



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:14 AM UTC

PDB ID : 6DD7 / pdb_00006dd7
Title : Crystal structure of plant UVB photoreceptor UVR8 from in situ serial Laue diffraction
Authors : Ren, Z.
Deposited on : 2018-05-09
Resolution : 2.00 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

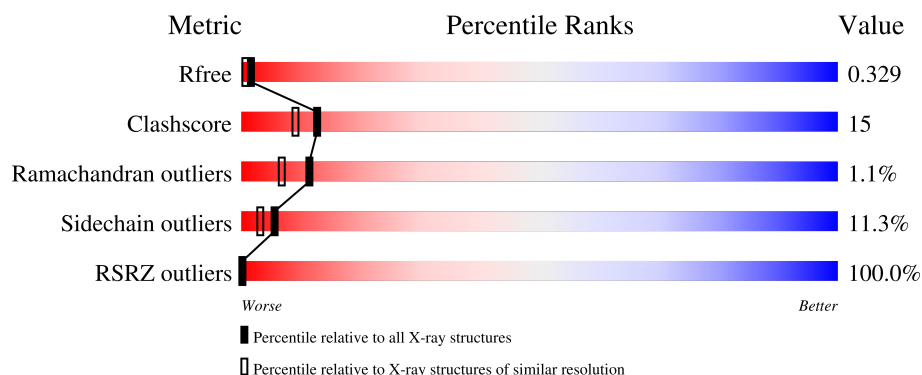
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	377	98% 60% 32% 5% ..
1	B	377	98% 68% 27% ..
1	C	377	98% 69% 25% ..
1	D	377	98% 65% 29% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12160 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 Ultraviolet-B receptor UVR8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2793	1741	505	534	13			
1	B	368	Total	C	N	O	S	0	0	0
			2793	1741	505	534	13			
1	C	368	Total	C	N	O	S	0	0	0
			2793	1741	505	534	13			
1	D	368	Total	C	N	O	S	0	0	0
			2793	1741	505	534	13			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	LEU	-	expression tag	UNP Q9FN03
A	383	GLU	-	expression tag	UNP Q9FN03
A	384	HIS	-	expression tag	UNP Q9FN03
A	385	HIS	-	expression tag	UNP Q9FN03
A	386	HIS	-	expression tag	UNP Q9FN03
A	387	HIS	-	expression tag	UNP Q9FN03
A	388	HIS	-	expression tag	UNP Q9FN03
A	389	HIS	-	expression tag	UNP Q9FN03
B	382	LEU	-	expression tag	UNP Q9FN03
B	383	GLU	-	expression tag	UNP Q9FN03
B	384	HIS	-	expression tag	UNP Q9FN03
B	385	HIS	-	expression tag	UNP Q9FN03
B	386	HIS	-	expression tag	UNP Q9FN03
B	387	HIS	-	expression tag	UNP Q9FN03
B	388	HIS	-	expression tag	UNP Q9FN03
B	389	HIS	-	expression tag	UNP Q9FN03
C	382	LEU	-	expression tag	UNP Q9FN03
C	383	GLU	-	expression tag	UNP Q9FN03
C	384	HIS	-	expression tag	UNP Q9FN03
C	385	HIS	-	expression tag	UNP Q9FN03
C	386	HIS	-	expression tag	UNP Q9FN03

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Chain	Residue	Modelled	Actual	Comment	Reference
C	387	HIS	-	expression tag	UNP Q9FN03
C	388	HIS	-	expression tag	UNP Q9FN03
C	389	HIS	-	expression tag	UNP Q9FN03
D	382	LEU	-	expression tag	UNP Q9FN03
D	383	GLU	-	expression tag	UNP Q9FN03
D	384	HIS	-	expression tag	UNP Q9FN03
D	385	HIS	-	expression tag	UNP Q9FN03
D	386	HIS	-	expression tag	UNP Q9FN03
D	387	HIS	-	expression tag	UNP Q9FN03
D	388	HIS	-	expression tag	UNP Q9FN03
D	389	HIS	-	expression tag	UNP Q9FN03

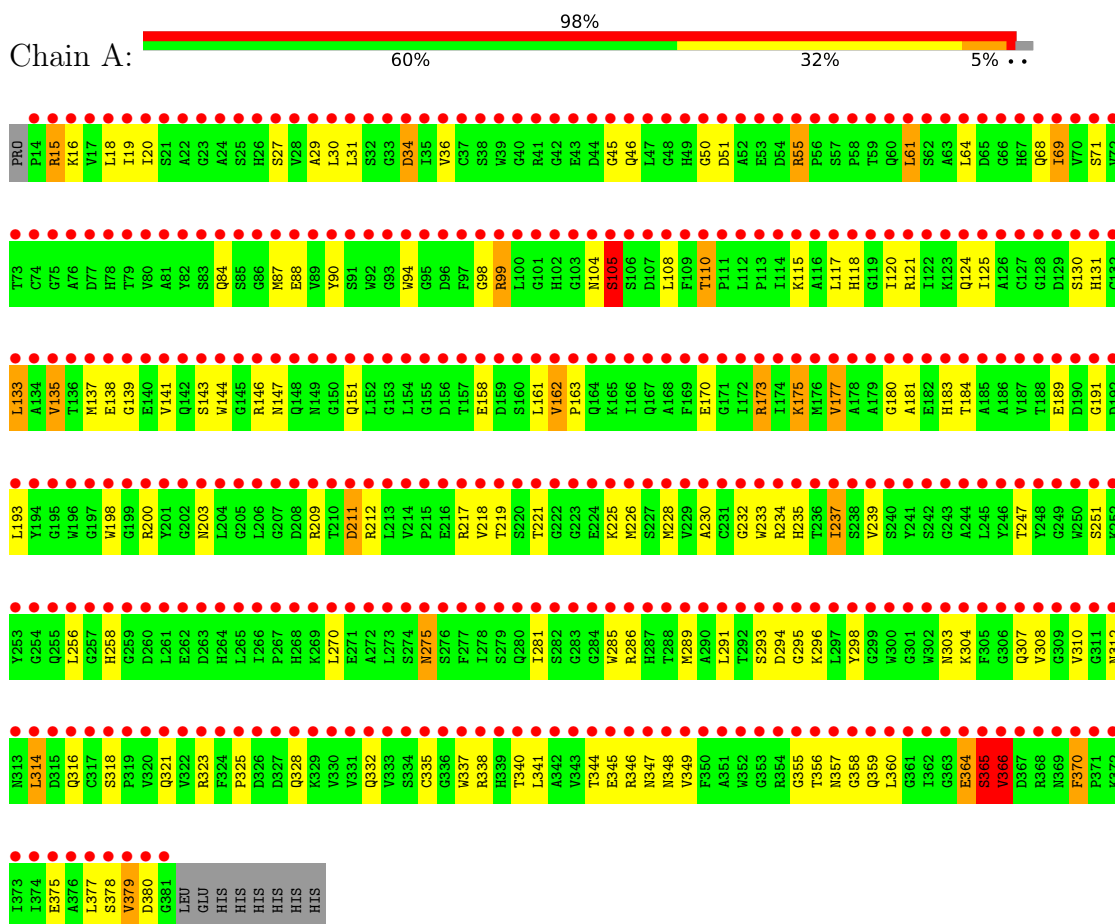
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	200	Total 200	O 200	0	0
2	B	306	Total 306	O 306	0	0
2	C	276	Total 276	O 276	0	0
2	D	206	Total 206	O 206	0	0

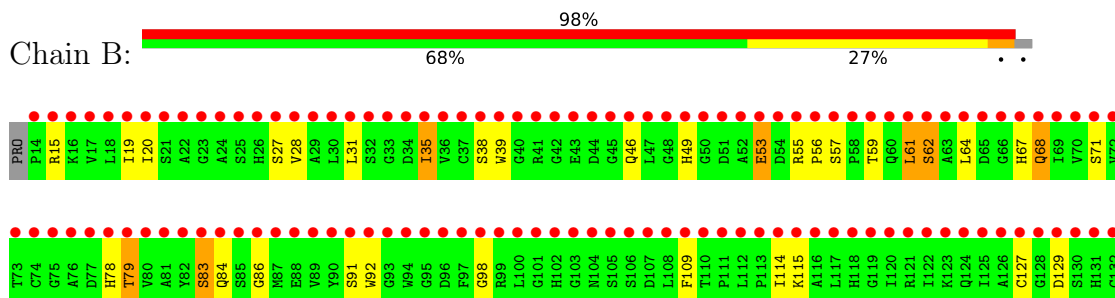
3 Residue-property plots

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: Ultraviolet-B receptor UVR8

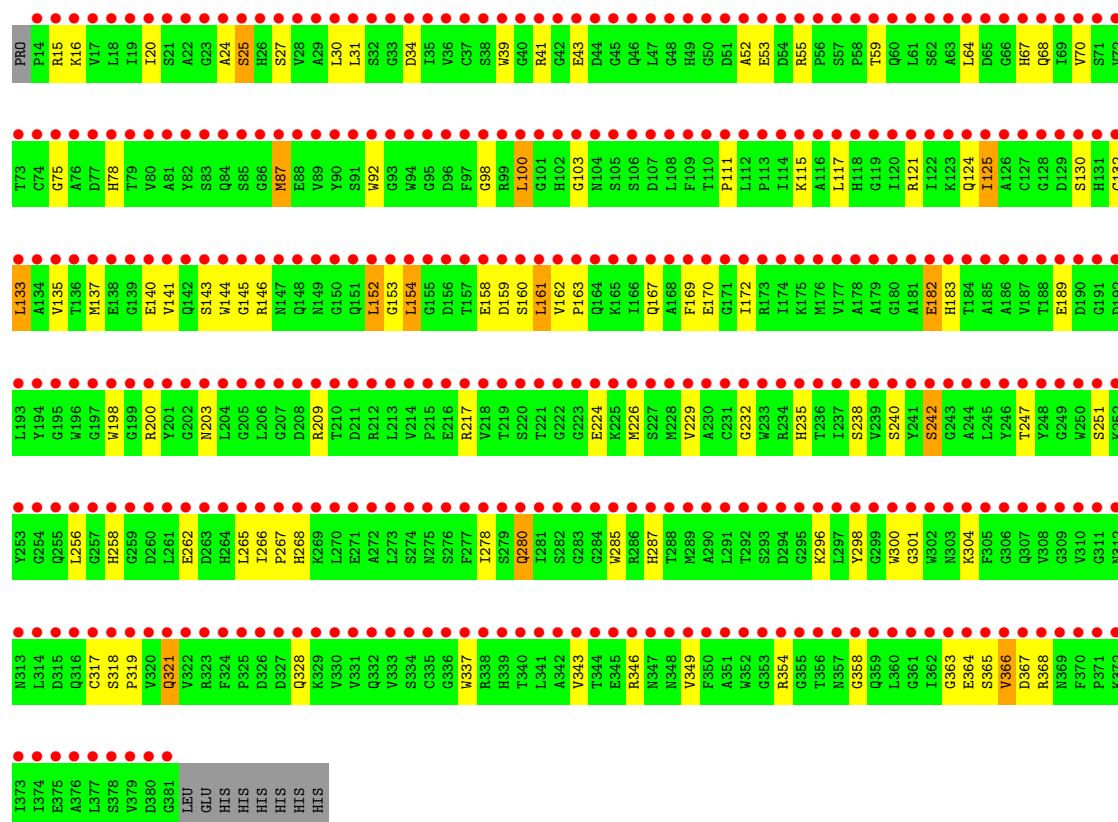


• Molecule 1: Ultraviolet-B receptor UVR8





• Molecule 1: Ultraviolet-B receptor UVR8



• Molecule 1: Ultraviolet-B receptor UVR8





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.20Å 80.30Å 190.00Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	47.33 – 2.00 47.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.6 (47.33-2.00) 87.2 (47.33-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.68 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.254 , 0.328 0.254 , 0.329	Depositor DCC
R_{free} test set	5010 reflections (3.25%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 106.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.42	EDS
Total number of atoms	12160	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5245e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [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	0.37	0/2860	0.62	2/3877 (0.1%)
1	B	0.46	0/2860	0.66	0/3877
1	C	0.44	0/2860	0.68	0/3877
1	D	0.35	0/2860	0.56	0/3877
All	All	0.41	0/11440	0.63	2/15508 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	SER	CA-C-N	5.34	131.31	121.70
1	A	365	SER	C-N-CA	5.34	131.31	121.70

There are no chirality outliers.

