Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:41 am BST

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

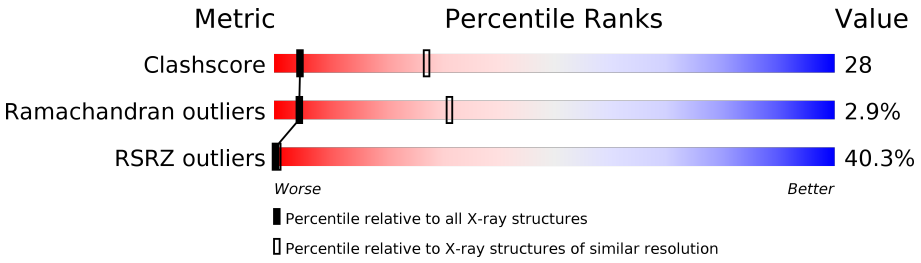
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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 on 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.

Mol	Chain	Length	Quality of chain
1	A	385	30% 50% 15% • 34%
1	B	385	22% 44% 19% • 35%
1	C	385	26% 46% 16% • 36%
1	D	385	26% 52% 12% • 34%
1	E	385	26% 45% 20% • 34%
1	F	385	28% 43% 19% • 36%
1	G	385	25% 46% 15% • 36%

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.

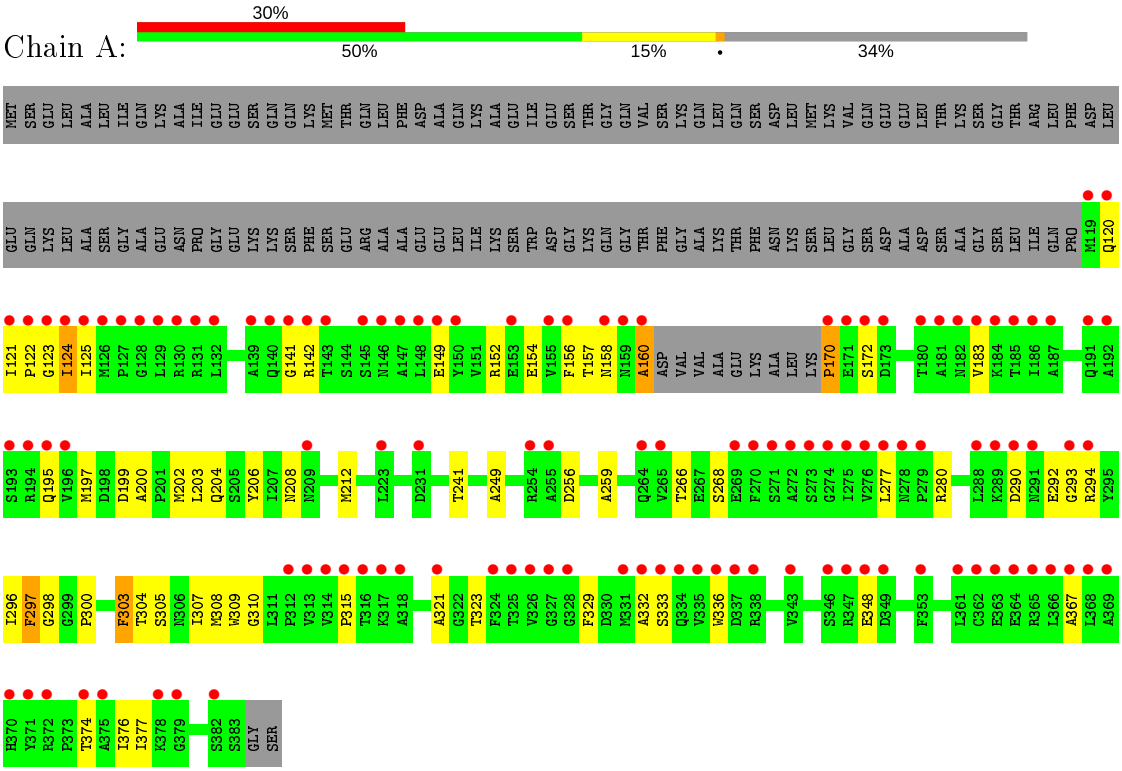
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	0	0	0
			1260	748	256	256			
1	B	250	Total	C	N	O	0	0	0
			1231	731	250	250			
1	C	248	Total	C	N	O	0	0	0
			1221	725	248	248			
1	D	254	Total	C	N	O	0	0	0
			1250	742	254	254			
1	E	255	Total	C	N	O	0	0	0
			1255	745	255	255			
1	F	248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

These plots are drawn for all protein, RNA and DNA 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.

