



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2017 – 04:19 AM EDT

PDB ID : 2RKW
Title : Intermediate position of ATP on its trail to the binding pocket inside the subunit B mutant R416W of the energy converter A1Ao ATP synthase
Authors : Kumar, A.; Manimekalai, M.S.S.; Balakrishna, A.M.; Hunke, C.; Gruber, G.
Deposited on : unknown
Resolution : 2.81 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

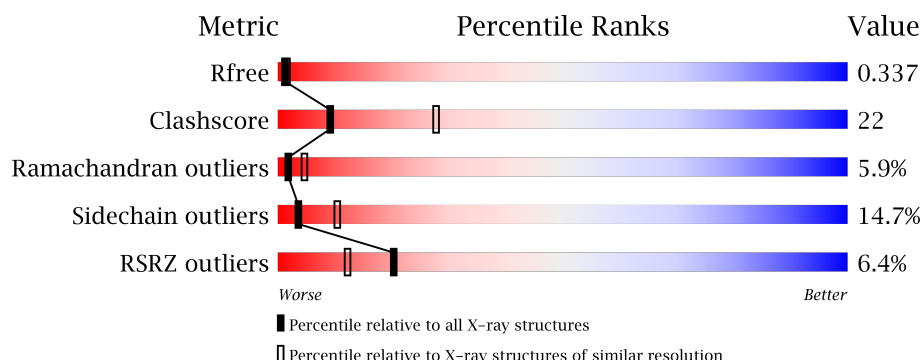
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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}	100719	2917 (2.84-2.80)
Clashscore	112137	3382 (2.84-2.80)
Ramachandran outliers	110173	3324 (2.84-2.80)
Sidechain outliers	110143	3326 (2.84-2.80)
RSRZ outliers	101464	2948 (2.84-2.80)

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	469	<div> <div>6%</div> <div> <div></div> <div>52%</div> <div>29%</div> <div>9%</div> <div>10%</div> </div> </div>
1	B	469	<div> <div>5%</div> <div> <div></div> <div>48%</div> <div>32%</div> <div>8%</div> <div>10%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6512 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 V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3257	2066	561	619	11			
1	B	422	Total	C	N	O	S	0	0	0
			3255	2062	562	620	11			

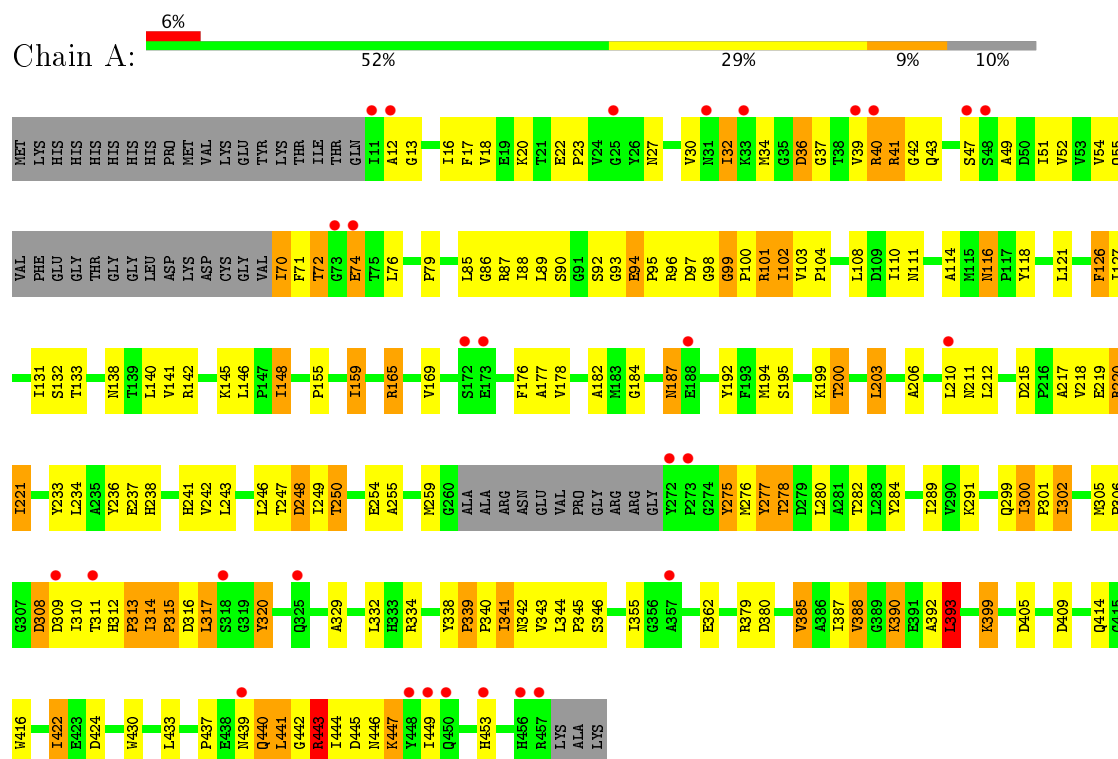
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	EXPRESSION TAG	UNP Q60187
A	-7	LYS	-	EXPRESSION TAG	UNP Q60187
A	-6	HIS	-	EXPRESSION TAG	UNP Q60187
A	-5	HIS	-	EXPRESSION TAG	UNP Q60187
A	-4	HIS	-	EXPRESSION TAG	UNP Q60187
A	-3	HIS	-	EXPRESSION TAG	UNP Q60187
A	-2	HIS	-	EXPRESSION TAG	UNP Q60187
A	-1	HIS	-	EXPRESSION TAG	UNP Q60187
A	0	PRO	-	EXPRESSION TAG	UNP Q60187
A	2	VAL	ALA	SEE REMARK 999	UNP Q60187
A	416	TRP	ARG	ENGINEERED	UNP Q60187
B	-8	MET	-	EXPRESSION TAG	UNP Q60187
B	-7	LYS	-	EXPRESSION TAG	UNP Q60187
B	-6	HIS	-	EXPRESSION TAG	UNP Q60187
B	-5	HIS	-	EXPRESSION TAG	UNP Q60187
B	-4	HIS	-	EXPRESSION TAG	UNP Q60187
B	-3	HIS	-	EXPRESSION TAG	UNP Q60187
B	-2	HIS	-	EXPRESSION TAG	UNP Q60187
B	-1	HIS	-	EXPRESSION TAG	UNP Q60187
B	0	PRO	-	EXPRESSION TAG	UNP Q60187
B	2	VAL	ALA	SEE REMARK 999	UNP Q60187
B	416	TRP	ARG	ENGINEERED	UNP Q60187

