



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:55 AM UTC

PDB ID : 6J32 / pdb_00006j32
Title : Crystal Structure Analysis of the Glycotransferase of kitacinnamycin
Authors : Shi, J.; Liu, C.L.; Zhang, B.; Guo, W.J.; Zhu, J.P.; Xu, X.; Xu, Q.; Jiao, R.H.;
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Deposited on : 2019-01-03
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

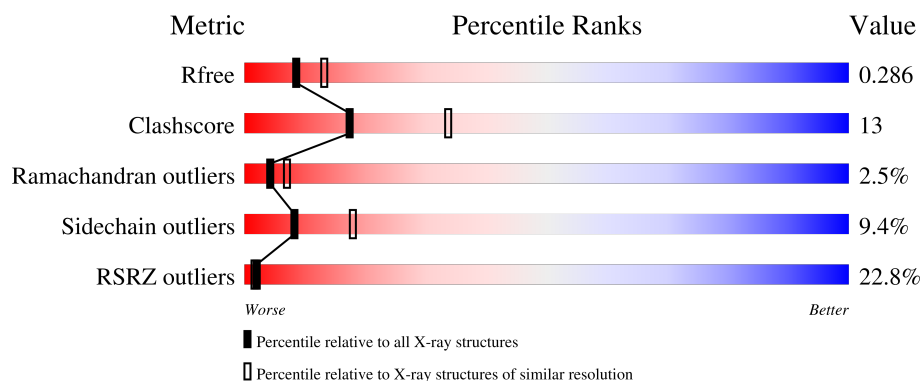
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of 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	399	19% 68% 22% 6% . .
1	B	399	24% 66% 25% 6% .
1	C	399	21% 72% 20% . .
1	D	399	25% 70% 21% 6% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11972 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 Kcn28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2953	1870	530	542	11			
1	B	386	Total	C	N	O	S	0	0	0
			2940	1861	525	544	10			
1	C	385	Total	C	N	O	S	0	0	0
			2942	1860	526	545	11			
1	D	385	Total	C	N	O	S	0	0	0
			2970	1878	534	547	11			

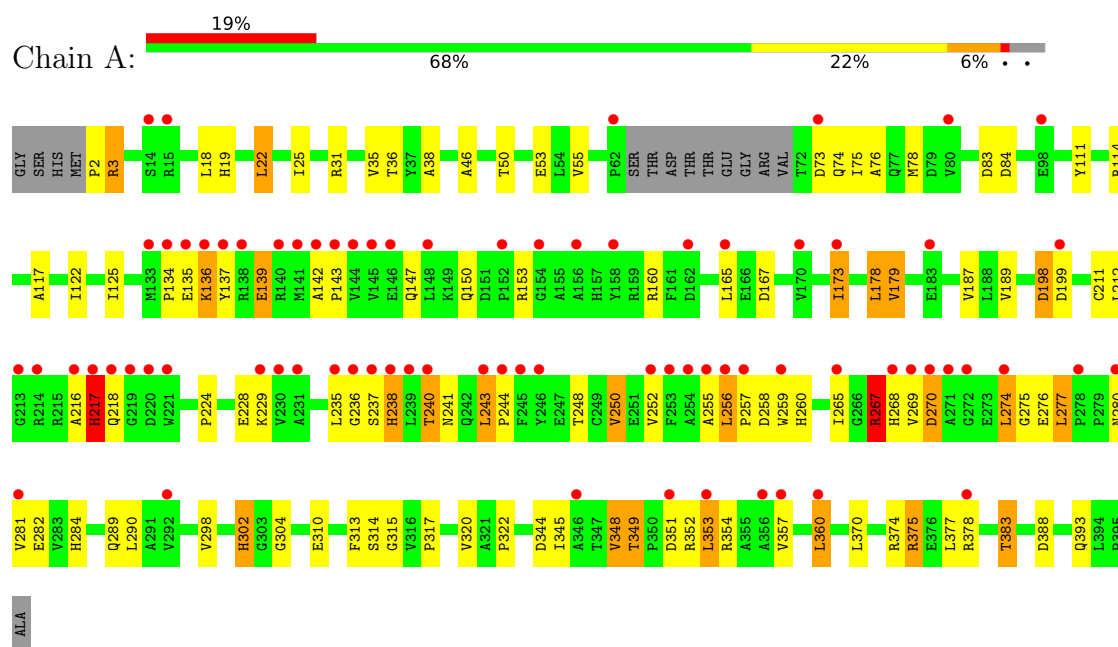
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	36	Total	O	0	0
			36	36		
2	B	54	Total	O	0	0
			54	54		
2	C	30	Total	O	0	0
			30	30		
2	D	47	Total	O	0	0
			47	47		

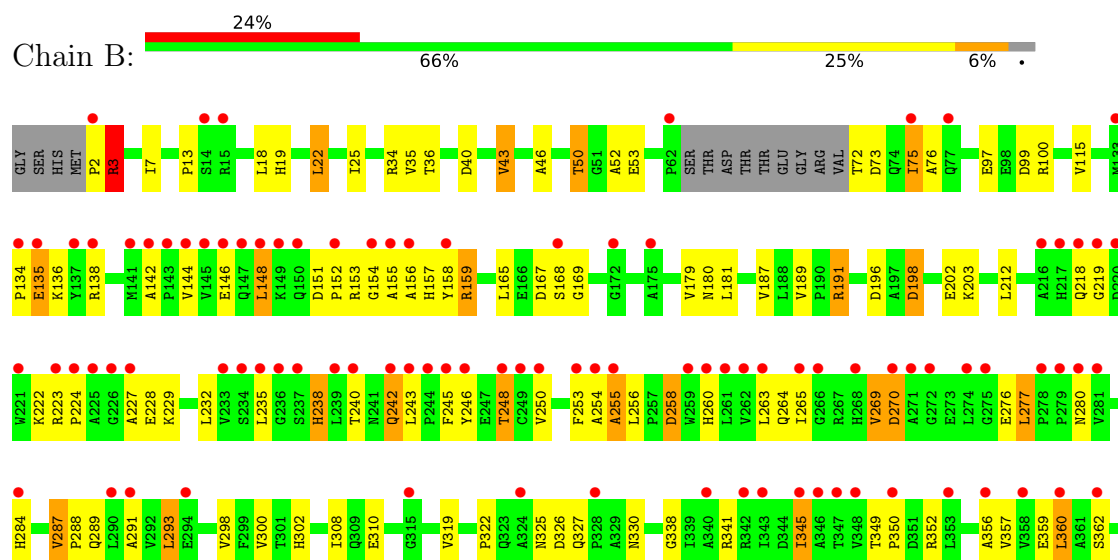
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Kcn28