There are no planarity outliers.

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	2793	0	2670	99	0
1	B	2793	0	2670	85	0
1	C	2793	0	2670	74	0
1	D	2793	0	2670	79	0
2	A	200	0	0	15	0
2	B	306	0	0	40	0
2	C	276	0	0	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	206	0	0	24	0
All	All	12160	0	10680	332	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 15.

All (332) 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:A:348:ASN:HD22	1:A:378:SER:HB2	1.29	0.95
1:D:200:ARG:NH2	2:D:404:HOH:O	2.05	0.89
1:C:145:GLY:O	2:C:401:HOH:O	1.90	0.89
1:D:76:ALA:O	2:D:401:HOH:O	1.93	0.87
1:B:98:GLY:O	2:B:401:HOH:O	1.96	0.84
1:D:182:GLU:OE2	2:D:402:HOH:O	1.95	0.83
1:C:158:GLU:O	2:C:402:HOH:O	1.98	0.81
1:A:61:LEU:HG	1:A:64:LEU:HD12	1.61	0.80
1:B:20:ILE:O	2:B:402:HOH:O	1.97	0.80
1:D:183:HIS:ND1	2:D:407:HOH:O	2.13	0.79
1:C:285:TRP:HB2	1:C:337:TRP:HA	1.65	0.79
1:A:121:ARG:HG3	1:A:137:MET:HB2	1.66	0.78
1:B:149:ASN:ND2	2:B:407:HOH:O	2.11	0.78
1:A:133:LEU:HD13	1:A:143:SER:HB3	1.66	0.77
1:B:127:CYS:O	2:B:403:HOH:O	2.01	0.77
1:B:129:ASP:O	2:B:404:HOH:O	2.02	0.76
1:C:160:SER:N	2:C:401:HOH:O	2.16	0.75
1:D:59:THR:OG1	2:D:403:HOH:O	2.03	0.75
1:A:294:ASP:OD1	2:A:401:HOH:O	2.05	0.74
1:D:192:ASP:OD1	1:D:217:ARG:NH1	2.21	0.73
1:C:301:GLY:O	2:C:404:HOH:O	2.07	0.72
1:A:293:SER:OG	2:A:403:HOH:O	2.07	0.72
1:A:316:GLN:OE1	2:A:402:HOH:O	2.07	0.71
1:B:364:GLU:O	1:B:366:VAL:N	2.24	0.71
1:B:366:VAL:O	2:B:405:HOH:O	2.08	0.71
1:B:203:ASN:ND2	2:B:415:HOH:O	2.24	0.70
1:D:64:LEU:O	2:D:405:HOH:O	2.10	0.70
1:A:275:ASN:OD1	1:A:275:ASN:N	2.23	0.69
1:A:379:VAL:O	2:A:404:HOH:O	2.11	0.69
1:B:175:LYS:NZ	1:B:227:SER:O	2.27	0.68
1:C:217:ARG:NH1	2:C:410:HOH:O	2.25	0.68
1:C:301:GLY:N	2:C:404:HOH:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:MET:HE1	1:C:121:ARG:HG2	1.75	0.68
1:D:27:SER:HB2	1:D:341:LEU:HD11	1.76	0.68
1:B:67:HIS:NE2	2:B:420:HOH:O	2.28	0.67
1:D:328:GLN:HB3	1:D:346:ARG:HH11	1.60	0.66
1:C:64:LEU:O	2:C:405:HOH:O	2.12	0.66
1:B:55:ARG:NE	2:B:408:HOH:O	2.23	0.66
1:B:115:LYS:NZ	2:B:411:HOH:O	2.19	0.66
1:A:365:SER:HA	1:A:366:VAL:HG12	1.77	0.66
1:D:253:TYR:OH	2:D:408:HOH:O	2.13	0.66
1:D:78:HIS:ND1	2:D:416:HOH:O	2.29	0.65
1:D:181:ALA:HB2	1:D:233:TRP:CD1	2.31	0.65
1:A:124:GLN:HE22	1:A:177:VAL:H	1.43	0.64
1:B:53:GLU:O	2:B:408:HOH:O	2.15	0.64
1:D:152:LEU:HB3	1:D:154:LEU:HG	1.78	0.64
1:B:147:ASN:ND2	1:B:156:ASP:O	2.30	0.64
1:A:15:ARG:HH21	1:A:15:ARG:HB3	1.63	0.64
1:D:330:VAL:HA	1:D:344:THR:HA	1.79	0.63
1:B:216:GLU:HB2	2:B:469:HOH:O	1.99	0.63
1:A:94:TRP:O	1:A:99:ARG:HD2	1.98	0.62
1:B:238:SER:HB2	2:B:571:HOH:O	1.98	0.62
1:A:303:ASN:ND2	2:A:408:HOH:O	2.23	0.62
1:A:173:ARG:NH2	1:A:189:GLU:OE2	2.33	0.62
1:A:198:TRP:CZ2	1:A:200:ARG:HB2	2.35	0.62
1:A:378:SER:HB3	2:A:445:HOH:O	1.98	0.61
1:A:232:GLY:HA3	1:A:235:HIS:CE1	2.35	0.61
1:B:68:GLN:NE2	2:B:423:HOH:O	2.33	0.61
1:D:237:ILE:HG22	1:D:245:LEU:HD11	1.82	0.61
1:B:184:THR:O	2:B:410:HOH:O	2.16	0.61
1:B:253:TYR:OH	2:B:409:HOH:O	2.15	0.61
1:D:354:ARG:NH1	1:D:367:ASP:OD2	2.30	0.60
1:C:103:GLY:HA3	2:C:563:HOH:O	2.01	0.60
1:D:41:ARG:NH2	1:D:44:ASP:OD2	2.34	0.60
1:D:285:TRP:HB2	1:D:337:TRP:HA	1.83	0.60
1:D:367:ASP:OD1	1:D:367:ASP:N	2.32	0.60
1:B:232:GLY:HA3	1:B:235:HIS:CE1	2.37	0.60
1:B:262:GLU:HG2	2:B:617:HOH:O	2.01	0.59
1:D:54:ASP:O	1:D:55:ARG:HD3	2.02	0.59
1:D:270:LEU:HD22	2:D:417:HOH:O	2.02	0.59
1:C:167:GLN:HB2	2:C:597:HOH:O	2.02	0.59
1:B:251:SER:OG	2:B:406:HOH:O	2.17	0.59
1:C:296:LYS:HG2	2:C:467:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:LYS:NZ	2:D:420:HOH:O	2.34	0.59
1:C:55:ARG:NE	2:C:418:HOH:O	2.36	0.59
1:A:193:LEU:HD22	1:A:226:MET:HG3	1.84	0.59
1:C:343:VAL:HG22	1:C:349:VAL:HG22	1.84	0.59
1:D:351:ALA:N	2:D:423:HOH:O	2.36	0.58
1:A:146:ARG:NH2	2:A:418:HOH:O	2.36	0.58
1:A:144:TRP:HB3	1:A:163:PRO:HA	1.84	0.58
1:D:196:TRP:HB3	1:D:215:PRO:HA	1.84	0.57
1:B:338:ARG:NH1	2:B:424:HOH:O	2.33	0.57
1:B:98:GLY:HA3	1:B:161:LEU:HD23	1.87	0.57
1:D:180:GLY:HA3	1:D:183:HIS:CE1	2.39	0.57
1:C:132:CYS:C	1:C:133:LEU:HD22	2.29	0.57
1:B:193:LEU:HD13	2:B:571:HOH:O	2.04	0.56
1:D:323:ARG:O	2:D:409:HOH:O	2.17	0.56
1:A:19:ILE:HD11	2:A:535:HOH:O	2.05	0.56
1:D:227:SER:HB2	1:D:241:TYR:CE2	2.41	0.56
1:D:52:ALA:HB2	1:D:109:PHE:HE2	1.71	0.56
1:D:226:MET:O	2:D:410:HOH:O	2.18	0.55
1:C:169:PHE:HD1	1:C:172:ILE:HD12	1.71	0.55
1:B:328:GLN:HB3	1:B:346:ARG:HE	1.72	0.55
1:C:68:GLN:HG3	2:C:522:HOH:O	2.07	0.55
1:D:287:HIS:HA	1:D:301:GLY:HA3	1.88	0.55
1:C:226:MET:HE2	1:C:238:SER:HB2	1.89	0.55
1:D:39:TRP:HB3	1:D:58:PRO:HA	1.88	0.55
1:B:38:SER:OG	1:B:49:HIS:NE2	2.37	0.55
1:D:350:PHE:HB3	2:D:423:HOH:O	2.06	0.54
1:C:140:GLU:HA	2:C:424:HOH:O	2.08	0.54
1:B:227:SER:HB3	1:B:241:TYR:CE1	2.42	0.54
1:A:144:TRP:CE3	1:A:163:PRO:HB3	2.43	0.54
1:C:15:ARG:NH2	2:C:417:HOH:O	2.35	0.54
1:A:211:ASP:O	1:A:212:ARG:HD3	2.07	0.54
1:A:356:THR:C	1:A:358:GLY:H	2.16	0.54
1:B:181:ALA:HB2	1:B:233:TRP:CD1	2.43	0.53
1:C:98:GLY:HA3	1:C:161:LEU:HD12	1.89	0.53
1:A:161:LEU:N	2:A:423:HOH:O	2.40	0.53
1:C:247:THR:HB	1:C:256:LEU:HD22	1.89	0.53
1:B:217:ARG:NH1	2:B:438:HOH:O	2.42	0.53
1:C:268:HIS:ND1	2:C:414:HOH:O	2.32	0.53
1:A:286:ARG:NH1	1:D:107:ASP:OD2	2.36	0.53
1:A:296:LYS:HD2	2:A:511:HOH:O	2.08	0.53
1:C:167:GLN:HG3	2:C:618:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:VAL:HG21	1:D:349:VAL:HG21	1.91	0.53
1:B:19:ILE:HD12	1:B:71:SER:HA	1.92	0.52
1:B:78:HIS:HB2	1:B:92:TRP:O	2.09	0.52
1:B:323:ARG:HG3	1:B:323:ARG:HH11	1.75	0.52
1:A:34:ASP:CG	1:A:68:GLN:HA	2.33	0.52
1:A:84:GLN:OE1	2:A:406:HOH:O	2.19	0.52
1:C:30:LEU:HD11	1:C:34:ASP:HA	1.90	0.52
1:A:338:ARG:NH2	2:A:405:HOH:O	2.16	0.52
1:C:280:GLN:NE2	2:C:420:HOH:O	2.37	0.52
1:C:232:GLY:HA3	1:C:235:HIS:CE1	2.45	0.52
1:D:370:PHE:HD1	1:D:370:PHE:H	1.58	0.52
1:C:43:GLU:HA	1:C:52:ALA:HB1	1.91	0.52
1:B:304:LYS:NZ	2:B:429:HOH:O	2.36	0.51
1:D:258:HIS:N	2:D:421:HOH:O	2.35	0.51
1:A:193:LEU:HG	1:A:218:VAL:HG21	1.93	0.51
1:C:280:GLN:HG2	2:C:521:HOH:O	2.10	0.51
1:D:188:THR:OG1	1:D:190:ASP:OD2	2.27	0.51
1:A:19:ILE:HA	1:A:332:GLN:OE1	2.11	0.50
1:C:247:THR:OG1	1:C:258:HIS:NE2	2.44	0.50
1:D:16:LYS:HG2	1:D:347:ASN:CG	2.37	0.50
1:D:220:SER:HB3	2:D:547:HOH:O	2.11	0.50
1:D:263:ASP:OD2	2:D:411:HOH:O	2.19	0.50
1:A:15:ARG:HB3	1:A:15:ARG:NH2	2.26	0.50
1:A:181:ALA:HB2	1:A:233:TRP:CD1	2.47	0.50
1:A:303:ASN:OD1	1:A:308:VAL:N	2.34	0.50
1:D:210:THR:HG22	1:D:211:ASP:O	2.12	0.50
1:A:291:LEU:HD11	1:A:295:GLY:HA2	1.93	0.50
1:A:124:GLN:NE2	1:A:177:VAL:O	2.45	0.49
1:C:55:ARG:NH1	1:C:59:THR:HG21	2.26	0.49
1:A:124:GLN:HG2	1:A:125:ILE:N	2.27	0.49
1:A:16:LYS:HG3	1:A:347:ASN:OD1	2.11	0.49
1:D:297:LEU:HD23	1:D:322:VAL:HG21	1.94	0.49
1:D:356:THR:HG23	2:D:466:HOH:O	2.11	0.49
1:B:232:GLY:N	1:B:235:HIS:O	2.39	0.49
1:C:121:ARG:NH2	2:C:432:HOH:O	2.45	0.49
1:A:365:SER:HA	1:A:366:VAL:CB	2.42	0.49
1:B:46:GLN:O	1:B:79:THR:OG1	2.29	0.49
1:A:139:GLY:HA3	1:A:173:ARG:NH1	2.28	0.49
1:B:227:SER:HB3	1:B:241:TYR:HE1	1.78	0.49
1:A:298:TYR:CE1	1:A:321:GLN:HB3	2.48	0.49
1:A:98:GLY:HA3	1:A:161:LEU:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:GLU:HB2	1:C:198:TRP:HB2	1.95	0.48
1:A:173:ARG:CZ	1:A:173:ARG:HB3	2.44	0.48
1:A:105:SER:O	2:D:408:HOH:O	2.20	0.48
1:B:291:LEU:CD1	1:B:330:VAL:HB	2.43	0.48
1:B:323:ARG:HG2	2:B:560:HOH:O	2.12	0.48
1:A:365:SER:HA	1:A:366:VAL:CG1	2.42	0.48
1:B:217:ARG:NE	2:B:433:HOH:O	2.39	0.48
1:C:298:TYR:CE2	1:C:321:GLN:HB2	2.49	0.48
1:D:251:SER:HB3	1:D:262:GLU:O	2.13	0.48
1:D:295:GLY:HA3	1:D:329:LYS:HB3	1.95	0.48
