



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:20 PM UTC

PDB ID : 2W99 / pdb_00002w99
Title : Crystal Structure of CDK4 in complex with a D-type cyclin
Authors : Day, P.J.; Cleasby, A.; Tickle, I.J.; Reilly, M.O.; Coyle, J.E.; Holding, F.P.;
McMenamin, R.L.; Yon, J.; Chopra, R.; Lengauer, C.; Jhoti, H.
Deposited on : 2009-01-22
Resolution : 2.80 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

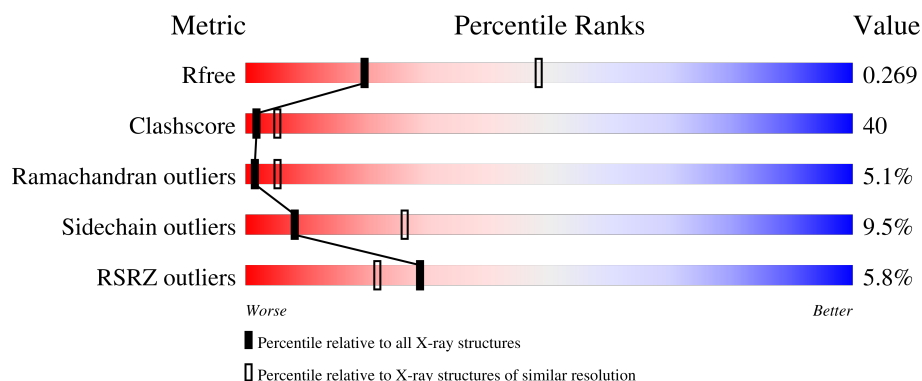
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 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	271	54% 34% 9%
2	B	306	9% 29% 53% 10% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4385 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 G1/S-SPECIFIC CYCLIN-D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1960	1246	333	360	21			

- Molecule 2 is a protein called CELL DIVISION PROTEIN KINASE 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	291	Total	C	N	O	S	0	0	0
			2299	1472	403	413	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	43	GLU	GLY	engineered mutation	UNP P11802
B	44	GLU	GLY	engineered mutation	UNP P11802
B	172	ALA	THR	engineered mutation	UNP P11802

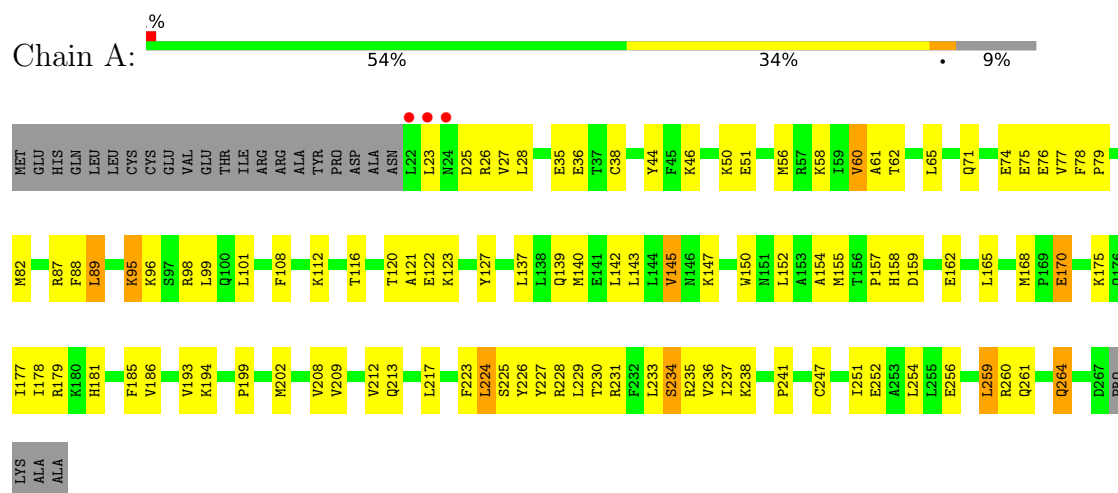
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total	O	0	0
			100	100		
3	B	26	Total	O	0	0
			26	26		

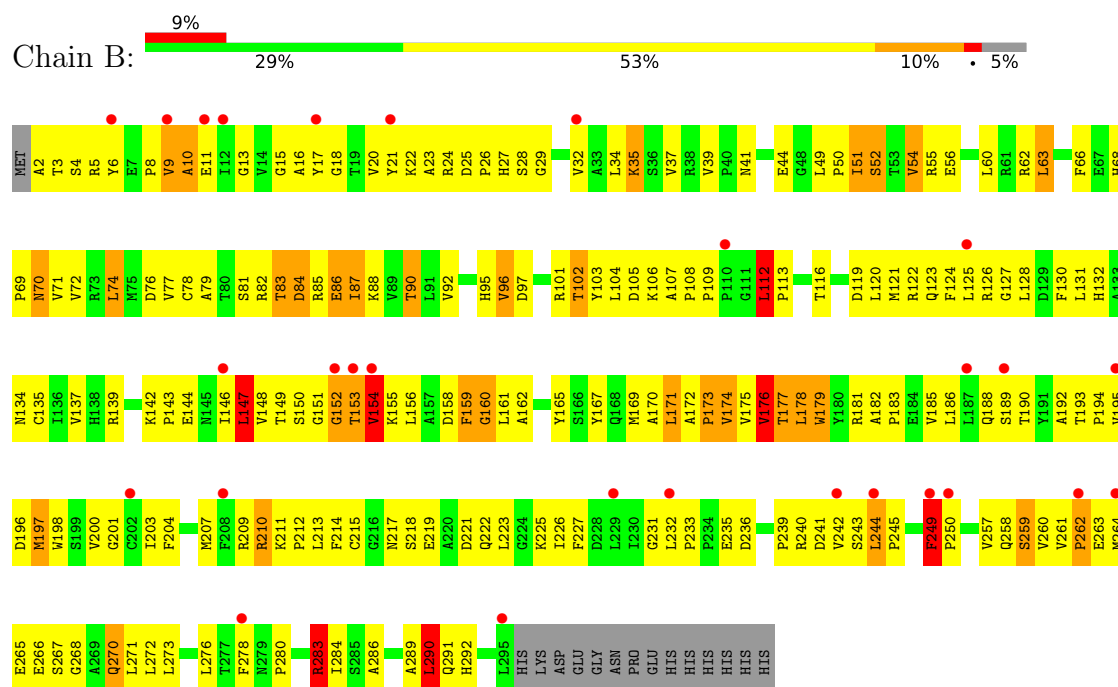
3 Residue-property plots

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: G1/S-SPECIFIC CYCLIN-D1



• Molecule 2: CELL DIVISION PROTEIN KINASE 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.02Å 64.68Å 188.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.49 – 2.80 94.37 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (94.49-2.80) 98.4 (94.37-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.82Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.213 , 0.270 (Not available) , 0.269	Depositor DCC
R_{free} test set	845 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	64.0	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 106.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4385	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 5.18% 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	0.37	0/1993	0.73	0/2691
2	B	0.32	0/2358	0.82	7/3209 (0.2%)
All	All	0.34	0/4351	0.78	7/5900 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	86	GLU	N-CA-C	6.23	118.54	108.32
2	B	147	LEU	N-CA-C	5.73	117.55	108.79
2	B	171	LEU	N-CA-C	-5.44	106.56	114.12
2	B	244	LEU	CA-C-N	5.19	126.33	119.84
