HA	1:E:76:THR:CB	2.52	0.40
1:H:91:THR:HG22	1:H:112:LEU:HD13	2.03	0.40
2:K:81:GLU:O	2:K:83:ALA:N	2.54	0.40
2:F:9:SER:O	2:F:105:THR:HA	2.21	0.40
3:R:55:ILE:HG22	3:R:59:ILE:CD1	2.51	0.40
2:F:66:GLY:HA2	2:F:70:GLU:O	2.22	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	219/231 (95%)	187 (85%)	28 (13%)	4 (2%)	6	31
1	C	219/231 (95%)	189 (86%)	26 (12%)	4 (2%)	6	31
1	E	219/231 (95%)	187 (85%)	28 (13%)	4 (2%)	6	31
1	G	219/231 (95%)	190 (87%)	25 (11%)	4 (2%)	6	31
1	H	219/231 (95%)	187 (85%)	28 (13%)	4 (2%)	6	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	219/231 (95%)	190 (87%)	25 (11%)	4 (2%)	6	31
2	B	215/217 (99%)	188 (87%)	14 (6%)	13 (6%)	1	8
2	D	215/217 (99%)	188 (87%)	14 (6%)	13 (6%)	1	8
2	F	215/217 (99%)	188 (87%)	14 (6%)	13 (6%)	1	8
2	I	215/217 (99%)	188 (87%)	14 (6%)	13 (6%)	1	8
2	K	215/217 (99%)	188 (87%)	14 (6%)	13 (6%)	1	8
2	L	215/217 (99%)	188 (87%)	15 (7%)	12 (6%)	1	10
3	M	55/115 (48%)	46 (84%)	7 (13%)	2 (4%)	2	17
3	N	55/115 (48%)	48 (87%)	5 (9%)	2 (4%)	2	17
3	O	55/115 (48%)	47 (86%)	6 (11%)	2 (4%)	2	17
3	P	55/115 (48%)	46 (84%)	7 (13%)	2 (4%)	2	17
3	Q	55/115 (48%)	46 (84%)	7 (13%)	2 (4%)	2	17
3	R	55/115 (48%)	47 (86%)	6 (11%)	2 (4%)	2	17
All	All	2934/3378 (87%)	2538 (86%)	283 (10%)	113 (4%)	2	15

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	174	SER
2	D	174	SER
2	F	174	SER
2	I	174	SER
2	K	174	SER
2	L	174	SER
3	M	29	PRO
3	N	29	PRO
3	O	29	PRO
3	P	29	PRO
3	Q	29	PRO
3	R	29	PRO
1	A	130	PRO
2	B	28	SER
2	B	32	TRP
2	B	76	SER
2	B	141	ASN
1	C	130	PRO
1	C	148	ASP

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Mol	Chain	Res	Type
2	D	28	SER
2	D	76	SER
2	D	141	ASN
1	E	130	PRO
1	E	148	ASP
2	F	28	SER
2	F	76	SER
2	F	94	ALA
2	F	141	ASN
1	G	130	PRO
1	H	130	PRO
1	H	148	ASP
2	I	28	SER
2	I	76	SER
2	I	141	ASN
1	J	130	PRO
1	J	148	ASP
2	K	28	SER
2	K	76	SER
2	K	94	ALA
2	K	141	ASN
2	L	28	SER
2	L	76	SER
2	L	141	ASN
1	A	148	ASP
1	A	220	CYS
2	B	30	SER
2	B	51	ALA
2	B	82	ASP
2	B	130	SER
2	B	207	PRO
2	D	30	SER
2	D	32	TRP
2	D	82	ASP
2	D	94	ALA
2	D	130	SER
1	E	220	CYS
2	F	30	SER
2	F	32	TRP
2	F	82	ASP
2	F	130	SER
2	F	207	PRO

