



# Full wwPDB X-ray Structure Validation Report i

Jun 12, 2024 – 08:16 PM EDT

PDB ID : 3QPR  
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](mailto: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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) i) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.20.1  
EDS : 2.36.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

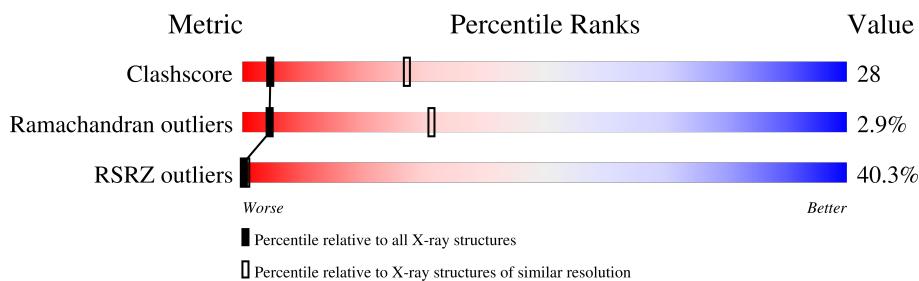
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

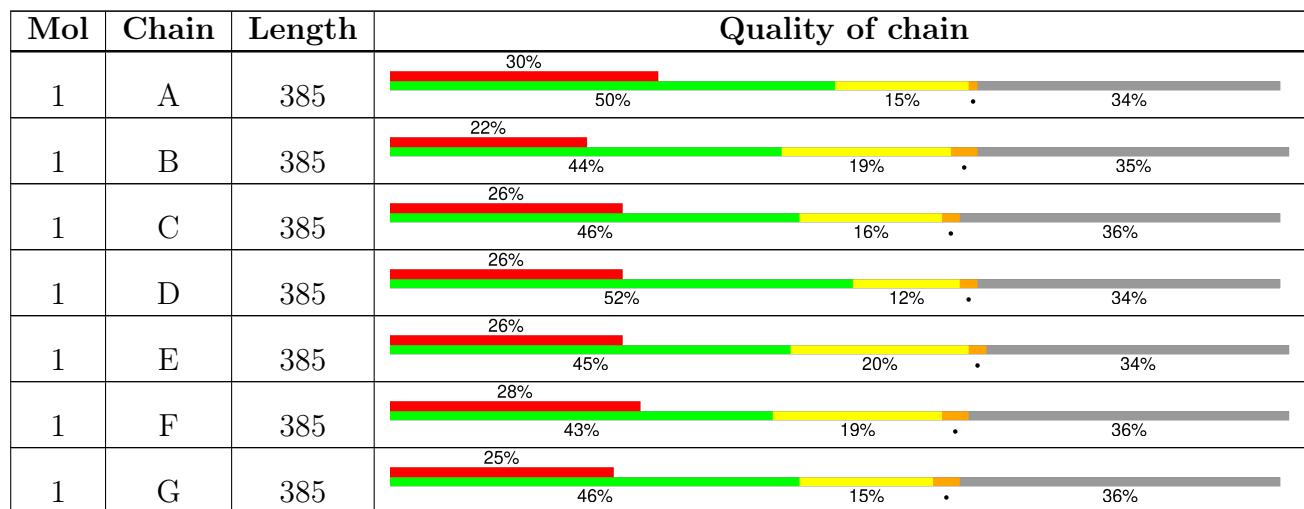
The reported resolution of this entry is 5.20 Å.

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	141614	1006 (6.56-3.84)
Ramachandran outliers	138981	1173 (6.60-3.80)
RSRZ outliers	127900	1008 (6.64-3.74)

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 <=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.



## 2 Entry composition [\(i\)](#)

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.

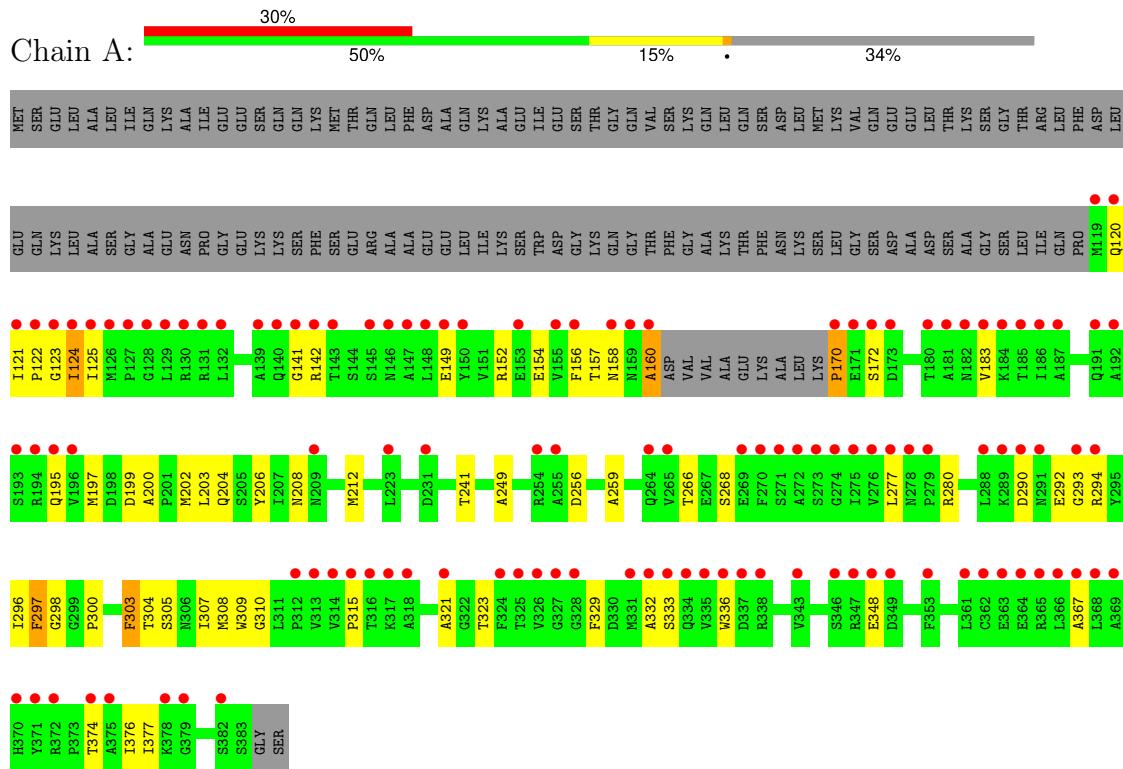
- Molecule 1 is a protein called Major capsid protein.

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

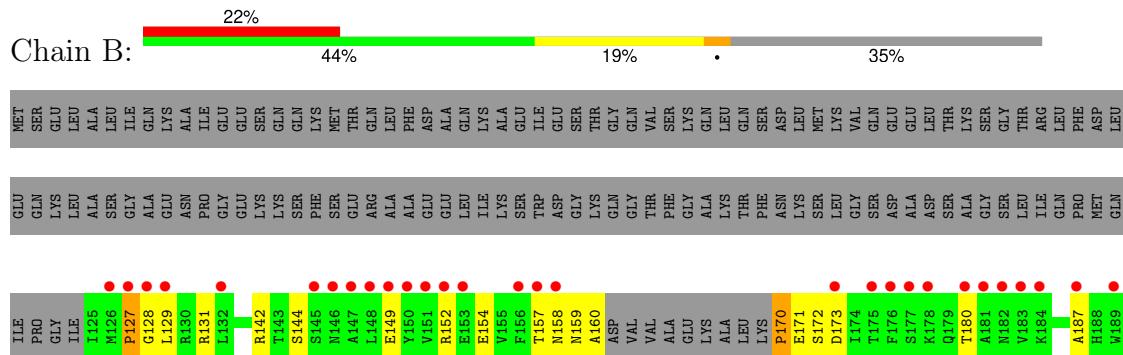
### 3 Residue-property plots

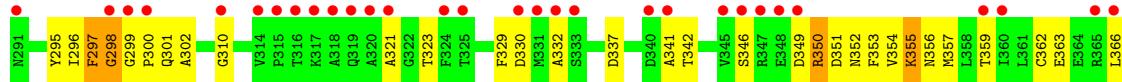
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

