



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:36 AM UTC

PDB ID : 1Q9J / pdb_00001q9j
Title : Structure of polyketide synthase associated protein 5 from Mycobacterium tuberculosis
Authors : Buglino, J.; Onwueme, K.C.; Quadri, L.E.; Lima, C.D.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2003-08-25
Resolution : 2.75 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

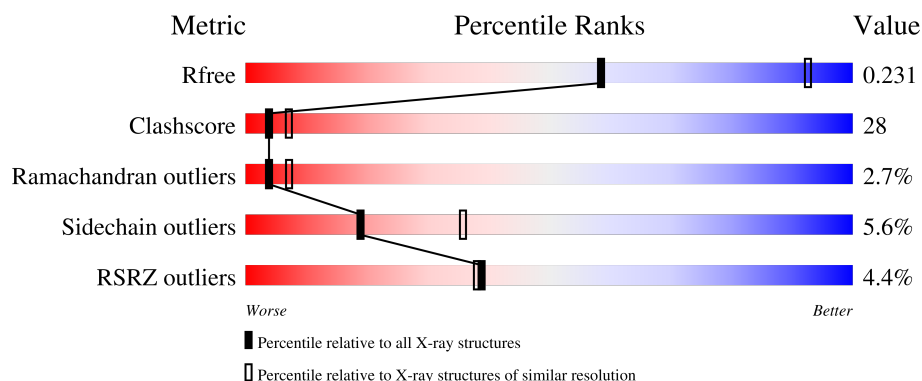
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	422	5% 49% 38% 5% • 8%
1	B	422	4% 52% 39% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6225 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 Polyketide synthase associated protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			2962	1893	495	560	14			
1	B	399	Total	C	N	O	S	0	0	0
			3037	1939	508	577	13			

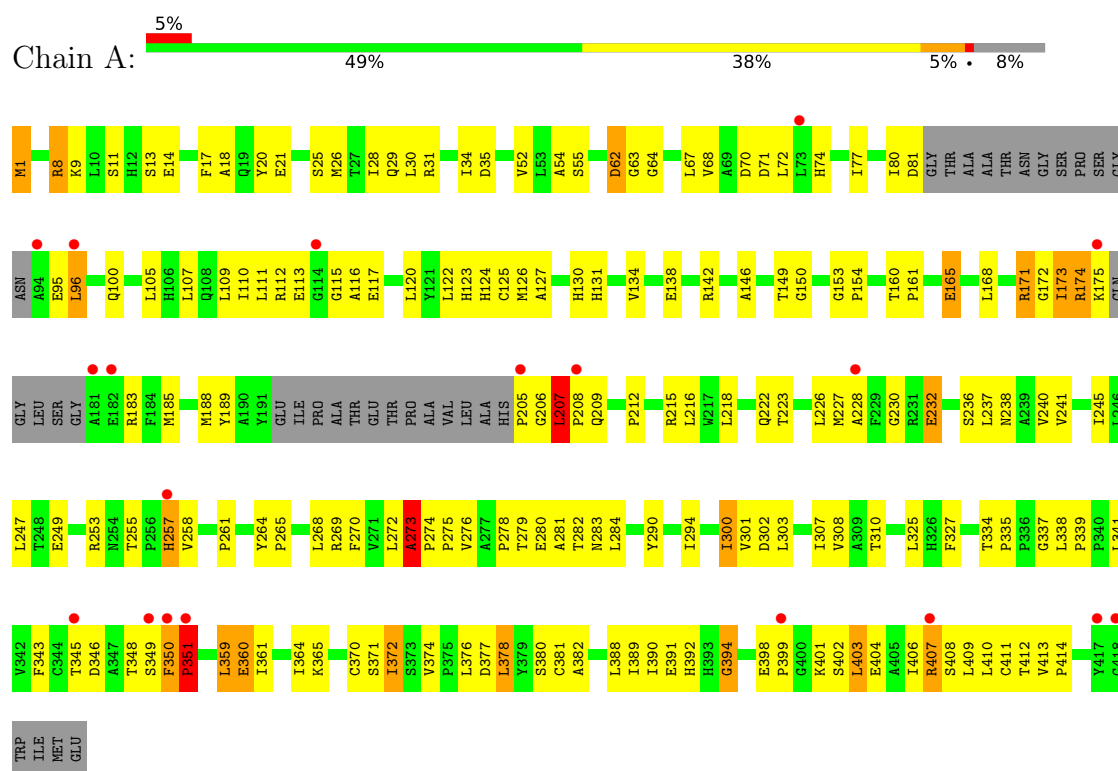
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total	O	0	0
			90	90		
2	B	136	Total	O	0	0
			136	136		