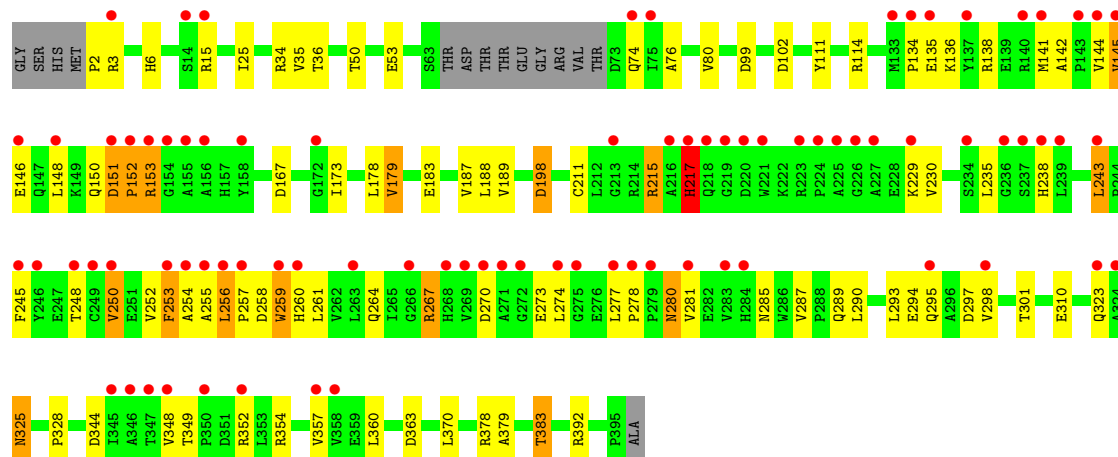
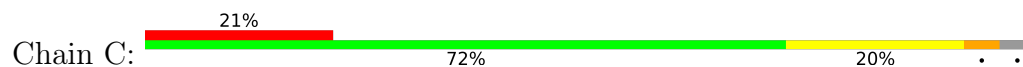


• Molecule 1: Kcn28

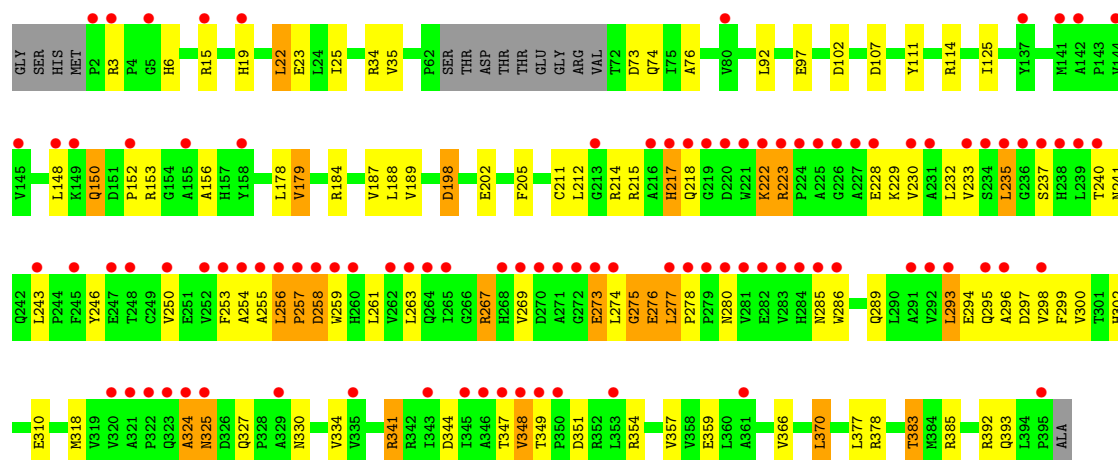




• Molecule 1: Kcn28



• Molecule 1: Kcn28



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	242.90Å 242.90Å 242.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.12 – 2.50 70.12 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (70.12-2.50) 99.3 (70.12-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.269 , 0.285 0.269 , 0.286	Depositor DCC
R_{free} test set	4100 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.009 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11972	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.90% 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	0.17	0/3025	0.49	0/4132
1	B	0.20	0/3011	0.52	0/4116
1	C	0.18	0/3013	0.51	2/4117 (0.0%)
1	D	0.23	0/3042	0.54	1/4153 (0.0%)
All	All	0.20	0/12091	0.51	3/16518 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	235	LEU	N-CA-C	-5.62	107.01	112.97
1	C	152	PRO	CA-C-N	5.22	131.51	121.54
1	C	152	PRO	C-N-CA	5.22	131.51	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2953	0	2918	72	0
1	B	2940	0	2887	86	0
1	C	2942	0	2893	64	0
1	D	2970	0	2941	77	0
2	A	36	0	0	3	0
2	B	54	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	30	0	0	7	0
2	D	47	0	0	13	0
All	All	11972	0	11639	294	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 13.