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Mol	Chain	Res	Type
1	G	148	ASP
2	I	30	SER
2	I	32	TRP
2	I	82	ASP
2	I	94	ALA
2	I	130	SER
1	J	220	CYS
2	K	30	SER
2	K	32	TRP
2	K	51	ALA
2	K	82	ASP
2	K	130	SER
2	L	30	SER
2	L	32	TRP
2	L	51	ALA
2	L	82	ASP
2	L	94	ALA
2	L	130	SER
2	L	207	PRO
1	A	30	SER
2	B	29	ILE
2	B	94	ALA
1	C	30	SER
1	C	220	CYS
2	D	29	ILE
2	D	207	PRO
1	E	30	SER
2	F	29	ILE
2	F	51	ALA
1	G	220	CYS
1	H	30	SER
1	H	220	CYS
2	I	29	ILE
2	I	207	PRO
1	J	30	SER
2	K	29	ILE
2	K	207	PRO
2	L	29	ILE
3	M	30	ASN
3	N	30	ASN
3	O	30	ASN
3	P	30	ASN

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Mol	Chain	Res	Type
3	Q	30	ASN
3	R	30	ASN
2	D	51	ALA
2	I	51	ALA
1	G	30	SER
2	F	77	GLY
2	B	77	GLY
2	I	77	GLY
2	D	77	GLY
2	K	77	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/192 (95%)	149 (82%)	33 (18%)	2	8
1	C	182/192 (95%)	150 (82%)	32 (18%)	2	9
1	E	182/192 (95%)	147 (81%)	35 (19%)	1	8
1	G	182/192 (95%)	148 (81%)	34 (19%)	1	8
1	H	182/192 (95%)	147 (81%)	35 (19%)	1	8
1	J	182/192 (95%)	149 (82%)	33 (18%)	2	8
2	B	184/185 (100%)	153 (83%)	31 (17%)	2	10
2	D	184/185 (100%)	152 (83%)	32 (17%)	2	9
2	F	184/185 (100%)	152 (83%)	32 (17%)	2	9
2	I	184/185 (100%)	154 (84%)	30 (16%)	2	11
2	K	184/185 (100%)	153 (83%)	31 (17%)	2	10
2	L	184/185 (100%)	154 (84%)	30 (16%)	2	11
3	M	53/101 (52%)	46 (87%)	7 (13%)	4	17
3	N	53/101 (52%)	45 (85%)	8 (15%)	3	13
3	O	53/101 (52%)	46 (87%)	7 (13%)	4	17
3	P	53/101 (52%)	47 (89%)	6 (11%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	53/101 (52%)	45 (85%)	8 (15%)	3	13
3	R	53/101 (52%)	45 (85%)	8 (15%)	3	13
All	All	2514/2868 (88%)	2082 (83%)	432 (17%)	2	9

All (432) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	13	THR
1	A	21	THR
1	A	25	SER
1	A	29	LEU
1	A	34	LEU
1	A	35	ASN
1	A	57	SER
1	A	62	SER
1	A	67	ARG
1	A	73	THR
1	A	76	THR
1	A	77	VAL
1	A	78	THR
1	A	82	THR
1	A	91	THR
1	A	104	PHE
1	A	117	SER
1	A	120	THR
1	A	142	LEU
1	A	144	CYS
1	A	147	LYS
1	A	152	GLU
1	A	173	VAL
1	A	174	LEU
1	A	182	LEU
1	A	183	SER
1	A	193	LEU
1	A	195	THR
1	A	196	GLN
1	A	197	THR
1	A	199	ILE
1	A	212	ASP
2	B	1	GLU

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Mol	Chain	Res	Type
2	B	2	LEU
2	B	12	SER
2	B	18	THR
2	B	27	GLN
2	B	32	TRP
2	B	33	LEU
2	B	34	SER
2	B	42	GLN
2	B	53	ASN
2	B	63	MET
2	B	65	SER
2	B	69	THR
2	B	75	ILE
2	B	76	SER
2	B	78	VAL
2	B	80	ARG
2	B	85	THR
2	B	109	ILE
2	B	112	THR
2	B	125	ASP
2	B	128	LEU
2	B	135	VAL
2	B	136	VAL
2	B	138	LEU
2	B	150	GLN
2	B	163	GLN
2	B	172	LYS
2	B	175	THR
2	B	179	SER
2	B	184	LEU
1	C	11	LEU
1	C	13	THR
1	C	21	THR
1	C	25	SER
1	C	29	LEU
1	C	34	LEU
1	C	35	ASN
1	C	57	SER
1	C	62	SER
1	C	67	ARG
1	C	71	SER
1	C	73	THR

