



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:04 PM EDT

PDB ID : 3QPR / pdb_00003qpr
Title : HK97 Prohead I encapsidating inactive virally encoded protease
Authors : Huang, R.K.; Khayat, R.; Lee, K.K.; Gertsman, I.; Duda, R.L.; Hendrix, R.W.; Johnson, J.E.
Deposited on : 2011-02-14
Resolution : 5.20 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

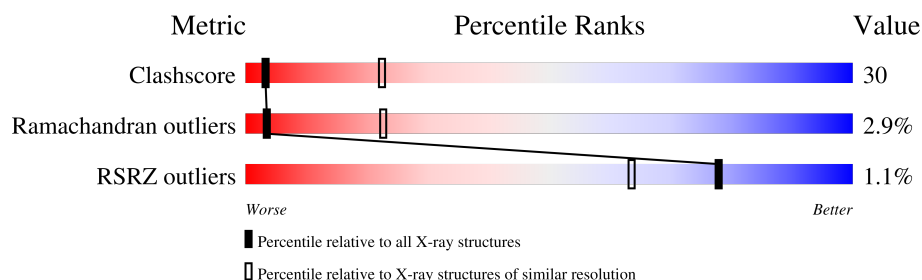
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.20 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))
Clashscore	190562	1066 (6.38-4.00)
Ramachandran outliers	187476	1004 (6.46-3.94)
RSRZ outliers	180081	1006 (6.38-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	385	% 48% 16% • 34%
1	B	385	2% 42% 19% • 35%
1	C	385	44% 17% • 36%
1	D	385	% 50% 13% • 34%
1	E	385	% 42% 21% • 34%
1	F	385	% 39% 21% 5% 36%
1	G	385	42% 17% 5% 36%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8654 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.

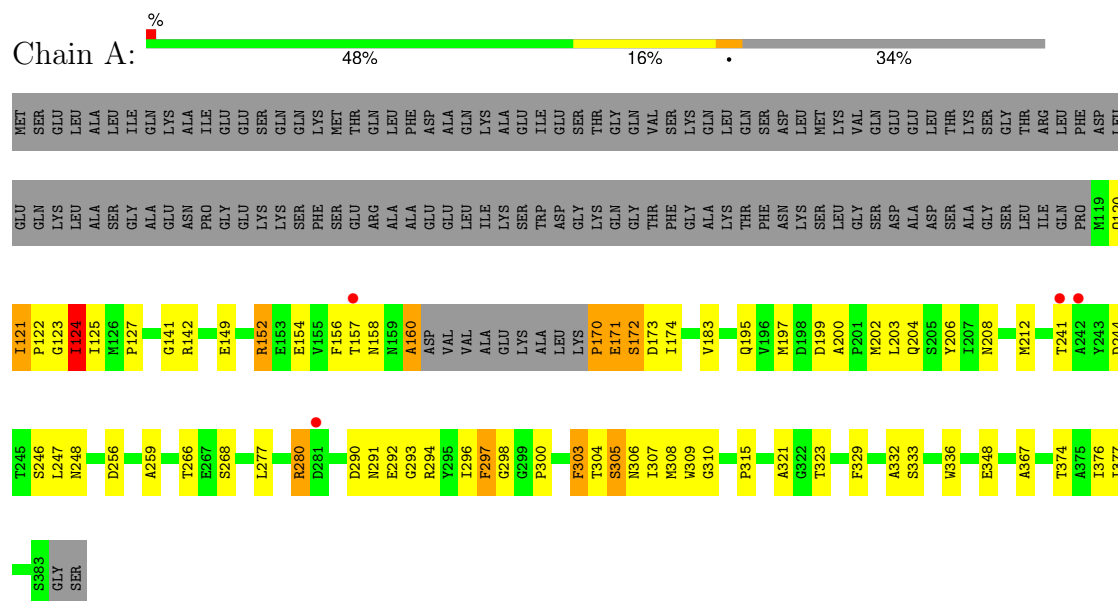
- Molecule 1 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	0	0	0
			1260	748	256	256			
1	B	250	Total	C	N	O	0	0	0
			1231	731	250	250			
1	C	248	Total	C	N	O	0	0	0
			1221	725	248	248			
1	D	254	Total	C	N	O	0	0	0
			1250	742	254	254			
1	E	255	Total	C	N	O	0	0	0
			1255	745	255	255			
1	F	248	Total	C	N	O	0	0	0
			1221	725	248	248			
1	G	247	Total	C	N	O	0	0	0
			1216	722	247	247			