All (294) 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:D:257:PRO:O	1:D:259:TRP:N	1.85	1.08
1:D:256:LEU:HD21	1:D:354:ARG:HH12	1.24	1.00
1:C:352:ARG:NH1	2:C:401:HOH:O	1.94	0.99
1:B:158:TYR:H	1:B:159:ARG:NH1	1.62	0.98
1:D:73:ASP:OD2	1:D:153:ARG:NH1	2.01	0.94
1:B:158:TYR:HB2	1:B:159:ARG:HE	1.36	0.90
1:B:229:LYS:NZ	2:B:401:HOH:O	1.97	0.89
1:D:6:HIS:N	1:D:102:ASP:OD2	2.05	0.88
1:D:258:ASP:OD1	2:D:401:HOH:O	1.95	0.83
1:D:107:ASP:OD1	2:D:402:HOH:O	1.96	0.82
1:D:215:ARG:NH1	2:D:407:HOH:O	2.14	0.81
1:A:19:HIS:HA	1:A:22:LEU:HD22	1.61	0.80
1:A:84:ASP:OD2	2:A:401:HOH:O	2.00	0.80
1:C:253:PHE:HA	1:C:256:LEU:HD12	1.65	0.79
1:C:294:GLU:OE1	2:C:403:HOH:O	2.01	0.78
1:D:97:GLU:OE1	2:D:403:HOH:O	2.01	0.77
1:D:359:GLU:OE2	2:D:404:HOH:O	2.01	0.77
1:B:158:TYR:CD2	1:B:159:ARG:NH1	2.53	0.77
1:B:156:ALA:N	1:B:159:ARG:HH21	1.82	0.76
1:A:360:LEU:O	2:A:402:HOH:O	2.03	0.76
1:B:158:TYR:HD2	1:B:159:ARG:HH11	1.29	0.76
1:D:385:ARG:NH1	2:D:406:HOH:O	2.10	0.75
1:B:167:ASP:OD2	1:D:217:HIS:ND1	2.19	0.75
1:C:298:VAL:HG11	1:C:357:VAL:HG13	1.68	0.74
1:A:267:ARG:HG2	1:A:268:HIS:H	1.50	0.74
1:B:19:HIS:HA	1:B:22:LEU:HD22	1.67	0.74
1:C:183:GLU:OE2	2:C:404:HOH:O	2.05	0.73
1:D:19:HIS:HA	1:D:22:LEU:HD22	1.70	0.73
1:D:215:ARG:O	2:D:405:HOH:O	2.07	0.73
1:B:158:TYR:H	1:B:159:ARG:CZ	2.01	0.72
1:C:289:GLN:NE2	1:C:310:GLU:OE1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:VAL:HG21	1:A:353:LEU:HD23	1.71	0.71
1:B:258:ASP:OD1	1:B:258:ASP:N	2.18	0.71
1:C:229:LYS:HB2	1:C:259:TRP:CD1	2.25	0.71
1:A:83:ASP:OD1	1:A:160:ARG:NH2	2.23	0.71
1:B:298:VAL:HG11	1:B:357:VAL:HG13	1.72	0.70
1:A:289:GLN:NE2	1:A:310:GLU:OE1	2.23	0.70
1:C:301:THR:OG1	2:C:405:HOH:O	2.09	0.70
1:A:256:LEU:O	1:A:280:ASN:ND2	2.24	0.70
1:C:2:PRO:HG2	1:C:3:ARG:NH1	2.06	0.70
1:D:341:ARG:NH2	1:D:359:GLU:OE1	2.22	0.70
1:C:34:ARG:NH2	1:C:99:ASP:OD2	2.20	0.69
1:A:236:GLY:H	1:A:302:HIS:H	1.38	0.69
1:C:114:ARG:NH1	1:C:178:LEU:HA	2.07	0.69
1:B:158:TYR:HD2	1:B:159:ARG:NH1	1.88	0.69
1:A:298:VAL:HG11	1:A:357:VAL:HG13	1.75	0.68
1:D:240:THR:OG1	1:D:246:TYR:OH	2.08	0.68
1:B:235:LEU:HD22	1:B:240:THR:HB	1.76	0.68
1:D:256:LEU:HD21	1:D:354:ARG:NH1	2.05	0.68
1:C:258:ASP:O	2:C:406:HOH:O	2.12	0.67
1:B:168:SER:OG	2:B:402:HOH:O	2.14	0.66
1:D:184:ARG:NH1	2:D:410:HOH:O	2.24	0.65
1:A:75:ILE:HG21	1:A:153:ARG:HB3	1.78	0.65
1:D:222:LYS:HB2	1:D:222:LYS:NZ	2.12	0.64
1:C:15:ARG:N	2:C:402:HOH:O	2.30	0.64
1:B:269:VAL:HG13	1:B:270:ASP:H	1.63	0.64
1:B:191:ARG:NH2	1:B:202:GLU:OE2	2.31	0.64
1:C:256:LEU:HD13	1:C:259:TRP:HE3	1.63	0.64
1:A:237:SER:HB2	1:A:304:GLY:HA3	1.78	0.63
1:A:235:LEU:HD22	1:A:240:THR:HB	1.81	0.63
1:D:156:ALA:O	2:D:408:HOH:O	2.15	0.63
1:D:325:ASN:OD1	1:D:325:ASN:N	2.31	0.63
1:A:198:ASP:OD1	1:A:198:ASP:N	2.30	0.62
1:B:223:ARG:NH1	1:B:227:ALA:O	2.32	0.62
1:B:253:PHE:O	1:B:255:ALA:N	2.29	0.62
1:A:136:LYS:HA	1:A:139:GLU:OE2	2.01	0.61
1:C:135:GLU:HG3	1:C:135:GLU:O	2.01	0.61
1:A:143:PRO:O	1:A:147:GLN:N	2.25	0.61
1:A:349:THR:HG22	1:A:352:ARG:H	1.65	0.60
1:B:157:HIS:H	1:B:159:ARG:NH2	1.99	0.60
1:A:265:ILE:HG12	1:A:284:HIS:O	2.02	0.59
1:B:169:GLY:O	2:B:403:HOH:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:GLY:C	1:B:159:ARG:NH2	2.60	0.59
1:C:267:ARG:HA	1:C:285:ASN:HB3	1.84	0.59
1:D:253:PHE:O	1:D:280:ASN:ND2	2.35	0.59
1:C:254:ALA:HA	1:C:280:ASN:HD21	1.69	0.57
1:B:155:ALA:C	1:B:159:ARG:HH21	2.12	0.57
1:C:151:ASP:C	1:C:153:ARG:H	2.11	0.57
1:C:243:LEU:H	1:C:243:LEU:HD22	1.69	0.57
1:A:374:ARG:HH21	1:A:378:ARG:HH22	1.52	0.57
1:B:75:ILE:HG21	1:B:153:ARG:HD3	1.86	0.56
1:B:341:ARG:NH2	1:B:359:GLU:OE1	2.36	0.56
1:C:261:LEU:HB3	1:C:281:VAL:HG22	1.85	0.56
1:A:344:ASP:O	1:A:348:VAL:HG12	2.04	0.56
1:B:157:HIS:N	1:B:159:ARG:NH2	2.53	0.56
1:B:245:PHE:CD1	1:B:345:ILE:HG12	2.40	0.56
1:D:150:GLN:H	1:D:150:GLN:CD	2.11	0.56
1:B:138:ARG:NH1	1:B:180:ASN:HD22	2.03	0.56
1:D:215:ARG:HB3	2:D:405:HOH:O	2.05	0.56
1:B:34:ARG:NH2	1:B:99:ASP:OD2	2.30	0.55
1:C:278:PRO:HB2	1:C:280:ASN:ND2	2.21	0.55
1:C:250:VAL:HG21	1:C:274:LEU:HD12	1.88	0.55
1:C:280:ASN:H	1:C:280:ASN:HD22	1.52	0.55
1:A:25:ILE:HG23	1:A:35:VAL:HG11	1.88	0.54
1:A:217:HIS:O	1:A:218:GLN:HG2	2.08	0.54
1:B:156:ALA:N	1:B:159:ARG:NH2	2.52	0.54
1:A:136:LYS:O	1:A:139:GLU:HG2	2.08	0.54
1:B:338:GLY:O	1:B:369:ARG:NH1	2.41	0.54
1:B:158:TYR:N	1:B:159:ARG:CZ	2.70	0.54
1:D:230:VAL:HB	1:D:296:ALA:HA	1.89	0.54
1:C:6:HIS:N	1:C:102:ASP:OD2	2.29	0.54
1:B:362:SER:HA	2:B:401:HOH:O	2.08	0.53
1:B:159:ARG:NE	1:B:159:ARG:H	2.07	0.53
1:B:218:GLN:HB3	1:B:288:PRO:HB3	1.89	0.53
1:D:229:LYS:HA	1:D:297:ASP:OD2	2.07	0.53
1:D:289:GLN:NE2	1:D:310:GLU:OE1	2.38	0.53
1:B:224:PRO:HG2	1:B:260:HIS:CD2	2.44	0.53
1:B:3:ARG:NH2	2:B:412:HOH:O	2.41	0.52
1:A:257:PRO:C	1:A:259:TRP:H	2.17	0.52
1:C:363:ASP:OD2	2:C:407:HOH:O	2.19	0.52
1:C:256:LEU:HD13	1:C:259:TRP:CE3	2.44	0.52
1:D:302:HIS:HD2	1:D:327:GLN:HE21	1.56	0.52
1:D:302:HIS:HD2	1:D:327:GLN:NE2	2.06	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ILE:HG23	1:B:35:VAL:HG11	1.90	0.52
1:C:245:PHE:HE2	1:C:348:VAL:HG21	1.75	0.52
1:D:198:ASP:OD1	1:D:198:ASP:N	2.29	0.52
1:D:246:TYR:CD1	1:D:263:LEU:HD11	2.45	0.52
1:C:229:LYS:HA	1:C:297:ASP:OD2	2.11	0.51
1:C:215:ARG:HG3	1:C:217:HIS:H	1.76	0.51
1:A:114:ARG:NH1	1:A:178:LEU:HA	2.26	0.51
1:A:73:ASP:OD1	1:A:74:GLN:N	2.38	0.51
1:C:280:ASN:ND2	1:C:281:VAL:HG23	2.26	0.51
1:B:265:ILE:HG12	1:B:284:HIS:O	2.11	0.51
1:C:260:HIS:ND1	1:C:280:ASN:O	2.44	0.51
1:B:3:ARG:NH1	1:B:396:ALA:O	2.40	0.50
1:D:73:ASP:OD1	1:D:74:GLN:N	2.44	0.50
1:C:280:ASN:HD22	1:C:280:ASN:N	2.08	0.50
1:A:139:GLU:HA	1:A:142:ALA:HB2	1.93	0.50
1:B:50:THR:HG22	1:B:52:ALA:H	1.75	0.50
1:D:378:ARG:NH2	2:D:417:HOH:O	2.43	0.50
1:B:158:TYR:HB2	1:B:159:ARG:NE	2.14	0.50
1:A:313:PHE:O	2:A:403:HOH:O	2.19	0.50
1:D:187:VAL:HG12	1:D:189:VAL:HG22	1.93	0.50
1:A:2:PRO:HB2	1:A:3:ARG:HD2	1.93	0.50
1:B:245:PHE:CG	1:B:345:ILE:HG12	2.47	0.50
1:D:256:LEU:O	1:D:280:ASN:ND2	2.32	0.49
1:B:289:GLN:NE2	1:B:310:GLU:OE1	2.39	0.49
1:D:324:ALA:N	1:D:327:GLN:OE1	2.37	0.49
1:B:151:ASP:OD1	1:B:152:PRO:HD2	2.12	0.49
1:D:25:ILE:HG23	1:D:35:VAL:HG11	1.95	0.49
1:D:237:SER:HB2	1:D:302:HIS:HE2	1.77	0.49
1:A:236:GLY:N	1:A:302:HIS:HB2	2.27	0.49
1:B:269:VAL:HG13	1:B:270:ASP:N	2.27	0.49
1:C:141:MET:O	1:C:145:VAL:HG13	2.12	0.49
1:A:224:PRO:HG2	1:A:260:HIS:CD2	2.48	0.49
1:B:248:THR:HG22	1:B:350:PRO:HG3	1.93	0.49
1:D:15:ARG:CZ	1:D:19:HIS:HB2	2.43	0.49
1:B:284:HIS:HB2	1:B:287:VAL:HG12	1.95	0.48
1:A:135:GLU:HB3	1:A:199:ASP:O	2.13	0.48
1:A:229:LYS:HB2	1:A:259:TRP:NE1	2.27	0.48
1:D:125:ILE:HD11	1:D:393:GLN:HG3	1.95	0.48
