



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:23 PM GMT

PDB ID : 4I5S
Title : Structure and function of sensor histidine kinase
Authors : Cai, Y.
Deposited on : 2012-11-28
Resolution : 3.30 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

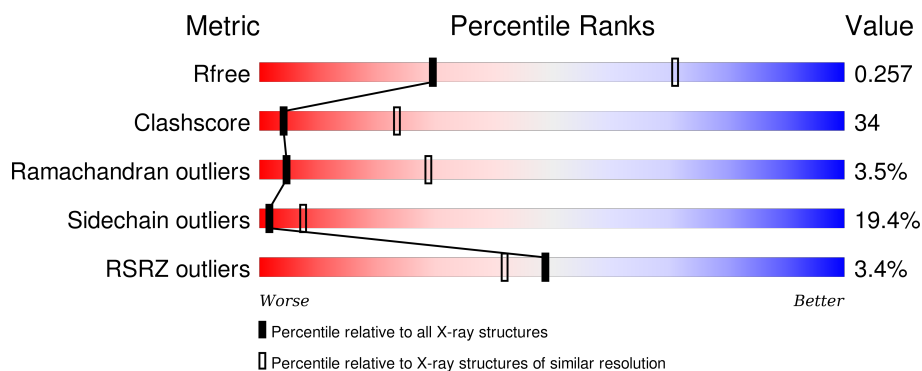
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	450	 2% 33% 38% 12% • 16%
1	B	450	 4% 38% 38% 11% • 12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6233 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 Putative histidine kinase CovS; VicK-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			3045	1905	523	608	9			
1	B	395	Total	C	N	O	S	0	0	0
			3188	1999	545	635	9			



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.12Å 153.12Å 125.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.62 – 3.30 36.62 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (36.62-3.30) 99.6 (36.62-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 3.32Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.230 , 0.270 0.209 , 0.257	Depositor DCC
R_{free} test set	1450 reflections (5.64%)	DCC
Wilson B-factor (Å ²)	111.3	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 115.4	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 25736 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6233	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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	0.27	0/3082	0.51	0/4164
1	B	0.28	0/3230	0.49	0/4366
All	All	0.28	0/6312	0.50	0/8530

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	3045	0	3049	224	0
1	B	3188	0	3183	219	0
All	All	6233	0	6232	421	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 34.