2	B	244	LEU	C-N-CA	5.19	126.33	119.84
2	B	66	PHE	N-CA-C	-5.14	107.40	113.97
2	B	170	ALA	N-CA-C	-5.11	106.82	113.16

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	1960	0	2014	94	0
2	B	2299	0	2310	260	0
3	A	100	0	0	6	0
3	B	26	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4385	0	4324	345	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 40.

All (345) 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:112:LYS:HD2	2:B:51:ILE:HD12	1.30	1.13
2:B:96:VAL:HB	2:B:147:LEU:HD12	1.32	1.11
2:B:112:LEU:HB2	2:B:113:PRO:HA	1.41	1.00
2:B:96:VAL:HG11	2:B:147:LEU:HB2	1.41	0.98
2:B:193:THR:HG22	2:B:194:PRO:HD3	1.45	0.96
2:B:32:VAL:HG11	2:B:92:VAL:HG13	1.51	0.91
2:B:182:ALA:HB3	2:B:185:VAL:HG23	1.50	0.90
2:B:173:PRO:HB2	2:B:174:VAL:HG22	1.53	0.89
1:A:259:LEU:HD13	1:A:260:ARG:N	1.90	0.86
2:B:240:ARG:HB2	2:B:241:ASP:HB2	1.59	0.85
1:A:259:LEU:HD13	1:A:260:ARG:H	1.38	0.85
2:B:173:PRO:HB2	2:B:174:VAL:CB	2.08	0.83
1:A:95:LYS:NZ	1:A:95:LYS:H	1.77	0.83
2:B:107:ALA:HB1	2:B:209:ARG:HH11	1.42	0.81
2:B:51:ILE:O	2:B:55:ARG:HG3	1.80	0.81
2:B:96:VAL:CB	2:B:147:LEU:HD12	2.11	0.81
2:B:32:VAL:CG1	2:B:92:VAL:HG13	2.11	0.81
2:B:9:VAL:HG23	2:B:10:ALA:H	1.45	0.80
2:B:63:LEU:HD21	2:B:134:ASN:HD22	1.46	0.80
2:B:123:GLN:HE21	2:B:154:VAL:HG22	1.44	0.79
2:B:173:PRO:HB2	2:B:174:VAL:CG2	2.11	0.79
2:B:172:ALA:N	2:B:173:PRO:HD3	1.99	0.78
1:A:228:ARG:HD3	1:A:231:ARG:HG3	1.65	0.78
2:B:173:PRO:HB2	2:B:174:VAL:HG13	1.66	0.77
2:B:72:VAL:HG22	2:B:156:LEU:O	1.84	0.77
2:B:112:LEU:HB2	2:B:113:PRO:CA	2.14	0.77
2:B:124:PHE:HE2	2:B:200:VAL:HG13	1.47	0.77
2:B:207:MET:O	2:B:209:ARG:HA	1.85	0.76
1:A:23:LEU:O	1:A:27:VAL:HG22	1.86	0.76
2:B:261:VAL:O	2:B:263:GLU:HA	1.87	0.75
1:A:120:THR:HG21	3:A:2057:HOH:O	1.87	0.75
1:A:228:ARG:HA	1:A:228:ARG:NE	2.02	0.75
2:B:107:ALA:HB1	2:B:209:ARG:NH1	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:THR:O	2:B:106:LYS:HG2	1.87	0.74
2:B:146:ILE:C	2:B:147:LEU:HD23	2.12	0.74
1:A:112:LYS:HD2	2:B:51:ILE:CD1	2.14	0.73
2:B:173:PRO:CB	2:B:174:VAL:HG22	2.18	0.73
1:A:168:MET:HE2	1:A:229:LEU:HD11	1.72	0.72
2:B:9:VAL:HG23	2:B:10:ALA:N	2.05	0.72
2:B:204:PHE:HA	2:B:207:MET:HE2	1.72	0.71
2:B:186:LEU:HD23	2:B:219:GLU:HG3	1.70	0.71
2:B:186:LEU:HD23	2:B:219:GLU:CG	2.21	0.71
2:B:87:ILE:HD12	2:B:88:LYS:N	2.06	0.70
2:B:173:PRO:HB2	2:B:174:VAL:CG1	2.20	0.70
2:B:69:PRO:O	2:B:155:LYS:HD3	1.92	0.70
2:B:2:ALA:HB1	2:B:3:THR:HA	1.72	0.69
2:B:203:ILE:O	2:B:207:MET:HG3	1.91	0.69
1:A:58:LYS:O	1:A:62:THR:HG23	1.93	0.69
2:B:68:HIS:ND1	2:B:69:PRO:HD2	2.08	0.69