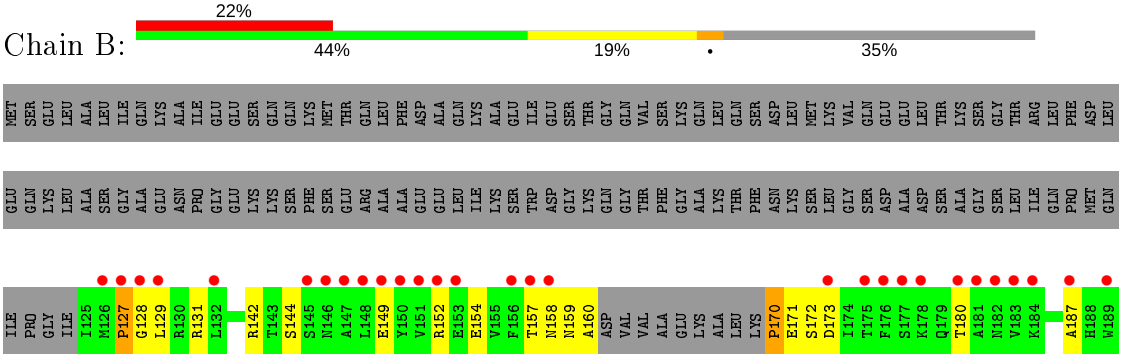
- Molecule 1: Major capsid protein

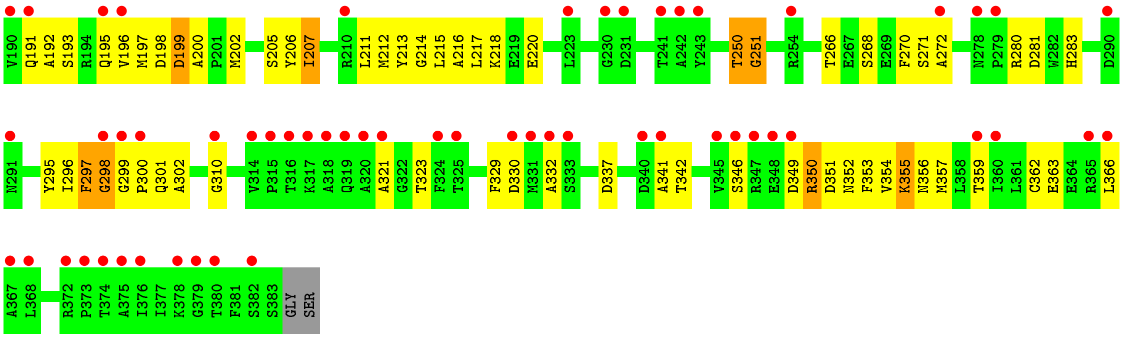
Chain A:



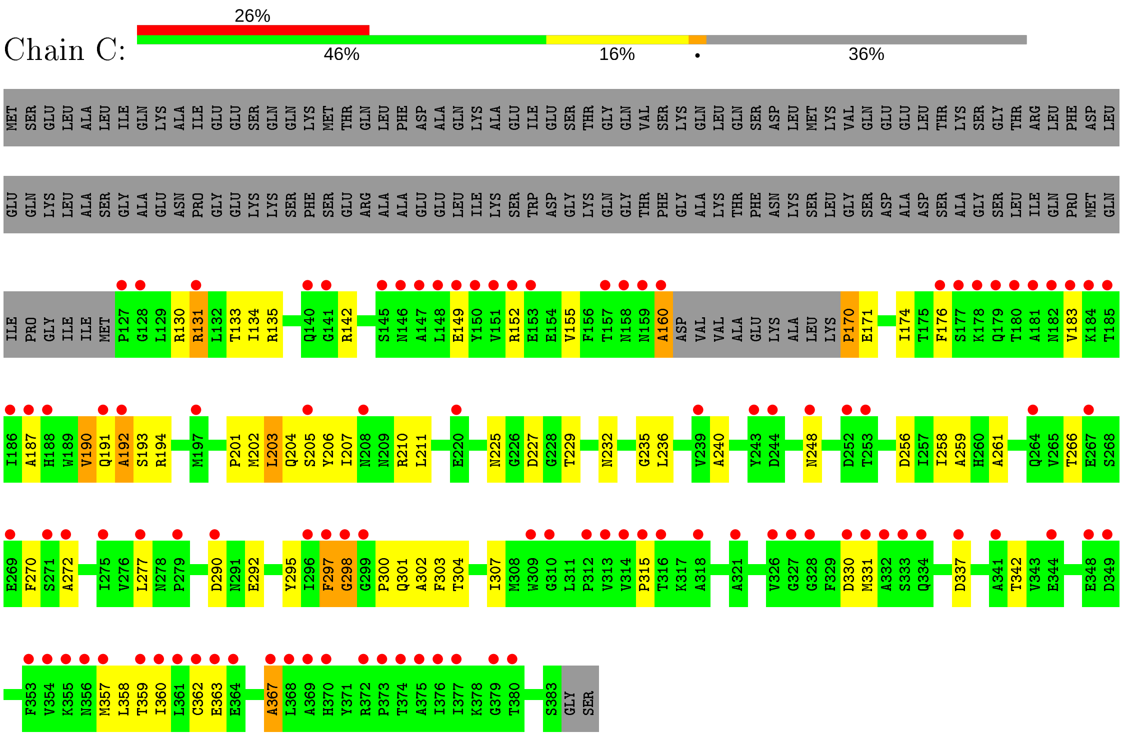
- Molecule 1: Major capsid protein

Chain B:

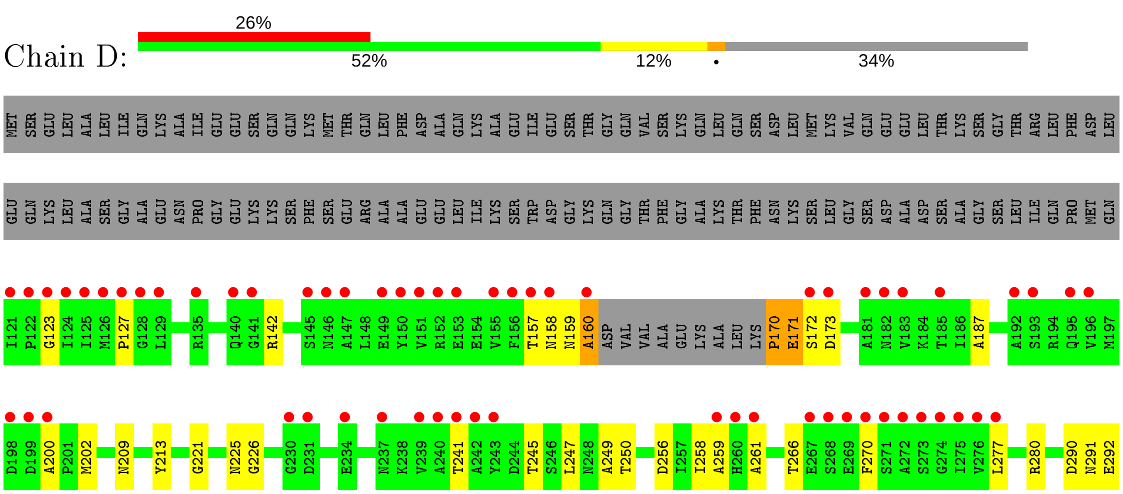


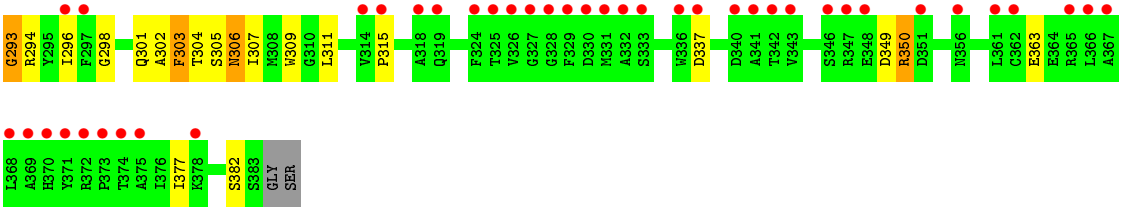


- Molecule 1: Major capsid protein



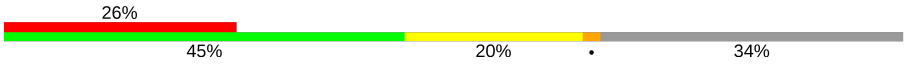
- Molecule 1: Major capsid protein

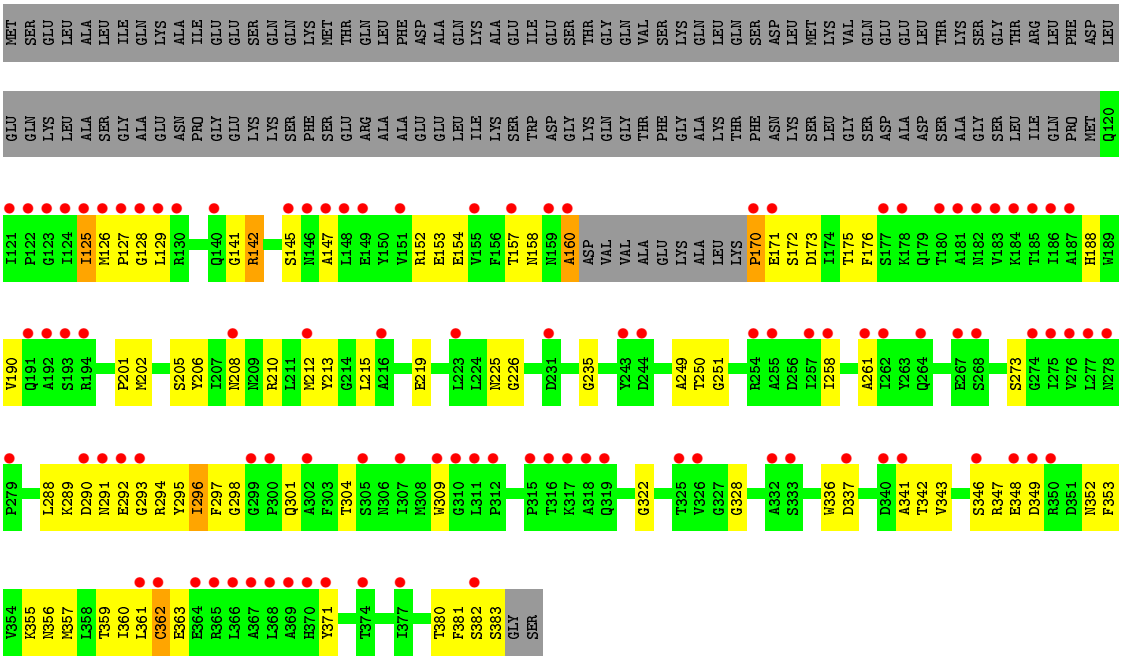




