



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:24 PM GMT

PDB ID : 1FGU
Title : SSDNA-BINDING DOMAIN OF THE LARGE SUBUNIT OF REPLICATION PROTEIN A
Authors : Bochkareva, E.; Belegu, V.; Korolev, S.; Bochkarev, A.
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
<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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

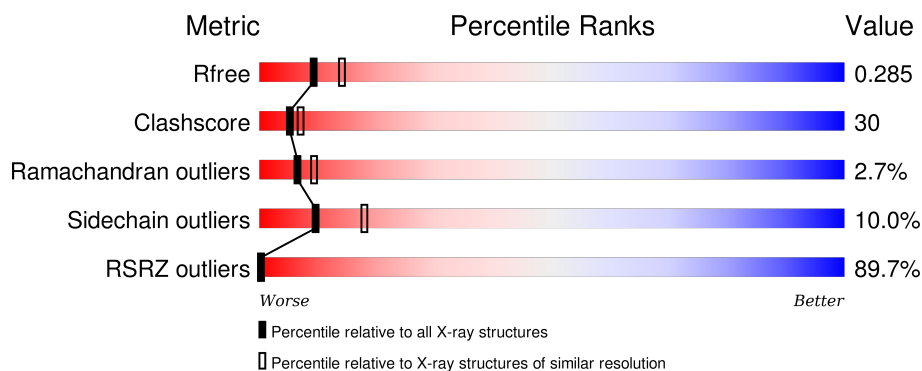
1 Overall quality at a glance

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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>91%</div> <div>54% 35% 8% .</div> </div>
1	B	252	<div> <div>81%</div> <div>43% 43% 8% 6%</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

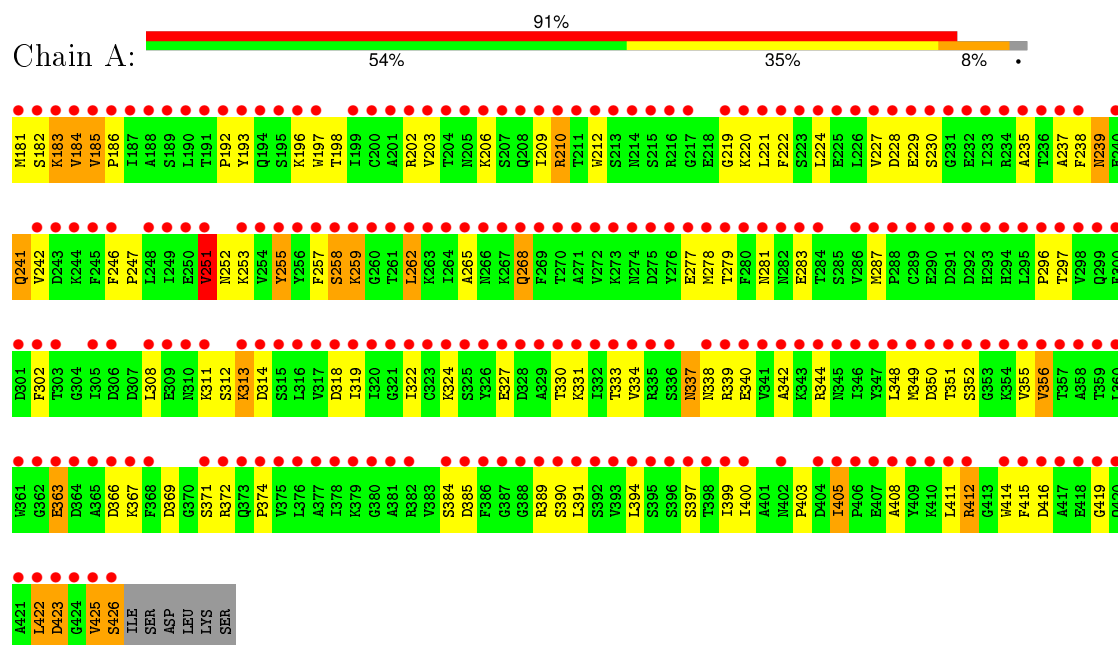
- Molecule 2 is water.

