



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:17 AM GMT

PDB ID : 3OOC
Title : Crystal structure of the membrane fusion protein CusB from Escherichia coli
Authors : Su, C.-C.; Yang, F.; Long, F.; Reyon, D.; Routh, M.D.; Kuo, D.W.; Mokhtari, A.K.; Van Ornam, J.D.; Rabe, K.L.; Hoy, J.A.; Lee, Y.J.; Rajashankar, K.R.; Yu, E.W.
Deposited on : 2010-08-30
Resolution : 3.40 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

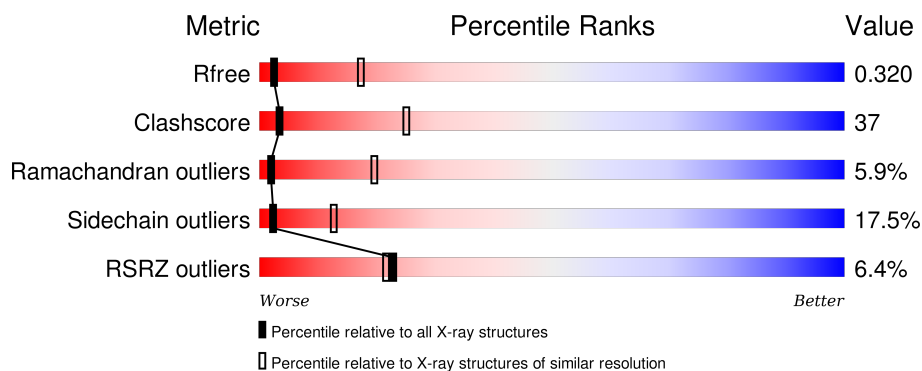
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	413	 4% 28% 35% 10% 28%
1	B	413	 5% 28% 33% 9% • 28%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4548 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 Cation efflux system protein cusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2274	1448	392	429	5			
1	B	297	Total	C	N	O	S	0	0	0
			2274	1448	392	429	5			

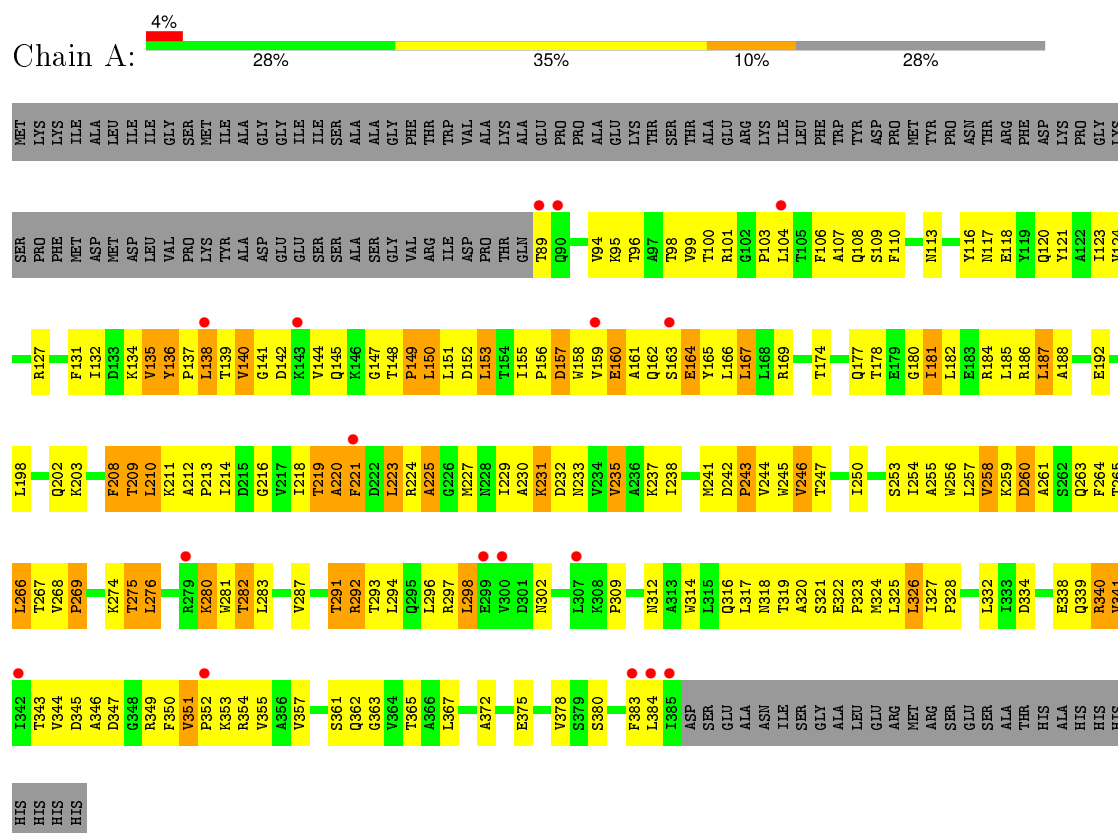
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	HIS	-	EXPRESSION TAG	UNP P77239
A	409	HIS	-	EXPRESSION TAG	UNP P77239
A	410	HIS	-	EXPRESSION TAG	UNP P77239
A	411	HIS	-	EXPRESSION TAG	UNP P77239
A	412	HIS	-	EXPRESSION TAG	UNP P77239
A	413	HIS	-	EXPRESSION TAG	UNP P77239
B	408	HIS	-	EXPRESSION TAG	UNP P77239
B	409	HIS	-	EXPRESSION TAG	UNP P77239
B	410	HIS	-	EXPRESSION TAG	UNP P77239
B	411	HIS	-	EXPRESSION TAG	UNP P77239
B	412	HIS	-	EXPRESSION TAG	UNP P77239
B	413	HIS	-	EXPRESSION TAG	UNP P77239

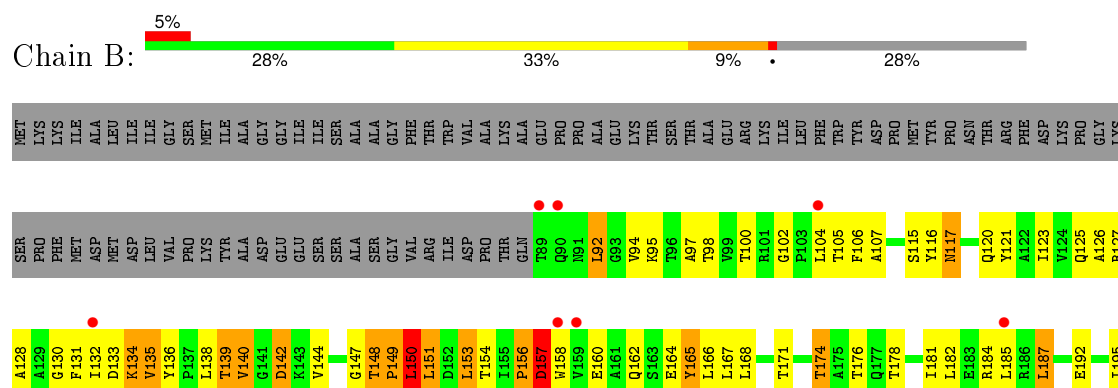
3 Residue-property plots

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: Cation efflux system protein cusB



• Molecule 1: Cation efflux system protein cusB





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	84.96Å 113.24Å 258.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.10 – 3.40 47.10 – 3.40	Depositor EDS
% Data completeness (in resolution range)	89.3 (47.10-3.40) 98.0 (47.10-3.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.261 , 0.318 0.272 , 0.320	Depositor DCC
R_{free} test set	867 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	132.2	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 145.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 17209 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4548	wwPDB-VP
Average B, all atoms (Å ²)	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.85% 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	0.24	0/2313	0.50	0/3152
1	B	0.25	0/2313	0.50	0/3152
All	All	0.25	0/4626	0.50	0/6304

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2274	0	2343	166	0
