



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:59 PM GMT

PDB ID : 5D1Y
Title : Low resolution crystal structure of human ribonucleotide reductase alpha6 hexamer in complex with dATP
Authors : Ando, N.; Li, H.; Brignole, E.J.; Thompson, S.; McLaughlin, M.I.; Page, J.; Asturias, F.; Stubbe, J.; Drennan, C.L.
Deposited on : 2015-08-04
Resolution : 9.01 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

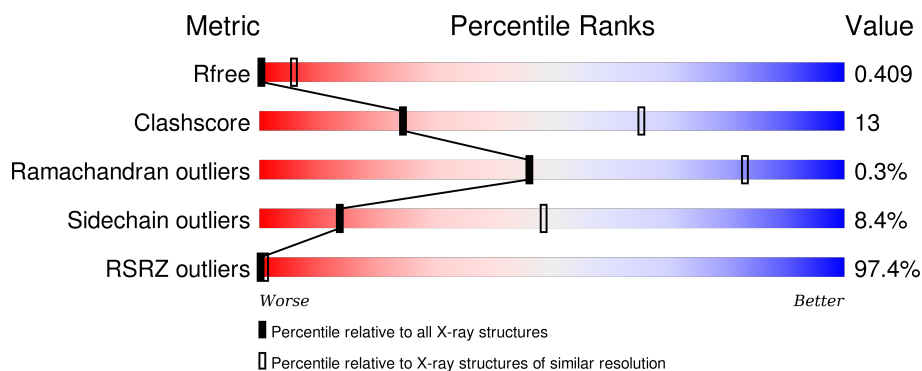
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 9.01 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}	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	812	<div> <div>85%</div> <div> <div>70%</div> <div>16%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	812	<div> <div>89%</div> <div> <div>73%</div> <div>16%</div> <div>•</div> <div>9%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11328 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 Ribonucleoside-diphosphate reductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	714	Total	C	N	O	S	0	0	0
			5577	3567	926	1052	32			
1	B	738	Total	C	N	O	S	0	0	0
			5751	3669	968	1080	34			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P23921
A	-18	GLY	-	expression tag	UNP P23921
A	-17	SER	-	expression tag	UNP P23921
A	-16	SER	-	expression tag	UNP P23921
A	-15	HIS	-	expression tag	UNP P23921
A	-14	HIS	-	expression tag	UNP P23921
A	-13	HIS	-	expression tag	UNP P23921
A	-12	HIS	-	expression tag	UNP P23921
A	-11	HIS	-	expression tag	UNP P23921
A	-10	HIS	-	expression tag	UNP P23921
A	-9	SER	-	expression tag	UNP P23921
A	-8	SER	-	expression tag	UNP P23921
A	-7	GLY	-	expression tag	UNP P23921
A	-6	LEU	-	expression tag	UNP P23921
A	-5	VAL	-	expression tag	UNP P23921
A	-4	PRO	-	expression tag	UNP P23921
A	-3	ARG	-	expression tag	UNP P23921
A	-2	GLY	-	expression tag	UNP P23921
A	-1	SER	-	expression tag	UNP P23921
A	0	HIS	-	expression tag	UNP P23921
B	-19	MET	-	initiating methionine	UNP P23921
B	-18	GLY	-	expression tag	UNP P23921
B	-17	SER	-	expression tag	UNP P23921
B	-16	SER	-	expression tag	UNP P23921
B	-15	HIS	-	expression tag	UNP P23921

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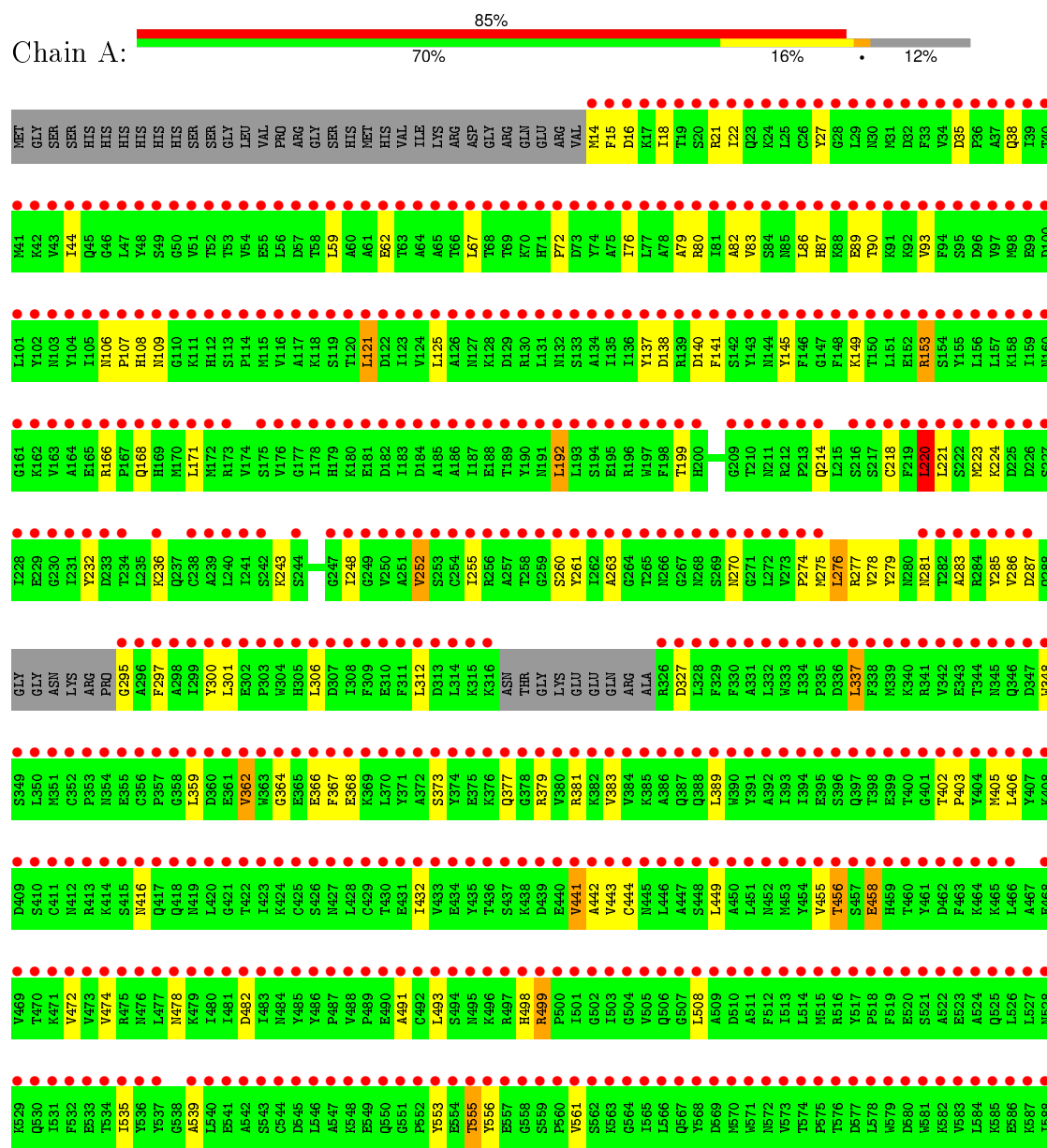
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P23921
B	-13	HIS	-	expression tag	UNP P23921
B	-12	HIS	-	expression tag	UNP P23921
B	-11	HIS	-	expression tag	UNP P23921
B	-10	HIS	-	expression tag	UNP P23921
B	-9	SER	-	expression tag	UNP P23921
B	-8	SER	-	expression tag	UNP P23921
B	-7	GLY	-	expression tag	UNP P23921
B	-6	LEU	-	expression tag	UNP P23921
B	-5	VAL	-	expression tag	UNP P23921
B	-4	PRO	-	expression tag	UNP P23921
B	-3	ARG	-	expression tag	UNP P23921
B	-2	GLY	-	expression tag	UNP P23921
B	-1	SER	-	expression tag	UNP P23921
B	0	HIS	-	expression tag	UNP P23921

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Ribonucleoside-diphosphate reductase large subunit





GLU	W581	I641	F701	GLU
LYS	K582	I642	I702	LYS
VAL	V583	R643	D703	VAL
SER	L584	D644	Q704	SER
LYS	K585	L645	S705	LYS
GLU	E586	T646	Q706	GLU
GLU	K587	E647	S707	GLU
GLU	I588	R648	L708	GLU
LYS	K590	G649	N709	LYS
GLU	Y591	L650	I710	GLU
ARG	G592	W651	H711	ARG
ASN	I593	H652	I712	ASN
THR	R594	E653	A713	THR
ALA	N595	E654	E714	ALA
ALA	S596	M655	P715	ALA
MET	L597	R656	N716	MET
VAL	L598	N657	Y717	VAL
CYS	I599	Q658	G718	CYS
SER	A600	I659	K719	SER
LEU	P601	I660	L720	LEU
GLU	M602	A661	T721	GLU
ASN	P603	G662	S722	ASN
ARG	T604	N663	M723	ARG
ASP	A605	G664	H724	ASP
GLU	S606	S665	F725	GLU
CYS	T607	I666	Y726	CYS
LEU	A608	Q667	G727	LEU
MET	Q609	S668	W728	MET
CYS	I610	I669	K729	CYS
GLY	L611	P670	Q730	GLY
SER	G612	E671	G731	SER
LYS	N613	L672	L732	LYS
GLU	M614	P673	K733	GLU
ASN	E615	D674	T734	ASN
LYS	S616	D675	G735	LYS
GLU	I617	L676	M736	GLU
LYS	E618	K677	Y737	LYS
ASN	P619	Q678	Y738	ASN
GLU	Y620	L679	L739	GLU
LYS	T621	Y680	R740	LYS
GLU	S622	K681	T741	GLU
LYS	N623	T682	R742	LYS
GLU	I624	V683	PRO	GLU
LYS	Y625	W684	ALA	LYS
GLU	T626	E685	ALA	GLU
LYS	R627	I686	ASN	LYS
GLU	G628	S687	PRO	GLU
LYS	V629	Q688	ILE	LYS
LEU	I630	K689	GLN	LEU
SER	SER	T690	PHE	SER
LYS	G632	V691	THR	LYS
GLU	E633	L692	LEU	GLU
LYS	F634	K693	ASN	LYS
GLU	Q635	M694	LYS	GLU
LYS	I636	A695	GLU	LYS
LYS	V637	A696	LYS	LYS
ASP	M638	E697	LEU	ASP
GLU	P639	H698	LYS	GLU
GLU	H640	G699	ASP	GLU
		A700	LYS	

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	356.01Å 356.01Å 356.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.90 – 9.01 75.90 – 8.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (75.90-9.01) 85.6 (75.90-8.55)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 8.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.405 , 0.426 0.388 , 0.409	Depositor DCC
R_{free} test set	535 reflections (9.97%)	DCC
Wilson B-factor (Å ²)	386.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.62 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 7071 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	11328	wwPDB-VP
Average B, all atoms (Å ²)	633.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.44% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.52	0/5699	0.63	3/7751 (0.0%)
1	B	0.45	0/5876	0.60	1/7986 (0.0%)
All	All	0.49	0/11575	0.61	4/15737 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	LEU	CA-CB-CG	7.02	131.46	115.30
1	A	499	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	220	LEU	CA-CB-CG	5.90	128.86	115.30
1	A	508	LEU	CA-CB-CG	5.29	127.48	115.30

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	5577	0	5412	199	28
1	B	5751	0	5584	185	14
All	All	11328	0	10996	288	28

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 13.