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

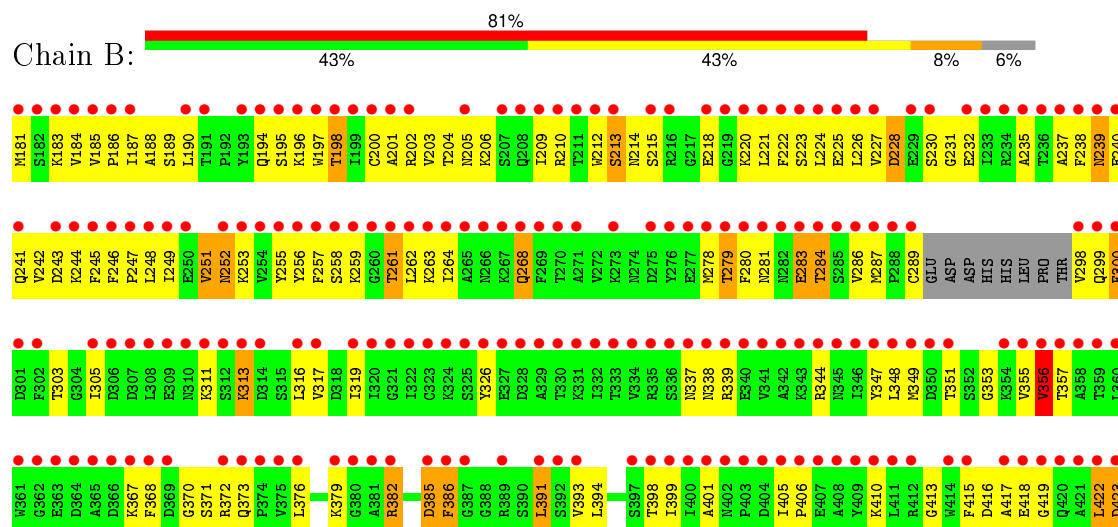
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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	1865 reflections (8.90%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 22677 reflections (0.004%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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($^{\circ}$)	Ideal($^{\circ}$)
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

Continued on next page...

Continued from previous page...

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:B:417:ALA:O	1:B:418:GLU:HG3	1.93	0.69
1:A:369:ASP:OD2	1:A:371:SER:HB2	1.91	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:B:337:ASN:HD21	1:B:339:ARG:CG	2.08	0.67
1:A:253:LYS:HB2	1:A:255:TYR:CE2	2.30	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:B:268:GLN:NE2	1:B:268:GLN:H	1.89	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:A:203:VAL:O	1:A:251:VAL:O	2.16	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:425:VAL:CG1	1:B:426:SER:H	1.98	0.62
1:B:278:MET:HG2	1:B:279:THR:N	2.13	0.62
1:B:337:ASN:ND2	1:B:339:ARG:H	1.98	0.62
1:B:181:MET:CE	1:B:183:LYS:HE2	2.29	0.62
1:B:209:ILE:HD11	1:B:246:PHE:CD1	2.34	0.62
1:A:181:MET:HG3	1:A:181:MET:O	1.98	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:MET:HG3	1:B:181:MET:O	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:B:188:ALA:HB3	1:B:230:SER:HB2	1.86	0.58
1:A:209:ILE:HD13	1:A:242:VAL:CG1	2.34	0.58
1:A:265:ALA:CB	1:A:277:GLU:HG3	2.35	0.57
1:A:363:GLU:OE2	1:A:367:LYS:HD3	2.05	0.56
1:A:311:LYS:O	1:A:389:ARG:NH2	2.34	0.56
1:B:201:ALA:HB1	1:B:227:VAL:O	2.06	0.56
1:A:212:TRP:CZ2	1:A:219:GLY:HA3	2.41	0.56
1:B:188:ALA:CB	1:B:230:SER:HB2	2.35	0.56
1:A:415:PHE:O	1:A:419:GLY:N	2.39	0.55
1:A:313:LYS:HE2	1:A:314:ASP:OD1	2.05	0.55
1:A:265:ALA:HB2	1:A:277:GLU:HG3	1.89	0.55
1:A:192:PRO:O	1:A:193:TYR:HB2	2.07	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:337:ASN:ND2	1:B:338:ASN:N	2.56	0.54
1:B:235:ALA:HA	1:B:278:MET:O	2.07	0.54
1:B:196:LYS:HD3	1:B:197:TRP:H	1.67	0.54
1:B:185:VAL:HG22	1:B:189:SER:OG	2.08	0.54
1:A:296:PRO:HB3	1:A:405:ILE:HD11	1.90	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