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Mol	Chain	Res	Type
1	C	76	THR
1	C	77	VAL
1	C	78	THR
1	C	82	THR
1	C	91	THR
1	C	104	PHE
1	C	117	SER
1	C	120	THR
1	C	142	LEU
1	C	144	CYS
1	C	147	LYS
1	C	173	VAL
1	C	174	LEU
1	C	182	LEU
1	C	183	SER
1	C	193	LEU
1	C	195	THR
1	C	196	GLN
1	C	199	ILE
1	C	212	ASP
2	D	1	GLU
2	D	2	LEU
2	D	12	SER
2	D	18	THR
2	D	27	GLN
2	D	32	TRP
2	D	33	LEU
2	D	34	SER
2	D	42	GLN
2	D	53	ASN
2	D	56	SER
2	D	63	MET
2	D	65	SER
2	D	69	THR
2	D	75	ILE
2	D	76	SER
2	D	78	VAL
2	D	80	ARG
2	D	85	THR
2	D	109	ILE
2	D	112	THR
2	D	125	ASP

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Mol	Chain	Res	Type
2	D	128	LEU
2	D	135	VAL
2	D	136	VAL
2	D	138	LEU
2	D	150	GLN
2	D	163	GLN
2	D	172	LYS
2	D	175	THR
2	D	179	SER
2	D	184	LEU
1	E	1	GLN
1	E	11	LEU
1	E	13	THR
1	E	21	THR
1	E	25	SER
1	E	29	LEU
1	E	34	LEU
1	E	35	ASN
1	E	43	LYS
1	E	57	SER
1	E	62	SER
1	E	67	ARG
1	E	73	THR
1	E	76	THR
1	E	77	VAL
1	E	78	THR
1	E	82	THR
1	E	91	THR
1	E	104	PHE
1	E	117	SER
1	E	120	THR
1	E	142	LEU
1	E	144	CYS
1	E	147	LYS
1	E	152	GLU
1	E	173	VAL
1	E	174	LEU
1	E	182	LEU
1	E	183	SER
1	E	193	LEU
1	E	195	THR
1	E	196	GLN

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Mol	Chain	Res	Type
1	E	197	THR
1	E	199	ILE
1	E	212	ASP
2	F	1	GLU
2	F	2	LEU
2	F	12	SER
2	F	18	THR
2	F	27	GLN
2	F	32	TRP
2	F	33	LEU
2	F	34	SER
2	F	42	GLN
2	F	53	ASN
2	F	63	MET
2	F	65	SER
2	F	69	THR
2	F	75	ILE
2	F	76	SER
2	F	78	VAL
2	F	80	ARG
2	F	85	THR
2	F	109	ILE
2	F	112	THR
2	F	125	ASP
2	F	128	LEU
2	F	135	VAL
2	F	136	VAL
2	F	138	LEU
2	F	150	GLN
2	F	163	GLN
2	F	172	LYS
2	F	175	THR
2	F	178	LEU
2	F	179	SER
2	F	184	LEU
1	G	11	LEU
1	G	13	THR
1	G	21	THR
1	G	25	SER
1	G	29	LEU
1	G	34	LEU
1	G	35	ASN

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Mol	Chain	Res	Type
1	G	57	SER
1	G	62	SER
1	G	67	ARG
1	G	71	SER
1	G	73	THR
1	G	76	THR
1	G	77	VAL
1	G	78	THR
1	G	82	THR
1	G	91	THR
1	G	104	PHE
1	G	117	SER
1	G	120	THR
1	G	142	LEU
1	G	144	CYS
1	G	147	LYS
1	G	152	GLU
1	G	173	VAL
1	G	174	LEU
1	G	182	LEU
1	G	183	SER
1	G	193	LEU
1	G	195	THR
1	G	196	GLN
1	G	197	THR
1	G	199	ILE
1	G	212	ASP
1	H	1	GLN
1	H	11	LEU
1	H	13	THR
1	H	21	THR
1	H	25	SER
1	H	29	LEU
1	H	34	LEU
1	H	35	ASN
1	H	57	SER
1	H	62	SER
1	H	67	ARG
1	H	71	SER
1	H	73	THR
1	H	76	THR
1	H	77	VAL