All (421) 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:209:ARG:HH11	1:A:209:ARG:HG2	1.28	0.94
1:B:142:ILE:HG22	1:B:143:LEU:H	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TYR:HD2	1:A:149:THR:H	1.16	0.92
1:B:127:LEU:HA	1:B:165:ARG:HD3	1.53	0.89
1:A:121:ASP:HA	1:A:124:GLN:HE21	1.38	0.86
1:A:311:ILE:HG22	1:A:349:VAL:HB	1.58	0.85
1:B:158:PRO:HB3	1:B:177:ARG:HA	1.58	0.85
1:B:433:TYR:CG	1:B:434:GLU:N	2.42	0.84
1:B:32:TYR:HE2	1:B:36:LYS:HG2	1.42	0.83
1:B:239:THR:HA	1:B:243:ALA:HB2	1.59	0.83
1:A:219:LEU:HD11	1:A:261:ILE:HD11	1.59	0.82
1:A:209:ARG:NH1	1:A:209:ARG:HG2	1.91	0.81
1:A:314:TYR:HB3	1:A:352:THR:HA	1.62	0.81
1:A:162:LEU:HD11	1:A:173:THR:HG22	1.62	0.81
1:A:371:ILE:HG13	1:A:372:PRO:HA	1.64	0.80
1:A:184:GLU:H	1:A:184:GLU:CD	1.85	0.79
1:A:314:TYR:HD1	1:A:314:TYR:O	1.63	0.79
1:A:110:THR:HG22	1:A:116:ILE:HA	1.65	0.78
1:B:281:LEU:HD11	1:B:320:TRP:HB3	1.66	0.78
1:B:149:THR:O	1:B:153:LEU:HD23	1.84	0.77
1:B:167:GLU:OE2	1:B:167:GLU:N	2.18	0.77
1:B:280:GLU:O	1:B:282:THR:HG22	1.85	0.77
1:B:388:LYS:HA	1:B:389:ALA:HB3	1.64	0.77
1:A:148:TYR:HD2	1:A:149:THR:N	1.83	0.76
1:A:100:LEU:HD23	1:A:103:MET:HE1	1.68	0.76
1:B:374:LYS:N	1:B:374:LYS:HD2	2.00	0.76
1:B:173:THR:H	1:B:199:THR:HG22	1.51	0.75
1:B:385:ARG:HD3	1:B:388:LYS:HD2	1.67	0.75
1:B:181:ASN:HB2	1:B:192:ILE:HG13	1.70	0.74
1:A:171:PHE:H	1:A:171:PHE:HD2	1.34	0.74
1:A:344:PRO:HD2	1:A:367:GLN:HB3	1.69	0.73
1:A:209:ARG:CG	1:A:209:ARG:HH11	2.00	0.73
1:A:382:ARG:HD2	1:A:383:PHE:CE2	2.24	0.72
1:A:177:ARG:NH1	1:B:196:HIS:HE1	1.87	0.72
1:A:229:TYR:CE1	1:A:297:GLN:HG2	2.23	0.72
1:A:371:ILE:HG23	1:A:372:PRO:HA	1.70	0.71
1:A:292:LEU:HD22	1:A:311:ILE:HD12	1.73	0.71
1:B:125:LYS:HD2	1:B:125:LYS:N	2.04	0.71
1:A:316:ASP:O	1:A:317:LYS:HE3	1.89	0.70
1:B:310:ILE:HD12	1:B:348:LYS:HG2	1.73	0.70
1:A:314:TYR:CD1	1:A:314:TYR:O	2.44	0.70
1:A:369:LEU:HB3	1:A:421:GLU:HG3	1.71	0.70
1:B:81:VAL:O	1:B:85:THR:HG23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ARG:NH2	1:B:271:ASP:OD2	2.26	0.68
1:B:412:LYS:O	1:B:412:LYS:HD3	1.94	0.68
1:A:229:TYR:O	1:A:233:LEU:HB3	1.92	0.68
1:B:264:LEU:HD12	1:B:399:LEU:HD11	1.76	0.68
1:A:281:LEU:HD23	1:A:322:GLU:HG3	1.75	0.68
1:A:334:ASN:O	1:A:337:ASN:HB2	1.94	0.68
1:B:388:LYS:HD3	1:B:390:ARG:HG2	1.76	0.68
1:A:128:ASN:HB2	1:A:165:ARG:O	1.94	0.68
1:A:255:ASN:OD1	1:B:227:LYS:NZ	2.28	0.67
1:B:101:SER:HA	1:B:120:ASN:HB2	1.77	0.67
1:A:386:VAL:HG13	1:B:272:ASN:ND2	2.10	0.67
1:A:314:TYR:N	1:A:315:PRO:HD2	2.09	0.67
1:A:229:TYR:CD1	1:A:297:GLN:HG2	2.29	0.66
1:A:371:ILE:HG23	1:A:372:PRO:CA	2.25	0.66
1:A:277:LEU:HD12	1:A:410:GLN:HB3	1.77	0.66
1:A:281:LEU:HD11	1:A:320:TRP:HB3	1.77	0.66
1:B:182:ARG:NH1	1:B:186:GLY:O	2.29	0.66
1:B:127:LEU:HA	1:B:165:ARG:CD	2.26	0.66
1:A:110:THR:O	1:A:190:GLY:HA3	1.96	0.66
1:B:224:THR:HA	1:B:227:LYS:HG2	1.76	0.66
1:B:403:ILE:H	1:B:403:ILE:HD12	1.61	0.65
1:B:314:TYR:H	1:B:315:PRO:HD2	1.60	0.65
1:B:153:LEU:HD13	1:B:180:LEU:HD21	1.77	0.65
1:B:115:LYS:HA	1:B:138:ASN:HA	1.77	0.65
1:A:250:SER:O	1:A:254:THR:HG23	1.96	0.65
1:B:44:LEU:HD11	1:B:72:VAL:HG22	1.79	0.65
1:A:41:VAL:O	1:A:45:ASN:HB2	1.96	0.65
1:A:277:LEU:HD23	1:A:278:ASP:H	1.62	0.65
1:B:269:ARG:HB3	1:B:275:SER:HB2	1.78	0.64
1:B:142:ILE:HG22	1:B:143:LEU:N	2.10	0.64
1:A:314:TYR:N	1:A:315:PRO:CD	2.60	0.64
1:A:338:ASN:HB3	1:A:399:LEU:CD2	2.27	0.64
1:B:156:LYS:O	1:B:156:LYS:HD2	1.98	0.64
1:A:163:THR:HB	1:A:165:ARG:CG	2.28	0.63
1:A:371:ILE:HD13	1:A:419:SER:O	1.98	0.63
1:B:281:LEU:HD23	1:B:322:GLU:HG2	1.80	0.63
1:B:243:ALA:HB3	1:B:244:PRO:HD3	1.81	0.63
1:B:288:MET:HE2	1:B:292:LEU:HD11	1.81	0.63
1:B:299:GLN:HE22	1:B:309:GLU:HG3	1.62	0.62
1:B:32:TYR:CE2	1:B:36:LYS:HG2	2.30	0.62
