



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:37 am BST

PDB ID : 1FGU
Title : SSDNA-BINDING DOMAIN OF THE LARGE SUBUNIT OF REPLICATION PROTEIN A
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Deposited on : 2000-07-28
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

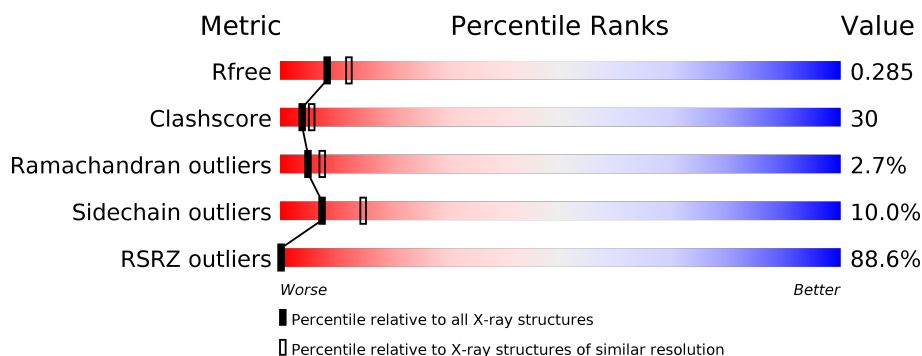
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	252	<div> <div>89%</div> <div> <div>54%</div> <div>35%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	252	<div> <div>81%</div> <div> <div>43%</div> <div>43%</div> <div>8%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3825 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 REPLICATION PROTEIN A 70 KDA DNA-BINDING SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1930	1216	326	381	7			
1	B	238	Total	C	N	O	S	0	0	0
			1863	1176	314	366	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	MET	-	INITIATING METHIONINE	UNP P27694
B	181	MET	-	INITIATING METHIONINE	UNP P27694

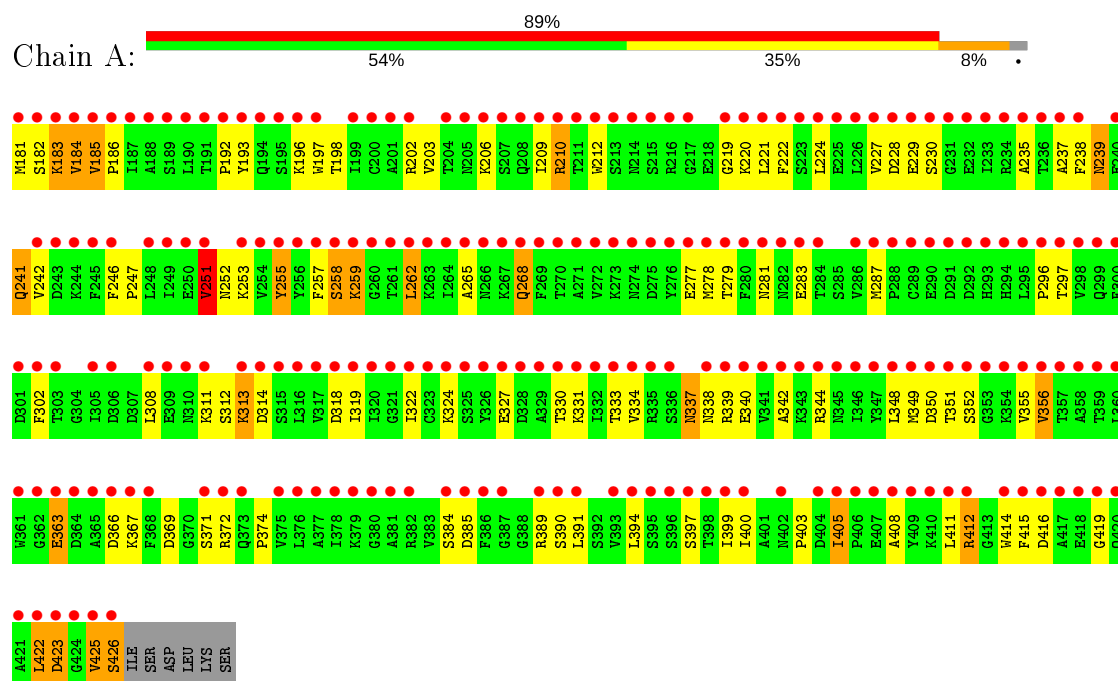
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total	O	0	0
			22	22		
2	B	10	Total	O	0	0
			10	10		

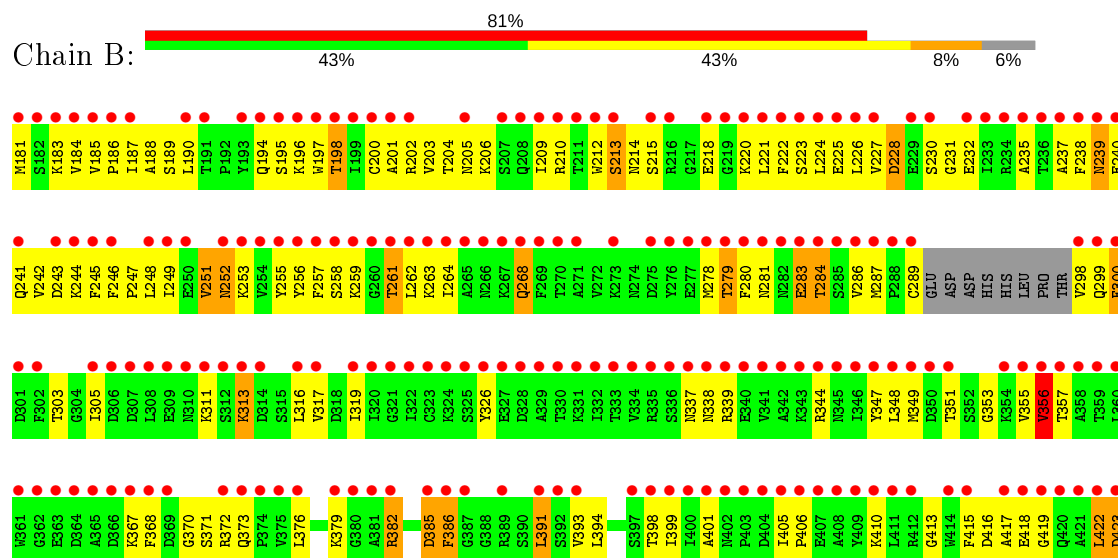
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: REPLICATION PROTEIN A 70 KDA DNA-BINDING SUBUNIT