Continued on next page...

Continued from previous page...

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:333:THR:HA	1:A:340:GLU:HA	1.92	0.51
1:A:327:GLU:HB2	2:A:19:HOH:O	2.11	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:B:337:ASN:HD22	1:B:338:ASN:H	1.58	0.50
1:A:222:PHE:HE2	1:A:237:ALA:HB3	1.74	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:406:PRO:HG2	2:B:10:HOH:O	2.12	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: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: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:319:ILE:HD13	1:B:391:LEU:CD2	2.43	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: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:B:255:TYR:HB2	1:B:257:PHE:CZ	2.49	0.47
1:A:308:LEU:HA	1:A:308:LEU:HD23	1.62	0.47

Continued on next page...

Continued from previous page...

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:303:THR:O	1:B:319:ILE:HG22	2.15	0.47
1:B:300:PHE:CD1	1:B:300:PHE:N	2.82	0.47
1:B:244:LYS:HD3	1:B:245:PHE:CE1	2.50	0.46
1:A:394:LEU:N	1:A:397:SER:OG	2.48	0.46
1:A:229:GLU:O	1:A:229:GLU:HG2	2.13	0.46
1:A:337:ASN:HB2	1:A:338:ASN:H	1.53	0.46
1:B:205:ASN:O	1:B:224:LEU:HA	2.14	0.46
1:B:212:TRP:HZ3	1:B:214:ASN:ND2	2.13	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:425:VAL:O	1:B:426:SER:C	2.55	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: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:B:224:LEU:HD11	1:B:249:ILE:HD12	1.99	0.45
1:A:181:MET:CE	1:A:287:MET:SD	3.05	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:385:ASP:O	1:B:386:PHE:C	2.55	0.44
1:B:316:LEU:CD2	1:B:382:ARG:HD3	2.44	0.44
1:A:324:LYS:HD2	1:A:423:ASP:HB3	1.98	0.44
1:A:351:THR:HG22	1:A:414:TRP:CG	2.52	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:B:246:PHE:CB	1:B:247:PRO:HD3	2.31	0.44
1:A:235:ALA:HA	1:A:278:MET:O	2.17	0.44
1:B:382:ARG:HB2	1:B:394:LEU:HD11	1.99	0.44
1:A:184:VAL:HA	1:A:198:THR:HG22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:MET:SD	1:B:280:PHE:CE1	3.04	0.44
1:A:182:SER:HA	1:A:184:VAL:HG12	1.99	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:B:196:LYS:HD2	2:B:13:HOH:O	2.20	0.42
1:A:302:PHE:HA	1:A:318:ASP:O	2.20	0.42
1:B:319:ILE:HD11	1:B:391:LEU:HD23	1.99	0.42
1:B:300:PHE:HD2	1:B:379:LYS:HB2	1.84	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:384:SER:O	1:A:389:ARG:HA	2.19	0.42
1:A:202:ARG:NH1	1:A:252:ASN:O	2.52	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:B:228:ASP:OD1	1:B:230:SER:OG	2.32	0.41
1:A:351:THR:HG22	1:A:414:TRP:CD2	2.56	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:416:ASP:OD1	1:B:416:ASP:OD2	2.39	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

Continued on next page...

Continued from previous page...