2:B:153:THR:O	2:B:154:VAL:HG22	1.93	0.69
2:B:143:PRO:HD3	2:B:203:ILE:HD11	1.75	0.68
2:B:265:GLU:HG2	2:B:266:GLU:H	1.59	0.68
1:A:88:PHE:CE1	1:A:147:LYS:HG3	2.28	0.68
1:A:260:ARG:HD3	1:A:261:GLN:N	2.09	0.68
1:A:112:LYS:O	2:B:55:ARG:NH1	2.27	0.67
2:B:218:SER:HB3	2:B:221:ASP:HB2	1.77	0.67
1:A:228:ARG:CD	1:A:231:ARG:HG3	2.25	0.67
2:B:211:LYS:HB3	2:B:212:PRO:CD	2.24	0.67
2:B:271:LEU:HD13	2:B:292:HIS:ND1	2.10	0.67
2:B:124:PHE:CE2	2:B:200:VAL:HG13	2.29	0.67
2:B:160:GLY:O	2:B:162:ALA:N	2.28	0.67
2:B:235:GLU:HB3	2:B:236:ASP:HA	1.76	0.66
2:B:257:VAL:HG21	2:B:273:LEU:HG	1.77	0.66
2:B:235:GLU:OE1	2:B:235:GLU:N	2.29	0.65
2:B:173:PRO:HB2	2:B:174:VAL:CA	2.26	0.65
2:B:213:LEU:O	2:B:213:LEU:HD22	1.96	0.65
2:B:8:PRO:HA	2:B:23:ALA:HB2	1.77	0.65
2:B:15:GLY:O	2:B:18:GLY:N	2.30	0.65
2:B:193:THR:CG2	2:B:194:PRO:HD3	2.22	0.64
2:B:178:LEU:O	2:B:222:GLN:NE2	2.28	0.64
2:B:123:GLN:NE2	2:B:153:THR:O	2.30	0.64
2:B:176:VAL:O	2:B:178:LEU:N	2.30	0.63
2:B:284:ILE:HD13	2:B:289:ALA:HB2	1.80	0.63
2:B:173:PRO:CB	2:B:174:VAL:HG13	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:ALA:HB1	2:B:194:PRO:HD2	1.81	0.63
1:A:108:PHE:O	1:A:112:LYS:HG3	1.98	0.63
2:B:76:ASP:OD1	2:B:77:VAL:N	2.30	0.63
2:B:173:PRO:HG2	2:B:174:VAL:HG22	1.81	0.62
2:B:79:ALA:HB1	2:B:87:ILE:CD1	2.29	0.62
2:B:218:SER:HB3	2:B:221:ASP:CB	2.30	0.62
2:B:63:LEU:CD2	2:B:134:ASN:HD22	2.10	0.62
1:A:256:GLU:O	1:A:259:LEU:HD12	2.00	0.62
2:B:6:TYR:CE2	2:B:92:VAL:HG21	2.34	0.62
2:B:81:SER:O	2:B:87:ILE:HA	1.99	0.62
2:B:171:LEU:C	2:B:173:PRO:HD3	2.24	0.62
2:B:34:LEU:CD2	2:B:92:VAL:HG22	2.30	0.61
1:A:79:PRO:HG3	1:A:158:HIS:CE1	2.35	0.61
1:A:120:THR:HG22	1:A:123:LYS:H	1.65	0.61
2:B:127:GLY:O	2:B:131:LEU:HD13	1.99	0.61
2:B:79:ALA:HB1	2:B:87:ILE:HD11	1.81	0.61
2:B:171:LEU:HB3	2:B:173:PRO:HG3	1.82	0.61
2:B:171:LEU:HD23	2:B:171:LEU:O	2.00	0.61
1:A:228:ARG:HA	1:A:228:ARG:HE	1.65	0.61
2:B:85:ARG:O	2:B:86:GLU:HG3	2.00	0.61
1:A:56:MET:O	1:A:60:VAL:HG23	2.01	0.60
2:B:181:ARG:HG3	2:B:185:VAL:HG11	1.83	0.60
1:A:193:VAL:HG22	3:A:2080:HOH:O	2.02	0.60
2:B:51:ILE:N	2:B:51:ILE:HD13	2.17	0.60
2:B:121:MET:CG	2:B:207:MET:HE1	2.31	0.60
1:A:71:GLN:NE2	1:A:127:TYR:OH	2.30	0.60
2:B:210:ARG:NH1	3:B:2025:HOH:O	2.27	0.59
2:B:123:GLN:NE2	2:B:154:VAL:HG22	2.17	0.59
2:B:52:SER:O	2:B:56:GLU:HG2	2.03	0.59
2:B:209:ARG:H	2:B:210:ARG:HG3	1.68	0.59
1:A:35:GLU:CD	1:A:199:PRO:HB2	2.27	0.59
1:A:170:GLU:OE1	1:A:225:SER:HB2	2.02	0.59
1:A:95:LYS:H	1:A:95:LYS:HZ2	1.51	0.59
2:B:25:ASP:O	2:B:29:GLY:N	2.28	0.59
2:B:70:ASN:ND2	2:B:127:GLY:N	2.50	0.59