1:A:71:LEU:HD21	1:B:44:LEU:HD23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ARG:HB2	1:B:212:VAL:HG11	1.81	0.62
1:A:49:ARG:HD2	1:A:52:ILE:HD12	1.80	0.62
1:A:211:PHE:O	1:A:215:VAL:HG22	1.99	0.62
1:A:421:GLU:N	1:A:421:GLU:OE1	2.32	0.62
1:B:163:THR:O	1:B:172:ILE:HG22	1.99	0.61
1:B:232:ALA:O	1:B:237:ALA:HB3	2.01	0.61
1:B:356:THR:HG23	1:B:361:ILE:HD11	1.80	0.61
1:B:44:LEU:CD1	1:B:72:VAL:HG22	2.31	0.61
1:A:338:ASN:HB3	1:A:399:LEU:HD22	1.81	0.61
1:A:338:ASN:HA	1:A:341:LYS:HB3	1.82	0.61
1:A:148:TYR:CD2	1:A:149:THR:N	2.69	0.61
1:A:114:GLY:HA3	1:A:139:ILE:HD11	1.81	0.61
1:B:422:GLY:HA2	1:B:423:GLU:O	2.01	0.61
1:B:61:LYS:O	1:B:61:LYS:HD3	2.00	0.60
1:B:168:TYR:CG	1:B:169:ASP:N	2.65	0.60
1:A:143:LEU:HB3	1:A:145:ASP:OD2	2.01	0.60
1:B:327:LYS:O	1:B:330:GLN:HB2	2.01	0.60
1:A:102:TYR:HE2	1:B:182:ARG:HB2	1.66	0.60
1:A:316:ASP:CG	1:A:317:LYS:H	2.05	0.60
1:A:89:LEU:HD12	1:B:89:LEU:HB3	1.83	0.59
1:B:62:VAL:HG12	1:B:64:ASP:H	1.68	0.59
1:B:341:LYS:HZ3	1:B:388:LYS:HD3	1.67	0.59
1:B:287:PHE:CZ	1:B:291:ILE:HD11	2.37	0.59
1:B:422:GLY:HA2	1:B:423:GLU:C	2.21	0.59
1:A:107:VAL:H	1:A:120:ASN:ND2	1.99	0.59
1:B:66:SER:O	1:B:69:SER:HB3	2.03	0.59
1:B:373:LYS:H	1:B:373:LYS:HD2	1.68	0.58
1:A:48:VAL:O	1:A:52:ILE:HG13	2.02	0.58
1:B:371:ILE:HD13	1:B:379:ILE:HD13	1.86	0.58
1:B:142:ILE:HB	1:B:145:ASP:OD2	2.03	0.58
1:A:288:MET:HG3	1:A:292:LEU:HD12	1.85	0.58
1:A:196:HIS:HD2	1:B:175:ARG:HH12	1.51	0.58
1:B:320:TRP:N	1:B:434:GLU:HG2	2.19	0.58
1:B:197:ASP:OD1	1:B:199:THR:HG23	2.03	0.57
1:A:93:LYS:O	1:A:97:THR:HG22	2.04	0.57
1:B:383:PHE:CZ	1:B:399:LEU:HD21	2.38	0.57
1:A:100:LEU:HA	1:A:103:MET:HE2	1.86	0.57
1:B:73:ASN:HA	1:B:76:ASN:HB2	1.87	0.57
1:A:150:TYR:O	1:A:154:ILE:HG13	2.04	0.57
1:A:243:ALA:N	1:A:244:PRO:HD2	2.19	0.57
1:B:219:LEU:O	1:B:222:PRO:HD2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LYS:HB3	1:A:407:ILE:HD13	1.87	0.57
1:B:131:ARG:O	1:B:135:LEU:HG	2.04	0.57
1:A:124:GLN:OE1	1:A:131:ARG:N	2.38	0.57
1:B:32:TYR:HD2	1:B:32:TYR:O	1.88	0.57
1:B:163:THR:HG21	1:B:165:ARG:CZ	2.35	0.56
1:B:210:LEU:O	1:B:210:LEU:HG	2.02	0.56
1:A:127:LEU:HA	1:A:165:ARG:HD3	1.86	0.56
1:A:335:ILE:HG23	1:A:427:PHE:CD2	2.39	0.56
1:B:379:ILE:HD11	1:B:417:ALA:HB2	1.87	0.56
1:B:407:ILE:O	1:B:410:GLN:HB2	2.06	0.56
1:B:227:LYS:O	1:B:231:GLU:HB2	2.06	0.56
1:A:238:LEU:O	1:A:240:GLU:N	2.38	0.56
1:A:376:LEU:O	1:A:379:ILE:HG12	2.05	0.56
1:B:385:ARG:NE	1:B:390:ARG:HH22	2.04	0.56
1:B:115:LYS:NZ	1:B:135:LEU:O	2.36	0.56
1:B:314:TYR:N	1:B:315:PRO:HD2	2.21	0.56
1:A:202:GLU:O	1:A:206:ARG:HG2	2.06	0.56
1:A:60:LEU:HD12	1:A:76:ASN:OD1	2.06	0.56
1:B:32:TYR:C	1:B:32:TYR:HD2	2.10	0.55
1:A:314:TYR:HB3	1:A:352:THR:CA	2.35	0.55
1:A:102:TYR:CE2	1:B:182:ARG:HB2	2.41	0.55
1:A:181:ASN:HB3	1:A:189:SER:HB2	1.87	0.55
1:B:168:TYR:CD1	1:B:169:ASP:N	2.75	0.55
1:A:210:LEU:HA	1:A:386:VAL:HG21	1.89	0.55
1:B:250:SER:O	1:B:254:THR:HG23	2.06	0.55
1:A:288:MET:HE1	1:A:362:LEU:HD11	1.89	0.55
1:A:110:THR:HA	1:A:117:THR:HG23	1.88	0.55
1:B:142:ILE:CG2	1:B:143:LEU:H	2.15	0.55
1:A:164:ARG:C	1:A:166:ASP:H	2.09	0.55
1:A:89:LEU:CD1	1:B:89:LEU:HB3	2.37	0.55
1:A:163:THR:HB	1:A:165:ARG:HG2	1.89	0.54
1:A:214:ASN:HB3	1:A:264:LEU:HD13	1.89	0.54
1:A:180:LEU:N	1:A:180:LEU:HD22	2.22	0.54
1:A:113:SER:O	1:A:149:THR:HG21	2.06	0.54
1:A:244:PRO:HA	1:B:238:LEU:HD21	1.90	0.54
1:B:217:HIS:CD2	1:B:217:HIS:C	2.80	0.54
1:B:32:TYR:C	1:B:32:TYR:CD2	2.81	0.54
1:A:257:MET:HE3	1:B:223:LEU:HD11	1.89	0.54
1:A:380:PHE:CD1	1:A:405:LYS:HD2	2.42	0.54
1:B:203:LYS:HA	1:B:206:ARG:HH12	1.73	0.54
1:A:331:VAL:HG13	1:A:404:ALA:HB1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:GLY:O	1:B:348:LYS:HB2	2.07	0.53
1:A:312:ARG:HG2	1:A:312:ARG:O	2.08	0.53