1	B	2274	0	2343	180	0
All	All	4548	0	4686	339	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 37.

All (339) 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:ALA:HB2	1:A:281:TRP:CD1	2.04	0.93
1:B:107:ALA:HB2	1:B:362:GLN:HE21	1.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ILE:HG23	1:A:233:ASN:HB2	1.54	0.89
1:B:166:LEU:HD22	1:B:202:GLN:HG3	1.52	0.89
1:B:340:ARG:HB3	1:B:353:LYS:O	1.76	0.85
1:B:147:GLY:O	1:B:211:LYS:HB3	1.79	0.82
1:B:207:ARG:HH11	1:B:207:ARG:CG	1.92	0.82
1:B:147:GLY:HA3	1:B:212:ALA:HB3	1.61	0.81
1:B:95:LYS:HB3	1:B:380:SER:HB3	1.60	0.81
1:B:182:LEU:HD21	1:B:199:ILE:HD11	1.62	0.81
1:B:278:ILE:HD12	1:B:278:ILE:H	1.47	0.80
1:B:181:ILE:HD12	1:B:184:ARG:HE	1.48	0.79
1:B:206:THR:HG23	1:B:207:ARG:H	1.48	0.79
1:B:126:ALA:O	1:B:232:ASP:HA	1.81	0.79
1:B:207:ARG:HH11	1:B:207:ARG:HG3	1.47	0.78
1:B:340:ARG:HG2	1:B:354:ARG:HA	1.65	0.77
1:A:132:ILE:HD11	1:A:229:ILE:HD11	1.64	0.77
1:A:223:LEU:HB3	1:A:227:MET:SD	2.25	0.77
1:B:244:VAL:HG12	1:B:300:VAL:HB	1.69	0.75
1:A:343:THR:HB	1:A:351:VAL:HG13	1.69	0.74
1:B:154:THR:HG22	1:B:207:ARG:HD2	1.70	0.74
1:A:255:ALA:O	1:A:258:VAL:HG23	1.86	0.74
1:A:384:LEU:HD23	1:A:384:LEU:H	1.52	0.74
1:B:218:ILE:H	1:B:218:ILE:HD12	1.52	0.74
1:B:107:ALA:HB2	1:B:362:GLN:NE2	2.02	0.73
1:A:106:PHE:CD2	1:B:253:SER:HA	2.22	0.73
1:B:144:VAL:HG13	1:B:218:ILE:HD11	1.68	0.73
1:A:138:LEU:HB2	1:A:221:PHE:CE1	2.24	0.72
1:B:379:SER:O	1:B:380:SER:HB2	1.87	0.72
1:B:167:LEU:HD12	1:B:168:LEU:N	2.05	0.72
1:A:117:ASN:HD21	1:A:243:PRO:HG2	1.55	0.71
1:A:138:LEU:HB2	1:A:221:PHE:HE1	1.56	0.71
1:A:265:THR:HB	1:A:316:GLN:HG3	1.73	0.70
1:A:136:TYR:HB3	1:A:137:PRO:HD2	1.73	0.69
1:A:103:PRO:HB3	1:A:321:SER:O	1.93	0.69
1:A:347:ASP:HB2	1:A:349:ARG:HG2	1.74	0.69
1:A:166:LEU:HD22	1:A:202:GLN:HG2	1.72	0.69
1:B:343:THR:HB	1:B:351:VAL:HG13	1.73	0.69
1:A:334:ASP:HB3	1:A:339:GLN:HA	1.75	0.69
1:A:147:GLY:HA3	1:A:212:ALA:HB3	1.74	0.69
1:A:287:VAL:HG12	1:A:294:LEU:HD21	1.73	0.69
1:A:332:LEU:HA	1:A:341:VAL:CG1	2.23	0.69
1:B:148:THR:OG1	1:B:149:PRO:HD3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:TRP:O	1:B:162:GLN:HG3	1.94	0.68
1:B:207:ARG:HG3	1:B:207:ARG:NH1	2.09	0.67
1:A:144:VAL:HG13	1:A:218:ILE:HD11	1.77	0.67
1:B:280:LYS:HG2	1:B:299:GLU:CB	2.25	0.66
1:A:242:ASP:HB3	1:A:243:PRO:HD3	1.76	0.66
1:B:139:THR:O	1:B:140:VAL:HB	1.95	0.66
1:B:249:ALA:HB1	1:B:293:THR:HG21	1.78	0.66
1:B:319:THR:HG22	1:B:320:ALA:N	2.10	0.66
1:A:291:THR:HG22	1:A:292:ARG:H	1.62	0.65
1:A:261:ALA:HB2	1:A:281:TRP:HD1	1.56	0.65
1:A:332:LEU:HA	1:A:341:VAL:HG12	1.78	0.65