2:B:150:SER:O	2:B:152:GLY:N	2.36	0.59
2:B:242:VAL:HG22	2:B:243:SER:H	1.68	0.58
2:B:34:LEU:HD22	2:B:92:VAL:HG22	1.84	0.58
1:A:162:GLU:OE2	1:A:179:ARG:HD3	2.03	0.58
2:B:125:LEU:HB3	2:B:290:LEU:HD12	1.86	0.58
2:B:120:LEU:C	2:B:120:LEU:HD23	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:VAL:HG21	1:A:99:LEU:HG	1.85	0.58
2:B:74:LEU:HD21	2:B:77:VAL:HG22	1.87	0.57
2:B:270:GLN:HA	2:B:270:GLN:HE21	1.69	0.57
2:B:159:PHE:N	2:B:159:PHE:CD1	2.71	0.57
1:A:60:VAL:HG21	1:A:99:LEU:CD2	2.35	0.56
2:B:154:VAL:HG23	2:B:154:VAL:O	2.05	0.56
2:B:249:PHE:CB	2:B:250:PRO:HD3	2.36	0.56
1:A:112:LYS:CD	2:B:51:ILE:HD12	2.19	0.56
2:B:35:LYS:HE2	2:B:158:ASP:OD1	2.06	0.56
2:B:192:ALA:O	2:B:195:VAL:HG22	2.06	0.56
2:B:173:PRO:CG	2:B:174:VAL:HG22	2.35	0.56
1:A:36:GLU:HB3	3:A:2009:HOH:O	2.06	0.55
2:B:25:ASP:CG	2:B:28:SER:HB3	2.32	0.55
2:B:290:LEU:HD23	2:B:290:LEU:O	2.07	0.55
1:A:25:ASP:OD2	1:A:26:ARG:N	2.41	0.54
2:B:20:VAL:HG23	2:B:20:VAL:O	2.07	0.54
2:B:20:VAL:HG12	2:B:35:LYS:HG3	1.89	0.54
2:B:71:VAL:HG12	2:B:159:PHE:HE2	1.73	0.54
2:B:272:LEU:O	2:B:272:LEU:HD12	2.07	0.54
2:B:128:LEU:HD13	2:B:128:LEU:C	2.33	0.54
2:B:262:PRO:HA	2:B:263:GLU:CB	2.36	0.54
1:A:224:LEU:HA	1:A:226:TYR:CD1	2.43	0.54
2:B:123:GLN:HG2	2:B:154:VAL:CG2	2.38	0.54
2:B:262:PRO:HA	2:B:263:GLU:HB2	1.90	0.54
2:B:8:PRO:HA	2:B:23:ALA:CB	2.38	0.54
2:B:51:ILE:HG21	2:B:55:ARG:NH2	2.23	0.54
1:A:259:LEU:C	1:A:259:LEU:HD22	2.33	0.53
2:B:128:LEU:HD12	2:B:286:ALA:HB1	1.90	0.53
1:A:139:GLN:HG3	2:B:82:ARG:HH12	1.74	0.53
1:A:75:GLU:OE1	1:A:75:GLU:N	2.36	0.53
1:A:79:PRO:HG3	1:A:158:HIS:HE1	1.73	0.53
2:B:109:PRO:HB3	2:B:112:LEU:HD12	1.90	0.53
2:B:211:LYS:HB3	2:B:212:PRO:HD2	1.90	0.53
2:B:97:ASP:H	2:B:149:THR:HA	1.74	0.52
2:B:175:VAL:C	2:B:176:VAL:HG23	2.33	0.52
1:A:228:ARG:HG2	1:A:231:ARG:NH1	2.24	0.52
2:B:4:SER:C	2:B:6:TYR:H	2.18	0.52
2:B:233:PRO:HG2	2:B:278:PHE:CD2	2.44	0.52
1:A:95:LYS:H	1:A:95:LYS:CE	2.22	0.52
1:A:224:LEU:HA	1:A:226:TYR:HD1	1.75	0.52
1:A:74:GLU:O	1:A:77:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:LEU:HD22	2:B:173:PRO:HG3	1.92	0.52
2:B:188:GLN:HG2	2:B:240:ARG:O	2.10	0.52
2:B:242:VAL:HG22	2:B:243:SER:N	2.24	0.52
1:A:168:MET:HE1	1:A:208:VAL:HG11	1.92	0.51
2:B:197:MET:HE2	2:B:200:VAL:HG21	1.92	0.51
2:B:39:VAL:HG23	2:B:87:ILE:HG23	1.92	0.51
2:B:108:PRO:N	2:B:109:PRO:CD	2.73	0.51
2:B:214:PHE:CZ	2:B:226:ILE:HA	2.45	0.51
2:B:2:ALA:CB	2:B:3:THR:HA	2.32	0.51
2:B:128:LEU:HD11	2:B:132:HIS:CE1	2.45	0.51
2:B:289:ALA:O	2:B:291:GLN:N	2.43	0.51
1:A:27:VAL:HG23	1:A:28:LEU:N	2.26	0.51