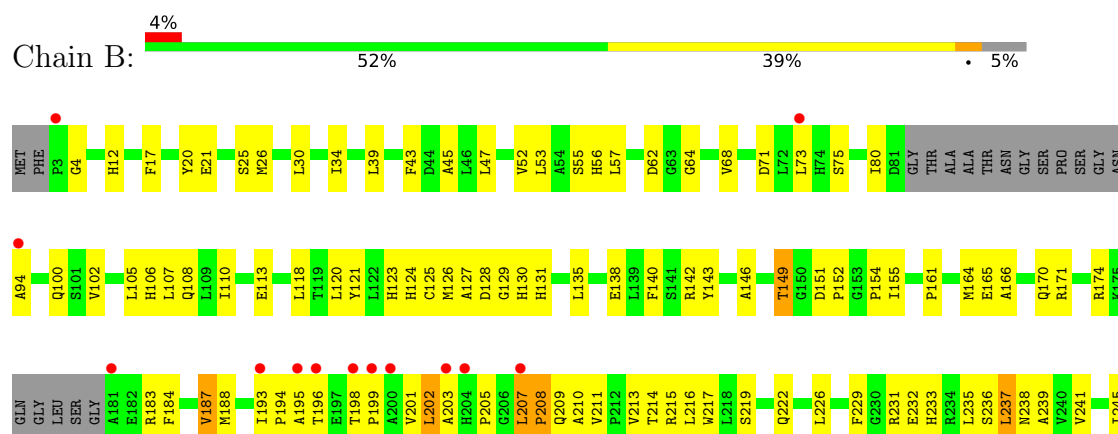
3 Residue-property plots

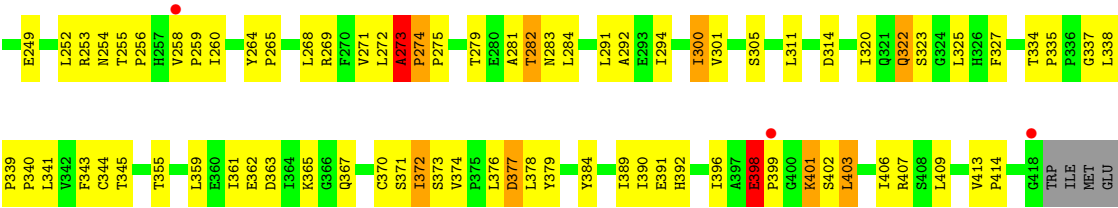
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Polyketide synthase associated protein 5



- Molecule 1: Polyketide synthase associated protein 5





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	172.98Å 172.98Å 80.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.75 20.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	93.7 (20.00-2.75) 93.5 (20.00-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.75Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.295 0.231 , 0.231	Depositor DCC
R_{free} test set	1172 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6225	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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	0.51	0/3032	0.95	10/4142 (0.2%)
1	B	0.52	0/3110	0.93	7/4255 (0.2%)
All	All	0.52	0/6142	0.94	17/8397 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	ALA	CA-C-N	-7.96	112.18	120.38
1	B	273	ALA	C-N-CA	-7.96	112.18	120.38
1	A	273	ALA	CA-C-N	-7.16	113.01	120.38
1	A	273	ALA	C-N-CA	-7.16	113.01	120.38
1	A	232	GLU	N-CA-C	-6.17	105.06	112.59
1	A	207	LEU	CA-C-N	6.08	126.56	119.99
1	A	207	LEU	C-N-CA	6.08	126.56	119.99
1	B	274	PRO	N-CA-C	-5.61	103.85	110.70
1	B	398	GLU	CA-C-N	5.40	125.74	119.47
1	B	398	GLU	C-N-CA	5.40	125.74	119.47
1	B	271	VAL	CB-CA-C	-5.35	106.36	111.44
1	A	67	LEU	N-CA-C	-5.24	99.24	108.20
1	A	394	GLY	N-CA-C	5.23	116.92	111.95
1	B	377	ASP	N-CA-C	-5.21	98.73	107.32
1	A	308	VAL	CB-CA-C	-5.20	105.23	112.04
1	A	153	GLY	CA-C-N	5.02	124.92	119.85
1	A	153	GLY	C-N-CA	5.02	124.92	119.85

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	2962	0	2938	180	0
1	B	3037	0	3011	159	0
2	A	90	0	0	7	0
2	B	136	0	0	7	12
All	All	6225	0	5949	339	12

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 28.