1:D:211:CYS:HA	1:D:383:THR:HG22	1.95	0.48
1:A:349:THR:HG23	1:A:351:ASP:H	1.78	0.48
1:B:223:ARG:NH1	1:B:228:GLU:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:PRO:HG2	1:B:260:HIS:NE2	2.28	0.48
1:C:252:VAL:HG13	1:C:354:ARG:HB3	1.94	0.48
1:D:289:GLN:O	1:D:293:LEU:HB2	2.14	0.48
1:C:258:ASP:N	1:C:258:ASP:OD1	2.47	0.48
1:A:117:ALA:HB1	1:A:122:ILE:O	2.13	0.48
1:B:73:ASP:HB3	1:B:76:ALA:HB3	1.96	0.48
1:B:232:LEU:HD23	1:B:293:LEU:HD13	1.95	0.48
1:B:325:ASN:O	1:B:326:ASP:HB2	2.13	0.48
1:D:237:SER:HB2	1:D:302:HIS:NE2	2.29	0.48
1:A:173:ILE:HG21	1:A:178:LEU:HB3	1.96	0.47
1:C:173:ILE:HD13	1:C:178:LEU:HB2	1.94	0.47
1:C:253:PHE:O	1:C:255:ALA:N	2.40	0.47
1:C:198:ASP:OD1	1:C:198:ASP:N	2.32	0.47
1:A:229:LYS:HB2	1:A:259:TRP:CD1	2.48	0.47
1:D:232:LEU:HD23	1:D:293:LEU:HD13	1.96	0.47
1:A:375:ARG:HD2	1:C:379:ALA:HA	1.95	0.47
1:B:264:GLN:HB2	1:B:287:VAL:HG13	1.97	0.47
1:A:187:VAL:HG12	1:A:189:VAL:HG22	1.96	0.47
1:D:150:GLN:OE1	1:D:150:GLN:N	2.25	0.47
1:A:211:CYS:HA	1:A:383:THR:HG22	1.96	0.47
1:A:75:ILE:HD13	1:A:153:ARG:HB2	1.96	0.47
1:A:74:GLN:HG2	1:A:78:MET:HE3	1.97	0.47
1:C:134:PRO:C	1:C:136:LYS:H	2.23	0.47
1:D:178:LEU:O	1:D:179:VAL:HB	2.15	0.47
1:C:142:ALA:O	1:C:146:GLU:HG3	2.16	0.46
1:A:216:ALA:O	1:A:218:GLN:N	2.48	0.46
1:C:142:ALA:O	1:C:145:VAL:HG22	2.15	0.46
1:D:254:ALA:C	1:D:256:LEU:H	2.22	0.46
1:A:36:THR:HG22	1:A:53:GLU:HB3	1.96	0.46
1:B:308:ILE:HD12	1:B:330:ASN:HB3	1.97	0.46
1:C:325:ASN:O	1:C:328:PRO:HD2	2.15	0.46
1:B:97:GLU:OE1	1:B:100:ARG:NH2	2.40	0.46
1:C:25:ILE:HB	1:C:50:THR:HG21	1.98	0.46
1:C:151:ASP:N	1:C:152:PRO:HD3	2.30	0.46
1:B:159:ARG:H	1:B:159:ARG:CD	2.24	0.46
1:B:300:VAL:HG22	1:B:319:VAL:HB	1.98	0.46
1:D:351:ASP:HA	1:D:354:ARG:HG2	1.97	0.46
1:A:160:ARG:HA	1:B:219:GLY:HA2	1.97	0.46
1:A:73:ASP:H	1:A:76:ALA:HB3	1.80	0.46
1:D:178:LEU:HD13	1:D:179:VAL:HG23	1.98	0.46
1:D:228:GLU:HB2	1:D:258:ASP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:HD21	1:B:46:ALA:HB3	1.98	0.45
1:A:282:GLU:HB2	1:D:152:PRO:HG3	1.98	0.45
1:C:245:PHE:O	1:C:248:THR:OG1	2.29	0.45
1:D:111:TYR:CG	1:D:179:VAL:HG22	2.50	0.45
1:A:250:VAL:HG21	1:A:274:LEU:HD21	1.97	0.45
1:D:240:THR:HG1	1:D:246:TYR:HH	1.35	0.45
1:C:111:TYR:CD1	1:C:179:VAL:HG22	2.52	0.45
1:C:187:VAL:HG12	1:C:189:VAL:HG22	1.98	0.45
1:D:298:VAL:HG11	1:D:357:VAL:HG13	1.98	0.45
1:B:148:LEU:O	1:B:154:GLY:HA3	2.16	0.45
1:C:2:PRO:HG2	1:C:3:ARG:HH12	1.81	0.44
1:D:347:THR:OG1	1:D:348:VAL:N	2.50	0.44
1:D:294:GLU:C	1:D:295:GLN:HE21	2.26	0.44
1:C:229:LYS:HB2	1:C:259:TRP:HD1	1.80	0.44
1:C:25:ILE:HG23	1:C:35:VAL:HG11	1.99	0.44
1:B:276:GLU:O	1:B:277:LEU:HB2	2.18	0.44
1:C:211:CYS:HA	1:C:383:THR:HG22	1.99	0.44
1:B:187:VAL:HG12	1:B:189:VAL:HG22	2.00	0.44
1:D:344:ASP:O	1:D:348:VAL:HG13	2.18	0.44
1:B:256:LEU:O	1:B:280:ASN:ND2	2.51	0.44
1:A:267:ARG:HD2	1:A:267:ARG:N	2.33	0.44
1:B:36:THR:HG22	1:B:53:GLU:HB3	1.99	0.44
1:D:257:PRO:C	1:D:259:TRP:N	2.66	0.43
1:B:151:ASP:O	1:B:154:GLY:N	2.51	0.43
1:D:76:ALA:HB2	1:D:153:ARG:HH22	1.83	0.43
1:A:268:HIS:O	1:A:270:ASP:N	2.52	0.43
1:A:250:VAL:HG22	1:A:281:VAL:HG11	1.99	0.43
1:B:212:LEU:O	1:B:383:THR:HG21	2.18	0.43
1:C:270:ASP:HA	1:C:285:ASN:OD1	2.19	0.43
1:A:315:GLY:C	1:A:370:LEU:HD13	2.43	0.43
1:C:36:THR:HG22	1:C:53:GLU:HB2	2.01	0.43
1:A:276:GLU:O	1:A:277:LEU:HB2	2.19	0.43
1:C:259:TRP:CH2	1:C:357:VAL:HG12	2.53	0.43
1:A:125:ILE:HD11	1:A:393:GLN:HG3	2.00	0.43
1:A:317:PRO:HB2	1:A:360:LEU:HG	2.00	0.43
1:B:198:ASP:OD2	1:B:198:ASP:N	2.47	0.43
1:D:274:LEU:O	1:D:276:GLU:N	2.51	0.43
1:D:275:GLY:O	1:D:276:GLU:HB2	2.19	0.43
1:A:228:GLU:CD	1:A:258:ASP:HB3	2.43	0.42
1:B:138:ARG:NH1	1:B:180:ASN:ND2	2.67	0.42
1:C:267:ARG:CA	1:C:285:ASN:HB3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:ASP:O	1:C:348:VAL:HG13	2.19	0.42
1:B:142:ALA:O	1:B:146:GLU:HG3	2.19	0.42
1:D:212:LEU:O	1:D:383:THR:HG21	2.18	0.42
1:A:111:TYR:CD2	1:A:179:VAL:HG22	2.54	0.42
1:A:212:LEU:O	1:A:383:THR:HG21	2.18	0.42
1:D:366:VAL:O	1:D:370:LEU:HD22	2.20	0.42
1:A:255:ALA:O	1:A:257:PRO:HD3	2.20	0.42
1:D:299:PHE:O	1:D:318:MET:HA	2.19	0.42
1:C:150:GLN:C	1:C:152:PRO:HD3	2.45	0.42
1:D:253:PHE:CG	1:D:261:LEU:HB2	2.54	0.42
1:D:202:GLU:HA	1:D:205:PHE:O	2.19	0.42
1:A:31:ARG:NH1	1:A:388:ASP:OD1	2.41	0.42
1:A:250:VAL:HG11	1:A:274:LEU:HD21	2.00	0.42
1:D:277:LEU:HA	1:D:278:PRO:HD3	1.92	0.42
1:C:76:ALA:O	1:C:80:VAL:HG23	2.19	0.42
1:B:134:PRO:HG2	1:B:196:ASP:HB2	2.01	0.42
1:C:230:VAL:HB	1:C:295:GLN:O	2.19	0.42
1:D:23:GLU:OE1	2:D:409:HOH:O	2.21	0.42
1:D:233:VAL:HG22	1:D:300:VAL:HB	2.01	0.42
1:B:13:PRO:HG3	1:B:40:ASP:HB3	2.01	0.41
1:B:167:ASP:OD2	1:D:217:HIS:CE1	2.73	0.41
1:C:111:TYR:CG	1:C:179:VAL:HG22	2.55	0.41
1:C:392:ARG:HD2	1:C:392:ARG:HA	1.89	0.41
1:D:255:ALA:O	1:D:257:PRO:HD3	2.20	0.41
1:B:2:PRO:HB2	1:B:3:ARG:H	1.70	0.41
1:B:115:VAL:HG11	1:B:168:SER:HB3	2.02	0.41
1:D:114:ARG:HD3	1:D:178:LEU:CD2	2.50	0.41
1:A:252:VAL:HG21	1:A:353:LEU:HB3	2.02	0.41
1:B:158:TYR:CB	1:B:159:ARG:HH11	2.34	0.41
1:B:7:ILE:O	1:B:35:VAL:HA	2.21	0.41
1:B:356:ALA:O	1:B:360:LEU:HB2	2.21	0.41
1:A:114:ARG:HH11	1:A:178:LEU:HA	1.86	0.41
1:B:302:HIS:O	1:B:327:GLN:HB3	2.21	0.41
1:A:243:LEU:N	1:A:244:PRO:HD2	2.35	0.41
1:B:13:PRO:HG3	1:B:40:ASP:CB	2.50	0.41
1:B:135:GLU:OE2	1:B:181:LEU:HD13	2.21	0.41
1:B:288:PRO:HB2	1:B:291:ALA:HB3	2.02	0.41
1:C:135:GLU:OE1	1:C:138:ARG:HG3	2.20	0.41
1:A:38:ALA:HA	1:A:55:VAL:O	2.21	0.41
1:A:136:LYS:HB2	1:A:136:LYS:HE2	1.62	0.41
1:A:229:LYS:HB2	1:A:259:TRP:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ARG:HA	2:D:432:HOH:O	2.21	0.41
1:D:330:ASN:O	1:D:334:VAL:HG22	2.21	0.41
1:A:257:PRO:HA	1:A:280:ASN:HD21	1.86	0.40
1:B:302:HIS:O	1:B:322:PRO:HA	2.21	0.40
1:A:134:PRO:HD2	1:A:137:TYR:HB3	2.03	0.40
1:A:237:SER:O	1:A:238:HIS:HB2	2.22	0.40
1:B:242:GLN:CD	1:B:242:GLN:N	2.80	0.40
1:B:246:TYR:CD1	1:B:263:LEU:HD11	2.55	0.40
1:B:253:PHE:C	1:B:255:ALA:N	2.78	0.40
1:A:320:VAL:HG12	1:A:322:PRO:HD3	2.03	0.40
1:D:223:ARG:HG3	1:D:230:VAL:HG21	2.03	0.40
1:A:18:LEU:HD21	1:A:46:ALA:HB3	2.03	0.40
1:B:18:LEU:HD22	1:B:43:VAL:HG21	2.03	0.40
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.84	0.40
1:D:111:TYR:CD2	1:D:179:VAL:HG22	2.56	0.40
1:D:235:LEU:HG	1:D:302:HIS:HB3	2.03	0.40
1:D:257:PRO:HB2	1:D:258:ASP:H	1.60	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	381/399 (96%)	354 (93%)	20 (5%)	7 (2%)	6	12
1	B	382/399 (96%)	355 (93%)	20 (5%)	7 (2%)	6	12
1	C	381/399 (96%)	345 (91%)	26 (7%)	10 (3%)	4	7
1	D	381/399 (96%)	351 (92%)	16 (4%)	14 (4%)	2	3
All	All	1525/1596 (96%)	1405 (92%)	82 (5%)	38 (2%)	4	7