All (288) 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:261:TYR:HB2	1:B:108:HIS:CE1	1.10	1.62
1:B:83:VAL:CG1	1:B:141:PHE:HD1	1.16	1.59
1:B:86:LEU:HD13	1:B:148:PHE:CE1	1.39	1.54
1:A:281:ASN:CG	1:B:281:ASN:HB3	1.23	1.53
1:B:90:THR:CG2	1:B:140:ASP:OD1	1.63	1.43
1:A:261:TYR:CB	1:B:108:HIS:HE1	1.30	1.42
1:A:285:TYR:CD1	1:B:278:VAL:CG1	1.85	1.41
1:A:261:TYR:CB	1:B:108:HIS:CE1	2.03	1.38
1:A:106:ASN:HD22	1:B:263:ALA:CB	1.35	1.37
1:A:285:TYR:CE1	1:B:278:VAL:HG11	1.58	1.36
1:B:83:VAL:CG1	1:B:141:PHE:CD1	2.07	1.35
1:A:285:TYR:CD1	1:B:278:VAL:HG11	1.08	1.35
1:A:281:ASN:ND2	1:B:281:ASN:HB3	1.44	1.32
1:A:285:TYR:CE1	1:B:232:TYR:CZ	2.20	1.28
1:A:86:LEU:CD1	1:A:140:ASP:HB2	1.64	1.27
1:A:86:LEU:HD11	1:A:140:ASP:CB	1.67	1.25
1:B:90:THR:HG23	1:B:166:ARG:CB	1.68	1.23
1:A:90:THR:CB	1:A:137:TYR:CB	2.03	1.23
1:A:90:THR:CA	1:A:137:TYR:HB2	1.70	1.21
1:A:72:PRO:HG3	1:A:646:THR:CG2	1.70	1.21
1:A:281:ASN:CG	1:B:281:ASN:CB	2.09	1.20
1:B:90:THR:CG2	1:B:166:ARG:HD3	1.60	1.19
1:A:90:THR:HA	1:A:137:TYR:CB	1.72	1.18
1:A:232:TYR:OH	1:B:286:VAL:HB	1.05	1.18
1:A:89:GLU:O	1:A:166:ARG:NH1	1.78	1.17
1:A:90:THR:CA	1:A:137:TYR:CB	2.20	1.17
1:B:90:THR:HG22	1:B:166:ARG:HD3	1.17	1.16
1:B:83:VAL:HG12	1:B:141:PHE:HD1	1.04	1.15
1:A:236:LYS:HD2	1:B:236:LYS:HD2	1.18	1.14
1:A:232:TYR:OH	1:B:286:VAL:CB	1.95	1.13
1:B:86:LEU:CD1	1:B:148:PHE:CE1	2.31	1.12
1:A:232:TYR:CZ	1:B:286:VAL:HB	1.85	1.10
1:B:83:VAL:HG13	1:B:141:PHE:CD1	1.86	1.10
1:A:106:ASN:ND2	1:B:263:ALA:HB2	1.63	1.09
1:A:106:ASN:ND2	1:B:263:ALA:CB	2.12	1.09
1:A:236:LYS:HZ2	1:B:236:LYS:NZ	1.52	1.07
1:A:261:TYR:OH	1:B:104:TYR:HE2	1.38	1.07
1:A:281:ASN:CB	1:B:281:ASN:HB3	1.84	1.06
1:A:86:LEU:CD1	1:A:140:ASP:CB	2.28	1.06
1:B:123:ILE:CD1	1:B:180:LYS:HG2	1.86	1.05
1:A:236:LYS:NZ	1:B:236:LYS:HZ3	1.52	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ALA:HB1	1:B:113:SER:HB3	1.40	1.04
1:A:72:PRO:HG3	1:A:646:THR:HG21	1.35	1.04
1:A:90:THR:HB	1:A:137:TYR:CB	1.83	1.04
1:B:83:VAL:HG12	1:B:141:PHE:CD1	1.79	1.02
1:A:90:THR:CB	1:A:137:TYR:HB2	1.79	1.02
1:A:263:ALA:HB1	1:B:113:SER:CB	1.90	1.01
1:B:90:THR:CG2	1:B:166:ARG:CD	2.40	0.99
1:B:90:THR:CG2	1:B:166:ARG:HB3	1.91	0.99
1:A:275:MET:O	1:B:285:TYR:CE2	2.16	0.98
1:A:261:TYR:OH	1:B:104:TYR:CE2	2.11	0.98
1:A:106:ASN:HD22	1:B:263:ALA:HB2	1.16	0.98
1:A:106:ASN:HD22	1:B:263:ALA:CA	1.77	0.97
1:A:90:THR:HA	1:A:137:TYR:HB3	1.43	0.97
1:B:83:VAL:HG13	1:B:141:PHE:HD1	1.22	0.97
1:A:86:LEU:HD11	1:A:140:ASP:HB2	0.98	0.97
1:A:285:TYR:CD1	1:B:232:TYR:OH	2.14	0.97
1:A:281:ASN:ND2	1:B:281:ASN:CB	2.25	0.96
1:A:285:TYR:CE1	1:B:232:TYR:OH	2.17	0.96
1:B:90:THR:HG23	1:B:166:ARG:HB3	0.95	0.95
1:A:106:ASN:ND2	1:B:263:ALA:CA	2.30	0.95
1:A:72:PRO:HG2	1:A:646:THR:HB	1.47	0.94
1:A:90:THR:HB	1:A:137:TYR:HB2	1.46	0.93
1:A:87:HIS:CD2	1:A:138:ASP:OD1	2.22	0.92
1:A:106:ASN:ND2	1:B:263:ALA:HA	1.84	0.92
1:A:90:THR:CA	1:A:137:TYR:HB3	1.90	0.91
1:A:72:PRO:CG	1:A:646:THR:HB	1.99	0.91
1:A:108:HIS:CB	1:B:261:TYR:CB	2.49	0.90
1:A:108:HIS:CB	1:B:261:TYR:CD1	2.53	0.90
1:B:86:LEU:HD13	1:B:148:PHE:CZ	2.07	0.89
1:B:90:THR:HG21	1:B:140:ASP:CG	1.91	0.89
1:A:275:MET:HA	1:B:285:TYR:HE2	1.37	0.87
1:A:285:TYR:CD1	1:B:278:VAL:HG13	2.10	0.87
1:A:236:LYS:HD2	1:B:236:LYS:CD	2.04	0.87
1:A:108:HIS:CB	1:B:261:TYR:CG	2.57	0.87
1:B:86:LEU:CD1	1:B:148:PHE:HE1	1.77	0.87
1:B:86:LEU:HD13	1:B:148:PHE:HE1	1.12	0.86
1:A:109:ASN:HD21	1:B:263:ALA:CB	1.88	0.86
1:A:277:ARG:HH12	1:B:284:ARG:CZ	1.88	0.86
1:A:86:LEU:HD21	1:A:138:ASP:O	1.77	0.85
1:A:285:TYR:CE1	1:B:232:TYR:CE2	2.66	0.84
1:A:236:LYS:NZ	1:B:236:LYS:NZ	2.15	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:MET:HA	1:B:285:TYR:CE2	2.14	0.82
1:A:72:PRO:HG3	1:A:646:THR:CB	2.09	0.82
1:B:90:THR:HG23	1:B:166:ARG:CG	2.08	0.82
1:A:285:TYR:HE1	1:B:232:TYR:CZ	1.97	0.81
1:A:275:MET:CA	1:B:285:TYR:HE2	1.93	0.81
1:B:90:THR:HG21	1:B:140:ASP:OD1	0.67	0.80
1:A:281:ASN:CB	1:B:281:ASN:CB	2.57	0.79
1:A:261:TYR:CD1	1:B:106:ASN:CB	2.67	0.77
1:A:86:LEU:HD11	1:A:140:ASP:CA	2.14	0.77
1:A:109:ASN:ND2	1:B:263:ALA:HB2	1.99	0.77
1:A:263:ALA:HB1	1:B:113:SER:OG	1.84	0.76
1:A:281:ASN:HB3	1:B:281:ASN:CB	2.16	0.75
1:B:223:MET:HG2	1:B:255:ILE:HD11	1.69	0.75
1:A:72:PRO:CG	1:A:646:THR:CB	2.63	0.75
1:A:62:GLU:CG	1:A:145:TYR:CE1	2.65	0.75
1:A:109:ASN:HD21	1:B:263:ALA:HB2	1.54	0.73
1:B:448:SER:HB3	1:B:602:MET:CE	2.17	0.73
1:B:196:ARG:HG2	1:B:611:LEU:HD22	1.71	0.73
1:B:83:VAL:HG11	1:B:141:PHE:HD1	1.46	0.72
1:A:106:ASN:HD22	1:B:263:ALA:HB1	1.51	0.72
1:A:86:LEU:CD2	1:A:138:ASP:O	2.37	0.72
1:B:123:ILE:HD13	1:B:180:LYS:HG2	1.70	0.72
1:A:261:TYR:CE1	1:B:106:ASN:CB	2.73	0.71
1:B:90:THR:CG2	1:B:166:ARG:CG	2.67	0.71
1:A:285:TYR:CD1	1:B:232:TYR:CZ	2.72	0.70
1:B:402:THR:HB	1:B:403:PRO:HA	1.74	0.68
1:A:108:HIS:CB	1:B:261:TYR:HB3	2.22	0.68
1:A:261:TYR:CB	1:B:108:HIS:ND1	2.57	0.67
1:B:448:SER:HB3	1:B:602:MET:HE1	1.75	0.66
1:A:279:TYR:HE2	1:B:285:TYR:HH	1.40	0.66
1:A:416:ASN:OD1	1:A:561:VAL:HG13	1.95	0.66
1:A:285:TYR:HE1	1:B:232:TYR:CE2	2.09	0.66
1:B:123:ILE:HD13	1:B:180:LYS:CG	2.26	0.66
1:A:478:ASN:HD22	1:A:499:ARG:HH11	1.44	0.65
1:A:285:TYR:CE1	1:B:278:VAL:CG1	2.50	0.65
1:A:281:ASN:HB3	1:B:281:ASN:HB2	1.77	0.64
1:B:123:ILE:HD11	1:B:180:LYS:HG2	1.80	0.64
1:A:87:HIS:HD2	1:A:138:ASP:OD1	1.76	0.63
1:A:223:MET:HG2	1:A:255:ILE:HD11	1.79	0.63
1:A:498:HIS:ND1	1:A:555:THR:HG21	2.14	0.63
1:A:285:TYR:HE2	1:B:275:MET:HA	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ASN:HB3	1:B:274:PRO:HG2	1.80	0.62
1:B:218:CYS:HB3	1:B:444:CYS:SG	2.40	0.62
1:A:283:ALA:HB1	1:A:295:GLY:O	2.00	0.62
1:A:482:ASP:OD2	1:A:499:ARG:NH2	2.32	0.62
1:B:220:LEU:HG	1:B:442:ALA:HB3	1.82	0.61
1:A:285:TYR:OH	1:B:231:ILE:CG2	2.49	0.61
1:B:83:VAL:HG12	1:B:141:PHE:CE1	2.34	0.61
1:B:226:ASP:OD1	1:B:256:ARG:HD2	2.00	0.61
1:A:281:ASN:OD1	1:B:281:ASN:CG	2.39	0.60
1:A:90:THR:HA	1:A:137:TYR:HB2	1.46	0.60
1:B:645:LEU:HD21	1:B:672:ILE:HD12	1.83	0.60
1:B:123:ILE:CD1	1:B:180:LYS:CG	2.70	0.60
1:B:221:LEU:HD13	1:B:248:ILE:HG21	1.84	0.59
1:A:62:GLU:HG2	1:A:145:TYR:CE1	2.36	0.59
1:A:87:HIS:NE2	1:A:138:ASP:OD1	2.34	0.59
1:B:415:SER:O	1:B:418:GLN:HB2	2.02	0.59
1:A:86:LEU:CD1	1:A:140:ASP:HB3	2.28	0.59
1:A:153:ARG:HB2	1:A:153:ARG:HH11	1.66	0.59
1:A:277:ARG:HH12	1:B:284:ARG:NH2	2.00	0.59
1:A:90:THR:C	1:A:137:TYR:HB2	2.22	0.59
1:A:277:ARG:NH1	1:B:284:ARG:CZ	2.61	0.59
1:A:86:LEU:HD13	1:A:140:ASP:CB	2.29	0.59
1:B:245:ALA:HB2	1:B:288:GLN:OE1	2.03	0.58
1:A:281:ASN:CG	1:B:281:ASN:CG	2.62	0.58
1:A:72:PRO:CG	1:A:646:THR:CG2	2.62	0.57
1:A:236:LYS:HZ2	1:B:236:LYS:HZ3	0.70	0.57
1:A:456:THR:HG23	1:A:458:GLU:H	1.68	0.57
1:A:285:TYR:CB	1:B:278:VAL:HG13	2.34	0.57
1:A:248:ILE:HD12	1:A:297:PHE:CE2	2.40	0.57
1:A:72:PRO:CG	1:A:646:THR:HG21	2.22	0.57
1:A:456:THR:CG2	1:A:458:GLU:H	2.17	0.57
1:B:3:VAL:HG22	1:B:13:VAL:HG22	1.87	0.57
1:A:275:MET:C	1:B:285:TYR:HE2	2.07	0.57
1:B:535:ILE:HG22	1:B:599:ILE:HD12	1.86	0.57
1:A:82:ALA:O	1:A:141:PHE:CD1	2.59	0.56
1:B:324:ARG:HG3	1:B:326:ARG:NH2	2.20	0.56
1:A:478:ASN:ND2	1:A:499:ARG:HH11	2.04	0.56
1:A:637:VAL:HG22	1:A:642:LEU:HB2	1.88	0.56
1:A:86:LEU:CD1	1:A:140:ASP:C	2.73	0.55
1:A:108:HIS:CB	1:B:261:TYR:HB2	2.35	0.55
1:A:362:VAL:HG22	1:A:366:GLU:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:HG3	1:A:646:THR:HG22	1.78	0.55
1:A:263:ALA:CB	1:B:113:SER:OG	2.54	0.54
1:A:109:ASN:ND2	1:B:263:ALA:CB	2.59	0.53
1:A:637:VAL:HG13	1:A:642:LEU:HD22	1.90	0.53
1:A:261:TYR:CZ	1:B:104:TYR:HE2	2.24	0.53
1:A:285:TYR:CD1	1:B:232:TYR:CE2	2.97	0.53
1:B:221:LEU:HD13	1:B:248:ILE:CG2	2.38	0.53
1:A:275:MET:CE	1:A:276:LEU:HD13	2.38	0.53
1:A:402:THR:HB	1:A:403:PRO:HA	1.90	0.53
1:A:275:MET:CA	1:B:285:TYR:CE2	2.82	0.53
1:A:478:ASN:HD22	1:A:499:ARG:NH1	2.07	0.53
1:B:130:ARG:CG	1:B:130:ARG:HH11	2.22	0.53
1:A:153:ARG:HB2	1:A:153:ARG:NH1	2.23	0.52
1:A:86:LEU:HD13	1:A:140:ASP:C	2.29	0.52
1:A:27:TYR:O	1:A:80:ARG:NH2	2.39	0.52
1:A:655:MET:HE3	1:A:672:ILE:HD11	1.92	0.51
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.10	0.51
1:B:223:MET:HE2	1:B:231:ILE:HG12	1.91	0.51
1:A:275:MET:HE2	1:A:276:LEU:HD13	1.91	0.51
1:B:362:VAL:CG1	1:B:367:PHE:HA	2.40	0.51
1:A:655:MET:CE	1:A:672:ILE:HD11	2.41	0.51
1:B:482:ASP:OD2	1:B:499:ARG:NH2	2.44	0.51
1:A:281:ASN:ND2	1:B:281:ASN:CA	2.73	0.50
1:B:287:ASP:HB3	1:B:294:PRO:HA	1.94	0.50
1:B:441:VAL:O	1:B:491:ALA:HA	2.11	0.50
1:B:90:THR:HG22	1:B:166:ARG:CD	2.11	0.50
1:A:221:LEU:CD1	1:A:248:ILE:HG23	2.42	0.50
1:A:260:SER:OG	1:A:381:ARG:NH2	2.44	0.50
1:A:109:ASN:HD21	1:B:263:ALA:HB3	1.72	0.49
1:A:275:MET:C	1:B:285:TYR:CE2	2.81	0.49
1:B:86:LEU:HD23	1:B:140:ASP:O	2.12	0.49
1:A:232:TYR:CZ	1:B:286:VAL:CB	2.78	0.49
1:A:261:TYR:HD1	1:B:106:ASN:CB	2.23	0.49
1:A:261:TYR:CG	1:B:108:HIS:CE1	2.95	0.49
1:A:553:TYR:CE1	1:A:555:THR:HG22	2.47	0.49
1:A:121:LEU:HD22	1:A:125:LEU:HG	1.93	0.49
1:A:285:TYR:CE1	1:B:232:TYR:CE1	2.92	0.49
1:B:448:SER:HB3	1:B:602:MET:HE3	1.93	0.49
1:B:83:VAL:HG11	1:B:141:PHE:CD1	2.31	0.49
1:A:535:ILE:HG22	1:A:599:ILE:HD12	1.95	0.49
1:B:627:ARG:HB2	1:B:636:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:HIS:O	1:A:655:MET:HB3	2.12	0.49
1:A:86:LEU:HD13	1:A:140:ASP:HB3	1.94	0.48
1:B:27:TYR:O	1:B:80:ARG:NH2	2.46	0.48
1:A:621:THR:HA	1:A:683:VAL:HG12	1.95	0.48
1:A:416:ASN:CG	1:A:561:VAL:HG13	2.35	0.48
1:B:356:CYS:HB3	1:B:374:TYR:CD1	2.49	0.47
1:A:364:GLY:O	1:A:368:GLU:HG3	2.14	0.47
1:A:18:ILE:O	1:A:22:ILE:HG12	2.14	0.47
1:A:277:ARG:NH1	1:B:284:ARG:NH2	2.62	0.47
1:A:35:ASP:HB3	1:A:38:GLN:HG3	1.96	0.47
1:A:285:TYR:CZ	1:B:232:TYR:CZ	2.96	0.46
1:A:232:TYR:OH	1:B:286:VAL:CA	2.61	0.46
1:A:86:LEU:HD12	1:A:140:ASP:HB2	1.83	0.46
1:A:90:THR:OG1	1:A:138:ASP:N	2.47	0.46
1:B:627:ARG:HB2	1:B:636:ILE:CD1	2.46	0.46
1:A:86:LEU:CD1	1:A:140:ASP:CA	2.86	0.46
1:B:341:ARG:HD2	1:B:347:ASP:O	2.16	0.46
1:B:90:THR:HA	1:B:166:ARG:HG2	0.81	0.46
1:A:278:VAL:N	1:B:285:TYR:CD2	2.82	0.46
1:A:362:VAL:HG13	1:A:367:PHE:HA	1.98	0.46
1:B:1:MET:HE3	1:B:47:LEU:HD12	1.96	0.46
1:B:556:TYR:HE2	1:B:561:VAL:CG2	2.29	0.45
1:B:86:LEU:CD2	1:B:140:ASP:O	2.64	0.45
1:A:300:TYR:HE2	1:A:406:LEU:HD13	1.81	0.45
1:B:603:PRO:HD3	1:B:707:SER:OG	2.16	0.45
1:A:90:THR:HA	1:A:137:TYR:CG	2.47	0.45
1:B:319:GLY:HA3	1:B:324:ARG:NH1	2.32	0.45
1:B:406:LEU:HD22	1:B:426:SER:HB2	1.99	0.45
1:B:256:ARG:HG3	1:B:354:ASN:HB2	1.99	0.45
1:B:416:ASN:CG	1:B:561:VAL:HG13	2.36	0.45
1:A:106:ASN:HA	1:A:107:PRO:HD3	1.83	0.45
1:A:474:VAL:HG21	1:A:539:ALA:HA	1.99	0.45
1:A:285:TYR:OH	1:B:231:ILE:HG22	2.18	0.44
1:B:275:MET:CE	1:B:276:LEU:HD13	2.47	0.44
1:B:284:ARG:HD2	1:B:327:ASP:OD2	2.17	0.44
1:A:76:ILE:O	1:A:80:ARG:HG3	2.18	0.44
1:B:715:PRO:HG3	1:B:741:THR:HG21	1.98	0.44
1:A:218:CYS:SG	1:A:432:ILE:HG13	2.58	0.44
1:B:140:ASP:OD2	1:B:168:GLN:HG2	2.18	0.44
1:A:285:TYR:OH	1:B:231:ILE:HG21	2.16	0.44
1:B:454:TYR:HB2	1:B:461:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ILE:HG13	1:B:444:CYS:SG	2.58	0.44
1:B:251:ALA:HB2	1:B:425:CYS:HB3	1.99	0.44
1:B:482:ASP:CG	1:B:499:ARG:HH22	2.20	0.44
1:B:90:THR:CB	1:B:166:ARG:CG	2.80	0.44
1:B:221:LEU:CD1	1:B:248:ILE:CG2	2.95	0.43
1:A:199:THR:HG21	1:A:607:THR:HB	2.00	0.43
1:A:278:VAL:HA	1:B:285:TYR:HB2	1.54	0.43
1:B:223:MET:HE3	1:B:231:ILE:HA	1.99	0.43
1:B:405:MET:HG3	1:B:724:HIS:CE1	2.53	0.43
1:A:270:ASN:HB3	1:A:274:PRO:HG3	2.01	0.42
1:A:261:TYR:CZ	1:B:104:TYR:CE2	3.02	0.42
1:A:62:GLU:HG3	1:A:145:TYR:CE1	2.50	0.42
1:A:362:VAL:CG1	1:A:367:PHE:HA	2.49	0.42
1:A:243:LYS:HD2	1:B:228:ILE:HG22	2.01	0.42
1:A:261:TYR:HB3	1:B:108:HIS:ND1	2.33	0.42
1:A:236:LYS:HZ3	1:B:236:LYS:NZ	2.11	0.42
1:A:82:ALA:O	1:A:141:PHE:CE1	2.73	0.42
1:B:300:TYR:HE2	1:B:406:LEU:HD13	1.84	0.42
1:A:275:MET:O	1:B:285:TYR:HE2	1.77	0.41
1:A:306:LEU:HD22	1:A:381:ARG:HG2	2.02	0.41
1:A:593:ILE:HD12	1:A:595:ASN:O	2.20	0.41
1:A:220:LEU:HG	1:A:442:ALA:HB3	2.02	0.41
1:A:441:VAL:HG22	1:A:491:ALA:HB2	2.01	0.41
1:A:405:MET:HG3	1:A:724:HIS:CE1	2.56	0.41
1:B:123:ILE:HD12	1:B:180:LYS:HG2	1.86	0.41
1:B:441:VAL:HG13	1:B:490:GLU:HB2	2.01	0.41
1:A:192:LEU:HD23	1:A:472:VAL:HG11	2.02	0.41
1:B:35:ASP:O	1:B:38:GLN:HB2	2.21	0.41
1:B:130:ARG:CG	1:B:130:ARG:NH1	2.82	0.41
1:A:79:ALA:O	1:A:83:VAL:HG23	2.21	0.41
1:A:553:TYR:HE1	1:A:555:THR:HG22	1.85	0.41
1:A:362:VAL:HG13	1:A:367:PHE:CA	2.50	0.41
1:A:337:LEU:HD13	1:A:348:TRP:HZ3	1.86	0.41
1:A:261:TYR:HH	1:B:104:TYR:HE2	0.56	0.41
1:B:221:LEU:CD1	1:B:248:ILE:HG23	2.51	0.41
1:A:710:ILE:HG12	1:A:736:MET:HG3	2.03	0.41
1:A:285:TYR:CE2	1:B:275:MET:HA	2.50	0.40
1:A:223:MET:CE	1:A:252:VAL:HG22	2.52	0.40
1:A:90:THR:HG22	1:A:137:TYR:HB3	1.08	0.40
1:B:196:ARG:HG2	1:B:611:LEU:CD2	2.46	0.40
1:A:373:SER:O	1:A:377:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:TYR:HE2	1:A:561:VAL:HG22	1.87	0.40