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:348:THR:HG22	1:A:382:ALA:HA	1.41	1.02
1:A:52:VAL:HG23	2:A:423:HOH:O	1.70	0.91
1:A:26:MET:HE2	1:A:364:ILE:HG23	1.51	0.91
1:A:273:ALA:CB	1:A:274:PRO:HD2	2.01	0.90
1:B:300:ILE:HD12	1:B:300:ILE:H	1.33	0.90
1:B:282:THR:HG22	1:B:283:ASN:ND2	1.88	0.89
1:A:371:SER:O	1:A:374:VAL:HG23	1.71	0.88
1:B:216:LEU:HD22	1:B:407:ARG:HH21	1.39	0.86
1:A:282:THR:HG22	1:A:283:ASN:ND2	1.93	0.83
1:A:392:HIS:HB2	1:A:403:LEU:HD13	1.60	0.82
1:A:52:VAL:HG21	1:A:161:PRO:HD2	1.61	0.81
1:A:34:ILE:HG21	1:A:109:LEU:HD21	1.63	0.81
1:B:273:ALA:HB3	1:B:274:PRO:HD3	1.63	0.80
1:A:216:LEU:HG	1:A:403:LEU:HD23	1.63	0.80
1:A:269:ARG:HE	1:A:278:PRO:HA	1.47	0.80
1:A:273:ALA:HB1	1:A:274:PRO:CD	2.13	0.79
1:B:210:ALA:HB1	1:B:367:GLN:NE2	1.98	0.78
1:B:199:PRO:HA	2:B:439:HOH:O	1.84	0.78
1:B:164:MET:HE2	1:B:268:LEU:HD12	1.65	0.77
1:B:164:MET:HG3	1:B:284:LEU:HD12	1.68	0.76
1:A:55:SER:HB2	1:A:68:VAL:O	1.84	0.76
1:A:20:TYR:HD2	1:A:374:VAL:HG22	1.51	0.76
1:A:273:ALA:HB1	1:A:274:PRO:HD2	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLU:HA	1:A:100:GLN:OE1	1.85	0.76
1:B:273:ALA:CB	1:B:274:PRO:HD3	2.16	0.75
1:A:273:ALA:O	1:A:274:PRO:C	2.27	0.75
1:B:209:GLN:OE1	1:B:372:ILE:HG23	1.85	0.75
1:B:57:LEU:HD12	1:B:100:GLN:HB2	1.68	0.75
1:B:26:MET:HG2	2:B:424:HOH:O	1.86	0.74
1:A:218:LEU:HD11	1:A:407:ARG:HH22	1.52	0.74
1:A:273:ALA:CB	1:A:274:PRO:CD	2.65	0.74
1:A:370:CYS:HB2	1:A:374:VAL:HG21	1.67	0.74
1:B:107:LEU:HD11	1:B:118:LEU:HD11	1.70	0.72
1:A:226:LEU:HD21	1:A:410:LEU:HD22	1.71	0.72
1:B:273:ALA:HB3	1:B:274:PRO:CD	2.20	0.71
1:A:112:ARG:HB2	1:A:115:GLY:O	1.89	0.71
1:A:273:ALA:HB3	1:A:274:PRO:HD2	1.71	0.71
1:A:238:ASN:HB3	1:A:346:ASP:OD1	1.91	0.70
1:A:247:LEU:HD23	1:A:294:ILE:HD13	1.73	0.69
1:A:348:THR:CG2	1:A:382:ALA:HA	2.21	0.69
1:B:334:THR:HG23	1:B:341:LEU:CD1	2.23	0.69
1:B:127:ALA:HB1	1:B:131:HIS:HB3	1.74	0.68
1:B:131:HIS:CE1	1:B:279:THR:HG22	2.29	0.68
1:B:20:TYR:HD2	1:B:374:VAL:HG22	1.59	0.68
1:B:171:ARG:NE	1:B:274:PRO:HD2	2.09	0.68
1:A:26:MET:HE2	1:A:364:ILE:CG2	2.22	0.68
1:B:56:HIS:HB3	1:B:102:VAL:O	1.94	0.67
1:B:138:GLU:O	1:B:142:ARG:HG3	1.94	0.67
1:A:168:LEU:HD22	1:A:173:ILE:HD12	1.77	0.67
1:B:174:ARG:HH11	1:B:174:ARG:HG2	1.60	0.67
1:B:259:PRO:HB2	1:B:291:LEU:HD11	1.76	0.67
1:A:265:PRO:HG3	1:A:345:THR:HG23	1.77	0.66
1:A:269:ARG:NE	1:A:278:PRO:HA	2.08	0.66
1:B:335:PRO:HG2	1:B:338:LEU:HD12	1.75	0.66
1:A:390:ILE:HG22	1:A:403:LEU:HD11	1.78	0.66
1:A:215:ARG:HD2	1:A:391:GLU:OE1	1.96	0.66
1:B:231:ARG:C	1:B:233:HIS:H	2.04	0.65
1:A:334:THR:HG23	1:A:341:LEU:HD13	1.79	0.65
1:A:272:LEU:O	1:A:273:ALA:O	2.13	0.65
1:B:52:VAL:HG21	1:B:161:PRO:CD	2.26	0.65
1:B:130:HIS:HD2	1:B:269:ARG:HD2	1.62	0.64
1:A:228:ALA:HA	2:A:427:HOH:O	1.95	0.64
1:A:138:GLU:O	1:A:142:ARG:HG3	1.98	0.64
1:B:273:ALA:CB	1:B:274:PRO:CD	2.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:HD23	1:B:126:MET:HE2	1.80	0.64
1:B:201:VAL:HG11	1:B:372:ILE:HG22	1.80	0.63
1:B:207:LEU:HB2	1:B:208:PRO:HD3	1.80	0.63
1:A:189:TYR:HE2	2:A:463:HOH:O	1.82	0.63
1:A:183:ARG:HH12	1:A:310:THR:HG21	1.62	0.62
1:B:12:HIS:HB3	2:B:433:HOH:O	1.99	0.62
1:B:30:LEU:HD21	1:B:140:PHE:HE2	1.65	0.62
1:A:168:LEU:HB3	1:A:173:ILE:HB	1.82	0.62
1:A:335:PRO:HG2	1:A:338:LEU:HD12	1.82	0.62
1:A:338:LEU:HD23	1:A:339:PRO:HD2	1.81	0.62
1:B:146:ALA:HB2	1:B:152:PRO:HB3	1.81	0.62
1:A:398:GLU:HB3	1:A:401:LYS:HB2	1.82	0.62
1:B:20:TYR:CD2	1:B:374:VAL:HG22	2.35	0.62
1:A:218:LEU:HD21	1:A:407:ARG:NH2	2.16	0.61
1:A:223:THR:HG22	1:A:227:MET:HE2	1.81	0.61
1:A:350:PHE:N	1:A:351:PRO:HD3	2.15	0.61
1:A:218:LEU:HD11	1:A:407:ARG:NH2	2.15	0.61
1:A:31:ARG:HA	1:A:115:GLY:HA3	1.81	0.60
1:B:193:ILE:HD12	1:B:339:PRO:HA	1.81	0.60
1:A:100:GLN:HG2	1:A:123:HIS:CE1	2.36	0.60
1:B:268:LEU:HB2	1:B:284:LEU:HG	1.83	0.60
1:A:95:GLU:O	1:A:96:LEU:HB2	2.00	0.60