• Molecule 1: REPLICATION PROTEIN A 70 KDA DNA-BINDING SUBUNIT



G424		
V425		
S426		
ILE	SER	ASP
	LEU	LYS
		SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.50 Å 84.86 Å 119.11 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 28.99 – 1.87	Depositor EDS
% Data completeness (in resolution range)	86.2 (20.00-2.50) 39.2 (28.99-1.87)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 1.87 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.215 , 0.281 0.225 , 0.285	Depositor DCC
R_{free} test set	1987 reflections (8.76%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3825	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.98	0/1966	1.08	8/2659 (0.3%)
1	B	0.80	0/1895	0.98	4/2559 (0.2%)
All	All	0.90	0/3861	1.03	12/5218 (0.2%)

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

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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	344	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	B	356	VAL	CB-CA-C	-6.35	99.34	111.40
1	B	349	MET	CG-SD-CE	-6.27	90.17	100.20
1	A	344	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	399	ILE	CB-CA-C	-5.83	99.93	111.60
1	B	424	GLY	N-CA-C	-5.79	98.62	113.10
1	A	210	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	356	VAL	CB-CA-C	-5.44	101.07	111.40
1	A	183	LYS	N-CA-C	-5.31	96.66	111.00
1	A	349	MET	CA-CB-CG	5.24	122.21	113.30
1	B	422	LEU	N-CA-C	5.11	124.78	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1930	0	1903	96	0
1	B	1863	0	1849	139	0
2	A	22	0	0	1	0
2	B	10	0	0	3	0
All	All	3825	0	3752	230	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 30.

