



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:04 AM UTC

PDB ID : 2FRP / pdb_00002frp
Title : Bacteriophage HK97 Expansion Intermediate IV
Authors : Gan, L.; Speir, J.A.; Conway, J.F.; Lander, G.; Cheng, N.; Firek, B.A.; Hendrix, R.W.; Duda, R.L.; Liljas, L.; Johnson, J.E.
Deposited on : 2006-01-19
Resolution : 7.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

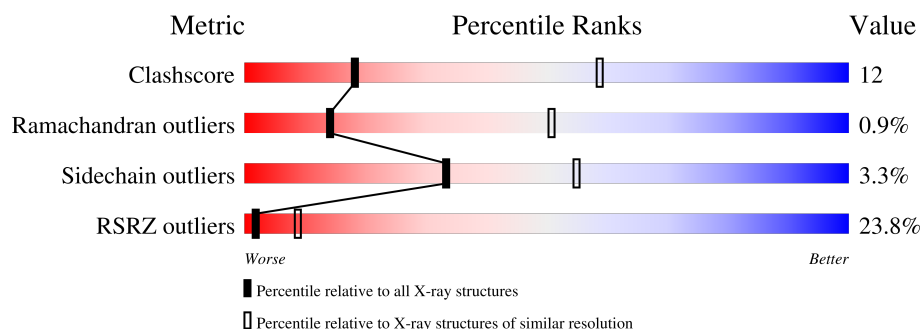
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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

Mol	Chain	Length	Quality of chain
1	A	282	26% 70% 28% ..
1	B	282	23% 72% 26% ..
1	C	282	23% 77% 22% .
1	D	282	20% 73% 24% ..
1	E	282	21% 72% 26% ..
1	F	282	21% 61% 28% 9%
1	G	282	27% 57% 26% 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14631 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.

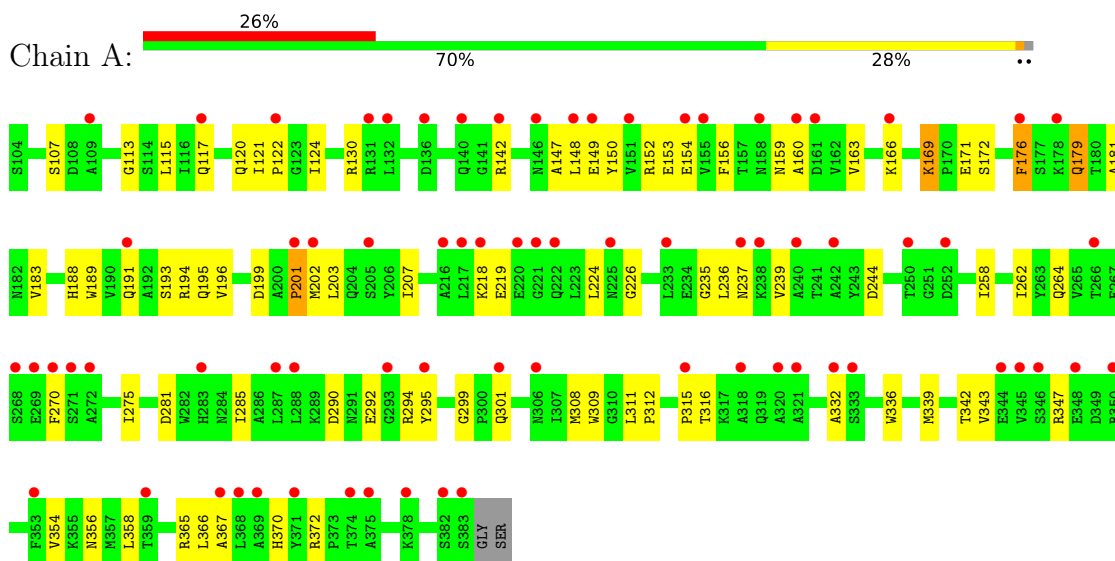
- Molecule 1 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	B	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	C	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	D	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	E	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	F	256	Total	C	N	O	S	0	0	0
			1986	1241	349	388	8			
1	G	243	Total	C	N	O	S	0	0	0
			1890	1181	333	368	8			

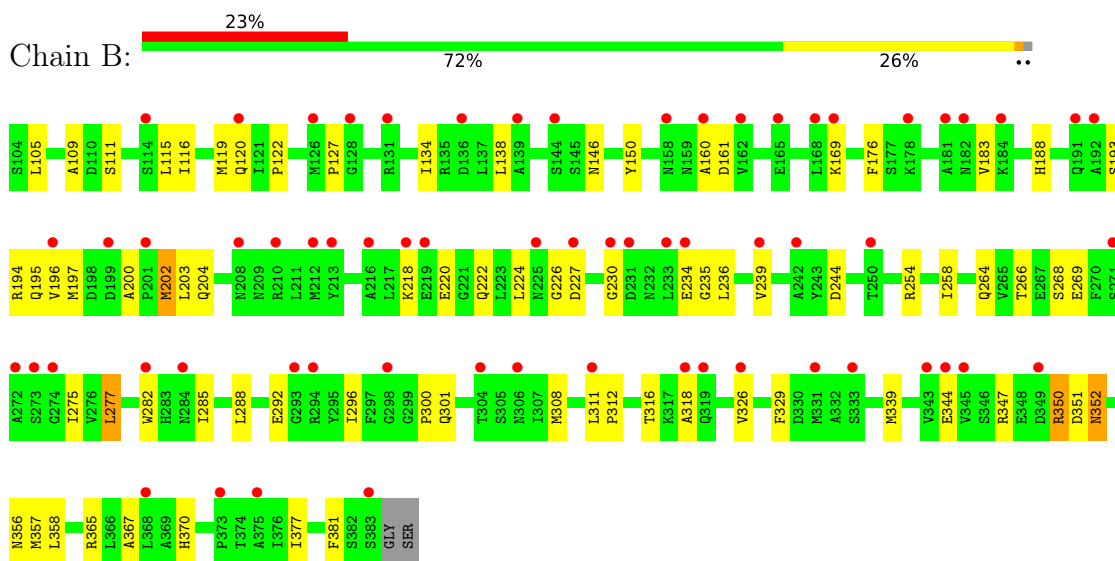
3 Residue-property plots

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.