1:A:208:PRO:HA	1:A:371:SER:HA	1.81	0.60
1:A:174:ARG:HD3	1:A:174:ARG:N	2.17	0.60
1:A:168:LEU:HD22	1:A:173:ILE:CD1	2.32	0.59
1:A:300:ILE:HG22	1:A:301:VAL:N	2.16	0.59
1:A:377:ASP:OD1	1:A:392:HIS:HE1	1.85	0.59
1:B:43:PHE:CE2	1:B:47:LEU:HD11	2.37	0.59
1:B:52:VAL:HG21	1:B:161:PRO:HD2	1.84	0.59
1:A:237:LEU:O	1:A:241:VAL:HG23	2.02	0.59
1:B:55:SER:HB2	1:B:68:VAL:O	2.03	0.58
1:A:77:ILE:HG22	1:A:107:LEU:HD23	1.85	0.58
1:B:105:LEU:HD11	1:B:120:LEU:HD11	1.85	0.58
1:B:203:ALA:CB	1:B:209:GLN:HG3	2.33	0.58
1:B:45:ALA:HA	1:B:155:ILE:HD11	1.86	0.57
1:A:8:ARG:NH1	1:A:161:PRO:O	2.34	0.57
1:A:215:ARG:HH12	1:A:365:LYS:HA	1.69	0.57
1:B:282:THR:HG22	1:B:283:ASN:HD22	1.65	0.57
1:A:218:LEU:HD21	1:A:407:ARG:CZ	2.34	0.57
1:B:171:ARG:NH1	1:B:171:ARG:HG3	2.19	0.57
1:B:203:ALA:HB1	1:B:209:GLN:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:CYS:O	1:A:282:THR:HG21	2.05	0.56
1:A:249:GLU:HB3	1:A:253:ARG:HE	1.69	0.56
1:A:290:TYR:CE2	1:A:307:ILE:HG12	2.40	0.56
1:B:396:ILE:HB	1:B:399:PRO:HG3	1.87	0.56
1:A:398:GLU:N	1:A:399:PRO:HD3	2.20	0.56
1:A:409:LEU:O	1:A:413:VAL:HG23	2.06	0.56
1:A:21:GLU:HG3	1:A:205:PRO:HB2	1.86	0.56
1:A:282:THR:CG2	1:A:283:ASN:ND2	2.68	0.56
1:B:171:ARG:HG3	1:B:171:ARG:HH11	1.69	0.56
1:B:215:ARG:HD2	1:B:391:GLU:OE2	2.06	0.55
1:A:264:TYR:HB2	1:A:265:PRO:HD2	1.87	0.55
1:A:348:THR:HA	1:A:382:ALA:CB	2.35	0.55
1:B:21:GLU:HA	1:B:100:GLN:OE1	2.06	0.55
1:B:149:THR:C	1:B:151:ASP:H	2.14	0.55
1:B:334:THR:HG23	1:B:341:LEU:HD12	1.88	0.55
1:A:174:ARG:HD3	1:A:174:ARG:H	1.71	0.55
1:B:392:HIS:HB2	1:B:403:LEU:HD13	1.88	0.55
1:A:349:SER:O	1:A:350:PHE:HB2	2.07	0.54
1:B:21:GLU:HG2	1:B:100:GLN:CD	2.32	0.54
1:B:202:LEU:HG	2:B:506:HOH:O	2.06	0.54
1:A:34:ILE:HG21	1:A:109:LEU:CD2	2.35	0.54
1:B:171:ARG:HE	1:B:274:PRO:HD2	1.72	0.54
1:A:376:LEU:O	1:A:394:GLY:HA3	2.08	0.54
1:B:52:VAL:HG21	1:B:161:PRO:HD3	1.88	0.54
1:A:28:ILE:HG23	1:A:361:ILE:HG23	1.89	0.54
1:A:404:GLU:HA	1:A:407:ARG:HB2	1.89	0.54
1:A:111:LEU:HA	1:A:116:ALA:HB2	1.91	0.53
1:B:236:SER:O	1:B:239:ALA:HB3	2.08	0.53
1:A:413:VAL:N	1:A:414:PRO:HD2	2.23	0.53
1:B:292:ALA:HB1	1:B:294:ILE:HD11	1.91	0.53
1:B:409:LEU:HD12	1:B:413:VAL:HG23	1.91	0.53
1:B:219:SER:OG	1:B:222:GLN:HG3	2.09	0.52
1:A:9:LYS:NZ	1:A:64:GLY:HA3	2.23	0.52
1:B:164:MET:HE2	1:B:268:LEU:CD1	2.36	0.52
1:B:211:VAL:HG11	1:B:376:LEU:HD23	1.91	0.52
1:A:8:ARG:HH11	1:A:160:THR:HG22	1.74	0.52
1:A:80:ILE:HG22	1:A:81:ASP:N	2.25	0.52
1:B:254:ASN:C	1:B:256:PRO:HD3	2.35	0.52
1:A:171:ARG:NH1	1:A:274:PRO:O	2.33	0.52
1:A:123:HIS:HD2	1:A:125:CYS:H	1.58	0.52
1:B:43:PHE:CD1	1:B:107:LEU:HD22	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:HD12	1:B:106:HIS:H	1.75	0.52
1:A:72:LEU:N	1:A:72:LEU:HD12	2.24	0.52
1:A:282:THR:HG22	1:A:283:ASN:HD22	1.73	0.52
1:B:323:SER:OG	1:B:325:LEU:HG	2.10	0.52
1:B:377:ASP:OD1	1:B:392:HIS:HE1	1.93	0.52
1:A:26:MET:HE3	1:A:365:LYS:O	2.10	0.51
1:A:276:VAL:HA	1:A:280:GLU:OE1	2.10	0.51
1:A:125:CYS:O	1:A:282:THR:CG2	2.58	0.51
1:A:110:ILE:O	1:A:116:ALA:HB1	2.11	0.51
1:A:131:HIS:HD2	1:A:281:ALA:O	1.93	0.51
1:A:343:PHE:HB3	1:A:378:LEU:HD12	1.91	0.51
1:B:80:ILE:HD13	1:B:94:ALA:N	2.25	0.51
1:B:413:VAL:N	1:B:414:PRO:HD2	2.26	0.51
1:A:183:ARG:NH1	1:A:310:THR:HG21	2.24	0.51
1:A:168:LEU:HB2	2:A:435:HOH:O	2.10	0.51
1:A:218:LEU:HD12	1:A:388:LEU:HB3	1.93	0.50
1:A:402:SER:O	1:A:406:ILE:HG13	2.12	0.50
1:A:149:THR:HG22	1:A:150:GLY:H	1.77	0.50
1:A:216:LEU:HD13	1:A:407:ARG:HG3	1.94	0.50
1:A:268:LEU:HB2	1:A:284:LEU:HG	1.93	0.50
1:A:52:VAL:HB	1:A:126:MET:HE1	1.93	0.50
1:B:207:LEU:O	1:B:371:SER:HA	2.11	0.50
1:B:260:ILE:HD12	1:B:294:ILE:HD13	1.94	0.50
1:A:74:HIS:HB2	2:A:483:HOH:O	2.12	0.50
1:A:247:LEU:HA	1:A:294:ILE:HD13	1.93	0.50
1:A:390:ILE:HG22	1:A:403:LEU:CD1	2.42	0.49
1:B:402:SER:O	1:B:406:ILE:HG13	2.12	0.49
1:A:13:SER:HB3	1:A:165:GLU:OE1	2.12	0.49
1:A:218:LEU:HD12	1:A:388:LEU:HD23	1.93	0.49