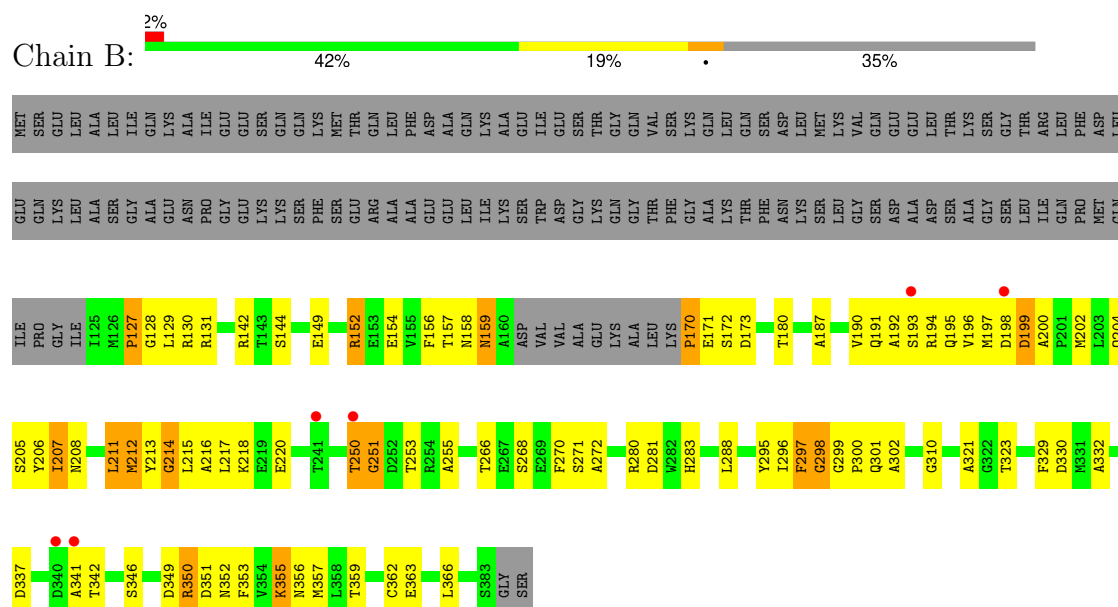
3 Residue-property plots

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: Major capsid protein

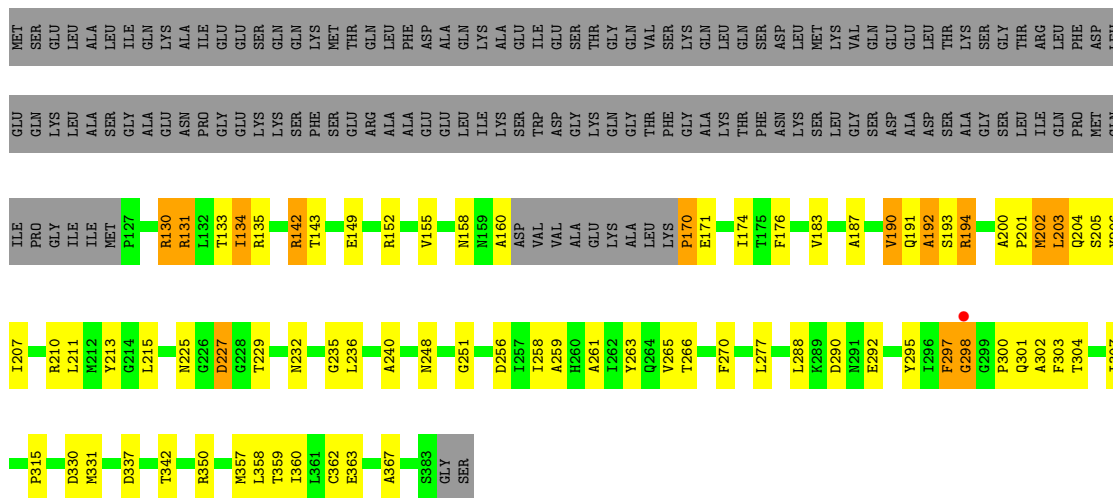


• Molecule 1: Major capsid protein



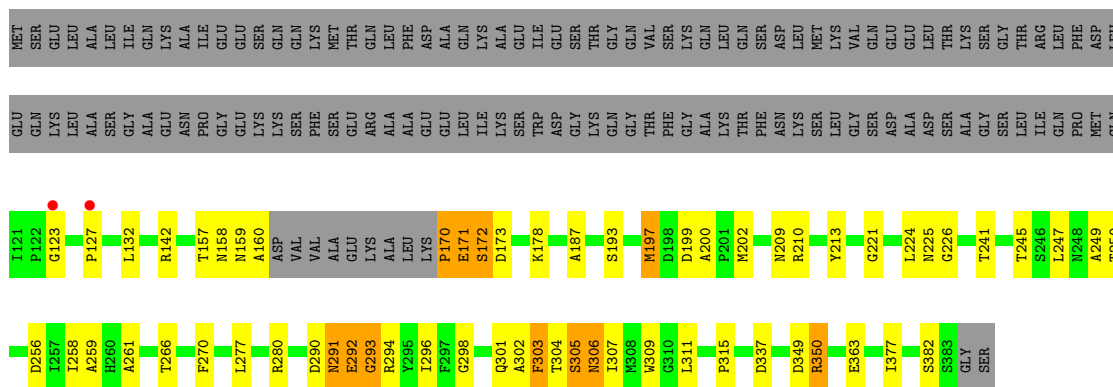
- Molecule 1: Major capsid protein

Chain C:



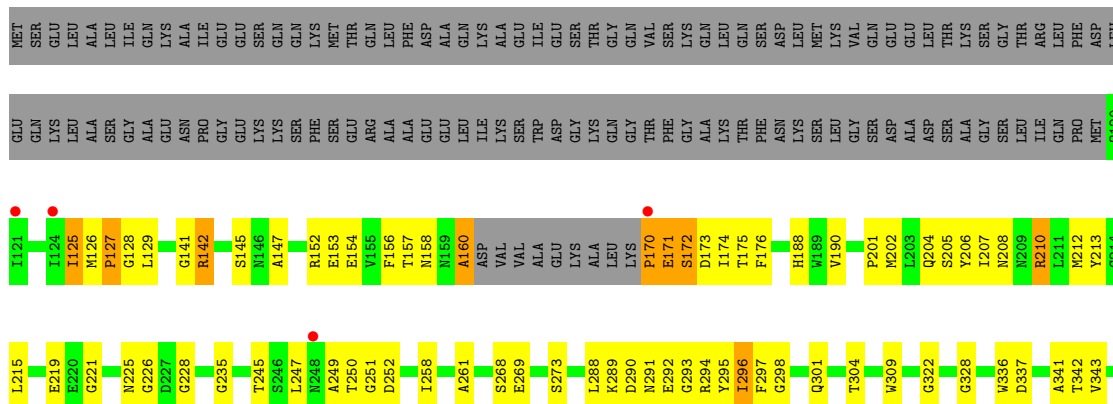
- Molecule 1: Major capsid protein

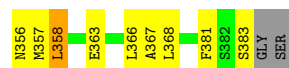
Chain D:



- Molecule 1: Major capsid protein

Chain E:





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	560.12Å 560.12Å 560.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 5.20 45.00 – 5.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (45.00-5.20) 77.3 (45.00-5.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 5.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.461 , 0.467 0.390 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	175.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 417.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	0.125 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.60	EDS
Total number of atoms	8654	wwPDB-VP
Average B, all atoms (Å ²)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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	0.64	1/1259 (0.1%)	1.43	34/1749 (1.9%)
1	B	0.67	1/1230 (0.1%)	1.40	21/1709 (1.2%)
1	C	0.54	1/1220 (0.1%)	1.27	16/1695 (0.9%)
1	D	0.54	0/1249	1.37	18/1735 (1.0%)
1	E	0.51	0/1254	1.40	20/1742 (1.1%)
1	F	0.72	1/1220 (0.1%)	1.54	37/1695 (2.2%)
1	G	0.62	0/1215	1.71	44/1688 (2.6%)
All	All	0.61	4/8647 (0.0%)	1.45	190/12013 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	MET	C-N	-9.41	1.22	1.33
1	C	288	LEU	C-N	7.19	1.42	1.33
1	B	190	VAL	C-N	-6.66	1.24	1.33
1	F	134	ILE	CA-CB	-5.10	1.47	1.54