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:B:184:VAL:HG12	1:B:198:THR:OG1	2.20	0.40
1:A:322:ILE:O	1:A:348:LEU:HA	2.21	0.40
1:B:258:SER:C	1:B:259:LYS:HG3	2.40	0.40
1:A:422:LEU:O	1:A:423:ASP:HB3	2.20	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%)	6	8
1	B	234/252 (93%)	204 (87%)	24 (10%)	6 (3%)	7	10
All	All	478/504 (95%)	422 (88%)	43 (9%)	13 (3%)	6	9

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

Continued on next page...

Continued from previous page...

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%)	10	19
1	B	207/221 (94%)	186 (90%)	21 (10%)	9	17
All	All	422/442 (96%)	380 (90%)	42 (10%)	9	18

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

Continued on next page...

Continued from previous page...

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%)	4.15	229 (93%) 0 0	29, 44, 77, 108	0
1	B	238/252 (94%)	4.56	205 (86%) 0 0	29, 61, 91, 107	0
All	All	484/504 (96%)	4.35	434 (89%) 0 0	29, 52, 89, 108	0

All (434) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	260	GLY	17.4
1	B	200	CYS	17.2
1	A	420	GLN	14.2
1	B	425	VAL	13.8
1	B	248	LEU	12.8
1	B	312	SER	12.7
1	A	425	VAL	12.5
1	B	419	GLY	12.0
1	A	200	CYS	11.8
1	A	426	SER	11.8
1	B	257	PHE	11.5
1	B	339	ARG	11.5
1	B	289	CYS	11.3
1	A	195	SER	10.6
1	B	280	PHE	10.3
1	B	199	ILE	10.2
1	B	372	ARG	9.9
1	B	286	VAL	9.8
1	B	216	ARG	9.8
1	A	335	ARG	9.7
1	A	185	VAL	9.5
1	B	184	VAL	9.5
1	B	185	VAL	9.4
1	B	250	GLU	8.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	387	GLY	8.7
1	B	232	GLU	8.5
1	B	421	ALA	8.3
1	A	256	TYR	8.2
1	B	195	SER	8.1
1	A	183	LYS	8.1
1	A	422	LEU	8.1
1	B	310	ASN	7.9
1	B	211	THR	7.9
1	B	376	LEU	7.8
1	B	202	ARG	7.8
1	B	273	LYS	7.7
1	B	212	TRP	7.6
1	B	409	TYR	7.6
1	B	196	LYS	7.4
1	B	391	LEU	7.4
1	B	338	ASN	7.4
1	B	422	LEU	7.3
1	A	372	ARG	7.3
1	A	282	ASN	7.3
1	B	299	GLN	7.3
1	B	190	LEU	7.3
1	B	298	VAL	7.0
1	B	361	TRP	7.0
1	A	190	LEU	7.0
1	A	418	GLU	6.9
1	A	341	VAL	6.9
1	A	280	PHE	6.8
1	A	221	LEU	6.8
1	A	324	LYS	6.8
1	B	418	GLU	6.7
1	A	326	TYR	6.7
1	B	238	PHE	6.7
1	B	227	VAL	6.7
1	A	263	LYS	6.6
1	B	265	ALA	6.6
1	A	424	GLY	6.6
1	A	216	ARG	6.6
1	B	300	PHE	6.5
1	B	404	ASP	6.5
1	A	224	LEU	6.5