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	VAL
1	A	238	HIS
1	A	267	ARG
1	A	275	GLY
1	B	179	VAL
1	B	254	ALA
1	B	255	ALA
1	C	179	VAL
1	C	217	HIS
1	C	325	ASN
1	D	179	VAL
1	D	218	GLN
1	D	258	ASP
1	D	267	ARG
1	D	275	GLY
1	D	276	GLU
1	D	348	VAL
1	B	269	VAL
1	C	153	ARG
1	D	241	ASN
1	D	257	PRO
1	D	273	GLU
1	A	277	LEU
1	C	257	PRO
1	D	277	LEU
1	B	238	HIS
1	C	74	GLN
1	C	151	ASP
1	D	3	ARG
1	D	214	ARG
1	D	324	ALA
1	A	217	HIS
1	B	3	ARG
1	B	277	LEU
1	C	238	HIS
1	A	269	VAL
1	C	253	PHE
1	C	277	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	308/323 (95%)	275 (89%)	33 (11%)	6	13
1	B	304/323 (94%)	271 (89%)	33 (11%)	6	13
1	C	307/323 (95%)	282 (92%)	25 (8%)	11	23
1	D	312/323 (97%)	287 (92%)	25 (8%)	11	24
All	All	1231/1292 (95%)	1115 (91%)	116 (9%)	8	18