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	125	ILE	N-CA-C	19.33	129.05	110.30
1	G	297	PHE	N-CA-C	-19.00	86.10	112.13
1	G	207	ILE	N-CA-C	15.30	125.11	110.42
1	A	298	GLY	N-CA-C	14.98	135.37	115.59
1	D	250	THR	N-CA-C	14.43	127.05	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	228	GLY	N-CA-C	13.29	133.66	115.32
1	D	123	GLY	N-CA-C	-12.64	92.50	112.85
1	B	355	LYS	N-CA-C	-12.48	97.36	111.71
1	F	349	ASP	N-CA-C	12.35	128.50	110.10
1	G	136	ASP	N-CA-C	-11.83	98.85	113.28
1	F	250	THR	N-CA-C	-11.64	95.11	110.24
1	B	250	THR	N-CA-C	11.54	125.10	111.02
1	D	157	THR	N-CA-C	-10.87	95.58	110.68
1	E	157	THR	N-CA-C	-10.84	95.61	110.68
1	F	157	THR	N-CA-C	-10.84	95.61	110.68
1	B	157	THR	N-CA-C	-10.84	95.61	110.68
1	C	297	PHE	N-CA-C	-10.76	93.90	109.18
1	G	210	ARG	N-CA-C	10.74	127.99	111.56
1	G	132	LEU	N-CA-C	-10.73	98.12	112.72
1	G	227	ASP	N-CA-C	10.49	126.21	113.41
1	G	296	ILE	N-CA-C	10.06	130.27	109.34
1	E	125	ILE	CB-CA-C	-9.89	99.45	111.81
1	E	126	MET	N-CA-C	9.73	131.31	109.81
1	A	125	ILE	N-CA-C	-9.61	97.18	109.58
1	A	348	GLU	N-CA-C	9.61	125.96	107.71
1	D	305	SER	N-CA-C	-9.59	100.83	111.28
1	C	170	PRO	N-CA-C	-9.48	92.95	112.47
1	G	207	ILE	CB-CA-C	-9.48	99.84	111.97
1	B	250	THR	CB-CA-C	-9.45	95.89	110.92
1	G	281	ASP	N-CA-C	-9.25	101.77	112.87
1	C	194	ARG	N-CA-C	9.09	121.19	111.28
1	B	128	GLY	N-CA-C	-9.08	91.65	113.18
1	A	303	PHE	N-CA-C	9.01	122.06	111.71
1	G	355	LYS	N-CA-C	-8.97	91.57	108.17
1	C	307	ILE	N-CA-C	-8.93	96.04	108.27
1	G	296	ILE	CB-CA-C	-8.91	96.67	111.29
1	G	209	ASN	CB-CA-C	8.91	125.12	110.24
1	G	288	LEU	CA-C-N	-8.87	109.64	122.94
1	G	288	LEU	C-N-CA	-8.87	109.64	122.94
1	F	212	MET	O-C-N	8.79	131.23	122.09
1	A	157	THR	N-CA-C	-8.56	97.44	110.70
1	F	257	ILE	CB-CA-C	-8.45	101.24	111.81
1	G	197	MET	N-CA-C	8.43	128.75	110.80
1	D	172	SER	N-CA-C	-8.23	103.75	113.21
1	F	204	GLN	N-CA-C	-8.06	101.18	111.02
1	E	207	ILE	N-CA-C	8.02	118.80	110.62
1	A	122	PRO	N-CA-C	-7.92	97.52	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	331	MET	N-CA-CB	-7.90	98.38	111.49
1	G	157	THR	N-CA-C	-7.80	101.51	111.02
1	A	348	GLU	CB-CA-C	-7.73	100.39	111.76
1	G	135	ARG	N-CA-C	7.73	120.60	111.71
1	G	298	GLY	N-CA-C	7.72	131.47	113.18
1	B	211	LEU	N-CA-C	7.66	120.75	111.40
1	C	227	ASP	N-CA-C	-7.66	97.53	109.25
1	A	303	PHE	CB-CA-C	-7.66	96.47	110.63
1	G	194	ARG	N-CA-C	7.65	120.74	111.40
1	A	297	PHE	CB-CA-C	-7.56	95.92	110.35
1	F	356	ASN	N-CA-C	-7.56	98.27	109.15
1	F	348	GLU	CB-CA-C	7.53	125.41	110.42
1	F	332	ALA	N-CA-CB	-7.50	100.53	110.88
1	B	272	ALA	N-CA-C	7.50	120.95	108.73
1	A	307	ILE	CB-CA-C	-7.48	99.74	110.82
1	F	143	THR	CB-CA-C	-7.42	96.63	111.91
1	F	349	ASP	N-CA-CB	-7.29	98.54	109.69
1	B	130	ARG	N-CA-C	-7.18	104.26	112.87
1	D	226	GLY	N-CA-C	7.10	130.01	113.18
1	A	121	ILE	N-CA-C	7.08	115.16	108.15
1	E	210	ARG	N-CA-C	7.02	118.94	111.28
1	G	272	ALA	CB-CA-C	-6.95	97.76	109.65
1	F	172	SER	N-CA-C	-6.92	105.64	112.97
1	G	172	SER	N-CA-C	-6.91	105.65	112.97
1	C	330	ASP	CB-CA-C	6.89	122.39	110.68
1	A	124	ILE	N-CA-C	6.81	123.50	109.34
1	F	258	ILE	N-CA-C	-6.79	102.11	111.89
1	D	178	LYS	N-CA-C	-6.77	101.60	110.53
1	A	280	ARG	N-CA-C	6.64	122.27	111.37
1	B	214	GLY	N-CA-C	-6.63	104.56	113.24
1	C	143	THR	N-CA-CB	-6.59	101.15	111.56
1	D	197	MET	N-CA-C	6.55	121.19	111.04
1	C	251	GLY	N-CA-C	6.53	123.40	114.92
1	A	127	PRO	CB-CA-C	-6.48	100.88	111.56
1	G	133	THR	CB-CA-C	-6.47	109.12	116.63
1	E	172	SER	N-CA-C	-6.45	105.70	112.93
1	A	172	SER	N-CA-C	-6.45	105.71	112.93
1	D	193	SER	N-CA-C	6.41	118.83	110.43
1	G	132	LEU	N-CA-CB	6.40	120.65	110.22
1	G	155	VAL	CB-CA-C	-6.39	100.81	111.29
1	G	350	ARG	N-CA-C	6.38	118.02	108.31
1	D	132	LEU	N-CA-CB	-6.35	100.80	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	170	PRO	N-CA-C	6.33	125.52	112.47
1	F	170	PRO	N-CA-C	6.33	125.52	112.47
1	A	170	PRO	N-CA-C	6.32	125.50	112.47
1	G	170	PRO	N-CA-C	6.32	125.48	112.47
1	G	173	ASP	N-CA-C	-6.32	102.38	110.53
1	B	204	GLN	N-CA-C	6.29	121.69	111.37
1	F	173	ASP	N-CA-C	-6.28	102.43	110.53
1	B	298	GLY	N-CA-C	-6.23	99.62	110.71
1	F	251	GLY	N-CA-C	6.20	123.60	115.36
1	G	137	LEU	N-CA-CB	-6.19	100.75	110.46
1	D	291	ASN	N-CA-C	-6.16	104.36	113.72
1	C	202	MET	N-CA-C	6.16	117.99	111.28
1	F	294	ARG	N-CA-CB	-6.13	100.21	111.37
1	G	273	SER	N-CA-CB	-6.13	101.51	110.40
1	A	120	GLN	CB-CA-C	-6.12	97.19	111.09
1	E	201	PRO	N-CA-CB	6.09	110.03	103.33
1	F	366	LEU	CB-CA-C	-6.09	97.04	111.65
1	F	273	SER	CB-CA-C	6.08	119.24	109.02
1	B	271	SER	CB-CA-C	-6.07	99.89	111.48
1	B	212	MET	N-CA-C	-6.06	104.36	110.97
1	F	331	MET	N-CA-C	6.05	120.25	112.26
1	C	201	PRO	N-CA-CB	5.99	109.92	103.33
1	F	250	THR	CB-CA-C	5.98	120.23	109.64
1	E	204	GLN	N-CA-C	5.97	117.79	111.28
1	E	252	ASP	N-CA-C	-5.96	101.65	110.48
1	A	149	GLU	CB-CA-C	-5.91	98.90	109.71
1	F	145	SER	CB-CA-C	-5.89	99.38	110.51
1	G	290	ASP	N-CA-C	-5.87	101.59	110.28
1	G	209	ASN	N-CA-CB	-5.87	100.47	110.33
1	E	127	PRO	CB-CA-C	5.86	121.22	111.56
1	E	142	ARG	N-CA-CB	-5.80	101.32	110.77
1	D	350	ARG	N-CA-CB	5.79	120.28	110.49
1	A	333	SER	N-CA-CB	5.77	119.70	111.05
1	F	134	ILE	CB-CA-C	-5.76	101.85	111.29
1	F	144	SER	N-CA-CB	-5.75	102.94	110.88
1	A	171	GLU	N-CA-C	-5.73	98.54	108.52
1	E	171	GLU	N-CA-C	-5.73	98.54	108.52
1	F	355	LYS	N-CA-C	-5.73	99.84	109.07
1	G	171	GLU	N-CA-C	-5.72	98.57	108.52
1	F	171	GLU	N-CA-C	-5.72	98.57	108.52
1	B	366	LEU	CB-CA-C	-5.71	98.09	109.79
1	D	249	ALA	CB-CA-C	-5.70	101.54	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	250	THR	N-CA-C	-5.69	104.28	111.11
1	E	293	GLY	N-CA-C	-5.66	99.77	113.18
1	D	171	GLU	N-CA-CB	5.65	120.04	110.49
1	B	159	ASN	N-CA-C	-5.65	103.18	110.19
1	F	135	ARG	N-CA-C	-5.65	105.00	112.34
1	F	350	ARG	CB-CA-C	-5.62	110.11	116.63
1	G	135	ARG	CB-CA-C	-5.62	100.23	110.63
1	B	194	ARG	N-CA-C	5.59	119.80	113.15
1	A	248	ASN	N-CA-C	-5.58	102.75	110.35
1	G	174	ILE	N-CA-C	5.57	115.88	107.80
1	F	174	ILE	N-CA-C	5.55	115.85	107.80
1	A	160	ALA	N-CA-C	5.55	122.07	109.81
1	B	288	LEU	O-C-N	-5.55	116.59	123.36
1	G	160	ALA	N-CA-C	5.54	122.06	109.81
1	F	160	ALA	N-CA-C	5.54	122.04	109.81
1	A	305	SER	N-CA-C	-5.52	99.04	110.80
1	E	381	PHE	N-CA-C	-5.52	101.48	109.59
1	E	160	ALA	N-CA-C	5.50	121.97	109.81
1	C	142	ARG	CB-CA-C	-5.50	100.58	111.91
1	A	149	GLU	N-CA-C	5.49	117.85	108.90
1	G	366	LEU	CB-CA-C	-5.48	100.43	111.17
1	C	158	ASN	N-CA-C	5.46	117.41	109.71
1	F	253	THR	CB-CA-C	-5.43	100.84	109.80
1	E	174	ILE	N-CA-C	5.43	115.91	107.99
1	F	298	GLY	N-CA-C	5.43	122.75	115.59
1	A	307	ILE	N-CA-CB	-5.39	104.97	112.52
1	A	174	ILE	N-CA-C	5.37	115.83	107.99
1	D	210	ARG	N-CA-C	5.37	119.78	111.56
1	F	152	ARG	CA-C-N	-5.37	111.29	121.54
1	F	152	ARG	C-N-CA	-5.37	111.29	121.54
1	G	131	ARG	N-CA-C	-5.35	100.52	109.24
1	F	129	LEU	N-CA-C	-5.34	107.31	113.88
1	G	280	ARG	CB-CA-C	-5.34	100.92	110.70
1	B	152	ARG	CA-C-N	-5.33	111.36	121.54
1	B	152	ARG	C-N-CA	-5.33	111.36	121.54
1	A	152	ARG	CA-C-N	-5.32	111.37	121.54
1	A	152	ARG	C-N-CA	-5.32	111.37	121.54
1	F	272	ALA	CB-CA-C	-5.32	100.56	109.65
1	A	291	ASN	N-CA-C	-5.30	107.18	113.38
1	A	333	SER	N-CA-C	-5.30	101.70	109.81
1	C	130	ARG	N-CA-C	5.28	122.04	110.80
1	E	221	GLY	N-CA-C	-5.28	106.25	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	350	ARG	CB-CA-C	-5.24	110.51	116.54
1	G	273	SER	N-CA-C	5.23	120.14	113.55
1	G	300	PRO	N-CA-C	-5.23	105.30	113.78
1	A	307	ILE	N-CA-C	5.16	116.33	108.80
1	A	306	ASN	N-CA-C	-5.13	99.41	108.08
1	F	360	ILE	CB-CA-C	-5.11	103.22	110.83
1	D	292	GLU	N-CA-C	-5.10	100.99	108.99
1	G	358	LEU	N-CA-CB	-5.09	103.34	111.43
1	E	349	ASP	N-CA-C	5.06	117.56	110.23
1	D	224	LEU	N-CA-C	5.05	117.76	111.24
1	A	247	LEU	N-CA-C	5.04	117.55	111.40
1	B	272	ALA	N-CA-CB	-5.04	102.20	110.42
1	D	250	THR	CB-CA-C	-5.03	103.16	110.95
1	G	158	ASN	CB-CA-C	-5.03	110.39	117.23
1	A	122	PRO	CB-CA-C	-5.03	106.26	113.09
1	B	251	GLY	N-CA-C	5.01	127.83	113.30
1	C	200	ALA	N-CA-C	5.00	116.19	109.83