1:B:61:LEU:HD13	1:B:64:LEU:HD12	1.95	0.48
1:A:348:ASN:HA	1:A:378:SER:HB2	1.96	0.48
1:A:289:MET:HE3	1:A:340:THR:HG21	1.96	0.47
1:A:310:VAL:HG23	1:A:312:ASN:ND2	2.28	0.47
1:B:231:CYS:HB2	2:B:439:HOH:O	2.14	0.47
1:A:233:TRP:HB2	1:A:285:TRP:HA	1.96	0.47
1:B:285:TRP:HB2	1:B:337:TRP:HA	1.96	0.47
1:A:247:THR:OG1	1:A:258:HIS:NE2	2.47	0.47
1:B:28:VAL:HG21	1:B:79:THR:CG2	2.45	0.47
1:B:364:GLU:HA	2:B:567:HOH:O	2.13	0.47
1:A:348:ASN:HD22	1:A:378:SER:CB	2.13	0.47
1:A:365:SER:OG	1:A:366:VAL:O	2.20	0.47
1:B:67:HIS:O	1:B:83:SER:OG	2.32	0.47
1:D:203:ASN:OD1	1:D:203:ASN:N	2.39	0.47
1:C:266:ILE:HB	1:C:267:PRO:HD2	1.97	0.47
1:D:19:ILE:HD12	1:D:71:SER:HA	1.96	0.47
1:C:121:ARG:NH1	2:C:436:HOH:O	2.47	0.47
1:D:14:PRO:N	1:D:16:LYS:HE3	2.30	0.46
1:A:234:ARG:HH21	1:D:97:PHE:HZ	1.62	0.46
1:B:270:LEU:HD12	1:B:270:LEU:HA	1.68	0.46
1:B:372:LYS:NZ	2:B:447:HOH:O	2.48	0.46
1:B:148:GLN:HE22	1:C:200:ARG:NH1	2.13	0.46
1:B:265:LEU:HD22	2:B:662:HOH:O	2.16	0.46
1:A:325:PRO:O	1:A:328:GLN:HG3	2.15	0.46
1:B:109:PHE:CZ	1:C:304:LYS:HE2	2.50	0.46
1:C:226:MET:HA	1:C:240:SER:HA	1.96	0.46
1:A:230:ALA:HB2	1:A:281:ILE:HG13	1.98	0.46
1:B:255:GLN:N	2:B:406:HOH:O	2.49	0.46
1:D:169:PHE:CE1	1:D:174:ILE:HD11	2.50	0.46
1:A:110:THR:HG23	2:A:449:HOH:O	2.15	0.46
1:A:370:PHE:HD1	1:A:370:PHE:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:HIS:HA	1:B:353:GLY:HA3	1.97	0.46
1:A:27:SER:HB3	1:A:341:LEU:HD11	1.98	0.46
1:C:146:ARG:HA	1:C:159:ASP:OD1	2.16	0.46
1:D:322:VAL:HB	2:D:563:HOH:O	2.15	0.46
1:A:237:ILE:HG23	1:A:247:THR:HG22	1.98	0.46
1:C:27:SER:HB2	1:C:39:TRP:CE2	2.51	0.45
1:D:147:ASN:CG	1:D:152:LEU:HB2	2.42	0.45
1:D:210:THR:HB	1:D:212:ARG:HH12	1.80	0.45
1:C:24:ALA:HA	1:C:337:TRP:CG	2.51	0.45
1:B:133:LEU:HD13	1:B:143:SER:HB3	1.98	0.45
1:B:291:LEU:HD11	1:B:330:VAL:HB	1.98	0.45
1:B:317:CYS:HB3	2:B:564:HOH:O	2.14	0.45
1:A:64:LEU:HD22	1:A:69:ILE:HD11	1.98	0.45
1:A:16:LYS:HD2	1:A:18:LEU:CD2	2.47	0.45
1:D:258:HIS:HE1	1:D:268:HIS:O	2.00	0.45
1:C:287:HIS:HA	1:C:301:GLY:HA3	1.99	0.45
1:D:173:ARG:O	1:D:189:GLU:HG2	2.17	0.45
1:B:84:GLN:N	2:B:442:HOH:O	2.50	0.45
1:A:46:GLN:OE1	1:A:46:GLN:N	2.33	0.44
1:A:104:ASN:O	1:A:161:LEU:HD22	2.17	0.44
1:A:203:ASN:HB3	1:A:234:ARG:O	2.17	0.44
1:C:167:GLN:HB3	2:C:444:HOH:O	2.17	0.44
1:D:16:LYS:HG2	1:D:347:ASN:ND2	2.31	0.44
1:B:114:ILE:HA	2:B:456:HOH:O	2.16	0.44
1:C:92:TRP:CE3	1:C:111:PRO:HG3	2.53	0.44
1:C:135:VAL:HG22	1:C:141:VAL:HG22	2.00	0.44
1:D:227:SER:HB2	1:D:241:TYR:CD2	2.52	0.44
1:A:50:GLY:HA2	1:A:110:THR:HG22	2.00	0.44
1:C:130:SER:OG	1:C:146:ARG:HB3	2.16	0.44
1:D:50:GLY:HA2	1:D:110:THR:HG23	1.99	0.44
1:A:87:MET:CE	1:A:121:ARG:HB3	2.48	0.44
1:B:133:LEU:HD21	1:B:184:THR:HG21	1.99	0.44
1:B:174:ILE:HA	1:B:188:THR:HA	1.99	0.44
1:B:304:LYS:HE2	2:B:537:HOH:O	2.18	0.44
1:C:152:LEU:HB3	1:C:154:LEU:HD22	1.99	0.44
1:B:209:ARG:NH2	2:B:448:HOH:O	2.49	0.44
1:C:285:TRP:HB2	1:C:337:TRP:CA	2.43	0.44
1:A:87:MET:HE3	1:A:121:ARG:HB3	1.99	0.44
1:D:251:SER:HB2	1:D:256:LEU:HG	1.99	0.44
1:C:100:LEU:HB2	2:C:497:HOH:O	2.17	0.44
1:C:209:ARG:NH1	1:C:265:LEU:HD11	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:HD13	1:A:36:VAL:HG22	2.00	0.44
1:B:91:SER:C	1:B:92:TRP:HE3	2.26	0.44
1:B:257:GLY:C	1:B:270:LEU:HD11	2.43	0.44
1:B:352:TRP:HB3	1:B:371:PRO:HA	2.00	0.44
1:C:25:SER:HB2	1:C:41:ARG:HB3	1.99	0.44
1:C:183:HIS:CG	1:C:203:ASN:HD22	2.36	0.44
1:C:133:LEU:HD13	1:C:143:SER:CB	2.47	0.43
1:D:69:ILE:HD13	1:D:83:SER:HB2	1.99	0.43
1:B:31:LEU:HB2	1:B:35:ILE:HB	2.00	0.43
1:A:131:HIS:CD2	1:A:151:GLN:HB2	2.53	0.43
1:A:314:LEU:HD12	1:A:314:LEU:HA	1.88	0.43
1:B:38:SER:C	1:B:39:TRP:HE3	2.26	0.43
1:A:304:LYS:NZ	2:A:407:HOH:O	2.20	0.43
1:C:367:ASP:O	1:C:368:ARG:HD3	2.17	0.43
1:C:287:HIS:HB2	1:C:300:TRP:O	2.18	0.43
1:A:358:GLY:O	1:A:360:LEU:N	2.52	0.43
1:D:207:GLY:HA2	1:D:265:LEU:HB2	1.99	0.43
1:B:142:GLN:HG2	1:B:165:LYS:HA	2.00	0.43
1:A:358:GLY:C	1:A:360:LEU:H	2.26	0.43
1:D:201:TYR:CD2	1:D:250:TRP:CG	3.06	0.43
1:D:201:TYR:HD2	1:D:250:TRP:HB2	1.84	0.43
1:A:175:LYS:HB3	1:A:189:GLU:HG2	2.00	0.43
1:D:20:ILE:HD12	1:D:341:LEU:HB2	2.01	0.43
1:A:46:GLN:H	1:A:46:GLN:CD	2.24	0.42
1:A:135:VAL:HG13	1:A:141:VAL:HG22	1.99	0.42
1:B:55:ARG:HA	1:B:55:ARG:HD3	1.79	0.42
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.84	0.42
1:A:30:LEU:O	1:A:31:LEU:HD23	2.19	0.42
1:A:88:GLU:HG3	1:A:118:HIS:HB2	2.01	0.42
1:A:348:ASN:HD21	1:A:380:ASP:H	1.67	0.42
1:B:362:ILE:H	1:B:362:ILE:HG13	1.70	0.42
1:C:24:ALA:HA	1:C:337:TRP:CD1	2.55	0.42
1:D:226:MET:HE1	1:D:246:TYR:CD1	2.54	0.42
1:A:298:TYR:HA	1:A:321:GLN:HA	2.01	0.42
1:B:250:TRP:CZ2	1:B:252:LYS:HD2	2.53	0.42
1:B:251:SER:HB2	1:B:256:LEU:CD1	2.49	0.42
1:D:47:LEU:HD12	2:D:462:HOH:O	2.19	0.42
1:D:321:GLN:O	2:D:413:HOH:O	2.21	0.42
1:B:198:TRP:CH2	1:B:200:ARG:HB2	2.55	0.42
1:D:143:SER:OG	1:D:154:LEU:HD21	2.20	0.42
1:A:180:GLY:HA3	1:A:183:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ASP:HA	2:B:545:HOH:O	2.19	0.42
1:D:239:VAL:HG22	1:D:245:LEU:HD13	2.01	0.42
1:A:191:GLY:HA3	1:A:225:LYS:HB3	2.02	0.42
1:A:147:ASN:HB3	1:A:158:GLU:C	2.45	0.42
1:B:147:ASN:O	1:B:157:THR:HA	2.19	0.42
1:D:251:SER:HB2	1:D:256:LEU:CG	2.50	0.42
1:D:306:GLY:HA3	1:D:369:ASN:HB3	2.01	0.42
1:C:278:ILE:HD13	1:C:278:ILE:HA	1.84	0.42
1:C:366:VAL:C	2:C:438:HOH:O	2.63	0.42
1:A:55:ARG:HG2	1:A:55:ARG:HH11	1.85	0.42
1:C:133:LEU:HD13	1:C:143:SER:HB2	2.02	0.42
1:C:224:GLU:OE1	1:C:242:SER:HB3	2.20	0.42
1:C:226:MET:HE2	1:C:238:SER:CB	2.49	0.42
1:B:219:THR:N	2:B:440:HOH:O	2.42	0.41
1:D:75:GLY:HA3	1:D:78:HIS:CE1	2.55	0.41
1:D:227:SER:HB2	1:D:241:TYR:HE2	1.84	0.41
1:A:117:LEU:HA	1:A:120:ILE:HD12	2.02	0.41
1:A:162:VAL:HG22	1:A:163:PRO:HD2	2.02	0.41
1:B:221:THR:HG22	1:B:267:PRO:HG2	2.02	0.41
1:C:75:GLY:HA3	1:C:78:HIS:CE1	2.55	0.41
1:D:348:ASN:OD1	1:D:378:SER:HB3	2.21	0.41
1:B:28:VAL:HG21	1:B:79:THR:HG23	2.03	0.41
1:C:153:GLY:O	2:C:406:HOH:O	2.22	0.41
1:C:358:GLY:HA2	2:C:528:HOH:O	2.19	0.41
1:A:234:ARG:N	2:A:432:HOH:O	2.54	0.41
1:A:20:ILE:HG22	1:A:29:ALA:HB2	2.02	0.41
1:A:104:ASN:OD1	1:A:105:SER:N	2.53	0.41
1:A:200:ARG:O	1:A:209:ARG:HD3	2.21	0.41
1:A:285:TRP:HB2	1:A:337:TRP:HA	2.01	0.41
1:B:158:GLU:HA	2:B:544:HOH:O	2.21	0.41
1:A:251:SER:HB2	1:A:256:LEU:HG	2.02	0.41
1:B:196:TRP:N	2:B:410:HOH:O	2.41	0.41
1:C:209:ARG:NH2	1:D:262:GLU:HB3	2.36	0.41
1:D:294:ASP:HB3	2:D:551:HOH:O	2.21	0.41
1:A:303:ASN:OD1	1:A:307:GLN:N	2.54	0.41
1:D:54:ASP:C	1:D:55:ARG:HD3	2.46	0.41
1:A:356:THR:C	1:A:358:GLY:N	2.79	0.41
1:B:55:ARG:HA	1:B:56:PRO:HD3	1.90	0.41
1:C:34:ASP:HB3	2:C:435:HOH:O	2.21	0.41
1:C:328:GLN:H	1:C:328:GLN:HG2	1.66	0.41
1:B:115:LYS:HD3	2:B:627:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LEU:HD23	1:C:117:LEU:HA	1.84	0.40
1:B:62:SER:C	1:B:64:LEU:H	2.28	0.40
1:C:67:HIS:HB2	2:C:405:HOH:O	2.21	0.40
1:A:355:GLY:HA3	1:A:360:LEU:HD12	2.02	0.40
1:B:204:LEU:HD12	2:B:418:HOH:O	2.20	0.40
1:C:144:TRP:CE3	1:C:163:PRO:HG3	2.56	0.40
1:C:154:LEU:HD12	1:C:154:LEU:HA	1.77	0.40
1:D:54:ASP:OD1	2:D:414:HOH:O	2.22	0.40
1:D:170:GLU:OE1	1:D:170:GLU:HA	2.21	0.40
1:A:45:GLY:N	1:A:46:GLN:OE1	2.54	0.40
1:B:228:MET:HB2	1:B:239:VAL:HB	2.03	0.40
1:C:124:GLN:HG2	1:C:125:ILE:N	2.36	0.40
1:C:319:PRO:CG	2:C:645:HOH:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/377 (97%)	336 (92%)	23 (6%)	7 (2%)	6	3
1	B	366/377 (97%)	337 (92%)	26 (7%)	3 (1%)	16	11
1	C	366/377 (97%)	343 (94%)	19 (5%)	4 (1%)	11	7
1	D	366/377 (97%)	335 (92%)	29 (8%)	2 (0%)	24	21
All	All	1464/1508 (97%)	1351 (92%)	97 (7%)	16 (1%)	11	7