All (230) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:VAL:HG12	1:B:426:SER:H	1.24	0.98
1:A:425:VAL:HG12	1:A:426:SER:H	1.30	0.95
1:B:196:LYS:HD3	1:B:197:TRP:N	1.84	0.93
1:A:268:GLN:HE21	1:A:268:GLN:H	0.95	0.93
1:B:246:PHE:HB3	1:B:247:PRO:HD3	1.50	0.92
1:B:268:GLN:HE21	1:B:268:GLN:H	1.12	0.91
1:B:313:LYS:HD2	1:B:385:ASP:HB2	1.52	0.90
1:B:337:ASN:HD21	1:B:339:ARG:HG2	1.42	0.85
1:A:412:ARG:HD3	1:B:416:ASP:HB2	1.60	0.83
1:A:268:GLN:HE21	1:A:268:GLN:N	1.76	0.83
1:A:222:PHE:CE2	1:A:237:ALA:HB3	2.15	0.82
1:A:268:GLN:NE2	1:A:268:GLN:H	1.77	0.82
1:B:425:VAL:HG12	1:B:426:SER:N	1.94	0.81
1:A:185:VAL:HG22	1:A:186:PRO:HD2	1.63	0.79
1:B:202:ARG:HD3	1:B:252:ASN:ND2	1.99	0.77
1:B:316:LEU:HD21	1:B:382:ARG:HD3	1.66	0.76
1:B:268:GLN:HE21	1:B:268:GLN:N	1.84	0.74
1:A:425:VAL:HG12	1:A:426:SER:N	2.01	0.74
1:A:412:ARG:HD3	1:B:416:ASP:CB	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LYS:HG2	1:B:385:ASP:OD2	1.88	0.73
1:B:185:VAL:CG2	1:B:186:PRO:HD2	2.18	0.72
1:B:337:ASN:ND2	1:B:339:ARG:N	2.38	0.72
1:B:405:ILE:HB	1:B:406:PRO:HD2	1.72	0.71
1:B:203:VAL:O	1:B:251:VAL:O	2.09	0.70
1:A:412:ARG:HG2	1:B:413:GLY:HA2	1.74	0.70
1:A:369:ASP:OD2	1:A:371:SER:HB2	1.91	0.69
1:B:417:ALA:O	1:B:418:GLU:HG3	1.93	0.69
1:B:196:LYS:HE2	1:B:259:LYS:HG2	1.74	0.68
1:B:222:PHE:HD2	1:B:242:VAL:HG22	1.58	0.68
1:B:202:ARG:HG3	1:B:253:LYS:O	1.94	0.68
1:B:305:ILE:HG23	1:B:356:VAL:HG22	1.77	0.67
1:B:278:MET:SD	1:B:280:PHE:HE1	2.16	0.67
1:A:253:LYS:HB2	1:A:255:TYR:CE2	2.30	0.67
1:B:337:ASN:HD21	1:B:339:ARG:CG	2.08	0.67
1:B:225:GLU:O	1:B:226:LEU:HD23	1.94	0.67
1:B:205:ASN:HB2	1:B:225:GLU:HB3	1.77	0.66
1:A:238:PHE:O	1:A:241:GLN:HG2	1.96	0.65
1:A:412:ARG:HG2	1:B:413:GLY:CA	2.26	0.65
1:B:181:MET:HE3	1:B:183:LYS:HE2	1.77	0.65
1:B:202:ARG:HD3	1:B:252:ASN:HD21	1.60	0.64
1:A:425:VAL:O	1:A:426:SER:HB2	1.96	0.64
1:A:203:VAL:O	1:A:251:VAL:O	2.16	0.64
1:B:181:MET:HE3	1:B:181:MET:HA	1.79	0.64
1:B:256:TYR:HB2	1:B:287:MET:HG2	1.79	0.64
1:B:268:GLN:NE2	1:B:268:GLN:H	1.89	0.64
1:B:281:ASN:OD1	1:B:283:GLU:HG3	1.97	0.64
1:B:203:VAL:HG21	1:B:249:ILE:CG2	2.28	0.64
1:B:382:ARG:HG2	1:B:382:ARG:HH11	1.63	0.64
1:B:337:ASN:ND2	1:B:339:ARG:HG2	2.11	0.63
1:A:425:VAL:CG1	1:A:426:SER:H	2.08	0.63
1:B:313:LYS:CD	1:B:385:ASP:HB2	2.26	0.63
1:B:281:ASN:O	1:B:284:THR:HB	2.00	0.62
1:B:278:MET:HG2	1:B:279:THR:N	2.13	0.62
1:B:425:VAL:CG1	1:B:426:SER:H	1.98	0.62
1:B:181:MET:CE	1:B:183:LYS:HE2	2.29	0.62
1:B:337:ASN:ND2	1:B:339:ARG:H	1.98	0.62
1:A:181:MET:HG3	1:A:181:MET:O	1.98	0.62
1:B:209:ILE:HD11	1:B:246:PHE:CD1	2.34	0.62
1:A:405:ILE:HG22	1:A:408:ALA:H	1.64	0.61
1:B:311:LYS:HG3	1:B:317:VAL:HG11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:MET:O	1:B:181:MET:HG3	2.02	0.60
1:B:319:ILE:CD1	1:B:391:LEU:HD23	2.31	0.60
1:B:196:LYS:HZ2	1:B:198:THR:HG22	1.67	0.60
1:B:222:PHE:CD2	1:B:242:VAL:HG22	2.37	0.60
1:A:206:LYS:HG3	1:A:224:LEU:HD23	1.84	0.60
1:B:185:VAL:HG22	1:B:186:PRO:HD2	1.83	0.59
1:B:196:LYS:NZ	1:B:198:THR:HG22	2.18	0.59
1:B:214:ASN:OD1	1:B:215:SER:N	2.36	0.58
1:A:209:ILE:HD13	1:A:242:VAL:CG1	2.34	0.58
1:B:188:ALA:HB3	1:B:230:SER:HB2	1.86	0.58
1:A:265:ALA:CB	1:A:277:GLU:HG3	2.35	0.57
1:A:311:LYS:O	1:A:389:ARG:NH2	2.34	0.56
1:A:363:GLU:OE2	1:A:367:LYS:HD3	2.05	0.56
1:A:212:TRP:CZ2	1:A:219:GLY:HA3	2.41	0.56
1:B:201:ALA:HB1	1:B:227:VAL:O	2.06	0.56
1:B:188:ALA:CB	1:B:230:SER:HB2	2.35	0.56