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Mol	Chain	Res	Type
1	H	78	THR
1	H	82	THR
1	H	91	THR
1	H	104	PHE
1	H	117	SER
1	H	120	THR
1	H	142	LEU
1	H	144	CYS
1	H	147	LYS
1	H	152	GLU
1	H	173	VAL
1	H	174	LEU
1	H	182	LEU
1	H	183	SER
1	H	193	LEU
1	H	195	THR
1	H	196	GLN
1	H	197	THR
1	H	199	ILE
1	H	212	ASP
2	I	1	GLU
2	I	2	LEU
2	I	12	SER
2	I	18	THR
2	I	27	GLN
2	I	32	TRP
2	I	33	LEU
2	I	34	SER
2	I	42	GLN
2	I	53	ASN
2	I	63	MET
2	I	65	SER
2	I	69	THR
2	I	75	ILE
2	I	76	SER
2	I	78	VAL
2	I	80	ARG
2	I	85	THR
2	I	109	ILE
2	I	112	THR
2	I	125	ASP
2	I	128	LEU

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Mol	Chain	Res	Type
2	I	135	VAL
2	I	136	VAL
2	I	150	GLN
2	I	163	GLN
2	I	172	LYS
2	I	175	THR
2	I	179	SER
2	I	184	LEU
1	J	1	GLN
1	J	11	LEU
1	J	13	THR
1	J	21	THR
1	J	25	SER
1	J	29	LEU
1	J	34	LEU
1	J	35	ASN
1	J	57	SER
1	J	62	SER
1	J	67	ARG
1	J	73	THR
1	J	76	THR
1	J	77	VAL
1	J	78	THR
1	J	82	THR
1	J	91	THR
1	J	104	PHE
1	J	117	SER
1	J	120	THR
1	J	142	LEU
1	J	144	CYS
1	J	147	LYS
1	J	173	VAL
1	J	174	LEU
1	J	182	LEU
1	J	183	SER
1	J	193	LEU
1	J	195	THR
1	J	196	GLN
1	J	197	THR
1	J	199	ILE
1	J	212	ASP
2	K	1	GLU

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Mol	Chain	Res	Type
2	K	2	LEU
2	K	12	SER
2	K	18	THR
2	K	27	GLN
2	K	32	TRP
2	K	33	LEU
2	K	34	SER
2	K	42	GLN
2	K	53	ASN
2	K	63	MET
2	K	65	SER
2	K	69	THR
2	K	75	ILE
2	K	78	VAL
2	K	80	ARG
2	K	85	THR
2	K	109	ILE
2	K	112	THR
2	K	125	ASP
2	K	128	LEU
2	K	135	VAL
2	K	136	VAL
2	K	138	LEU
2	K	150	GLN
2	K	163	GLN
2	K	172	LYS
2	K	175	THR
2	K	178	LEU
2	K	179	SER
2	K	184	LEU
2	L	1	GLU
2	L	2	LEU
2	L	12	SER
2	L	18	THR
2	L	27	GLN
2	L	32	TRP
2	L	33	LEU
2	L	34	SER
2	L	42	GLN
2	L	53	ASN
2	L	63	MET
2	L	65	SER

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Mol	Chain	Res	Type
2	L	69	THR
2	L	75	ILE
2	L	78	VAL
2	L	80	ARG
2	L	85	THR
2	L	109	ILE
2	L	112	THR
2	L	125	ASP
2	L	128	LEU
2	L	135	VAL
2	L	136	VAL
2	L	138	LEU
2	L	150	GLN
2	L	163	GLN
2	L	172	LYS
2	L	175	THR
2	L	179	SER
2	L	184	LEU
3	M	11	ASP
3	M	20	LYS
3	M	22	LEU
3	M	30	ASN
3	M	34	THR
3	M	49	GLN
3	M	64	LEU
3	N	10	GLU
3	N	11	ASP
3	N	20	LYS
3	N	22	LEU
3	N	30	ASN
3	N	34	THR
3	N	49	GLN
3	N	64	LEU
3	O	10	GLU
3	O	20	LYS
3	O	22	LEU
3	O	30	ASN
3	O	34	THR
3	O	49	GLN
3	O	64	LEU
3	P	20	LYS
3	P	22	LEU