All (28) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:TYR:CD1	1:A:27:TYR:CD1[22_554]	0.73	1.47
1:A:27:TYR:CG	1:A:27:TYR:CE1[22_554]	0.90	1.30
1:A:27:TYR:CE2	1:A:27:TYR:CZ[22_554]	1.07	1.13
1:A:27:TYR:CD2	1:A:27:TYR:CZ[22_554]	1.15	1.05
1:A:27:TYR:CD2	1:A:27:TYR:CE1[22_554]	1.27	0.93
1:A:27:TYR:CE2	1:A:27:TYR:CE2[22_554]	1.27	0.93
1:A:27:TYR:CG	1:A:27:TYR:CD1[22_554]	1.45	0.75
1:A:14:MET:CE	1:B:15:PHE:O[9_555]	1.67	0.53
1:A:27:TYR:CD2	1:A:27:TYR:OH[22_554]	1.67	0.53
1:A:27:TYR:CD1	1:A:27:TYR:CE1[22_554]	1.69	0.51
1:A:14:MET:CE	1:B:15:PHE:C[9_555]	1.69	0.51
1:A:27:TYR:CE2	1:A:27:TYR:OH[22_554]	1.78	0.42
1:A:16:ASP:CB	1:B:14:MET:CG[9_555]	1.79	0.41
1:A:14:MET:CG	1:B:15:PHE:CA[9_555]	1.82	0.38
1:A:14:MET:N	1:B:16:ASP:OD2[9_555]	1.84	0.36
1:A:14:MET:CG	1:B:15:PHE:CD2[9_555]	1.86	0.34
1:A:27:TYR:CZ	1:A:27:TYR:CZ[22_554]	1.93	0.27
1:A:14:MET:CB	1:B:15:PHE:C[9_555]	1.95	0.25
1:A:15:PHE:CD2	1:B:13:VAL:O[9_555]	1.96	0.24
1:A:14:MET:SD	1:B:15:PHE:CG[9_555]	2.03	0.17
1:A:14:MET:CG	1:B:15:PHE:C[9_555]	2.04	0.16
1:A:27:TYR:CG	1:A:27:TYR:CZ[22_554]	2.04	0.16
1:A:14:MET:SD	1:B:15:PHE:CA[9_555]	2.05	0.15
1:A:27:TYR:CB	1:A:27:TYR:CE1[22_554]	2.06	0.14
1:A:14:MET:N	1:B:16:ASP:CG[9_555]	2.08	0.12
1:A:14:MET:CB	1:B:15:PHE:CB[9_555]	2.09	0.11
1:A:14:MET:SD	1:B:15:PHE:CD2[9_555]	2.10	0.10
1:A:27:TYR:CE1	1:A:27:TYR:CE2[22_554]	2.12	0.08