1:A:313:LYS:HE2	1:A:314:ASP:OD1	2.05	0.55
1:A:415:PHE:O	1:A:419:GLY:N	2.39	0.55
1:A:192:PRO:O	1:A:193:TYR:HB2	2.07	0.55
1:A:265:ALA:HB2	1:A:277:GLU:HG3	1.89	0.55
1:B:337:ASN:HD22	1:B:338:ASN:N	2.04	0.55
1:B:382:ARG:HG2	1:B:382:ARG:NH1	2.22	0.55
1:A:210:ARG:O	1:A:220:LYS:HA	2.06	0.55
1:B:209:ILE:HG13	1:B:246:PHE:CZ	2.42	0.55
1:B:246:PHE:HB3	1:B:247:PRO:CD	2.32	0.55
1:B:185:VAL:HG23	1:B:186:PRO:HD2	1.86	0.55
1:B:393:VAL:HG11	1:B:399:ILE:HD11	1.87	0.55
1:A:246:PHE:HB3	1:A:247:PRO:HD3	1.87	0.54
1:A:246:PHE:N	1:A:247:PRO:HD2	2.23	0.54
1:B:194:GLN:OE1	1:B:197:TRP:HB3	2.07	0.54
1:B:235:ALA:HA	1:B:278:MET:O	2.07	0.54
1:B:337:ASN:ND2	1:B:338:ASN:N	2.56	0.54
1:A:296:PRO:HB3	1:A:405:ILE:HD11	1.90	0.54
1:B:185:VAL:HG22	1:B:189:SER:OG	2.08	0.54
1:B:196:LYS:HD3	1:B:197:TRP:H	1.67	0.54
1:A:246:PHE:HB3	1:A:247:PRO:CD	2.39	0.53
1:A:337:ASN:HD22	1:A:339:ARG:H	1.55	0.53
1:B:203:VAL:HG21	1:B:249:ILE:HG23	1.90	0.52
1:B:227:VAL:HG22	1:B:232:GLU:HB3	1.92	0.52
1:B:213:SER:HB2	1:B:218:GLU:OE2	2.09	0.52
1:A:237:ALA:HB1	1:A:241:GLN:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:PHE:O	1:B:419:GLY:N	2.43	0.51
1:A:348:LEU:O	1:A:355:VAL:HA	2.11	0.51
1:A:196:LYS:HG2	1:A:197:TRP:N	2.25	0.51
1:A:206:LYS:HG3	1:A:224:LEU:CD2	2.40	0.51
1:A:327:GLU:HB2	2:A:19:HOH:O	2.11	0.51
1:A:333:THR:HA	1:A:340:GLU:HA	1.92	0.51
1:B:184:VAL:HA	1:B:198:THR:O	2.10	0.51
1:B:185:VAL:HG22	1:B:186:PRO:CD	2.41	0.51
1:A:228:ASP:OD1	1:A:228:ASP:C	2.48	0.51
1:B:319:ILE:HD13	1:B:391:LEU:HD23	1.93	0.50
1:A:222:PHE:HE2	1:A:237:ALA:HB3	1.74	0.50
1:B:337:ASN:HD22	1:B:338:ASN:H	1.58	0.50
1:B:305:ILE:CG2	1:B:356:VAL:HG22	2.40	0.50
1:B:337:ASN:HD21	1:B:339:ARG:CB	2.24	0.50
1:A:184:VAL:HA	1:A:198:THR:O	2.12	0.49
1:B:196:LYS:CE	1:B:259:LYS:HG2	2.41	0.49
1:A:350:ASP:HA	1:A:411:LEU:HD21	1.94	0.49
1:B:196:LYS:NZ	1:B:258:SER:OG	2.42	0.49
1:B:376:LEU:HD23	1:B:401:ALA:HA	1.95	0.49
1:B:181:MET:CE	1:B:181:MET:HA	2.43	0.49
1:B:256:TYR:CE1	1:B:289:CYS:HB2	2.48	0.49
1:B:406:PRO:HG2	2:B:10:HOH:O	2.12	0.49
1:A:196:LYS:HE3	1:A:259:LYS:HD3	1.95	0.48
1:A:400:ILE:HG21	1:A:403:PRO:HB3	1.94	0.48
1:B:196:LYS:HD3	1:B:196:LYS:C	2.31	0.48
1:B:206:LYS:NZ	1:B:246:PHE:O	2.44	0.48
1:A:184:VAL:HA	1:A:198:THR:CG2	2.43	0.48
1:B:238:PHE:O	1:B:241:GLN:HG2	2.13	0.48
1:B:319:ILE:HD13	1:B:391:LEU:CD2	2.43	0.48
1:B:252:ASN:HD22	1:B:252:ASN:C	2.17	0.48
1:B:212:TRP:CZ3	1:B:214:ASN:ND2	2.81	0.48
1:B:240:GLU:O	1:B:243:ASP:HB2	2.14	0.48
1:B:257:PHE:CD2	1:B:286:VAL:HG22	2.49	0.48
1:B:372:ARG:O	1:B:373:GLN:C	2.52	0.48
1:A:313:LYS:O	1:A:314:ASP:HB2	2.14	0.47
1:A:331:LYS:HD3	1:A:340:GLU:OE2	2.14	0.47
1:B:252:ASN:ND2	1:B:252:ASN:C	2.66	0.47
1:A:385:ASP:OD2	1:A:389:ARG:CD	2.63	0.47
1:A:333:THR:HG22	1:A:334:VAL:N	2.29	0.47
1:A:308:LEU:HA	1:A:308:LEU:HD23	1.62	0.47
1:B:255:TYR:HB2	1:B:257:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:GLY:O	1:B:425:VAL:O	2.33	0.47
1:B:300:PHE:CD1	1:B:300:PHE:N	2.82	0.47
1:B:303:THR:O	1:B:319:ILE:HG22	2.15	0.47
1:A:229:GLU:O	1:A:229:GLU:HG2	2.13	0.46
1:A:394:LEU:N	1:A:397:SER:OG	2.48	0.46
1:B:244:LYS:HD3	1:B:245:PHE:CE1	2.50	0.46
1:A:337:ASN:HB2	1:A:338:ASN:H	1.53	0.46
1:B:212:TRP:HZ3	1:B:214:ASN:ND2	2.13	0.46
1:B:205:ASN:O	1:B:224:LEU:HA	2.14	0.46
1:A:389:ARG:HG3	1:A:390:SER:N	2.30	0.46
1:B:256:TYR:HB2	1:B:287:MET:CG	2.44	0.46
1:A:350:ASP:HA	1:A:411:LEU:CD2	2.46	0.46
1:A:259:LYS:HB2	1:A:259:LYS:HE3	1.78	0.45