1:B:347:ASP:HB2	1:B:349:ARG:HG2	1.78	0.65
1:B:280:LYS:HG2	1:B:299:GLU:HB3	1.78	0.64
1:A:132:ILE:HD11	1:A:229:ILE:CD1	2.26	0.64
1:B:134:LYS:O	1:B:135:VAL:HB	1.98	0.64
1:B:377:VAL:HG22	1:B:378:VAL:H	1.63	0.64
1:A:340:ARG:HB3	1:A:355:VAL:H	1.63	0.63
1:A:150:LEU:HD21	1:A:212:ALA:HB2	1.81	0.63
1:B:255:ALA:O	1:B:258:VAL:HG23	1.98	0.62
1:A:140:VAL:O	1:A:140:VAL:HG12	2.00	0.62
1:B:342:ILE:HD12	1:B:350:PHE:HB3	1.81	0.62
1:A:160:GLU:HG3	1:A:161:ALA:N	2.15	0.62
1:A:94:VAL:HG12	1:A:95:LYS:O	2.00	0.62
1:B:156:PRO:O	1:B:158:TRP:N	2.33	0.62
1:A:187:LEU:HD12	1:A:188:ALA:N	2.15	0.61
1:B:203:LYS:HD3	1:B:203:LYS:O	1.99	0.61
1:B:197:ARG:HB2	1:B:205:GLN:NE2	2.15	0.61
1:A:165:TYR:HB2	1:A:181:ILE:CD1	2.30	0.61
1:A:241:MET:O	1:A:302:ASN:HB3	2.01	0.61
1:B:269:PRO:HD2	1:B:312:ASN:O	2.01	0.61
1:B:338:GLU:CG	1:B:340:ARG:HD2	2.31	0.61
1:B:279:ARG:HG2	1:B:299:GLU:O	2.00	0.61
1:B:332:LEU:HA	1:B:341:VAL:HG12	1.82	0.60
1:B:316:GLN:HG3	1:B:316:GLN:O	2.01	0.60
1:A:231:LYS:HG3	1:A:232:ASP:H	1.66	0.60
1:A:101:ARG:NH2	1:A:325:LEU:HD21	2.16	0.60
1:A:229:ILE:HG22	1:A:230:ALA:N	2.15	0.60
1:A:150:LEU:HB3	1:A:151:LEU:HD23	1.84	0.60
1:A:282:THR:HG23	1:A:297:ARG:HB3	1.84	0.60
1:B:231:LYS:HG3	1:B:232:ASP:N	2.17	0.59
1:B:132:ILE:HD11	1:B:229:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ARG:CG	1:B:354:ARG:HA	2.29	0.59
1:B:165:TYR:HB2	1:B:181:ILE:HG21	1.83	0.59
1:A:340:ARG:HG2	1:A:354:ARG:HA	1.84	0.59
1:A:283:LEU:HD21	1:A:294:LEU:HD13	1.83	0.59
1:B:261:ALA:HB2	1:B:281:TRP:CD1	2.38	0.59
1:B:379:SER:O	1:B:380:SER:CB	2.51	0.59
1:B:150:LEU:O	1:B:151:LEU:HB3	2.01	0.59
1:A:338:GLU:HB2	1:A:340:ARG:HH12	1.67	0.59
1:A:253:SER:HA	1:B:106:PHE:CD2	2.38	0.59
1:A:220:ALA:O	1:A:221:PHE:HB2	2.03	0.58
1:A:218:ILE:HD12	1:A:218:ILE:H	1.68	0.58
1:A:149:PRO:O	1:A:150:LEU:HB2	2.03	0.58
1:A:162:GLN:HG2	1:A:185:LEU:HD21	1.86	0.58
1:A:267:THR:CG2	1:A:314:TRP:HB2	2.34	0.58
1:B:244:VAL:O	1:B:245:TRP:HD1	1.87	0.58
1:A:357:VAL:HG23	1:B:285:PRO:HG2	1.85	0.58
1:B:219:THR:O	1:B:220:ALA:HB3	2.04	0.58
1:A:246:VAL:HG22	1:A:298:LEU:HB3	1.85	0.57
1:B:280:LYS:HG3	1:B:281:TRP:N	2.19	0.57
1:A:117:ASN:HB3	1:A:245:TRP:CE2	2.39	0.57
1:B:276:LEU:HD23	1:B:276:LEU:N	2.20	0.57
1:B:147:GLY:CA	1:B:212:ALA:HB3	2.32	0.57
1:A:287:VAL:O	1:A:287:VAL:HG23	2.05	0.57
1:A:338:GLU:HB2	1:A:340:ARG:NH1	2.19	0.57
1:A:113:ASN:O	1:A:246:VAL:HA	2.03	0.57
1:A:158:TRP:O	1:A:162:GLN:HG3	2.04	0.56
1:B:125:GLN:HA	1:B:233:ASN:O	2.05	0.56
1:B:231:LYS:HG3	1:B:232:ASP:H	1.70	0.56
1:B:117:ASN:N	1:B:117:ASN:OD1	2.34	0.56
1:B:231:LYS:CG	1:B:232:ASP:N	2.67	0.56