1:B:415:ILE:HA	1:B:428:THR:O	2.09	0.53
1:A:284:PHE:HE2	1:A:362:LEU:HD12	1.72	0.53
1:B:388:LYS:HA	1:B:389:ALA:CB	2.32	0.53
1:A:415:ILE:HG23	1:A:415:ILE:O	2.09	0.53
1:A:369:LEU:HD13	1:A:421:GLU:HG3	1.91	0.53
1:B:158:PRO:CB	1:B:177:ARG:HA	2.36	0.52
1:B:299:GLN:NE2	1:B:309:GLU:HG3	2.24	0.52
1:A:128:ASN:CG	1:A:128:ASN:O	2.48	0.52
1:A:238:LEU:O	1:A:239:THR:C	2.47	0.52
1:A:277:LEU:HD21	1:A:411:HIS:HE1	1.73	0.52
1:A:276:HIS:O	1:A:327:LYS:NZ	2.30	0.52
1:A:284:PHE:CE2	1:A:362:LEU:HD12	2.44	0.52
1:B:433:TYR:CD1	1:B:434:GLU:N	2.78	0.52
1:B:153:LEU:HD13	1:B:180:LEU:CD2	2.39	0.52
1:B:414:PHE:CD1	1:B:415:ILE:N	2.73	0.52
1:A:288:MET:O	1:A:292:LEU:HB2	2.10	0.52
1:A:173:THR:HG21	1:A:202:GLU:HG3	1.91	0.52
1:B:195:LEU:HD12	1:B:195:LEU:N	2.24	0.52
1:B:203:LYS:HA	1:B:206:ARG:NH1	2.24	0.52
1:B:92:GLU:HA	1:B:95:ARG:NH1	2.24	0.52
1:A:371:ILE:HD11	1:A:373:LYS:NZ	2.25	0.51
1:B:93:LYS:HE3	1:B:94:ASN:OD1	2.10	0.51
1:A:107:VAL:H	1:A:120:ASN:HD21	1.58	0.51
1:B:356:THR:HG23	1:B:361:ILE:CD1	2.40	0.51
1:B:291:ILE:HD13	1:B:329:THR:HG23	1.92	0.51
1:A:390:ARG:HD3	1:B:269:ARG:HH12	1.75	0.51
1:B:242:VAL:HB	1:B:246:PHE:CE2	2.44	0.51
1:B:282:THR:CG2	1:B:323:ILE:HG12	2.40	0.51
1:A:310:ILE:O	1:A:312:ARG:NH2	2.43	0.51
1:B:218:GLU:HG3	1:B:260:MET:HE1	1.91	0.51
1:B:188:ILE:HD12	1:B:188:ILE:N	2.26	0.51
1:A:257:MET:O	1:A:261:ILE:HG12	2.10	0.51
1:A:164:ARG:NH1	1:A:171:PHE:HB3	2.25	0.51
1:B:62:VAL:HG13	1:B:69:SER:OG	2.10	0.51
1:A:301:GLN:HA	1:A:302:GLN:HB2	1.94	0.50
1:A:162:LEU:CD1	1:A:173:THR:HG22	2.39	0.50
1:A:380:PHE:HB3	1:A:405:LYS:HD3	1.93	0.50
1:A:388:LYS:HG2	1:A:389:ALA:H	1.76	0.50
1:A:47:LYS:HD3	1:A:60:LEU:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:HD12	1:A:69:SER:N	2.27	0.50
1:B:112:ARG:H	1:B:112:ARG:NH1	2.09	0.50
1:B:148:TYR:O	1:B:152:ASP:HB2	2.11	0.50
1:A:288:MET:CE	1:A:362:LEU:HD11	2.41	0.50
1:A:164:ARG:C	1:A:166:ASP:N	2.64	0.50
1:B:376:LEU:HD11	1:B:417:ALA:O	2.11	0.50
1:A:205:GLU:OE1	1:B:208:ARG:NH1	2.44	0.50
1:B:399:LEU:O	1:B:401:LEU:N	2.45	0.50
1:A:157:THR:OG1	1:A:159:GLU:HG3	2.11	0.50
1:A:348:LYS:N	1:A:348:LYS:HD2	2.26	0.50
1:A:292:LEU:CD2	1:A:311:ILE:HD12	2.42	0.50
1:A:317:LYS:O	1:A:318:SER:HB3	2.12	0.50
1:A:315:PRO:HG3	1:A:353:MET:HE2	1.94	0.49
1:A:207:GLU:HB3	1:A:268:SER:HB3	1.93	0.49
1:A:129:VAL:HG13	1:A:130:THR:O	2.12	0.49
1:A:242:VAL:C	1:A:244:PRO:HD2	2.32	0.49
1:B:173:THR:H	1:B:199:THR:CG2	2.22	0.49
1:B:352:THR:HG23	1:B:363:SER:OG	2.13	0.49
1:A:102:TYR:CD1	1:A:102:TYR:N	2.80	0.49
1:B:155:THR:O	1:B:157:THR:N	2.46	0.49
1:B:310:ILE:HB	1:B:348:LYS:HA	1.94	0.49
1:B:162:LEU:HD22	1:B:162:LEU:O	2.13	0.49
1:B:379:ILE:HD11	1:B:417:ALA:CB	2.43	0.48
1:A:197:ASP:OD1	1:A:199:THR:HG22	2.12	0.48
1:B:173:THR:HG23	1:B:199:THR:HA	1.94	0.48
1:A:155:THR:O	1:A:156:LYS:C	2.51	0.48
1:A:369:LEU:HB3	1:A:421:GLU:CG	2.42	0.48
1:B:173:THR:HG23	1:B:199:THR:HG22	1.95	0.48
1:B:341:LYS:HZ3	1:B:390:ARG:HG2	1.79	0.48
1:B:92:GLU:HG2	1:B:95:ARG:HH12	1.77	0.48
1:A:155:THR:OG1	1:A:157:THR:HG22	2.14	0.48
1:B:357:ASP:OD2	1:B:357:ASP:N	2.46	0.48
1:A:301:GLN:HA	1:A:302:GLN:CB	2.43	0.48
1:A:221:THR:N	1:A:222:PRO:HD2	2.29	0.48
1:A:315:PRO:HB3	1:A:353:MET:HE3	1.96	0.48
1:A:331:VAL:HG22	1:A:404:ALA:HA	1.95	0.48
1:B:43:GLN:O	1:B:46:ALA:HB3	2.14	0.48
1:B:29:PHE:C	1:B:29:PHE:CD2	2.87	0.48
1:B:208:ARG:O	1:B:211:PHE:HB3	2.14	0.48
1:B:154:ILE:HG13	1:B:155:THR:N	2.29	0.48
1:A:239:THR:HG22	1:A:241:SER:OG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LYS:NZ	1:A:398:GLY:O	2.47	0.48
1:B:420:GLU:C	1:B:422:GLY:H	2.16	0.48
1:A:371:ILE:CG2	1:A:372:PRO:HA	2.39	0.47
1:A:335:ILE:CD1	1:A:429:ILE:HD11	2.44	0.47
1:B:180:LEU:HD22	1:B:180:LEU:HA	1.63	0.47
1:B:164:ARG:O	1:B:166:ASP:N	2.47	0.47