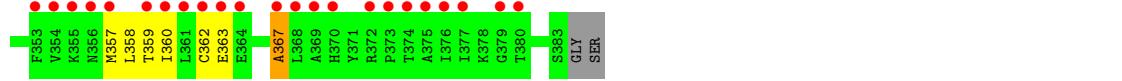
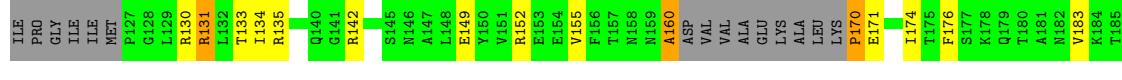
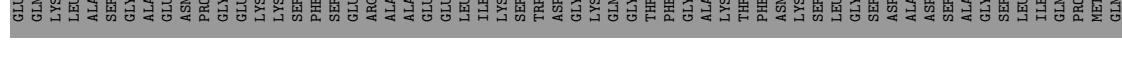


- Molecule 1: Major capsid protein



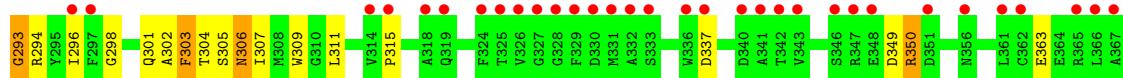


- Molecule 1: Major capsid protein

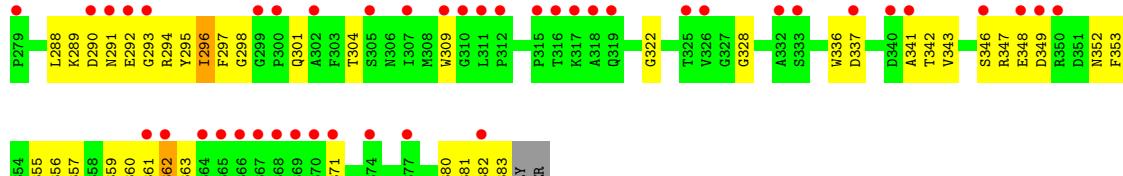


- Molecule 1: Major capsid protein

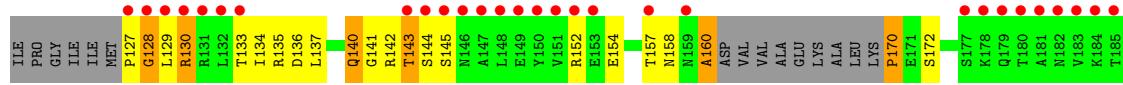


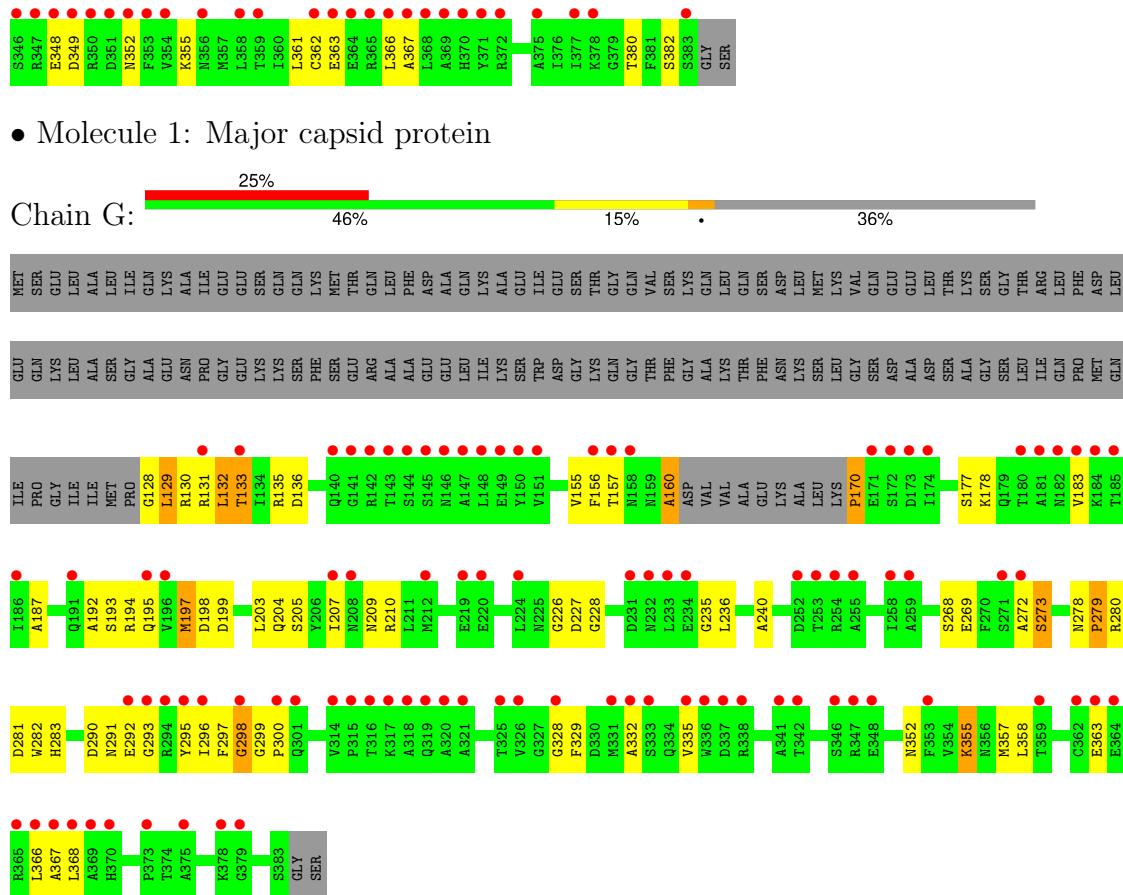


- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein





## 4 Data and refinement statistics i

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	560.12Å    560.12Å    560.12Å 90.00°    90.00°    90.00°	Depositor
Resolution (Å)	45.00 – 5.20 44.56 – 5.19	Depositor EDS
% Data completeness (in resolution range)	(Not available) (45.00-5.20) 77.1 (44.56-5.19)	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 <sup>2</sup> )	175.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 298.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.32$ , $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	0.125 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.73	EDS
Total number of atoms	8654	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

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	0.39	1/1259 (0.1%)	0.94	15/1749 (0.9%)
1	B	0.42	0/1230	0.90	11/1709 (0.6%)
1	C	0.34	0/1220	0.80	9/1695 (0.5%)
1	D	0.35	0/1249	0.85	8/1735 (0.5%)
1	E	0.32	0/1254	0.81	9/1742 (0.5%)
1	F	0.43	0/1220	1.07	19/1695 (1.1%)
1	G	0.38	0/1215	1.10	22/1688 (1.3%)
All	All	0.38	1/8647 (0.0%)	0.93	93/12013 (0.8%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	MET	C-N	-5.26	1.22	1.34