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	364	GLU

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Mol	Chain	Res	Type
1	B	365	SER
1	C	364	GLU
1	C	365	SER
1	A	105	SER
1	A	366	VAL
1	C	363	GLY
1	D	24	ALA
1	B	15	ARG
1	B	86	GLY
1	C	366	VAL
1	A	357	ASN
1	A	359	GLN
1	D	380	ASP
1	A	365	SER

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	291/300 (97%)	246 (84%)	45 (16%)	2	1
1	B	291/300 (97%)	264 (91%)	27 (9%)	8	5
1	C	291/300 (97%)	262 (90%)	29 (10%)	7	4
1	D	291/300 (97%)	260 (89%)	31 (11%)	6	4
All	All	1164/1200 (97%)	1032 (89%)	132 (11%)	5	3

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	34	ASP
1	A	51	ASP
1	A	55	ARG
1	A	61	LEU
1	A	69	ILE
1	A	71	SER

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Mol	Chain	Res	Type
1	A	90	TYR
1	A	105	SER
1	A	108	LEU
1	A	110	THR
1	A	115	LYS
1	A	130	SER
1	A	133	LEU
1	A	135	VAL
1	A	138	GLU
1	A	162	VAL
1	A	170	GLU
1	A	173	ARG
1	A	175	LYS
1	A	177	VAL
1	A	184	THR
1	A	211	ASP
1	A	217	ARG
1	A	219	THR
1	A	221	THR
1	A	228	MET
1	A	237	ILE
1	A	239	VAL
1	A	270	LEU
1	A	275	ASN
1	A	314	LEU
1	A	318	SER
1	A	323	ARG
1	A	335	CYS
1	A	344	THR
1	A	345	GLU
1	A	346	ARG
1	A	349	VAL
1	A	364	GLU
1	A	365	SER
1	A	366	VAL
1	A	370	PHE
1	A	375	GLU
1	A	379	VAL
1	B	27	SER
1	B	35	ILE
1	B	53	GLU
1	B	57	SER

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Mol	Chain	Res	Type
1	B	59	THR
1	B	61	LEU
1	B	62	SER
1	B	68	GLN
1	B	79	THR
1	B	83	SER
1	B	133	LEU
1	B	137	MET
1	B	174	ILE
1	B	184	THR
1	B	252	LYS
1	B	265	LEU
1	B	280	GLN
1	B	281	ILE
1	B	293	SER
1	B	294	ASP
1	B	318	SER
1	B	326	ASP
1	B	341	LEU
1	B	357	ASN
1	B	362	ILE
1	B	370	PHE
1	B	379	VAL
1	C	16	LYS
1	C	20	ILE
1	C	25	SER
1	C	31	LEU
1	C	53	GLU
1	C	70	VAL
1	C	87	MET
1	C	100	LEU
1	C	115	LYS
1	C	125	ILE
1	C	133	LEU
1	C	137	MET
1	C	152	LEU
1	C	154	LEU
1	C	161	LEU
1	C	162	VAL
1	C	170	GLU
1	C	182	GLU
1	C	189	GLU

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Mol	Chain	Res	Type
1	C	229	VAL
1	C	242	SER
1	C	251	SER
1	C	262	GLU
1	C	280	GLN
1	C	317	CYS
1	C	318	SER
1	C	321	GLN
1	C	346	ARG
1	C	354	ARG
1	D	16	LYS
1	D	25	SER
1	D	53	GLU
1	D	54	ASP
1	D	55	ARG
1	D	57	SER
1	D	62	SER
1	D	70	VAL
1	D	85	SER
1	D	124	GLN
1	D	135	VAL
1	D	142	GLN
1	D	161	LEU
1	D	203	ASN
1	D	214	VAL
1	D	216	GLU
1	D	265	LEU
1	D	269	LYS
1	D	270	LEU
1	D	291	LEU
1	D	294	ASP
1	D	310	VAL
1	D	314	LEU
1	D	320	VAL
1	D	322	VAL
1	D	341	LEU
1	D	356	THR
1	D	367	ASP
1	D	370	PHE
1	D	374	ILE
1	D	379	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	313	ASN
1	A	328	GLN
1	A	348	ASN
1	B	67	HIS
1	B	142	GLN
1	B	164	GLN
1	C	164	GLN
1	C	203	ASN
1	C	347	ASN
1	C	357	ASN
1	D	235	HIS
1	D	264	HIS
1	D	268	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	368/377 (97%)	12.23	368 (100%) 0 0	40, 53, 84, 106	0
1	B	368/377 (97%)	9.20	368 (100%) 0 0	17, 33, 58, 81	0
1	C	368/377 (97%)	8.46	368 (100%) 0 0	16, 30, 52, 76	0
1	D	368/377 (97%)	11.60	368 (100%) 0 0	38, 50, 68, 89	0
All	All	1472/1508 (97%)	10.37	1472 (100%) 0 0	16, 44, 69, 106	0

All (1472) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	172	ILE	34.5
1	A	360	LEU	27.0
1	D	174	ILE	25.0
1	D	362	ILE	24.9
1	A	145	GLY	24.9
1	B	59	THR	23.5
1	D	128	GLY	23.3
1	D	47	LEU	22.2
1	D	62	SER	22.2
1	A	82	TYR	21.9
1	D	364	GLU	21.2
1	A	35	ILE	21.2
1	D	250	TRP	20.9
1	D	308	VAL	20.5
1	A	59	THR	20.5
1	A	15	ARG	20.3
1	A	214	VAL	19.6
1	A	114	ILE	19.5
1	A	155	GLY	19.3
1	C	171	GLY	19.2
1	D	185	ALA	19.2

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Mol	Chain	Res	Type	RSRZ
1	C	381	GLY	18.9
1	A	36	VAL	18.7
1	D	14	PRO	18.5
1	A	19	ILE	18.5
1	B	381	GLY	18.4
1	C	309	GLY	18.4
1	D	331	VAL	18.3
1	A	14	PRO	18.1
1	A	290	ALA	18.1
1	C	243	GLY	18.1
1	A	30	LEU	18.1
1	A	195	GLY	18.0
1	D	309	GLY	18.0
1	D	177	VAL	17.9
1	D	374	ILE	17.8
1	A	313	ASN	17.8
1	A	122	ILE	17.8
1	D	256	LEU	17.7
1	D	349	VAL	17.6
1	A	40	GLY	17.5
1	B	360	LEU	17.5
1	D	119	GLY	17.4
1	B	36	VAL	17.3
1	A	100	LEU	17.3
1	A	138	GLU	17.2
1	A	70	VAL	17.2
1	A	80	VAL	17.2
1	A	189	GLU	17.2
1	C	290	ALA	17.1
1	C	361	GLY	17.0
1	A	172	ILE	16.8
1	A	380	ASP	16.8
1	C	375	GLU	16.8
1	A	174	ILE	16.7
1	A	245	LEU	16.7
1	C	172	ILE	16.7
1	A	316	GLN	16.7
1	A	29	ALA	16.6
1	C	331	VAL	16.6
1	A	199	GLY	16.6
1	A	68	GLN	16.5
1	A	63	ALA	16.4

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Mol	Chain	Res	Type	RSRZ
1	D	244	ALA	16.4
1	D	70	VAL	16.4
1	D	214	VAL	16.3
1	A	119	GLY	16.3
1	A	81	ALA	16.3
1	D	302	TRP	16.2
1	D	186	ALA	16.2
1	A	256	LEU	16.2
1	A	149	ASN	16.2
1	B	98	GLY	16.2
1	D	215	PRO	16.2
1	A	340	THR	16.2
1	D	298	TYR	16.2
1	A	274	SER	16.1
1	A	198	TRP	16.1
1	A	308	VAL	16.1
1	A	246	TYR	16.0
1	A	266	ILE	16.0
1	A	20	ILE	16.0
1	B	14	PRO	15.9
1	A	376	ALA	15.9
1	A	350	PHE	15.9
1	A	188	THR	15.8
1	A	204	LEU	15.8
1	A	33	GLY	15.8
1	D	152	LEU	15.8
1	A	327	ASP	15.8
1	D	344	THR	15.7
1	A	93	GLY	15.7
1	A	38	SER	15.7
1	A	241	TYR	15.6
1	A	361	GLY	15.6
1	D	154	LEU	15.6
1	A	109	PHE	15.6
1	D	207	GLY	15.6
1	B	379	VAL	15.6
1	D	381	GLY	15.5
1	A	64	LEU	15.5
1	A	44	ASP	15.5
1	A	301	GLY	15.4
1	D	375	GLU	15.4
1	D	360	LEU	15.3