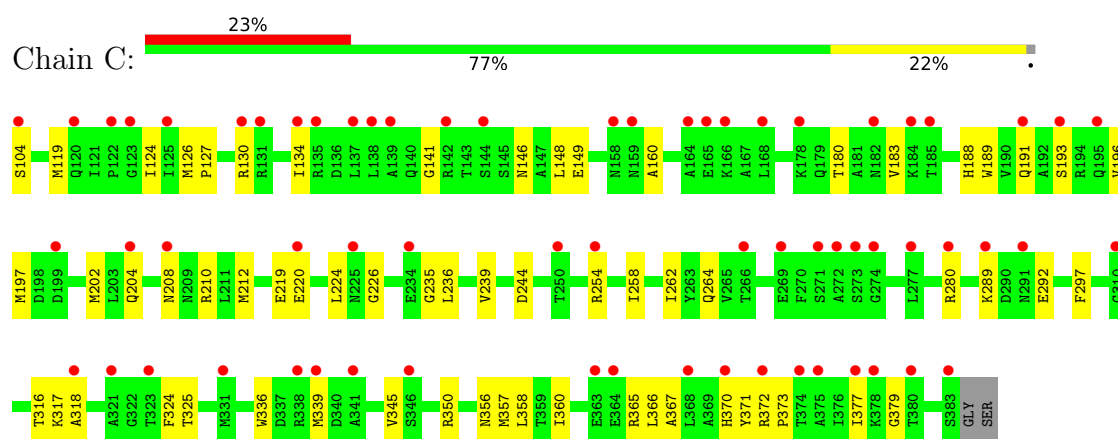
• Molecule 1: Major capsid protein



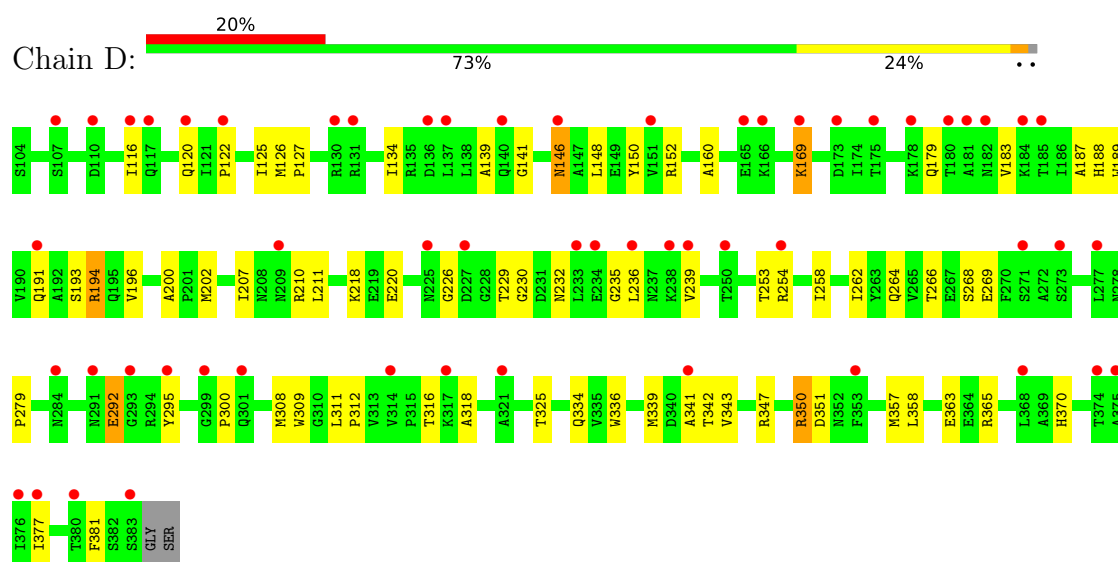
• Molecule 1: Major capsid protein



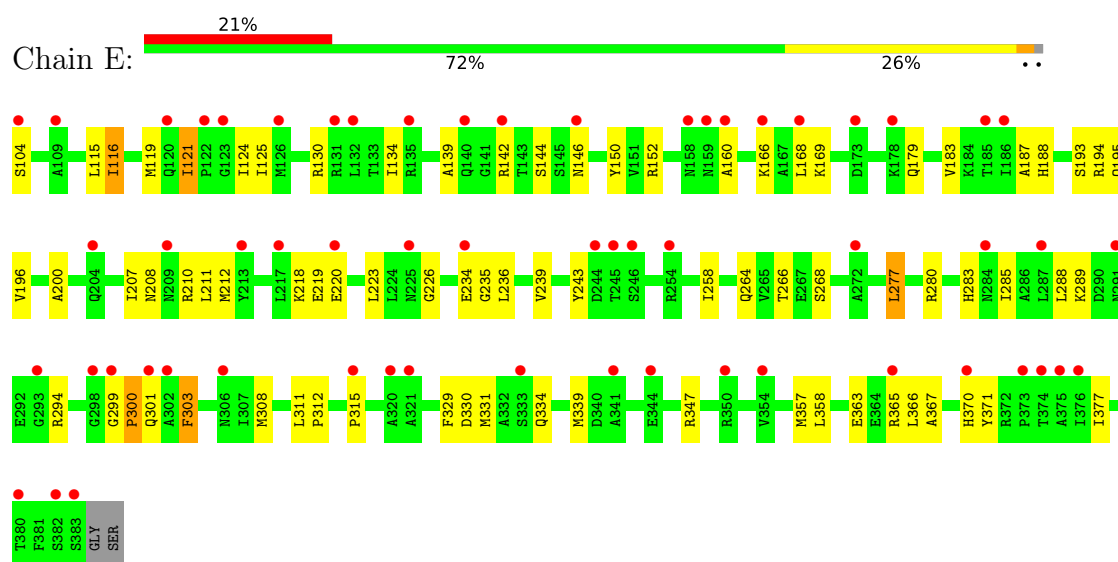
• Molecule 1: Major capsid protein



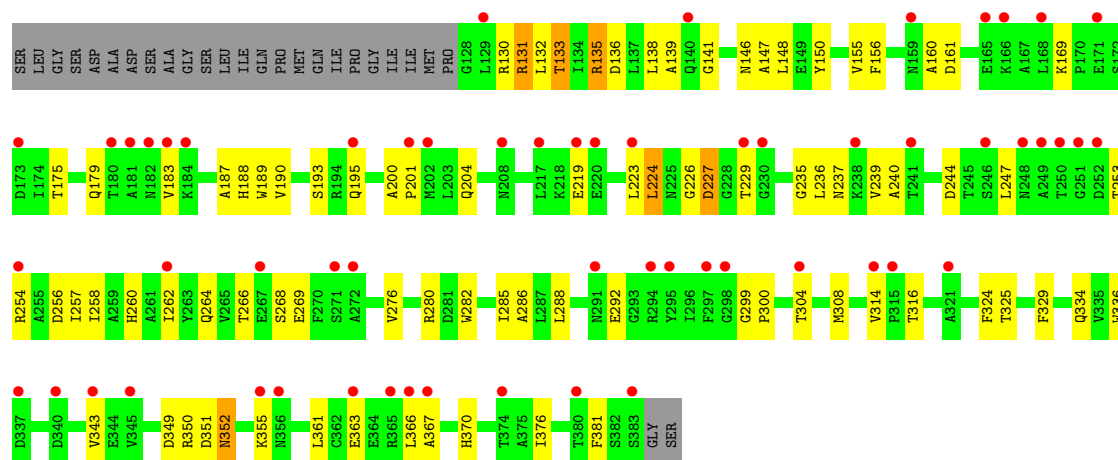
- Molecule 1: Major capsid protein



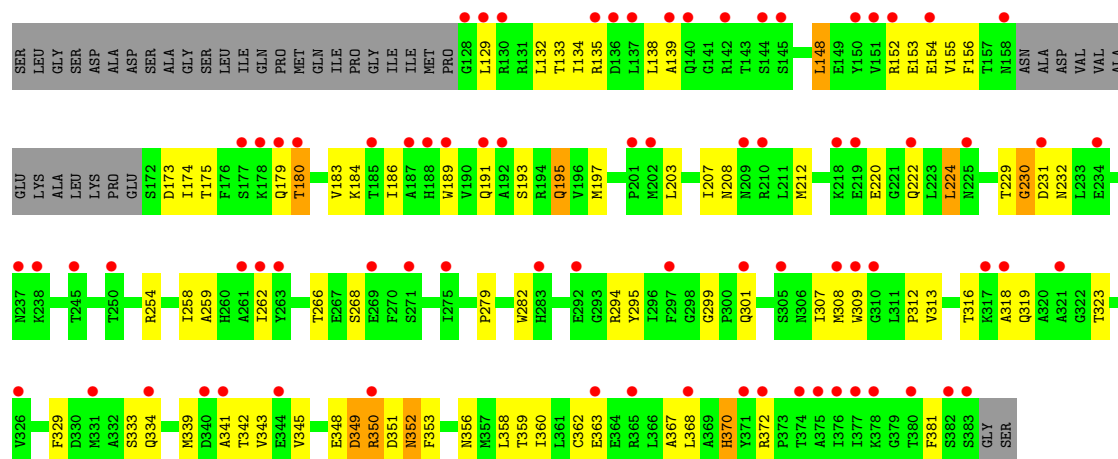
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	1008.97Å 1008.97Å 728.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 7.50 40.00 – 7.50	Depositor EDS
% Data completeness (in resolution range)	64.7 (40.00-7.50) 64.7 (40.00-7.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 7.33Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.421 , (Not available) 0.339 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	152.2	Xtriage
Anisotropy	0.757	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.18	EDS
Total number of atoms	14631	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	1/2188 (0.0%)	0.83	3/2969 (0.1%)
1	B	0.36	1/2188 (0.0%)	0.83	3/2969 (0.1%)
1	C	0.33	1/2188 (0.0%)	0.82	3/2969 (0.1%)
1	D	0.35	1/2188 (0.0%)	0.83	3/2969 (0.1%)
1	E	0.31	0/2188	0.86	6/2969 (0.2%)
1	F	0.31	0/2020	0.85	4/2740 (0.1%)
1	G	0.65	2/1922 (0.1%)	0.99	8/2605 (0.3%)
All	All	0.39	6/14882 (0.0%)	0.86	30/20190 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	180	THR	C-N	-23.25	0.94	1.33
1	B	356	ASN	CG-ND2	9.36	1.52	1.33
1	G	148	LEU	C-N	7.76	1.45	1.33
1	D	169	LYS	CE-NZ	7.02	1.70	1.49
1	A	356	ASN	CG-ND2	5.55	1.45	1.33
1	C	356	ASN	CG-ND2	5.09	1.44	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	148	LEU	O-C-N	16.17	143.00	123.27
1	G	148	LEU	CA-C-N	-13.12	103.36	122.77
1	G	148	LEU	C-N-CA	-13.12	103.36	122.77
1	E	299	GLY	CA-C-N	8.81	130.86	119.84
1	E	299	GLY	C-N-CA	8.81	130.86	119.84
1	G	180	THR	O-C-N	-7.89	114.12	123.27
1	F	200	ALA	CA-C-N	7.33	127.68	119.32
1	F	200	ALA	C-N-CA	7.33	127.68	119.32
1	D	350	ARG	CB-CA-C	-6.78	108.75	116.54
1	A	372	ARG	CA-C-N	6.39	126.08	119.56
1	A	372	ARG	C-N-CA	6.39	126.08	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	200	ALA	CA-C-N	5.95	125.16	118.97
1	D	200	ALA	C-N-CA	5.95	125.16	118.97
1	A	332	ALA	N-CA-C	5.92	117.81	111.36
1	B	200	ALA	CA-C-N	5.74	125.20	119.24
1	B	200	ALA	C-N-CA	5.74	125.20	119.24
1	C	372	ARG	CA-C-N	5.71	125.24	119.19
1	C	372	ARG	C-N-CA	5.71	125.24	119.19
1	B	350	ARG	CB-CA-C	-5.61	110.09	116.54
1	F	299	GLY	CA-C-N	5.57	126.80	119.84
1	F	299	GLY	C-N-CA	5.57	126.80	119.84
1	G	180	THR	CA-C-N	5.49	130.48	122.85
1	G	180	THR	C-N-CA	5.49	130.48	122.85
1	E	200	ALA	CA-C-N	5.49	125.57	119.32
1	E	200	ALA	C-N-CA	5.49	125.57	119.32
1	G	299	GLY	CA-C-N	5.47	125.14	119.56
1	G	299	GLY	C-N-CA	5.47	125.14	119.56
1	E	121	ILE	CA-C-N	5.36	125.66	119.93
1	E	121	ILE	C-N-CA	5.36	125.66	119.93
1	C	350	ARG	CB-CA-C	-5.18	110.58	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2151	0	2119	56	0
1	B	2151	0	2119	58	0
1	C	2151	0	2119	52	0
1	D	2151	0	2119	56	0
1	E	2151	0	2119	53	0
1	F	1986	0	1951	66	0
1	G	1890	0	1850	58	0
All	All	14631	0	14396	351	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 12.