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Mol	Chain	Res	Type
3	P	30	ASN
3	P	34	THR
3	P	49	GLN
3	P	64	LEU
3	Q	10	GLU
3	Q	11	ASP
3	Q	20	LYS
3	Q	22	LEU
3	Q	30	ASN
3	Q	34	THR
3	Q	49	GLN
3	Q	64	LEU
3	R	10	GLU
3	R	14	LYS
3	R	20	LYS
3	R	22	LEU
3	R	30	ASN
3	R	34	THR
3	R	49	GLN
3	R	64	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
2	B	37	GLN
2	B	150	GLN
2	B	201	HIS
2	B	202	GLN
1	C	1	GLN
1	C	203	ASN
2	D	37	GLN
2	D	150	GLN
2	D	163	GLN
2	D	169	GLN
2	D	201	HIS
2	D	202	GLN
1	E	1	GLN
1	E	203	ASN
1	E	208	ASN
2	F	37	GLN
2	F	150	GLN

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Mol	Chain	Res	Type
2	F	169	GLN
2	F	201	HIS
2	F	202	GLN
1	G	1	GLN
1	G	203	ASN
1	H	1	GLN
1	H	203	ASN
1	H	208	ASN
2	I	37	GLN
2	I	127	GLN
2	I	150	GLN
2	I	169	GLN
2	I	201	HIS
1	J	1	GLN
1	J	39	GLN
1	J	203	ASN
1	J	208	ASN
2	K	37	GLN
2	K	38	GLN
2	K	127	GLN
2	K	169	GLN
2	K	201	HIS
2	K	202	GLN
2	L	37	GLN
2	L	127	GLN
2	L	150	GLN
2	L	201	HIS
2	L	202	GLN
3	M	24	GLN
3	M	51	GLN
3	N	24	GLN
3	N	51	GLN
3	O	24	GLN
3	O	51	GLN
3	P	24	GLN
3	P	49	GLN
3	P	51	GLN
3	Q	24	GLN
3	Q	49	GLN
3	Q	51	GLN
3	R	24	GLN
3	R	51	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	221/231 (95%)	-0.92	0 100 100	75, 114, 192, 246	0
1	C	221/231 (95%)	-0.59	0 100 100	102, 173, 235, 263	0
1	E	221/231 (95%)	-0.82	0 100 100	78, 118, 191, 251	0
1	G	221/231 (95%)	-0.56	1 (0%) 87 75	100, 175, 246, 265	0
1	H	221/231 (95%)	-0.88	0 100 100	67, 113, 195, 224	0
1	J	221/231 (95%)	-0.86	0 100 100	74, 119, 201, 236	0
2	B	217/217 (100%)	-0.89	0 100 100	73, 116, 189, 208	0
2	D	217/217 (100%)	-0.70	0 100 100	98, 156, 248, 263	0
2	F	217/217 (100%)	-0.81	0 100 100	74, 113, 200, 229	0
2	I	217/217 (100%)	-0.66	0 100 100	88, 149, 251, 283	0
2	K	217/217 (100%)	-0.81	0 100 100	75, 116, 188, 222	0
2	L	217/217 (100%)	-0.88	0 100 100	76, 116, 186, 211	0
3	M	57/115 (49%)	-0.68	0 100 100	109, 164, 278, 284	0
3	N	57/115 (49%)	-0.75	0 100 100	96, 155, 287, 298	0
3	O	57/115 (49%)	-0.59	0 100 100	97, 151, 278, 287	0
3	P	57/115 (49%)	-0.54	0 100 100	119, 165, 276, 280	0
3	Q	57/115 (49%)	-0.79	0 100 100	98, 151, 275, 277	0
3	R	57/115 (49%)	-0.64	0 100 100	95, 156, 274, 280	0
All	All	2970/3378 (87%)	-0.77	1 (0%) 100 100	67, 129, 236, 298	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	187	THR	2.5

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.