1:A:348:THR:HG22	1:A:382:ALA:CA	2.28	0.49
1:A:1:MET:HA	2:A:425:HOH:O	2.12	0.49
1:B:34:ILE:HD12	1:B:34:ILE:N	2.27	0.49
1:B:258:VAL:O	1:B:258:VAL:HG13	2.12	0.49
1:A:105:LEU:HD13	1:A:122:LEU:HD13	1.94	0.49
1:B:231:ARG:C	1:B:233:HIS:N	2.70	0.49
1:B:355:THR:HG21	1:B:361:ILE:HG13	1.94	0.49
1:B:265:PRO:HD3	1:B:327:PHE:CZ	2.47	0.49
1:A:127:ALA:HB1	1:A:131:HIS:HB3	1.95	0.48
1:A:149:THR:HG22	1:A:150:GLY:N	2.28	0.48
1:A:207:LEU:HA	1:A:208:PRO:HD3	1.67	0.48
1:B:207:LEU:CB	1:B:208:PRO:HD3	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:PHE:CE1	1:B:107:LEU:HB2	2.48	0.48
1:B:126:MET:O	1:B:282:THR:HG23	2.14	0.48
1:A:142:ARG:NH2	1:A:154:PRO:O	2.46	0.48
1:B:146:ALA:O	1:B:149:THR:O	2.32	0.48
1:A:230:GLY:C	1:A:232:GLU:H	2.22	0.48
1:B:174:ARG:HG2	1:B:174:ARG:NH1	2.28	0.48
1:A:218:LEU:HG	1:A:407:ARG:NH1	2.29	0.47
1:A:130:HIS:HD2	1:A:269:ARG:HD2	1.80	0.47
1:A:20:TYR:O	1:A:21:GLU:C	2.58	0.47
1:A:30:LEU:HB3	1:A:359:LEU:HD21	1.96	0.47
1:A:350:PHE:N	1:A:351:PRO:CD	2.77	0.47
1:A:381:CYS:HA	1:A:389:ILE:O	2.14	0.47
1:B:131:HIS:HD2	1:B:281:ALA:O	1.96	0.47
1:A:370:CYS:CB	1:A:374:VAL:HG21	2.41	0.47
1:B:131:HIS:CD2	1:B:279:THR:HA	2.49	0.47
1:A:257:HIS:HB2	2:A:454:HOH:O	2.14	0.47
1:B:106:HIS:HB2	1:B:121:TYR:HB2	1.96	0.47
1:A:212:PRO:HG2	1:A:394:GLY:C	2.39	0.47
1:B:25:SER:HA	1:B:120:LEU:O	2.14	0.47
1:B:107:LEU:CD1	1:B:118:LEU:HD11	2.44	0.47
1:B:398:GLU:HB2	1:B:401:LYS:HE3	1.97	0.47
1:B:143:TYR:CE2	1:B:359:LEU:HD12	2.50	0.47
1:B:213:VAL:HG12	1:B:214:THR:N	2.30	0.47
1:A:206:GLY:O	1:A:207:LEU:C	2.58	0.46
1:B:255:THR:O	1:B:258:VAL:HG12	2.15	0.46
1:A:52:VAL:CG1	1:A:126:MET:HE1	2.45	0.46
1:A:274:PRO:HA	1:A:275:PRO:HD2	1.78	0.46
1:B:143:TYR:HE2	1:B:359:LEU:HD12	1.79	0.46
1:A:18:ALA:HA	1:A:100:GLN:OE1	2.16	0.46
1:A:34:ILE:N	1:A:34:ILE:HD12	2.30	0.46
1:A:390:ILE:HD11	1:A:410:LEU:HD12	1.98	0.46
1:A:161:PRO:HB3	1:A:279:THR:O	2.16	0.46
1:A:276:VAL:HG13	1:A:280:GLU:CD	2.41	0.46
1:B:194:PRO:O	1:B:196:THR:N	2.46	0.46
1:B:17:PHE:CD2	1:B:124:HIS:HB3	2.50	0.46
1:B:164:MET:HB2	1:B:283:ASN:O	2.16	0.46
1:A:134:VAL:HG21	1:A:278:PRO:HB2	1.98	0.46
1:B:264:TYR:HB2	1:B:265:PRO:HD2	1.98	0.46
1:A:35:ASP:C	1:A:35:ASP:OD2	2.58	0.46
1:A:226:LEU:HD22	1:A:410:LEU:HB3	1.97	0.46
1:A:146:ALA:O	1:A:149:THR:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LEU:HD11	1:B:301:VAL:HG13	1.98	0.46
1:B:373:SER:O	1:B:374:VAL:C	2.58	0.46
1:B:71:ASP:HB2	1:B:73:LEU:HD13	1.98	0.45
1:B:282:THR:CG2	1:B:283:ASN:ND2	2.69	0.45
1:A:183:ARG:HH12	1:A:310:THR:CG2	2.27	0.45
1:A:236:SER:O	1:A:240:VAL:HG23	2.17	0.45
1:A:265:PRO:HB3	1:A:327:PHE:CD2	2.51	0.45
1:B:30:LEU:HD21	1:B:140:PHE:CE2	2.50	0.45
1:B:311:LEU:HD12	1:B:320:ILE:HD11	1.98	0.45
1:B:370:CYS:HB2	1:B:374:VAL:HG21	1.98	0.45
1:A:189:TYR:CD1	1:A:337:GLY:HA3	2.52	0.45
1:A:212:PRO:HG2	1:A:394:GLY:O	2.17	0.45
1:A:265:PRO:HD3	1:A:327:PHE:CZ	2.51	0.45
1:A:388:LEU:HD12	1:A:389:ILE:H	1.82	0.45
1:B:245:ILE:HG12	1:B:406:ILE:HD13	1.99	0.45
1:B:292:ALA:HB1	1:B:294:ILE:CD1	2.47	0.45
1:B:226:LEU:O	1:B:229:PHE:HB3	2.16	0.45
1:B:238:ASN:HB3	2:B:499:HOH:O	2.17	0.44
1:B:260:ILE:HB	1:B:292:ALA:HB3	2.00	0.44
1:A:261:PRO:HG2	1:A:341:LEU:HA	1.99	0.44
1:B:183:ARG:NH2	1:B:314:ASP:OD2	2.41	0.44
1:B:241:VAL:O	1:B:245:ILE:HG13	2.16	0.44
1:A:9:LYS:HZ1	1:A:64:GLY:HA3	1.82	0.44
1:A:171:ARG:HG2	1:A:273:ALA:HB3	1.99	0.44
1:A:327:PHE:HE2	1:A:345:THR:HG1	1.65	0.44
1:B:334:THR:HA	1:B:341:LEU:HD13	1.99	0.44
1:A:209:GLN:HG3	1:A:372:ILE:HG12	1.98	0.44
1:A:29:GLN:OE1	1:A:117:GLU:HG2	2.17	0.44
1:A:17:PHE:CD2	1:A:124:HIS:HB3	2.53	0.43
1:A:62:ASP:C	1:A:64:GLY:H	2.26	0.43
1:B:73:LEU:HD12	1:B:73:LEU:H	1.82	0.43
1:A:255:THR:O	1:A:258:VAL:HG22	2.18	0.43
1:B:56:HIS:CE1	1:B:68:VAL:HB	2.53	0.43
1:B:300:ILE:H	1:B:300:ILE:CD1	2.08	0.43
1:B:108:GLN:OE1	1:B:110:ILE:HD11	2.18	0.43
1:B:184:PHE:O	1:B:187:VAL:HG23	2.18	0.43