All (351) 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:D:169:LYS:CE	1:D:169:LYS:NZ	1.70	1.50
1:F:224:LEU:HD11	1:F:276:VAL:HG11	1.53	0.89
1:G:345:VAL:HB	1:G:358:LEU:HD21	1.56	0.88
1:G:316:THR:HG22	1:G:318:ALA:H	1.41	0.85
1:G:138:LEU:HD23	1:G:329:PHE:HB3	1.56	0.84
1:A:218:LYS:HE2	1:B:161:ASP:OD1	1.77	0.83
1:G:319:GLN:HE21	1:G:323:THR:HB	1.43	0.83
1:B:218:LYS:HE3	1:B:222:GLN:NE2	1.95	0.81
1:G:229:THR:HG23	1:G:230:GLY:H	1.45	0.81
1:B:339:MET:HE2	1:B:365:ARG:HG3	1.65	0.77
1:G:368:LEU:HG	1:G:370:HIS:HE1	1.52	0.74
1:A:153:GLU:HA	1:A:176:PHE:HB3	1.70	0.73
1:F:133:THR:HG22	1:F:136:ASP:H	1.53	0.73
1:E:194:ARG:HH12	1:E:347:ARG:NE	1.86	0.72
1:C:219:GLU:HG3	1:C:366:LEU:HD11	1.70	0.72
1:E:218:LYS:HE2	1:F:161:ASP:OD1	1.89	0.72
1:D:316:THR:HG22	1:D:318:ALA:H	1.54	0.71
1:E:121:ILE:HD12	1:F:150:TYR:HB3	1.73	0.71
1:C:149:GLU:HG2	1:C:180:THR:HG22	1.72	0.71
1:G:148:LEU:O	1:G:180:THR:HA	1.90	0.70
1:C:197:MET:HE1	1:C:204:GLN:HB2	1.72	0.70
1:E:130:ARG:HA	1:F:269:GLU:HG2	1.72	0.70
1:A:179:GLN:HE21	1:A:179:GLN:HA	1.55	0.70
1:D:127:PRO:HD2	1:D:210:ARG:HH21	1.57	0.70
1:A:347:ARG:HB3	1:A:358:LEU:HD12	1.74	0.68
1:F:236:LEU:HD23	1:F:370:HIS:HE1	1.58	0.68
1:D:254:ARG:HB3	1:D:381:PHE:HE2	1.59	0.68
1:A:124:ILE:HD11	1:B:176:PHE:HE2	1.60	0.66
1:A:188:HIS:ND1	1:B:160:ALA:HB2	2.10	0.66
1:A:339:MET:HE2	1:A:365:ARG:HG3	1.78	0.66
1:B:226:GLY:H	1:B:235:GLY:HA3	1.61	0.66
1:C:339:MET:HE2	1:C:365:ARG:HG3	1.76	0.66
1:G:368:LEU:HG	1:G:370:HIS:CE1	2.31	0.66
1:A:244:ASP:HB2	1:A:264:GLN:NE2	2.11	0.65
1:A:130:ARG:HA	1:B:269:GLU:HG2	1.79	0.65
1:F:130:ARG:C	1:F:132:LEU:H	2.05	0.64
1:G:193:SER:HB2	1:G:195:GLN:NE2	2.13	0.64
1:B:301:GLN:HE22	1:C:297:PHE:HA	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:THR:HG23	1:F:135:ARG:HB3	1.79	0.63
1:A:160:ALA:HB2	1:F:188:HIS:ND1	2.14	0.63
1:B:218:LYS:HE3	1:B:222:GLN:HE21	1.63	0.63
1:B:183:VAL:HG22	1:B:367:ALA:HB2	1.81	0.63
1:C:189:TRP:HZ3	1:C:191:GLN:HB2	1.65	0.62
1:G:183:VAL:HG22	1:G:367:ALA:HB2	1.81	0.62
1:E:193:SER:HB3	1:E:196:VAL:HG23	1.81	0.61
1:A:226:GLY:H	1:A:235:GLY:HA3	1.64	0.61
1:D:239:VAL:HG21	1:D:370:HIS:CD2	2.36	0.61
1:B:218:LYS:CE	1:B:222:GLN:NE2	2.64	0.61
1:B:239:VAL:HG21	1:B:370:HIS:CD2	2.36	0.60
1:F:286:ALA:HB1	1:F:304:THR:HG21	1.84	0.60
1:A:236:LEU:HD23	1:A:370:HIS:HE1	1.66	0.60
1:B:275:ILE:HG23	1:B:326:VAL:HG22	1.82	0.60
1:F:244:ASP:HB3	1:F:247:LEU:HG	1.83	0.60
1:D:229:THR:HG22	1:D:232:ASN:HD22	1.66	0.60
1:D:236:LEU:HD23	1:D:370:HIS:HE1	1.65	0.59
1:F:244:ASP:HB2	1:F:264:GLN:NE2	2.17	0.59
1:A:239:VAL:HG21	1:A:370:HIS:CD2	2.38	0.59
1:B:316:THR:HG22	1:B:318:ALA:H	1.68	0.59
1:G:189:TRP:CD1	1:G:189:TRP:H	2.19	0.59
1:E:264:GLN:HB3	1:E:377:ILE:HD13	1.85	0.59
1:G:134:ILE:HD12	1:G:220:GLU:HG2	1.84	0.58
1:B:197:MET:HE1	1:B:204:GLN:HA	1.84	0.58
1:G:254:ARG:HB3	1:G:381:PHE:HZ	1.68	0.58
1:B:347:ARG:HB3	1:B:358:LEU:HD12	1.85	0.58
1:D:189:TRP:HZ3	1:D:191:GLN:HB2	1.67	0.58
1:C:226:GLY:HA3	1:C:235:GLY:H	1.69	0.58
1:F:183:VAL:HG22	1:F:367:ALA:HB2	1.84	0.58
1:C:104:SER:HB3	1:E:166:LYS:NZ	2.18	0.58
1:D:339:MET:HE2	1:D:365:ARG:HG3	1.84	0.58
1:F:138:LEU:HD23	1:F:329:PHE:HB3	1.86	0.58
1:C:130:ARG:HA	1:D:269:GLU:HG2	1.86	0.57
1:E:183:VAL:HG22	1:E:367:ALA:HB2	1.84	0.57
1:F:133:THR:CG2	1:F:136:ASP:H	2.17	0.57
1:A:336:TRP:HB2	1:A:367:ALA:HB3	1.87	0.57
1:D:264:GLN:HB3	1:D:377:ILE:HD13	1.86	0.57
1:A:189:TRP:HZ3	1:A:191:GLN:HB2	1.69	0.57
1:E:119:MET:HB3	1:F:148:LEU:HD23	1.87	0.57
1:A:189:TRP:CD1	1:B:169:LYS:HB2	2.38	0.57
1:E:239:VAL:HG21	1:E:370:HIS:CD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:LEU:HD23	1:B:370:HIS:HE1	1.69	0.56
1:C:236:LEU:HD23	1:C:370:HIS:HE1	1.70	0.56
1:D:146:ASN:O	1:D:183:VAL:HG12	2.04	0.56
1:E:243:TYR:HA	1:E:264:GLN:HE22	1.70	0.56
1:C:316:THR:HG22	1:C:318:ALA:H	1.68	0.56
1:D:134:ILE:HB	1:D:220:GLU:HG3	1.88	0.56
1:E:116:ILE:HD12	1:F:146:ASN:HB2	1.86	0.56
1:E:187:ALA:HB2	1:E:363:GLU:HA	1.87	0.55
1:F:150:TYR:CE1	1:F:179:GLN:HB2	2.41	0.55
1:G:156:PHE:CD1	1:G:174:ILE:HG12	2.41	0.55
1:A:188:HIS:CE1	1:B:160:ALA:HB2	2.42	0.55
1:D:139:ALA:HB3	1:D:334:GLN:HB2	1.88	0.55
1:B:193:SER:HB3	1:B:196:VAL:HG23	1.89	0.55
1:F:239:VAL:HG21	1:F:370:HIS:CD2	2.41	0.55
1:C:141:GLY:O	1:C:336:TRP:HA	2.07	0.55
1:F:227:ASP:HB3	1:F:229:THR:HG22	1.88	0.55
1:F:350:ARG:HG3	1:F:351:ASP:H	1.72	0.55
1:E:188:HIS:ND1	1:F:160:ALA:HB2	2.22	0.54
1:B:264:GLN:HB3	1:B:377:ILE:HD13	1.90	0.54
1:C:188:HIS:ND1	1:D:160:ALA:HB2	2.23	0.54
1:A:193:SER:HB3	1:A:196:VAL:HG23	1.89	0.54
1:C:183:VAL:HG22	1:C:367:ALA:HB2	1.90	0.54
1:B:244:ASP:HB2	1:B:264:GLN:NE2	2.23	0.54
1:D:339:MET:HE1	1:D:363:GLU:HG3	1.90	0.54
1:E:210:ARG:HB3	1:F:156:PHE:HE2	1.73	0.53
1:A:142:ARG:NH1	1:A:142:ARG:HB3	2.23	0.53
1:B:218:LYS:CE	1:B:222:GLN:HE21	2.21	0.53
1:A:107:SER:O	1:A:113:GLY:HA3	2.07	0.53
1:G:132:LEU:HD13	1:G:312:PRO:HB3	1.90	0.53
1:F:201:PRO:O	1:F:204:GLN:HB3	2.08	0.53
1:B:352:ASN:HA	1:B:357:MET:HB2	1.91	0.53
1:D:141:GLY:O	1:D:336:TRP:HA	2.08	0.53
1:F:236:LEU:HD23	1:F:370:HIS:CE1	2.42	0.53
1:D:254:ARG:HB3	1:D:381:PHE:CE2	2.43	0.53
1:E:266:THR:C	1:E:268:SER:H	2.17	0.53
1:E:188:HIS:HB3	1:F:160:ALA:HA	1.91	0.52
1:C:239:VAL:HG21	1:C:370:HIS:CD2	2.44	0.52
1:F:224:LEU:HD23	1:F:237:ASN:ND2	2.23	0.52
1:D:229:THR:CG2	1:D:232:ASN:HD22	2.22	0.52
1:G:153:GLU:HG3	1:G:372:ARG:NH1	2.25	0.52