1:B:298:VAL:HG12	1:B:299:GLN:H	1.81	0.45
1:A:181:MET:HE2	1:A:287:MET:SD	2.56	0.45
1:A:221:LEU:C	1:A:221:LEU:HD12	2.36	0.45
1:B:253:LYS:HD3	1:B:253:LYS:HA	1.63	0.45
1:A:385:ASP:OD2	1:A:389:ARG:HD2	2.17	0.45
1:B:206:LYS:CE	1:B:246:PHE:CE2	2.99	0.45
1:B:326:TYR:CE2	1:B:370:GLY:HA3	2.52	0.45
1:B:425:VAL:O	1:B:426:SER:C	2.55	0.45
1:B:227:VAL:HG13	1:B:231:GLY:O	2.17	0.45
1:B:244:LYS:O	1:B:248:LEU:HG	2.17	0.45
1:A:181:MET:CE	1:A:287:MET:SD	3.05	0.45
1:B:224:LEU:HD11	1:B:249:ILE:HD12	1.99	0.45
1:B:221:LEU:HA	1:B:237:ALA:O	2.16	0.45
1:B:220:LYS:HG2	1:B:239:ASN:HA	1.99	0.45
1:B:316:LEU:CD2	1:B:382:ARG:HD3	2.44	0.44
1:B:385:ASP:O	1:B:386:PHE:C	2.55	0.44
1:A:351:THR:HG22	1:A:414:TRP:CG	2.52	0.44
1:A:324:LYS:HD2	1:A:423:ASP:HB3	1.98	0.44
1:A:228:ASP:OD1	1:A:230:SER:N	2.50	0.44
1:B:187:ILE:O	1:B:190:LEU:HG	2.17	0.44
1:A:333:THR:HG22	1:A:334:VAL:O	2.17	0.44
1:A:192:PRO:HB3	1:A:262:LEU:O	2.18	0.44
1:B:263:LYS:HG3	1:B:264:ILE:O	2.17	0.44
1:B:261:THR:O	1:B:262:LEU:HD23	2.18	0.44
1:A:235:ALA:HA	1:A:278:MET:O	2.17	0.44
1:B:246:PHE:CB	1:B:247:PRO:HD3	2.31	0.44
1:A:184:VAL:HA	1:A:198:THR:HG22	1.99	0.44
1:B:382:ARG:HB2	1:B:394:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:SER:HA	1:A:184:VAL:HG12	1.99	0.44
1:B:278:MET:SD	1:B:280:PHE:CE1	3.04	0.44
1:B:205:ASN:HB2	1:B:225:GLU:CB	2.48	0.43
1:B:391:LEU:HD12	1:B:391:LEU:HA	1.92	0.43
1:A:333:THR:HG23	1:A:339:ARG:O	2.19	0.43
1:B:200:CYS:HA	1:B:255:TYR:O	2.17	0.43
1:B:257:PHE:HD2	1:B:286:VAL:HG22	1.83	0.43
1:B:347:TYR:HE2	1:B:357:THR:HG1	1.61	0.43
1:A:212:TRP:CH2	1:A:219:GLY:HA3	2.54	0.43
1:B:351:THR:C	1:B:353:GLY:N	2.72	0.43
1:B:210:ARG:O	1:B:220:LYS:HA	2.19	0.42
1:B:410:LYS:HB3	1:B:410:LYS:HE2	1.76	0.42
1:A:302:PHE:HA	1:A:318:ASP:O	2.20	0.42
1:B:196:LYS:HD2	2:B:13:HOH:O	2.20	0.42
1:B:300:PHE:HD2	1:B:379:LYS:HB2	1.84	0.42
1:B:319:ILE:HD11	1:B:391:LEU:HD23	1.99	0.42
1:B:417:ALA:C	1:B:418:GLU:HG3	2.40	0.42
1:A:281:ASN:OD1	1:A:283:GLU:HG3	2.20	0.42
1:A:297:THR:O	1:A:297:THR:HG22	2.20	0.42
1:A:196:LYS:HG2	1:A:197:TRP:H	1.85	0.42
1:A:422:LEU:C	1:A:423:ASP:OD2	2.58	0.42
1:A:202:ARG:NH1	1:A:252:ASN:O	2.52	0.42
1:A:384:SER:O	1:A:389:ARG:HA	2.19	0.42
1:A:220:LYS:HG2	1:A:239:ASN:HA	2.01	0.41
1:A:239:ASN:O	1:A:242:VAL:HB	2.20	0.41
1:A:319:ILE:HD11	1:A:348:LEU:HD12	2.02	0.41
1:A:185:VAL:CG2	1:A:186:PRO:HD2	2.44	0.41
1:B:298:VAL:CG1	1:B:299:GLN:H	2.30	0.41
1:B:422:LEU:HD13	2:B:8:HOH:O	2.18	0.41
1:A:183:LYS:O	1:A:198:THR:HG22	2.20	0.41
1:A:198:THR:OG1	1:A:258:SER:HB3	2.20	0.41
1:A:198:THR:HA	1:A:257:PHE:O	2.21	0.41
1:A:351:THR:HG22	1:A:414:TRP:CD2	2.56	0.41
1:B:228:ASP:OD1	1:B:230:SER:OG	2.32	0.41
1:A:405:ILE:HG21	1:A:405:ILE:HD13	1.68	0.41
1:A:422:LEU:O	1:A:423:ASP:CB	2.69	0.41
1:A:241:GLN:HE21	1:A:241:GLN:H	1.69	0.41
1:A:198:THR:HA	1:A:258:SER:HB3	2.02	0.41
1:A:330:THR:O	1:A:342:ALA:HA	2.21	0.41
1:B:367:LYS:O	1:B:368:PHE:C	2.56	0.41
1:A:416:ASP:OD1	1:B:416:ASP:OD2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:VAL:HG12	1:B:228:ASP:N	2.37	0.40
1:B:348:LEU:O	1:B:355:VAL:HA	2.21	0.40
1:A:322:ILE:O	1:A:348:LEU:HA	2.21	0.40
1:B:184:VAL:HG12	1:B:198:THR:OG1	2.20	0.40
1:A:422:LEU:O	1:A:423:ASP:HB3	2.20	0.40
1:B:258:SER:C	1:B:259:LYS:HG3	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	244/252 (97%)	218 (89%)	19 (8%)	7 (3%)	4	6
1	B	234/252 (93%)	204 (87%)	24 (10%)	6 (3%)	5	8
All	All	478/504 (95%)	422 (88%)	43 (9%)	13 (3%)	5	7