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	362	CYS	Mainchain

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	1260	0	595	46	0
1	B	1231	0	583	84	0
1	C	1221	0	580	54	0
1	D	1250	0	591	44	0
1	E	1255	0	593	76	0
1	F	1221	0	580	67	0
1	G	1216	0	578	55	0
All	All	8654	0	4100	389	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 30.

All (389) 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:B:158:ASN:CB	1:B:172:SER:HA	1.21	1.57
1:B:158:ASN:CB	1:B:172:SER:CA	2.08	1.31
1:E:202:MET:HA	1:F:142:ARG:O	1.26	1.26
1:B:193:SER:CB	1:C:149:GLU:CB	2.14	1.26
1:A:293:GLY:O	1:C:298:GLY:CA	1.84	1.24
1:A:293:GLY:O	1:C:298:GLY:HA2	1.07	1.20
1:B:192:ALA:O	1:B:357:MET:CB	1.91	1.18
1:E:152:ARG:CB	1:E:371:TYR:HA	1.77	1.15
1:E:202:MET:CA	1:F:142:ARG:O	1.93	1.15
1:D:293:GLY:HA3	1:F:298:GLY:HA2	1.18	1.12
1:B:212:MET:O	1:B:215:LEU:N	1.83	1.10
1:B:250:THR:CB	1:B:251:GLY:HA3	1.78	1.10
1:A:202:MET:HA	1:B:142:ARG:O	1.50	1.09
1:E:202:MET:CB	1:F:143:THR:HA	1.83	1.07
1:D:293:GLY:CA	1:F:298:GLY:HA2	1.85	1.06
1:E:152:ARG:CB	1:E:371:TYR:O	2.02	1.06
1:G:194:ARG:HA	1:G:197:MET:CB	1.88	1.03
1:G:132:LEU:CB	1:G:136:ASP:CB	2.41	0.99
1:C:192:ALA:O	1:C:358:LEU:N	1.97	0.98
1:A:200:ALA:HB1	1:B:144:SER:H	1.30	0.95
1:E:202:MET:CB	1:F:142:ARG:O	2.16	0.94
1:A:293:GLY:C	1:C:298:GLY:HA2	1.93	0.93
1:E:152:ARG:CB	1:E:371:TYR:CA	2.45	0.93
1:B:170:PRO:C	1:B:172:SER:CB	2.43	0.91
1:D:293:GLY:C	1:F:298:GLY:HA3	1.97	0.90
1:B:250:THR:CB	1:B:251:GLY:CA	2.49	0.88
1:D:293:GLY:C	1:F:298:GLY:CA	2.47	0.88
1:B:127:PRO:C	1:B:129:LEU:H	1.82	0.87
1:G:187:ALA:HB2	1:G:363:GLU:HA	1.56	0.87
1:G:352:ASN:O	1:G:355:LYS:O	1.94	0.85
1:C:183:VAL:HA	1:C:367:ALA:HB2	1.58	0.85
1:G:290:ASP:C	1:G:292:GLU:H	1.80	0.85
1:B:202:MET:CB	1:C:142:ARG:O	2.24	0.85
1:E:125:ILE:CB	1:E:212:MET:CB	2.56	0.84
1:A:141:GLY:O	1:A:336:TRP:HA	1.77	0.83
1:D:293:GLY:HA3	1:F:298:GLY:CA	2.04	0.83
1:E:343:VAL:HA	1:E:361:LEU:O	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:SER:HA	1:C:358:LEU:H	1.44	0.82
1:E:152:ARG:CB	1:E:371:TYR:C	2.52	0.82
1:F:134:ILE:O	1:F:137:LEU:N	2.10	0.82
1:G:128:GLY:C	1:G:130:ARG:N	2.30	0.81
1:G:192:ALA:O	1:G:358:LEU:N	2.10	0.81
1:G:290:ASP:C	1:G:292:GLU:N	2.35	0.81
1:F:253:THR:O	1:F:254:ARG:C	2.21	0.81
1:F:342:THR:O	1:F:362:CYS:HA	1.79	0.81
1:G:129:LEU:C	1:G:131:ARG:H	1.87	0.81
1:B:193:SER:HA	1:B:357:MET:CB	2.10	0.81
1:B:170:PRO:O	1:B:172:SER:CB	2.30	0.80
1:B:207:ILE:O	1:B:211:LEU:CB	2.28	0.80
1:E:356:ASN:CB	1:E:357:MET:HA	2.09	0.80
1:C:187:ALA:HB2	1:C:363:GLU:HA	1.65	0.79
1:A:183:VAL:HA	1:A:367:ALA:HB2	1.66	0.76
1:F:226:GLY:H	1:F:235:GLY:HA3	1.51	0.76
1:A:308:MET:C	1:A:310:GLY:H	1.93	0.76
1:D:171:GLU:C	1:D:173:ASP:H	1.94	0.76
1:B:212:MET:O	1:B:213:TYR:C	2.28	0.75
1:B:296:ILE:C	1:B:298:GLY:N	2.42	0.74
1:E:382:SER:O	1:E:383:SER:CB	2.35	0.74
1:B:296:ILE:C	1:B:298:GLY:H	1.93	0.74
1:C:190:VAL:O	1:C:360:ILE:N	2.20	0.74
1:D:293:GLY:C	1:F:298:GLY:HA2	2.13	0.73
1:E:127:PRO:CB	1:E:213:TYR:HA	2.17	0.73
1:E:154:GLU:N	1:E:175:THR:O	2.22	0.72
1:F:249:ALA:O	1:F:250:THR:C	2.32	0.72
1:A:296:ILE:O	1:A:297:PHE:CB	2.37	0.72
1:E:142:ARG:HA	1:E:337:ASP:H	1.53	0.72
1:B:296:ILE:O	1:B:298:GLY:N	2.23	0.72
1:B:171:GLU:CA	1:B:172:SER:CB	2.69	0.71
1:B:202:MET:CA	1:C:142:ARG:O	2.39	0.71
1:F:129:LEU:O	1:F:130:ARG:CB	2.39	0.71
1:G:128:GLY:C	1:G:130:ARG:H	1.97	0.70
1:G:278:ASN:O	1:G:280:ARG:N	2.24	0.70
1:B:159:ASN:O	1:B:172:SER:CB	2.39	0.70
1:F:141:GLY:O	1:F:336:TRP:HA	1.91	0.70
1:D:209:ASN:O	1:D:213:TYR:CB	2.40	0.69
1:A:123:GLY:O	1:A:124:ILE:CB	2.40	0.69
1:E:346:SER:O	1:E:359:THR:CB	2.41	0.69
1:D:305:SER:O	1:D:307:ILE:N	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:MET:O	1:C:205:SER:N	2.27	0.68
1:B:216:ALA:O	1:B:217:LEU:C	2.34	0.68
1:E:342:THR:O	1:E:362:CYS:HA	1.93	0.68
1:E:352:ASN:O	1:E:355:LYS:N	2.27	0.68
1:G:193:SER:O	1:G:197:MET:CB	2.42	0.67
1:E:205:SER:CB	1:F:140:GLN:O	2.43	0.67
1:E:153:GLU:HA	1:E:175:THR:O	1.95	0.67
1:B:158:ASN:CB	1:B:172:SER:N	2.57	0.67
1:C:225:ASN:HA	1:C:235:GLY:HA3	1.77	0.66
1:F:211:LEU:O	1:F:214:GLY:N	2.28	0.66
1:G:131:ARG:C	1:G:133:THR:H	2.00	0.65
1:A:308:MET:C	1:A:310:GLY:N	2.54	0.65
1:F:134:ILE:O	1:F:136:ASP:N	2.30	0.65
1:F:342:THR:O	1:F:362:CYS:CA	2.45	0.65