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	22	LEU
1	A	50	THR
1	A	136	LYS
1	A	139	GLU
1	A	150	GLN
1	A	165	LEU
1	A	167	ASP
1	A	173	ILE
1	A	178	LEU
1	A	198	ASP
1	A	217	HIS
1	A	240	THR
1	A	241	ASN
1	A	243	LEU
1	A	248	THR
1	A	250	VAL
1	A	256	LEU
1	A	267	ARG
1	A	270	ASP
1	A	274	LEU
1	A	290	LEU
1	A	302	HIS
1	A	314	SER
1	A	345	ILE
1	A	348	VAL
1	A	349	THR
1	A	353	LEU

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Mol	Chain	Res	Type
1	A	354	ARG
1	A	360	LEU
1	A	375	ARG
1	A	377	LEU
1	A	383	THR
1	B	3	ARG
1	B	22	LEU
1	B	43	VAL
1	B	50	THR
1	B	72	THR
1	B	75	ILE
1	B	135	GLU
1	B	136	LYS
1	B	144	VAL
1	B	148	LEU
1	B	159	ARG
1	B	165	LEU
1	B	191	ARG
1	B	198	ASP
1	B	203	LYS
1	B	222	LYS
1	B	238	HIS
1	B	242	GLN
1	B	243	LEU
1	B	248	THR
1	B	250	VAL
1	B	258	ASP
1	B	270	ASP
1	B	287	VAL
1	B	293	LEU
1	B	345	ILE
1	B	349	THR
1	B	352	ARG
1	B	360	LEU
1	B	371	SER
1	B	374	ARG
1	B	377	LEU
1	B	383	THR
1	C	144	VAL
1	C	145	VAL
1	C	167	ASP
1	C	188	LEU