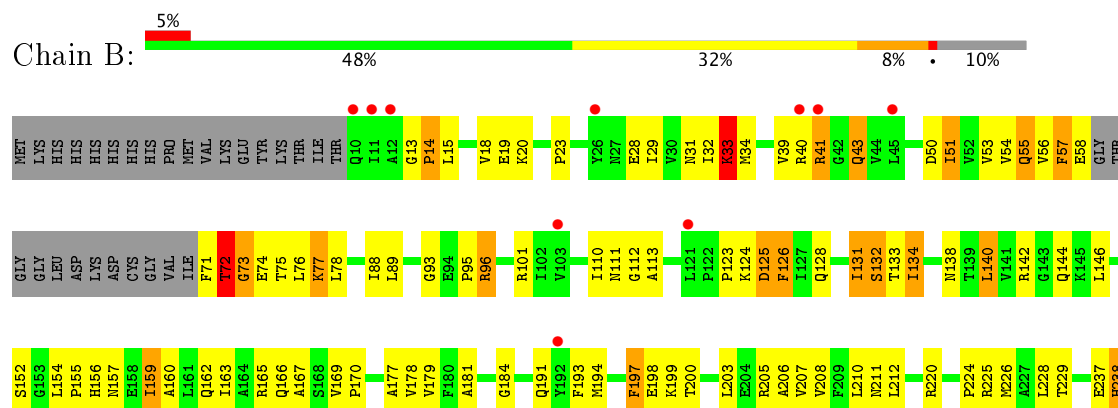
3 Residue-property plots

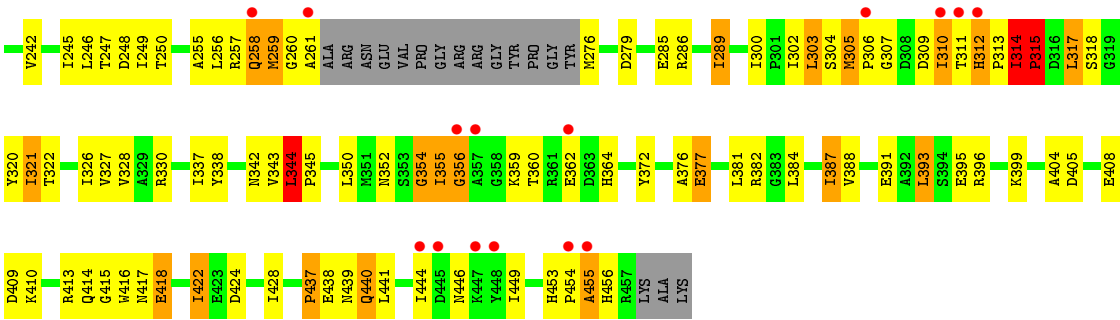
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: V-type ATP synthase beta chain



• Molecule 1: V-type ATP synthase beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.05Å 96.09Å 129.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.73 – 2.81 34.15 – 2.81	Depositor EDS
% Data completeness (in resolution range)	86.9 (34.73-2.81) 86.9 (34.15-2.81)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.271 , 0.330 0.269 , 0.337	Depositor DCC
R_{free} test set	1032 reflections (5.45%)	DCC
Wilson B-factor (Å ²)	80.2	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6512	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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 [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	0.39	0/3320	0.63	1/4504 (0.0%)
1	B	0.41	0/3316	0.63	0/4497
All	All	0.40	0/6636	0.63	1/9001 (0.0%)

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	B	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	393	LEU	CA-CB-CG	5.48	127.90	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	314	ILE	Peptide
1	B	315	PRO	Peptide
1	B	344	LEU	Peptide

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	3257	0	3259	130	0
1	B	3255	0	3257	166	0
All	All	6512	0	6516	288	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 22.