1:G:183:VAL:HA	1:G:367:ALA:HB2	1.79	0.64
1:E:226:GLY:H	1:E:235:GLY:HA3	1.63	0.64
1:E:304:THR:CB	1:F:309:TRP:O	2.45	0.64
1:D:296:ILE:C	1:D:298:GLY:H	2.05	0.64
1:B:171:GLU:N	1:B:172:SER:CB	2.60	0.64
1:A:308:MET:O	1:A:310:GLY:N	2.31	0.64
1:G:128:GLY:O	1:G:130:ARG:N	2.31	0.64
1:G:128:GLY:O	1:G:129:LEU:C	2.40	0.63
1:G:291:ASN:C	1:G:293:GLY:H	2.05	0.63
1:F:203:LEU:O	1:F:204:GLN:C	2.39	0.63
1:F:292:GLU:O	1:F:294:ARG:N	2.30	0.63
1:E:296:ILE:O	1:E:298:GLY:O	2.16	0.62
1:F:133:THR:O	1:F:134:ILE:C	2.42	0.62
1:B:171:GLU:HA	1:B:172:SER:C	2.24	0.62
1:B:353:PHE:O	1:B:356:ASN:HA	1.99	0.62
1:E:125:ILE:O	1:E:208:ASN:O	2.18	0.62
1:E:206:TYR:O	1:E:210:ARG:CB	2.47	0.62
1:C:192:ALA:O	1:C:357:MET:C	2.42	0.62
1:B:351:ASP:O	1:B:355:LYS:N	2.23	0.61
1:E:349:ASP:O	1:E:353:PHE:CB	2.48	0.61
1:A:280:ARG:HA	1:B:310:GLY:HA3	1.82	0.61
1:E:202:MET:HA	1:F:142:ARG:C	2.19	0.61
1:D:302:ALA:O	1:D:304:THR:N	2.33	0.61
1:A:293:GLY:O	1:C:298:GLY:HA3	1.94	0.60
1:E:127:PRO:CB	1:E:213:TYR:CA	2.78	0.60
1:F:266:THR:HA	1:F:270:PHE:O	2.01	0.60
1:A:156:PHE:C	1:A:158:ASN:H	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:ASP:O	1:D:350:ARG:C	2.43	0.60
1:B:191:GLN:HA	1:B:359:THR:HA	1.84	0.60
1:D:302:ALA:O	1:D:305:SER:N	2.35	0.59
1:B:195:GLN:C	1:B:197:MET:H	2.11	0.59
1:B:171:GLU:HA	1:B:172:SER:CB	2.31	0.59
1:D:200:ALA:C	1:D:202:MET:H	2.11	0.59
1:G:329:PHE:HA	1:G:332:ALA:HB3	1.85	0.59
1:D:241:THR:O	1:D:377:ILE:HA	2.03	0.59
1:E:348:GLU:C	1:E:353:PHE:CB	2.75	0.59
1:A:300:PRO:HA	1:A:303:PHE:CB	2.33	0.59
1:E:288:LEU:O	1:E:295:TYR:HA	2.03	0.59
1:E:348:GLU:O	1:E:353:PHE:CB	2.52	0.58
1:G:187:ALA:CB	1:G:363:GLU:HA	2.30	0.58
1:E:290:ASP:C	1:E:292:GLU:H	2.11	0.58
1:G:278:ASN:O	1:G:279:PRO:C	2.46	0.58
1:B:299:GLY:O	1:B:302:ALA:N	2.37	0.58
1:G:195:GLN:C	1:G:197:MET:H	2.12	0.58
1:E:153:GLU:CA	1:E:175:THR:O	2.52	0.58
1:B:342:THR:O	1:B:362:CYS:HA	2.03	0.58
1:E:347:ARG:O	1:E:353:PHE:CB	2.52	0.58
1:G:226:GLY:H	1:G:235:GLY:HA3	1.68	0.58
1:D:301:GLN:O	1:D:302:ALA:C	2.47	0.58
1:A:202:MET:CA	1:B:142:ARG:O	2.39	0.57
1:E:296:ILE:C	1:E:298:GLY:N	2.61	0.57
1:F:134:ILE:C	1:F:136:ASP:N	2.56	0.57
1:A:156:PHE:C	1:A:158:ASN:N	2.60	0.57
1:B:205:SER:O	1:B:206:TYR:C	2.46	0.57
1:G:194:ARG:C	1:G:197:MET:H	2.13	0.57
1:B:299:GLY:O	1:B:300:PRO:C	2.48	0.57
1:B:198:ASP:O	1:B:200:ALA:N	2.38	0.57
1:E:125:ILE:C	1:E:212:MET:CB	2.77	0.57
1:G:290:ASP:O	1:G:292:GLU:N	2.38	0.56
1:E:273:SER:N	1:E:328:GLY:HA2	2.20	0.56
1:F:134:ILE:O	1:F:135:ARG:C	2.48	0.56
1:C:227:ASP:O	1:C:232:ASN:CB	2.53	0.56
1:C:266:THR:HA	1:C:270:PHE:O	2.05	0.56
1:F:142:ARG:HA	1:F:337:ASP:H	1.69	0.56
1:G:194:ARG:O	1:G:197:MET:N	2.39	0.56
1:G:352:ASN:O	1:G:355:LYS:C	2.49	0.56
1:G:335:VAL:HA	1:G:368:LEU:HA	1.88	0.56
1:E:289:LYS:HA	1:E:294:ARG:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:225:ASN:HA	1:F:235:GLY:HA3	1.88	0.55
1:G:194:ARG:CA	1:G:197:MET:CB	2.75	0.55
1:B:193:SER:CA	1:B:357:MET:CB	2.82	0.55
1:G:129:LEU:C	1:G:131:ARG:N	2.57	0.55
1:G:278:ASN:O	1:G:281:ASP:N	2.40	0.55
1:B:192:ALA:C	1:B:357:MET:CB	2.78	0.55
1:B:299:GLY:C	1:B:301:GLN:N	2.61	0.55
1:D:170:PRO:O	1:D:171:GLU:C	2.48	0.55
1:D:277:LEU:O	1:D:315:PRO:HA	2.06	0.55
1:G:280:ARG:C	1:G:282:TRP:N	2.56	0.55
1:F:249:ALA:C	1:F:250:THR:O	2.41	0.55
1:A:290:ASP:C	1:A:292:GLU:H	2.13	0.54
1:G:197:MET:O	1:G:199:ASP:N	2.36	0.54
1:B:129:LEU:C	1:B:131:ARG:N	2.64	0.54
1:E:153:GLU:HA	1:E:176:PHE:HA	1.88	0.54
1:A:156:PHE:O	1:A:158:ASN:N	2.37	0.54
1:E:127:PRO:CB	1:E:213:TYR:N	2.71	0.54
1:D:303:PHE:HA	1:D:306:ASN:CB	2.37	0.54
1:E:225:ASN:HA	1:E:235:GLY:HA3	1.88	0.54
1:D:290:ASP:C	1:D:292:GLU:H	2.16	0.54
1:F:134:ILE:C	1:F:136:ASP:H	2.15	0.54
1:D:305:SER:C	1:D:307:ILE:H	2.15	0.54
1:B:280:ARG:O	1:B:281:ASP:C	2.51	0.54
1:G:290:ASP:O	1:G:293:GLY:N	2.41	0.53
1:E:290:ASP:C	1:E:292:GLU:N	2.66	0.53
1:A:200:ALA:HB1	1:B:144:SER:N	2.11	0.53
1:E:249:ALA:O	1:E:250:THR:C	2.51	0.53
1:E:296:ILE:O	1:E:297:PHE:C	2.52	0.53
1:F:253:THR:O	1:F:256:ASP:N	2.42	0.53
1:E:273:SER:H	1:E:328:GLY:HA2	1.74	0.53
1:F:158:ASN:CB	1:F:172:SER:HA	2.39	0.53
1:A:290:ASP:C	1:A:292:GLU:N	2.65	0.52
1:B:346:SER:CB	1:B:349:ASP:CB	2.87	0.52
1:B:171:GLU:HA	1:B:173:ASP:N	2.25	0.52
1:E:158:ASN:CB	1:E:172:SER:HA	2.39	0.52