1:B:341:LYS:NZ	1:B:390:ARG:HG2	2.29	0.47
1:A:233:LEU:O	1:A:233:LEU:HG	2.14	0.47
1:B:156:LYS:HD2	1:B:156:LYS:C	2.35	0.47
1:A:257:MET:CE	1:B:223:LEU:HD11	2.45	0.47
1:B:388:LYS:HB3	1:B:390:ARG:HG3	1.97	0.47
1:A:312:ARG:HD2	1:A:350:THR:HG23	1.96	0.47
1:B:155:THR:O	1:B:156:LYS:HG3	2.14	0.47
1:A:99:ILE:HD11	1:B:109:ALA:HB2	1.97	0.47
1:A:105:ASP:N	1:A:105:ASP:OD1	2.46	0.47
1:B:403:ILE:HD12	1:B:403:ILE:N	2.28	0.47
1:A:177:ARG:NH1	1:B:196:HIS:CE1	2.75	0.47
1:B:222:PRO:HB2	1:B:257:MET:SD	2.55	0.47
1:A:359:GLN:HG3	1:A:432:PRO:C	2.36	0.47
1:A:371:ILE:HG22	1:A:421:GLU:OE2	2.14	0.47
1:B:68:LEU:HD22	1:B:68:LEU:HA	1.75	0.47
1:A:102:TYR:HD1	1:A:102:TYR:N	2.13	0.47
1:A:265:LEU:HD11	1:B:216:SER:OG	2.16	0.47
1:B:134:ALA:O	1:B:137:CYS:HB2	2.15	0.47
1:B:272:ASN:C	1:B:273:GLN:HG2	2.36	0.46
1:B:361:ILE:N	1:B:361:ILE:HD12	2.30	0.46
1:B:219:LEU:C	1:B:222:PRO:HD2	2.36	0.46
1:B:163:THR:CG2	1:B:165:ARG:HG3	2.45	0.46
1:B:400:GLY:N	1:B:403:ILE:HD13	2.30	0.46
1:A:275:SER:C	1:A:276:HIS:CG	2.89	0.46
1:A:163:THR:HB	1:A:165:ARG:HG3	1.96	0.46
1:A:200:GLU:HG2	1:A:201:GLN:N	2.31	0.45
1:A:371:ILE:CG1	1:A:372:PRO:HA	2.39	0.45
1:B:224:THR:HA	1:B:227:LYS:CG	2.45	0.45
1:B:233:LEU:HD11	1:B:246:PHE:HB3	1.96	0.45
1:A:142:ILE:HG22	1:A:142:ILE:O	2.16	0.45
1:A:371:ILE:HG23	1:A:372:PRO:N	2.31	0.45
1:B:375:ASP:N	1:B:375:ASP:OD1	2.50	0.45
1:B:229:TYR:CE1	1:B:249:VAL:HG11	2.51	0.45
1:B:168:TYR:C	1:B:170:GLU:H	2.19	0.45
1:B:315:PRO:HD3	1:B:353:MET:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:THR:C	1:B:157:THR:N	2.70	0.45
1:B:151:ASN:OD1	1:B:151:ASN:C	2.55	0.45
1:B:151:ASN:HA	1:B:154:ILE:HG12	1.98	0.45
1:A:260:MET:HE3	1:A:330:GLN:HG2	1.99	0.45
1:B:388:LYS:CA	1:B:389:ALA:HB3	2.40	0.45
1:A:226:VAL:HG21	1:A:254:THR:HG22	1.98	0.45
1:A:162:LEU:HD13	1:A:162:LEU:HA	1.64	0.45
1:A:316:ASP:CG	1:A:317:LYS:N	2.70	0.45
1:A:115:LYS:HG3	1:A:137:CYS:O	2.17	0.45
1:B:130:THR:O	1:B:131:ARG:C	2.55	0.45
1:A:380:PHE:CD1	1:A:405:LYS:HB2	2.52	0.45
1:B:175:ARG:HD2	1:B:196:HIS:HB3	1.99	0.45
1:B:223:LEU:HA	1:B:223:LEU:HD12	1.73	0.44
1:A:386:VAL:HG12	1:A:387:ASP:OD1	2.18	0.44
1:B:143:LEU:O	1:B:144:ASP:C	2.55	0.44
1:B:319:VAL:C	1:B:434:GLU:HG2	2.38	0.44
1:A:81:VAL:CG1	1:A:82:PHE:N	2.80	0.44
1:A:207:GLU:O	1:A:210:LEU:HB3	2.17	0.44
1:A:61:LYS:NZ	1:A:61:LYS:HB2	2.32	0.44
1:A:409:LYS:NZ	1:A:414:PHE:HA	2.32	0.44
1:A:209:ARG:HG2	1:B:272:ASN:ND2	2.32	0.44
1:A:105:ASP:OD2	1:A:196:HIS:HD2	2.01	0.44
1:A:124:GLN:HB3	1:A:129:VAL:O	2.18	0.44
1:B:412:LYS:HD3	1:B:412:LYS:C	2.38	0.44
1:B:104:THR:O	1:B:122:MET:HG2	2.17	0.44
1:B:335:ILE:CG2	1:B:364:ILE:HD12	2.47	0.44
1:A:196:HIS:CD2	1:B:175:ARG:HH12	2.32	0.44
1:B:109:ALA:HB3	1:B:118:VAL:HB	1.99	0.44
1:A:400:GLY:O	1:A:401:LEU:HD12	2.18	0.44
1:B:365:SER:HA	1:B:426:THR:HB	2.00	0.44
1:A:153:LEU:HD22	1:A:188:ILE:HG21	2.00	0.44
1:A:130:THR:OG1	1:A:133:GLN:HG3	2.18	0.44
1:B:214:ASN:O	1:B:218:GLU:HB2	2.18	0.44
1:A:348:LYS:O	1:A:366:ASP:HA	2.17	0.44
1:A:218:GLU:O	1:A:260:MET:HE1	2.18	0.44
1:A:164:ARG:O	1:A:166:ASP:N	2.51	0.43
1:B:231:GLU:O	1:B:235:ASP:HB2	2.18	0.43
1:B:91:GLN:O	1:B:95:ARG:HG3	2.18	0.43
1:A:120:ASN:O	1:A:124:GLN:HG3	2.18	0.43
1:A:56:TYR:CE1	1:A:83:ARG:HD3	2.53	0.43
1:B:62:VAL:HG12	1:B:64:ASP:N	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ILE:N	1:B:30:LEU:HD12	2.32	0.43
1:B:163:THR:HG22	1:B:165:ARG:HG3	2.01	0.43
1:A:121:ASP:O	1:A:124:GLN:HB2	2.18	0.43
1:A:243:ALA:N	1:A:244:PRO:CD	2.82	0.43
1:B:214:ASN:HB3	1:B:383:PHE:CD1	2.54	0.43
1:B:153:LEU:CD1	1:B:180:LEU:HD21	2.46	0.43
1:B:385:ARG:HG2	1:B:388:LYS:NZ	2.33	0.43
1:A:150:TYR:CD1	1:A:154:ILE:HD11	2.54	0.43
1:B:145:ASP:O	1:B:146:ASP:HB2	2.19	0.43
1:B:285:THR:OG1	1:B:315:PRO:HB2	2.19	0.43