1:G:254:ARG:HB3	1:G:381:PHE:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ILE:HB	1:C:220:GLU:HG3	1.91	0.52
1:C:188:HIS:HB3	1:D:160:ALA:HA	1.91	0.51
1:C:208:ASN:O	1:C:212:MET:HG2	2.10	0.51
1:G:208:ASN:O	1:G:212:MET:HG2	2.10	0.51
1:C:244:ASP:HB2	1:C:264:GLN:NE2	2.25	0.51
1:D:226:GLY:H	1:D:235:GLY:HA3	1.76	0.51
1:A:166:LYS:HE3	1:E:104:SER:HB2	1.92	0.51
1:E:258:ILE:HD12	1:E:308:MET:HE1	1.92	0.51
1:G:197:MET:HE2	1:G:360:ILE:HD11	1.92	0.51
1:A:224:LEU:HD13	1:A:237:ASN:HD22	1.76	0.51
1:E:223:LEU:O	1:E:236:LEU:HD13	2.11	0.51
1:G:154:GLU:HB2	1:G:175:THR:HB	1.93	0.51
1:D:193:SER:HB3	1:D:196:VAL:HG23	1.93	0.50
1:F:343:VAL:HA	1:F:361:LEU:O	2.12	0.50
1:E:236:LEU:HD12	1:E:370:HIS:HE1	1.77	0.50
1:F:282:TRP:O	1:F:285:ILE:HB	2.11	0.50
1:A:258:ILE:O	1:A:262:ILE:HG13	2.12	0.50
1:F:351:ASP:HB3	1:F:355:LYS:HD3	1.93	0.50
1:B:188:HIS:HB3	1:C:160:ALA:HA	1.94	0.50
1:D:139:ALA:HB3	1:D:334:GLN:CB	2.41	0.50
1:F:226:GLY:H	1:F:235:GLY:HA3	1.75	0.50
1:A:218:LYS:O	1:A:218:LYS:HG3	2.12	0.50
1:B:188:HIS:ND1	1:C:160:ALA:HB2	2.27	0.50
1:B:282:TRP:HZ3	1:B:308:MET:HE2	1.77	0.50
1:E:226:GLY:H	1:E:235:GLY:HA3	1.77	0.49
1:A:163:VAL:HG21	1:A:169:LYS:HG3	1.95	0.49
1:C:124:ILE:N	1:C:124:ILE:HD12	2.27	0.49
1:E:168:LEU:HD23	1:E:169:LYS:N	2.27	0.49
1:G:191:GLN:OE1	1:G:350:ARG:NH1	2.45	0.49
1:B:115:LEU:N	1:B:115:LEU:HD12	2.27	0.49
1:D:116:ILE:HG21	1:E:146:ASN:HB2	1.93	0.49
1:D:120:GLN:O	1:D:122:PRO:HD3	2.12	0.49
1:D:150:TYR:CE1	1:D:179:GLN:HB2	2.48	0.49
1:D:189:TRP:CZ3	1:D:191:GLN:HB2	2.48	0.49
1:G:133:THR:HG22	1:G:135:ARG:H	1.76	0.49
1:E:139:ALA:O	1:E:334:GLN:HG3	2.13	0.49
1:A:120:GLN:O	1:A:122:PRO:HD3	2.12	0.49
1:D:347:ARG:HG2	1:D:358:LEU:CD1	2.43	0.49
1:F:132:LEU:HB3	1:F:314:VAL:HG12	1.94	0.49
1:C:119:MET:HB3	1:D:148:LEU:HD23	1.94	0.49
1:C:292:GLU:HG2	1:D:292:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:139:ALA:HB3	1:G:334:GLN:CB	2.42	0.48
1:A:194:ARG:CZ	1:A:347:ARG:NH1	2.76	0.48
1:G:186:ILE:HG21	1:G:222:GLN:HG3	1.95	0.48
1:B:288:LEU:O	1:B:296:ILE:HG12	2.14	0.48
1:C:345:VAL:HG12	1:C:360:ILE:HG12	1.94	0.48
1:D:254:ARG:O	1:D:258:ILE:HD12	2.13	0.48
1:A:169:LYS:HB3	1:F:189:TRP:HD1	1.77	0.48
1:E:219:GLU:HG3	1:E:366:LEU:HD11	1.94	0.48
1:D:188:HIS:ND1	1:E:160:ALA:HB2	2.28	0.48
1:E:124:ILE:HG22	1:E:125:ILE:N	2.28	0.48
1:A:121:ILE:HG13	1:B:150:TYR:HB3	1.95	0.48
1:C:104:SER:HB3	1:E:166:LYS:HZ2	1.78	0.48
1:C:264:GLN:HB3	1:C:377:ILE:HD13	1.94	0.48
1:B:119:MET:HB3	1:C:148:LEU:HD23	1.96	0.48
1:D:218:LYS:O	1:D:218:LYS:HG3	2.14	0.48
1:E:283:HIS:NE2	1:F:260:HIS:HA	2.28	0.48
1:C:130:ARG:HD2	1:C:317:LYS:HB2	1.96	0.47
1:D:188:HIS:CE1	1:E:160:ALA:HB2	2.49	0.47
1:D:194:ARG:NH2	1:D:347:ARG:NH2	2.62	0.47
1:G:153:GLU:HG3	1:G:372:ARG:CZ	2.44	0.47
1:G:139:ALA:HB3	1:G:334:GLN:HB2	1.96	0.47
1:G:349:ASP:OD1	1:G:350:ARG:HG2	2.15	0.47
1:B:218:LYS:NZ	1:B:222:GLN:NE2	2.62	0.47
1:A:160:ALA:HA	1:F:188:HIS:HB3	1.97	0.47
1:B:282:TRP:CZ3	1:B:308:MET:HE2	2.49	0.46
1:F:133:THR:CG2	1:F:135:ARG:HB3	2.43	0.46
1:A:292:GLU:HG3	1:B:292:GLU:HG2	1.95	0.46
1:D:350:ARG:HB3	1:D:351:ASP:H	1.44	0.46
1:A:219:GLU:HG3	1:A:366:LEU:HD11	1.98	0.46
1:A:224:LEU:HD13	1:A:237:ASN:ND2	2.30	0.46
1:B:266:THR:C	1:B:268:SER:H	2.22	0.46
1:G:229:THR:HG23	1:G:230:GLY:N	2.21	0.46
1:G:258:ILE:O	1:G:262:ILE:HG13	2.15	0.46
1:B:258:ILE:HD11	1:B:381:PHE:HZ	1.81	0.46
1:D:258:ILE:O	1:D:262:ILE:HG13	2.16	0.46
1:D:342:THR:HG22	1:D:343:VAL:N	2.30	0.46
1:F:139:ALA:O	1:F:334:GLN:HG3	2.16	0.46
1:B:236:LEU:HD23	1:B:370:HIS:CE1	2.49	0.46
1:F:258:ILE:O	1:F:262:ILE:HG13	2.16	0.46
1:C:324:PHE:CZ	1:C:379:GLY:HA3	2.50	0.46
1:D:341:ALA:HA	1:D:363:GLU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:ILE:O	1:F:288:LEU:HG	2.16	0.46
1:A:150:TYR:HE2	1:A:181:ALA:HB2	1.80	0.46
1:G:229:THR:CG2	1:G:232:ASN:HD22	2.29	0.46
1:A:172:SER:O	1:F:190:VAL:HG22	2.15	0.46
1:F:155:VAL:H	1:F:175:THR:HB	1.81	0.45
1:B:138:LEU:HD23	1:B:329:PHE:HB3	1.99	0.45
1:G:350:ARG:HG2	1:G:350:ARG:H	1.47	0.45
1:A:188:HIS:HB3	1:B:160:ALA:HA	1.98	0.45
1:E:234:GLU:HG2	1:E:239:VAL:CG2	2.46	0.45
1:G:155:VAL:H	1:G:175:THR:HB	1.81	0.45
1:B:116:ILE:HG21	1:C:146:ASN:HB2	1.98	0.45
1:D:236:LEU:HD23	1:D:370:HIS:CE1	2.48	0.45
1:E:285:ILE:O	1:E:288:LEU:HG	2.16	0.45
1:C:325:THR:HA	1:C:377:ILE:O	2.16	0.45
1:E:329:PHE:C	1:E:331:MET:H	2.24	0.45
1:F:156:PHE:CD1	1:F:156:PHE:C	2.95	0.45
1:D:295:TYR:CE1	1:D:300:PRO:HG3	2.51	0.45
1:G:339:MET:HE1	1:G:363:GLU:HG3	1.99	0.45
1:D:207:ILE:O	1:D:211:LEU:HD23	2.17	0.45
1:A:258:ILE:HG21	1:A:275:ILE:HD13	1.98	0.45
1:B:134:ILE:HD12	1:B:220:GLU:CG	2.47	0.45
1:F:258:ILE:HD12	1:F:308:MET:HE1	1.99	0.45
1:A:154:GLU:H	1:A:176:PHE:HA	1.82	0.44
1:A:156:PHE:C	1:A:156:PHE:CD1	2.94	0.44
1:D:266:THR:C	1:D:268:SER:H	2.25	0.44
1:B:120:GLN:O	1:B:122:PRO:HD3	2.17	0.44
1:C:124:ILE:HD12	1:C:124:ILE:H	1.81	0.44
1:D:229:THR:HG23	1:D:230:GLY:N	2.32	0.44
1:B:134:ILE:HD12	1:B:220:GLU:HG2	1.98	0.44
1:A:347:ARG:HB3	1:A:358:LEU:CD1	2.46	0.44
1:C:254:ARG:O	1:C:258:ILE:HD13	2.17	0.44
1:F:193:SER:OG	1:F:195:GLN:HG2	2.18	0.44
1:G:282:TRP:CE3	1:G:313:VAL:HG11	2.53	0.44
1:B:194:ARG:HD2	1:B:347:ARG:NH1	2.32	0.44
1:B:285:ILE:O	1:B:288:LEU:HG	2.17	0.44
1:D:191:GLN:HG2	1:D:357:MET:HE3	1.99	0.44
1:E:130:ARG:HA	1:F:269:GLU:CG	2.44	0.44
1:A:290:ASP:OD2	1:A:294:ARG:HB2	2.17	0.44