1:G:280:ARG:C	1:G:282:TRP:H	2.16	0.52
1:E:145:SER:C	1:E:147:ALA:H	2.18	0.52
1:C:194:ARG:CB	1:C:358:LEU:CB	2.87	0.52
1:G:268:SER:O	1:G:269:GLU:CB	2.58	0.52
1:A:266:THR:C	1:A:268:SER:H	2.18	0.52
1:D:245:THR:C	1:D:247:LEU:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ASP:O	1:B:199:ASP:C	2.51	0.52
1:C:152:ARG:O	1:C:176:PHE:HA	2.10	0.52
1:A:142:ARG:O	1:F:202:MET:CB	2.58	0.52
1:A:158:ASN:CB	1:A:172:SER:HA	2.39	0.52
1:G:280:ARG:O	1:G:283:HIS:N	2.42	0.52
1:A:266:THR:C	1:A:268:SER:N	2.67	0.51
1:A:304:THR:O	1:A:305:SER:C	2.52	0.51
1:A:321:ALA:C	1:A:323:THR:H	2.19	0.51
1:C:142:ARG:HA	1:C:337:ASP:H	1.74	0.51
1:D:305:SER:C	1:D:307:ILE:N	2.66	0.51
1:E:141:GLY:O	1:E:336:TRP:HA	2.10	0.51
1:G:203:LEU:C	1:G:205:SER:H	2.18	0.51
1:C:300:PRO:O	1:C:301:GLN:C	2.53	0.51
1:E:190:VAL:O	1:E:360:ILE:CB	2.58	0.51
1:C:202:MET:O	1:C:204:GLN:N	2.43	0.51
1:D:158:ASN:CB	1:D:172:SER:HA	2.41	0.51
1:A:329:PHE:HA	1:A:332:ALA:HB3	1.93	0.51
1:B:216:ALA:O	1:B:217:LEU:O	2.29	0.51
1:E:294:ARG:O	1:E:295:TYR:C	2.53	0.51
1:F:301:GLN:O	1:F:302:ALA:C	2.54	0.51
1:A:203:LEU:O	1:A:204:GLN:C	2.54	0.50
1:G:131:ARG:C	1:G:133:THR:N	2.65	0.50
1:F:127:PRO:O	1:F:128:GLY:C	2.54	0.50
1:B:329:PHE:HA	1:B:332:ALA:HB3	1.94	0.50
1:C:133:THR:O	1:C:135:ARG:N	2.45	0.50
1:D:266:THR:HA	1:D:270:PHE:O	2.11	0.50
1:E:226:GLY:N	1:E:235:GLY:HA3	2.27	0.50
1:C:130:ARG:O	1:C:131:ARG:O	2.30	0.50
1:E:356:ASN:CB	1:E:357:MET:CA	2.84	0.50
1:C:206:TYR:O	1:C:210:ARG:N	2.44	0.50
1:B:195:GLN:C	1:B:197:MET:N	2.68	0.50
1:D:296:ILE:C	1:D:298:GLY:N	2.70	0.50
1:E:188:HIS:O	1:E:362:CYS:N	2.41	0.50
1:F:194:ARG:HA	1:F:197:MET:CB	2.42	0.50
1:E:205:SER:CB	1:F:141:GLY:CA	2.90	0.49
1:B:212:MET:O	1:B:214:GLY:N	2.45	0.49
1:A:200:ALA:C	1:A:202:MET:H	2.20	0.49
1:E:141:GLY:C	1:E:336:TRP:HA	2.36	0.49
1:B:195:GLN:O	1:B:197:MET:N	2.45	0.49
1:C:202:MET:CB	1:D:142:ARG:H	2.25	0.49
1:C:301:GLN:O	1:C:302:ALA:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:295:TYR:CB	1:G:298:GLY:O	2.61	0.49
1:B:355:LYS:O	1:B:356:ASN:CB	2.61	0.49
1:F:212:MET:O	1:F:215:LEU:N	2.46	0.49
1:B:352:ASN:HA	1:B:357:MET:O	2.14	0.48
1:E:205:SER:CB	1:F:141:GLY:HA2	2.43	0.48
1:C:227:ASP:C	1:C:229:THR:H	2.21	0.48
1:B:187:ALA:HB2	1:B:363:GLU:HA	1.96	0.48
1:C:300:PRO:C	1:C:302:ALA:N	2.68	0.48
1:A:374:THR:C	1:A:376:ILE:H	2.21	0.48
1:B:329:PHE:O	1:B:330:ASP:C	2.54	0.48
1:C:202:MET:C	1:C:204:GLN:N	2.70	0.48
1:E:292:GLU:O	1:E:294:ARG:N	2.47	0.48
1:B:296:ILE:O	1:B:297:PHE:C	2.54	0.48
1:F:204:GLN:O	1:F:205:SER:C	2.56	0.48
1:F:257:ILE:C	1:F:259:ALA:N	2.69	0.48
1:B:212:MET:O	1:B:215:LEU:CA	2.59	0.48
1:G:129:LEU:O	1:G:131:ARG:N	2.47	0.48
1:G:156:PHE:O	1:G:157:THR:C	2.56	0.48
1:B:280:ARG:O	1:B:283:HIS:N	2.45	0.48
1:D:142:ARG:HA	1:D:337:ASP:H	1.79	0.48
1:B:158:ASN:CB	1:B:172:SER:H	2.27	0.47
1:B:295:TYR:CB	1:B:298:GLY:O	2.61	0.47
1:B:349:ASP:O	1:B:350:ARG:C	2.56	0.47
1:G:273:SER:H	1:G:328:GLY:HA2	1.78	0.47
1:C:290:ASP:C	1:C:292:GLU:N	2.69	0.47
1:C:295:TYR:CB	1:C:297:PHE:O	2.62	0.47
1:G:177:SER:O	1:G:178:LYS:C	2.56	0.47
1:C:207:ILE:HA	1:C:211:LEU:CB	2.45	0.47
1:D:290:ASP:C	1:D:292:GLU:N	2.72	0.47
1:E:128:GLY:O	1:E:129:LEU:CB	2.62	0.47
1:G:197:MET:C	1:G:199:ASP:H	2.22	0.47
1:B:127:PRO:C	1:B:129:LEU:N	2.53	0.47
1:B:142:ARG:HA	1:B:337:ASP:H	1.79	0.47
1:C:302:ALA:O	1:C:303:PHE:C	2.57	0.47
1:E:341:ALA:HA	1:E:363:GLU:O	2.15	0.47
1:A:292:GLU:C	1:A:294:ARG:H	2.23	0.47
1:B:217:LEU:O	1:B:218:LYS:C	2.57	0.47
1:D:293:GLY:CA	1:F:298:GLY:CA	2.66	0.47
1:F:343:VAL:HA	1:F:361:LEU:O	2.15	0.46
1:G:131:ARG:O	1:G:133:THR:N	2.41	0.46
1:G:299:GLY:O	1:G:300:PRO:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:THR:O	1:C:362:CYS:HA	2.15	0.46
1:D:301:GLN:C	1:D:303:PHE:N	2.66	0.46
1:A:197:MET:C	1:A:199:ASP:H	2.24	0.46
1:F:257:ILE:O	1:F:258:ILE:C	2.59	0.46
1:A:121:ILE:C	1:A:123:GLY:N	2.73	0.46
1:F:227:ASP:C	1:F:229:THR:H	2.23	0.46
1:B:266:THR:C	1:B:268:SER:H	2.24	0.46
1:G:280:ARG:C	1:G:283:HIS:H	2.23	0.46
1:A:256:ASP:O	1:A:259:ALA:HB3	2.16	0.46
1:F:204:GLN:O	1:F:206:TYR:N	2.49	0.46
1:F:226:GLY:N	1:F:235:GLY:HA3	2.25	0.46
1:C:277:LEU:O	1:C:315:PRO:HA	2.16	0.46
1:D:171:GLU:C	1:D:173:ASP:N	2.64	0.46
1:F:253:THR:O	1:F:255:ALA:N	2.48	0.46
1:B:299:GLY:O	1:B:301:GLN:N	2.49	0.46