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	297	PHE	N-CA-C	-9.22	86.10	111.00
1	A	298	GLY	N-CA-C	8.91	135.37	113.10
1	B	128	GLY	N-CA-C	-8.58	91.65	113.10
1	D	123	GLY	N-CA-C	-8.24	92.50	113.10
1	G	272	ALA	CB-CA-C	-8.23	97.76	110.10
1	G	228	GLY	N-CA-C	8.22	133.66	113.10
1	E	126	MET	N-CA-C	7.52	131.31	111.00
1	F	348	GLU	CB-CA-C	7.50	125.41	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	296	ILE	CB-CA-C	-7.46	96.67	111.60
1	C	170	PRO	N-CA-C	-7.37	92.95	112.10
1	G	209	ASN	CB-CA-C	7.36	125.12	110.40
1	G	298	GLY	N-CA-C	7.35	131.47	113.10
1	A	297	PHE	CB-CA-C	-7.24	95.92	110.40
1	G	355	LYS	N-CA-C	-7.20	91.57	111.00
1	G	296	ILE	N-CA-C	7.14	130.27	111.00
1	A	303	PHE	CB-CA-C	-6.97	96.47	110.40
1	F	366	LEU	CB-CA-C	-6.93	97.04	110.20
1	F	332	ALA	N-CA-CB	-6.84	100.53	110.10
1	C	331	MET	N-CA-CB	-6.79	98.38	110.60
1	D	226	GLY	N-CA-C	6.77	130.01	113.10
1	F	349	ASP	N-CA-CB	-6.70	98.54	110.60
1	E	125	ILE	N-CA-C	6.69	129.05	111.00
1	G	133	THR	N-CA-CB	6.63	122.91	110.30
1	A	120	GLN	CB-CA-C	-6.61	97.19	110.40
1	G	197	MET	N-CA-C	6.57	128.75	111.00
1	F	349	ASP	N-CA-C	6.48	128.50	111.00
1	B	366	LEU	CB-CA-C	-6.37	98.09	110.20
1	F	272	ALA	CB-CA-C	-6.36	100.56	110.10
1	C	297	PHE	N-CA-C	-6.33	93.90	111.00
1	G	210	ARG	N-CA-C	6.29	127.99	111.00
1	F	249	ALA	CB-CA-C	6.19	119.38	110.10
1	A	333	SER	N-CA-CB	6.13	119.70	110.50
1	E	125	ILE	CB-CA-C	-6.07	99.45	111.60
1	C	330	ASP	CB-CA-C	6.00	122.39	110.40
1	G	273	SER	N-CA-CB	-5.99	101.51	110.50
1	D	250	THR	N-CA-C	5.94	127.05	111.00
1	A	307	ILE	CB-CA-C	-5.93	99.74	111.60
1	B	251	GLY	N-CA-C	5.89	127.83	113.10
1	F	250	THR	N-CA-C	-5.88	95.11	111.00
1	G	207	ILE	CB-CA-C	-5.88	99.84	111.60
1	B	250	THR	CB-CA-C	-5.82	95.89	111.60
1	A	249	ALA	CB-CA-C	-5.81	101.38	110.10
1	B	160	ALA	N-CA-CB	-5.80	101.98	110.10
1	F	294	ARG	N-CA-CB	-5.77	100.21	110.60
1	A	149	GLU	CB-CA-C	-5.75	98.90	110.40
1	D	157	THR	N-CA-C	-5.71	95.58	111.00
1	D	249	ALA	CB-CA-C	-5.71	101.54	110.10
1	E	157	THR	N-CA-C	-5.70	95.61	111.00
1	B	157	THR	N-CA-C	-5.70	95.61	111.00
1	F	157	THR	N-CA-C	-5.70	95.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	145	SER	CB-CA-C	-5.64	99.38	110.10
1	B	272	ALA	N-CA-CB	-5.64	102.20	110.10
1	G	227	ASP	N-CA-C	5.63	126.21	111.00
1	G	209	ASN	N-CA-CB	-5.63	100.47	110.60
1	A	122	PRO	N-CA-C	-5.61	97.52	112.10
1	E	201	PRO	N-CA-CB	5.61	110.03	103.30
1	G	155	VAL	CB-CA-C	-5.58	100.81	111.40
1	F	143	THR	CB-CA-C	-5.54	96.63	111.60
1	A	348	GLU	N-CA-C	5.54	125.96	111.00
1	C	307	ILE	N-CA-C	-5.54	96.04	111.00
1	C	201	PRO	N-CA-CB	5.51	109.92	103.30
1	B	298	GLY	N-CA-C	-5.39	99.62	113.10
1	B	271	SER	CB-CA-C	-5.38	99.89	110.10
1	D	350	ARG	N-CA-CB	5.38	120.28	110.60
1	E	293	GLY	N-CA-C	-5.33	99.77	113.10
1	F	212	MET	O-C-N	5.33	131.23	122.70
1	C	272	ALA	CB-CA-C	-5.26	102.22	110.10
1	D	171	GLU	N-CA-CB	5.25	120.04	110.60
1	D	160	ALA	N-CA-CB	-5.23	102.77	110.10
1	G	207	ILE	N-CA-C	5.23	125.11	111.00
1	B	250	THR	N-CA-C	5.22	125.10	111.00
1	C	367	ALA	N-CA-CB	-5.20	102.81	110.10
1	F	257	ILE	CB-CA-C	-5.18	101.24	111.60
1	E	170	PRO	N-CA-C	5.16	125.52	112.10
1	F	170	PRO	N-CA-C	5.16	125.52	112.10
1	E	142	ARG	N-CA-CB	-5.16	101.32	110.60
1	C	160	ALA	N-CA-CB	-5.15	102.88	110.10
1	A	170	PRO	N-CA-C	5.15	125.50	112.10
1	G	170	PRO	N-CA-C	5.15	125.48	112.10
1	G	366	LEU	CB-CA-C	-5.14	100.43	110.20
1	F	367	ALA	N-CA-CB	-5.14	102.90	110.10
1	F	140	GLN	CB-CA-C	-5.13	100.14	110.40
1	F	160	ALA	N-CA-CB	-5.12	102.93	110.10
1	G	132	LEU	N-CA-CB	5.12	120.65	110.40
1	A	125	ILE	N-CA-C	-5.12	97.18	111.00
1	A	160	ALA	N-CA-CB	-5.11	102.95	110.10
1	G	160	ALA	N-CA-CB	-5.10	102.96	110.10
1	G	135	ARG	CB-CA-C	-5.08	100.23	110.40
1	E	160	ALA	N-CA-CB	-5.07	103.00	110.10
1	B	355	LYS	N-CA-C	-5.05	97.36	111.00
1	F	144	SER	N-CA-CB	-5.04	102.94	110.50
1	A	157	THR	N-CA-C	-5.02	97.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	GLU	CB-CA-C	-5.00	100.39	110.40

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	42	0
1	B	1231	0	583	78	0
1	C	1221	0	580	49	0
1	D	1250	0	591	44	0
1	E	1255	0	593	71	0
1	F	1221	0	580	63	0
1	G	1216	0	578	50	0
All	All	8654	0	4100	361	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 28.

