WORLDWIDE wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:12 AM GMT

PDB ID	:	2W9Z
Title	:	CRYSTAL STRUCTURE OF CDK4 IN COMPLEX WITH A D-TYPE CY-CLIN
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	:	2009-01-30
Resolution	:	2.45 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:

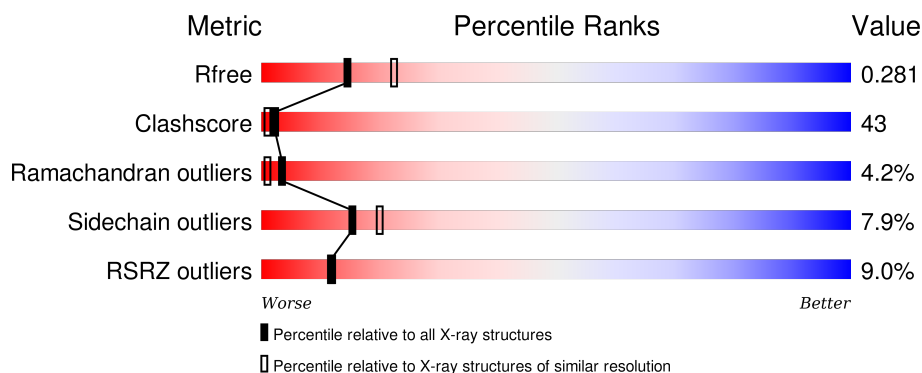|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	Percentile Ranks	Value
Rfree		0.281
Clashscore		43
Ramachandran outliers		4.2%
Sidechain outliers		7.9%
RSRZ outliers		9.0%

Worse　　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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 <=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	257	5% 60% 31% 5% ·
2	B	306	12% 35% 46% 9% · 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4462 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	2	0
			1970	1253	333	362	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	287	Total	C	N	O	S	0	0	0
			2270	1454	399	406	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	152	Total	O	0	0
			152	152		
3	B	70	Total	O	0	0
			70	70		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: G1/S-SPECIFIC CYCLIN-D1
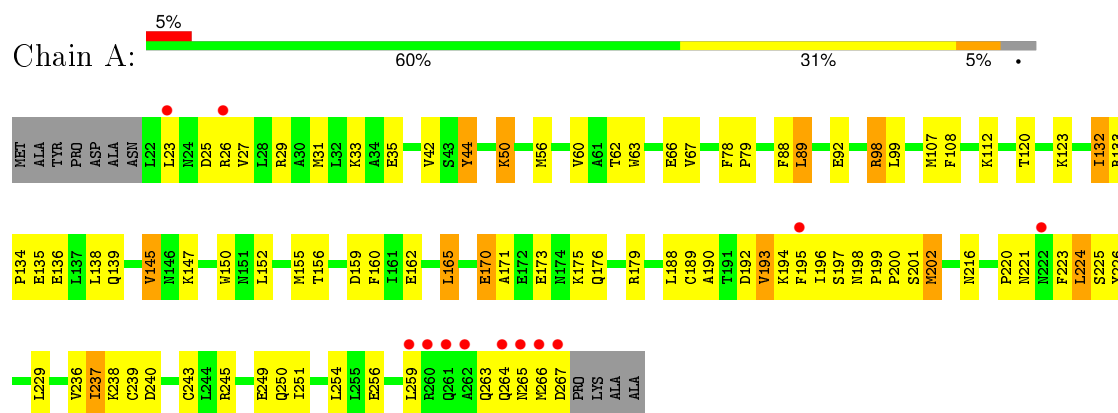
- Molecule 2: CELL DIVISION PROTEIN KINASE 4
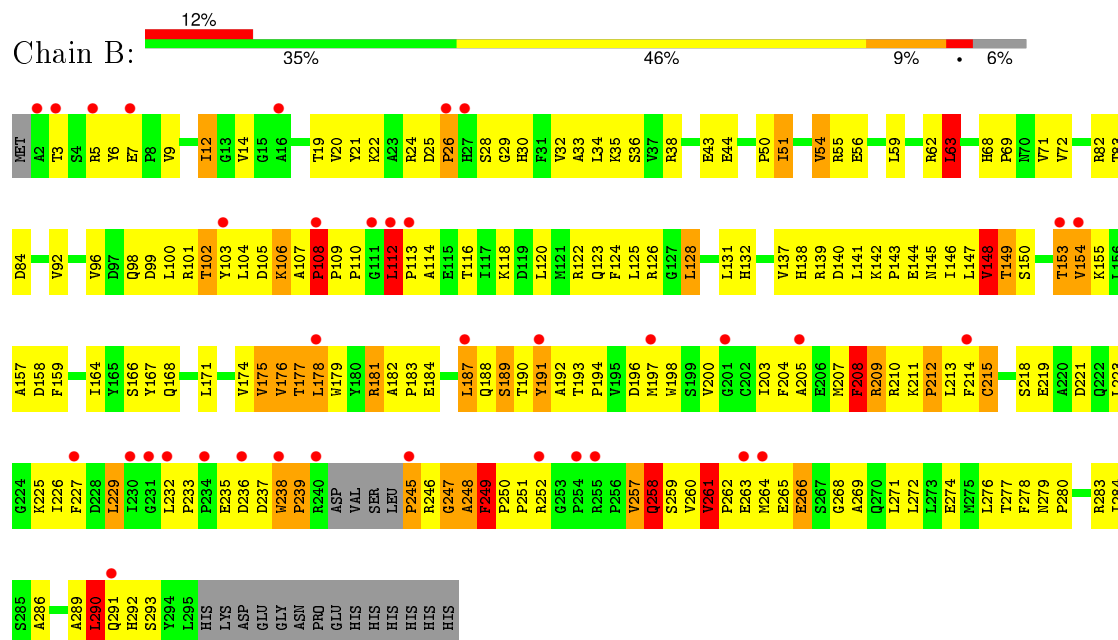
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.20Å 65.01Å 188.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.49 – 2.45 94.35 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.8 (94.49-2.45) 98.0 (94.35-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.51 (at 2.45Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.225 , 0.272 0.233 , 0.281	Depositor DCC
R_{free} test set	1291 reflections (5.19%)	DCC
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 88.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 26174 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4462	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.31	0/2009	0.45	0/2712
2	B	0.27	0/2328	0.61	5/3165 (0.2%)
All	All	0.29	0/4337	0.54	5/5877 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	238	TRP	C-N-CD	-12.93	92.16	120.60
2	B	112	LEU	C-N-CD	-8.53	101.84	120.60
2	B	108	PRO	C-N-CD	-7.23	104.69	120.60
2	B	247	GLY	N-CA-C	-5.66	98.94	113.10
2	B	261	VAL	C-N-CD	-5.54	108.41	120.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	208	PHE	Peptide
2	B	209	ARG	Peptide
2	B	248	ALA	Peptide
2	B	258	GLN	Peptide