2:B:212:PRO:HB2	2:B:215:CYS:SG	2.51	0.51
2:B:271:LEU:HD13	2:B:292:HIS:CG	2.46	0.51
2:B:212:PRO:HB2	2:B:215:CYS:HB3	1.93	0.51
2:B:240:ARG:HB2	2:B:241:ASP:CB	2.35	0.51
1:A:61:ALA:HB2	1:A:82:MET:CE	2.41	0.51
1:A:202:MET:CE	1:A:247:CYS:HB2	2.41	0.50
2:B:289:ALA:C	2:B:291:GLN:H	2.19	0.50
2:B:235:GLU:CB	2:B:236:ASP:HA	2.38	0.50
1:A:194:LYS:NZ	1:A:247:CYS:SG	2.82	0.50
2:B:150:SER:C	2:B:152:GLY:H	2.20	0.50
2:B:212:PRO:CB	2:B:215:CYS:HB3	2.41	0.50
2:B:197:MET:HE3	2:B:197:MET:HA	1.94	0.49
2:B:272:LEU:HD12	2:B:276:LEU:HG	1.93	0.49
2:B:193:THR:N	2:B:194:PRO:CD	2.76	0.49
1:A:157:PRO:HG2	1:A:186:VAL:HG13	1.94	0.48
1:A:209:VAL:HG23	1:A:233:LEU:HD12	1.95	0.48
2:B:178:LEU:CD2	2:B:181:ARG:HB2	2.43	0.48
2:B:198:TRP:HB2	2:B:283:ARG:NH1	2.28	0.48
2:B:74:LEU:HD21	2:B:77:VAL:CG2	2.43	0.48
2:B:213:LEU:HD13	2:B:214:PHE:CD1	2.49	0.48
1:A:226:TYR:CG	1:A:227:TYR:N	2.81	0.48
2:B:232:LEU:C	2:B:232:LEU:HD23	2.37	0.48
2:B:122:ARG:O	2:B:126:ARG:HG3	2.13	0.48
1:A:38:CYS:O	1:A:87:ARG:HD2	2.13	0.48
2:B:197:MET:O	2:B:200:VAL:HB	2.13	0.48
1:A:157:PRO:HG2	1:A:186:VAL:CG1	2.43	0.48
2:B:96:VAL:CG1	2:B:97:ASP:N	2.76	0.48
2:B:167:TYR:HB3	3:B:2006:HOH:O	2.13	0.48
1:A:142:LEU:HD21	2:B:49:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:GLY:O	2:B:17:TYR:N	2.46	0.47
2:B:244:LEU:N	2:B:245:PRO:HD3	2.28	0.47
2:B:4:SER:O	2:B:6:TYR:N	2.38	0.47
2:B:121:MET:HG3	2:B:207:MET:HE1	1.96	0.47
2:B:149:THR:HG23	2:B:150:SER:N	2.29	0.47
2:B:209:ARG:O	2:B:209:ARG:HG3	2.14	0.47
2:B:232:LEU:HD12	2:B:250:PRO:O	2.14	0.47
2:B:258:GLN:HA	2:B:261:VAL:HG23	1.96	0.47
2:B:70:ASN:HD22	2:B:127:GLY:CA	2.27	0.47
2:B:134:ASN:O	2:B:135:CYS:HB2	2.15	0.47
2:B:258:GLN:CD	2:B:258:GLN:H	2.22	0.47
2:B:2:ALA:HB1	2:B:3:THR:CA	2.43	0.47
2:B:68:HIS:ND1	2:B:69:PRO:CD	2.77	0.47
2:B:194:PRO:O	2:B:197:MET:N	2.44	0.47
2:B:79:ALA:CB	2:B:87:ILE:HD11	2.44	0.47
2:B:124:PHE:HD1	2:B:156:LEU:HD21	1.79	0.47
2:B:173:PRO:CB	2:B:174:VAL:CA	2.93	0.47
2:B:213:LEU:CD1	2:B:214:PHE:CD1	2.98	0.47
2:B:13:GLY:O	2:B:20:VAL:HG22	2.15	0.47
1:A:101:LEU:HG	1:A:140:MET:HG3	1.96	0.47
2:B:257:VAL:O	2:B:261:VAL:HG22	2.14	0.47
1:A:61:ALA:HB2	1:A:82:MET:HE1	1.96	0.46
1:A:95:LYS:HB3	3:A:2042:HOH:O	2.14	0.46
1:A:230:THR:O	1:A:234:SER:OG	2.29	0.46
1:A:236:VAL:O	1:A:238:LYS:HD2	2.15	0.46
2:B:50:PRO:O	2:B:54:VAL:HG13	2.16	0.46
2:B:71:VAL:HG21	2:B:131:LEU:CD1	2.46	0.46
2:B:70:ASN:ND2	2:B:127:GLY:CA	2.79	0.46
2:B:267:SER:O	2:B:270:GLN:N	2.48	0.46
1:A:145:VAL:CG1	1:A:150:TRP:CE2	2.98	0.46
2:B:201:GLY:HA2	2:B:204:PHE:HB3	1.97	0.46