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:B:71:PHE:HA	1:B:72:THR:HB	1.21	1.16
1:B:41:ARG:HB3	1:B:56:VAL:CG2	1.87	1.05
1:A:314:ILE:HB	1:A:315:PRO:HA	1.38	1.04
1:B:71:PHE:HA	1:B:72:THR:CB	1.87	1.03
1:A:99:GLY:H	1:A:100:PRO:HD3	1.20	1.02
1:A:339:PRO:HB2	1:A:340:PRO:HA	1.48	0.95
1:B:343:VAL:O	1:B:345:PRO:HD2	1.67	0.94
1:B:41:ARG:CB	1:B:56:VAL:HG21	1.97	0.94
1:B:156:HIS:HD2	1:B:302:ILE:HD12	1.33	0.93
1:B:41:ARG:HB3	1:B:56:VAL:HG21	1.48	0.90
1:B:312:HIS:HB3	1:B:313:PRO:C	1.91	0.90
1:A:94:GLU:HB3	1:A:95:PRO:HD3	1.54	0.90
1:B:134:ILE:HD11	1:B:140:LEU:HB2	1.55	0.89
1:B:248:ASP:H	1:B:302:ILE:HG12	1.37	0.87
1:B:289:ILE:H	1:B:289:ILE:HD12	1.39	0.87
1:A:99:GLY:H	1:A:100:PRO:CD	1.87	0.85
1:A:249:ILE:HD11	1:A:301:PRO:HB2	1.58	0.84
1:B:56:VAL:HG22	1:B:57:PHE:H	1.41	0.84
1:B:77:LYS:H	1:B:77:LYS:HD3	1.43	0.83
1:A:311:THR:C	1:A:313:PRO:HD2	1.99	0.82
1:B:156:HIS:CD2	1:B:302:ILE:HD12	2.13	0.81
1:A:339:PRO:HB2	1:A:340:PRO:CA	2.11	0.80
1:B:152:SER:HB2	1:B:306:PRO:HA	1.63	0.80
1:B:220:ARG:HD2	1:B:255:ALA:HB2	1.64	0.79
1:B:142:ARG:NH2	1:B:169:VAL:HB	1.99	0.78
1:B:142:ARG:HH21	1:B:169:VAL:HB	1.47	0.78
1:A:145:LYS:HD3	1:A:284:TYR:O	1.84	0.78
1:A:444:ILE:HG13	1:A:449:ILE:HD11	1.66	0.77
1:B:310:ILE:HG13	1:B:311:THR:H	1.49	0.76
1:A:99:GLY:N	1:A:100:PRO:HD3	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ASP:H	1:B:302:ILE:CG1	2.00	0.75
1:A:131:ILE:HA	1:A:414:GLN:HE22	1.52	0.75
1:B:71:PHE:CA	1:B:72:THR:CB	2.63	0.74
1:B:315:PRO:CG	1:B:317:LEU:HD13	2.17	0.74
1:B:41:ARG:HB3	1:B:56:VAL:HG22	1.67	0.74
1:B:179:VAL:HG22	1:B:207:VAL:HG22	1.69	0.73
1:A:314:ILE:HB	1:A:315:PRO:CA	2.17	0.73
1:B:184:GLY:H	1:B:211:ASN:HD22	1.37	0.73
1:B:197:PHE:O	1:B:199:LYS:N	2.22	0.73
1:B:354:GLY:HA2	1:B:359:LYS:HD2	1.71	0.72
1:A:184:GLY:H	1:A:211:ASN:HD22	1.36	0.72
1:B:71:PHE:CA	1:B:72:THR:HB	2.08	0.72
1:A:339:PRO:HB3	1:A:341:ILE:HD13	1.71	0.72
1:A:146:LEU:O	1:A:300:ILE:HD12	1.91	0.71
1:B:54:VAL:HG13	1:B:55:GLN:N	2.06	0.70
1:A:440:GLN:OE1	1:A:441:LEU:HB2	1.91	0.70
1:B:41:ARG:HB2	1:B:56:VAL:HG21	1.72	0.70
1:A:312:HIS:N	1:A:313:PRO:HD2	2.07	0.68
1:A:422:ILE:H	1:A:422:ILE:HD13	1.58	0.67
1:B:33:LYS:HG3	1:B:74:GLU:HA	1.77	0.67
1:B:343:VAL:C	1:B:345:PRO:HD2	2.15	0.67
1:B:309:ASP:OD2	1:B:314:ILE:HG23	1.95	0.66
1:B:315:PRO:HG2	1:B:317:LEU:HD13	1.75	0.66
1:A:443:ARG:HG3	1:A:444:ILE:HG23	1.76	0.66
1:B:250:THR:HG21	1:B:304:SER:O	1.95	0.66
1:B:71:PHE:N	1:B:72:THR:HG1	1.94	0.66
1:A:17:PHE:HB2	1:A:110:ILE:HD11	1.78	0.66
1:A:192:TYR:HA	1:A:195:SER:OG	1.95	0.65
1:B:32:ILE:HG12	1:B:73:GLY:HA3	1.76	0.65
1:A:155:PRO:O	1:A:159:ILE:HG23	1.97	0.65
1:B:51:ILE:HG21	1:B:76:LEU:HD22	1.78	0.64
1:B:409:ASP:O	1:B:413:ARG:HB3	1.97	0.64
1:A:86:GLY:HA2	1:A:203:LEU:O	1.97	0.64
1:A:133:THR:OG1	1:A:341:ILE:HD11	1.97	0.63
1:B:166:GLN:NE2	1:B:417:ASN:O	2.31	0.63
1:B:146:LEU:O	1:B:300:ILE:HG22	1.98	0.63
1:B:33:LYS:HZ2	1:B:75:THR:HG22	1.62	0.63
1:A:343:VAL:HA	1:A:346:SER:HB2	1.81	0.62
1:A:93:GLY:O	1:A:94:GLU:HB2	1.98	0.62
1:B:260:GLY:O	1:B:276:MET:N	2.33	0.62
1:B:309:ASP:OD1	1:B:312:HIS:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:PHE:O	1:B:142:ARG:NH1	2.34	0.61