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	706/812 (87%)	683 (97%)	21 (3%)	2 (0%)	46	83
1	B	730/812 (90%)	700 (96%)	28 (4%)	2 (0%)	46	83
All	All	1436/1624 (88%)	1383 (96%)	49 (3%)	4 (0%)	46	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	LYS
1	B	224	LYS
1	A	737	TYR
1	B	601	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	592/710 (83%)	545 (92%)	47 (8%)	15	51
1	B	607/710 (86%)	553 (91%)	54 (9%)	12	44
All	All	1199/1420 (84%)	1098 (92%)	101 (8%)	14	48

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	44	ILE

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Mol	Chain	Res	Type
1	A	59	LEU
1	A	67	LEU
1	A	93	VAL
1	A	121	LEU
1	A	149	LYS
1	A	153	ARG
1	A	171	LEU
1	A	192	LEU
1	A	214	GLN
1	A	220	LEU
1	A	252	VAL
1	A	276	LEU
1	A	286	VAL
1	A	287	ASP
1	A	301	LEU
1	A	312	LEU
1	A	327	ASP
1	A	337	LEU
1	A	359	LEU
1	A	362	VAL
1	A	379	ARG
1	A	383	VAL
1	A	389	LEU
1	A	441	VAL
1	A	443	VAL
1	A	444	CYS
1	A	449	LEU
1	A	455	VAL
1	A	456	THR
1	A	458	GLU
1	A	493	LEU
1	A	555	THR
1	A	606	SER
1	A	637	VAL
1	A	653	GLU
1	A	679	LEU
1	A	692	LEU
1	A	693	LYS
1	A	703	ASP
1	A	708	LEU
1	A	716	ASN
1	A	720	LEU

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Mol	Chain	Res	Type
1	A	739	LEU
1	A	741	THR
1	A	742	ARG
1	B	3	VAL
1	B	12	ARG
1	B	47	LEU
1	B	56	LEU
1	B	59	LEU
1	B	67	LEU
1	B	80	ARG
1	B	93	VAL
1	B	108	HIS
1	B	121	LEU
1	B	130	ARG
1	B	149	LYS
1	B	171	LEU
1	B	180	LYS
1	B	192	LEU
1	B	217	SER
1	B	218	CYS
1	B	220	LEU
1	B	225	ASP
1	B	252	VAL
1	B	256	ARG
1	B	276	LEU
1	B	286	VAL
1	B	301	LEU
1	B	312	LEU
1	B	316	LYS
1	B	318	THR
1	B	337	LEU
1	B	359	LEU
1	B	361	GLU
1	B	362	VAL
1	B	365	GLU
1	B	380	VAL
1	B	381	ARG
1	B	389	LEU
1	B	441	VAL
1	B	449	LEU
1	B	455	VAL
1	B	493	LEU

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Mol	Chain	Res	Type
1	B	508	LEU
1	B	516	ARG
1	B	543	SER
1	B	561	VAL
1	B	602	MET
1	B	615	GLU
1	B	627	ARG
1	B	648	ARG
1	B	671	GLU
1	B	678	GLN
1	B	679	LEU
1	B	692	LEU
1	B	708	LEU
1	B	723	MET
1	B	739	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	106	ASN
1	A	160	ASN
1	A	266	ASN
1	B	108	HIS
1	B	270	ASN
1	B	281	ASN

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 carbohydrates 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	B	1
1	A	1







All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	90:THR	C	91:LYS	N	11.08
1	B	90:THR	C	91:LYS	N	5.88

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	714/812 (87%)	15.87	691 (96%)  	631, 631, 660, 660	0
1	B	738/812 (90%)	17.88	723 (97%)  	631, 631, 642, 642	0
All	All	1452/1624 (89%)	16.89	1414 (97%)  	631, 631, 660, 660	0

All (1414) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	682	THR	75.2
1	B	495	ASN	63.1
1	A	677	LYS	61.0
1	B	359	LEU	60.7
1	B	335	PRO	59.2
1	B	538	GLY	58.7
1	B	592	GLY	58.1
1	A	415	SER	56.8
1	A	416	ASN	56.2
1	B	567	GLN	54.4
1	A	367	PHE	52.2
1	A	666	ILE	51.9
1	B	680	TYR	51.3
1	A	495	ASN	51.1
1	B	539	ALA	50.7
1	B	494	SER	50.3
1	B	360	ASP	50.2
1	A	405	MET	50.0
1	B	736	MET	49.3
1	B	595	ASN	49.1
1	B	336	ASP	48.9
1	B	682	THR	48.8
1	B	543	SER	48.8
1	B	500	PRO	48.6

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Mol	Chain	Res	Type	RSRZ
1	B	703	ASP	48.1
1	A	334	ILE	47.3
1	B	544	CYS	47.0
1	B	676	LEU	46.4
1	B	623	ASN	46.2
1	B	655	MET	46.1
1	A	619	PRO	46.0
1	A	359	LEU	45.4
1	B	358	GLY	45.4
1	B	356	CYS	45.2
1	B	405	MET	45.1
1	A	680	TYR	45.1
1	A	403	PRO	45.1
1	A	672	ILE	44.9
1	A	669	ILE	44.5
1	A	408	LYS	44.4
1	B	683	VAL	44.4
1	A	667	GLN	44.3
1	A	412	ASN	44.0
1	A	417	GLN	43.9
1	A	676	LEU	43.9
1	B	638	ASN	43.9
1	A	679	LEU	43.9
1	A	681	LYS	43.4
1	A	665	SER	43.0
1	B	498	HIS	42.7
1	B	672	ILE	42.7
1	A	650	LEU	42.6
1	B	553	TYR	42.5
1	A	335	PRO	42.2
1	A	559	SER	41.7
1	B	417	GLN	41.7
1	A	651	TRP	41.2
1	B	552	PRO	41.1
1	A	331	ALA	40.6
1	B	671	GLU	40.6
1	B	596	SER	40.6
1	B	534	THR	40.4
1	A	664	GLY	40.2
1	A	332	LEU	40.2
1	B	408	LYS	40.2
1	B	679	LEU	39.9

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Mol	Chain	Res	Type	RSRZ
1	B	216	SER	39.9
1	B	677	LYS	39.3
1	B	542	ALA	39.2
1	A	409	ASP	38.9
1	A	675	ASP	38.6
1	B	599	ILE	38.5
1	A	411	CYS	38.3
1	B	593	ILE	38.3
1	A	673	PRO	38.1
1	B	481	ILE	37.9
1	B	337	LEU	37.9
1	B	341	ARG	37.8
1	A	356	CYS	37.8
1	B	598	LEU	37.8
1	B	692	LEU	37.8
1	B	664	GLY	37.7
1	A	656	LYS	37.5
1	A	560	PRO	37.2
1	B	367	PHE	36.9
1	A	685	GLU	36.9
1	A	655	MET	36.9
1	B	416	ASN	36.5
1	A	407	TYR	36.4
1	B	434	GLU	36.4
1	A	668	SER	36.3
1	B	415	SER	36.3
1	B	669	ILE	36.3
1	B	334	ILE	36.2
1	B	536	TYR	36.1
1	B	535	ILE	36.0
1	B	619	PRO	36.0
1	B	547	ALA	36.0
1	B	556	TYR	35.9
1	B	597	LEU	35.7
1	B	665	SER	35.7
1	B	470	THR	35.7
1	B	650	LEU	35.6
1	A	623	ASN	35.6
1	A	406	LEU	35.2
1	B	652	HIS	35.1
1	B	409	ASP	34.9
1	A	434	GLU	34.9