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Mol	Chain	Res	Type
1	C	198	ASP
1	C	215	ARG
1	C	217	HIS
1	C	235	LEU
1	C	243	LEU
1	C	250	VAL
1	C	256	LEU
1	C	259	TRP
1	C	264	GLN
1	C	267	ARG
1	C	273	GLU
1	C	280	ASN
1	C	287	VAL
1	C	290	LEU
1	C	293	LEU
1	C	323	GLN
1	C	349	THR
1	C	360	LEU
1	C	370	LEU
1	C	378	ARG
1	C	383	THR
1	D	22	LEU
1	D	92	LEU
1	D	148	LEU
1	D	150	GLN
1	D	188	LEU
1	D	198	ASP
1	D	217	HIS
1	D	222	LYS
1	D	223	ARG
1	D	243	LEU
1	D	250	VAL
1	D	256	LEU
1	D	267	ARG
1	D	269	VAL
1	D	273	GLU
1	D	285	ASN
1	D	286	TRP
1	D	293	LEU
1	D	325	ASN
1	D	341	ARG
1	D	349	THR

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Mol	Chain	Res	Type
1	D	370	LEU
1	D	377	LEU
1	D	383	THR
1	D	392	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	HIS
1	B	180	ASN
1	B	217	HIS
1	B	285	ASN
1	C	147	GLN
1	C	280	ASN
1	D	19	HIS
1	D	242	GLN
1	D	295	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 oligosaccharides 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	385/399 (96%)	1.06	76 (19%) 3 2	42, 74, 146, 207	0
1	B	386/399 (96%)	1.18	95 (24%) 2 1	41, 72, 142, 224	0
1	C	385/399 (96%)	1.21	82 (21%) 2 2	52, 82, 150, 216	0
1	D	385/399 (96%)	1.27	99 (25%) 1 1	42, 77, 148, 197	0
All	All	1541/1596 (96%)	1.18	352 (22%) 2 2	41, 77, 148, 224	0