1:B:258:VAL:O	1:B:259:LYS:HB2	2.05	0.56
1:A:276:LEU:N	1:A:276:LEU:HD23	2.20	0.56
1:A:124:VAL:O	1:A:235:VAL:HG22	2.06	0.56
1:A:134:LYS:O	1:A:135:VAL:HB	2.06	0.56
1:A:229:ILE:HD12	1:A:229:ILE:N	2.21	0.56
1:A:120:GLN:O	1:A:120:GLN:HG3	2.06	0.56
1:B:261:ALA:HB2	1:B:281:TRP:HD1	1.70	0.55
1:B:329:SER:HA	1:B:365:THR:HG23	1.88	0.55
1:B:251:PRO:O	1:B:254:ILE:HG22	2.07	0.55
1:A:117:ASN:ND2	1:A:243:PRO:HG2	2.22	0.55
1:B:195:ILE:O	1:B:199:ILE:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:PHE:CD1	1:B:208:PHE:N	2.72	0.55
1:A:123:ILE:O	1:A:123:ILE:HD12	2.07	0.55
1:A:256:TRP:CE2	1:B:321:SER:HA	2.42	0.54
1:B:205:GLN:OE1	1:B:205:GLN:HA	2.06	0.54
1:A:334:ASP:CB	1:A:339:GLN:HA	2.37	0.54
1:B:270:ALA:O	1:B:271:ARG:C	2.45	0.54
1:A:208:PHE:CD1	1:A:208:PHE:N	2.75	0.54
1:A:127:ARG:HD2	1:A:127:ARG:N	2.23	0.54
1:A:144:VAL:CG1	1:A:218:ILE:HD11	2.37	0.54
1:A:99:VAL:HG22	1:A:327:ILE:HG22	1.88	0.54
1:B:135:VAL:O	1:B:136:TYR:HB2	2.07	0.54
1:B:148:THR:CB	1:B:149:PRO:HD3	2.38	0.54
1:B:127:ARG:O	1:B:128:ALA:HB3	2.08	0.54
1:B:329:SER:HB2	1:B:364:VAL:HA	1.89	0.54
1:B:319:THR:HG22	1:B:320:ALA:H	1.73	0.54
1:A:165:TYR:HB2	1:A:181:ILE:HD11	1.88	0.54
1:B:153:LEU:N	1:B:153:LEU:HD13	2.23	0.54
1:A:340:ARG:HB3	1:A:354:ARG:HA	1.91	0.53
1:B:147:GLY:HA3	1:B:212:ALA:CB	2.37	0.53
1:B:242:ASP:HB3	1:B:243:PRO:HD3	1.90	0.53
1:A:104:LEU:O	1:A:320:ALA:HA	2.08	0.53
1:B:230:ALA:H	1:B:233:ASN:ND2	2.07	0.53
1:A:156:PRO:O	1:A:159:VAL:HG22	2.09	0.53
1:A:155:ILE:HD12	1:A:158:TRP:CE3	2.44	0.53
1:B:230:ALA:O	1:B:231:LYS:C	2.48	0.53
1:A:186:ARG:HG2	1:A:192:GLU:OE1	2.09	0.53
1:B:230:ALA:HB3	1:B:233:ASN:HD21	1.75	0.52
1:B:222:ASP:O	1:B:223:LEU:HG	2.08	0.52
1:A:319:THR:HG22	1:A:320:ALA:H	1.73	0.52
1:A:317:LEU:HD12	1:A:318:ASN:H	1.73	0.52
1:B:339:GLN:C	1:B:340:ARG:HG3	2.29	0.52
1:B:150:LEU:HD13	1:B:212:ALA:HB2	1.92	0.52
1:A:155:ILE:O	1:A:159:VAL:HG13	2.10	0.52
1:B:266:LEU:HD22	1:B:315:LEU:HD13	1.90	0.52
1:B:319:THR:CG2	1:B:320:ALA:N	2.72	0.52
1:A:229:ILE:CG2	1:A:230:ALA:N	2.73	0.52
1:A:136:TYR:HB3	1:A:137:PRO:CD	2.39	0.52
1:B:372:ALA:O	1:B:375:GLU:HB2	2.10	0.52
1:B:345:ASP:C	1:B:347:ASP:H	2.13	0.51
1:B:210:LEU:C	1:B:210:LEU:HD12	2.30	0.51
1:B:154:THR:CG2	1:B:207:ARG:HD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASP:C	1:A:347:ASP:H	2.14	0.51
1:B:115:SER:HB3	1:B:245:TRP:O	2.11	0.51
1:A:152:ASP:HA	1:A:209:THR:HA	1.92	0.51
1:B:158:TRP:HB3	1:B:162:GLN:HE21	1.76	0.51
1:B:116:TYR:CE1	1:B:309:PRO:HG2	2.46	0.51
1:B:218:ILE:HD12	1:B:218:ILE:N	2.25	0.51
1:B:178:THR:O	1:B:181:ILE:HG22	2.11	0.50
1:A:340:ARG:HB2	1:A:353:LYS:O	2.11	0.50