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Mol	Chain	Res	Type	RSRZ
1	B	357	PRO	34.8
1	A	644	ASP	34.8
1	B	695	ALA	34.7
1	A	78	ALA	34.6
1	A	358	GLY	34.6
1	B	715	PRO	34.5
1	B	338	PHE	34.5
1	B	562	SER	34.4
1	B	448	SER	34.3
1	B	506	GLN	34.1
1	B	561	VAL	34.1
1	A	645	LEU	34.1
1	B	445	ASN	34.1
1	B	333	TRP	34.0
1	B	443	VAL	33.9
1	A	553	TYR	33.9
1	A	352	CYS	33.9
1	B	666	ILE	33.8
1	A	621	THR	33.8
1	A	443	VAL	33.6
1	B	499	ARG	33.6
1	B	449	LEU	33.4
1	A	69	THR	33.2
1	B	537	TYR	33.1
1	B	702	ILE	33.1
1	A	518	PRO	33.1
1	A	561	VAL	33.1
1	A	724	HIS	33.0
1	B	474	VAL	32.9
1	A	653	GLU	32.7
1	B	378	GLY	32.5
1	B	620	TYR	32.5
1	B	513	ILE	32.5
1	B	339	MET	32.4
1	B	501	ILE	32.3
1	B	698	ARG	32.2
1	A	596	SER	32.2
1	A	683	VAL	32.2
1	A	678	GLN	32.1
1	B	503	ILE	32.1
1	B	700	ALA	32.1
1	A	671	GLU	32.0

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Mol	Chain	Res	Type	RSRZ
1	A	397	GLN	32.0
1	A	652	HIS	32.0
1	B	710	ILE	31.9
1	B	555	THR	31.9
1	B	735	GLY	31.9
1	A	727	GLY	31.8
1	A	567	GLN	31.8
1	B	423	ILE	31.7
1	B	670	PRO	31.7
1	A	670	PRO	31.5
1	B	704	GLN	31.5
1	B	659	ILE	31.4
1	B	675	ASP	31.3
1	B	502	GLY	31.2
1	B	379	ARG	31.2
1	A	34	VAL	31.2
1	A	300	TYR	30.9
1	A	357	PRO	30.8
1	B	426	SER	30.8
1	B	407	TYR	30.8
1	B	723	MET	30.7
1	B	691	VAL	30.6
1	B	386	ALA	30.5
1	B	594	ARG	30.5
1	A	509	ALA	30.4
1	A	659	ILE	30.3
1	A	674	ASP	30.3
1	B	551	GLY	30.3
1	A	556	TYR	30.1
1	B	410	SER	30.1
1	B	724	HIS	30.1
1	A	519	PHE	30.0
1	B	406	LEU	30.0
1	B	587	LYS	30.0
1	A	686	ILE	29.9
1	B	588	ILE	29.8
1	A	353	PRO	29.7
1	A	57	ASP	29.7
1	B	411	CYS	29.7
1	B	601	PRO	29.6
1	B	673	PRO	29.6
1	A	410	SER	29.6

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Mol	Chain	Res	Type	RSRZ
1	A	513	ILE	29.5
1	A	364	GLY	29.5
1	B	658	GLN	29.5
1	B	473	VAL	29.4
1	B	570	MET	29.3
1	B	505	VAL	29.3
1	B	215	LEU	29.3
1	B	345	ASN	29.2
1	A	430	THR	29.1
1	B	559	SER	29.1
1	B	739	LEU	29.1
1	B	540	LEU	29.0
1	B	491	ALA	28.9
1	B	614	ASN	28.8
1	B	706	GLN	28.8
1	B	404	TYR	28.7
1	A	734	THR	28.7
1	B	425	CYS	28.7
1	A	404	TYR	28.7
1	B	654	GLU	28.7
1	A	333	TRP	28.6
1	A	595	ASN	28.6
1	A	494	SER	28.6
1	A	426	SER	28.5
1	B	640	HIS	28.4
1	A	691	VAL	28.4
1	B	331	ALA	28.3
1	A	82	ALA	28.2
1	B	504	GLY	28.2
1	B	533	GLU	28.1
1	A	26	CYS	28.0
1	B	478	ASN	28.0
1	B	560	PRO	27.9
1	B	412	ASN	27.9
1	B	430	THR	27.8
1	A	568	TYR	27.8
1	A	396	SER	27.7
1	B	484	ASN	27.6
1	B	34	VAL	27.5
1	A	380	VAL	27.4
1	B	734	THR	27.4
1	A	433	VAL	27.4

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Mol	Chain	Res	Type	RSRZ
1	B	584	LEU	27.4
1	B	467	ALA	27.3
1	A	706	GLN	27.3
1	B	347	ASP	27.2
1	B	711	HIS	27.2
1	A	622	SER	27.2
1	A	368	GLU	27.1
1	A	662	CYS	27.1
1	A	390	TRP	27.1
1	B	433	VAL	27.1
1	B	616	SER	27.1
1	B	342	VAL	27.0
1	A	77	LEU	27.0
1	A	733	LYS	26.9
1	A	705	SER	26.9
1	B	699	GLY	26.9
1	A	574	THR	26.8
1	B	403	PRO	26.7
1	B	364	GLY	26.7
1	A	684	TRP	26.6
1	B	516	ARG	26.6
1	A	575	PRO	26.5
1	A	499	ARG	26.4
1	A	657	ASN	26.4
1	B	515	MET	26.4
1	A	422	THR	26.3
1	B	532	PHE	26.3
1	A	735	GLY	26.2
1	A	61	ALA	26.1
1	A	721	THR	26.1
1	B	708	LEU	26.1
1	A	339	MET	26.0
1	B	600	ALA	26.0
1	A	402	THR	26.0
1	B	422	THR	25.9
1	A	498	HIS	25.9
1	B	727	GLY	25.9
1	B	390	TRP	25.8
1	B	688	GLN	25.8
1	B	371	TYR	25.7
1	B	472	VAL	25.6
1	B	432	ILE	25.5

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Mol	Chain	Res	Type	RSRZ
1	B	480	ILE	25.5
1	A	360	ASP	25.4
1	B	694	MET	25.4
1	A	72	PRO	25.3
1	B	554	GLU	25.2
1	B	414	LYS	25.2
1	B	528	ASN	25.2
1	A	312	LEU	25.2
1	B	213	PRO	25.0
1	B	566	LEU	25.0
1	B	497	ARG	25.0
1	B	622	SER	24.9
1	A	506	GLN	24.9
1	A	663	ASN	24.9
1	A	566	LEU	24.8
1	B	701	PHE	24.8
1	B	355	GLU	24.8
1	A	401	GLY	24.8
1	B	332	LEU	24.7
1	A	658	GLN	24.7
1	B	352	CYS	24.7
1	B	402	THR	24.7
1	B	419	ASN	24.6
1	A	351	MET	24.5
1	B	617	ILE	24.5
1	B	375	GLU	24.5
1	A	414	LYS	24.4
1	B	461	TYR	24.4
1	A	423	ILE	24.4
1	B	365	GLU	24.4
1	B	656	LYS	24.4
1	B	512	PHE	24.3
1	A	336	ASP	24.3
1	B	436	THR	24.3
1	A	720	LEU	24.3
1	B	705	SER	24.2
1	B	720	LEU	24.2
1	A	257	ALA	24.2
1	B	618	GLU	24.1
1	B	517	TYR	24.1
1	A	736	MET	24.1
1	B	330	PHE	24.1

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Mol	Chain	Res	Type	RSRZ
1	B	524	ALA	24.0
1	B	340	LYS	23.9
1	B	440	GLU	23.9
1	B	681	LYS	23.9
1	B	712	ILE	23.9
1	A	646	THR	23.9
1	B	733	LYS	23.8
1	A	450	ALA	23.8
1	B	477	LEU	23.8
1	A	641	LEU	23.8
1	B	450	ALA	23.8
1	B	713	ALA	23.7
1	B	351	MET	23.7
1	B	510	ASP	23.7
1	A	81	ILE	23.7
1	A	620	TYR	23.7
1	B	444	CYS	23.7
1	B	621	THR	23.7
1	B	511	ALA	23.7
1	A	570	MET	23.6
1	A	638	ASN	23.6
1	A	614	ASN	23.6
1	A	728	TRP	23.6
1	A	302	GLU	23.6
1	A	436	THR	23.5
1	B	304	TRP	23.5
1	B	457	SER	23.5
1	B	649	GLY	23.5
1	B	518	PRO	23.5
1	A	496	LYS	23.4
1	B	387	GLN	23.3
1	B	462	ASP	23.2
1	B	662	CYS	23.2
1	A	695	ALA	23.2
1	A	419	ASN	23.2
1	B	374	TYR	23.2
1	A	427	ASN	23.1
1	A	616	SER	23.1
1	B	346	GLN	23.1
1	A	97	VAL	23.0
1	A	520	GLU	23.0
1	B	362	VAL	23.0

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Mol	Chain	Res	Type	RSRZ
1	B	644	ASP	23.0
1	A	432	ILE	22.9
1	A	425	CYS	22.9
1	A	58	THR	22.9
1	A	703	ASP	22.9
1	A	85	ASN	22.9
1	B	519	PHE	22.9
1	B	709	ASN	22.8
1	A	601	PRO	22.8
1	B	427	ASN	22.8
1	B	648	ARG	22.8
1	A	741	THR	22.8
1	A	371	TYR	22.8
1	A	725	PHE	22.8
1	A	654	GLU	22.7
1	A	732	LEU	22.6
1	B	645	LEU	22.6
1	B	541	GLU	22.6
1	A	700	ALA	22.6
1	B	685	GLU	22.5
1	B	586	GLU	22.5
1	A	562	SER	22.5
1	B	388	GLN	22.5
1	A	555	THR	22.4
1	B	348	TRP	22.4
1	B	455	VAL	22.4
1	B	385	LYS	22.3
1	A	255	ILE	22.3
1	B	531	ILE	22.3
1	B	199	THR	22.3
1	B	442	ALA	22.2
1	A	707	SER	22.2
1	B	651	TRP	22.2
1	B	26	CYS	22.2
1	B	641	LEU	22.1
1	A	505	VAL	22.1
1	A	713	ALA	22.1
1	B	452	ASN	22.1
1	A	442	ALA	22.1
1	B	571	TRP	22.1
1	A	349	SER	22.0
1	A	690	THR	22.0

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Mol	Chain	Res	Type	RSRZ
1	A	418	GLN	22.0
1	B	380	VAL	21.9
1	A	370	LEU	21.9
1	B	302	GLU	21.9
1	B	397	GLN	21.9
1	B	546	LEU	21.9
1	B	431	GLU	21.8
1	B	696	ALA	21.8
1	B	466	LEU	21.7
1	A	393	ILE	21.7
1	B	389	LEU	21.7
1	A	311	PHE	21.7
1	A	337	LEU	21.7
1	A	381	ARG	21.7
1	A	304	TRP	21.7
1	B	392	ALA	21.6
1	B	421	GLY	21.6
1	A	375	GLU	21.6
1	B	30	ASN	21.6
1	A	739	LEU	21.6
1	A	435	TYR	21.6
1	A	387	GLN	21.6
1	A	711	HIS	21.5
1	B	72	PRO	21.5
1	A	660	ILE	21.5
1	A	507	GLY	21.4
1	B	485	TYR	21.4
1	B	564	GLY	21.4
1	B	424	LYS	21.4
1	A	510	ASP	21.3
1	B	690	THR	21.3
1	A	362	VAL	21.3
1	B	368	GLU	21.3
1	B	363	TRP	21.3
1	B	441	VAL	21.2
1	B	456	THR	21.2
1	A	394	ILE	21.2
1	B	530	GLN	21.2
1	B	344	THR	21.2
1	A	74	TYR	21.1
1	B	353	PRO	21.1
1	B	483	ILE	21.1