1:B:156:HIS:HD2	1:B:302:ILE:CD1	2.12	0.60
1:A:329:ALA:HB2	1:A:342:ASN:HB2	1.82	0.60
1:A:332:LEU:HB3	1:A:340:PRO:HB2	1.83	0.60
1:B:54:VAL:HG13	1:B:55:GLN:H	1.66	0.60
1:B:259:MET:HG2	1:B:312:HIS:CE1	2.37	0.60
1:B:276:MET:HA	1:B:279:ASP:HB3	1.83	0.60
1:B:312:HIS:CB	1:B:313:PRO:CA	2.80	0.60
1:B:39:VAL:HG22	1:B:40:ARG:N	2.17	0.60
1:A:250:THR:HG23	1:A:317:LEU:HD11	1.82	0.60
1:A:387:ILE:HG13	1:B:112:GLY:HA3	1.83	0.59
1:A:310:ILE:HG13	1:A:313:PRO:HG3	1.84	0.59
1:B:181:ALA:HB3	1:B:246:LEU:HD23	1.84	0.59
1:A:40:ARG:HA	1:A:40:ARG:NE	2.16	0.59
1:A:306:PRO:HB3	1:A:310:ILE:HD11	1.84	0.59
1:A:30:VAL:O	1:A:42:GLY:HA3	2.02	0.59
1:B:77:LYS:N	1:B:77:LYS:HD3	2.16	0.59
1:A:306:PRO:HB2	1:A:313:PRO:HB3	1.86	0.58
1:B:32:ILE:C	1:B:39:VAL:HG21	2.24	0.58
1:B:312:HIS:HB3	1:B:313:PRO:CA	2.34	0.58
1:B:404:ALA:O	1:B:408:GLU:HG2	2.04	0.58
1:B:155:PRO:O	1:B:159:ILE:HG23	2.04	0.57
1:B:381:LEU:HD23	1:B:384:LEU:HD21	1.86	0.57
1:B:382:ARG:HH22	1:B:408:GLU:CD	2.08	0.57
1:B:32:ILE:CD1	1:B:72:THR:HG23	2.35	0.56
1:A:442:GLY:C	1:A:444:ILE:H	2.08	0.56
1:A:18:VAL:HB	1:A:52:VAL:HG23	1.87	0.56
1:A:96:ARG:NH2	1:A:215:ASP:OD1	2.37	0.56
1:A:234:LEU:O	1:A:238:HIS:HB2	2.06	0.56
1:B:20:LYS:HE2	1:B:23:PRO:HA	1.87	0.56
1:B:453:HIS:O	1:B:455:ALA:N	2.35	0.56
1:B:258:GLN:HB3	1:B:259:MET:HG3	1.88	0.56
1:B:124:LYS:O	1:B:142:ARG:HB2	2.06	0.56
1:B:360:THR:HB	1:B:422:ILE:HG21	1.88	0.55
1:A:246:LEU:CD1	1:A:299:GLN:HE21	2.18	0.55
1:B:438:GLU:O	1:B:440:GLN:N	2.35	0.55
1:B:258:GLN:HG3	1:B:259:MET:HE3	1.88	0.55
1:B:312:HIS:CG	1:B:314:ILE:HG22	2.42	0.55
1:A:442:GLY:O	1:A:444:ILE:HG12	2.06	0.55
1:B:157:ASN:OD1	1:B:247:THR:OG1	2.21	0.55
1:A:211:ASN:ND2	1:A:220:ARG:HG3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ASN:O	1:A:447:LYS:HG2	2.07	0.55
1:B:312:HIS:CB	1:B:313:PRO:C	2.72	0.55
1:A:314:ILE:HG21	1:B:330:ARG:HE	1.72	0.54
1:A:233:TYR:O	1:A:237:GLU:HB2	2.07	0.54
1:B:89:LEU:HB3	1:B:93:GLY:HA2	1.88	0.54
1:B:54:VAL:CG1	1:B:55:GLN:N	2.70	0.54
1:B:152:SER:CB	1:B:306:PRO:HA	2.36	0.54
1:B:54:VAL:CG1	1:B:55:GLN:H	2.21	0.54
1:B:152:SER:O	1:B:330:ARG:NH2	2.42	0.53
1:A:79:PRO:HG3	1:A:101:ARG:HH12	1.72	0.53
1:A:126:PHE:HA	1:A:141:VAL:HA	1.90	0.53
1:B:32:ILE:HG12	1:B:73:GLY:CA	2.38	0.53
1:A:278:THR:O	1:A:282:THR:HG23	2.08	0.53
1:B:437:PRO:HB2	1:B:440:GLN:HE22	1.72	0.53
1:B:128:GLN:O	1:B:167:ALA:HA	2.09	0.53
1:B:384:LEU:O	1:B:388:VAL:HG22	2.09	0.53
1:B:387:ILE:HG13	1:B:388:VAL:HG13	1.90	0.53
1:B:41:ARG:HG2	1:B:57:PHE:O	2.08	0.53
1:A:248:ASP:OD1	1:A:248:ASP:C	2.47	0.52
1:B:256:LEU:O	1:B:257:ARG:C	2.47	0.52
1:A:127:ILE:HB	1:A:140:LEU:HD23	1.91	0.52
1:A:306:PRO:HG2	1:A:313:PRO:HA	1.92	0.52
1:B:32:ILE:HG21	1:B:73:GLY:HA3	1.92	0.52
1:A:312:HIS:N	1:A:313:PRO:CD	2.73	0.52
1:B:162:GLN:HE22	1:B:338:TYR:HE2	1.56	0.52
1:B:417:ASN:O	1:B:418:GLU:C	2.48	0.52
1:B:228:LEU:HD13	1:B:286:ARG:HB2	1.92	0.51
1:B:309:ASP:HB3	1:B:313:PRO:HA	1.92	0.51
1:A:380:ASP:HB3	1:B:285:GLU:HG2	1.92	0.51
1:A:339:PRO:CB	1:A:341:ILE:HD13	2.40	0.51
1:B:128:GLN:NE2	1:B:422:ILE:H	2.09	0.51
1:A:345:PRO:HG3	1:B:318:SER:HB2	1.93	0.51
1:B:343:VAL:O	1:B:345:PRO:CD	2.52	0.51
1:B:31:ASN:HA	1:B:41:ARG:O	2.11	0.51