All (361) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:152:ARG:CB	1:E:371:TYR:CA	2.45	0.93
1:A:293:GLY:C	1:C:298:GLY:HA2	1.93	0.89
1:B:250:THR:CB	1:B:251:GLY:CA	2.49	0.88
1:B:170:PRO:C	1:B:172:SER:CB	2.43	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:B:202:MET:CB	1:C:142:ARG:O	2.24	0.85
1:D:293:GLY:C	1:F:298:GLY:HA3	1.97	0.85
1:E:125:ILE:CB	1:E:212:MET:CB	2.56	0.84
1:G:290:ASP:C	1:G:292:GLU:H	1.80	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
1:B:127:PRO:C	1:B:129:LEU:H	1.82	0.82
1:C:193:SER:HA	1:C:358:LEU:H	1.44	0.82
1:D:293:GLY:C	1:F:298:GLY:CA	2.47	0.82
1:F:134:ILE:O	1:F:137:LEU:N	2.10	0.82
1:G:192:ALA:O	1:G:358:LEU:N	2.10	0.81
1:F:342:THR:O	1:F:362:CYS:HA	1.79	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:E:152:ARG:CB	1:E:371:TYR:C	2.52	0.77
1:G:128:GLY:C	1:G:130:ARG:N	2.30	0.77
1:F:253:THR:O	1:F:254:ARG:C	2.21	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:290:ASP:C	1:G:292:GLU:N	2.35	0.77
1:G:129:LEU:C	1:G:131:ARG:H	1.87	0.77
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:E:382:SER:O	1:E:383:SER:CB	2.35	0.74
1:C:190:VAL:O	1:C:360:ILE:N	2.20	0.74
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: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:296:ILE:C	1:B:298:GLY:N	2.42	0.71
1:B:171:GLU:CA	1:B:172:SER:CB	2.69	0.71
1:B:296:ILE:C	1:B:298:GLY:H	1.93	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:A:308:MET:C	1:A:310:GLY:H	1.93	0.70
1:B:212:MET:O	1:B:213:TYR:C	2.28	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:D:171:GLU:C	1:D:173:ASP:H	1.94	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:293:GLY:C	1:F:298:GLY:HA2	2.13	0.69
1:D:305:SER:O	1:D:307:ILE:N	2.23	0.69
1:C:202:MET:O	1:C:205:SER:N	2.27	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:F:249:ALA:O	1:F:250:THR:C	2.32	0.68
1:G:193:SER:O	1:G:197:MET:CB	2.42	0.67
1:D:293:GLY:CA	1:F:298:GLY:CA	2.66	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:G:128:GLY:C	1:G:130:ARG:H	1.97	0.66
1:F:211:LEU:O	1:F:214:GLY:N	2.28	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:216:ALA:O	1:B:217:LEU:C	2.34	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: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: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:D:302:ALA:O	1:D:304:THR:N	2.33	0.61
1:G:131:ARG:C	1:G:133:THR:H	2.00	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:308:MET:C	1:A:310:GLY:N	2.54	0.60
1:G:291:ASN:C	1:G:293:GLY:H	2.05	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:171:GLU:HA	1:B:172:SER:CB	2.31	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: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:128:GLY:O	1:G:129:LEU:C	2.40	0.58
1:G:187:ALA:CB	1:G:363:GLU:HA	2.30	0.58
1:F:203:LEU:O	1:F:204:GLN:C	2.39	0.58
1:G:280:ARG:C	1:G:282:TRP:N	2.56	0.58
1:B:299:GLY:O	1:B:302:ALA:N	2.37	0.58
1:E:153:GLU:CA	1:E:175:THR:O	2.52	0.58
1:D:296:ILE:C	1:D:298:GLY:H	2.05	0.58
1:F:133:THR:O	1:F:134:ILE:C	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:MET:CA	1:B:142:ARG:O	2.39	0.57
1:B:171:GLU:HA	1:B:172:SER:C	2.24	0.57
1:B:127:PRO:C	1:B:129:LEU:N	2.53	0.57
1:C:192:ALA:O	1:C:357:MET:C	2.42	0.57
1:B:198:ASP:O	1:B:200:ALA:N	2.38	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: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:F:134:ILE:C	1:F:136:ASP:N	2.56	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
1:A:156:PHE:C	1:A:158:ASN:H	2.09	0.55
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:D:349:ASP:O	1:D:350:ARG:C	2.43	0.55
1:G:129:LEU:C	1:G:131:ARG:N	2.57	0.55
1:B:193:SER:CA	1:B:357:MET:CB	2.82	0.55
1:G:278:ASN:O	1:G:281:ASP:N	2.40	0.55
1:A:156:PHE:C	1:A:158:ASN:N	2.60	0.55
1:D:277:LEU:O	1:D:315:PRO:HA	2.06	0.55
1:G:197:MET:O	1:G:199:ASP:N	2.36	0.54
1:E:153:GLU:HA	1:E:176:PHE:HA	1.88	0.54
1:E:348:GLU:C	1:E:353:PHE:CB	2.75	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:E:290:ASP:C	1:E:292:GLU:H	2.11	0.54
1:G:278:ASN:O	1:G:279:PRO:C	2.46	0.54
1:D:200:ALA:C	1:D:202:MET:H	2.11	0.53
1:G:195:GLN:C	1:G:197:MET:H	2.12	0.53
1:G:290:ASP:O	1:G:293:GLY:N	2.41	0.53
1:B:195:GLN:C	1:B:197:MET:H	2.11	0.53
1:D:301:GLN:O	1:D:302:ALA:C	2.47	0.53
1:A:200:ALA:HB1	1:B:144:SER:N	2.11	0.53
1:E:296:ILE:C	1:E:298:GLY:N	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:ASN:CB	1:F:172:SER:HA	2.39	0.53
1:B:205:SER:O	1:B:206:TYR:C	2.46	0.52
1:B:346:SER:CB	1:B:349:ASP:CB	2.87	0.52
1:G:194:ARG:C	1:G:197:MET:H	2.13	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:C:194:ARG:CB	1:C:358:LEU:CB	2.87	0.52
1:B:299:GLY:O	1:B:300:PRO:C	2.48	0.52
1:E:125:ILE:C	1:E:212:MET:CB	2.77	0.52
1:G:268:SER:O	1:G:269:GLU:CB	2.58	0.52
1:B:299:GLY:C	1:B:301:GLN:N	2.61	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:F:134:ILE:O	1:F:135:ARG:C	2.48	0.52
1:G:280:ARG:O	1:G:283:HIS:N	2.42	0.52
1:C:142:ARG:HA	1:C:337:ASP:H	1.74	0.51
1:E:141:GLY:O	1:E:336:TRP:HA	2.10	0.51
1:G:352:ASN:O	1:G:355:LYS:C	2.49	0.51
1:E:190:VAL:O	1:E:360:ILE:CB	2.58	0.51
1:D:171:GLU:C	1:D:173:ASP:N	2.64	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:A:290:ASP:C	1:A:292:GLU:H	2.13	0.50
1:E:202:MET:HA	1:F:142:ARG:C	2.19	0.50
1:B:212:MET:O	1:B:214:GLY:N	2.45	0.50
1:A:290:ASP:C	1:A:292:GLU:N	2.65	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:D:170:PRO:O	1:D:171:GLU:C	2.48	0.50
1:F:249:ALA:C	1:F:250:THR:O	2.41	0.50
1:E:188:HIS:O	1:E:362:CYS:N	2.41	0.50
1:B:129:LEU:C	1:B:131:ARG:N	2.64	0.50
1:F:194:ARG:HA	1:F:197:MET:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:SER:CB	1:F:141:GLY:CA	2.90	0.49
1:F:134:ILE:C	1:F:136:ASP:H	2.15	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:D:305:SER:C	1:D:307:ILE:H	2.15	0.49
1:B:280:ARG:O	1:B:281:ASP:C	2.51	0.49
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:D:305:SER:C	1:D:307:ILE:N	2.66	0.48
1:E:205:SER:CB	1:F:141:GLY:HA2	2.43	0.48
1:B:187:ALA:HB2	1:B:363:GLU:HA	1.96	0.48
1:E:249:ALA:O	1:E:250:THR:C	2.51	0.48
1:E:292:GLU:O	1:E:294:ARG:N	2.47	0.48
1:A:266:THR:C	1:A:268:SER:N	2.67	0.48
1:B:212:MET:O	1:B:215:LEU:CA	2.59	0.48
1:E:296:ILE:O	1:E:297:PHE:C	2.52	0.48
1:E:290:ASP:C	1:E:292:GLU:N	2.66	0.48
1:G:129:LEU:O	1:G:131:ARG:N	2.47	0.48
1:G:280:ARG:C	1:G:282:TRP:H	2.16	0.48
1:A:266:THR:C	1:A:268:SER:H	2.18	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:D:290:ASP:C	1:D:292:GLU:H	2.16	0.47
1:E:145:SER:C	1:E:147:ALA:H	2.18	0.47
1:G:273:SER:H	1:G:328:GLY:HA2	1.78	0.47
1:C:295:TYR:CB	1:C:297:PHE:O	2.62	0.47
1:C:207:ILE:HA	1:C:211:LEU:CB	2.45	0.47
1:D:245:THR:C	1:D:247:LEU:H	2.17	0.47
1:E:128:GLY:O	1:E:129:LEU:CB	2.62	0.47
1:B:198:ASP:O	1:B:199:ASP:C	2.51	0.47
1:B:142:ARG:HA	1:B:337:ASP:H	1.79	0.47
1:E:341:ALA:HA	1:E:363:GLU:O	2.15	0.47
1:A:304:THR:O	1:A:305:SER:C	2.52	0.47
1:G:203:LEU:C	1:G:205:SER:H	2.18	0.47
1:C:300:PRO:O	1:C:301:GLN:C	2.53	0.46
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