1	B	261	THR	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	182	SER	6.5
1	B	336	SER	6.5
1	A	368	PHE	6.5
1	B	208	GLN	6.5
1	A	339	ARG	6.5
1	A	405	ILE	6.4
1	B	399	ILE	6.4
1	A	191	THR	6.3
1	B	415	PHE	6.3
1	A	400	ILE	6.3
1	A	212	TRP	6.2
1	A	348	LEU	6.2
1	A	382	ARG	6.1
1	B	356	VAL	6.1
1	B	420	GLN	6.1
1	A	347	TYR	6.1
1	B	264	ILE	6.0
1	B	271	ALA	6.0
1	A	240	GLU	6.0
1	A	210	ARG	6.0
1	A	421	ALA	6.0
1	B	331	LYS	5.9
1	A	182	SER	5.9
1	A	391	LEU	5.9
1	A	264	ILE	5.9
1	A	222	PHE	5.9
1	A	211	THR	5.8
1	A	377	ALA	5.8
1	B	382	ARG	5.8
1	B	256	TYR	5.7
1	B	267	LYS	5.7
1	A	188	ALA	5.7
1	A	289	CYS	5.7
1	A	365	ALA	5.7
1	B	332	ILE	5.7
1	B	407	GLU	5.7
1	B	326	TYR	5.6
1	B	340	GLU	5.6
1	A	340	GLU	5.6
1	B	225	GLU	5.6
1	B	269	PHE	5.5
1	A	351	THR	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	361	TRP	5.5
1	A	360	LEU	5.5
1	B	301	ASP	5.5
1	A	302	PHE	5.4
1	B	283	GLU	5.4
1	A	276	TYR	5.4
1	A	336	SER	5.4
1	A	220	LYS	5.4
1	A	367	LYS	5.4
1	B	197	TRP	5.3
1	A	197	TRP	5.3
1	A	265	ALA	5.3
1	B	285	SER	5.3
1	B	226	LEU	5.3
1	A	243	ASP	5.3
1	A	253	LYS	5.3
1	A	306	ASP	5.2
1	A	355	VAL	5.2
1	B	347	TYR	5.2
1	B	346	ILE	5.2
1	A	286	VAL	5.2
1	B	366	ASP	5.2
1	A	250	GLU	5.2
1	A	346	ILE	5.2
1	B	320	ILE	5.2
1	A	233	ILE	5.1
1	A	254	VAL	5.1
1	A	310	ASN	5.1
1	A	342	ALA	5.1
1	B	355	VAL	5.1
1	B	364	ASP	5.1
1	A	296	PRO	5.1
1	A	314	ASP	5.1
1	B	302	PHE	5.1
1	B	412	ARG	5.0
1	A	385	ASP	5.0
1	B	426	SER	5.0
1	B	323	CYS	5.0
1	B	311	LYS	5.0
1	A	410	LYS	4.9
1	A	384	SER	4.9
1	B	309	GLU	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	255	TYR	4.9
1	B	215	SER	4.8
1	B	223	SER	4.8
1	B	344	ARG	4.8
1	A	199	ILE	4.8
1	B	209	ILE	4.8
1	B	224	LEU	4.8
1	B	389	ARG	4.8
1	B	220	LYS	4.8
1	B	249	ILE	4.7
1	B	213	SER	4.7
1	B	348	LEU	4.7
1	B	234	ARG	4.7
1	A	419	GLY	4.7
1	A	230	SER	4.7
1	B	367	LYS	4.7
1	B	229	GLU	4.7
1	B	243	ASP	4.6
1	B	306	ASP	4.6
1	A	387	GLY	4.6
1	A	334	VAL	4.6
1	B	317	VAL	4.6
1	A	189	SER	4.6
1	A	320	ILE	4.6
1	A	323	CYS	4.5
1	A	319	ILE	4.5
1	B	218	GLU	4.5
1	A	357	THR	4.5
1	A	343	LYS	4.5
1	B	282	ASN	4.5
1	B	365	ALA	4.5
1	A	415	PHE	4.5
1	B	316	LEU	4.4
1	A	408	ALA	4.4
1	A	354	LYS	4.4
1	A	300	PHE	4.4
1	B	414	TRP	4.4
1	A	187	ILE	4.4
1	A	331	LYS	4.4
1	A	292	ASP	4.4