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Mol	Chain	Res	Type	RSRZ
1	B	353	GLY	15.3
1	D	278	ILE	15.3
1	D	192	ASP	15.3
1	A	377	LEU	15.3
1	A	120	ILE	15.3
1	B	145	GLY	15.3
1	D	171	GLY	15.3
1	B	122	ILE	15.2
1	A	344	THR	15.2
1	A	112	LEU	15.2
1	A	118	HIS	15.2
1	D	301	GLY	15.1
1	D	44	ASP	15.1
1	A	98	GLY	15.1
1	A	135	VAL	15.1
1	D	330	VAL	15.1
1	A	213	LEU	15.1
1	D	204	LEU	15.1
1	D	312	ASN	15.1
1	C	271	GLU	15.1
1	D	324	PHE	15.0
1	D	40	GLY	15.0
1	D	75	GLY	15.0
1	A	352	TRP	15.0
1	A	28	VAL	14.9
1	A	181	ALA	14.9
1	D	287	HIS	14.9
1	A	314	LEU	14.9
1	D	311	GLY	14.9
1	A	161	LEU	14.8
1	D	273	LEU	14.8
1	D	293	SER	14.8
1	D	36	VAL	14.8
1	D	206	LEU	14.7
1	D	299	GLY	14.7
1	A	39	TRP	14.7
1	A	107	ASP	14.7
1	A	291	LEU	14.7
1	A	113	PRO	14.7
1	A	355	GLY	14.7
1	A	285	TRP	14.7
1	D	48	GLY	14.7

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Mol	Chain	Res	Type	RSRZ
1	D	139	GLY	14.7
1	D	297	LEU	14.7
1	A	169	PHE	14.6
1	D	255	GLN	14.6
1	C	221	THR	14.6
1	A	69	ILE	14.6
1	D	199	GLY	14.6
1	A	193	LEU	14.5
1	A	278	ILE	14.5
1	A	87	MET	14.5
1	A	236	THR	14.5
1	A	275	ASN	14.5
1	B	82	TYR	14.5
1	A	139	GLY	14.5
1	A	191	GLY	14.5
1	A	322	VAL	14.5
1	B	380	ASP	14.4
1	A	17	VAL	14.4
1	B	35	ILE	14.4
1	A	369	ASN	14.4
1	D	122	ILE	14.4
1	D	201	TYR	14.4
1	C	320	VAL	14.4
1	D	221	THR	14.3
1	A	334	SER	14.3
1	A	187	VAL	14.3
1	D	352	TRP	14.3
1	D	314	LEU	14.3
1	B	134	ALA	14.2
1	A	374	ILE	14.2
1	D	111	PRO	14.2
1	B	363	GLY	14.2
1	D	168	ALA	14.2
1	A	320	VAL	14.2
1	D	41	ARG	14.1
1	D	237	ILE	14.1
1	A	365	SER	14.1
1	A	270	LEU	14.1
1	D	238	SER	14.1
1	A	175	LYS	14.1
1	A	76	ALA	14.1
1	A	265	LEU	14.1

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Mol	Chain	Res	Type	RSRZ
1	D	85	SER	14.1
1	A	330	VAL	14.0
1	C	348	ASN	14.0
1	A	108	LEU	14.0
1	A	194	TYR	14.0
1	C	370	PHE	14.0
1	D	156	ASP	14.0
1	A	110	THR	14.0
1	D	305	PHE	14.0
1	D	366	VAL	14.0
1	A	58	PRO	14.0
1	C	14	PRO	14.0
1	A	254	GLY	14.0
1	B	93	GLY	14.0
1	A	341	LEU	13.9
1	D	220	SER	13.9
1	D	113	PRO	13.9
1	C	282	SER	13.9
1	B	28	VAL	13.9
1	B	87	MET	13.9
1	B	218	VAL	13.9
1	D	333	VAL	13.8
1	B	79	THR	13.8
1	D	371	PRO	13.8
1	A	261	LEU	13.8
1	B	31	LEU	13.8
1	C	317	CYS	13.8
1	D	190	ASP	13.8
1	D	310	VAL	13.7
1	A	268	HIS	13.7
1	B	346	ARG	13.7
1	D	59	THR	13.7
1	B	243	GLY	13.6
1	D	315	ASP	13.6
1	C	360	LEU	13.6
1	C	246	TYR	13.6
1	D	295	GLY	13.6
1	A	251	SER	13.6
1	D	133	LEU	13.6
1	D	303	ASN	13.6
1	D	367	ASP	13.6
1	A	61	LEU	13.6

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Mol	Chain	Res	Type	RSRZ
1	A	354	ARG	13.6
1	D	39	TRP	13.5
1	A	141	VAL	13.5
1	C	308	VAL	13.5
1	A	271	GLU	13.5
1	A	97	PHE	13.5
1	A	269	LYS	13.5
1	B	366	VAL	13.5
1	A	83	SER	13.5
1	D	285	TRP	13.4
1	D	377	LEU	13.4
1	A	229	VAL	13.4
1	D	28	VAL	13.4
1	C	323	ARG	13.4
1	D	354	ARG	13.4
1	D	89	VAL	13.4
1	A	152	LEU	13.4
1	C	347	ASN	13.4
1	C	266	ILE	13.4
1	A	127	CYS	13.3
1	D	242	SER	13.3
1	B	376	ALA	13.3
1	A	106	SER	13.3
1	D	378	SER	13.3
1	A	323	ARG	13.3
1	D	320	VAL	13.2
1	D	155	GLY	13.2
1	B	189	GLU	13.2
1	A	351	ALA	13.2
1	D	90	TYR	13.2
1	D	132	CYS	13.2
1	B	371	PRO	13.2
1	A	196	TRP	13.1
1	A	297	LEU	13.1
1	D	363	GLY	13.1
1	A	47	LEU	13.1
1	A	233	TRP	13.1
1	D	198	TRP	13.1
1	A	279	SER	13.1
1	B	169	PHE	13.1
1	A	117	LEU	13.1
1	D	69	ILE	13.1

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Mol	Chain	Res	Type	RSRZ
1	A	136	THR	13.1
1	D	370	PHE	13.1
1	B	241	TYR	13.0
1	D	180	GLY	13.0
1	C	313	ASN	13.0
1	D	323	ARG	13.0
1	B	47	LEU	13.0
1	B	266	ILE	13.0
1	D	355	GLY	13.0
1	D	92	TRP	13.0
1	D	246	TYR	13.0
1	A	277	PHE	13.0
1	B	370	PHE	13.0
1	A	66	GLY	13.0
1	A	249	GLY	13.0
1	A	250	TRP	13.0
1	D	84	GLN	13.0
1	D	338	ARG	13.0
1	D	368	ARG	13.0
1	A	133	LEU	13.0
1	C	305	PHE	13.0
1	A	240	SER	12.9
1	A	18	LEU	12.9
1	B	64	LEU	12.9
1	A	309	GLY	12.9
1	A	373	ILE	12.9
1	B	121	ARG	12.9
1	C	324	PHE	12.9
1	A	32	SER	12.9
1	D	379	VAL	12.9
1	C	59	THR	12.9
1	C	344	THR	12.9
1	D	274	SER	12.9
1	B	254	GLY	12.9
1	A	121	ARG	12.9
1	A	168	ALA	12.9
1	D	33	GLY	12.9
1	D	80	VAL	12.8
1	A	288	THR	12.8
1	D	325	PRO	12.8
1	B	85	SER	12.8
1	A	370	PHE	12.8

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Mol	Chain	Res	Type	RSRZ
1	D	42	GLY	12.8
1	C	152	LEU	12.8
1	C	157	THR	12.8
1	B	65	ASP	12.8
1	A	197	GLY	12.8
1	A	219	THR	12.8
1	B	70	VAL	12.8
1	B	80	VAL	12.8
1	A	298	TYR	12.7
1	A	328	GLN	12.7
1	C	362	ILE	12.7
1	A	257	GLY	12.7
1	D	161	LEU	12.7
1	A	56	PRO	12.7
1	C	162	VAL	12.7
1	A	31	LEU	12.6
1	A	357	ASN	12.6
1	D	251	SER	12.6
1	A	89	VAL	12.6
1	D	19	ILE	12.6
1	A	217	ARG	12.6
1	A	95	GLY	12.6
1	D	347	ASN	12.6
1	D	348	ASN	12.6
1	D	291	LEU	12.6
1	A	326	ASP	12.6
1	B	204	LEU	12.6
1	A	84	GLN	12.5
1	A	125	ILE	12.5
1	D	343	VAL	12.5
1	D	275	ASN	12.5
1	A	167	GLN	12.5
1	A	50	GLY	12.5
1	C	278	ILE	12.5
1	A	131	HIS	12.5
1	A	367	ASP	12.5
1	B	192	ASP	12.5
1	A	116	ALA	12.5
1	B	375	GLU	12.5
1	A	287	HIS	12.5
1	B	20	ILE	12.5
1	C	366	VAL	12.5

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Mol	Chain	Res	Type	RSRZ
1	B	58	PRO	12.5
1	C	154	LEU	12.5
1	B	335	CYS	12.4
1	A	310	VAL	12.4
1	B	42	GLY	12.4
1	B	68	GLN	12.4
1	D	97	PHE	12.4
1	D	277	PHE	12.4
1	A	253	TYR	12.4
1	C	64	LEU	12.4
1	D	263	ASP	12.4
1	D	229	VAL	12.4
1	D	134	ALA	12.3
1	B	172	ILE	12.3
1	D	365	SER	12.3
1	D	31	LEU	12.3
1	A	343	VAL	12.3
1	A	379	VAL	12.3
1	C	17	VAL	12.3
1	D	357	ASN	12.3
1	B	265	LEU	12.3
1	D	270	LEU	12.3
1	A	46	GLN	12.3
1	A	207	GLY	12.3
1	B	170	GLU	12.2
1	B	105	SER	12.2
1	A	223	GLY	12.2
1	C	18	LEU	12.2
1	D	112	LEU	12.2
1	B	91	SER	12.2
1	B	274	SER	12.2
1	C	237	ILE	12.2
1	B	301	GLY	12.2
1	D	241	TYR	12.2
1	A	166	ILE	12.2
1	D	281	ILE	12.2
1	C	133	LEU	12.2
1	D	61	LEU	12.2
1	C	15	ARG	12.1
1	A	91	SER	12.1
1	B	57	SER	12.1
1	A	137	MET	12.1

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Mol	Chain	Res	Type	RSRZ
1	D	253	TYR	12.1
1	B	310	VAL	12.1
1	D	100	LEU	12.1
1	C	327	ASP	12.1
1	D	148	GLN	12.1
1	A	222	GLY	12.1
1	A	362	ILE	12.1
1	C	33	GLY	12.1
1	C	301	GLY	12.1
1	D	300	TRP	12.1
1	D	329	LYS	12.1
1	A	134	ALA	12.1
1	C	275	ASN	12.1
1	A	79	THR	12.1
1	A	364	GLU	12.0
1	A	348	ASN	12.0
1	A	190	ASP	12.0
1	D	327	ASP	12.0
1	A	258	HIS	12.0
1	A	220	SER	12.0
1	D	240	SER	12.0
1	D	350	PHE	12.0
1	B	69	ILE	12.0
1	A	55	ARG	11.9
1	A	90	TYR	11.9
1	D	356	THR	11.9
1	A	260	ASP	11.9
1	A	86	GLY	11.9
1	A	311	GLY	11.9
1	D	127	CYS	11.9
1	D	276	SER	11.9
1	D	29	ALA	11.9
1	B	196	TRP	11.9
1	A	158	GLU	11.9
1	B	278	ILE	11.8
1	A	226	MET	11.8
1	A	363	GLY	11.8
1	B	37	CYS	11.8
1	C	37	CYS	11.8
1	A	94	TRP	11.8
1	D	46	GLN	11.8
1	C	254	GLY	11.8