1:D:309:TRP:C	1:D:311:LEU:H	2.24	0.46
1:B:341:ALA:HA	1:B:363:GLU:O	2.16	0.45
1:F:288:LEU:O	1:F:295:TYR:HA	2.16	0.45
1:B:266:THR:HA	1:B:270:PHE:O	2.16	0.45
1:E:295:TYR:C	1:E:296:ILE:O	2.59	0.45
1:B:321:ALA:C	1:B:323:THR:H	2.24	0.45
1:C:142:ARG:HA	1:C:337:ASP:N	2.31	0.45
1:C:155:VAL:HA	1:C:174:ILE:HA	1.99	0.45
1:C:202:MET:O	1:C:203:LEU:C	2.58	0.45
1:C:227:ASP:C	1:C:229:THR:N	2.75	0.45
1:D:302:ALA:O	1:D:303:PHE:C	2.59	0.45
1:A:277:LEU:O	1:A:315:PRO:HA	2.16	0.45
1:B:149:GLU:HA	1:B:180:THR:HA	1.99	0.45
1:C:133:THR:O	1:C:134:ILE:C	2.60	0.45
1:C:290:ASP:C	1:C:292:GLU:H	2.25	0.45
1:E:171:GLU:C	1:E:173:ASP:H	2.24	0.45
1:B:352:ASN:CB	1:B:357:MET:O	2.65	0.44
1:C:133:THR:C	1:C:135:ARG:N	2.72	0.44
1:C:263:TYR:C	1:C:265:VAL:N	2.75	0.44
1:G:249:ALA:O	1:G:250:THR:C	2.60	0.44
1:A:171:GLU:C	1:A:173:ASP:H	2.24	0.44
1:D:258:ILE:O	1:D:261:ALA:HB3	2.17	0.44
1:G:355:LYS:O	1:G:356:ASN:C	2.60	0.44
1:A:200:ALA:CB	1:B:144:SER:H	2.15	0.44
1:D:197:MET:C	1:D:199:ASP:H	2.26	0.44
1:E:352:ASN:O	1:E:355:LYS:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:ASP:O	1:E:292:GLU:N	2.51	0.44
1:F:227:ASP:C	1:F:229:THR:N	2.73	0.44
1:G:347:ARG:C	1:G:349:ASP:H	2.26	0.44
1:F:236:LEU:O	1:F:240:ALA:N	2.50	0.44
1:E:258:ILE:O	1:E:261:ALA:HB3	2.18	0.44
1:A:244:ASP:C	1:A:246:SER:H	2.26	0.43
1:D:187:ALA:HB2	1:D:363:GLU:CB	2.48	0.43
1:D:293:GLY:O	1:F:298:GLY:HA3	2.15	0.43
1:B:202:MET:HA	1:C:142:ARG:O	2.16	0.43
1:B:351:ASP:O	1:B:352:ASN:C	2.61	0.43
1:C:302:ALA:O	1:C:304:THR:O	2.37	0.43
1:F:263:TYR:C	1:F:265:VAL:N	2.75	0.43
1:F:193:SER:C	1:F:195:GLN:H	2.27	0.43
1:A:241:THR:O	1:A:377:ILE:HA	2.17	0.43
1:E:301:GLN:O	1:E:304:THR:N	2.52	0.43
1:D:280:ARG:CB	1:E:309:TRP:O	2.67	0.43
1:G:195:GLN:C	1:G:197:MET:N	2.71	0.43
1:C:191:GLN:HA	1:C:359:THR:HA	2.00	0.42
1:D:221:GLY:O	1:D:225:ASN:N	2.47	0.42
1:A:152:ARG:O	1:A:154:GLU:N	2.53	0.42
1:F:152:ARG:O	1:F:154:GLU:N	2.53	0.42
1:B:152:ARG:O	1:B:154:GLU:N	2.53	0.42
1:C:258:ILE:O	1:C:261:ALA:HB3	2.20	0.42
1:E:245:THR:C	1:E:247:LEU:H	2.27	0.42
1:E:322:GLY:O	1:E:380:THR:HA	2.19	0.42
1:B:217:LEU:O	1:B:220:GLU:N	2.53	0.42
1:D:256:ASP:O	1:D:259:ALA:HB3	2.20	0.42
1:B:352:ASN:O	1:B:356:ASN:N	2.53	0.42
1:A:202:MET:O	1:A:206:TYR:N	2.51	0.42
1:G:352:ASN:CB	1:G:357:MET:O	2.66	0.42
1:E:156:PHE:C	1:E:158:ASN:N	2.78	0.42
1:A:244:ASP:C	1:A:246:SER:N	2.78	0.41
1:C:301:GLN:O	1:C:304:THR:N	2.53	0.41
1:B:253:THR:C	1:B:255:ALA:H	2.28	0.41
1:C:256:ASP:O	1:C:259:ALA:HB3	2.20	0.41
1:E:215:LEU:O	1:E:219:GLU:N	2.48	0.41
1:D:294:ARG:N	1:F:298:GLY:CA	2.82	0.41
1:F:308:MET:O	1:F:311:LEU:N	2.53	0.41
1:B:207:ILE:O	1:B:208:ASN:C	2.63	0.41
1:B:213:TYR:O	1:B:214:GLY:C	2.62	0.41
1:A:266:THR:O	1:A:268:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ALA:CB	1:C:363:GLU:HA	2.43	0.41
1:D:294:ARG:N	1:F:298:GLY:HA3	2.35	0.41
1:F:352:ASN:O	1:F:355:LYS:O	2.39	0.41
1:E:226:GLY:C	1:E:228:GLY:N	2.78	0.41
1:F:187:ALA:HB2	1:F:363:GLU:HA	2.02	0.41
1:G:211:LEU:O	1:G:212:MET:C	2.64	0.41
1:B:171:GLU:C	1:B:173:ASP:H	2.28	0.41
1:D:290:ASP:O	1:D:291:ASN:CB	2.67	0.41
1:E:322:GLY:HA2	1:E:381:PHE:CB	2.51	0.41
1:B:193:SER:CB	1:C:149:GLU:C	2.94	0.41
1:G:236:LEU:O	1:G:240:ALA:N	2.54	0.41
1:G:381:PHE:C	1:G:383:SER:H	2.29	0.41
1:A:200:ALA:C	1:A:202:MET:N	2.79	0.40
1:B:156:PHE:C	1:B:158:ASN:N	2.78	0.40
1:C:236:LEU:O	1:C:240:ALA:HB2	2.21	0.40
1:F:263:TYR:C	1:F:265:VAL:H	2.29	0.40
1:F:253:THR:C	1:F:255:ALA:N	2.74	0.40
1:E:268:SER:O	1:E:269:GLU:C	2.64	0.40
1:E:127:PRO:N	1:E:212:MET:CB	2.85	0.40
1:F:223:LEU:O	1:F:224:LEU:C	2.63	0.40
1:F:322:GLY:O	1:F:380:THR:CB	2.70	0.40
1:C:213:TYR:C	1:C:215:LEU:N	2.78	0.40
1:E:127:PRO:CB	1:E:212:MET:C	2.95	0.40
1:E:296:ILE:O	1:E:298:GLY:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	254/385 (66%)	194 (76%)	54 (21%)	6 (2%)	4 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	248/385 (64%)	194 (78%)	47 (19%)	7 (3%)	4	24
1	C	246/385 (64%)	200 (81%)	36 (15%)	10 (4%)	2	17
1	D	252/385 (66%)	205 (81%)	39 (16%)	8 (3%)	3	21
1	E	253/385 (66%)	215 (85%)	33 (13%)	5 (2%)	6	30
1	F	246/385 (64%)	201 (82%)	36 (15%)	9 (4%)	2	19
1	G	245/385 (64%)	201 (82%)	38 (16%)	6 (2%)	4	26
All	All	1744/2695 (65%)	1410 (81%)	283 (16%)	51 (3%)	3	23