2:B:207:MET:C	2:B:209:ARG:HA	2.40	0.46
2:B:9:VAL:N	2:B:22:LYS:O	2.38	0.45
2:B:101:ARG:C	2:B:103:TYR:N	2.73	0.45
2:B:150:SER:C	2:B:152:GLY:N	2.73	0.45
1:A:228:ARG:CG	1:A:231:ARG:HG3	2.46	0.45
1:A:60:VAL:HG21	1:A:99:LEU:CG	2.47	0.45
2:B:108:PRO:HG2	2:B:109:PRO:HD3	1.98	0.45
1:A:213:GLN:O	1:A:217:LEU:HD13	2.16	0.45
2:B:51:ILE:CG2	2:B:55:ARG:NH2	2.79	0.45
2:B:71:VAL:CG1	2:B:159:PHE:HE2	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ARG:O	1:A:264:GLN:HG3	2.17	0.45
1:A:95:LYS:HZ3	1:A:98:ARG:HH11	1.65	0.45
2:B:240:ARG:CB	2:B:241:ASP:CB	2.95	0.45
2:B:24:ARG:O	2:B:26:PRO:HD3	2.17	0.45
1:A:228:ARG:HD3	1:A:231:ARG:NE	2.33	0.44
2:B:108:PRO:CG	2:B:109:PRO:HD3	2.47	0.44
2:B:112:LEU:CB	2:B:113:PRO:HA	2.30	0.44
2:B:227:PHE:CE2	2:B:233:PRO:HD2	2.52	0.44
2:B:249:PHE:HB2	2:B:250:PRO:HD3	1.99	0.44
2:B:183:PRO:HB2	2:B:278:PHE:CE1	2.52	0.44
2:B:280:PRO:HA	2:B:283:ARG:HD3	1.99	0.44
1:A:152:LEU:C	1:A:154:ALA:H	2.25	0.44
2:B:68:HIS:CD2	2:B:130:PHE:CG	3.06	0.44
2:B:149:THR:CG2	2:B:150:SER:N	2.79	0.44
2:B:240:ARG:CB	2:B:241:ASP:CA	2.95	0.44
1:A:185:PHE:CD2	1:A:251:ILE:CG2	3.00	0.44
2:B:172:ALA:N	2:B:173:PRO:CD	2.74	0.44
2:B:171:LEU:HD22	2:B:173:PRO:HB3	1.99	0.44
2:B:197:MET:CE	2:B:200:VAL:HG21	2.47	0.44
1:A:150:TRP:HZ2	2:B:79:ALA:HB2	1.82	0.44
2:B:242:VAL:O	2:B:243:SER:HB2	2.18	0.44
2:B:259:SER:OG	2:B:260:VAL:N	2.51	0.44
1:A:228:ARG:NE	1:A:228:ARG:CA	2.78	0.44
2:B:62:ARG:O	2:B:62:ARG:HG2	2.16	0.44
2:B:192:ALA:CB	2:B:194:PRO:HD2	2.48	0.44
2:B:240:ARG:CB	2:B:241:ASP:HB2	2.40	0.44
1:A:88:PHE:HE1	1:A:147:LYS:HG3	1.77	0.44
2:B:35:LYS:HB2	2:B:35:LYS:NZ	2.32	0.44
1:A:170:GLU:O	1:A:175:LYS:HE3	2.18	0.43
2:B:21:TYR:CD1	2:B:34:LEU:HB2	2.52	0.43
2:B:71:VAL:HG11	2:B:131:LEU:HD11	2.00	0.43
1:A:202:MET:HE3	1:A:202:MET:HB3	1.90	0.43
2:B:212:PRO:HB2	2:B:215:CYS:CB	2.48	0.43
1:A:51:GLU:OE1	1:A:96:LYS:HG2	2.18	0.43
1:A:121:ALA:N	2:B:44:GLU:OE2	2.29	0.43
2:B:51:ILE:HG22	2:B:55:ARG:CZ	2.48	0.43
2:B:123:GLN:O	2:B:126:ARG:HB2	2.18	0.43
2:B:142:LYS:O	2:B:146:ILE:HG13	2.19	0.43
2:B:71:VAL:CG1	2:B:131:LEU:HD11	2.47	0.43
2:B:139:ARG:NH2	2:B:162:ALA:HB1	2.32	0.43
2:B:4:SER:C	2:B:6:TYR:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:THR:O	2:B:116:THR:HG22	2.18	0.43
1:A:194:LYS:CE	1:A:247:CYS:SG	3.07	0.43
2:B:105:ASP:C	2:B:107:ALA:H	2.27	0.43
1:A:177:ILE:O	1:A:181:HIS:ND1	2.52	0.43
2:B:137:VAL:HG13	2:B:196:ASP:HB2	1.99	0.43
2:B:149:THR:HG23	2:B:150:SER:OG	2.18	0.43
2:B:260:VAL:O	2:B:260:VAL:HG22	2.17	0.43
1:A:28:LEU:HD12	1:A:28:LEU:O	2.18	0.43
2:B:71:VAL:CG1	2:B:159:PHE:CE2	3.02	0.43