1:B:280:LYS:HG2	1:B:299:GLU:HB2	1.93	0.50
1:A:274:LYS:O	1:A:275:THR:HG23	2.12	0.50
1:B:178:THR:O	1:B:182:LEU:HD13	2.11	0.50
1:B:117:ASN:ND2	1:B:120:GLN:HB2	2.26	0.50
1:A:250:ILE:O	1:A:293:THR:HA	2.11	0.50
1:B:184:ARG:HB3	1:B:184:ARG:NH1	2.26	0.50
1:A:95:LYS:HG2	1:A:96:THR:H	1.77	0.50
1:A:150:LEU:CD2	1:A:212:ALA:HB2	2.41	0.50
1:B:319:THR:CG2	1:B:320:ALA:H	2.25	0.50
1:A:181:ILE:O	1:A:181:ILE:HD12	2.11	0.50
1:A:372:ALA:O	1:A:375:GLU:HB2	2.12	0.50
1:A:230:ALA:O	1:A:231:LYS:C	2.49	0.49
1:A:181:ILE:C	1:A:181:ILE:HD12	2.32	0.49
1:B:131:PHE:HA	1:B:227:MET:O	2.12	0.49
1:B:302:ASN:ND2	1:B:307:LEU:HB2	2.27	0.49
1:A:244:VAL:HG12	1:A:245:TRP:N	2.28	0.49
1:A:132:ILE:HD13	1:A:227:MET:HB2	1.95	0.49
1:B:264:PHE:HE1	1:B:281:TRP:CD1	2.30	0.49
1:B:332:LEU:HA	1:B:341:VAL:CG1	2.42	0.49
1:A:162:GLN:O	1:A:165:TYR:HB3	2.13	0.49
1:B:181:ILE:CD1	1:B:184:ARG:HE	2.22	0.49
1:A:148:THR:N	1:A:149:PRO:HD3	2.28	0.49
1:B:154:THR:HG22	1:B:207:ARG:HB3	1.95	0.48
1:B:181:ILE:HD12	1:B:184:ARG:NE	2.23	0.48
1:A:250:ILE:O	1:A:294:LEU:N	2.44	0.48
1:A:147:GLY:O	1:A:211:LYS:HB3	2.13	0.48
1:B:181:ILE:HA	1:B:184:ARG:NE	2.29	0.48
1:B:167:LEU:O	1:B:171:THR:HG23	2.14	0.48
1:B:187:LEU:O	1:B:187:LEU:HD12	2.13	0.48
1:B:288:ASP:HB2	1:B:293:THR:HB	1.94	0.48
1:B:162:GLN:HG2	1:B:185:LEU:HD21	1.96	0.48
1:B:104:LEU:HD13	1:B:326:LEU:HD11	1.96	0.48
1:A:340:ARG:CB	1:A:354:ARG:HA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ILE:HG12	1:B:254:ILE:O	2.13	0.47
1:A:263:GLN:HB2	1:A:318:ASN:HB2	1.95	0.47
1:B:92:LEU:CD1	1:B:92:LEU:H	2.27	0.47
1:B:229:ILE:HG23	1:B:233:ASN:HB2	1.96	0.47
1:B:244:VAL:HG13	1:B:245:TRP:N	2.28	0.47
1:B:245:TRP:CE2	1:B:297:ARG:HD3	2.50	0.47
1:A:283:LEU:HD21	1:A:294:LEU:CD1	2.44	0.47
1:A:153:LEU:N	1:A:153:LEU:HD13	2.29	0.47
1:A:223:LEU:HB3	1:A:227:MET:CE	2.44	0.47
1:A:244:VAL:HG12	1:A:245:TRP:H	1.78	0.47
1:A:256:TRP:CD2	1:A:257:LEU:HD22	2.49	0.47
1:A:131:PHE:HA	1:A:227:MET:O	2.15	0.47
1:B:97:ALA:HB3	1:B:328:PRO:HG2	1.97	0.47
1:B:121:TYR:CD2	1:B:121:TYR:C	2.88	0.47
1:B:132:ILE:HG22	1:B:133:ASP:N	2.29	0.47
1:A:269:PRO:HD2	1:A:312:ASN:O	2.15	0.47
1:A:334:ASP:HB2	1:A:338:GLU:O	2.15	0.47
1:B:264:PHE:HE1	1:B:281:TRP:CG	2.33	0.47
1:B:278:ILE:CG2	1:B:298:LEU:HB3	2.45	0.47
1:A:256:TRP:CE3	1:B:322:GLU:HG2	2.49	0.47
1:B:338:GLU:HG3	1:B:340:ARG:HD2	1.96	0.46
1:B:206:THR:HG23	1:B:207:ARG:N	2.26	0.46
1:A:384:LEU:H	1:A:384:LEU:CD2	2.26	0.46
1:A:163:SER:HA	1:A:166:LEU:HD12	1.96	0.46
1:A:294:LEU:HD11	1:B:359:GLN:OE1	2.15	0.46
1:B:92:LEU:H	1:B:92:LEU:HD13	1.80	0.46
1:B:105:THR:HA	1:B:319:THR:O	2.15	0.46