1:F:266:THR:C	1:F:268:SER:H	2.25	0.44
1:C:226:GLY:H	1:C:235:GLY:HA3	1.81	0.44
1:F:349:ASP:O	1:F:352:ASN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLU:HG2	1:B:239:VAL:CG2	2.48	0.44
1:C:191:GLN:HG2	1:C:357:MET:HE3	2.00	0.44
1:B:275:ILE:HG22	1:B:277:LEU:HD11	1.99	0.43
1:F:130:ARG:C	1:F:132:LEU:N	2.73	0.43
1:G:203:LEU:O	1:G:207:ILE:HG13	2.17	0.43
1:G:266:THR:C	1:G:268:SER:H	2.26	0.43
1:B:301:GLN:NE2	1:C:297:PHE:HA	2.32	0.43
1:E:208:ASN:O	1:E:212:MET:HG2	2.18	0.43
1:E:303:PHE:HD2	1:E:303:PHE:HA	1.70	0.43
1:G:352:ASN:O	1:G:356:ASN:N	2.51	0.43
1:D:254:ARG:HH21	1:D:381:PHE:HB3	1.83	0.43
1:F:131:ARG:HH21	1:F:316:THR:HA	1.84	0.43
1:A:152:ARG:CZ	1:A:179:GLN:HG3	2.48	0.43
1:F:244:ASP:HB2	1:F:264:GLN:HE22	1.83	0.43
1:G:279:PRO:HD3	1:G:316:THR:O	2.18	0.43
1:D:325:THR:HA	1:D:377:ILE:O	2.18	0.43
1:G:138:LEU:HD22	1:G:333:SER:O	2.18	0.43
1:E:119:MET:HB3	1:F:148:LEU:CD2	2.49	0.43
1:F:187:ALA:HB2	1:F:363:GLU:HA	2.01	0.43
1:B:119:MET:HB3	1:C:148:LEU:CD2	2.49	0.43
1:A:153:GLU:CA	1:A:176:PHE:HB3	2.45	0.43
1:A:199:ASP:O	1:A:201:PRO:HD3	2.19	0.43
1:C:239:VAL:HG12	1:C:373:PRO:HB3	2.01	0.43
1:D:264:GLN:HB3	1:D:377:ILE:CD1	2.48	0.43
1:G:152:ARG:HB3	1:G:153:GLU:H	1.60	0.43
1:B:258:ILE:HD11	1:B:381:PHE:CZ	2.54	0.43
1:E:116:ILE:H	1:E:116:ILE:HG12	1.71	0.43
1:A:342:THR:HG22	1:A:343:VAL:N	2.34	0.42
1:C:208:ASN:C	1:C:210:ARG:H	2.27	0.42
1:F:254:ARG:HB3	1:F:381:PHE:HE2	1.84	0.42
1:C:189:TRP:CZ3	1:C:191:GLN:HB2	2.51	0.42
1:C:258:ILE:O	1:C:262:ILE:HG13	2.19	0.42
1:C:289:LYS:NZ	1:D:253:THR:HG23	2.35	0.42
1:F:219:GLU:HG3	1:F:366:LEU:HD11	2.01	0.42
1:C:193:SER:HB3	1:C:196:VAL:HG23	2.01	0.42
1:E:264:GLN:HE21	1:E:377:ILE:HG12	1.83	0.42
1:C:264:GLN:HB3	1:C:377:ILE:CD1	2.49	0.42
1:D:187:ALA:HB3	1:E:169:LYS:HE2	2.02	0.42
1:G:152:ARG:HG2	1:G:370:HIS:O	2.19	0.42
1:B:350:ARG:HB3	1:B:351:ASP:H	1.47	0.42
1:D:295:TYR:HE1	1:D:300:PRO:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:MET:HG2	1:D:309:TRP:CD1	2.54	0.42
1:D:311:LEU:HA	1:D:312:PRO:HD3	1.91	0.42
1:G:319:GLN:NE2	1:G:323:THR:HB	2.24	0.42
1:B:311:LEU:HA	1:B:312:PRO:HD3	1.89	0.42
1:G:152:ARG:NE	1:G:179:GLN:HG3	2.35	0.42
1:A:159:ASN:H	1:A:172:SER:HB3	1.84	0.42
1:E:150:TYR:CE1	1:E:179:GLN:HB2	2.55	0.42
1:F:350:ARG:HG3	1:F:351:ASP:N	2.35	0.42
1:A:171:GLU:HB2	1:F:189:TRP:CZ2	2.55	0.42
1:B:254:ARG:O	1:B:258:ILE:HD13	2.19	0.42
1:E:134:ILE:HB	1:E:220:GLU:HG3	2.02	0.42
1:C:371:TYR:CD1	1:C:371:TYR:N	2.88	0.42
1:G:139:ALA:O	1:G:334:GLN:HB2	2.20	0.42
1:G:212:MET:HE1	1:G:341:ALA:HB3	2.01	0.42
1:G:224:LEU:HD21	1:G:319:GLN:OE1	2.20	0.42
1:G:259:ALA:HA	1:G:262:ILE:HD12	2.02	0.42
1:G:308:MET:HG2	1:G:309:TRP:CD1	2.55	0.42
1:B:277:LEU:HD12	1:B:277:LEU:N	2.34	0.41
1:G:348:GLU:H	1:G:348:GLU:HG2	1.75	0.41
1:G:135:ARG:HG3	1:G:135:ARG:HH11	1.85	0.41
1:C:126:MET:HA	1:C:127:PRO:HD3	1.90	0.41
1:A:203:LEU:O	1:A:207:ILE:HG13	2.20	0.41
1:G:203:LEU:HD21	1:G:207:ILE:HD11	2.02	0.41
1:A:308:MET:HG2	1:A:309:TRP:CD1	2.55	0.41
1:C:197:MET:HG3	1:C:358:LEU:HD23	2.02	0.41
1:E:311:LEU:HA	1:E:312:PRO:HD3	1.92	0.41
1:E:339:MET:HB3	1:E:365:ARG:HG3	2.02	0.41
1:A:281:ASP:O	1:A:285:ILE:HG13	2.20	0.41
1:A:311:LEU:HA	1:A:312:PRO:HD3	1.91	0.41
1:E:207:ILE:O	1:E:211:LEU:HD13	2.21	0.41
1:F:276:VAL:HB	1:F:325:THR:HB	2.03	0.41
1:A:354:VAL:O	1:A:354:VAL:HG12	2.21	0.41
1:B:109:ALA:C	1:B:111:SER:H	2.29	0.41
1:C:371:TYR:H	1:C:371:TYR:HD1	1.69	0.41
1:E:234:GLU:HG2	1:E:239:VAL:HG22	2.01	0.41
1:F:133:THR:HG22	1:F:136:ASP:CG	2.46	0.41
1:F:253:THR:OG1	1:F:256:ASP:HB2	2.21	0.41
1:G:193:SER:HB2	1:G:195:GLN:HE21	1.85	0.41
1:G:294:ARG:HD3	1:G:295:TYR:H	1.85	0.41
1:G:342:THR:HG22	1:G:343:VAL:N	2.36	0.41
1:F:223:LEU:O	1:F:236:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:236:LEU:HD22	1:F:376:ILE:HD13	2.03	0.41
1:B:119:MET:HE1	1:C:336:TRP:CZ3	2.56	0.41
1:D:126:MET:HA	1:D:127:PRO:HD3	1.93	0.41
1:E:357:MET:HG3	1:E:358:LEU:H	1.85	0.41
1:F:257:ILE:O	1:F:260:HIS:HB2	2.21	0.41
1:G:351:ASP:O	1:G:353:PHE:N	2.54	0.41
1:A:147:ALA:HA	1:A:183:VAL:HG23	2.03	0.40
1:A:176:PHE:CD1	1:A:176:PHE:N	2.89	0.40
1:B:202:MET:HG2	1:B:203:LEU:N	2.36	0.40
1:E:187:ALA:HB3	1:F:169:LYS:HE2	2.03	0.40
1:E:194:ARG:NH1	1:E:347:ARG:NE	2.63	0.40
1:A:258:ILE:N	1:A:258:ILE:HD12	2.36	0.40
1:A:295:TYR:HB2	1:A:299:GLY:HA2	2.03	0.40
1:B:234:GLU:HG2	1:B:239:VAL:HG23	2.03	0.40
1:D:125:ILE:HD13	1:E:371:TYR:HB3	2.04	0.40
1:D:226:GLY:N	1:D:235:GLY:HA3	2.35	0.40
1:E:289:LYS:HA	1:E:294:ARG:O	2.21	0.40
1:C:183:VAL:HG13	1:C:366:LEU:O	2.22	0.40
1:C:197:MET:CE	1:C:204:GLN:HB2	2.45	0.40
1:F:141:GLY:O	1:F:336:TRP:HA	2.22	0.40
1:G:184:LYS:HD3	1:G:231:ASP:C	2.46	0.40
1:G:358:LEU:HD23	1:G:359:THR:N	2.36	0.40
1:E:277:LEU:O	1:E:315:PRO:HA	2.22	0.40
1:F:147:ALA:HA	1:F:183:VAL:HG23	2.02	0.40
1:F:324:PHE:HB3	1:F:381:PHE:HE1	1.84	0.40
1:G:343:VAL:HG22	1:G:362:CYS:SG	2.61	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	278/282 (99%)	249 (90%)	27 (10%)	2 (1%)	18	56
1	B	278/282 (99%)	252 (91%)	22 (8%)	4 (1%)	9	40
1	C	278/282 (99%)	258 (93%)	20 (7%)	0	100	100
1	D	278/282 (99%)	256 (92%)	22 (8%)	0	100	100
1	E	278/282 (99%)	246 (88%)	29 (10%)	3 (1%)	11	46
1	F	254/282 (90%)	229 (90%)	21 (8%)	4 (2%)	7	38
1	G	239/282 (85%)	208 (87%)	27 (11%)	4 (2%)	7	36
All	All	1883/1974 (95%)	1698 (90%)	168 (9%)	17 (1%)	14	51