• Molecule 1: Major capsid protein

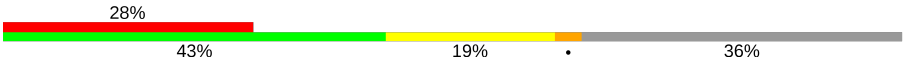
Chain E:

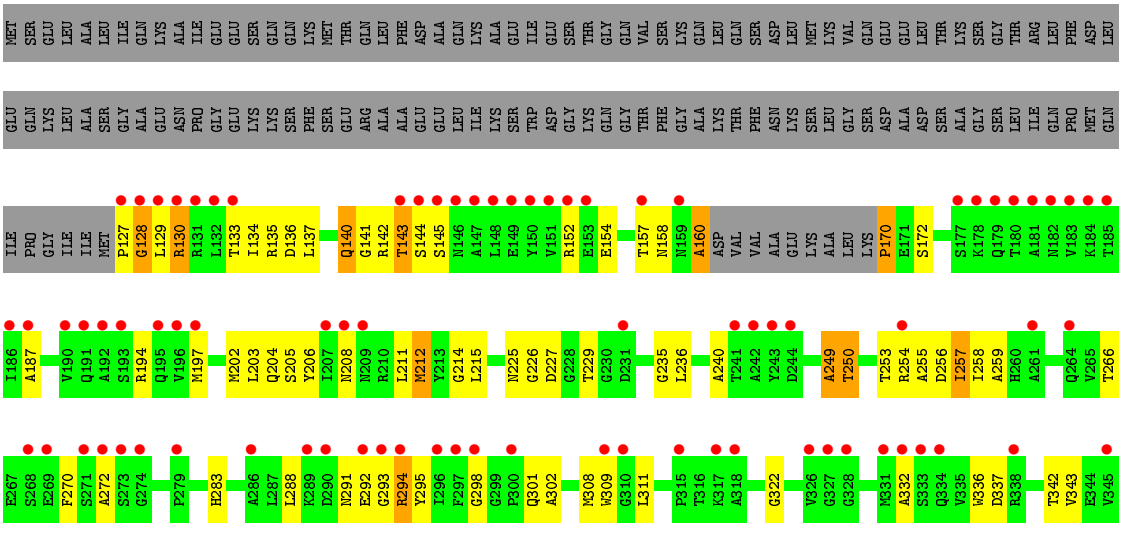


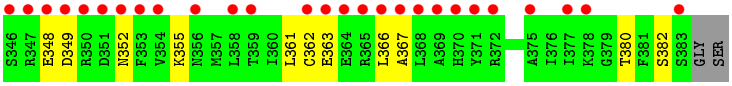


• Molecule 1: Major capsid protein

Chain F:

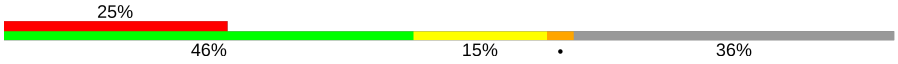


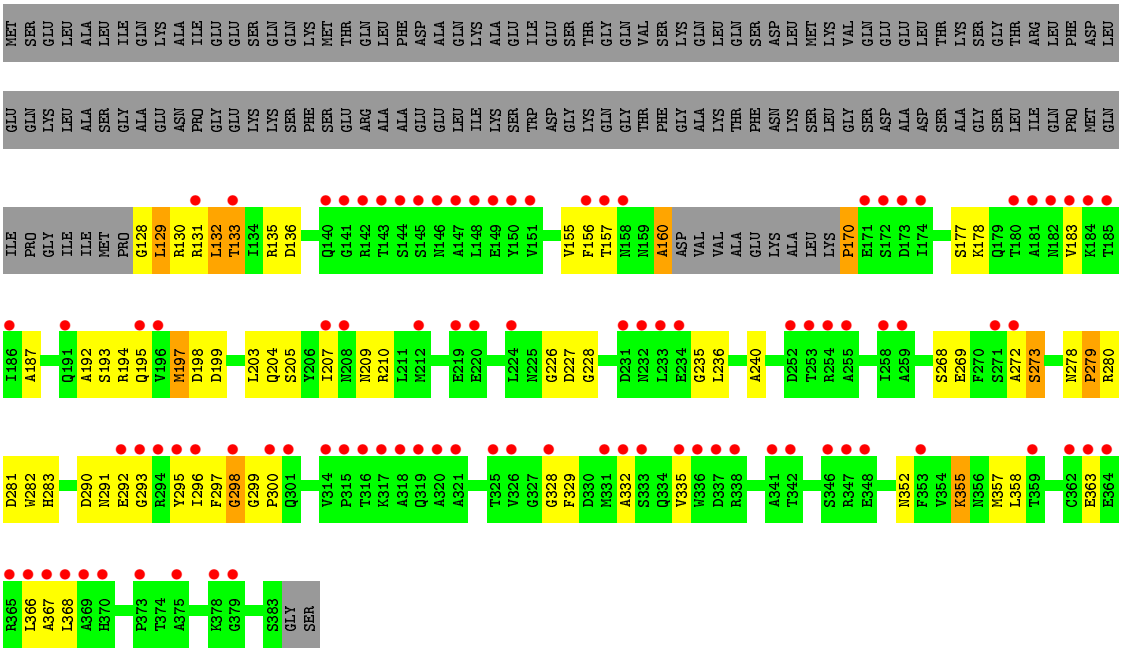




- Molecule 1: Major capsid protein

Chain G:





4 Data and refinement statistics (i)

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 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
$< I/\sigma(I) >$ [1]	1.72 (at 5.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.461 , 0.467 0.387 , (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)	0.34 , 298.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.16$	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^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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.39	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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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

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:305:SER:O	1:D:307:ILE:N	2.23	0.69
1:D:293:GLY:C	1:F:298:GLY:HA2	2.13	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:206:TYR:O	1:E:210:ARG:CB	2.47	0.62
1:E:125:ILE:O	1:E:208:ASN:O	2.18	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:227:ASP:C	1:F:229:THR:N	2.73	0.41
1:F:187:ALA:HB2	1:F:363:GLU:HA	2.02	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 carbohydrates 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, 95^{th} 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%)	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	121, 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	15.0
1	B	149	GLU	14.2
1	B	147	ALA	13.6
1	B	182	ASN	13.3
1	B	146	ASN	12.2
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	11.5
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	C	147	ALA	9.5
1	F	149	GLU	9.5
1	F	191	GLN	9.5
1	E	124	ILE	9.4
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	9.1
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	8.1
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	C	314	VAL	7.8
1	F	151	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	7.3
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	6.6
1	F	128	GLY	6.5
1	B	183	VAL	6.5
1	A	367	ALA	6.5
1	E	310	GLY	6.5
1	B	190	VAL	6.5
1	A	141	GLY	6.4
1	D	147	ALA	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	B	127	PRO	6.1
1	C	187	ALA	6.1
1	G	181	ALA	6.1
1	D	121	ILE	6.0
1	A	124	ILE	6.0
1	C	145	SER	6.0
1	F	354	VAL	6.0
1	B	177	SER	6.0
1	F	145	SER	5.9
1	G	332	ALA	5.9
1	C	356	ASN	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	E	193	SER	5.8