1:B:64:ASP:HA	1:B:65:ASN:HA	1.47	0.43
1:A:210:LEU:HA	1:A:386:VAL:CG2	2.48	0.43
1:B:175:ARG:HD3	1:B:177:ARG:HG3	2.01	0.43
1:A:313:ASP:C	1:A:315:PRO:HD2	2.39	0.43
1:B:224:THR:O	1:B:227:LYS:HG3	2.18	0.43
1:B:223:LEU:HD13	1:B:257:MET:SD	2.59	0.43
1:A:338:ASN:HB3	1:A:399:LEU:HD23	2.01	0.42
1:A:89:LEU:HB3	1:B:89:LEU:HD13	2.00	0.42
1:A:248:LYS:NZ	1:B:234:ASP:OD2	2.42	0.42
1:A:120:ASN:ND2	1:A:123:ALA:H	2.17	0.42
1:A:43:GLN:O	1:A:46:ALA:HB3	2.18	0.42
1:A:380:PHE:CG	1:A:405:LYS:HD2	2.54	0.42
1:B:111:ASP:HB2	1:B:112:ARG:NH1	2.34	0.42
1:A:366:ASP:O	1:A:424:GLY:HA3	2.19	0.42
1:A:105:ASP:OD2	1:A:196:HIS:CD2	2.72	0.42
1:B:32:TYR:O	1:B:35:TYR:HB3	2.20	0.42
1:B:287:PHE:CZ	1:B:291:ILE:CD1	3.02	0.42
1:A:376:LEU:HB3	1:A:377:PRO:HD3	2.01	0.42
1:A:287:PHE:CE1	1:A:328:MET:HB3	2.53	0.42
1:B:315:PRO:O	1:B:316:ASP:HB2	2.19	0.42
1:A:180:LEU:N	1:A:180:LEU:CD2	2.82	0.42
1:A:415:ILE:HA	1:A:428:THR:O	2.19	0.42
1:B:336:LEU:O	1:B:340:ILE:HD13	2.19	0.42
1:A:162:LEU:HD13	1:A:173:THR:HA	2.01	0.42
1:B:142:ILE:HB	1:B:145:ASP:OD1	2.20	0.42
1:A:149:THR:HG22	1:A:153:LEU:HD12	2.01	0.42
1:A:233:LEU:HB2	1:A:246:PHE:HD1	1.85	0.42
1:B:353:MET:HE2	1:B:353:MET:HB3	1.84	0.42
1:A:174:LEU:HD23	1:A:197:ASP:HA	2.01	0.42
1:A:431:LEU:HA	1:A:432:PRO:HD3	1.82	0.42
1:A:341:LYS:HE2	1:A:342:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLU:OE1	1:B:206:ARG:NH2	2.52	0.42
1:A:229:TYR:HE1	1:A:297:GLN:HG2	1.82	0.41
1:A:278:ASP:OD2	1:A:278:ASP:C	2.58	0.41
1:B:234:ASP:C	1:B:236:GLY:H	2.22	0.41
1:B:431:LEU:HA	1:B:432:PRO:HD3	1.94	0.41
1:B:163:THR:HG21	1:B:165:ARG:NE	2.35	0.41
1:A:81:VAL:HG12	1:A:82:PHE:N	2.34	0.41
1:A:197:ASP:C	1:A:197:ASP:OD1	2.58	0.41
1:B:141:ASP:O	1:B:142:ILE:HD13	2.19	0.41
1:B:401:LEU:HD23	1:B:401:LEU:HA	1.91	0.41
1:A:405:LYS:HG3	1:A:415:ILE:CG2	2.50	0.41
1:A:68:LEU:HD12	1:A:68:LEU:C	2.41	0.41
1:B:142:ILE:HB	1:B:145:ASP:CG	2.40	0.41
1:A:195:LEU:N	1:A:195:LEU:HD23	2.35	0.41
1:B:279:VAL:HG12	1:B:323:ILE:C	2.40	0.41
1:B:124:GLN:NE2	1:B:131:ARG:HG3	2.35	0.41
1:A:370:GLY:HA3	1:A:419:SER:OG	2.20	0.41
1:A:47:LYS:HE3	1:A:57:THR:HG23	2.02	0.41
1:A:368:GLY:C	1:A:369:LEU:HD23	2.40	0.41
1:B:166:ASP:HA	1:B:167:GLU:OE2	2.20	0.41
1:B:63:GLU:O	1:B:64:ASP:C	2.59	0.41
1:B:126:GLN:O	1:B:165:ARG:HD2	2.20	0.41
1:A:368:GLY:O	1:A:369:LEU:HD23	2.20	0.41
1:A:371:ILE:HG22	1:A:421:GLU:CD	2.41	0.41
1:A:281:LEU:HD22	1:A:321:ILE:C	2.41	0.41
1:A:155:THR:O	1:A:156:LYS:HG3	2.21	0.41
1:B:234:ASP:C	1:B:236:GLY:N	2.73	0.41
1:A:309:GLU:HA	1:A:347:GLY:N	2.36	0.41
1:B:44:LEU:HD12	1:B:60:LEU:HD12	2.03	0.41
1:A:138:ASN:OD1	1:A:139:ILE:HD12	2.21	0.41
1:A:167:GLU:HG3	1:A:167:GLU:H	1.67	0.41
1:A:371:ILE:HG13	1:A:372:PRO:CA	2.42	0.40
1:B:387:ASP:O	1:B:389:ALA:HB3	2.21	0.40
1:A:120:ASN:N	1:A:120:ASN:HD22	2.19	0.40
1:A:314:TYR:CG	1:A:352:THR:HB	2.56	0.40
1:A:59:LYS:HG2	1:A:76:ASN:HB3	2.03	0.40
1:A:253:GLU:OE2	1:A:256:ARG:NH1	2.53	0.40
1:B:272:ASN:HB2	1:B:274:THR:HG23	2.02	0.40
1:B:238:LEU:HD12	1:B:239:THR:HG23	2.04	0.40
1:B:282:THR:HG23	1:B:323:ILE:HG12	2.04	0.40
1:A:405:LYS:HA	1:A:415:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:HG2	1:A:112:ARG:H	1.62	0.40
1:B:239:THR:HG22	1:B:243:ALA:HB1	2.03	0.40
1:A:277:LEU:HD23	1:A:278:ASP:N	2.33	0.40
1:B:205:GLU:O	1:B:209:ARG:HG3	2.20	0.40
1:B:209:ARG:O	1:B:212:VAL:HG22	2.22	0.40
1:B:216:SER:O	1:B:217:HIS:C	2.59	0.40
1:B:332:ILE:HD11	1:B:362:LEU:HD11	2.04	0.40
1:A:129:VAL:HG11	1:A:134:ALA:HB2	2.03	0.40
1:B:264:LEU:HD12	1:B:399:LEU:CD1	2.50	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	372/450 (83%)	315 (85%)	44 (12%)	13 (4%)	4	29
1	B	389/450 (86%)	322 (83%)	53 (14%)	14 (4%)	4	28
All	All	761/900 (85%)	637 (84%)	97 (13%)	27 (4%)	4	29