1:B:273:ALA:O	1:B:274:PRO:C	2.58	0.43
1:A:222:GLN:NE2	1:A:411:CYS:SG	2.91	0.43
1:A:185:MET:HA	1:A:188:MET:HG2	2.01	0.43
1:A:268:LEU:HB3	1:A:272:LEU:HG	1.99	0.43
1:B:149:THR:C	1:B:151:ASP:N	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LEU:CD2	1:B:407:ARG:HH21	2.22	0.43
1:B:300:ILE:HD11	2:B:425:HOH:O	2.18	0.43
1:A:273:ALA:O	1:A:275:PRO:N	2.51	0.43
1:B:193:ILE:CD1	1:B:340:PRO:HD3	2.49	0.43
1:B:53:LEU:HD13	1:B:105:LEU:HD22	2.01	0.42
1:B:135:LEU:HD23	1:B:135:LEU:HA	1.75	0.42
1:B:166:ALA:O	1:B:170:GLN:HB2	2.19	0.42
1:B:258:VAL:O	1:B:258:VAL:CG1	2.67	0.42
1:A:226:LEU:HD13	1:A:410:LEU:O	2.19	0.42
1:A:272:LEU:C	1:A:273:ALA:O	2.62	0.42
1:B:130:HIS:CD2	1:B:269:ARG:HD2	2.48	0.42
1:B:209:GLN:CD	1:B:372:ILE:HG23	2.45	0.42
1:A:11:SER:OG	1:A:14:GLU:HG3	2.19	0.42
1:A:209:GLN:CG	1:A:372:ILE:HG12	2.50	0.42
1:B:107:LEU:HD11	1:B:118:LEU:CD1	2.44	0.42
1:B:252:LEU:HD11	1:B:402:SER:HB3	2.02	0.42
1:B:253:ARG:C	1:B:255:THR:H	2.28	0.42
1:A:8:ARG:NH1	1:A:160:THR:HG22	2.35	0.42
1:A:31:ARG:CA	1:A:115:GLY:HA3	2.49	0.42
1:B:378:LEU:HD12	1:B:379:TYR:H	1.84	0.42
1:A:35:ASP:OD2	1:A:35:ASP:O	2.37	0.42
1:B:217:TRP:CZ3	1:B:389:ILE:HD11	2.54	0.42
1:A:54:ALA:O	1:A:70:ASP:HB2	2.20	0.42
1:B:142:ARG:NH2	1:B:154:PRO:O	2.53	0.42
1:B:322:GLN:HE21	1:B:322:GLN:HB3	1.58	0.42
1:A:407:ARG:NH2	1:A:410:LEU:HB2	2.35	0.42
1:B:45:ALA:HA	1:B:155:ILE:CD1	2.50	0.42
1:A:407:ARG:HG2	1:A:407:ARG:HH11	1.85	0.41
1:B:123:HIS:HD2	1:B:125:CYS:SG	2.43	0.41
1:A:25:SER:HA	1:A:120:LEU:O	2.20	0.41
1:A:174:ARG:H	1:A:174:ARG:CD	2.32	0.41
1:A:134:VAL:HG21	1:A:278:PRO:CB	2.51	0.41
1:A:348:THR:O	1:A:349:SER:HB2	2.20	0.41
1:B:273:ALA:HB1	1:B:274:PRO:HD3	1.99	0.41
1:B:105:LEU:CD1	1:B:120:LEU:HD11	2.51	0.41
1:B:210:ALA:HB1	1:B:367:GLN:HE21	1.82	0.41
1:B:216:LEU:HG	1:B:403:LEU:HD23	2.03	0.41
1:B:390:ILE:O	1:B:403:LEU:HD21	2.20	0.41
1:A:245:ILE:HG12	1:A:406:ILE:HD13	2.03	0.41
1:A:359:LEU:O	1:A:360:GLU:HG3	2.20	0.41
1:B:188:MET:HA	1:B:337:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLU:O	1:B:253:ARG:HG3	2.21	0.41
1:A:126:MET:HE3	1:A:126:MET:HB3	1.94	0.41
1:A:172:GLY:O	1:A:173:ILE:C	2.63	0.41
1:A:255:THR:HB	1:A:258:VAL:HG21	2.03	0.41
1:B:237:LEU:HD23	1:B:237:LEU:HA	1.87	0.41
1:B:268:LEU:HB3	1:B:272:LEU:HG	2.03	0.41
1:A:303:LEU:O	1:A:307:ILE:HG13	2.20	0.41
1:B:73:LEU:HD12	1:B:73:LEU:N	2.35	0.41
1:A:30:LEU:C	1:A:115:GLY:HA3	2.46	0.41
1:A:30:LEU:O	1:A:115:GLY:HA3	2.20	0.41
1:A:123:HIS:CD2	1:A:125:CYS:H	2.38	0.41
1:B:231:ARG:O	1:B:233:HIS:N	2.52	0.41
1:A:31:ARG:HA	1:A:115:GLY:CA	2.49	0.41
1:B:128:ASP:OD2	1:B:283:ASN:HA	2.20	0.41
1:B:249:GLU:O	1:B:253:ARG:HD2	2.20	0.41
1:B:343:PHE:O	1:B:378:LEU:HD12	2.21	0.41
1:B:128:ASP:O	1:B:129:GLY:C	2.64	0.41
1:A:126:MET:O	1:A:127:ALA:HB2	2.21	0.40
1:A:185:MET:HA	1:A:188:MET:CG	2.51	0.40
1:B:384:TYR:HE1	2:B:449:HOH:O	2.03	0.40
1:A:173:ILE:H	1:A:173:ILE:HG13	1.61	0.40
1:B:274:PRO:HA	1:B:275:PRO:HD2	1.95	0.40
1:B:110:ILE:HD12	1:B:110:ILE:N	2.37	0.40
1:B:210:ALA:HB1	1:B:367:GLN:HE22	1.83	0.40
1:B:215:ARG:NH2	1:B:217:TRP:HZ2	2.20	0.40
1:B:362:GLU:O	1:B:363:ASP:HB2	2.21	0.40
1:B:344:CYS:HA	1:B:379:TYR:O	2.21	0.40
1:A:74:HIS:ND1	1:A:74:HIS:C	2.79	0.40
1:A:412:THR:C	1:A:414:PRO:HD2	2.46	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:533:HOH:O	2:B:556:HOH:O[4_555]	1.31	0.89
2:B:538:HOH:O	2:B:545:HOH:O[4_555]	1.33	0.87
2:B:534:HOH:O	2:B:570:HOH:O[4_555]	1.37	0.83
2:B:532:HOH:O	2:B:554:HOH:O[4_555]	1.40	0.80
2:B:571:HOH:O	2:B:571:HOH:O[4_555]	1.48	0.72
2:B:557:HOH:O	2:B:567:HOH:O[4_555]	1.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:535:HOH:O	2:B:571:HOH:O[4_555]	1.69	0.51
2:B:530:HOH:O	2:B:558:HOH:O[4_555]	1.81	0.39
2:B:552:HOH:O	2:B:567:HOH:O[4_555]	1.88	0.32
2:B:558:HOH:O	2:B:566:HOH:O[4_555]	1.88	0.32
2:B:527:HOH:O	2:B:538:HOH:O[4_555]	2.06	0.14
2:B:559:HOH:O	2:B:559:HOH:O[4_555]	2.11	0.09