1:A:343:THR:O	1:A:350:PHE:HA	2.16	0.46
1:B:250:ILE:O	1:B:293:THR:HA	2.16	0.45
1:B:144:VAL:CG1	1:B:218:ILE:HD11	2.42	0.45
1:A:319:THR:HG22	1:A:320:ALA:N	2.31	0.45
1:B:174:THR:C	1:B:176:THR:H	2.19	0.45
1:B:202:GLN:O	1:B:202:GLN:HG2	2.16	0.45
1:B:117:ASN:HD21	1:B:243:PRO:HG2	1.82	0.45
1:A:135:VAL:HG21	1:A:225:ALA:H	1.82	0.45
1:B:377:VAL:HG22	1:B:378:VAL:N	2.29	0.45
1:A:139:THR:O	1:A:140:VAL:HB	2.17	0.45
1:A:124:VAL:HG22	1:A:213:PRO:HD3	1.98	0.45
1:B:308:LYS:HD3	1:B:311:MET:CE	2.46	0.45
1:B:156:PRO:O	1:B:157:ASP:C	2.55	0.45
1:A:157:ASP:N	1:A:157:ASP:OD2	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ALA:C	1:B:257:LEU:H	2.20	0.45
1:A:340:ARG:HG2	1:A:354:ARG:HG3	1.98	0.44
1:B:133:ASP:O	1:B:134:LYS:HB3	2.18	0.44
1:A:219:THR:HG23	1:A:237:LYS:HG3	1.98	0.44
1:A:187:LEU:HD12	1:A:188:ALA:H	1.82	0.44
1:B:321:SER:O	1:B:322:GLU:C	2.53	0.44
1:B:317:LEU:HD12	1:B:318:ASN:H	1.83	0.44
1:B:252:GLU:HG2	1:B:292:ARG:HB3	2.00	0.44
1:A:149:PRO:HB2	1:A:150:LEU:H	1.46	0.44
1:A:177:GLN:O	1:A:181:ILE:HG23	2.18	0.44
1:B:130:GLY:O	1:B:228:ASN:HA	2.18	0.44
1:A:139:THR:O	1:A:140:VAL:CB	2.65	0.44
1:B:104:LEU:HG	1:B:361:SER:HB3	2.00	0.44
1:B:120:GLN:HG3	1:B:240:GLY:HA3	1.99	0.43
1:A:264:PHE:CZ	1:A:296:LEU:HD21	2.52	0.43
1:A:351:VAL:HA	1:A:352:PRO:HD3	1.89	0.43
1:A:124:VAL:HG12	1:A:124:VAL:O	2.18	0.43
1:A:148:THR:N	1:A:149:PRO:CD	2.82	0.43
1:A:123:ILE:H	1:A:123:ILE:HG13	1.66	0.43
1:B:192:GLU:O	1:B:196:ARG:HG3	2.18	0.43
1:A:340:ARG:HA	1:A:355:VAL:HG22	1.99	0.43
1:A:254:ILE:O	1:A:254:ILE:HG22	2.17	0.43
1:A:344:VAL:HG12	1:A:346:ALA:H	1.84	0.43
1:B:142:ASP:N	1:B:142:ASP:OD2	2.51	0.43
1:A:116:TYR:CD1	1:A:309:PRO:HG2	2.53	0.43
1:B:203:LYS:O	1:B:204:ILE:HB	2.19	0.43
1:B:165:TYR:CE2	1:B:182:LEU:HD11	2.54	0.43
1:B:218:ILE:CD1	1:B:218:ILE:H	2.28	0.42
1:B:102:GLY:O	1:B:323:PRO:HA	2.18	0.42
1:A:180:GLY:O	1:A:184:ARG:HG3	2.19	0.42
1:A:198:LEU:HD12	1:A:203:LYS:O	2.19	0.42
1:A:324:MET:O	1:A:326:LEU:HD23	2.19	0.42
1:B:245:TRP:CH2	1:B:297:ARG:CZ	3.02	0.42
1:A:361:SER:O	1:A:362:GLN:HB2	2.19	0.42
1:A:339:GLN:HE21	1:A:357:VAL:HG22	1.85	0.42
1:B:256:TRP:CE2	1:B:257:LEU:HD22	2.55	0.42
1:B:153:LEU:HD11	1:B:210:LEU:HD23	2.02	0.42
1:B:266:LEU:HA	1:B:266:LEU:HD13	1.74	0.42
1:A:167:LEU:HD12	1:A:167:LEU:C	2.39	0.42
1:B:117:ASN:HB3	1:B:245:TRP:CE2	2.55	0.42
1:B:219:THR:O	1:B:220:ALA:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ASP:OD1	1:A:209:THR:HB	2.19	0.42
1:A:280:LYS:HE2	1:A:281:TRP:O	2.19	0.42
1:A:213:PRO:HB2	1:A:214:ILE:HG23	2.01	0.42
1:A:210:LEU:O	1:A:210:LEU:HD12	2.20	0.42
1:A:212:ALA:HA	1:A:213:PRO:HD3	1.91	0.42