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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:A:321:ALA:C	1:A:323:THR:H	2.19	0.46
1:B:195:GLN:C	1:B:197:MET:N	2.68	0.46
1:E:294:ARG:O	1:E:295:TYR:C	2.53	0.46
1:A:256:ASP:O	1:A:259:ALA:HB3	2.16	0.46
1:D:301:GLN:C	1:D:303:PHE:N	2.66	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:F:301:GLN:O	1:F:302:ALA:C	2.54	0.46
1:A:203:LEU:O	1:A:204:GLN:C	2.54	0.46
1:C:277:LEU:O	1:C:315:PRO:HA	2.16	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:B:341:ALA:HA	1:B:363:GLU:O	2.16	0.45
1:F:127:PRO:O	1:F:128:GLY:C	2.54	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:C:142:ARG:HA	1:C:337:ASP:N	2.31	0.45
1:D:296:ILE:C	1:D:298:GLY:N	2.70	0.45
1:C:155:VAL:HA	1:C:174:ILE:HA	1.99	0.45
1:A:200:ALA:C	1:A:202:MET:H	2.20	0.45
1:C:300:PRO:C	1:C:302:ALA:N	2.68	0.45
1:C:290:ASP:C	1:C:292:GLU:N	2.69	0.45
1:E:141:GLY:C	1:E:336:TRP:HA	2.36	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:G:299:GLY:O	1:G:300:PRO:C	2.54	0.45
1:B:352:ASN:CB	1:B:357:MET:O	2.65	0.44
1:C:202:MET:C	1:C:204:GLN:N	2.70	0.44
1:D:258:ILE:O	1:D:261:ALA:HB3	2.17	0.44
1:G:131:ARG:C	1:G:133:THR:N	2.65	0.44
1:A:200:ALA:CB	1:B:144:SER:H	2.15	0.44
1:C:301:GLN:O	1:C:302:ALA:C	2.56	0.44
1:E:352:ASN:O	1:E:355:LYS:CB	2.66	0.44
1:E:290:ASP:O	1:E:292:GLU:N	2.51	0.44
1:F:257:ILE:C	1:F:259:ALA:N	2.69	0.44
1:F:236:LEU:O	1:F:240:ALA:N	2.50	0.44
1:C:227:ASP:C	1:C:229:THR:H	2.21	0.44
1:E:258:ILE:O	1:E:261:ALA:HB3	2.18	0.44
1:G:195:GLN:C	1:G:197:MET:N	2.71	0.43
1:B:192:ALA:C	1:B:357:MET:CB	2.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:329:PHE:O	1:B:330:ASP:C	2.54	0.43
1:A:374:THR:C	1:A:376:ILE:H	2.21	0.43
1:B:202:MET:HA	1:C:142:ARG:O	2.16	0.43
1:F:204:GLN:O	1:F:205:SER:C	2.56	0.43
1:B:296:ILE:O	1:B:297:PHE:C	2.54	0.43
1:C:302:ALA:O	1:C:304:THR:O	2.37	0.43
1:G:156:PHE:O	1:G:157:THR:C	2.56	0.43
1:B:349:ASP:O	1:B:350:ARG:C	2.56	0.43
1:A:241:THR:O	1:A:377:ILE:HA	2.17	0.43
1:D:290:ASP:C	1:D:292:GLU:N	2.72	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:C:191:GLN:HA	1:C:359:THR:HA	2.00	0.42
1:G:177:SER:O	1:G:178:LYS:C	2.56	0.42
1:D:221:GLY:O	1:D:225:ASN:N	2.47	0.42
1:C:133:THR:C	1:C:135:ARG:N	2.72	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:B:354:VAL:C	1:B:356:ASN:N	2.72	0.42
1:C:258:ILE:O	1:C:261:ALA:HB3	2.20	0.42
1:C:302:ALA:O	1:C:303:PHE:C	2.57	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:A:292:GLU:C	1:A:294:ARG:H	2.23	0.42
1:B:217:LEU:O	1:B:218:LYS:C	2.57	0.42
1:D:256:ASP:O	1:D:259:ALA:HB3	2.20	0.42
1:G:291:ASN:C	1:G:293:GLY:N	2.73	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:C:301:GLN:O	1:C:304:THR:N	2.53	0.41
1:A:197:MET:C	1:A:199:ASP:H	2.24	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:F:227:ASP:C	1:F:229:THR:H	2.23	0.41
1:F:257:ILE:O	1:F:258:ILE:C	2.59	0.41
1:A:121:ILE:C	1:A:123:GLY:N	2.73	0.41
1:D:294:ARG:N	1:F:298:GLY:CA	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:MET:O	1:F:311:LEU:N	2.53	0.41
1:B:266:THR:C	1:B:268:SER:H	2.24	0.41
1:G:280:ARG:C	1:G:283:HIS:H	2.23	0.41
1:A:266:THR:O	1:A:268:SER:N	2.53	0.41
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:D:200:ALA:C	1:D:202:MET:N	2.73	0.41
1:F:187:ALA:HB2	1:F:363:GLU:HA	2.02	0.41
1:F:227:ASP:C	1:F:229:THR:N	2.73	0.41
1:D:290:ASP:O	1:D:291:ASN:CB	2.67	0.41
1:D:309:TRP:C	1:D:311:LEU:H	2.24	0.41
1:E:322:GLY:HA2	1:E:381:PHE:CB	2.51	0.41
1:F:249:ALA:O	1:F:250:THR:O	2.38	0.41
1:G:236:LEU:O	1:G:240:ALA:N	2.54	0.41
1:E:295:TYR:C	1:E:296:ILE:O	2.59	0.41
1:B:321:ALA:C	1:B:323:THR:H	2.24	0.40
1:C:236:LEU:O	1:C:240:ALA:HB2	2.21	0.40
1:C:202:MET:O	1:C:203:LEU:C	2.58	0.40
1:C:227:ASP:C	1:C:229:THR:N	2.75	0.40
1:D:302:ALA:O	1:D:303:PHE:C	2.59	0.40
1:E:127:PRO:N	1:E:212:MET:CB	2.85	0.40
1:F:322:GLY:O	1:F:380:THR:CB	2.70	0.40
1:E:171:GLU:C	1:E:173:ASP:H	2.24	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%)	6 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	248/385 (64%)	194 (78%)	47 (19%)	7 (3%)	5 32
1	C	246/385 (64%)	200 (81%)	36 (15%)	10 (4%)	3 24
1	D	252/385 (66%)	205 (81%)	39 (16%)	8 (3%)	4 29
1	E	253/385 (66%)	215 (85%)	33 (13%)	5 (2%)	7 39
1	F	246/385 (64%)	201 (82%)	36 (15%)	9 (4%)	3 27
1	G	245/385 (64%)	201 (82%)	38 (16%)	6 (2%)	6 35
All	All	1744/2695 (65%)	1410 (81%)	283 (16%)	51 (3%)	4 31

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 monosaccharides 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 i

### 6.1 Protein, DNA and RNA chains i

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	256/385 (66%)	2.25	117 (45%) 0   0	118, 145, 169, 195	0
1	B	250/385 (64%)	1.94	86 (34%) 0   1	118, 149, 175, 187	0
1	C	248/385 (64%)	2.00	101 (40%) 0   0	120, 150, 174, 189	0
1	D	254/385 (65%)	2.00	102 (40%) 0   1	118, 149, 170, 188	0
1	E	255/385 (66%)	1.90	101 (39%) 0   1	120, 152, 173, 203	0
1	F	248/385 (64%)	2.32	107 (43%) 0   0	123, 147, 170, 191	0
1	G	247/385 (64%)	1.88	95 (38%) 0   1	122, 149, 172, 193	0
All	All	1758/2695 (65%)	2.04	709 (40%) 0   0	118, 149, 173, 203	0