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Mol	Chain	Res	Type	RSRZ
1	D	188	THR	11.8
1	A	173	ARG	11.8
1	C	123	LYS	11.8
1	D	76	ALA	11.8
1	D	123	LYS	11.8
1	A	154	LEU	11.8
1	D	17	VAL	11.8
1	B	194	TYR	11.8
1	B	51	ASP	11.8
1	B	118	HIS	11.8
1	D	282	SER	11.8
1	C	343	VAL	11.8
1	A	157	THR	11.7
1	A	209	ARG	11.7
1	B	217	ARG	11.7
1	D	120	ILE	11.7
1	A	92	TRP	11.7
1	D	72	VAL	11.7
1	A	16	LYS	11.7
1	D	294	ASP	11.7
1	D	257	GLY	11.7
1	D	58	PRO	11.7
1	D	296	LYS	11.7
1	C	261	LEU	11.7
1	A	159	ASP	11.6
1	C	244	ALA	11.6
1	A	27	SER	11.6
1	A	252	LYS	11.6
1	A	292	THR	11.6
1	A	300	TRP	11.6
1	A	101	GLY	11.6
1	C	134	ALA	11.6
1	A	273	LEU	11.6
1	A	325	PRO	11.6
1	B	219	THR	11.6
1	A	212	ARG	11.6
1	A	302	TRP	11.6
1	B	275	ASN	11.6
1	C	141	VAL	11.6
1	D	50	GLY	11.6
1	A	160	SER	11.5
1	D	15	ARG	11.5

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Mol	Chain	Res	Type	RSRZ
1	B	114	ILE	11.5
1	C	245	LEU	11.5
1	D	266	ILE	11.5
1	A	34	ASP	11.5
1	B	345	GLU	11.5
1	D	182	GLU	11.5
1	B	198	TRP	11.5
1	A	342	ALA	11.5
1	B	214	VAL	11.5
1	D	243	GLY	11.5
1	D	144	TRP	11.5
1	D	35	ILE	11.5
1	D	175	LYS	11.5
1	C	187	VAL	11.5
1	D	286	ARG	11.5
1	D	181	ALA	11.5
1	D	216	GLU	11.5
1	B	166	ILE	11.5
1	A	225	LYS	11.4
1	B	225	LYS	11.4
1	D	140	GLU	11.4
1	B	221	THR	11.4
1	C	356	THR	11.4
1	B	330	VAL	11.4
1	A	171	GLY	11.4
1	D	118	HIS	11.4
1	D	103	GLY	11.4
1	A	208	ASP	11.4
1	A	221	THR	11.4
1	D	290	ALA	11.4
1	D	373	ILE	11.4
1	A	375	GLU	11.4
1	D	269	LYS	11.3
1	A	45	GLY	11.3
1	D	249	GLY	11.3
1	D	326	ASP	11.3
1	D	189	GLU	11.3
1	D	262	GLU	11.3
1	B	213	LEU	11.3
1	C	222	GLY	11.3
1	A	321	GLN	11.3
1	A	371	PRO	11.3

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Mol	Chain	Res	Type	RSRZ
1	B	73	THR	11.3
1	A	345	GLU	11.3
1	D	224	GLU	11.3
1	B	272	ALA	11.3
1	A	239	VAL	11.3
1	B	137	MET	11.2
1	A	366	VAL	11.2
1	B	188	THR	11.2
1	B	140	GLU	11.2
1	B	229	VAL	11.2
1	D	228	MET	11.2
1	D	169	PHE	11.2
1	B	92	TRP	11.2
1	B	290	ALA	11.2
1	C	168	ALA	11.2
1	A	347	ASN	11.2
1	D	346	ARG	11.2
1	A	130	SER	11.2
1	C	377	LEU	11.2
1	A	144	TRP	11.2
1	D	313	ASN	11.2
1	A	215	PRO	11.1
1	A	88	GLU	11.1
1	A	24	ALA	11.1
1	A	244	ALA	11.1
1	C	306	GLY	11.1
1	C	312	ASN	11.1
1	D	337	TRP	11.1
1	C	82	TYR	11.1
1	D	328	GLN	11.1
1	A	192	ASP	11.1
1	B	66	GLY	11.1
1	B	108	LEU	11.1
1	D	82	TYR	11.1
1	D	126	ALA	11.1
1	D	272	ALA	11.1
1	B	222	GLY	11.0
1	D	101	GLY	11.0
1	D	361	GLY	11.0
1	A	183	HIS	11.0
1	D	125	ILE	11.0
1	A	162	VAL	11.0

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Mol	Chain	Res	Type	RSRZ
1	B	309	GLY	11.0
1	C	207	GLY	11.0
1	D	358	GLY	11.0
1	A	264	HIS	11.0
1	D	110	THR	11.0
1	A	48	GLY	11.0
1	D	43	GLU	11.0
1	B	215	PRO	11.0
1	D	231	CYS	11.0
1	B	368	ARG	11.0
1	B	328	GLN	11.0
1	A	299	GLY	11.0
1	B	295	GLY	11.0
1	A	201	TYR	11.0
1	B	81	ALA	11.0
1	A	358	GLY	10.9
1	B	230	ALA	10.9
1	D	94	TRP	10.9
1	A	156	ASP	10.9
1	D	87	MET	10.9
1	D	130	SER	10.9
1	A	353	GLY	10.9
1	A	381	GLY	10.9
1	B	201	TYR	10.9
1	D	247	THR	10.9
1	B	119	GLY	10.9
1	D	178	ALA	10.9
1	A	43	GLU	10.9
1	B	327	ASP	10.9
1	D	104	ASN	10.9
1	A	163	PRO	10.9
1	C	69	ILE	10.8
1	B	354	ARG	10.8
1	B	133	LEU	10.8
1	D	341	LEU	10.8
1	B	313	ASN	10.8
1	B	97	PHE	10.8
1	A	140	GLU	10.8
1	D	280	GLN	10.8
1	B	112	LEU	10.8
1	A	248	TYR	10.8
1	C	196	TRP	10.8

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Mol	Chain	Res	Type	RSRZ
1	B	171	GLY	10.8
1	D	45	GLY	10.8
1	C	235	HIS	10.8
1	D	121	ARG	10.8
1	D	288	THR	10.8
1	C	281	ILE	10.8
1	C	350	PHE	10.8
1	A	337	TRP	10.8
1	B	144	TRP	10.8
1	D	114	ILE	10.8
1	B	256	LEU	10.7
1	D	73	THR	10.7
1	A	75	GLY	10.7
1	A	164	GLN	10.7
1	A	349	VAL	10.7
1	B	152	LEU	10.7
1	A	339	HIS	10.7
1	B	34	ASP	10.7
1	B	240	SER	10.7
1	D	83	SER	10.7
1	D	22	ALA	10.7
1	A	335	CYS	10.7
1	A	206	LEU	10.7
1	C	270	LEU	10.7
1	B	45	GLY	10.6
1	A	49	HIS	10.6
1	A	78	HIS	10.6
1	B	86	GLY	10.6
1	A	333	VAL	10.6
1	D	108	LEU	10.6
1	B	250	TRP	10.6
1	C	250	TRP	10.6
1	D	150	GLY	10.6
1	C	35	ILE	10.6
1	A	85	SER	10.6
1	D	376	ALA	10.6
1	A	267	PRO	10.6
1	B	202	GLY	10.6
1	D	147	ASN	10.6
1	A	62	SER	10.5
1	A	227	SER	10.5
1	C	378	SER	10.5

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Mol	Chain	Res	Type	RSRZ
1	B	18	LEU	10.5
1	A	281	ILE	10.5
1	B	232	GLY	10.5
1	C	284	GLY	10.5
1	B	30	LEU	10.5
1	B	271	GLU	10.5
1	D	235	HIS	10.5
1	B	120	ILE	10.5
1	B	109	PHE	10.5
1	C	111	PRO	10.5
1	D	254	GLY	10.5
1	D	193	LEU	10.5
1	D	332	GLN	10.5
1	A	218	VAL	10.4
1	A	150	GLY	10.4
1	D	66	GLY	10.4
1	B	245	LEU	10.4
1	D	196	TRP	10.4
1	D	340	THR	10.4
1	B	154	LEU	10.4
1	D	67	HIS	10.4
1	D	167	GLN	10.4
1	D	226	MET	10.4
1	D	197	GLY	10.4
1	D	267	PRO	10.4
1	D	81	ALA	10.4
1	A	53	GLU	10.3
1	C	267	PRO	10.3
1	D	184	THR	10.3
1	A	305	PHE	10.3
1	D	57	SER	10.3
1	A	165	LYS	10.3
1	D	252	LYS	10.3
1	A	324	PHE	10.3
1	C	30	LEU	10.3
1	D	60	GLN	10.3
1	D	306	GLY	10.3
1	D	157	THR	10.3
1	D	63	ALA	10.3
1	C	97	PHE	10.3
1	C	277	PHE	10.3
1	A	124	GLN	10.3

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Mol	Chain	Res	Type	RSRZ
1	B	94	TRP	10.2
1	C	121	ARG	10.2
1	C	346	ARG	10.2
1	B	103	GLY	10.2
1	B	205	GLY	10.2
1	B	246	TYR	10.2
1	C	110	THR	10.2
1	C	135	VAL	10.2
1	D	268	HIS	10.2
1	D	353	GLY	10.2
1	D	248	TYR	10.2
1	B	110	THR	10.2
1	B	344	THR	10.2
1	D	109	PHE	10.2
1	B	141	VAL	10.2
1	A	37	CYS	10.2
1	B	56	PRO	10.2
1	C	380	ASP	10.2
1	B	365	SER	10.2
1	B	291	LEU	10.1
1	B	349	VAL	10.1
1	A	57	SER	10.1
1	A	378	SER	10.1
1	B	25	SER	10.1
1	D	55	ARG	10.1
1	B	237	ILE	10.1
1	A	186	ALA	10.1
1	C	169	PHE	10.1
1	C	330	VAL	10.1
1	D	205	GLY	10.1
1	A	71	SER	10.1
1	C	253	TYR	10.1
1	A	170	GLU	10.1
1	A	179	ALA	10.1
1	A	185	ALA	10.1
1	B	372	LYS	10.1
1	A	41	ARG	10.1
1	A	151	GLN	10.1
1	A	359	GLN	10.1
1	B	15	ARG	10.1
1	D	179	ALA	10.1
1	A	304	LYS	10.1

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Mol	Chain	Res	Type	RSRZ
1	A	259	GLY	10.1
1	D	86	GLY	10.1
1	C	125	ILE	10.0
1	C	186	ALA	10.0
1	C	241	TYR	10.0
1	C	368	ARG	10.0
1	A	60	GLN	10.0
1	D	217	ARG	10.0
1	D	166	ILE	10.0
1	B	159	ASP	10.0
1	D	54	ASP	10.0
1	D	77	ASP	10.0
1	A	123	LYS	10.0
1	D	74	CYS	10.0
1	A	202	GLY	10.0
1	D	194	TYR	10.0
1	C	258	HIS	10.0
1	C	192	ASP	9.9
1	C	81	ALA	9.9
1	C	223	GLY	9.9
1	D	213	LEU	9.9
1	C	115	LYS	9.9
1	A	22	ALA	9.9
1	C	42	GLY	9.9
1	C	299	GLY	9.9
1	D	64	LEU	9.9
1	A	103	GLY	9.9
1	A	237	ILE	9.9
1	C	48	GLY	9.9
1	A	52	ALA	9.9
1	B	100	LEU	9.9
1	A	294	ASP	9.8
1	D	380	ASP	9.8
1	C	203	ASN	9.8
1	B	50	GLY	9.8
1	C	285	TRP	9.8
1	A	276	SER	9.8
1	D	372	LYS	9.8
1	D	170	GLU	9.8
1	B	302	TRP	9.8
1	D	30	LEU	9.8
1	B	113	PRO	9.8