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	300	PRO
1	F	352	ASN
1	G	352	ASN
1	E	330	ASP
1	G	224	LEU
1	A	201	PRO
1	B	127	PRO
1	B	230	GLY
1	F	131	ARG
1	G	349	ASP
1	B	352	ASN
1	E	144	SER
1	F	240	ALA
1	F	300	PRO
1	G	230	GLY
1	A	315	PRO
1	B	300	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	230/231 (100%)	218 (95%)	12 (5%)	21	42
1	B	230/231 (100%)	222 (96%)	8 (4%)	32	53
1	C	230/231 (100%)	227 (99%)	3 (1%)	61	74
1	D	230/231 (100%)	224 (97%)	6 (3%)	40	62
1	E	230/231 (100%)	220 (96%)	10 (4%)	26	47
1	F	211/231 (91%)	205 (97%)	6 (3%)	38	59
1	G	201/231 (87%)	194 (96%)	7 (4%)	32	53
All	All	1562/1617 (97%)	1510 (97%)	52 (3%)	33	55

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	117	GLN
1	A	148	LEU
1	A	149	GLU
1	A	169	LYS
1	A	176	PHE
1	A	179	GLN
1	A	195	GLN
1	A	202	MET
1	A	270	PHE
1	A	301	GLN
1	A	316	THR
1	B	105	LEU
1	B	146	ASN
1	B	195	GLN
1	B	202	MET
1	B	224	LEU
1	B	227	ASP
1	B	277	LEU
1	B	344	GLU
1	C	202	MET
1	C	224	LEU
1	C	280	ARG
1	D	146	ASN
1	D	152	ARG
1	D	194	ARG
1	D	202	MET
1	D	279	PRO
1	D	292	GLU