1:A:164:GLU:O	1:A:167:LEU:HG	2.19	0.42
1:B:212:ALA:HA	1:B:213:PRO:HD3	1.81	0.41
1:A:120:GLN:NE2	1:A:243:PRO:HD3	2.35	0.41
1:A:256:TRP:CE2	1:A:257:LEU:HD22	2.55	0.41
1:A:89:THR:HG22	1:A:383:PHE:CE1	2.54	0.41
1:B:340:ARG:HG2	1:B:354:ARG:CA	2.44	0.41
1:A:340:ARG:CG	1:A:354:ARG:HA	2.48	0.41
1:A:216:GLY:HA3	1:A:238:ILE:CG2	2.50	0.41
1:A:321:SER:O	1:A:322:GLU:C	2.57	0.41
1:A:287:VAL:HA	1:A:294:LEU:HD23	2.01	0.41
1:A:95:LYS:HB3	1:A:380:SER:HB3	2.02	0.41
1:B:361:SER:O	1:B:363:GLY:N	2.52	0.41
1:B:181:ILE:HA	1:B:184:ARG:HE	1.84	0.41
1:A:344:VAL:HG22	1:A:350:PHE:CD1	2.56	0.41
1:B:187:LEU:C	1:B:187:LEU:HD12	2.41	0.41
1:B:94:VAL:HG12	1:B:95:LYS:N	2.35	0.41
1:A:117:ASN:HB3	1:A:245:TRP:NE1	2.35	0.41
1:A:323:PRO:O	1:A:324:MET:HG3	2.20	0.41
1:B:238:ILE:HG22	1:B:239:GLN:N	2.35	0.41
1:B:343:THR:OG1	1:B:353:LYS:HG3	2.20	0.41
1:B:231:LYS:CG	1:B:232:ASP:H	2.30	0.41
1:A:110:PHE:N	1:A:110:PHE:CD2	2.89	0.41
1:B:283:LEU:O	1:B:285:PRO:HD3	2.21	0.41
1:B:97:ALA:O	1:B:377:VAL:HG12	2.20	0.41
1:B:202:GLN:O	1:B:202:GLN:CG	2.69	0.41
1:B:207:ARG:HH11	1:B:207:ARG:HG2	1.80	0.41
1:A:107:ALA:HA	1:A:317:LEU:O	2.20	0.41
1:B:241:MET:O	1:B:302:ASN:HB3	2.21	0.41
1:A:259:LYS:O	1:A:260:ASP:O	2.38	0.41
1:A:246:VAL:HG21	1:A:266:LEU:HD21	2.02	0.41
1:A:327:ILE:HD12	1:A:328:PRO:O	2.21	0.41
1:A:229:ILE:CG2	1:A:230:ALA:H	2.34	0.40
1:B:156:PRO:HB2	1:B:157:ASP:H	1.55	0.40
1:B:258:VAL:O	1:B:263:GLN:NE2	2.54	0.40
1:A:256:TRP:CD1	1:B:321:SER:HB3	2.55	0.40
1:A:152:ASP:C	1:A:153:LEU:HD13	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:VAL:HA	1:A:269:PRO:HD3	1.93	0.40
1:B:166:LEU:HD11	1:B:204:ILE:HG12	2.02	0.40
1:A:140:VAL:HG22	1:A:221:PHE:C	2.42	0.40
1:B:345:ASP:C	1:B:347:ASP:N	2.75	0.40
1:A:116:TYR:CE1	1:A:309:PRO:HG2	2.56	0.40
1:B:278:ILE:HG23	1:B:298:LEU:HB3	2.02	0.40
1:A:155:ILE:HA	1:A:156:PRO:HD3	1.81	0.40
1:B:185:LEU:HA	1:B:185:LEU:HD12	1.94	0.40
1:B:280:LYS:HE2	1:B:299:GLU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	295/413 (71%)	218 (74%)	60 (20%)	17 (6%)	2	20
1	B	295/413 (71%)	231 (78%)	46 (16%)	18 (6%)	2	18
All	All	590/826 (71%)	449 (76%)	106 (18%)	35 (6%)	2	19

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	140	VAL
1	A	149	PRO
1	A	150	LEU
1	A	221	PHE
1	A	225	ALA
1	A	231	LYS
1	A	258	VAL
1	A	260	ASP

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Mol	Chain	Res	Type
1	B	135	VAL
1	B	140	VAL
1	B	156	PRO
1	B	157	ASP
1	B	380	SER
1	A	141	GLY
1	A	223	LEU
1	B	150	LEU
1	B	204	ILE
1	B	223	LEU
1	B	231	LYS
1	A	220	ALA
1	A	243	PRO
1	B	134	LYS
1	B	206	THR
1	B	362	GLN
1	A	363	GLY
1	B	151	LEU