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	380/422 (90%)	336 (88%)	35 (9%)	9 (2%)	4	9
1	B	393/422 (93%)	339 (86%)	42 (11%)	12 (3%)	3	6
All	All	773/844 (92%)	675 (87%)	77 (10%)	21 (3%)	4	7

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	GLU
1	A	273	ALA
1	B	273	ALA
1	A	96	LEU
1	A	173	ILE
1	B	282	THR
1	A	372	ILE
1	B	205	PRO
1	B	207	LEU
1	B	232	GLU
1	A	257	HIS
1	A	351	PRO
1	B	75	SER
1	B	113	GLU

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Mol	Chain	Res	Type
1	B	195	ALA
1	B	208	PRO
1	B	401	LYS
1	A	350	PHE
1	B	4	GLY
1	A	63	GLY
1	B	64	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	324/348 (93%)	303 (94%)	21 (6%)	15	29
1	B	332/348 (95%)	316 (95%)	16 (5%)	23	44
All	All	656/696 (94%)	619 (94%)	37 (6%)	19	36

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	ARG
1	A	62	ASP
1	A	71	ASP
1	A	165	GLU
1	A	171	ARG
1	A	174	ARG
1	A	175	LYS
1	A	207	LEU
1	A	270	PHE
1	A	300	ILE
1	A	302	ASP
1	A	325	LEU
1	A	351	PRO
1	A	359	LEU
1	A	360	GLU