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Mol	Chain	Res	Type
1	E	115	LEU
1	E	116	ILE
1	E	142	ARG
1	E	152	ARG
1	E	195	GLN
1	E	277	LEU
1	E	280	ARG
1	E	300	PRO
1	E	301	GLN
1	E	303	PHE
1	F	133	THR
1	F	135	ARG
1	F	224	LEU
1	F	227	ASP
1	F	280	ARG
1	F	292	GLU
1	G	129	LEU
1	G	173	ASP
1	G	195	GLN
1	G	301	GLN
1	G	307	ILE
1	G	350	ARG
1	G	370	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	158	ASN
1	A	179	GLN
1	A	204	GLN
1	A	225	ASN
1	A	334	GLN
1	B	158	ASN
1	B	191	GLN
1	B	222	GLN
1	B	301	GLN
1	B	334	GLN
1	B	352	ASN
1	C	140	GLN
1	C	158	ASN
1	C	188	HIS

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Mol	Chain	Res	Type
1	C	222	GLN
1	C	334	GLN
1	D	158	ASN
1	D	195	GLN
1	D	222	GLN
1	D	232	ASN
1	D	334	GLN
1	E	117	GLN
1	E	158	ASN
1	E	191	GLN
1	E	208	ASN
1	E	306	ASN
1	E	352	ASN
1	F	146	ASN
1	F	158	ASN
1	F	222	GLN
1	F	237	ASN
1	F	260	HIS
1	F	306	ASN
1	F	334	GLN
1	G	195	GLN
1	G	232	ASN
1	G	260	HIS
1	G	264	GLN
1	G	283	HIS
1	G	306	ASN
1	G	319	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	180:THR	C	181:ALA	N	0.94

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	280/282 (99%)	1.40	73 (26%) 1 8	58, 58, 58, 58	0
1	B	280/282 (99%)	1.32	64 (22%) 2 9	54, 54, 54, 54	0
1	C	280/282 (99%)	1.40	65 (23%) 2 9	53, 53, 53, 53	0
1	D	280/282 (99%)	1.26	56 (20%) 3 10	54, 54, 54, 54	0
1	E	280/282 (99%)	1.27	59 (21%) 2 10	48, 48, 48, 48	0
1	F	256/282 (90%)	1.30	58 (22%) 2 9	61, 61, 61, 61	0
1	G	243/282 (86%)	1.56	77 (31%) 1 6	99, 99, 99, 99	0
All	All	1899/1974 (96%)	1.35	452 (23%) 2 9	48, 54, 99, 99	0