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	VAL
1	B	425	VAL
1	A	239	ASN
1	A	372	ARG
1	A	425	VAL
1	B	313	LYS
1	B	386	PHE
1	A	259	LYS
1	A	423	ASP
1	B	423	ASP
1	A	251	VAL
1	B	239	ASN

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Mol	Chain	Res	Type
1	A	422	LEU

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	215/221 (97%)	194 (90%)	21 (10%)	8	15
1	B	207/221 (94%)	186 (90%)	21 (10%)	7	14
All	All	422/442 (96%)	380 (90%)	42 (10%)	7	15

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	VAL
1	A	185	VAL
1	A	227	VAL
1	A	241	GLN
1	A	251	VAL
1	A	258	SER
1	A	262	LEU
1	A	268	GLN
1	A	279	THR
1	A	312	SER
1	A	313	LYS
1	A	337	ASN
1	A	352	SER
1	A	356	VAL
1	A	363	GLU
1	A	366	ASP
1	A	374	PRO
1	A	391	LEU
1	A	405	ILE
1	A	412	ARG
1	A	426	SER
1	B	195	SER

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Mol	Chain	Res	Type
1	B	198	THR
1	B	204	THR
1	B	213	SER
1	B	223	SER
1	B	228	ASP
1	B	252	ASN
1	B	261	THR
1	B	268	GLN
1	B	279	THR
1	B	283	GLU
1	B	284	THR
1	B	300	PHE
1	B	344	ARG
1	B	356	VAL
1	B	371	SER
1	B	382	ARG
1	B	385	ASP
1	B	391	LEU
1	B	398	THR
1	B	423	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	268	GLN
1	A	294	HIS
1	A	337	ASN
1	B	252	ASN
1	B	268	GLN
1	B	337	ASN
1	B	420	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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](#)

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	246/252 (97%)	3.98	225 (91%) 0 0	29, 44, 77, 108	0
1	B	238/252 (94%)	4.37	204 (85%) 0 0	29, 61, 91, 107	0
All	All	484/504 (96%)	4.17	429 (88%) 0 0	29, 52, 89, 108	0

All (429) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	260	GLY	16.7
1	B	200	CYS	16.5
1	A	420	GLN	13.7
1	B	425	VAL	13.2
1	B	248	LEU	12.5
1	B	312	SER	12.5
1	A	425	VAL	12.0
1	B	419	GLY	11.5
1	A	200	CYS	11.4
1	A	426	SER	11.3
1	B	257	PHE	11.2
1	B	339	ARG	11.1
1	B	289	CYS	10.8
1	A	195	SER	10.3
1	B	280	PHE	10.0
1	B	199	ILE	9.7
1	B	372	ARG	9.7
1	B	216	ARG	9.5
1	B	286	VAL	9.5
1	A	335	ARG	9.5
1	A	185	VAL	9.1
1	B	184	VAL	9.0
1	B	185	VAL	8.9
1	B	250	GLU	8.7

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Mol	Chain	Res	Type	RSRZ
1	B	387	GLY	8.3
1	B	232	GLU	8.2
1	B	195	SER	7.9
1	A	183	LYS	7.9
1	A	256	TYR	7.8
1	A	422	LEU	7.8
1	B	421	ALA	7.8
1	B	310	ASN	7.7
1	B	376	LEU	7.5
1	B	202	ARG	7.5
1	B	211	THR	7.5
1	B	273	LYS	7.4
1	B	212	TRP	7.3
1	B	409	TYR	7.3
1	B	196	LYS	7.2
1	A	372	ARG	7.1
1	B	391	LEU	7.1
1	B	338	ASN	7.1
1	A	282	ASN	7.1
1	B	299	GLN	7.0
1	B	422	LEU	7.0
1	B	190	LEU	7.0
1	B	361	TRP	6.8
1	A	190	LEU	6.7
1	A	418	GLU	6.7
1	B	298	VAL	6.7
1	A	280	PHE	6.6
1	A	324	LYS	6.6
1	A	341	VAL	6.6
1	A	221	LEU	6.5
1	A	326	TYR	6.5
1	B	418	GLU	6.5
1	A	263	LYS	6.5
1	B	238	PHE	6.5
1	B	265	ALA	6.3
1	B	227	VAL	6.3
1	B	336	SER	6.3
1	B	208	GLN	6.3
1	A	368	PHE	6.3
1	B	300	PHE	6.3
1	A	424	GLY	6.3
1	A	216	ARG	6.3