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Mol	Chain	Res	Type
1	A	378	LEU
1	A	380	SER
1	A	403	LEU
1	A	407	ARG
1	A	408	SER
1	B	39	LEU
1	B	62	ASP
1	B	149	THR
1	B	165	GLU
1	B	187	VAL
1	B	198	THR
1	B	202	LEU
1	B	237	LEU
1	B	300	ILE
1	B	305	SER
1	B	322	GLN
1	B	345	THR
1	B	365	LYS
1	B	372	ILE
1	B	398	GLU
1	B	403	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	123	HIS
1	A	130	HIS
1	A	209	GLN
1	A	222	GLN
1	A	233	HIS
1	A	238	ASN
1	A	317	ASN
1	A	322	GLN
1	A	392	HIS
1	B	56	HIS
1	B	106	HIS
1	B	123	HIS
1	B	130	HIS
1	B	131	HIS
1	B	158	GLN
1	B	170	GLN

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Mol	Chain	Res	Type
1	B	222	GLN
1	B	238	ASN
1	B	317	ASN
1	B	322	GLN
1	B	367	GLN
1	B	387	GLN
1	B	392	HIS

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 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	388/422 (91%)	0.28	19 (4%) 35 34	33, 68, 113, 136	0
1	B	399/422 (94%)	0.07	16 (4%) 42 40	34, 62, 104, 147	0
All	All	787/844 (93%)	0.18	35 (4%) 39 38	33, 65, 111, 147	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	94	ALA	5.7
1	B	181	ALA	5.0
1	A	418	GLY	4.9
1	B	207	LEU	4.2
1	B	200	ALA	4.1
1	A	94	ALA	4.0
1	A	73	LEU	3.9
1	B	418	GLY	3.9
1	A	181	ALA	3.9
1	B	199	PRO	2.8
1	A	205	PRO	2.7
1	B	3	PRO	2.7
1	B	195	ALA	2.7
1	A	208	PRO	2.7
1	B	203	ALA	2.7
1	B	193	ILE	2.6
1	A	349	SER	2.4
1	A	175	LYS	2.3
1	A	182	GLU	2.3
1	A	350	PHE	2.3
1	A	345	THR	2.2
1	A	399	PRO	2.2
1	A	407	ARG	2.2
1	B	73	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	198	THR	2.2
1	B	258	VAL	2.2
1	B	399	PRO	2.1
1	A	114	GLY	2.1
1	B	196	THR	2.1
1	A	96	LEU	2.1
1	A	228	ALA	2.1
1	A	417	TYR	2.1
1	A	257	HIS	2.1
1	A	351	PRO	2.0
1	B	204	HIS	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.