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Mol	Chain	Res	Type	RSRZ
1	B	173	ARG	9.8
1	D	173	ARG	9.8
1	D	26	HIS	9.8
1	D	203	ASN	9.8
1	D	336	GLY	9.8
1	D	91	SER	9.8
1	A	73	THR	9.8
1	A	331	VAL	9.7
1	A	153	GLY	9.7
1	A	105	SER	9.7
1	D	38	SER	9.7
1	B	281	ILE	9.7
1	D	339	HIS	9.7
1	B	342	ALA	9.7
1	A	51	ASP	9.7
1	C	120	ILE	9.7
1	D	151	GLN	9.7
1	A	356	THR	9.7
1	B	352	TRP	9.7
1	B	355	GLY	9.7
1	B	84	GLN	9.7
1	D	245	LEU	9.7
1	A	307	GLN	9.6
1	D	271	GLU	9.6
1	D	117	LEU	9.6
1	D	304	LYS	9.6
1	B	101	GLY	9.6
1	C	336	GLY	9.6
1	A	263	ASP	9.6
1	C	118	HIS	9.6
1	B	136	THR	9.6
1	A	295	GLY	9.6
1	A	242	SER	9.6
1	A	332	GLN	9.6
1	B	62	SER	9.6
1	A	315	ASP	9.6
1	B	39	TRP	9.6
1	D	265	LEU	9.6
1	C	276	SER	9.6
1	B	324	PHE	9.6
1	B	316	GLN	9.5
1	C	280	GLN	9.5

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Mol	Chain	Res	Type	RSRZ
1	A	74	CYS	9.5
1	A	234	ARG	9.5
1	B	270	LEU	9.5
1	B	19	ILE	9.5
1	A	128	GLY	9.5
1	B	149	ASN	9.5
1	B	96	ASP	9.5
1	D	208	ASP	9.5
1	B	334	SER	9.5
1	D	71	SER	9.5
1	B	329	LYS	9.5
1	D	289	MET	9.5
1	B	29	ALA	9.5
1	C	354	ARG	9.5
1	C	219	THR	9.5
1	D	115	LYS	9.5
1	D	165	LYS	9.5
1	C	379	VAL	9.4
1	B	190	ASP	9.4
1	D	18	LEU	9.4
1	D	107	ASP	9.4
1	B	157	THR	9.4
1	B	311	GLY	9.4
1	B	336	GLY	9.4
1	C	357	ASN	9.4
1	D	316	GLN	9.4
1	A	146	ARG	9.4
1	A	296	LYS	9.4
1	B	261	LEU	9.4
1	D	79	THR	9.4
1	B	350	PHE	9.4
1	D	322	VAL	9.4
1	B	127	CYS	9.4
1	B	138	GLU	9.4
1	A	205	GLY	9.3
1	B	38	SER	9.3
1	C	238	SER	9.3
1	C	73	THR	9.3
1	D	93	GLY	9.3
1	D	153	GLY	9.3
1	A	286	ARG	9.3
1	A	115	LYS	9.3

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Mol	Chain	Res	Type	RSRZ
1	A	132	CYS	9.3
1	A	238	SER	9.3
1	C	337	TRP	9.3
1	A	21	SER	9.3
1	B	314	LEU	9.3
1	C	177	VAL	9.3
1	B	131	HIS	9.3
1	D	351	ALA	9.3
1	C	236	THR	9.3
1	C	218	VAL	9.3
1	D	162	VAL	9.3
1	C	32	SER	9.2
1	B	369	ASN	9.2
1	B	273	LEU	9.2
1	D	131	HIS	9.2
1	D	261	LEU	9.2
1	D	176	MET	9.2
1	D	27	SER	9.2
1	D	225	LYS	9.2
1	D	95	GLY	9.2
1	A	247	THR	9.2
1	D	239	VAL	9.2
1	B	60	GLN	9.2
1	C	96	ASP	9.2
1	B	175	LYS	9.2
1	C	45	GLY	9.2
1	B	323	ARG	9.2
1	B	187	VAL	9.2
1	D	65	ASP	9.2
1	D	187	VAL	9.2
1	A	303	ASN	9.2
1	A	184	THR	9.1
1	D	137	MET	9.1
1	A	306	GLY	9.1
1	D	145	GLY	9.1
1	B	317	CYS	9.1
1	C	231	CYS	9.1
1	B	373	ILE	9.1
1	B	283	GLY	9.1
1	A	77	ASP	9.1
1	D	292	THR	9.1
1	B	89	VAL	9.1

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Mol	Chain	Res	Type	RSRZ
1	A	312	ASN	9.1
1	A	111	PRO	9.1
1	B	249	GLY	9.1
1	C	283	GLY	9.1
1	D	230	ALA	9.1
1	C	365	SER	9.0
1	A	372	LYS	9.0
1	A	346	ARG	9.0
1	A	148	GLN	9.0
1	B	61	LEU	9.0
1	C	167	GLN	9.0
1	C	204	LEU	9.0
1	C	220	SER	9.0
1	A	232	GLY	9.0
1	D	20	ILE	9.0
1	B	67	HIS	9.0
1	B	206	LEU	9.0
1	C	215	PRO	9.0
1	C	326	ASP	9.0
1	D	234	ARG	9.0
1	D	149	ASN	9.0
1	D	233	TRP	9.0
1	C	329	LYS	9.0
1	B	364	GLU	9.0
1	D	158	GLU	9.0
1	A	338	ARG	9.0
1	C	68	GLN	8.9
1	B	277	PHE	8.9
1	B	24	ALA	8.9
1	B	377	LEU	8.9
1	C	300	TRP	8.9
1	A	231	CYS	8.9
1	B	55	ARG	8.9
1	B	223	GLY	8.9
1	D	135	VAL	8.9
1	C	142	GLN	8.9
1	C	138	GLU	8.9
1	B	44	ASP	8.9
1	B	280	GLN	8.9
1	D	141	VAL	8.9
1	D	116	ALA	8.9
1	C	47	LEU	8.9

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Mol	Chain	Res	Type	RSRZ
1	B	167	GLN	8.9
1	C	205	GLY	8.9
1	D	218	VAL	8.9
1	A	210	THR	8.9
1	B	182	GLU	8.9
1	B	340	THR	8.9
1	D	334	SER	8.8
1	A	280	GLN	8.8
1	C	249	GLY	8.8
1	A	67	HIS	8.8
1	D	258	HIS	8.8
1	C	92	TRP	8.8
1	B	155	GLY	8.8
1	D	319	PRO	8.8
1	B	125	ILE	8.8
1	C	19	ILE	8.8
1	B	341	LEU	8.8
1	C	264	HIS	8.8
1	C	41	ARG	8.8
1	C	145	GLY	8.8
1	D	212	ARG	8.8
1	B	210	THR	8.7
1	B	378	SER	8.7
1	B	362	ILE	8.7
1	D	88	GLU	8.7
1	B	116	ALA	8.7
1	B	168	ALA	8.7
1	B	244	ALA	8.7
1	D	223	GLY	8.7
1	C	349	VAL	8.7
1	D	210	THR	8.7
1	D	37	CYS	8.7
1	B	88	GLU	8.7
1	B	279	SER	8.7
1	D	143	SER	8.7
1	C	319	PRO	8.7
1	B	269	LYS	8.7
1	D	16	LYS	8.7
1	A	293	SER	8.7
1	C	85	SER	8.7
1	D	68	GLN	8.7
1	D	56	PRO	8.7

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Mol	Chain	Res	Type	RSRZ
1	A	224	GLU	8.7
1	A	129	ASP	8.7
1	C	80	VAL	8.7
1	A	126	ALA	8.6
1	C	225	LYS	8.6
1	C	198	TRP	8.6
1	A	143	SER	8.6
1	D	32	SER	8.6
1	C	84	GLN	8.6
1	C	358	GLY	8.6
1	B	179	ALA	8.6
1	C	291	LEU	8.6
1	C	144	TRP	8.6
1	C	274	SER	8.6
1	C	119	GLY	8.6
1	D	283	GLY	8.6
1	D	102	HIS	8.6
1	A	104	ASN	8.6
1	B	262	GLU	8.6
1	B	197	GLY	8.6
1	D	163	PRO	8.5
1	C	112	LEU	8.5
1	B	305	PHE	8.5
1	C	70	VAL	8.5
1	D	317	CYS	8.5
1	B	174	ILE	8.5
1	C	374	ILE	8.5
1	B	49	HIS	8.5
1	A	289	MET	8.5
1	C	314	LEU	8.5
1	C	136	THR	8.5
1	D	222	GLY	8.5
1	A	177	VAL	8.5
1	C	20	ILE	8.5
1	A	272	ALA	8.5
1	B	150	GLY	8.5
1	B	239	VAL	8.5
1	B	164	GLN	8.5
1	C	185	ALA	8.5
1	A	329	LYS	8.5
1	B	356	THR	8.5
1	B	191	GLY	8.4

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Mol	Chain	Res	Type	RSRZ
1	B	343	VAL	8.4
1	D	53	GLU	8.4
1	C	302	TRP	8.4
1	A	255	GLN	8.4
1	D	49	HIS	8.4
1	D	236	THR	8.4
1	A	99	ARG	8.4
1	B	294	ASP	8.4
1	C	311	GLY	8.4
1	D	260	ASP	8.4
1	C	248	TYR	8.4
1	D	342	ALA	8.4
1	C	233	TRP	8.4
1	A	200	ARG	8.4
1	C	260	ASP	8.4
1	D	98	GLY	8.4
1	D	259	GLY	8.4
1	C	325	PRO	8.3
1	C	342	ALA	8.3
1	D	307	GLN	8.3
1	D	200	ARG	8.3
1	C	247	THR	8.3
1	B	135	VAL	8.3
1	B	347	ASN	8.3
1	C	206	LEU	8.3
1	C	363	GLY	8.3
1	C	39	TRP	8.3
1	D	160	SER	8.3
1	B	126	ALA	8.3
1	C	24	ALA	8.3
1	D	211	ASP	8.3
1	C	209	ARG	8.3
1	C	54	ASP	8.3
1	D	34	ASP	8.3
1	B	374	ILE	8.3
1	D	99	ARG	8.2
1	A	228	MET	8.2
1	A	72	VAL	8.2
1	B	351	ALA	8.2
1	B	292	THR	8.2
1	B	297	LEU	8.2
1	A	25	SER	8.2

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Mol	Chain	Res	Type	RSRZ
1	C	240	SER	8.2
1	B	285	TRP	8.2
1	B	184	THR	8.2
1	C	201	TYR	8.2
1	C	321	GLN	8.2
1	C	74	CYS	8.2
1	C	58	PRO	8.2
1	C	173	ARG	8.2
1	C	122	ILE	8.2
1	C	213	LEU	8.2
1	D	232	GLY	8.2
1	D	335	CYS	8.2
1	B	264	HIS	8.2
1	B	260	ASP	8.1
1	D	146	ARG	8.1
1	B	320	VAL	8.1
1	C	188	THR	8.1
1	D	78	HIS	8.1
1	A	96	ASP	8.1
1	D	345	GLU	8.1
1	C	174	ILE	8.1
1	D	105	SER	8.1
1	B	41	ARG	8.1
1	B	129	ASP	8.1
1	C	268	HIS	8.1
1	B	307	GLN	8.1
1	C	194	TYR	8.1
1	C	165	LYS	8.1
1	A	23	GLY	8.0
1	C	184	THR	8.0
1	D	227	SER	8.0
1	B	300	TRP	8.0
1	A	42	GLY	8.0
1	C	178	ALA	8.0
1	C	224	GLU	8.0
1	A	65	ASP	8.0
1	B	83	SER	8.0
1	B	276	SER	8.0
1	B	148	GLN	8.0
1	B	22	ALA	8.0
1	A	230	ALA	8.0
1	C	57	SER	8.0