1	B	221	PHE
1	B	259	LYS
1	B	149	PRO
1	B	258	VAL
1	A	269	PRO
1	A	136	TYR
1	A	341	VAL
1	B	363	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	243/338 (72%)	201 (83%)	42 (17%)	2	13
1	B	243/338 (72%)	200 (82%)	43 (18%)	2	12
All	All	486/676 (72%)	401 (82%)	85 (18%)	2	13

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	THR
1	A	100	THR
1	A	108	GLN
1	A	109	SER
1	A	118	GLU
1	A	121	TYR
1	A	138	LEU
1	A	142	ASP
1	A	145	GLN
1	A	153	LEU
1	A	157	ASP
1	A	160	GLU
1	A	164	GLU
1	A	167	LEU
1	A	169	ARG
1	A	174	THR
1	A	178	THR
1	A	181	ILE
1	A	182	LEU
1	A	187	LEU
1	A	208	PHE
1	A	209	THR
1	A	210	LEU
1	A	219	THR
1	A	224	ARG
1	A	235	VAL
1	A	246	VAL
1	A	247	THR
1	A	266	LEU
1	A	275	THR
1	A	276	LEU
1	A	280	LYS
1	A	282	THR
1	A	291	THR
1	A	292	ARG
1	A	298	LEU
1	A	326	LEU
1	A	340	ARG
1	A	351	VAL
1	A	365	THR
1	A	367	LEU
1	A	378	VAL
1	B	92	LEU

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Mol	Chain	Res	Type
1	B	98	THR
1	B	100	THR
1	B	117	ASN
1	B	123	ILE
1	B	138	LEU
1	B	139	THR
1	B	142	ASP
1	B	148	THR
1	B	150	LEU
1	B	153	LEU
1	B	157	ASP
1	B	160	GLU
1	B	164	GLU
1	B	165	TYR
1	B	174	THR
1	B	187	LEU
1	B	204	ILE
1	B	206	THR
1	B	207	ARG
1	B	208	PHE
1	B	210	LEU
1	B	219	THR
1	B	224	ARG
1	B	232	ASP
1	B	239	GLN
1	B	241	MET
1	B	244	VAL
1	B	257	LEU
1	B	266	LEU
1	B	273	ASP
1	B	275	THR
1	B	276	LEU
1	B	278	ILE
1	B	282	THR
1	B	283	LEU
1	B	284	LEU
1	B	294	LEU
1	B	326	LEU
1	B	340	ARG
1	B	367	LEU
1	B	378	VAL
1	B	382	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	202	GLN
1	A	239	GLN
1	B	162	GLN
1	B	202	GLN
1	B	233	ASN
1	B	239	GLN
1	B	362	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	297/413 (71%)	0.57	17 (5%) 27 25	136, 169, 291, 372	0
1	B	297/413 (71%)	0.55	21 (7%) 19 18	133, 182, 279, 427	0
All	All	594/826 (71%)	0.56	38 (6%) 23 21	133, 175, 284, 427	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	ILE	7.7
1	B	90	GLN	5.4
1	B	337	SER	4.4
1	B	343	THR	3.7
1	B	158	TRP	3.5
1	A	352	PRO	3.5
1	A	384	LEU	3.2
1	B	89	THR	3.2
1	B	266	LEU	3.1
1	A	89	THR	3.0
1	B	159	VAL	2.9
1	A	143	LYS	2.9
1	B	202	GLN	2.9
1	A	221	PHE	2.8
1	B	285	PRO	2.7
1	A	307	LEU	2.6
1	A	90	GLN	2.6
1	B	381	GLY	2.5
1	B	104	LEU	2.5
1	B	185	LEU	2.4
1	B	350	PHE	2.3
1	B	371	LEU	2.3
1	A	279	ARG	2.3
1	B	300	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	300	VAL	2.2
1	B	301	ASP	2.2
1	B	223	LEU	2.2
1	A	342	ILE	2.2
1	B	352	PRO	2.1
1	B	307	LEU	2.1
1	A	159	VAL	2.1
1	B	279	ARG	2.1
1	A	163	SER	2.1
1	A	104	LEU	2.1
1	A	138	LEU	2.1
1	A	383	PHE	2.1
1	A	299	GLU	2.0
1	B	132	ILE	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.