2:B:101:ARG:HH12	2:B:144:GLU:HG3	1.84	0.43
1:A:226:TYR:CD2	1:A:226:TYR:C	2.96	0.42
1:A:120:THR:HG23	3:B:2011:HOH:O	2.19	0.42
2:B:122:ARG:HG3	2:B:290:LEU:HD23	2.01	0.42
2:B:183:PRO:HB2	2:B:278:PHE:HE1	1.84	0.42
2:B:223:LEU:HD23	2:B:223:LEU:O	2.19	0.42
2:B:60:LEU:CB	2:B:74:LEU:HD12	2.49	0.42
2:B:108:PRO:N	2:B:109:PRO:HD2	2.34	0.42
2:B:11:GLU:HA	2:B:21:TYR:HA	2.01	0.42
2:B:96:VAL:HG13	2:B:97:ASP:N	2.34	0.42
2:B:218:SER:HB3	2:B:221:ASP:HB3	2.02	0.42
2:B:264:MET:HE3	2:B:268:GLY:HA3	2.00	0.42
2:B:104:LEU:HD22	2:B:209:ARG:NH2	2.34	0.42
2:B:272:LEU:CD1	2:B:276:LEU:HG	2.50	0.42
1:A:95:LYS:NZ	1:A:95:LYS:N	2.57	0.42
2:B:37:VAL:HG23	2:B:165:TYR:CD2	2.54	0.42
2:B:105:ASP:C	2:B:107:ALA:N	2.78	0.42
2:B:41:ASN:HB3	2:B:85:ARG:H	1.84	0.42
2:B:60:LEU:HB2	2:B:74:LEU:HD12	2.02	0.42
2:B:101:ARG:C	2:B:103:TYR:H	2.28	0.42
2:B:139:ARG:HB2	2:B:139:ARG:NH1	2.34	0.42
2:B:177:THR:O	2:B:179:TRP:N	2.45	0.42
2:B:22:LYS:HD2	2:B:95:HIS:NE2	2.35	0.41
1:A:155:MET:HE1	1:A:159:ASP:HB3	2.02	0.41
2:B:78:CYS:HB3	2:B:90:THR:HG23	2.01	0.41
2:B:188:GLN:NE2	2:B:190:THR:CG2	2.83	0.41
2:B:123:GLN:HG2	2:B:154:VAL:HG22	2.02	0.41
2:B:63:LEU:CD2	2:B:134:ASN:ND2	2.79	0.41
1:A:46:LYS:NZ	3:A:2016:HOH:O	2.53	0.41
1:A:78:PHE:N	1:A:79:PRO:HD2	2.36	0.41
1:A:175:LYS:O	1:A:179:ARG:HB2	2.21	0.41
2:B:124:PHE:CE2	2:B:200:VAL:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:TYR:CE2	1:A:89:LEU:HB3	2.56	0.41
1:A:95:LYS:HZ2	1:A:95:LYS:N	2.16	0.41
1:A:228:ARG:HG3	1:A:231:ARG:HB2	2.03	0.41
1:A:237:ILE:O	1:A:237:ILE:HG22	2.21	0.41
2:B:265:GLU:HG2	2:B:266:GLU:HG2	2.03	0.41
1:A:120:THR:HG22	1:A:122:GLU:N	2.35	0.41
2:B:22:LYS:HD2	2:B:95:HIS:CE1	2.56	0.41
2:B:37:VAL:HB	2:B:165:TYR:CE2	2.56	0.41
1:A:123:LYS:HB2	1:A:123:LYS:HE3	1.84	0.40
2:B:37:VAL:HG23	2:B:165:TYR:CE2	2.56	0.40
1:A:23:LEU:HD23	1:A:23:LEU:HA	1.95	0.40
1:A:223:PHE:C	1:A:225:SER:H	2.29	0.40
1:A:241:PRO:HG2	3:A:2096:HOH:O	2.20	0.40
2:B:271:LEU:HD22	2:B:292:HIS:ND1	2.37	0.40
2:B:62:ARG:NH1	3:B:2014:HOH:O	2.44	0.40
2:B:210:ARG:NE	2:B:211:LYS:O	2.54	0.40
2:B:231:GLY:O	2:B:233:PRO:HD3	2.22	0.40
1:A:178:ILE:CD1	1:A:212:VAL:HG22	2.52	0.40
2:B:32:VAL:HG11	2:B:92:VAL:CG1	2.37	0.40
2:B:83:THR:O	2:B:84:ASP:C	2.64	0.40
2:B:221:ASP:O	2:B:225:LYS:HB2	2.22	0.40
2:B:222:GLN:HA	2:B:225:LYS:HB2	2.03	0.40
2:B:249:PHE:HD1	2:B:249:PHE:HA	1.70	0.40
1:A:139:GLN:HG3	2:B:82:ARG:NH1	2.36	0.40
2:B:54:VAL:CG2	2:B:55:ARG:N	2.84	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	244/271 (90%)	228 (93%)	15 (6%)	1 (0%)	30 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	289/306 (94%)	211 (73%)	52 (18%)	26 (9%)	0	1