1	A	399	ILE	4.4
1	B	210	ARG	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	417	ALA	4.3
1	A	206	LYS	4.3
1	B	221	LEU	4.3
1	B	246	PHE	4.3
1	A	248	LEU	4.3
1	A	344	ARG	4.3
1	A	193	TYR	4.3
1	B	330	THR	4.3
1	B	181	MET	4.3
1	A	366	ASP	4.2
1	A	244	LYS	4.2
1	A	261	THR	4.2
1	B	284	THR	4.2
1	A	209	ILE	4.2
1	A	257	PHE	4.2
1	B	270	THR	4.2
1	B	329	ALA	4.2
1	A	290	GLU	4.2
1	B	281	ASN	4.2
1	B	314	ASP	4.2
1	A	271	ALA	4.2
1	B	262	LEU	4.1
1	A	269	PHE	4.1
1	A	278	MET	4.1
1	B	307	ASP	4.1
1	B	324	LYS	4.1
1	A	313	LYS	4.1
1	B	322	ILE	4.1
1	A	329	ALA	4.1
1	A	414	TRP	4.0
1	B	386	PHE	4.0
1	A	349	MET	4.0
1	B	385	ASP	4.0
1	A	208	GLN	4.0
1	A	298	VAL	4.0
1	A	196	LYS	4.0
1	B	244	LYS	4.0
1	B	375	VAL	4.0
1	A	378	ILE	4.0
1	A	376	LEU	4.0
1	A	321	GLY	4.0
1	A	379	LYS	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	205	ASN	4.0
1	B	259	LYS	4.0
1	A	308	LEU	4.0
1	A	389	ARG	3.9
1	A	373	GLN	3.9
1	B	266	ASN	3.9
1	A	225	GLU	3.9
1	B	319	ILE	3.9
1	A	186	PRO	3.9
1	B	363	GLU	3.9
1	B	313	LYS	3.9
1	B	308	LEU	3.9
1	A	258	SER	3.9
1	A	417	ALA	3.9
1	A	283	GLU	3.9
1	A	394	LEU	3.9
1	A	407	GLU	3.8
1	A	194	GLN	3.8
1	B	275	ASP	3.8
1	B	288	PRO	3.8
1	B	358	ALA	3.8
1	A	266	ASN	3.8
1	B	335	ARG	3.8
1	A	332	ILE	3.8
1	A	201	ALA	3.8
1	B	368	PHE	3.8
1	B	341	VAL	3.8
1	A	359	THR	3.8
1	B	222	PHE	3.7
1	A	380	GLY	3.7
1	A	345	ASN	3.7
1	B	277	GLU	3.7
1	A	294	HIS	3.7
1	B	325	SER	3.7
1	A	229	GLU	3.7
1	A	356	VAL	3.7
1	B	241	GLN	3.7
1	B	398	THR	3.6
1	A	181	MET	3.6
1	A	217	GLY	3.6
1	B	343	LYS	3.6
1	A	288	PRO	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	297	THR	3.6
1	A	311	LYS	3.6
1	B	373	GLN	3.6
1	B	400	ILE	3.6
1	B	333	THR	3.5
1	B	245	PHE	3.5
1	B	369	ASP	3.5
1	A	226	LEU	3.5
1	B	374	PRO	3.5
1	A	284	THR	3.5
1	B	354	LYS	3.5
1	B	252	ASN	3.5
1	B	345	ASN	3.5
1	A	393	VAL	3.5
1	B	403	PRO	3.5
1	B	236	THR	3.5
1	B	381	ALA	3.5
1	A	363	GLU	3.5
1	A	262	LEU	3.5
1	B	410	LYS	3.5
1	A	322	ILE	3.5
1	B	305	ILE	3.5
1	A	227	VAL	3.5
1	A	325	SER	3.5
1	B	263	LYS	3.4
1	A	398	THR	3.4
1	A	238	PHE	3.4
1	B	233	ILE	3.4
1	A	251	VAL	3.3
1	A	423	ASP	3.3
1	B	321	GLY	3.3
1	B	193	TYR	3.3
1	A	236	THR	3.3
1	B	253	LYS	3.3
1	B	235	ALA	3.3
1	A	364	ASP	3.3
1	B	276	TYR	3.3
1	A	272	VAL	3.3
1	A	358	ALA	3.3