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Mol	Chain	Res	Type	RSRZ
1	B	261	THR	6.3
1	A	224	LEU	6.2
1	A	405	ILE	6.2
1	B	182	SER	6.2
1	A	339	ARG	6.2
1	B	404	ASP	6.1
1	B	415	PHE	6.1
1	B	399	ILE	6.1
1	A	191	THR	6.1
1	A	212	TRP	6.1
1	A	400	ILE	6.0
1	A	382	ARG	5.9
1	A	348	LEU	5.9
1	A	347	TYR	5.9
1	B	264	ILE	5.8
1	B	356	VAL	5.8
1	B	420	GLN	5.8
1	A	240	GLU	5.8
1	A	210	ARG	5.8
1	B	331	LYS	5.8
1	A	421	ALA	5.7
1	A	182	SER	5.7
1	B	271	ALA	5.7
1	A	264	ILE	5.7
1	A	391	LEU	5.7
1	A	222	PHE	5.7
1	A	211	THR	5.6
1	B	382	ARG	5.6
1	B	256	TYR	5.6
1	A	377	ALA	5.5
1	B	332	ILE	5.5
1	B	267	LYS	5.5
1	B	326	TYR	5.5
1	B	407	GLU	5.5
1	A	188	ALA	5.4
1	A	365	ALA	5.4
1	B	340	GLU	5.4
1	B	269	PHE	5.4
1	A	340	GLU	5.4
1	A	289	CYS	5.4
1	B	225	GLU	5.4
1	A	361	TRP	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	302	PHE	5.3
1	A	360	LEU	5.3
1	B	301	ASP	5.3
1	B	283	GLU	5.2
1	A	351	THR	5.2
1	A	220	LYS	5.2
1	A	276	TYR	5.2
1	A	336	SER	5.2
1	A	197	TRP	5.2
1	A	367	LYS	5.2
1	B	197	TRP	5.1
1	B	285	SER	5.1
1	A	243	ASP	5.1
1	B	347	TYR	5.1
1	A	265	ALA	5.1
1	A	253	LYS	5.0
1	B	226	LEU	5.0
1	B	346	ILE	5.0
1	A	355	VAL	5.0
1	A	346	ILE	5.0
1	B	320	ILE	5.0
1	A	250	GLU	4.9
1	A	306	ASP	4.9
1	A	310	ASN	4.9
1	B	366	ASP	4.9
1	B	302	PHE	4.9
1	A	233	ILE	4.9
1	A	286	VAL	4.9
1	A	296	PRO	4.9
1	B	311	LYS	4.9
1	A	342	ALA	4.9
1	B	412	ARG	4.9
1	B	355	VAL	4.9
1	B	364	ASP	4.8
1	A	254	VAL	4.8
1	A	314	ASP	4.8
1	B	426	SER	4.8
1	A	410	LYS	4.8
1	B	323	CYS	4.7
1	A	385	ASP	4.7
1	B	255	TYR	4.7
1	B	215	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	309	GLU	4.7
1	A	384	SER	4.7
1	B	223	SER	4.7
1	B	344	ARG	4.7
1	B	249	ILE	4.7
1	B	389	ARG	4.6
1	B	209	ILE	4.6
1	B	224	LEU	4.6
1	A	199	ILE	4.6
1	A	230	SER	4.6
1	B	229	GLU	4.6
1	B	234	ARG	4.5
1	B	367	LYS	4.5
1	B	348	LEU	4.5
1	B	220	LYS	4.5
1	B	213	SER	4.5
1	B	306	ASP	4.5
1	A	419	GLY	4.5
1	A	189	SER	4.4
1	B	317	VAL	4.4
1	A	334	VAL	4.4
1	A	320	ILE	4.4
1	B	243	ASP	4.4
1	A	387	GLY	4.4
1	A	343	LYS	4.3
1	A	415	PHE	4.3
1	A	319	ILE	4.3
1	A	323	CYS	4.3
1	B	316	LEU	4.3
1	B	218	GLU	4.3
1	B	282	ASN	4.3
1	A	357	THR	4.3
1	A	354	LYS	4.3
1	A	300	PHE	4.3
1	A	331	LYS	4.2
1	B	365	ALA	4.2
1	B	414	TRP	4.2
1	A	408	ALA	4.2
1	B	246	PHE	4.2
1	B	210	ARG	4.2
1	A	187	ILE	4.2
1	A	193	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	399	ILE	4.2
1	A	344	ARG	4.2
1	A	206	LYS	4.2
1	A	248	LEU	4.1
1	A	292	ASP	4.1
1	B	221	LEU	4.1
1	A	244	LYS	4.1
1	B	330	THR	4.1
1	B	417	ALA	4.1
1	A	261	THR	4.1
1	A	209	ILE	4.0
1	B	281	ASN	4.0
1	A	257	PHE	4.0
1	A	366	ASP	4.0
1	B	284	THR	4.0
1	B	329	ALA	4.0
1	B	314	ASP	4.0
1	A	290	GLU	4.0
1	B	181	MET	4.0
1	A	269	PHE	4.0
1	B	262	LEU	4.0
1	A	271	ALA	4.0
1	B	270	THR	3.9
1	B	307	ASP	3.9
1	B	324	LYS	3.9
1	B	386	PHE	3.9
1	A	196	LYS	3.9
1	A	313	LYS	3.9
1	B	322	ILE	3.9
1	A	278	MET	3.9
1	A	208	GLN	3.9
1	A	414	TRP	3.9
1	A	329	ALA	3.9
1	A	379	LYS	3.9
1	B	244	LYS	3.9
1	A	298	VAL	3.9
1	B	385	ASP	3.8
1	B	259	LYS	3.8
1	B	205	ASN	3.8
1	A	376	LEU	3.8
1	A	349	MET	3.8
1	A	378	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	313	LYS	3.8
1	B	266	ASN	3.8
1	A	373	GLN	3.8
1	A	321	GLY	3.8
1	B	375	VAL	3.8
1	A	225	GLU	3.8
1	A	389	ARG	3.7
1	B	319	ILE	3.7
1	B	363	GLU	3.7
1	A	308	LEU	3.7
1	B	308	LEU	3.7
1	B	335	ARG	3.7
1	A	258	SER	3.7
1	A	283	GLU	3.7