1:B:110:ILE:HG21	1:B:226:MET:HG2	1.93	0.51
1:A:70:ILE:HD12	1:A:71:PHE:H	1.75	0.51
1:A:316:ASP:HB2	1:B:330:ARG:HB2	1.92	0.51
1:B:310:ILE:HG13	1:B:311:THR:N	2.22	0.50
1:A:89:LEU:HD12	1:A:94:GLU:HG3	1.93	0.50
1:A:248:ASP:HB2	1:A:302:ILE:HG13	1.93	0.50
1:B:312:HIS:CD2	1:B:314:ILE:HG22	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLY:HA3	1:A:220:ARG:NH2	2.26	0.50
1:A:218:VAL:HA	1:A:221:ILE:CD1	2.42	0.50
1:A:299:GLN:NE2	1:A:320:TYR:OH	2.45	0.50
1:B:352:ASN:HA	1:B:355:ILE:HG21	1.94	0.50
1:A:182:ALA:HA	1:A:247:THR:O	2.12	0.50
1:B:33:LYS:NZ	1:B:75:THR:HG22	2.27	0.49
1:A:116:ASN:O	1:A:291:LYS:HE3	2.11	0.49
1:A:118:TYR:O	1:A:291:LYS:HE2	2.12	0.49
1:A:51:ILE:HD11	1:A:92:SER:HB2	1.94	0.49
1:A:54:VAL:HG12	1:A:55:GLN:N	2.28	0.49
1:B:289:ILE:HD12	1:B:289:ILE:N	2.17	0.49
1:B:260:GLY:HA3	1:B:261:ALA:C	2.32	0.49
1:B:446:ASN:HA	1:B:449:ILE:HG12	1.94	0.49
1:B:88:ILE:HG23	1:B:208:VAL:HB	1.94	0.49
1:B:384:LEU:HA	1:B:387:ILE:HG23	1.94	0.49
1:B:441:LEU:O	1:B:444:ILE:HG22	2.13	0.48
1:A:388:VAL:HG13	1:A:392:ALA:HB3	1.95	0.48
1:A:344:LEU:HB3	1:B:322:THR:HA	1.95	0.48
1:B:125:ASP:C	1:B:142:ARG:HH11	2.17	0.48
1:A:437:PRO:HB2	1:A:440:GLN:HG3	1.95	0.48
1:B:225:ARG:O	1:B:229:THR:OG1	2.20	0.48
1:A:275:TYR:HD1	1:A:277:TYR:O	1.97	0.48
1:A:301:PRO:HG3	1:A:320:TYR:CE2	2.49	0.48
1:B:327:VAL:HG21	1:B:345:PRO:HB2	1.96	0.48
1:B:154:LEU:HD13	1:B:328:VAL:HG12	1.95	0.48
1:A:148:ILE:HG22	1:A:300:ILE:HD11	1.96	0.48
1:A:87:ARG:NH1	1:A:97:ASP:OD2	2.47	0.48
1:B:126:PHE:HE1	1:B:170:PRO:HG2	1.79	0.48
1:B:165:ARG:HD2	1:B:200:THR:HG21	1.95	0.47
1:B:131:ILE:HG13	1:B:134:ILE:HG23	1.96	0.47
1:B:303:LEU:HB3	1:B:317:LEU:HD23	1.96	0.47
1:A:99:GLY:N	1:A:100:PRO:CD	2.64	0.47
1:B:321:ILE:HG13	1:B:321:ILE:O	2.14	0.47
1:A:131:ILE:HA	1:A:414:GLN:NE2	2.25	0.47
1:B:131:ILE:HG13	1:B:131:ILE:O	2.15	0.47
1:B:32:ILE:HD13	1:B:72:THR:HG23	1.96	0.47
1:A:399:LYS:HG3	1:A:437:PRO:HD3	1.96	0.47
1:A:442:GLY:C	1:A:444:ILE:N	2.68	0.47
1:A:390:LYS:HD3	1:B:58:GLU:HB3	1.96	0.47
1:B:312:HIS:HB3	1:B:314:ILE:N	2.29	0.47
1:B:391:GLU:C	1:B:393:LEU:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:TRP:HA	1:A:433:LEU:HD12	1.97	0.46
1:B:377:GLU:OE2	1:B:396:ARG:NH2	2.44	0.46
1:B:391:GLU:C	1:B:393:LEU:N	2.68	0.46
1:A:249:ILE:CD1	1:A:301:PRO:HB2	2.37	0.46
1:B:193:PHE:O	1:B:197:PHE:HD1	1.99	0.46
1:B:384:LEU:HB2	1:B:387:ILE:HG12	1.98	0.46
1:B:424:ASP:O	1:B:428:ILE:HG12	2.16	0.46
1:B:258:GLN:HA	1:B:258:GLN:NE2	2.30	0.45
1:B:160:ALA:O	1:B:163:ILE:HG12	2.15	0.45
1:B:191:GLN:HA	1:B:194:MET:HB3	1.98	0.45
1:A:344:LEU:HD21	1:A:379:ARG:HD3	1.99	0.45
1:B:184:GLY:N	1:B:211:ASN:HD22	2.10	0.45
1:B:310:ILE:CG1	1:B:311:THR:H	2.24	0.45
1:B:56:VAL:HG22	1:B:57:PHE:N	2.19	0.45
1:A:32:ILE:HB	1:A:74:GLU:O	2.17	0.45
1:A:108:LEU:HD22	1:A:114:ALA:HB1	1.98	0.45
1:A:236:TYR:O	1:A:237:GLU:HB2	2.15	0.45
1:A:47:SER:HA	1:A:52:VAL:HG12	1.98	0.45
1:B:39:VAL:HG22	1:B:40:ARG:H	1.81	0.45
1:A:316:ASP:OD1	1:B:330:ARG:N	2.46	0.45
1:A:177:ALA:HB3	1:A:242:VAL:HG22	2.00	0.44
1:A:249:ILE:HD11	1:A:301:PRO:CB	2.39	0.44
1:A:32:ILE:N	1:A:32:ILE:HD13	2.31	0.44
1:A:399:LYS:HE3	1:A:399:LYS:HB3	1.75	0.44
1:A:92:SER:HB3	1:A:219:GLU:CD	2.38	0.44