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Mol	Chain	Res	Type	RSRZ
1	B	147	ASN	7.9
1	C	332	GLN	7.9
1	D	318	SER	7.9
1	C	217	ARG	7.9
1	D	209	ARG	7.9
1	C	364	GLU	7.9
1	A	319	PRO	7.9
1	B	95	GLY	7.9
1	C	372	LYS	7.9
1	B	90	TYR	7.9
1	C	170	GLU	7.9
1	D	183	HIS	7.9
1	C	148	GLN	7.9
1	D	359	GLN	7.9
1	C	355	GLY	7.9
1	A	54	ASP	7.9
1	A	317	CYS	7.9
1	B	326	ASP	7.9
1	A	282	SER	7.9
1	A	147	ASN	7.9
1	A	368	ARG	7.8
1	B	227	SER	7.8
1	B	17	VAL	7.8
1	B	162	VAL	7.8
1	B	48	GLY	7.8
1	B	208	ASP	7.8
1	C	289	MET	7.8
1	D	284	GLY	7.8
1	B	32	SER	7.8
1	C	105	SER	7.8
1	C	127	CYS	7.8
1	C	316	GLN	7.8
1	A	178	ALA	7.8
1	C	89	VAL	7.8
1	B	16	LYS	7.8
1	C	351	ALA	7.7
1	B	77	ASP	7.7
1	C	65	ASP	7.7
1	D	142	GLN	7.7
1	C	91	SER	7.7
1	C	227	SER	7.7
1	A	262	GLU	7.7

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Mol	Chain	Res	Type	RSRZ
1	C	208	ASP	7.7
1	C	256	LEU	7.7
1	C	71	SER	7.7
1	B	33	GLY	7.7
1	B	139	GLY	7.7
1	B	361	GLY	7.7
1	C	338	ARG	7.7
1	A	182	GLU	7.6
1	A	176	MET	7.6
1	B	52	ALA	7.6
1	D	52	ALA	7.6
1	B	338	ARG	7.6
1	C	31	LEU	7.6
1	B	298	TYR	7.6
1	C	216	GLU	7.6
1	B	176	MET	7.6
1	D	202	GLY	7.6
1	B	308	VAL	7.6
1	B	195	GLY	7.6
1	C	334	SER	7.6
1	C	369	ASN	7.6
1	B	286	ARG	7.6
1	B	284	GLY	7.5
1	C	98	GLY	7.5
1	C	161	LEU	7.5
1	D	106	SER	7.5
1	C	229	VAL	7.5
1	D	138	GLU	7.5
1	C	226	MET	7.5
1	D	23	GLY	7.5
1	C	293	SER	7.5
1	B	177	VAL	7.5
1	C	139	GLY	7.5
1	B	63	ALA	7.5
1	C	76	ALA	7.5
1	B	339	HIS	7.5
1	A	142	GLN	7.5
1	C	46	GLN	7.5
1	D	129	ASP	7.4
1	A	26	HIS	7.4
1	A	235	HIS	7.4
1	C	304	LYS	7.4

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Mol	Chain	Res	Type	RSRZ
1	B	185	ALA	7.4
1	C	29	ALA	7.4
1	C	297	LEU	7.4
1	D	96	ASP	7.4
1	C	40	GLY	7.4
1	C	295	GLY	7.4
1	A	216	GLU	7.4
1	C	107	ASP	7.4
1	C	156	ASP	7.4
1	D	124	GLN	7.4
1	C	147	ASN	7.4
1	C	195	GLY	7.4
1	C	210	THR	7.4
1	C	303	ASN	7.3
1	C	191	GLY	7.3
1	D	191	GLY	7.3
1	C	287	HIS	7.3
1	B	267	PRO	7.3
1	B	228	MET	7.3
1	C	232	GLY	7.3
1	B	200	ARG	7.3
1	C	113	PRO	7.3
1	B	253	TYR	7.3
1	C	262	GLU	7.3
1	C	99	ARG	7.3
1	B	359	GLN	7.3
1	B	193	LEU	7.3
1	C	298	TYR	7.3
1	C	335	CYS	7.3
1	D	279	SER	7.3
1	C	376	ALA	7.2
1	C	150	GLY	7.2
1	B	158	GLU	7.2
1	C	333	VAL	7.2
1	A	102	HIS	7.2
1	C	175	LYS	7.2
1	B	337	TRP	7.2
1	A	283	GLY	7.2
1	B	43	GLU	7.2
1	B	146	ARG	7.2
1	C	353	GLY	7.2
1	B	296	LYS	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	336	GLY	7.1
1	C	151	GLN	7.1
1	C	273	LEU	7.1
1	C	373	ILE	7.1
1	A	203	ASN	7.1
1	C	190	ASP	7.1
1	D	159	ASP	7.1
1	C	359	GLN	7.1
1	B	325	PRO	7.1
1	B	117	LEU	7.1
1	B	123	LYS	7.1
1	B	255	GLN	7.1
1	D	164	GLN	7.1
1	C	94	TRP	7.0
1	C	108	LEU	7.0
1	B	104	ASN	7.0
1	B	165	LYS	7.0
1	B	242	SER	7.0
1	C	16	LYS	7.0
1	B	181	ALA	7.0
1	B	233	TRP	7.0
1	A	318	SER	7.0
1	A	243	GLY	7.0
1	B	75	GLY	7.0
1	D	264	HIS	7.0
1	B	142	GLN	7.0
1	C	100	LEU	6.9
1	D	369	ASN	6.9
1	B	315	ASP	6.9
1	C	269	LYS	6.9
1	B	226	MET	6.9
1	C	90	TYR	6.9
1	C	228	MET	6.9
1	B	23	GLY	6.9
1	B	235	HIS	6.9
1	D	219	THR	6.9
1	B	161	LEU	6.9
1	C	341	LEU	6.9
1	D	51	ASP	6.9
1	C	352	TRP	6.9
1	C	160	SER	6.9
1	D	21	SER	6.9

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Mol	Chain	Res	Type	RSRZ
1	C	93	GLY	6.9
1	B	71	SER	6.8
1	B	293	SER	6.8
1	B	348	ASN	6.8
1	C	78	HIS	6.8
1	B	186	ALA	6.8
1	C	214	VAL	6.8
1	B	130	SER	6.8
1	C	55	ARG	6.7
1	B	220	SER	6.7
1	B	163	PRO	6.7
1	A	180	GLY	6.7
1	C	36	VAL	6.6
1	C	86	GLY	6.6
1	B	209	ARG	6.6
1	B	74	CYS	6.6
1	C	294	ASP	6.6
1	C	265	LEU	6.6
1	D	25	SER	6.5
1	B	115	LYS	6.5
1	C	239	VAL	6.5
1	B	132	CYS	6.5
1	C	263	ASP	6.5
1	C	259	GLY	6.5
1	B	107	ASP	6.5
1	B	212	ARG	6.5
1	D	24	ALA	6.5
1	C	28	VAL	6.5
1	C	137	MET	6.5
1	B	203	ASN	6.5
1	B	251	SER	6.5
1	B	263	ASP	6.5
1	C	163	PRO	6.4
1	C	371	PRO	6.4
1	C	251	SER	6.4
1	C	87	MET	6.4
1	C	77	ASP	6.4
1	B	40	GLY	6.4
1	B	248	TYR	6.4
1	C	140	GLU	6.4
1	D	136	THR	6.4
1	B	282	SER	6.4

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Mol	Chain	Res	Type	RSRZ
1	C	279	SER	6.4
1	C	296	LYS	6.4
1	C	242	SER	6.3
1	C	288	THR	6.3
1	C	146	ARG	6.3
1	C	53	GLU	6.3
1	C	131	HIS	6.3
1	C	130	SER	6.3
1	C	286	ARG	6.3
1	B	143	SER	6.2
1	D	321	GLN	6.2
1	B	367	ASP	6.2
1	C	182	GLU	6.2
1	C	345	GLU	6.2
1	C	310	VAL	6.2
1	C	34	ASP	6.2
1	C	153	GLY	6.2
1	B	99	ARG	6.2
1	C	234	ARG	6.2
1	C	272	ALA	6.2
1	C	166	ILE	6.2
1	B	46	GLN	6.1
1	C	126	ALA	6.1
1	B	53	GLU	6.1
1	C	158	GLU	6.1
1	C	109	PHE	6.1
1	C	328	GLN	6.1
1	C	117	LEU	6.1
1	C	129	ASP	6.1
1	C	149	ASN	6.1
1	B	257	GLY	6.1
1	C	72	VAL	6.1
1	C	193	LEU	6.1
1	C	21	SER	6.1
1	B	236	THR	6.1
1	B	288	THR	6.1
1	B	224	GLU	6.0
1	B	151	GLN	6.0
1	B	247	THR	6.0
1	C	124	GLN	6.0
1	B	21	SER	6.0
1	C	102	HIS	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	321	GLN	6.0
1	C	176	MET	6.0
1	C	88	GLU	6.0
1	C	367	ASP	5.9
1	C	181	ALA	5.9
1	B	199	GLY	5.9
1	C	67	HIS	5.9
1	C	83	SER	5.9
1	B	156	ASP	5.9
1	C	200	ARG	5.9
1	B	102	HIS	5.9
1	C	339	HIS	5.9
1	B	289	MET	5.9
1	A	211	ASP	5.9
1	B	333	VAL	5.9
1	C	202	GLY	5.8
1	D	195	GLY	5.8
1	B	322	VAL	5.8
1	B	54	ASP	5.8
1	C	51	ASP	5.8
1	B	259	GLY	5.8
1	B	357	ASN	5.8
1	C	114	ILE	5.8
1	C	79	THR	5.8
1	B	106	SER	5.8
1	C	318	SER	5.8
1	B	78	HIS	5.7
1	C	22	ALA	5.6
1	C	197	GLY	5.6
1	C	189	GLU	5.6
1	B	178	ALA	5.6
1	B	238	SER	5.6
1	C	179	ALA	5.6
1	C	52	ALA	5.6
1	B	287	HIS	5.5
1	C	50	GLY	5.5
1	C	49	HIS	5.5
1	B	26	HIS	5.4
1	C	164	GLN	5.4
1	B	304	LYS	5.4
1	B	72	VAL	5.4
1	C	307	GLN	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	111	PRO	5.4
1	B	331	VAL	5.4
1	B	128	GLY	5.4
1	B	252	LYS	5.4
1	B	258	HIS	5.4
1	B	153	GLY	5.3
1	C	75	GLY	5.3
1	B	180	GLY	5.3
1	B	303	ASN	5.3
1	C	132	CYS	5.3
1	C	43	GLU	5.2
1	B	183	HIS	5.2
1	B	76	ALA	5.2
1	C	143	SER	5.2
1	C	211	ASP	5.2
1	B	268	HIS	5.2
1	B	211	ASP	5.2
1	C	159	ASP	5.1
1	C	116	ALA	5.1
1	B	124	GLN	5.1
1	B	306	GLY	5.1
1	B	234	ARG	5.0
1	B	216	GLU	5.0
1	C	212	ARG	5.0
1	C	62	SER	4.9
1	C	128	GLY	4.9
1	C	230	ALA	4.8
1	A	284	GLY	4.7
1	B	332	GLN	4.7
1	B	231	CYS	4.7
1	B	312	ASN	4.7
1	C	25	SER	4.7
1	C	292	THR	4.7
1	C	63	ALA	4.7
1	C	315	ASP	4.7
1	B	299	GLY	4.6
1	B	358	GLY	4.6
1	C	95	GLY	4.6
1	C	26	HIS	4.6
1	C	252	LYS	4.6
1	C	44	ASP	4.6
1	C	255	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	319	PRO	4.5
1	C	38	SER	4.5
1	C	103	GLY	4.3
1	C	23	GLY	4.2
1	C	180	GLY	4.2
1	C	199	GLY	4.2
1	C	61	LEU	4.2
1	C	104	ASN	4.1
1	C	60	GLN	4.1
1	C	340	THR	4.0
1	C	183	HIS	4.0
1	B	160	SER	3.9
1	B	318	SER	3.9
1	C	257	GLY	3.7
1	C	56	PRO	3.6
1	C	27	SER	3.6
1	C	106	SER	3.6
1	B	207	GLY	3.6
1	C	322	VAL	3.6
1	C	101	GLY	3.5
1	B	27	SER	3.5
1	C	155	GLY	3.3
1	C	66	GLY	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.