1	A	407	GLU	3.7
1	A	186	PRO	3.7
1	A	194	GLN	3.7
1	A	394	LEU	3.7
1	B	288	PRO	3.7
1	A	417	ALA	3.7
1	B	368	PHE	3.7
1	A	266	ASN	3.7
1	A	332	ILE	3.6
1	B	358	ALA	3.6
1	B	222	PHE	3.6
1	B	275	ASP	3.6
1	A	201	ALA	3.6
1	A	359	THR	3.6
1	B	341	VAL	3.6
1	A	294	HIS	3.6
1	A	229	GLU	3.6
1	B	277	GLU	3.6
1	A	345	ASN	3.6
1	B	325	SER	3.5
1	A	380	GLY	3.5
1	B	241	GLN	3.5
1	B	343	LYS	3.5
1	A	356	VAL	3.5
1	B	398	THR	3.4
1	B	373	GLN	3.4
1	A	311	LYS	3.4
1	B	333	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	245	PHE	3.4
1	A	297	THR	3.4
1	A	181	MET	3.4
1	B	354	LYS	3.4
1	A	226	LEU	3.4
1	B	369	ASP	3.4
1	A	217	GLY	3.4
1	B	252	ASN	3.4
1	B	345	ASN	3.4
1	A	284	THR	3.3
1	A	288	PRO	3.3
1	B	410	LYS	3.3
1	A	325	SER	3.3
1	A	262	LEU	3.3
1	B	305	ILE	3.3
1	B	400	ILE	3.3
1	B	263	LYS	3.3
1	B	374	PRO	3.3
1	B	236	THR	3.3
1	A	393	VAL	3.3
1	A	238	PHE	3.3
1	A	322	ILE	3.3
1	A	363	GLU	3.3
1	A	398	THR	3.3
1	B	381	ALA	3.3
1	A	227	VAL	3.3
1	B	403	PRO	3.2
1	B	193	TYR	3.2
1	B	253	LYS	3.2
1	A	423	ASP	3.2
1	A	236	THR	3.1
1	B	276	TYR	3.1
1	B	233	ILE	3.1
1	B	321	GLY	3.1
1	A	251	VAL	3.1
1	B	235	ALA	3.1
1	A	364	ASP	3.1
1	B	194	GLN	3.1
1	B	287	MET	3.1
1	A	293	HIS	3.1
1	A	272	VAL	3.1
1	A	358	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	404	ASP	3.1
1	A	219	GLY	3.1
1	A	223	SER	3.1
1	A	309	GLU	3.1
1	A	260	GLY	3.1
1	A	402	ASN	3.1
1	A	279	THR	3.1
1	A	409	TYR	3.0
1	B	424	GLY	3.0
1	B	423	ASP	3.0
1	A	350	ASP	3.0
1	A	412	ARG	3.0
1	A	291	ASP	3.0
1	A	277	GLU	3.0
1	B	237	ALA	3.0
1	B	239	ASN	3.0
1	B	393	VAL	3.0
1	B	402	ASN	3.0
1	A	305	ILE	3.0
1	B	279	THR	3.0
1	B	379	LYS	3.0
1	B	342	ALA	2.9
1	A	416	ASP	2.9
1	A	406	PRO	2.9
1	B	360	LEU	2.9
1	B	349	MET	2.9
1	A	397	SER	2.9
1	A	330	THR	2.9
1	B	327	GLU	2.8
1	A	232	GLU	2.8
1	A	301	ASP	2.8
1	A	327	GLU	2.8
1	A	287	MET	2.8
1	B	406	PRO	2.8
1	A	235	ALA	2.8
1	A	228	ASP	2.8
1	A	273	LYS	2.8
1	A	371	SER	2.8
1	B	380	GLY	2.8
1	A	375	VAL	2.8
1	B	240	GLU	2.8
1	A	299	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	234	ARG	2.8
1	A	215	SER	2.8
1	A	249	ILE	2.7
1	A	214	ASN	2.7
1	A	207	SER	2.7
1	A	268	GLN	2.7
1	A	205	ASN	2.7
1	A	242	VAL	2.7
1	A	295	LEU	2.7
1	B	230	SER	2.7
1	A	362	GLY	2.7
1	B	328	ASP	2.7
1	A	231	GLY	2.7
1	A	281	ASN	2.7
1	B	392	SER	2.6
1	B	219	GLY	2.6
1	B	201	ALA	2.6
1	B	408	ALA	2.6
1	A	318	ASP	2.6
1	A	411	LEU	2.6
1	B	186	PRO	2.6
1	A	270	THR	2.6
1	A	353	GLY	2.6
1	A	204	THR	2.6
1	A	333	THR	2.6
1	A	275	ASP	2.6
1	A	317	VAL	2.5
1	B	357	THR	2.5
1	B	337	ASN	2.5
1	A	184	VAL	2.5
1	A	390	SER	2.5
1	B	183	LYS	2.5
1	A	352	SER	2.5
1	A	381	ALA	2.5
1	A	237	ALA	2.5
1	B	334	VAL	2.5
1	A	259	LYS	2.5
1	B	191	THR	2.5
1	B	411	LEU	2.4
1	B	397	SER	2.4
1	B	405	ILE	2.4
1	A	255	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	350	ASP	2.4
1	B	362	GLY	2.4
1	B	351	THR	2.4
1	A	303	THR	2.3
1	B	359	THR	2.3
1	A	267	LYS	2.3
1	A	396	SER	2.3
1	A	274	ASN	2.3
1	A	328	ASP	2.3
1	B	198	THR	2.3
1	A	245	PHE	2.3
1	B	254	VAL	2.2
1	A	202	ARG	2.2
1	B	278	MET	2.2
1	A	246	PHE	2.2
1	A	192	PRO	2.2
1	B	258	SER	2.1
1	A	386	PHE	2.1
1	A	315	SER	2.1
1	A	338	ASN	2.1
1	A	213	SER	2.1
1	B	268	GLN	2.1
1	A	316	LEU	2.1
1	B	401	ALA	2.0
1	B	187	ILE	2.0
1	A	395	SER	2.0
1	B	207	SER	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

There are no such residues in this entry.