1:A:51:ILE:HG12	1:A:76:LEU:HD22	1.99	0.44
1:B:126:PHE:CE1	1:B:170:PRO:HG2	2.52	0.44
1:A:338:TYR:HA	1:A:339:PRO:C	2.38	0.44
1:A:339:PRO:CB	1:A:340:PRO:CA	2.92	0.44
1:A:405:ASP:O	1:A:409:ASP:HB2	2.18	0.44
1:A:94:GLU:HB3	1:A:95:PRO:CD	2.34	0.44
1:B:18:VAL:HG12	1:B:19:GLU:N	2.33	0.43
1:B:96:ARG:HH12	1:B:212:LEU:HG	1.83	0.43
1:A:233:TYR:O	1:A:236:TYR:O	2.36	0.43
1:A:315:PRO:HG2	1:A:317:LEU:HD21	2.00	0.43
1:A:390:LYS:HD2	1:A:390:LYS:H	1.83	0.43
1:B:32:ILE:HA	1:B:39:VAL:HG11	2.00	0.43
1:B:344:LEU:HD23	1:B:376:ALA:HB2	1.98	0.43
1:B:438:GLU:HG3	1:B:441:LEU:HD12	1.99	0.43
1:A:218:VAL:HA	1:A:221:ILE:HD13	1.99	0.43
1:A:103:VAL:HA	1:A:104:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:VAL:HG23	1:A:393:LEU:HD21	2.01	0.43
1:A:247:THR:HA	1:A:248:ASP:HA	1.68	0.43
1:B:177:ALA:O	1:B:242:VAL:HA	2.18	0.43
1:A:385:VAL:HG23	1:A:393:LEU:CD2	2.48	0.43
1:A:93:GLY:O	1:A:94:GLU:CB	2.64	0.43
1:B:110:ILE:HG13	1:B:111:ASN:N	2.34	0.43
1:B:72:THR:HA	1:B:73:GLY:HA3	1.71	0.43
1:B:337:ILE:HG22	1:B:413:ARG:NH2	2.34	0.43
1:A:338:TYR:CD1	1:A:339:PRO:O	2.71	0.43
1:A:178:VAL:O	1:A:206:ALA:HA	2.19	0.43
1:A:40:ARG:HA	1:A:40:ARG:CZ	2.47	0.43
1:B:238:HIS:HD1	1:B:238:HIS:N	2.17	0.43
1:A:34:MET:HB2	1:A:36:ASP:O	2.19	0.42
1:A:98:GLY:HA2	1:A:99:GLY:HA3	1.81	0.42
1:A:20:LYS:HE3	1:A:23:PRO:HA	2.01	0.42
1:B:159:ILE:HG22	1:B:338:TYR:CE1	2.54	0.42
1:A:187:ASN:OD1	1:A:187:ASN:N	2.51	0.42
1:A:138:ASN:OD1	1:A:346:SER:HB3	2.18	0.42
1:A:165:ARG:NH2	1:A:416:TRP:O	2.50	0.42
1:B:178:VAL:O	1:B:206:ALA:HA	2.20	0.42
1:A:88:ILE:HD13	1:A:194:MET:HG2	2.02	0.42
1:B:123:PRO:HG2	1:B:350:LEU:HD13	2.01	0.42
1:A:199:LYS:HG3	1:A:200:THR:N	2.35	0.42
1:B:144:GLN:HE21	1:B:146:LEU:HD13	1.84	0.42
1:B:248:ASP:N	1:B:302:ILE:HG12	2.18	0.42
1:A:176:PHE:CD1	1:A:241:HIS:O	2.73	0.41
1:A:132:SER:H	1:A:414:GLN:NE2	2.18	0.41
1:B:13:GLY:O	1:B:14:PRO:O	2.38	0.41
1:B:354:GLY:HA2	1:B:359:LYS:CD	2.45	0.41
1:B:414:GLN:HG3	1:B:418:GLU:HG3	2.00	0.41
1:A:217:ALA:HB1	1:A:259:MET:HG2	2.01	0.41
1:A:27:ASN:HD22	1:A:27:ASN:HA	1.63	0.41
1:B:132:SER:H	1:B:414:GLN:HE22	1.68	0.41
1:A:275:TYR:CD1	1:A:277:TYR:O	2.73	0.41
1:A:102:ILE:H	1:A:102:ILE:HG12	1.60	0.41
1:A:233:TYR:CZ	1:A:238:HIS:HE1	2.38	0.41
1:A:30:VAL:HA	1:A:72:THR:HG22	2.03	0.41
1:B:395:GLU:O	1:B:399:LYS:HD2	2.21	0.41
1:A:305:MET:HA	1:A:306:PRO:HD3	1.87	0.41
1:A:314:ILE:CB	1:A:315:PRO:CA	2.95	0.41
1:B:342:ASN:HA	1:B:342:ASN:HD22	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ILE:HG23	1:B:356:GLY:N	2.36	0.41
1:B:312:HIS:HB2	1:B:313:PRO:HA	2.02	0.40
1:B:415:GLY:C	1:B:417:ASN:N	2.75	0.40
1:A:16:ILE:HD13	1:A:111:ASN:OD1	2.22	0.40
1:A:121:LEU:CB	1:A:289:ILE:HD11	2.51	0.40
1:B:162:GLN:HA	1:B:165:ARG:NH1	2.37	0.40
1:B:220:ARG:O	1:B:224:PRO:HD3	2.21	0.40
1:B:305:MET:HA	1:B:306:PRO:HD3	1.88	0.40
1:B:355:ILE:HG13	1:B:364:HIS:ND1	2.36	0.40
1:B:384:LEU:O	1:B:388:VAL:CG2	2.69	0.40
1:B:410:LYS:HA	1:B:410:LYS:HD3	1.93	0.40
1:B:19:GLU:HA	1:B:51:ILE:HG22	2.03	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	416/469 (89%)	340 (82%)	54 (13%)	22 (5%)	2	6
1	B	416/469 (89%)	323 (78%)	66 (16%)	27 (6%)	1	3
All	All	832/938 (89%)	663 (80%)	120 (14%)	49 (6%)	2	5