All (709) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	127	PRO	16.6
1	A	127	PRO	15.5
1	A	126	MET	14.9
1	B	149	GLU	14.2
1	B	147	ALA	13.6
1	B	182	ASN	13.3
1	B	146	ASN	12.3
1	B	191	GLN	12.0
1	C	146	ASN	11.9
1	F	147	ALA	11.8
1	B	181	ALA	11.6
1	E	182	ASN	11.6
1	C	191	GLN	11.1
1	E	147	ALA	10.9
1	G	141	GLY	10.9
1	A	146	ASN	10.8
1	A	147	ALA	9.8

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Mol	Chain	Res	Type	RSRZ
1	D	126	MET	9.8
1	F	346	SER	9.7
1	F	191	GLN	9.5
1	C	147	ALA	9.5
1	F	149	GLU	9.5
1	E	124	ILE	9.5
1	G	182	ASN	9.3
1	B	150	TYR	9.2
1	B	148	LEU	9.2
1	A	125	ILE	9.2
1	F	146	ASN	9.1
1	F	242	ALA	9.0
1	A	191	GLN	9.0
1	G	146	ASN	8.9
1	G	142	ARG	8.9
1	D	271	SER	8.8
1	B	151	VAL	8.5
1	A	128	GLY	8.2
1	F	127	PRO	8.2
1	F	243	TYR	8.1
1	F	148	LEU	8.0
1	D	122	PRO	7.9
1	D	128	GLY	7.9
1	E	146	ASN	7.8
1	B	128	GLY	7.8
1	F	151	VAL	7.8
1	C	314	VAL	7.8
1	A	182	ASN	7.7
1	F	349	ASP	7.6
1	E	122	PRO	7.6
1	A	334	GLN	7.6
1	F	347	ARG	7.6
1	F	348	GLU	7.6
1	A	185	THR	7.5
1	C	140	GLN	7.4
1	C	315	PRO	7.4
1	D	272	ALA	7.3
1	G	149	GLU	7.3
1	F	350	ARG	7.2
1	E	183	VAL	7.2
1	F	150	TYR	7.2
1	F	178	LYS	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	368	LEU	7.2
1	F	195	GLN	7.1
1	A	160	ALA	7.0
1	G	183	VAL	7.0
1	E	123	GLY	6.9
1	F	181	ALA	6.9
1	F	359	THR	6.8
1	F	294	ARG	6.7
1	C	182	ASN	6.7
1	E	181	ALA	6.7
1	F	378	LYS	6.7
1	A	140	GLN	6.7
1	G	341	ALA	6.6
1	C	141	GLY	6.5
1	B	183	VAL	6.5
1	F	128	GLY	6.5
1	A	367	ALA	6.5
1	E	310	GLY	6.5
1	B	190	VAL	6.4
1	D	147	ALA	6.4
1	A	141	GLY	6.4
1	D	276	VAL	6.3
1	C	158	ASN	6.3
1	G	147	ALA	6.2
1	E	187	ALA	6.2
1	E	125	ILE	6.2
1	C	187	ALA	6.1
1	B	127	PRO	6.1
1	G	181	ALA	6.1
1	D	121	ILE	6.1
1	A	124	ILE	6.0
1	C	145	SER	6.0
1	B	177	SER	6.0
1	F	354	VAL	6.0
1	F	145	SER	5.9
1	C	356	ASN	5.9
1	G	332	ALA	5.9
1	D	341	ALA	5.9
1	E	279	PRO	5.9
1	B	176	PHE	5.8
1	A	315	PRO	5.8
1	G	232	ASN	5.8