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	PRO
1	A	167	GLU
1	A	239	THR
1	B	315	PRO
1	B	400	GLY
1	A	168	TYR
1	A	345	ASP
1	B	156	LYS
1	B	165	ARG

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Mol	Chain	Res	Type
1	B	168	TYR
1	B	347	GLY
1	A	238	LEU
1	B	169	ASP
1	A	66	SER
1	A	165	ARG
1	A	302	GLN
1	B	144	ASP
1	B	216	SER
1	B	345	ASP
1	A	227	LYS
1	A	318	SER
1	B	314	TYR
1	B	316	ASP
1	A	303	SER
1	B	164	ARG
1	B	344	PRO
1	A	314	TYR

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	348/413 (84%)	275 (79%)	73 (21%)	1	6
1	B	363/413 (88%)	298 (82%)	65 (18%)	2	10
All	All	711/826 (86%)	573 (81%)	138 (19%)	2	7

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	57	THR
1	A	60	LEU
1	A	68	LEU
1	A	80	GLU

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Mol	Chain	Res	Type
1	A	81	VAL
1	A	84	LEU
1	A	88	ASN
1	A	89	LEU
1	A	91	GLN
1	A	97	THR
1	A	103	MET
1	A	104	THR
1	A	105	ASP
1	A	112	ARG
1	A	120	ASN
1	A	137	CYS
1	A	139	ILE
1	A	142	ILE
1	A	148	TYR
1	A	152	ASP
1	A	156	LYS
1	A	157	THR
1	A	159	GLU
1	A	162	LEU
1	A	163	THR
1	A	164	ARG
1	A	167	GLU
1	A	169	ASP
1	A	171	PHE
1	A	173	THR
1	A	175	ARG
1	A	177	ARG
1	A	181	ASN
1	A	195	LEU
1	A	206	ARG
1	A	209	ARG
1	A	221	THR
1	A	233	LEU
1	A	238	LEU
1	A	240	GLU
1	A	242	VAL
1	A	254	THR
1	A	262	THR
1	A	267	LEU
1	A	268	SER
1	A	276	HIS