All (352) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	346	ALA	6.3
1	D	255	ALA	6.0
1	C	269	VAL	5.8
1	D	283	VAL	5.8
1	C	272	GLY	5.7
1	D	263	LEU	5.5
1	D	235	LEU	5.5
1	B	236	GLY	5.4
1	D	237	SER	5.4
1	D	265	ILE	5.2
1	C	259	TRP	5.2
1	C	346	ALA	5.1
1	C	237	SER	5.0
1	A	255	ALA	4.9
1	D	256	LEU	4.9
1	B	2	PRO	4.9
1	D	272	GLY	4.9
1	B	278	PRO	4.8
1	D	274	LEU	4.8
1	C	284	HIS	4.8
1	B	237	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	255	ALA	4.7
1	B	347	THR	4.7
1	D	271	ALA	4.7
1	A	254	ALA	4.7
1	C	256	LEU	4.7
1	B	156	ALA	4.6
1	D	346	ALA	4.6
1	A	137	TYR	4.4
1	C	274	LEU	4.4
1	C	283	VAL	4.4
1	D	324	ALA	4.4
1	C	257	PRO	4.4
1	B	218	GLN	4.4
1	B	152	PRO	4.4
1	B	271	ALA	4.3
1	D	233	VAL	4.3
1	A	272	GLY	4.3
1	B	219	GLY	4.3
1	C	219	GLY	4.3
1	D	239	LEU	4.3
1	D	269	VAL	4.2
1	B	254	ALA	4.2
1	C	145	VAL	4.2
1	D	345	ILE	4.1
1	A	238	HIS	4.1
1	B	158	TYR	4.1
1	B	272	GLY	4.1
1	A	219	GLY	4.1
1	D	281	VAL	4.1
1	B	345	ILE	4.0
1	C	239	LEU	4.0
1	C	254	ALA	4.0
1	A	243	LEU	4.0
1	C	243	LEU	4.0
1	A	235	LEU	3.9
1	D	259	TRP	3.9
1	A	259	TRP	3.9
1	A	218	GLN	3.9
1	D	236	GLY	3.9
1	D	277	LEU	3.9
1	A	265	ILE	3.9
1	D	221	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	237	SER	3.8
1	A	216	ALA	3.8
1	C	220	ASP	3.8
1	A	281	VAL	3.7
1	D	348	VAL	3.7
1	A	231	ALA	3.7
1	A	236	GLY	3.7
1	B	172	GLY	3.7
1	A	271	ALA	3.7
1	A	230	VAL	3.7
1	B	137	TYR	3.7
1	A	138	ARG	3.7
1	C	281	VAL	3.7
1	B	135	GLU	3.7
1	C	216	ALA	3.7
1	D	291	ALA	3.7
1	D	262	VAL	3.6
1	D	279	PRO	3.6
1	B	348	VAL	3.6
1	C	324	ALA	3.6
1	A	142	ALA	3.6
1	D	227	ALA	3.6
1	C	154	GLY	3.6
1	D	225	ALA	3.6
1	D	2	PRO	3.5
1	A	141	MET	3.5
1	A	269	VAL	3.5
1	D	335	VAL	3.5
1	C	268	HIS	3.5
1	B	145	VAL	3.5
1	C	134	PRO	3.5
1	C	158	TYR	3.5
1	B	144	VAL	3.4
1	D	218	GLN	3.4
1	B	240	THR	3.4
1	B	239	LEU	3.4
1	D	278	PRO	3.4
1	A	351	ASP	3.4
1	B	221	TRP	3.4
1	D	230	VAL	3.4
1	D	148	LEU	3.4
1	D	219	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	322	PRO	3.4
1	B	275	GLY	3.4
1	A	158	TYR	3.3
1	C	221	TRP	3.3
1	C	225	ALA	3.3
1	B	245	PHE	3.3
1	D	292	VAL	3.2
1	B	216	ALA	3.2
1	C	218	GLN	3.2
1	D	15	ARG	3.2
1	D	247	GLU	3.2
1	C	141	MET	3.2
1	C	266	GLY	3.2
1	B	362	SER	3.2
1	B	220	ASP	3.2
1	C	152	PRO	3.2
1	D	145	VAL	3.2
1	C	224	PRO	3.1
1	C	278	PRO	3.1
1	D	238	HIS	3.1
1	B	281	VAL	3.1
1	C	236	GLY	3.1
1	C	348	VAL	3.1
1	B	143	PRO	3.1
1	D	234	SER	3.1
1	D	226	GLY	3.1
1	A	244	PRO	3.1
1	D	224	PRO	3.1
1	A	239	LEU	3.1
1	C	275	GLY	3.1
1	B	250	VAL	3.1
1	D	144	VAL	3.1
1	D	320	VAL	3.1
1	A	146	GLU	3.1
1	D	253	PHE	3.1
1	B	154	GLY	3.1
1	B	235	LEU	3.0
1	B	141	MET	3.0
1	A	217	HIS	3.0
1	B	249	CYS	3.0
1	D	286	TRP	3.0
1	B	255	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	263	LEU	3.0
1	B	340	ALA	2.9
1	C	271	ALA	2.9
1	D	254	ALA	2.9
1	B	274	LEU	2.9
1	A	154	GLY	2.9
1	B	244	PRO	2.9
1	A	252	VAL	2.9
1	B	15	ARG	2.9
1	B	224	PRO	2.9
1	D	142	ALA	2.9
1	D	222	LYS	2.9
1	A	253	PHE	2.9
1	D	268	HIS	2.8
1	B	324	ALA	2.8
1	D	347	THR	2.8
1	B	155	ALA	2.8
1	C	277	LEU	2.8
1	B	242	GLN	2.8
1	D	295	GLN	2.8
1	A	213	GLY	2.8
1	B	315	GLY	2.8
1	D	217	HIS	2.8
1	B	265	ILE	2.8
1	B	243	LEU	2.8
1	B	133	MET	2.8
1	D	220	ASP	2.8
1	D	5	GLY	2.8
1	D	260	HIS	2.8
1	D	158	TYR	2.8
1	D	325	ASN	2.8
1	A	274	LEU	2.8
1	B	227	ALA	2.8
1	C	234	SER	2.7
1	C	350	PRO	2.7
1	B	150	GLN	2.7
1	A	73	ASP	2.7
1	A	173	ILE	2.7
1	D	252	VAL	2.7
1	C	148	LEU	2.7
1	C	223	ARG	2.7
1	B	284	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	226	GLY	2.7
1	C	250	VAL	2.7
1	B	148	LEU	2.7
1	D	293	LEU	2.7
1	D	216	ALA	2.7
1	B	268	HIS	2.7
1	A	162	ASP	2.7
1	D	231	ALA	2.7
1	C	279	PRO	2.6
1	D	257	PRO	2.6
1	A	148	LEU	2.6
1	B	147	GLN	2.6
1	D	152	PRO	2.6
1	B	280	ASN	2.6
1	D	243	LEU	2.6
1	A	143	PRO	2.6
1	B	134	PRO	2.6
1	A	133	MET	2.6
1	D	343	ILE	2.6
1	C	245	PHE	2.6
1	B	233	VAL	2.6
1	C	249	CYS	2.6
1	B	248	THR	2.6
1	A	15	ARG	2.5
1	B	138	ARG	2.5
1	A	278	PRO	2.5
1	C	352	ARG	2.5
1	C	133	MET	2.5
1	C	345	ILE	2.5
1	D	228	GLU	2.5
1	B	149	LYS	2.5
1	B	225	ALA	2.5
1	B	279	PRO	2.5
1	A	156	ALA	2.5
1	C	156	ALA	2.5
1	D	3	ARG	2.5
1	D	282	GLU	2.5
1	A	221	TRP	2.5
1	A	240	THR	2.5
1	B	14	SER	2.5
1	A	257	PRO	2.4
1	A	199	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	217	HIS	2.4
1	D	298	VAL	2.4
1	B	266	GLY	2.4
1	B	290	LEU	2.4
1	D	137	TYR	2.4
1	C	227	ALA	2.4
1	D	258	ASP	2.4
1	B	77	GLN	2.4
1	B	261	LEU	2.4
1	C	323	GLN	2.4
1	A	378	ARG	2.4
1	C	144	VAL	2.4
1	D	361	ALA	2.4
1	B	234	SER	2.4
1	C	226	GLY	2.4
1	B	343	ILE	2.4
1	C	217	HIS	2.4
1	A	245	PHE	2.4
1	A	144	VAL	2.4
1	C	155	ALA	2.4
1	A	134	PRO	2.3
1	A	145	VAL	2.3
1	A	356	ALA	2.3
1	B	328	PRO	2.3
1	C	295	GLN	2.3
1	D	264	GLN	2.3
1	A	353	LEU	2.3
1	A	246	TYR	2.3
1	B	146	GLU	2.3
1	A	62	PRO	2.3
1	B	350	PRO	2.3
1	D	155	ALA	2.3
1	A	183	GLU	2.3
1	C	137	TYR	2.3
1	C	357	VAL	2.3
1	C	3	ARG	2.3
1	D	223	ARG	2.3
1	C	238	HIS	2.3
1	D	141	MET	2.3
1	C	143	PRO	2.3
1	B	142	ALA	2.2
1	D	280	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	240	THR	2.2
1	D	19	HIS	2.2
1	A	135	GLU	2.2
1	C	140	ARG	2.2
1	B	260	HIS	2.2
1	A	165	LEU	2.2
1	A	256	LEU	2.2
1	A	80	VAL	2.2
1	D	350	PRO	2.2
1	C	229	LYS	2.2
1	A	14	SER	2.2
1	A	220	ASP	2.2
1	B	270	ASP	2.2
1	C	146	GLU	2.2
1	A	140	ARG	2.2
1	B	259	TRP	2.2
1	B	358	VAL	2.2
1	D	285	ASN	2.2
1	D	296	ALA	2.2
1	C	347	THR	2.2
1	D	213	GLY	2.2
1	A	214	ARG	2.2
1	B	262	VAL	2.1
1	D	250	VAL	2.1
1	B	356	ALA	2.1
1	D	284	HIS	2.1
1	D	323	GLN	2.1
1	B	353	LEU	2.1
1	C	263	LEU	2.1
1	B	246	TYR	2.1
1	B	294	GLU	2.1
1	C	135	GLU	2.1
1	A	270	ASP	2.1
1	A	229	LYS	2.1
1	B	253	PHE	2.1
1	C	253	PHE	2.1
1	C	260	HIS	2.1
1	B	175	ALA	2.1
1	D	321	ALA	2.1
1	A	152	PRO	2.1
1	D	245	PHE	2.1
1	A	357	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	74	GLN	2.1
1	A	346	ALA	2.1
1	B	291	ALA	2.1
1	D	329	ALA	2.1
1	A	280	ASN	2.1
1	A	360	LEU	2.1
1	B	360	LEU	2.1
1	C	172	GLY	2.1
1	D	349	THR	2.1
1	C	15	ARG	2.1
1	C	151	ASP	2.1
1	D	149	LYS	2.1
1	C	358	VAL	2.1
1	D	248	THR	2.1
1	D	273	GLU	2.1
1	A	136	LYS	2.1
1	C	246	TYR	2.1
1	A	268	HIS	2.1
1	C	298	VAL	2.0
1	B	223	ARG	2.0
1	C	153	ARG	2.0
1	D	353	LEU	2.0
1	A	98	GLU	2.0
1	C	75	ILE	2.0
1	C	270	ASP	2.0
1	B	62	PRO	2.0
1	B	168	SER	2.0
1	C	14	SER	2.0
1	A	170	VAL	2.0
1	A	292	VAL	2.0
1	B	342	ARG	2.0
1	D	80	VAL	2.0
1	C	213	GLY	2.0
1	B	75	ILE	2.0
1	C	248	THR	2.0
1	D	270	ASP	2.0
1	D	395	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 [i](#)

There are no oligosaccharides 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.