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Mol	Chain	Res	Type	RSRZ
1	G	367	ALA	5.8
1	E	193	SER	5.8
1	E	128	GLY	5.8
1	A	120	GLN	5.8
1	F	366	LEU	5.7
1	C	149	GLU	5.7
1	D	325	THR	5.7
1	A	181	ALA	5.7
1	A	333	SER	5.7
1	E	368	LEU	5.6
1	A	186	ILE	5.6
1	B	375	ALA	5.5
1	F	132	LEU	5.5
1	D	368	LEU	5.5
1	C	127	PRO	5.5
1	B	372	ARG	5.5
1	A	170	PRO	5.5
1	C	333	SER	5.5
1	D	347	ARG	5.5
1	F	372	ARG	5.4
1	G	365	ARG	5.4
1	A	369	ALA	5.4
1	F	365	ARG	5.4
1	F	184	LYS	5.4
1	G	318	ALA	5.4
1	G	272	ALA	5.4
1	C	153	GLU	5.3
1	C	313	VAL	5.3
1	D	146	ASN	5.3
1	C	368	LEU	5.3
1	A	336	TRP	5.2
1	A	335	VAL	5.2
1	F	345	VAL	5.2
1	A	314	VAL	5.2
1	E	325	THR	5.2
1	F	183	VAL	5.2
1	G	315	PRO	5.2
1	D	273	SER	5.2
1	A	148	LEU	5.2
1	F	364	GLU	5.2
1	F	182	ASN	5.1
1	A	325	THR	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	326	VAL	5.1
1	C	178	LYS	5.1
1	E	160	ALA	5.1
1	D	332	ALA	5.1
1	D	374	THR	5.1
1	C	332	ALA	5.0
1	G	140	GLN	5.0
1	D	151	VAL	5.0
1	F	332	ALA	5.0
1	C	128	GLY	5.0
1	F	367	ALA	5.0
1	A	289	LYS	5.0
1	A	172	SER	5.0
1	G	271	SER	4.9
1	D	367	ALA	4.9
1	G	317	LYS	4.9
1	E	318	ALA	4.9
1	F	331	MET	4.9
1	G	321	ALA	4.9
1	A	131	ARG	4.9
1	G	319	GLN	4.9
1	B	254	ARG	4.9
1	A	378	LYS	4.9
1	G	364	GLU	4.9
1	D	336	TRP	4.8
1	A	363	GLU	4.8
1	E	170	PRO	4.8
1	G	173	ASP	4.8
1	B	196	VAL	4.8
1	C	354	VAL	4.7
1	A	119	MET	4.7
1	F	196	VAL	4.7
1	G	331	MET	4.7
1	F	192	ALA	4.7
1	C	252	ASP	4.7
1	B	348	GLU	4.7
1	A	362	CYS	4.7
1	C	157	THR	4.7
1	G	366	LEU	4.7
1	G	336	TRP	4.6
1	C	183	VAL	4.6
1	G	252	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	373	PRO	4.6
1	E	316	THR	4.6
1	E	126	MET	4.6
1	E	148	LEU	4.5
1	D	370	HIS	4.5
1	E	145	SER	4.5
1	B	365	ARG	4.5
1	E	291	ASN	4.5
1	E	317	LYS	4.5
1	C	331	MET	4.5
1	F	179	GLN	4.5
1	B	341	ALA	4.5
1	D	231	ASP	4.5
1	D	274	GLY	4.5
1	A	195	GLN	4.5
1	F	368	LEU	4.5
1	A	275	ILE	4.4
1	A	274	GLY	4.4
1	C	192	ALA	4.4
1	F	272	ALA	4.4
1	A	155	VAL	4.4
1	A	347	ARG	4.4
1	D	371	TYR	4.4
1	C	148	LEU	4.4
1	A	187	ALA	4.4
1	A	326	VAL	4.4
1	C	369	ALA	4.4
1	C	298	GLY	4.4
1	A	123	GLY	4.4
1	D	330	ASP	4.4
1	E	326	VAL	4.4
1	A	122	PRO	4.4
1	D	155	VAL	4.4
1	G	337	ASP	4.4
1	E	293	GLY	4.4
1	A	173	ASP	4.4
1	F	269	GLU	4.4
1	F	185	THR	4.4
1	G	151	VAL	4.4
1	E	261	ALA	4.3
1	D	153	GLU	4.3
1	C	181	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	290	ASP	4.3
1	B	310	GLY	4.3
1	F	193	SER	4.3
1	F	129	LEU	4.3
1	E	290	ASP	4.3
1	A	276	VAL	4.3
1	E	349	ASP	4.2
1	E	364	GLU	4.2
1	F	208	ASN	4.2
1	E	341	ALA	4.2
1	A	349	ASP	4.2
1	D	124	ILE	4.2
1	A	159	ASN	4.2
1	A	145	SER	4.2
1	B	195	GLN	4.2
1	D	372	ARG	4.2
1	D	333	SER	4.2
1	F	377	ILE	4.2
1	F	157	THR	4.2
1	F	383	SER	4.2
1	C	341	ALA	4.2
1	D	123	GLY	4.2
1	D	373	PRO	4.2
1	E	127	PRO	4.2
1	F	293	GLY	4.2
1	A	192	ALA	4.2
1	G	145	SER	4.2
1	D	234	GLU	4.2
1	D	314	VAL	4.2
1	A	183	VAL	4.2
1	B	157	THR	4.2
1	F	180	THR	4.2
1	D	182	ASN	4.1
1	F	152	ARG	4.1
1	E	370	HIS	4.1
1	D	199	ASP	4.1
1	F	177	SER	4.1
1	D	346	SER	4.1
1	B	374	THR	4.1
1	G	347	ARG	4.1
1	B	145	SER	4.1
1	D	318	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	316	THR	4.1
1	G	378	LYS	4.1
1	F	231	ASP	4.1
1	A	129	LEU	4.0
1	G	150	TYR	4.0
1	C	159	ASN	4.0
1	A	149	GLU	4.0
1	G	368	LEU	4.0
1	D	369	ALA	4.0
1	D	173	ASP	4.0
1	D	158	ASN	4.0
1	C	297	PHE	4.0
1	B	230	GLY	4.0
1	G	320	ALA	4.0
1	B	346	SER	4.0
1	B	359	THR	3.9
1	C	373	PRO	3.9
1	D	196	VAL	3.9
1	A	313	VAL	3.9
1	D	269	GLU	3.9
1	D	242	ALA	3.9
1	D	331	MET	3.9
1	E	231	ASP	3.9
1	D	326	VAL	3.9
1	E	367	ALA	3.8
1	A	156	PHE	3.8
1	F	131	ARG	3.8
1	E	311	LEU	3.8
1	E	185	THR	3.8
1	E	319	GLN	3.8
1	A	196	VAL	3.8
1	B	180	THR	3.8
1	B	315	PRO	3.8
1	G	196	VAL	3.8
1	A	327	GLY	3.8
1	B	300	PRO	3.8
1	C	179	GLN	3.8
1	D	141	GLY	3.8
1	C	327	GLY	3.7
1	D	270	PHE	3.7
1	C	374	THR	3.7
1	B	299	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	315	PRO	3.7
1	B	317	LYS	3.7
1	C	337	ASP	3.7
1	E	171	GLU	3.7
1	A	379	GLY	3.7
1	C	367	ALA	3.7
1	E	180	THR	3.7
1	C	372	ARG	3.7
1	E	159	ASN	3.7
1	D	337	ASP	3.7
1	C	334	GLN	3.7
1	F	375	ALA	3.7
1	A	184	LYS	3.7
1	C	151	VAL	3.6
1	G	148	LEU	3.6
1	A	348	GLU	3.6
1	E	149	GLU	3.6
1	B	290	ASP	3.6
1	B	325	THR	3.6
1	B	382	SER	3.6
1	E	366	LEU	3.6
1	C	361	LEU	3.6
1	B	330	ASP	3.6
1	C	264	GLN	3.6
1	A	364	GLU	3.6
1	G	174	ILE	3.6
1	D	156	PHE	3.6
1	E	337	ASP	3.6
1	F	351	ASP	3.6
1	D	343	VAL	3.6
1	E	365	ARG	3.5
1	D	327	GLY	3.5
1	F	289	LYS	3.5
1	B	340	ASP	3.5
1	D	375	ALA	3.5
1	A	318	ALA	3.5
1	A	142	ARG	3.5
1	G	379	GLY	3.5
1	B	291	ASN	3.5
1	B	184	LYS	3.5
1	E	184	LYS	3.5
1	A	337	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	291	ASN	3.5
1	G	342	THR	3.5
1	F	356	ASN	3.5
1	D	240	ALA	3.5
1	C	379	GLY	3.5
1	B	379	GLY	3.5
1	G	184	LYS	3.5
1	B	318	ALA	3.4
1	A	139	ALA	3.4
1	B	279	PRO	3.4
1	D	319	GLN	3.4
1	F	133	THR	3.4
1	B	324	PHE	3.4
1	B	178	LYS	3.4
1	C	243	TYR	3.4
1	F	333	SER	3.4
1	G	346	SER	3.4
1	B	242	ALA	3.4
1	E	292	GLU	3.4
1	G	195	GLN	3.4
1	D	297	PHE	3.4
1	D	172	SER	3.4
1	C	208	ASN	3.3
1	G	143	THR	3.3
1	B	298	GLY	3.3
1	D	129	LEU	3.3
1	G	131	ARG	3.3
1	A	231	ASP	3.3
1	A	293	GLY	3.3
1	G	219	GLU	3.3
1	D	340	ASP	3.3
1	B	319	GLN	3.3
1	E	307	ILE	3.3
1	C	362	CYS	3.3
1	E	277	LEU	3.3
1	E	299	GLY	3.3
1	A	332	ALA	3.3
1	B	349	ASP	3.3
1	F	273	SER	3.3
1	F	317	LYS	3.3
1	A	331	MET	3.3
1	F	310	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	186	ILE	3.3
1	F	363	GLU	3.3
1	A	271	SER	3.2
1	G	296	ILE	3.2
1	A	375	ALA	3.2
1	A	372	ARG	3.2
1	C	160	ALA	3.2
1	C	355	LYS	3.2
1	F	369	ALA	3.2
1	A	193	SER	3.2
1	D	125	ILE	3.2