All (452) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	383	SER	11.1
1	B	304	THR	8.3
1	A	225	ASN	8.3
1	A	332	ALA	8.0
1	C	104	SER	7.7
1	C	274	GLY	7.6
1	F	183	VAL	6.8
1	C	122	PRO	6.8
1	B	191	GLN	6.3
1	F	171	GLU	6.1
1	A	367	ALA	6.1
1	A	271	SER	6.0
1	C	139	ALA	5.9
1	A	272	ALA	5.6
1	E	321	ALA	5.6
1	F	182	ASN	5.5
1	D	225	ASN	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	341	ALA	5.5
1	C	164	ALA	5.5
1	D	151	VAL	5.4
1	F	272	ALA	5.4
1	F	220	GLU	5.3
1	A	383	SER	5.2
1	G	140	GLN	5.2
1	E	291	ASN	5.2
1	G	375	ALA	5.1
1	F	230	GLY	5.1
1	F	298	GLY	5.0
1	A	368	LEU	4.9
1	C	273	SER	4.9
1	E	344	GLU	4.9
1	A	161	ASP	4.9
1	B	225	ASN	4.9
1	G	318	ALA	4.9
1	C	272	ALA	4.8
1	C	370	HIS	4.8
1	A	375	ALA	4.8
1	E	374	THR	4.7
1	F	249	ALA	4.7
1	C	339	MET	4.6
1	D	234	GLU	4.6
1	D	117	GLN	4.6
1	D	271	SER	4.5
1	A	270	PHE	4.5
1	D	239	VAL	4.5
1	A	178	LYS	4.5
1	F	254	ARG	4.5
1	E	380	THR	4.4
1	A	237	ASN	4.4
1	D	182	ASN	4.4
1	B	271	SER	4.4
1	G	188	HIS	4.4
1	G	310	GLY	4.4
1	A	233	LEU	4.4
1	F	202	MET	4.3
1	G	321	ALA	4.3
1	D	314	VAL	4.3
1	B	199	ASP	4.3
1	B	230	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	378	LYS	4.3
1	B	272	ALA	4.3
1	G	180	THR	4.2
1	G	231	ASP	4.2
1	G	130	ARG	4.2
1	G	144	SER	4.2
1	E	104	SER	4.2
1	G	185	THR	4.1
1	D	250	THR	4.1
1	G	151	VAL	4.1
1	G	187	ALA	4.0
1	D	166	LYS	4.0
1	G	158	ASN	4.0
1	G	382	SER	4.0
1	G	191	GLN	4.0
1	B	343	VAL	4.0
1	A	191	GLN	4.0
1	G	225	ASN	4.0
1	G	377	ILE	4.0
1	E	160	ALA	3.9
1	G	189	TRP	3.9
1	G	380	THR	3.9
1	D	317	LYS	3.9
1	D	140	GLN	3.9
1	A	242	ALA	3.9
1	A	345	VAL	3.9
1	C	166	LYS	3.9
1	F	365	ARG	3.9
1	F	129	LEU	3.9
1	G	177	SER	3.9
1	G	179	GLN	3.8
1	D	180	THR	3.7
1	E	375	ALA	3.7
1	D	376	ILE	3.7
1	E	370	HIS	3.7
1	C	271	SER	3.7
1	D	185	THR	3.7
1	G	341	ALA	3.7
1	B	213	TYR	3.7
1	G	234	GLU	3.7
1	C	199	ASP	3.7
1	E	140	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	340	ASP	3.7
1	F	173	ASP	3.6
1	F	271	SER	3.6
1	G	136	ASP	3.6
1	A	318	ALA	3.6
1	A	293	GLY	3.6
1	F	291	ASN	3.6
1	F	321	ALA	3.6
1	E	301	GLN	3.6
1	E	166	LYS	3.6
1	C	131	ARG	3.5
1	F	195	GLN	3.5
1	E	376	ILE	3.5
1	D	173	ASP	3.5
1	G	376	ILE	3.5
1	G	128	GLY	3.5
1	B	144	SER	3.5
1	A	238	LYS	3.5
1	B	282	TRP	3.4
1	C	234	GLU	3.4
1	B	333	SER	3.4
1	F	168	LEU	3.4
1	B	375	ALA	3.4
1	D	184	LYS	3.4
1	E	146	ASN	3.4
1	G	374	THR	3.4
1	B	182	ASN	3.4
1	C	123	GLY	3.4
1	E	293	GLY	3.4
1	E	298	GLY	3.4
1	B	368	LEU	3.3
1	C	375	ALA	3.3
1	D	131	ARG	3.3
1	G	202	MET	3.3
1	F	184	LYS	3.3
1	G	378	LYS	3.3
1	D	375	ALA	3.3
1	C	338	ARG	3.3
1	E	185	THR	3.3
1	F	356	ASN	3.3
1	B	169	LYS	3.3
1	A	146	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	254	ARG	3.2
1	B	128	GLY	3.2
1	G	297	PHE	3.2
1	F	367	ALA	3.2
1	G	305	SER	3.2
1	F	140	GLN	3.2
1	F	366	LEU	3.2
1	C	318	ALA	3.2
1	C	374	THR	3.2
1	E	234	GLU	3.2
1	G	237	ASN	3.2
1	G	301	GLN	3.2
1	C	363	GLU	3.1
1	B	250	THR	3.1
1	F	229	THR	3.1
1	A	117	GLN	3.1
1	A	151	VAL	3.1
1	G	283	HIS	3.1
1	D	165	GLU	3.1
1	F	267	GLU	3.1
1	G	363	GLU	3.1
1	F	383	SER	3.1
1	A	315	PRO	3.1
1	C	134	ILE	3.1
1	D	377	ILE	3.1
1	C	364	GLU	3.1
1	D	374	THR	3.1
1	E	350	ARG	3.1
1	E	373	PRO	3.1
1	F	262	ILE	3.1
1	C	144	SER	3.1
1	G	178	LYS	3.1
1	A	382	SER	3.0
1	C	168	LEU	3.0
1	F	181	ALA	3.0
1	A	333	SER	3.0
1	E	142	ARG	3.0
1	G	152	ARG	3.0
1	G	331	MET	3.0
1	A	222	GLN	3.0
1	C	142	ARG	3.0
1	C	254	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	180	THR	3.0
1	D	368	LEU	3.0
1	B	274	GLY	3.0
1	D	293	GLY	3.0
1	B	160	ALA	3.0
1	B	178	LYS	3.0
1	B	234	GLU	3.0
1	D	295	TYR	2.9
1	A	142	ARG	2.9
1	C	372	ARG	2.9
1	A	166	LYS	2.9
1	C	378	LYS	2.9
1	F	166	LYS	2.9
1	D	181	ALA	2.9
1	E	109	ALA	2.9
1	B	331	MET	2.9
1	C	125	ILE	2.9
1	F	159	ASN	2.9
1	A	160	ALA	2.9
1	G	308	MET	2.9
1	B	311	LEU	2.9
1	E	186	ILE	2.8
1	G	201	PRO	2.8
1	A	359	THR	2.8
1	D	107	SER	2.8
1	A	348	GLU	2.8
1	C	269	GLU	2.8
1	B	298	GLY	2.8
1	D	137	LEU	2.8
1	A	221	GLY	2.8
1	A	201	PRO	2.8
1	D	291	ASN	2.8
1	E	158	ASN	2.8
1	F	248	ASN	2.8
1	B	210	ARG	2.8
1	C	193	SER	2.8
1	F	165	GLU	2.8
1	A	369	ALA	2.8
1	B	136	ASP	2.8
1	B	192	ALA	2.8
1	B	318	ALA	2.8
1	B	349	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	306	ASN	2.8
1	G	238	LYS	2.8
1	F	374	THR	2.8
1	G	344	GLU	2.8
1	B	201	PRO	2.8
1	D	122	PRO	2.8
1	G	271	SER	2.8
1	G	222	GLN	2.7
1	C	377	ILE	2.7
1	G	350	ARG	2.7
1	F	355	LYS	2.7
1	F	241	THR	2.7
1	G	218	LYS	2.7
1	E	209	ASN	2.7
1	A	320	ALA	2.7
1	C	250	THR	2.7
1	D	383	SER	2.7
1	F	345	VAL	2.7
1	C	184	LYS	2.7
1	A	132	LEU	2.7
1	E	246	SER	2.7
1	A	344	GLU	2.7
1	A	202	MET	2.7
1	D	273	SER	2.7
1	G	261	ALA	2.7
1	C	225	ASN	2.7
1	C	368	LEU	2.7
1	D	277	LEU	2.7
1	G	368	LEU	2.7
1	E	299	GLY	2.7
1	A	353	PHE	2.7
1	E	173	ASP	2.6
1	G	263	TYR	2.6
1	B	239	VAL	2.6
1	C	323	THR	2.6
1	B	139	ALA	2.6
1	E	272	ALA	2.6
1	B	162	VAL	2.6
1	G	275	ILE	2.6
1	A	350	ARG	2.6
1	A	269	GLU	2.6
1	F	238	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	374	THR	2.6
1	B	168	LEU	2.6
1	F	294	ARG	2.6
1	E	122	PRO	2.6
1	E	244	ASP	2.6
1	G	309	TRP	2.6
1	A	140	GLN	2.6
1	B	293	GLY	2.6
1	D	238	LYS	2.6
1	D	299	GLY	2.6
1	A	240	ALA	2.6
1	C	137	LEU	2.6
1	B	273	SER	2.6
1	F	223	LEU	2.6
1	E	245	THR	2.6
1	C	346	SER	2.6
1	A	306	ASN	2.6
1	B	158	ASN	2.6
1	G	250	THR	2.6
1	F	314	VAL	2.5
1	D	321	ALA	2.5
1	E	178	LYS	2.5
1	E	168	LEU	2.5
1	F	217	LEU	2.5
1	A	321	ALA	2.5
1	B	319	GLN	2.5
1	D	116	ILE	2.5
1	C	165	GLU	2.5
1	F	337	ASP	2.5
1	E	204	GLN	2.5
1	F	219	GLU	2.5
1	D	284	ASN	2.5
1	B	294	ARG	2.5
1	G	135	ARG	2.5
1	D	175	THR	2.5
1	A	154	GLU	2.5
1	A	148	LEU	2.5
1	D	110	ASP	2.5
1	F	252	ASP	2.5
1	E	320	ALA	2.5
1	D	178	LYS	2.5
1	B	233	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	317	LYS	2.4
1	D	353	PHE	2.4
1	A	295	TYR	2.4
1	F	380	THR	2.4
1	G	245	THR	2.4
1	C	383	SER	2.4
1	E	131	ARG	2.4
1	E	220	GLU	2.4
1	A	216	ALA	2.4
1	B	284	ASN	2.4
1	A	155	VAL	2.4
1	C	135	ARG	2.4
1	A	220	GLU	2.4
1	C	185	THR	2.4
1	D	120	GLN	2.4
1	G	210	ARG	2.4
1	C	266	THR	2.4
1	A	217	LEU	2.4
1	G	142	ARG	2.4
1	B	184	LYS	2.4
1	C	208	ASN	2.4
1	A	176	PHE	2.4
1	A	346	SER	2.4
1	E	383	SER	2.4
1	B	231	ASP	2.4
1	G	326	VAL	2.4
1	C	289	LYS	2.4
1	E	284	ASN	2.4
1	E	315	PRO	2.3
1	C	130	ARG	2.3
1	F	201	PRO	2.3
1	F	315	PRO	2.3
1	A	149	GLU	2.3
1	C	120	GLN	2.3
1	C	220	GLU	2.3
1	F	251	GLY	2.3
1	E	341	ALA	2.3
1	B	131	ARG	2.3
1	E	354	VAL	2.3
1	F	297	PHE	2.3
1	A	109	ALA	2.3
1	C	182	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	363	GLU	2.3
1	D	227	ASP	2.3
1	C	321	ALA	2.3
1	C	380	THR	2.3
1	E	287	LEU	2.3
1	F	250	THR	2.3
1	A	268	SER	2.3
1	B	216	ALA	2.3
1	D	236	LEU	2.3
1	D	136	ASP	2.3
1	D	233	LEU	2.3
1	G	137	LEU	2.3
1	G	269	GLU	2.3
1	A	218	LYS	2.3
1	D	169	LYS	2.3
1	C	277	LEU	2.3
1	E	126	MET	2.3
1	G	372	ARG	2.3
1	E	159	ASN	2.2
1	D	380	THR	2.2
1	E	382	SER	2.2
1	A	287	LEU	2.2
1	B	181	ALA	2.2
1	C	138	LEU	2.2
1	E	302	ALA	2.2
1	F	343	VAL	2.2
1	E	225	ASN	2.2
1	G	262	ILE	2.2
1	A	205	SER	2.2
1	E	365	ARG	2.2
1	A	371	TYR	2.2
1	D	146	ASN	2.2
1	A	283	HIS	2.2
1	G	292	GLU	2.2
1	B	208	ASN	2.2
1	C	159	ASN	2.2
1	E	135	ARG	2.2
1	G	209	ASN	2.2
1	A	250	THR	2.2
1	B	219	GLU	2.2
1	B	344	GLU	2.2
1	E	217	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	150	TYR	2.2
1	D	130	ARG	2.2
1	G	145	SER	2.2
1	E	132	LEU	2.2
1	G	129	LEU	2.2
1	B	196	VAL	2.2
1	B	345	VAL	2.2
1	A	122	PRO	2.2
1	B	218	LYS	2.2
1	B	114	SER	2.2
1	F	246	SER	2.2
1	F	295	TYR	2.2
1	G	371	TYR	2.2
1	B	242	ALA	2.1
1	C	280	ARG	2.1
1	G	365	ARG	2.1
1	G	154	GLU	2.1
1	A	136	ASP	2.1
1	D	254	ARG	2.1
1	B	165	GLU	2.1
1	D	341	ALA	2.1
1	B	212	MET	2.1
1	C	291	ASN	2.1
1	D	209	ASN	2.1
1	C	191	GLN	2.1
1	C	195	GLN	2.1
1	C	310	GLY	2.1
1	B	326	VAL	2.1
1	F	208	ASN	2.1
1	G	192	ALA	2.1
1	B	383	SER	2.1
1	E	333	SER	2.1
1	C	331	MET	2.1
1	C	178	LYS	2.1
1	E	213	TYR	2.1
1	E	123	GLY	2.1
1	A	301	GLN	2.1
1	B	120	GLN	2.1
1	B	373	PRO	2.1
1	C	204	GLN	2.1
1	D	191	GLN	2.1
1	D	301	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	120	GLN	2.1
1	A	131	ARG	2.0
1	G	139	ALA	2.0
1	A	266	THR	2.0
1	E	306	ASN	2.0
1	F	304	THR	2.0
1	G	334	GLN	2.0
1	G	219	GLU	2.0
1	F	340	ASP	2.0
1	B	126	MET	2.0
1	A	288	LEU	2.0
1	A	252	ASP	2.0
1	B	227	ASP	2.0
1	A	158	ASN	2.0
1	C	158	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.