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Mol	Chain	Res	Type	RSRZ
1	G	232	ASN	5.8
1	G	367	ALA	5.8
1	E	128	GLY	5.8
1	A	120	GLN	5.8
1	F	366	LEU	5.7
1	A	181	ALA	5.7
1	A	333	SER	5.7
1	D	325	THR	5.7
1	C	149	GLU	5.7
1	E	368	LEU	5.6
1	A	186	ILE	5.6
1	B	375	ALA	5.6
1	B	372	ARG	5.5
1	F	132	LEU	5.5
1	C	127	PRO	5.5
1	D	368	LEU	5.5
1	A	170	PRO	5.5
1	C	333	SER	5.5
1	D	347	ARG	5.5
1	F	372	ARG	5.5
1	G	365	ARG	5.4
1	A	369	ALA	5.4
1	F	184	LYS	5.4
1	F	365	ARG	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	C	368	LEU	5.3
1	D	146	ASN	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	F	183	VAL	5.2
1	E	325	THR	5.2
1	G	315	PRO	5.2
1	A	148	LEU	5.2
1	F	364	GLU	5.2
1	F	182	ASN	5.2
1	D	273	SER	5.2
1	C	326	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	160	ALA	5.1
1	A	325	THR	5.1
1	C	178	LYS	5.1
1	D	332	ALA	5.1
1	D	374	THR	5.1
1	C	332	ALA	5.0
1	D	151	VAL	5.0
1	G	140	GLN	5.0
1	F	332	ALA	5.0
1	F	367	ALA	5.0
1	C	128	GLY	5.0
1	A	289	LYS	5.0
1	A	172	SER	4.9
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	319	GLN	4.9
1	G	321	ALA	4.9
1	A	131	ARG	4.9
1	B	254	ARG	4.9
1	G	364	GLU	4.9
1	A	378	LYS	4.9
1	D	336	TRP	4.9
1	E	170	PRO	4.8
1	A	363	GLU	4.8
1	G	173	ASP	4.8
1	C	354	VAL	4.8
1	B	196	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	B	348	GLU	4.7
1	C	252	ASP	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	B	365	ARG	4.5
1	D	370	HIS	4.5
1	E	148	LEU	4.5
1	E	145	SER	4.5
1	E	291	ASN	4.5
1	C	331	MET	4.5
1	E	317	LYS	4.5
1	F	179	GLN	4.5
1	B	341	ALA	4.5
1	D	231	ASP	4.5
1	F	368	LEU	4.5
1	A	195	GLN	4.5
1	D	274	GLY	4.5
1	F	272	ALA	4.4
1	C	192	ALA	4.4
1	A	155	VAL	4.4
1	A	275	ILE	4.4
1	D	371	TYR	4.4
1	A	274	GLY	4.4
1	A	187	ALA	4.4
1	C	369	ALA	4.4
1	A	347	ARG	4.4
1	C	148	LEU	4.4
1	A	123	GLY	4.4
1	C	298	GLY	4.4
1	E	326	VAL	4.4
1	A	326	VAL	4.4
1	D	155	VAL	4.4
1	D	330	ASP	4.4
1	A	122	PRO	4.4
1	E	293	GLY	4.4
1	F	185	THR	4.4
1	G	337	ASP	4.4
1	A	173	ASP	4.4
1	F	269	GLU	4.4
1	G	151	VAL	4.4
1	D	153	GLU	4.3
1	E	261	ALA	4.3
1	A	290	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	181	ALA	4.3
1	B	310	GLY	4.3
1	F	193	SER	4.3
1	E	290	ASP	4.3
1	F	129	LEU	4.3
1	A	276	VAL	4.3
1	E	349	ASP	4.3
1	F	208	ASN	4.3
1	E	341	ALA	4.2
1	E	364	GLU	4.2
1	A	349	ASP	4.2
1	D	124	ILE	4.2
1	A	159	ASN	4.2
1	D	372	ARG	4.2
1	A	145	SER	4.2
1	F	377	ILE	4.2
1	D	333	SER	4.2
1	F	157	THR	4.2
1	C	341	ALA	4.2
1	B	195	GLN	4.2
1	F	383	SER	4.2
1	F	293	GLY	4.2
1	D	373	PRO	4.2
1	D	123	GLY	4.2
1	E	127	PRO	4.2
1	D	234	GLU	4.2
1	D	314	VAL	4.2
1	A	192	ALA	4.2
1	G	145	SER	4.2
1	B	157	THR	4.2
1	A	183	VAL	4.2
1	F	180	THR	4.2
1	E	370	HIS	4.1
1	F	152	ARG	4.1
1	D	182	ASN	4.1
1	B	374	THR	4.1
1	F	177	SER	4.1
1	D	346	SER	4.1
1	D	199	ASP	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	G	150	TYR	4.0
1	A	129	LEU	4.0
1	C	159	ASN	4.0
1	A	149	GLU	4.0
1	G	368	LEU	4.0
1	D	173	ASP	4.0
1	D	369	ALA	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	C	373	PRO	3.9
1	B	359	THR	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	A	156	PHE	3.8
1	E	367	ALA	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	D	141	GLY	3.8
1	D	270	PHE	3.8
1	G	196	VAL	3.8
1	B	300	PRO	3.8
1	C	179	GLN	3.7
1	C	327	GLY	3.7
1	C	374	THR	3.7
1	A	327	GLY	3.7
1	B	299	GLY	3.7