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	GLU
1	A	313	PRO
1	A	314	ILE
1	A	339	PRO
1	B	14	PRO
1	B	33	LYS

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Mol	Chain	Res	Type
1	B	72	THR
1	B	197	PHE
1	B	198	GLU
1	B	310	ILE
1	B	312	HIS
1	B	315	PRO
1	B	344	LEU
1	A	49	ALA
1	A	72	THR
1	A	308	ASP
1	A	445	ASP
1	B	113	ALA
1	B	205	ARG
1	B	258	GLN
1	B	355	ILE
1	B	418	GLU
1	B	439	ASN
1	A	13	GLY
1	A	41	ARG
1	A	142	ARG
1	A	255	ALA
1	A	309	ASP
1	A	443	ARG
1	B	34	MET
1	B	73	GLY
1	B	101	ARG
1	B	437	PRO
1	B	455	ALA
1	A	90	SER
1	A	99	GLY
1	A	315	PRO
1	B	95	PRO
1	B	125	ASP
1	B	354	GLY
1	A	12	ALA
1	B	454	PRO
1	A	355	ILE
1	A	439	ASN
1	A	453	HIS
1	B	43	GLN
1	B	356	GLY
1	A	37	GLY

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Mol	Chain	Res	Type
1	B	307	GLY