1	B	287	MET	3.3
1	A	404	ASP	3.3
1	A	219	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	194	GLN	3.3
1	B	423	ASP	3.2
1	B	424	GLY	3.2
1	A	223	SER	3.2
1	A	293	HIS	3.2
1	A	309	GLU	3.2
1	A	260	GLY	3.2
1	A	279	THR	3.2
1	A	350	ASP	3.2
1	A	402	ASN	3.2
1	A	409	TYR	3.2
1	B	239	ASN	3.1
1	A	305	ILE	3.1
1	B	237	ALA	3.1
1	B	393	VAL	3.1
1	A	291	ASP	3.1
1	A	412	ARG	3.1
1	B	402	ASN	3.1
1	B	279	THR	3.1
1	A	277	GLU	3.1
1	B	342	ALA	3.1
1	B	379	LYS	3.1
1	A	287	MET	3.1
1	B	349	MET	3.0
1	A	416	ASP	3.0
1	A	406	PRO	3.0
1	B	406	PRO	3.0
1	B	360	LEU	3.0
1	B	380	GLY	3.0
1	B	240	GLU	3.0
1	A	330	THR	3.0
1	A	397	SER	3.0
1	A	235	ALA	3.0
1	A	375	VAL	3.0
1	B	327	GLU	3.0
1	A	228	ASP	3.0
1	A	301	ASP	3.0
1	A	232	GLU	3.0
1	A	327	GLU	3.0
1	A	215	SER	2.9
1	A	371	SER	2.9
1	A	234	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	273	LYS	2.9
1	A	249	ILE	2.9
1	A	299	GLN	2.9
1	A	214	ASN	2.9
1	A	362	GLY	2.9
1	A	205	ASN	2.8
1	A	242	VAL	2.8
1	B	328	ASP	2.8
1	A	207	SER	2.8
1	A	268	GLN	2.8
1	B	219	GLY	2.8
1	B	230	SER	2.8
1	A	295	LEU	2.8
1	A	231	GLY	2.8
1	B	186	PRO	2.8
1	B	201	ALA	2.8
1	A	281	ASN	2.8
1	B	408	ALA	2.8
1	B	392	SER	2.8
1	A	353	GLY	2.7
1	A	411	LEU	2.7
1	A	318	ASP	2.7
1	A	270	THR	2.7
1	A	275	ASP	2.7
1	A	204	THR	2.7
1	A	317	VAL	2.7
1	A	333	THR	2.7
1	B	357	THR	2.7
1	A	184	VAL	2.7
1	B	337	ASN	2.7
1	A	352	SER	2.7
1	A	381	ALA	2.7
1	B	183	LYS	2.7
1	A	390	SER	2.6
1	A	237	ALA	2.6
1	B	405	ILE	2.6
1	B	334	VAL	2.6
1	B	191	THR	2.6
1	B	411	LEU	2.6
1	A	259	LYS	2.6
1	B	397	SER	2.5
1	B	350	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	362	GLY	2.5
1	A	255	TYR	2.5
1	B	351	THR	2.5
1	A	303	THR	2.5
1	B	359	THR	2.5
1	A	267	LYS	2.4
1	B	198	THR	2.4
1	A	396	SER	2.4
1	A	328	ASP	2.4
1	A	274	ASN	2.4
1	B	278	MET	2.4
1	B	254	VAL	2.4
1	A	245	PHE	2.4
1	A	202	ARG	2.3
1	A	192	PRO	2.3
1	A	246	PHE	2.3
1	B	258	SER	2.2
1	A	338	ASN	2.2
1	A	315	SER	2.2
1	A	213	SER	2.2
1	B	187	ILE	2.2
1	A	386	PHE	2.2
1	B	401	ALA	2.2
1	B	268	GLN	2.2
1	A	316	LEU	2.2
1	B	207	SER	2.1
1	A	203	VAL	2.1
1	A	395	SER	2.1
1	A	388	GLY	2.1
1	A	392	SER	2.1
1	B	247	PRO	2.1
1	A	374	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

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.