All	All	533/577 (92%)	439 (82%)	67 (13%)	27 (5%)	1	5

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	10	ALA
2	B	16	ALA
2	B	161	LEU
2	B	177	THR
2	B	283	ARG
2	B	9	VAL
2	B	84	ASP
2	B	151	GLY
2	B	217	ASN
2	B	5	ARG
2	B	259	SER
2	B	290	LEU
2	B	262	PRO
1	A	224	LEU
2	B	63	LEU
2	B	102	THR
2	B	169	MET
2	B	173	PRO
2	B	189	SER
2	B	178	LEU
2	B	249	PHE
2	B	152	GLY
2	B	154	VAL
2	B	160	GLY
2	B	176	VAL
2	B	112	LEU
2	B	239	PRO

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	222/243 (91%)	204 (92%)	18 (8%)	11	33
2	B	250/264 (95%)	223 (89%)	27 (11%)	6	21
All	All	472/507 (93%)	427 (90%)	45 (10%)	8	26

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	60	VAL
1	A	65	LEU
1	A	76	GLU
1	A	89	LEU
1	A	95	LYS
1	A	116	THR
1	A	137	LEU
1	A	143	LEU
1	A	145	VAL
1	A	165	LEU
1	A	170	GLU
1	A	234	SER
1	A	235	ARG
1	A	252	GLU
1	A	254	LEU
1	A	259	LEU
1	A	264	GLN
2	B	27	HIS
2	B	35	LYS
2	B	51	ILE
2	B	52	SER
2	B	54	VAL
2	B	70	ASN
2	B	74	LEU
2	B	83	THR
2	B	87	ILE
2	B	90	THR
2	B	96	VAL
2	B	112	LEU
2	B	119	ASP
2	B	147	LEU
2	B	148	VAL
2	B	153	THR
2	B	154	VAL

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Mol	Chain	Res	Type
2	B	159	PHE
2	B	174	VAL
2	B	176	VAL
2	B	179	TRP
2	B	197	MET
2	B	210	ARG
2	B	249	PHE
2	B	270	GLN
2	B	283	ARG
2	B	290	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	71	GLN
1	A	139	GLN
1	A	158	HIS
1	A	176	GLN
1	A	198	ASN
1	A	216	ASN
1	A	261	GLN
1	A	264	GLN
2	B	41	ASN
2	B	70	ASN
2	B	98	GLN
2	B	123	GLN
2	B	134	ASN
2	B	188	GLN
2	B	258	GLN
2	B	270	GLN
2	B	291	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 oligosaccharides 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	246/271 (90%)	-0.19	3 (1%) 76 68	32, 51, 108, 157	0
2	B	291/306 (95%)	0.96	28 (9%) 13 10	59, 112, 151, 171	0
All	All	537/577 (93%)	0.43	31 (5%) 29 22	32, 87, 143, 171	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	295	LEU	4.7
2	B	12	ILE	3.9
2	B	21	TYR	3.8
2	B	264	MET	3.2
2	B	232	LEU	3.1
1	A	22	LEU	2.9
2	B	152	GLY	2.8
2	B	195	VAL	2.8
2	B	244	LEU	2.8
2	B	262	PRO	2.8
2	B	187	LEU	2.6
2	B	9	VAL	2.6
2	B	208	PHE	2.5
2	B	242	VAL	2.5
2	B	110	PRO	2.5
2	B	17	TYR	2.5
2	B	32	VAL	2.5
2	B	278	PHE	2.4
2	B	125	LEU	2.4
2	B	249	PHE	2.3
2	B	189	SER	2.2
2	B	154	VAL	2.2
1	A	23	LEU	2.2
2	B	153	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	11	GLU	2.1
2	B	202	CYS	2.1
2	B	6	TYR	2.1
2	B	146	ILE	2.0
2	B	250	PRO	2.0
2	B	229	LEU	2.0
1	A	24	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.