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Mol	Chain	Res	Type	RSRZ
1	B	668	SER	21.1
1	A	104	TYR	21.1
1	A	648	ARG	21.1
1	A	692	LEU	21.1
1	B	73	ASP	21.1
1	B	435	TYR	21.1
1	B	589	ALA	21.0
1	B	581	TRP	21.0
1	B	260	SER	21.0
1	A	606	SER	21.0
1	A	106	ASN	21.0
1	B	486	TYR	21.0
1	A	431	GLU	20.9
1	B	393	ILE	20.9
1	B	585	LYS	20.8
1	B	70	LYS	20.8
1	B	413	ARG	20.7
1	A	699	GLY	20.7
1	B	667	GLN	20.6
1	B	71	HIS	20.6
1	B	728	TRP	20.5
1	A	421	GLY	20.5
1	B	420	LEU	20.5
1	B	447	ALA	20.5
1	A	71	HIS	20.5
1	B	214	GLN	20.4
1	A	384	VAL	20.4
1	B	460	THR	20.4
1	A	260	SER	20.4
1	A	618	GLU	20.4
1	B	521	SER	20.4
1	A	70	LYS	20.4
1	A	253	SER	20.4
1	A	254	CYS	20.3
1	B	471	LYS	20.3
1	B	290	GLY	20.3
1	A	398	THR	20.3
1	B	463	PHE	20.3
1	A	688	GLN	20.3
1	A	382	LYS	20.2
1	A	617	ILE	20.2
1	A	383	VAL	20.1

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Mol	Chain	Res	Type	RSRZ
1	B	349	SER	20.1
1	B	451	LEU	20.0
1	A	30	ASN	20.0
1	B	507	GLY	20.0
1	B	653	GLU	19.9
1	A	113	SER	19.9
1	A	355	GLU	19.9
1	A	374	TYR	19.8
1	A	500	PRO	19.8
1	A	444	CYS	19.8
1	A	341	ARG	19.8
1	A	718	GLY	19.8
1	B	579	TRP	19.8
1	B	418	GLN	19.7
1	A	613	ASN	19.7
1	B	492	CYS	19.6
1	B	496	LYS	19.6
1	B	732	LEU	19.6
1	B	646	THR	19.6
1	B	590	LYS	19.6
1	B	469	VAL	19.5
1	B	548	LYS	19.5
1	A	68	THR	19.5
1	B	370	LEU	19.5
1	B	687	SER	19.5
1	B	686	ILE	19.4
1	B	300	TYR	19.4
1	B	475	ARG	19.4
1	B	523	GLU	19.4
1	A	372	ALA	19.3
1	A	712	ILE	19.3
1	B	657	ASN	19.3
1	B	693	LYS	19.3
1	A	363	TRP	19.3
1	B	68	THR	19.2
1	B	74	TYR	19.2
1	A	558	GLY	19.1
1	B	354	ASN	19.1
1	A	702	ILE	19.1
1	A	696	ALA	19.1
1	B	726	TYR	19.1
1	A	220	LEU	19.1

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Mol	Chain	Res	Type	RSRZ
1	B	684	TRP	19.1
1	B	545	ASP	19.1
1	B	707	SER	19.0
1	A	385	LYS	19.0
1	B	384	VAL	19.0
1	B	509	ALA	18.9
1	B	454	TYR	18.9
1	A	22	ILE	18.9
1	B	29	LEU	18.9
1	A	252	VAL	18.8
1	B	303	PRO	18.8
1	B	613	ASN	18.8
1	A	80	ARG	18.8
1	B	311	PHE	18.7
1	B	490	GLU	18.7
1	A	649	GLY	18.7
1	B	731	GLY	18.7
1	B	366	GLU	18.6
1	A	388	GLN	18.6
1	A	594	ARG	18.6
1	B	678	GLN	18.6
1	A	25	LEU	18.6
1	A	73	ASP	18.6
1	B	714	GLU	18.5
1	A	482	ASP	18.5
1	A	661	ALA	18.5
1	B	220	LEU	18.5
1	A	569	ASP	18.5
1	A	552	PRO	18.5
1	A	704	GLN	18.4
1	B	637	VAL	18.4
1	B	569	ASP	18.4
1	A	642	LEU	18.4
1	A	65	ALA	18.4
1	B	465	LYS	18.4
1	A	62	GLU	18.4
1	B	558	GLY	18.3
1	A	593	ILE	18.3
1	A	740	ARG	18.3
1	B	674	ASP	18.3
1	A	348	TRP	18.2
1	B	527	LEU	18.2

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Mol	Chain	Res	Type	RSRZ
1	B	697	GLU	18.2
1	A	516	ARG	18.2
1	A	251	ALA	18.2
1	A	600	ALA	18.2
1	B	576	THR	18.1
1	A	46	GLY	18.1
1	A	301	LEU	18.1
1	B	222	SER	18.1
1	B	557	GLU	18.1
1	A	354	ASN	18.1
1	B	361	GLU	18.0
1	B	737	TYR	18.0
1	A	497	ARG	18.0
1	A	607	THR	17.9
1	A	298	ALA	17.9
1	A	378	GLY	17.9
1	A	299	ILE	17.9
1	B	642	LEU	17.9
1	A	345	ASN	17.9
1	B	721	THR	17.8
1	A	369	LYS	17.8
1	A	624	ILE	17.8
1	B	401	GLY	17.8
1	B	312	LEU	17.8
1	A	715	PRO	17.8
1	B	31	MET	17.8
1	A	342	VAL	17.7
1	A	517	TYR	17.7
1	A	386	ALA	17.7
1	B	482	ASP	17.7
1	B	568	TYR	17.6
1	B	310	GLU	17.6
1	B	730	GLN	17.6
1	A	400	THR	17.6
1	A	99	GLU	17.6
1	A	140	ASP	17.5
1	A	634	PHE	17.5
1	B	725	PHE	17.5
1	A	64	ALA	17.5
1	B	738	TYR	17.4
1	B	313	ASP	17.4
1	B	394	ILE	17.4

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Mol	Chain	Res	Type	RSRZ
1	A	604	THR	17.4
1	A	84	SER	17.4
1	A	392	ALA	17.3
1	A	249	GLY	17.3
1	A	597	LEU	17.3
1	A	709	ASN	17.3
1	A	452	ASN	17.3
1	B	508	LEU	17.2
1	A	605	ALA	17.2
1	A	565	ILE	17.2
1	A	701	PHE	17.2
1	B	565	ILE	17.1
1	A	379	ARG	17.1
1	A	588	ILE	17.1
1	A	33	PHE	17.0
1	A	258	THR	17.0
1	A	344	THR	17.0
1	B	468	GLU	16.9
1	A	56	LEU	16.9
1	B	439	ASP	16.9
1	B	741	THR	16.9
1	B	624	ILE	16.9
1	B	184	ASP	16.9
1	A	100	ASP	16.9
1	B	459	HIS	16.8
1	B	663	ASN	16.8
1	B	36	PRO	16.8
1	A	554	GLU	16.8
1	B	257	ALA	16.7
1	B	520	GLU	16.7
1	A	637	VAL	16.7
1	B	210	THR	16.7
1	B	716	ASN	16.7
1	A	310	GLU	16.7
1	A	731	GLY	16.6
1	A	346	GLN	16.6
1	A	35	ASP	16.6
1	B	381	ARG	16.6
1	A	615	GLU	16.5
1	A	723	MET	16.5
1	A	424	LYS	16.5
1	A	571	TRP	16.5

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Mol	Chain	Res	Type	RSRZ
1	A	60	ALA	16.4
1	B	253	SER	16.4
1	B	740	ARG	16.4
1	A	32	ASP	16.4
1	B	476	ASN	16.4
1	B	525	GLN	16.4
1	A	719	LYS	16.3
1	B	591	TYR	16.3
1	B	514	LEU	16.3
1	B	611	LEU	16.3
1	A	710	ILE	16.3
1	A	24	LYS	16.2
1	A	694	MET	16.2
1	A	222	SER	16.2
1	A	572	ASN	16.2
1	B	251	ALA	16.1
1	A	521	SER	16.0
1	A	95	SER	16.0
1	A	79	ALA	16.0
1	B	261	TYR	16.0
1	B	487	PRO	15.9
1	A	742	ARG	15.9
1	A	635	GLN	15.9
1	A	399	GLU	15.8
1	B	661	ALA	15.8
1	A	640	HIS	15.8
1	A	350	LEU	15.8
1	B	377	GLN	15.8
1	B	198	PHE	15.7
1	A	96	ASP	15.7
1	A	226	ASP	15.6
1	A	338	PHE	15.5
1	B	608	ALA	15.5
1	A	573	VAL	15.5
1	A	347	ASP	15.5
1	B	343	GLU	15.4
1	A	330	PHE	15.4
1	A	708	LEU	15.4
1	B	722	SER	15.4
1	A	420	LEU	15.4
1	A	564	GLY	15.3
1	B	25	LEU	15.3

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Mol	Chain	Res	Type	RSRZ
1	A	738	TYR	15.3
1	B	65	ALA	15.3
1	B	219	PHE	15.2
1	A	103	ASN	15.2
1	A	389	LEU	15.2
1	B	718	GLY	15.2
1	A	481	ILE	15.2
1	B	221	LEU	15.2
1	B	35	ASP	15.2
1	A	256	ARG	15.2
1	A	395	GLU	15.1
1	A	31	MET	15.1
1	B	660	ILE	15.1
1	A	309	PHE	15.1
1	A	478	ASN	15.1
1	A	730	GLN	15.1
1	A	168	GLN	15.1
1	B	134	ALA	15.1
1	A	440	GLU	15.0
1	A	98	MET	15.0
1	A	448	SER	14.9
1	A	577	ASP	14.9
1	B	572	ASN	14.9
1	B	689	LYS	14.8
1	A	697	GLU	14.8
1	A	576	THR	14.8
1	A	101	LEU	14.8
1	B	69	THR	14.8
1	A	687	SER	14.8
1	B	639	PRO	14.7
1	A	21	ARG	14.7
1	A	492	CYS	14.7
1	A	698	ARG	14.7
1	A	693	LYS	14.7
1	B	117	ALA	14.7
1	B	625	TYR	14.7
1	A	592	GLY	14.6
1	B	580	ASP	14.6
1	B	266	ASN	14.6
1	B	77	LEU	14.6
1	A	451	LEU	14.6
1	A	504	GLY	14.5