1	G	370	HIS	3.2
1	A	346	SER	3.2
1	G	157	THR	3.2
1	D	183	VAL	3.2
1	D	277	LEU	3.2
1	A	272	ALA	3.2
1	B	243	TYR	3.2
1	F	353	PHE	3.2
1	D	185	THR	3.2
1	A	121	ILE	3.2
1	B	332	ALA	3.1
1	B	366	LEU	3.1
1	F	130	ARG	3.1
1	A	277	LEU	3.1
1	C	180	THR	3.1
1	G	328	GLY	3.1
1	G	369	ALA	3.1
1	A	254	ARG	3.1
1	C	375	ALA	3.1
1	D	140	GLN	3.1
1	D	195	GLN	3.1
1	F	153	GLU	3.1
1	B	368	LEU	3.1
1	A	180	THR	3.1
1	E	194	ARG	3.1
1	B	126	MET	3.1
1	E	276	VAL	3.1
1	D	237	ASN	3.0
1	G	231	ASP	3.0
1	D	267	GLU	3.0
1	F	292	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	177	SER	3.0
1	C	299	GLY	3.0
1	G	362	CYS	3.0
1	B	316	THR	3.0
1	B	333	SER	3.0
1	D	378	LYS	3.0
1	B	380	THR	3.0
1	D	275	ILE	3.0
1	G	363	GLU	3.0
1	G	335	VAL	3.0
1	F	297	PHE	3.0
1	E	178	LYS	3.0
1	G	156	PHE	3.0
1	G	180	THR	2.9
1	A	312	PRO	2.9
1	E	157	THR	2.9
1	A	382	SER	2.9
1	E	130	ARG	2.9
1	E	155	VAL	2.9
1	G	212	MET	2.9
1	C	348	GLU	2.9
1	D	193	SER	2.9
1	E	369	ALA	2.9
1	F	209	ASN	2.9
1	C	357	MET	2.9
1	C	275	ILE	2.9
1	A	264	GLN	2.9
1	B	321	ALA	2.9
1	C	150	TYR	2.9
1	G	233	LEU	2.9
1	E	151	VAL	2.9
1	G	298	GLY	2.9
1	F	207	ILE	2.9
1	E	191	GLN	2.9
1	F	264	GLN	2.9
1	G	255	ALA	2.9
1	G	375	ALA	2.9
1	E	278	ASN	2.9
1	F	143	THR	2.8
1	F	290	ASP	2.8
1	G	293	GLY	2.8
1	E	348	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	158	ASN	2.8
1	A	361	LEU	2.8
1	D	230	GLY	2.8
1	G	133	THR	2.8
1	C	360	ILE	2.8
1	D	348	GLU	2.8
1	E	243	TYR	2.8
1	G	220	GLU	2.8
1	D	328	GLY	2.8
1	E	309	TRP	2.8
1	C	370	HIS	2.8
1	A	143	THR	2.7
1	A	255	ALA	2.7
1	B	241	THR	2.7
1	F	197	MET	2.8
1	D	268	SER	2.7
1	E	244	ASP	2.7
1	C	296	ILE	2.7
1	C	377	ILE	2.7
1	F	286	ALA	2.7
1	A	366	LEU	2.7
1	F	271	SER	2.7
1	D	135	ARG	2.7
1	F	371	TYR	2.7
1	B	378	LYS	2.7
1	G	171	GLU	2.7
1	C	279	PRO	2.7
1	E	264	GLN	2.7
1	A	130	ARG	2.7
1	B	272	ALA	2.7
1	D	157	THR	2.7
1	F	254	ARG	2.7
1	B	129	LEU	2.7
1	G	314	VAL	2.7
1	G	353	PHE	2.7
1	F	268	SER	2.7
1	D	150	TYR	2.7
1	F	318	ALA	2.7
1	G	144	SER	2.7
1	G	359	THR	2.7
1	A	370	HIS	2.6
1	B	223	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	340	ASP	2.6
1	B	153	GLU	2.6
1	F	186	ILE	2.6
1	B	210	ARG	2.6
1	G	253	THR	2.6
1	A	343	VAL	2.6
1	B	231	ASP	2.6
1	C	267	GLU	2.6
1	F	362	CYS	2.6
1	G	208	ASN	2.6
1	D	362	CYS	2.6
1	E	268	SER	2.6
1	G	172	SER	2.6
1	B	331	MET	2.6
1	F	190	VAL	2.6
1	C	349	ASP	2.6
1	D	241	THR	2.6
1	C	176	PHE	2.6
1	D	192	ALA	2.6
1	E	312	PRO	2.6
1	D	315	PRO	2.6
1	A	316	THR	2.6
1	D	342	THR	2.6
1	A	321	ALA	2.5
1	B	187	ALA	2.5
1	C	271	SER	2.5
1	F	315	PRO	2.5
1	C	269	GLU	2.5
1	G	234	GLU	2.5
1	D	149	GLU	2.5
1	A	269	GLU	2.5
1	A	158	ASN	2.5
1	E	121	ILE	2.5
1	F	144	SER	2.5
1	C	330	ASP	2.5
1	A	265	VAL	2.5
1	E	371	TYR	2.5
1	A	317	LYS	2.5
1	A	338	ARG	2.5
1	A	294	ARG	2.5
1	C	253	THR	2.5
1	B	278	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	257	ILE	2.5
1	E	267	GLU	2.5
1	G	325	THR	2.5
1	F	279	PRO	2.5
1	D	181	ALA	2.5
1	A	194	ARG	2.5
1	E	361	LEU	2.5
1	D	152	ARG	2.4
1	F	338	ARG	2.4
1	E	346	SER	2.4
1	D	239	VAL	2.4
1	F	334	GLN	2.4
1	C	244	ASP	2.4
1	D	260	HIS	2.4
1	D	243	TYR	2.4
1	C	376	ILE	2.4
1	E	305	SER	2.4
1	A	365	ARG	2.4
1	B	156	PHE	2.4
1	F	244	ASP	2.4
1	E	177	SER	2.4
1	G	258	ILE	2.4
1	F	328	GLY	2.4
1	F	261	ALA	2.4
1	F	327	GLY	2.4
1	A	288	LEU	2.4
1	B	360	ILE	2.4
1	F	296	ILE	2.4
1	G	300	PRO	2.4
1	G	301	GLN	2.4
1	G	185	THR	2.4
1	B	320	ALA	2.4
1	C	205	SER	2.4
1	G	348	GLU	2.4
1	C	185	THR	2.4
1	A	279	PRO	2.4
1	G	254	ARG	2.4
1	D	296	ILE	2.4
1	E	374	THR	2.3
1	A	353	PHE	2.3
1	C	186	ILE	2.3
1	B	189	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	192	ALA	2.3
1	E	254	ARG	2.3
1	C	310	GLY	2.3
1	F	358	LEU	2.3
1	A	132	LEU	2.3
1	D	351	ASP	2.3
1	E	208	ASN	2.3
1	F	274	GLY	2.3
1	E	274	GLY	2.3
1	E	140	GLN	2.3
1	G	338	ARG	2.3
1	C	353	PHE	2.3
1	E	332	ALA	2.3
1	B	314	VAL	2.3
1	B	347	ARG	2.3
1	C	309	TRP	2.3
1	G	333	SER	2.3
1	C	316	THR	2.3
1	G	224	LEU	2.3
1	A	324	PHE	2.3
1	C	328	GLY	2.3
1	C	364	GLU	2.3
1	F	309	TRP	2.3
1	E	382	SER	2.3
1	F	370	HIS	2.3
1	A	273	SER	2.3
1	E	223	LEU	2.3
1	C	131	ARG	2.3
1	D	160	ALA	2.3
1	E	258	ILE	2.2
1	A	374	THR	2.2
1	A	223	LEU	2.2
1	D	200	ALA	2.2
1	B	175	THR	2.2
1	C	197	MET	2.2
1	B	376	ILE	2.2
1	B	173	ASP	2.2
1	A	209	ASN	2.2
1	C	220	GLU	2.2
1	A	278	ASN	2.2
1	C	363	GLU	2.2
1	E	300	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	132	LEU	2.2
1	E	362	CYS	2.2
1	C	152	ARG	2.2
1	E	302	ALA	2.2
1	F	241	THR	2.2
1	B	152	ARG	2.2
1	F	326	VAL	2.2
1	E	216	ALA	2.2
1	D	324	PHE	2.2
1	D	365	ARG	2.2
1	D	356	ASN	2.2
1	C	380	THR	2.2
1	C	312	PRO	2.2
1	C	344	GLU	2.2
1	D	329	PHE	2.2
1	G	292	GLU	2.2
1	B	367	ALA	2.2
1	A	270	PHE	2.1
1	C	277	LEU	2.1
1	G	207	ILE	2.1
1	C	188	HIS	2.1
1	E	275	ILE	2.1
1	E	377	ILE	2.1
1	E	350	ARG	2.1
1	A	153	GLU	2.1
1	F	159	ASN	2.1
1	A	328	GLY	2.1
1	D	198	ASP	2.1
1	D	145	SER	2.1
1	C	272	ALA	2.1
1	E	255	ALA	2.1
1	B	345	VAL	2.1
1	A	171	GLU	2.1
1	A	150	TYR	2.1
1	G	191	GLN	2.1
1	D	366	LEU	2.1
1	F	352	ASN	2.1
1	C	321	ALA	2.1
1	F	300	PRO	2.1
1	D	361	LEU	2.1
1	C	248	ASN	2.1
1	D	261	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	318	ALA	2.1
1	C	290	ASP	2.1
1	C	184	LYS	2.1
1	C	239	VAL	2.1
1	E	212	MET	2.1
1	E	262	ILE	2.1
1	E	129	LEU	2.1
1	G	295	TYR	2.1
1	E	333	SER	2.1
1	C	359	THR	2.1
1	G	326	VAL	2.1
1	G	186	ILE	2.0
1	G	259	ALA	2.0
1	A	371	TYR	2.0
1	F	298	GLY	2.0
1	F	187	ALA	2.0
1	G	294	ARG	2.0
1	B	158	ASN	2.0
1	G	373	PRO	2.0
1	D	259	ALA	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 monosaccharides 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.