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Mol	Chain	Res	Type
1	A	277	LEU
1	A	278	ASP
1	A	282	THR
1	A	287	PHE
1	A	290	TYR
1	A	304	THR
1	A	309	GLU
1	A	310	ILE
1	A	312	ARG
1	A	313	ASP
1	A	314	TYR
1	A	317	LYS
1	A	325	THR
1	A	350	THR
1	A	352	THR
1	A	360	LEU
1	A	363	SER
1	A	367	GLN
1	A	369	LEU
1	A	371	ILE
1	A	374	LYS
1	A	376	LEU
1	A	401	LEU
1	A	403	ILE
1	A	411	HIS
1	A	426	THR
1	B	29	PHE
1	B	30	LEU
1	B	32	TYR
1	B	49	ARG
1	B	61	LYS
1	B	67	ASP
1	B	68	LEU
1	B	71	LEU
1	B	84	LEU
1	B	85	THR
1	B	89	LEU
1	B	93	LYS
1	B	97	THR
1	B	100	LEU
1	B	104	THR
1	B	112	ARG

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Mol	Chain	Res	Type
1	B	125	LYS
1	B	128	ASN
1	B	130	THR
1	B	139	ILE
1	B	150	TYR
1	B	153	LEU
1	B	156	LYS
1	B	157	THR
1	B	159	GLU
1	B	160	ILE
1	B	162	LEU
1	B	164	ARG
1	B	166	ASP
1	B	169	ASP
1	B	171	PHE
1	B	173	THR
1	B	175	ARG
1	B	180	LEU
1	B	196	HIS
1	B	200	GLU
1	B	204	GLU
1	B	208	ARG
1	B	210	LEU
1	B	217	HIS
1	B	223	LEU
1	B	227	LYS
1	B	234	ASP
1	B	235	ASP
1	B	242	VAL
1	B	256	ARG
1	B	264	LEU
1	B	273	GLN
1	B	276	HIS
1	B	279	VAL
1	B	282	THR
1	B	285	THR
1	B	313	ASP
1	B	316	ASP
1	B	330	GLN
1	B	357	ASP
1	B	375	ASP
1	B	376	LEU

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Mol	Chain	Res	Type
1	B	378	LEU
1	B	397	THR
1	B	399	LEU
1	B	412	LYS
1	B	416	TRP
1	B	426	THR
1	B	430	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	B	196	HIS
1	B	217	HIS
1	B	272	ASN
1	B	299	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 ⓘ

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	380/450 (84%)	0.06	9 (2%) 62 55	95, 152, 216, 254	0
1	B	395/450 (87%)	0.09	17 (4%) 39 32	90, 137, 221, 263	0
All	All	775/900 (86%)	0.07	26 (3%) 49 42	90, 144, 220, 263	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	THR	5.5
1	B	233	LEU	3.9
1	B	238	LEU	3.8
1	B	165	ARG	3.6
1	A	37	ASN	3.4
1	B	244	PRO	2.8
1	A	319	VAL	2.7
1	B	147	SER	2.6
1	B	243	ALA	2.6
1	B	277	LEU	2.5
1	B	55	HIS	2.4
1	B	56	TYR	2.4
1	A	165	ARG	2.4
1	A	320	TRP	2.4
1	B	242	VAL	2.4
1	A	191	LEU	2.3
1	A	247	ILE	2.3
1	B	241	SER	2.3
1	B	170	GLU	2.3
1	B	168	TYR	2.2
1	A	148	TYR	2.2
1	A	374	LYS	2.2
1	B	150	TYR	2.2
1	B	28	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	238	LEU	2.1
1	B	344	PRO	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.