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Mol	Chain	Res	Type	RSRZ
1	B	298	ALA	14.5
1	B	717	TYR	14.5
1	B	578	LEU	14.5
1	B	229	GLU	14.5
1	B	489	PRO	14.5
1	B	369	LYS	14.5
1	B	209	GLY	14.5
1	B	183	ILE	14.4
1	B	437	SER	14.4
1	A	109	ASN	14.4
1	A	508	LEU	14.4
1	A	716	ASN	14.4
1	B	493	LEU	14.4
1	A	27	TYR	14.4
1	B	636	ILE	14.3
1	A	29	LEU	14.3
1	B	28	GLY	14.3
1	A	86	LEU	14.3
1	B	549	GLU	14.3
1	A	305	HIS	14.2
1	A	111	LYS	14.2
1	A	225	ASP	14.2
1	B	573	VAL	14.2
1	A	343	GLU	14.2
1	B	398	THR	14.2
1	B	106	ASN	14.2
1	B	217	SER	14.2
1	B	254	CYS	14.2
1	A	511	ALA	14.2
1	A	194	SER	14.1
1	A	737	TYR	14.1
1	A	167	PRO	14.1
1	B	32	ASP	14.1
1	A	23	GLN	14.1
1	A	269	SER	14.0
1	B	453	MET	14.0
1	B	400	THR	14.0
1	B	305	HIS	14.0
1	B	67	LEU	14.0
1	A	391	TYR	14.0
1	B	309	PHE	14.0
1	B	138	ASP	13.9

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Mol	Chain	Res	Type	RSRZ
1	A	115	MET	13.9
1	B	299	ILE	13.9
1	A	633	GLU	13.9
1	A	722	SER	13.9
1	B	119	SER	13.8
1	B	458	GLU	13.8
1	B	396	SER	13.8
1	B	719	LYS	13.8
1	A	66	THR	13.8
1	A	75	ALA	13.7
1	B	479	LYS	13.7
1	B	33	PHE	13.7
1	A	59	LEU	13.7
1	B	391	TYR	13.6
1	A	550	GLN	13.5
1	A	141	PHE	13.5
1	A	142	SER	13.5
1	A	603	PRO	13.5
1	A	114	PRO	13.4
1	A	373	SER	13.4
1	A	250	VAL	13.4
1	B	529	LYS	13.4
1	A	36	PRO	13.4
1	B	522	ALA	13.4
1	B	291	ASN	13.4
1	A	445	ASN	13.4
1	A	313	ASP	13.3
1	A	108	HIS	13.3
1	A	512	PHE	13.2
1	A	110	GLY	13.2
1	A	441	VAL	13.2
1	A	602	MET	13.1
1	B	66	THR	13.1
1	B	80	ARG	13.1
1	B	27	TYR	13.1
1	A	67	LEU	13.0
1	B	395	GLU	13.0
1	B	550	GLN	13.0
1	A	340	LYS	13.0
1	A	218	CYS	13.0
1	A	608	ALA	13.0
1	A	523	GLU	12.9

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Mol	Chain	Res	Type	RSRZ
1	B	263	ALA	12.9
1	A	107	PRO	12.8
1	A	303	PRO	12.8
1	B	113	SER	12.8
1	A	261	TYR	12.8
1	A	308	ILE	12.8
1	A	112	HIS	12.8
1	A	223	MET	12.8
1	B	250	VAL	12.8
1	A	429	CYS	12.7
1	B	383	VAL	12.7
1	B	114	PRO	12.7
1	B	256	ARG	12.7
1	A	437	SER	12.6
1	B	249	GLY	12.6
1	A	491	ALA	12.6
1	A	631	SER	12.5
1	A	55	GLU	12.5
1	B	350	LEU	12.5
1	B	607	THR	12.5
1	A	138	ASP	12.5
1	B	563	LYS	12.5
1	B	120	THR	12.5
1	B	160	ASN	12.4
1	B	488	VAL	12.4
1	B	604	THR	12.4
1	B	464	LYS	12.4
1	A	63	THR	12.3
1	B	88	LYS	12.3
1	A	361	GLU	12.3
1	B	211	ASN	12.3
1	A	533	GLU	12.2
1	A	259	GLY	12.2
1	B	180	LYS	12.2
1	B	615	GLU	12.1
1	B	323	GLN	12.1
1	B	372	ALA	12.1
1	A	453	MET	12.1
1	B	610	ILE	12.1
1	A	267	GLY	12.1
1	B	64	ALA	12.1
1	B	446	LEU	12.1

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Mol	Chain	Res	Type	RSRZ
1	A	413	ARG	12.1
1	A	449	LEU	12.1
1	A	198	PHE	12.1
1	A	166	ARG	12.0
1	A	726	TYR	12.0
1	B	602	MET	12.0
1	A	377	GLN	12.0
1	A	439	ASP	12.0
1	A	169	HIS	11.9
1	B	382	LYS	11.9
1	B	575	PRO	11.9
1	A	628	ARG	11.9
1	B	131	LEU	11.9
1	B	238	CYS	11.9
1	B	91	LYS	11.9
1	B	212	ARG	11.9
1	B	187	ILE	11.8
1	B	118	LYS	11.8
1	A	83	VAL	11.8
1	B	242	SER	11.7
1	B	204	THR	11.7
1	B	7	ASP	11.7
1	A	270	ASN	11.7
1	A	376	LYS	11.6
1	A	87	HIS	11.6
1	B	609	GLN	11.6
1	A	515	MET	11.6
1	A	587	LYS	11.6
1	A	717	TYR	11.6
1	B	583	VAL	11.6
1	A	484	ASN	11.6
1	A	316	LYS	11.6
1	B	108	HIS	11.6
1	B	123	ILE	11.6
1	A	525	GLN	11.5
1	B	218	CYS	11.5
1	B	200	HIS	11.5
1	A	45	GLN	11.5
1	A	557	GLU	11.5
1	A	271	GLY	11.5
1	B	115	MET	11.5
1	B	269	SER	11.5

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Mol	Chain	Res	Type	RSRZ
1	B	632	GLY	11.5
1	B	109	ASN	11.5
1	B	258	THR	11.4
1	A	19	THR	11.4
1	B	76	ILE	11.3
1	B	116	VAL	11.3
1	A	365	GLU	11.3
1	A	139	ARG	11.3
1	B	376	LYS	11.3
1	A	137	TYR	11.3
1	B	297	PHE	11.2
1	B	107	PRO	11.2
1	B	124	VAL	11.2
1	B	314	LEU	11.2
1	A	548	LYS	11.2
1	A	307	ASP	11.2
1	A	689	LYS	11.2
1	B	197	TRP	11.2
1	A	563	LYS	11.2
1	A	599	ILE	11.1
1	B	182	ASP	11.1
1	B	130	ARG	11.1
1	B	78	ALA	11.1
1	A	536	TYR	11.0
1	A	47	LEU	11.0
1	B	574	THR	11.0
1	A	647	GLU	11.0
1	A	729	LYS	11.0
1	A	632	GLY	11.0
1	A	229	GLU	11.0
1	B	307	ASP	11.0
1	A	20	SER	11.0
1	A	591	TYR	10.9
1	B	399	GLU	10.9
1	A	102	TYR	10.9
1	A	549	GLU	10.8
1	B	315	LYS	10.8
1	A	272	LEU	10.8
1	B	327	ASP	10.8
1	B	208	ALA	10.8
1	A	585	LYS	10.8
1	A	714	GLU	10.8

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Mol	Chain	Res	Type	RSRZ
1	A	611	LEU	10.7
1	B	283	ALA	10.7
1	A	196	ARG	10.7
1	A	90	THR	10.6
1	A	105	ILE	10.6
1	A	93	VAL	10.6
1	B	239	ALA	10.6
1	A	136	ILE	10.6
1	A	486	TYR	10.6
1	B	248	ILE	10.5
1	A	28	GLY	10.5
1	B	241	ILE	10.4
1	A	94	PHE	10.4
1	A	329	PHE	10.4
1	A	590	LYS	10.4
1	B	582	LYS	10.4
1	B	643	LYS	10.4
1	A	268	ASN	10.3
1	B	162	LYS	10.3
1	A	190	TYR	10.3
1	B	742	ARG	10.3
1	B	87	HIS	10.2
1	B	185	ALA	10.2
1	B	647	GLU	10.2
1	B	226	ASP	10.2
1	A	145	TYR	10.2
1	A	493	LEU	10.1
1	B	188	GLU	10.1
1	A	589	ALA	10.1
1	B	105	ILE	10.1
1	B	526	LEU	10.1
1	A	627	ARG	10.1
1	A	122	ASP	10.1
1	A	121	LEU	10.1
1	B	286	VAL	10.0
1	A	524	ALA	10.0
1	A	639	PRO	10.0
1	B	75	ALA	10.0
1	A	135	ILE	10.0
1	A	514	LEU	10.0
1	B	127	ASN	10.0
1	B	429	CYS	10.0

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Mol	Chain	Res	Type	RSRZ
1	B	308	ILE	9.9
1	A	165	GLU	9.9
1	B	191	ASN	9.9
1	A	116	VAL	9.9
1	B	122	ASP	9.8
1	B	373	SER	9.8
1	A	543	SER	9.8
1	A	522	ALA	9.8
1	B	181	GLU	9.8
1	A	197	TRP	9.8
1	B	39	ILE	9.8
1	A	643	LYS	9.7
1	B	179	HIS	9.7
1	A	545	ASP	9.7
1	A	581	TRP	9.7
1	B	189	THR	9.7
1	B	207	ASN	9.6
1	B	329	PHE	9.6
1	B	328	LEU	9.6
1	A	221	LEU	9.6
1	A	609	GLN	9.6
1	B	104	TYR	9.6
1	B	259	GLY	9.6
1	A	428	LEU	9.5
1	B	316	LYS	9.5
1	A	489	PRO	9.4
1	A	483	ILE	9.3
1	A	544	CYS	9.3
1	A	625	TYR	9.3
1	A	219	PHE	9.3
1	B	612	GLY	9.2
1	B	301	LEU	9.2
1	A	191	ASN	9.2
1	A	454	TYR	9.2
1	A	143	TYR	9.2
1	B	132	ASN	9.2
1	A	598	LEU	9.2
1	B	306	LEU	9.2
1	B	161	GLY	9.1
1	A	306	LEU	9.1
1	A	551	GLY	9.1
1	B	577	ASP	9.1

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Mol	Chain	Res	Type	RSRZ
1	B	103	ASN	9.1
1	B	635	GLN	9.0
1	A	266	ASN	9.0
1	A	119	SER	9.0
1	A	53	THR	9.0
1	A	76	ILE	9.0
1	B	322	GLU	9.0
1	A	630	LEU	9.0
1	B	237	GLN	8.9
1	B	225	ASP	8.9
1	B	84	SER	8.9
1	A	51	VAL	8.9
1	B	23	GLN	8.9
1	A	366	GLU	8.8
1	B	111	LYS	8.8
1	B	729	LYS	8.8
1	A	546	LEU	8.8
1	B	79	ALA	8.8
1	A	124	VAL	8.7
1	A	547	ALA	8.7
1	A	193	LEU	8.7
1	A	578	LEU	8.7
1	B	136	ILE	8.7
1	B	112	HIS	8.7
1	B	634	PHE	8.7
1	A	326	ARG	8.7
1	A	134	ALA	8.6
1	A	89	GLU	8.6
1	B	6	ARG	8.6
1	B	201	ALA	8.6
1	A	43	VAL	8.5
1	A	629	VAL	8.5
1	B	186	ALA	8.5
1	A	52	THR	8.5
1	A	189	THR	8.5
1	B	287	ASP	8.5
1	B	22	ILE	8.5
1	A	315	LYS	8.5
1	B	255	ILE	8.5
1	A	501	ILE	8.4
1	A	263	ALA	8.4
1	A	37	ALA	8.4