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

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Mol	Chain	Res	Type	RSRZ
1	E	184	LYS	3.5
1	F	356	ASN	3.5
1	G	342	THR	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	324	PHE	3.4
1	B	279	PRO	3.4
1	D	319	GLN	3.4
1	F	133	THR	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	172	SER	3.4
1	D	297	PHE	3.4
1	C	208	ASN	3.4
1	A	231	ASP	3.3
1	B	298	GLY	3.3
1	G	131	ARG	3.3
1	D	129	LEU	3.3
1	G	143	THR	3.3
1	A	293	GLY	3.3
1	G	219	GLU	3.3
1	B	319	GLN	3.3
1	D	340	ASP	3.3
1	E	307	ILE	3.3
1	E	299	GLY	3.3
1	C	362	CYS	3.3
1	E	277	LEU	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	372	ARG	3.2
1	A	375	ALA	3.2
1	C	355	LYS	3.2
1	C	160	ALA	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	G	157	THR	3.2
1	A	346	SER	3.2
1	D	183	VAL	3.2
1	D	277	LEU	3.2
1	B	243	TYR	3.2
1	A	272	ALA	3.2
1	F	353	PHE	3.2
1	D	185	THR	3.2
1	A	121	ILE	3.2
1	B	332	ALA	3.2
1	B	366	LEU	3.1
1	F	130	ARG	3.1
1	A	277	LEU	3.1
1	G	328	GLY	3.1
1	G	369	ALA	3.1
1	A	254	ARG	3.1
1	C	180	THR	3.1
1	C	375	ALA	3.1
1	D	140	GLN	3.1
1	B	368	LEU	3.1
1	D	195	GLN	3.1
1	F	153	GLU	3.1
1	A	180	THR	3.1
1	B	126	MET	3.1
1	E	194	ARG	3.1
1	D	237	ASN	3.1
1	E	276	VAL	3.1
1	D	267	GLU	3.0
1	F	292	GLU	3.0
1	G	231	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	177	SER	3.0
1	C	299	GLY	3.0
1	B	316	THR	3.0
1	G	362	CYS	3.0
1	B	333	SER	3.0
1	D	378	LYS	3.0
1	B	380	THR	3.0
1	F	297	PHE	3.0
1	G	363	GLU	3.0
1	D	275	ILE	3.0
1	G	335	VAL	3.0
1	G	156	PHE	3.0
1	E	178	LYS	3.0
1	E	157	THR	2.9
1	G	180	THR	2.9
1	E	130	ARG	2.9
1	A	382	SER	2.9
1	E	369	ALA	2.9
1	A	312	PRO	2.9
1	E	155	VAL	2.9
1	C	348	GLU	2.9
1	D	193	SER	2.9
1	G	212	MET	2.9
1	F	209	ASN	2.9
1	C	357	MET	2.9
1	C	275	ILE	2.9
1	B	321	ALA	2.9
1	A	264	GLN	2.9
1	C	150	TYR	2.9
1	G	233	LEU	2.9
1	G	298	GLY	2.9
1	F	207	ILE	2.9
1	E	151	VAL	2.9
1	F	264	GLN	2.9
1	E	191	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	E	348	GLU	2.8
1	G	158	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	293	GLY	2.8
1	D	348	GLU	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	G	220	GLU	2.8
1	E	243	TYR	2.8
1	C	370	HIS	2.8
1	D	328	GLY	2.8
1	E	309	TRP	2.8
1	B	241	THR	2.8
1	A	255	ALA	2.8
1	D	268	SER	2.8
1	F	197	MET	2.8
1	A	143	THR	2.7
1	E	244	ASP	2.7
1	F	286	ALA	2.7
1	C	296	ILE	2.7
1	C	377	ILE	2.7
1	F	271	SER	2.7
1	B	378	LYS	2.7
1	D	135	ARG	2.7
1	A	366	LEU	2.7
1	G	171	GLU	2.7
1	F	371	TYR	2.7
1	C	279	PRO	2.7
1	E	264	GLN	2.7
1	D	157	THR	2.7
1	B	272	ALA	2.7
1	G	314	VAL	2.7
1	A	130	ARG	2.7
1	B	129	LEU	2.7
1	F	254	ARG	2.7
1	G	353	PHE	2.7
1	F	268	SER	2.7
1	F	318	ALA	2.7
1	D	150	TYR	2.7
1	A	370	HIS	2.7
1	G	359	THR	2.7
1	G	144	SER	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	E	268	SER	2.6
1	F	362	CYS	2.6
1	G	208	ASN	2.6
1	D	362	CYS	2.6
1	G	172	SER	2.6
1	B	331	MET	2.6
1	C	349	ASP	2.6
1	D	241	THR	2.6
1	C	176	PHE	2.6
1	F	190	VAL	2.6
1	D	192	ALA	2.6