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	346/384 (90%)	293 (85%)	53 (15%)	3	9
1	B	346/384 (90%)	297 (86%)	49 (14%)	4	11
All	All	692/768 (90%)	590 (85%)	102 (15%)	3	10

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	32	ILE
1	A	36	ASP
1	A	39	VAL
1	A	40	ARG
1	A	41	ARG
1	A	43	GLN
1	A	70	ILE
1	A	74	GLU
1	A	85	LEU
1	A	101	ARG
1	A	102	ILE
1	A	116	ASN
1	A	126	PHE
1	A	148	ILE
1	A	159	ILE
1	A	165	ARG
1	A	169	VAL
1	A	187	ASN
1	A	200	THR
1	A	203	LEU
1	A	210	LEU

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Mol	Chain	Res	Type
1	A	212	LEU
1	A	220	ARG
1	A	221	ILE
1	A	243	LEU
1	A	248	ASP
1	A	250	THR
1	A	254	GLU
1	A	275	TYR
1	A	276	MET
1	A	277	TYR
1	A	278	THR
1	A	280	LEU
1	A	300	ILE
1	A	302	ILE
1	A	308	ASP
1	A	317	LEU
1	A	320	TYR
1	A	334	ARG
1	A	341	ILE
1	A	362	GLU
1	A	385	VAL
1	A	388	VAL
1	A	390	LYS
1	A	393	LEU
1	A	399	LYS
1	A	422	ILE
1	A	424	ASP
1	A	440	GLN
1	A	441	LEU
1	A	443	ARG
1	A	447	LYS
1	B	15	LEU
1	B	28	GLU
1	B	29	ILE
1	B	33	LYS
1	B	41	ARG
1	B	43	GLN
1	B	50	ASP
1	B	51	ILE
1	B	53	VAL
1	B	55	GLN
1	B	57	PHE

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Mol	Chain	Res	Type
1	B	72	THR
1	B	77	LYS
1	B	78	LEU
1	B	96	ARG
1	B	126	PHE
1	B	131	ILE
1	B	132	SER
1	B	133	THR
1	B	134	ILE
1	B	138	ASN
1	B	140	LEU
1	B	159	ILE
1	B	203	LEU
1	B	210	LEU
1	B	237	GLU
1	B	238	HIS
1	B	245	ILE
1	B	249	ILE
1	B	259	MET
1	B	289	ILE
1	B	303	LEU
1	B	305	MET
1	B	314	ILE
1	B	317	LEU
1	B	320	TYR
1	B	321	ILE
1	B	326	ILE
1	B	344	LEU
1	B	362	GLU
1	B	372	TYR
1	B	377	GLU
1	B	387	ILE
1	B	393	LEU
1	B	405	ASP
1	B	416	TRP
1	B	422	ILE
1	B	440	GLN
1	B	456	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	156	HIS
1	A	191	GLN
1	A	211	ASN
1	A	238	HIS
1	A	299	GLN
1	A	325	GLN
1	A	414	GLN
1	A	431	GLN
1	B	106	GLN
1	B	128	GLN
1	B	162	GLN
1	B	166	GLN
1	B	187	ASN
1	B	211	ASN
1	B	299	GLN
1	B	342	ASN
1	B	417	ASN
1	B	439	ASN
1	B	450	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	422/469 (89%)	0.35	29 (6%)	18 10	62, 76, 103, 109	0
1	B	422/469 (89%)	0.39	25 (5%)	23 15	64, 76, 93, 104	0
All	All	844/938 (89%)	0.37	54 (6%)	20 12	62, 76, 102, 109	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	ILE	8.4
1	B	455	ALA	5.5
1	B	261	ALA	5.5
1	B	357	ALA	5.3
1	B	11	ILE	4.8
1	A	74	GLU	4.7
1	B	312	HIS	4.0
1	B	311	THR	4.0
1	B	306	PRO	3.9
1	A	39	VAL	3.8
1	A	448	TYR	3.8
1	B	103	VAL	3.7
1	A	309	ASP	3.6
1	A	272	TYR	3.6
1	A	73	GLY	3.4
1	A	273	PRO	3.3
1	A	40	ARG	3.3
1	B	447	LYS	3.2
1	A	33	LYS	3.0
1	B	445	ASP	3.0
1	B	444	ILE	3.0
1	A	11	ILE	2.9
1	B	26	TYR	2.8
1	B	192	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	311	THR	2.7
1	B	10	GLN	2.7
1	B	121	LEU	2.6
1	A	449	ILE	2.6
1	A	439	ASN	2.5
1	B	356	GLY	2.5
1	A	457	ARG	2.5
1	A	318	SER	2.5
1	B	258	GLN	2.4
1	A	456	HIS	2.4
1	A	210	LEU	2.4
1	B	448	TYR	2.4
1	A	12	ALA	2.3
1	B	454	PRO	2.3
1	A	47	SER	2.3
1	A	188	GLU	2.3
1	A	173	GLU	2.2
1	B	12	ALA	2.2
1	A	31	ASN	2.2
1	A	453	HIS	2.1
1	B	362	GLU	2.1
1	B	40	ARG	2.1
1	A	450	GLN	2.1
1	A	325	GLN	2.1
1	A	25	GLY	2.1
1	B	41	ARG	2.1
1	A	48	SER	2.0
1	A	357	ALA	2.0
1	B	45	LEU	2.0
1	A	172	SER	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.