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Mol	Chain	Res	Type	RSRZ
1	B	95	SER	8.4
1	B	11	GLU	8.4
1	B	628	ARG	8.4
1	B	90	THR	8.4
1	B	268	ASN	8.3
1	A	530	GLN	8.3
1	A	227	SER	8.3
1	B	102	TYR	8.3
1	A	438	LYS	8.3
1	B	295	GLY	8.2
1	B	121	LEU	8.2
1	B	246	GLY	8.2
1	B	62	GLU	8.2
1	A	117	ALA	8.2
1	A	164	ALA	8.2
1	A	490	GLU	8.2
1	B	8	GLY	8.1
1	B	252	VAL	8.1
1	A	529	LYS	8.1
1	B	81	ILE	8.1
1	B	321	GLU	8.1
1	B	63	THR	8.1
1	B	626	THR	8.1
1	B	318	THR	8.1
1	A	92	LYS	8.0
1	A	120	THR	8.0
1	B	96	ASP	8.0
1	B	267	GLY	8.0
1	B	89	GLU	8.0
1	A	132	ASN	7.9
1	B	324	ARG	7.9
1	B	92	LYS	7.9
1	B	196	ARG	7.9
1	A	211	ASN	7.9
1	B	37	ALA	7.9
1	B	325	ALA	7.9
1	B	629	VAL	7.9
1	B	230	GLY	7.8
1	B	282	THR	7.8
1	A	457	SER	7.8
1	A	612	GLY	7.8
1	A	18	ILE	7.8

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Mol	Chain	Res	Type	RSRZ
1	B	133	SER	7.8
1	B	135	ILE	7.8
1	B	38	GLN	7.8
1	B	85	ASN	7.8
1	B	177	GLY	7.8
1	A	636	ILE	7.7
1	A	38	GLN	7.7
1	A	458	GLU	7.7
1	B	142	SER	7.7
1	B	223	MET	7.7
1	B	158	LYS	7.7
1	B	317	ASN	7.7
1	B	227	SER	7.7
1	B	203	PRO	7.7
1	A	610	ILE	7.7
1	B	176	VAL	7.6
1	B	101	LEU	7.6
1	B	100	ASP	7.6
1	A	224	LYS	7.6
1	B	192	LEU	7.6
1	A	184	ASP	7.5
1	B	10	GLN	7.5
1	A	50	GLY	7.5
1	B	166	ARG	7.5
1	A	528	ASN	7.5
1	B	234	THR	7.5
1	A	199	THR	7.4
1	A	284	ARG	7.4
1	B	178	ILE	7.4
1	B	233	ASP	7.4
1	A	91	LYS	7.4
1	B	99	GLU	7.4
1	A	39	ILE	7.3
1	B	319	GLY	7.3
1	A	118	LYS	7.3
1	A	262	ILE	7.3
1	A	479	LYS	7.3
1	A	626	THR	7.3
1	A	295	GLY	7.3
1	B	98	MET	7.3
1	A	159	ILE	7.3
1	B	633	GLU	7.2

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Mol	Chain	Res	Type	RSRZ
1	B	428	LEU	7.2
1	B	224	LYS	7.2
1	B	24	LYS	7.2
1	B	326	ARG	7.1
1	A	502	GLY	7.1
1	B	61	ALA	7.1
1	A	248	ILE	7.1
1	A	532	PHE	7.0
1	A	48	TYR	7.0
1	A	195	GLU	7.0
1	B	125	LEU	7.0
1	B	294	PRO	7.0
1	A	54	VAL	6.9
1	B	110	GLY	6.9
1	A	160	ASN	6.9
1	A	540	LEU	6.9
1	A	125	LEU	6.9
1	A	286	VAL	6.8
1	A	44	ILE	6.8
1	B	270	ASN	6.8
1	A	579	TRP	6.7
1	A	297	PHE	6.7
1	B	289	GLY	6.7
1	B	284	ARG	6.7
1	B	1	MET	6.7
1	B	438	LYS	6.7
1	A	461	TYR	6.6
1	B	240	LEU	6.6
1	A	283	ALA	6.6
1	B	21	ARG	6.6
1	B	243	LYS	6.6
1	A	216	SER	6.6
1	A	327	ASP	6.6
1	B	140	ASP	6.6
1	A	314	LEU	6.5
1	A	459	HIS	6.5
1	A	531	ILE	6.5
1	B	320	LYS	6.5
1	A	580	ASP	6.5
1	A	171	LEU	6.4
1	A	161	GLY	6.4
1	B	141	PHE	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	164	ALA	6.4
1	A	172	MET	6.4
1	A	187	ILE	6.4
1	A	40	THR	6.4
1	A	586	GLU	6.3
1	B	159	ILE	6.3
1	B	247	GLY	6.3
1	B	265	THR	6.3
1	B	86	LEU	6.3
1	A	534	THR	6.3
1	A	526	LEU	6.3
1	A	153	ARG	6.2
1	A	535	ILE	6.2
1	A	176	VAL	6.2
1	B	280	ASN	6.2
1	B	12	ARG	6.2
1	A	192	LEU	6.2
1	B	83	VAL	6.1
1	A	460	THR	6.1
1	A	182	ASP	6.0
1	A	584	LEU	6.0
1	B	262	ILE	6.0
1	A	88	LYS	6.0
1	B	264	GLY	6.0
1	B	244	SER	6.0
1	A	455	VAL	5.9
1	B	137	TYR	5.9
1	A	127	ASN	5.9
1	A	541	GLU	5.9
1	B	139	ARG	5.8
1	B	94	PHE	5.8
1	B	2	HIS	5.8
1	B	126	ALA	5.8
1	B	97	VAL	5.8
1	A	503	ILE	5.8
1	A	146	PHE	5.8
1	B	143	TYR	5.7
1	B	627	ARG	5.6
1	B	603	PRO	5.6
1	B	129	ASP	5.6
1	A	175	SER	5.6
1	B	202	SER	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	180	LYS	5.6
1	A	186	ALA	5.5
1	A	464	LYS	5.5
1	B	172	MET	5.5
1	A	217	SER	5.5
1	B	605	ALA	5.5
1	B	128	LYS	5.4
1	A	485	TYR	5.4
1	A	131	LEU	5.4
1	B	606	SER	5.4
1	A	447	ALA	5.4
1	A	158	LYS	5.4
1	B	82	ALA	5.4
1	A	480	ILE	5.4
1	A	527	LEU	5.3
1	B	40	THR	5.3
1	A	144	ASN	5.2
1	B	195	GLU	5.2
1	B	153	ARG	5.1
1	A	177	GLY	5.1
1	A	230	GLY	5.1
1	A	147	GLY	5.1
1	A	296	ALA	5.1
1	A	156	LEU	5.1
1	B	50	GLY	5.0
1	B	271	GLY	5.0
1	B	60	ALA	5.0
1	A	209	GLY	5.0
1	A	542	ALA	5.0
1	A	181	GLU	5.0
1	A	157	LEU	4.9
1	B	144	ASN	4.9
1	A	463	PHE	4.9
1	A	242	SER	4.8
1	A	170	MET	4.8
1	B	44	ILE	4.8
1	B	5	LYS	4.8
1	A	273	VAL	4.8
1	A	462	ASP	4.7
1	A	133	SER	4.7
1	A	476	ASN	4.7
1	A	487	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	173	ARG	4.6
1	A	188	GLU	4.6
1	B	296	ALA	4.6
1	A	130	ARG	4.6
1	A	213	PRO	4.6
1	A	210	THR	4.6
1	A	466	LEU	4.5
1	A	232	TYR	4.5
1	A	475	ARG	4.5
1	B	232	TYR	4.5
1	B	205	LEU	4.5
1	A	128	LYS	4.5
1	B	147	GLY	4.5
1	A	179	HIS	4.5
1	A	582	LYS	4.4
1	B	55	GLU	4.4
1	A	126	ALA	4.4
1	A	281	ASN	4.4
1	B	157	LEU	4.4
1	B	19	THR	4.4
1	B	165	GLU	4.4
1	A	42	LYS	4.4
1	B	41	MET	4.4
1	A	123	ILE	4.3
1	A	287	ASP	4.3
1	A	274	PRO	4.3
1	B	93	VAL	4.2
1	A	539	ALA	4.2
1	A	583	VAL	4.2
1	A	17	LYS	4.2
1	A	537	TYR	4.1
1	B	13	VAL	4.1
1	A	456	THR	4.1
1	A	474	VAL	4.1
1	A	228	ILE	4.0
1	A	41	MET	4.0
1	B	49	SER	3.9
1	A	178	ILE	3.9
1	A	183	ILE	3.9
1	B	236	LYS	3.8
1	A	488	VAL	3.8
1	A	214	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	468	GLU	3.8
1	B	190	TYR	3.8
1	B	146	PHE	3.8
1	B	9	ARG	3.8
1	A	264	GLY	3.8
1	B	48	TYR	3.7
1	B	43	VAL	3.7
1	B	150	THR	3.7
1	B	173	ARG	3.7
1	B	281	ASN	3.6
1	B	167	PRO	3.6
1	B	42	LYS	3.6
1	A	231	ILE	3.6
1	B	45	GLN	3.5
1	B	231	ILE	3.5
1	A	282	THR	3.5
1	B	46	GLY	3.5
1	A	163	VAL	3.5
1	B	272	LEU	3.4
1	B	57	ASP	3.4
1	A	328	LEU	3.4
1	A	244	SER	3.3
1	A	233	ASP	3.3
1	B	18	ILE	3.3
1	A	129	ASP	3.3
1	A	469	VAL	3.3
1	A	212	ARG	3.3
1	A	185	ALA	3.3
1	B	228	ILE	3.3
1	B	151	LEU	3.3
1	B	175	SER	3.2
1	B	154	SER	3.2
1	A	234	THR	3.2
1	B	152	GLU	3.2
1	A	151	LEU	3.2
1	B	47	LEU	3.2
1	A	446	LEU	3.2
1	A	49	SER	3.1
1	B	3	VAL	3.1
1	B	20	SER	3.0
1	A	265	THR	3.0
1	B	163	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	148	PHE	3.0
1	A	471	LYS	3.0
1	A	155	TYR	2.9
1	A	15	PHE	2.9
1	B	169	HIS	2.9
1	A	149	LYS	2.9
1	B	194	SER	2.9
1	A	14	MET	2.9
1	A	200	HIS	2.8
1	B	145	TYR	2.8
1	A	238	CYS	2.8
1	A	162	LYS	2.8
1	A	150	THR	2.7
1	A	154	SER	2.7
1	A	236	LYS	2.7
1	A	465	LYS	2.6
1	B	4	ILE	2.6
1	A	477	LEU	2.6
1	B	285	TYR	2.6
1	B	288	GLN	2.6
1	B	193	LEU	2.6
1	A	247	GLY	2.5
1	A	470	THR	2.5
1	B	156	LEU	2.5
1	B	59	LEU	2.5
1	B	155	TYR	2.5
1	B	52	THR	2.5
1	B	58	THR	2.5
1	B	15	PHE	2.4
1	A	240	LEU	2.3
1	B	168	GLN	2.3
1	A	473	VAL	2.3
1	A	152	GLU	2.2
1	A	472	VAL	2.2
1	B	148	PHE	2.2
1	B	206	PHE	2.2
1	A	239	ALA	2.2
1	A	275	MET	2.1
1	A	16	ASP	2.1
1	B	53	THR	2.1
1	A	241	ILE	2.1
1	B	149	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	273	VAL	2.1
1	B	235	LEU	2.0
1	A	285	TYR	2.0
1	B	14	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.