1	D	315	PRO	2.6
1	E	312	PRO	2.6
1	A	316	THR	2.6
1	A	321	ALA	2.5
1	C	271	SER	2.5
1	D	342	THR	2.5
1	F	315	PRO	2.5
1	B	187	ALA	2.5
1	C	269	GLU	2.5
1	D	149	GLU	2.5
1	G	234	GLU	2.5
1	A	269	GLU	2.5
1	A	158	ASN	2.5
1	F	144	SER	2.5
1	C	330	ASP	2.5
1	E	121	ILE	2.5
1	A	265	VAL	2.5
1	E	371	TYR	2.5
1	A	317	LYS	2.5
1	E	267	GLU	2.5
1	A	294	ARG	2.5
1	A	338	ARG	2.5
1	G	325	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	278	ASN	2.5
1	C	253	THR	2.5
1	E	257	ILE	2.5
1	F	279	PRO	2.5
1	D	152	ARG	2.5
1	D	181	ALA	2.5
1	A	194	ARG	2.5
1	F	338	ARG	2.4
1	E	361	LEU	2.4
1	D	239	VAL	2.4
1	E	346	SER	2.4
1	F	334	GLN	2.4
1	C	244	ASP	2.4
1	B	156	PHE	2.4
1	D	260	HIS	2.4
1	D	243	TYR	2.4
1	E	305	SER	2.4
1	C	376	ILE	2.4
1	E	177	SER	2.4
1	F	328	GLY	2.4
1	A	365	ARG	2.4
1	F	244	ASP	2.4
1	G	258	ILE	2.4
1	A	288	LEU	2.4
1	F	261	ALA	2.4
1	F	327	GLY	2.4
1	F	296	ILE	2.4
1	B	360	ILE	2.4
1	G	185	THR	2.4
1	B	320	ALA	2.4
1	G	300	PRO	2.4
1	C	205	SER	2.4
1	G	301	GLN	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	E	374	THR	2.4
1	C	186	ILE	2.3
1	D	296	ILE	2.3
1	C	310	GLY	2.3
1	E	192	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	353	PHE	2.3
1	E	254	ARG	2.3
1	B	189	TRP	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	F	358	LEU	2.3
1	E	274	GLY	2.3
1	E	140	GLN	2.3
1	C	353	PHE	2.3
1	E	332	ALA	2.3
1	G	338	ARG	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	A	324	PHE	2.3
1	C	316	THR	2.3
1	C	364	GLU	2.3
1	G	224	LEU	2.3
1	C	328	GLY	2.3
1	F	309	TRP	2.3
1	E	382	SER	2.3
1	F	370	HIS	2.3
1	E	223	LEU	2.3
1	A	273	SER	2.3
1	C	131	ARG	2.3
1	D	160	ALA	2.3
1	E	258	ILE	2.2
1	A	223	LEU	2.2
1	A	374	THR	2.2
1	B	376	ILE	2.2
1	B	173	ASP	2.2
1	C	197	MET	2.2
1	D	200	ALA	2.2
1	B	175	THR	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	C	152	ARG	2.2
1	E	302	ALA	2.2
1	F	241	THR	2.2
1	E	362	CYS	2.2
1	F	326	VAL	2.2
1	B	152	ARG	2.2
1	D	324	PHE	2.2
1	E	216	ALA	2.2
1	D	365	ARG	2.2
1	D	356	ASN	2.2
1	C	380	THR	2.2
1	B	367	ALA	2.2
1	C	312	PRO	2.2
1	A	270	PHE	2.2
1	C	277	LEU	2.2
1	C	344	GLU	2.2
1	G	292	GLU	2.2
1	D	329	PHE	2.1
1	E	350	ARG	2.1
1	E	377	ILE	2.1
1	G	207	ILE	2.1
1	A	153	GLU	2.1
1	E	275	ILE	2.1
1	F	159	ASN	2.1
1	C	188	HIS	2.1
1	D	145	SER	2.1
1	C	272	ALA	2.1
1	A	328	GLY	2.1
1	A	150	TYR	2.1
1	E	255	ALA	2.1
1	D	198	ASP	2.1
1	G	191	GLN	2.1
1	F	300	PRO	2.1
1	A	171	GLU	2.1
1	B	345	VAL	2.1
1	C	321	ALA	2.1
1	D	366	LEU	2.1
1	F	352	ASN	2.1
1	C	248	ASN	2.1
1	D	361	LEU	2.1
1	C	318	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	261	ALA	2.1
1	C	290	ASP	2.1
1	C	239	VAL	2.1
1	C	184	LYS	2.1
1	E	212	MET	2.1
1	E	262	ILE	2.1
1	E	333	SER	2.1
1	E	129	LEU	2.1
1	G	295	TYR	2.1
1	G	326	VAL	2.1
1	C	359	THR	2.1
1	G	186	ILE	2.0
1	A	371	TYR	2.0
1	G	259	ALA	2.0
1	F	298	GLY	2.0
1	B	158	ASN	2.0
1	F	187	ALA	2.0
1	G	294	ARG	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 carbohydrates 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.