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ILE
1	A	170	PRO
1	A	208	ASN
1	B	170	PRO
1	B	350	ARG
1	C	131	ARG
1	C	160	ALA
1	C	170	PRO
1	D	127	PRO
1	E	170	PRO
1	E	296	ILE
1	F	170	PRO
1	G	170	PRO
1	G	198	ASP
1	G	279	PRO
1	A	195	GLN
1	A	309	TRP
1	B	297	PHE
1	C	203	LEU
1	F	128	GLY
1	F	130	ARG
1	F	293	GLY
1	B	127	PRO
1	B	196	VAL
1	B	199	ASP
1	C	171	GLU
1	D	303	PHE
1	D	306	ASN
1	E	291	ASN

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Mol	Chain	Res	Type
1	F	382	SER
1	G	129	LEU
1	C	134	ILE
1	D	160	ALA
1	F	208	ASN
1	G	204	GLN
1	C	298	GLY
1	D	159	ASN
1	D	382	SER
1	F	283	HIS
1	F	291	ASN
1	A	160	ALA
1	C	192	ALA
1	C	248	ASN
1	E	160	ALA
1	F	160	ALA
1	G	160	ALA
1	D	170	PRO
1	D	293	GLY
1	B	207	ILE
1	C	190	VAL
1	E	251	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	256/385 (66%)	-0.24	4 (1%) 70 57	118, 145, 169, 195	0
1	B	250/385 (64%)	-0.29	6 (2%) 59 49	118, 149, 175, 187	0
1	C	248/385 (64%)	-0.27	1 (0%) 88 77	120, 150, 174, 189	0
1	D	254/385 (65%)	-0.26	2 (0%) 82 69	118, 149, 170, 188	0
1	E	255/385 (66%)	-0.31	4 (1%) 70 57	120, 152, 173, 203	0
1	F	248/385 (64%)	-0.30	2 (0%) 82 69	123, 147, 170, 191	0
1	G	247/385 (64%)	-0.25	0 100 100	122, 149, 172, 193	0
All	All	1758/2695 (65%)	-0.27	19 (1%) 78 63	118, 149, 173, 203	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	198	ASP	4.0
1	E	121	ILE	3.9
1	B	241	THR	3.8
1	C	298	GLY	3.7
1	A	241	THR	3.3
1	D	123	GLY	3.1
1	F	345	VAL	3.0
1	B	250	THR	2.8
1	B	193	SER	2.8
1	D	127	PRO	2.7
1	A	242	ALA	2.7
1	B	341	ALA	2.7
1	B	340	ASP	2.5
1	E	248	ASN	2.5
1	E	124	ILE	2.4
1	F	251	GLY	2.4
1	A	281	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	170	PRO	2.3
1	A	157	THR	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.