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	1970	0	2027	91	0
2	B	2270	0	2281	286	0
3	A	152	0	0	3	0
3	B	70	0	0	4	0
All	All	4462	0	4308	371	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 43.

All (371) 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)
2:B:258:GLN:HB3	2:B:261:VAL:HG22	1.23	1.13
2:B:218:SER:HB3	2:B:221:ASP:HB2	1.24	1.08
2:B:235:GLU:HB3	2:B:236:ASP:HA	1.44	0.99
2:B:193:THR:HG22	2:B:194:PRO:HD3	1.44	0.98
2:B:175:VAL:HG12	2:B:176:VAL:H	1.30	0.96
2:B:209:ARG:HH21	2:B:260:VAL:HG13	1.29	0.96
2:B:258:GLN:CB	2:B:261:VAL:HG22	1.98	0.93
2:B:258:GLN:HB3	2:B:261:VAL:CG2	1.98	0.92
2:B:183:PRO:HB2	2:B:278:PHE:HE1	1.34	0.91
2:B:218:SER:CB	2:B:221:ASP:HB2	1.99	0.91
2:B:205:ALA:HB2	2:B:272:LEU:HD21	1.53	0.90
2:B:258:GLN:HA	2:B:261:VAL:H	1.34	0.90
2:B:213:LEU:HD21	2:B:229:LEU:HD12	1.52	0.90
2:B:261:VAL:HG23	2:B:262:PRO:HA	1.54	0.90
2:B:183:PRO:HB2	2:B:278:PHE:CE1	2.06	0.89
2:B:71:VAL:HG13	2:B:159:PHE:CE1	2.07	0.89
2:B:112:LEU:HB2	2:B:113:PRO:HA	1.56	0.88
2:B:143:PRO:HD3	2:B:203:ILE:HD11	1.54	0.88
1:A:98:ARG:HG2	1:A:98:ARG:HH11	1.36	0.87
2:B:109:PRO:HB3	2:B:112:LEU:HD12	1.57	0.87
2:B:123:GLN:HE21	2:B:154:VAL:HG22	1.36	0.87
2:B:123:GLN:NE2	2:B:154:VAL:HG22	1.90	0.85
2:B:124:PHE:CE2	2:B:200:VAL:HG13	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:PHE:CZ	2:B:200:VAL:HG22	2.12	0.84
2:B:261:VAL:HG23	2:B:262:PRO:CA	2.08	0.84
2:B:174:VAL:HB	2:B:175:VAL:HG23	1.63	0.81
2:B:246:ARG:HB3	2:B:247:GLY:HA3	1.62	0.81
2:B:232:LEU:HD23	2:B:233:PRO:N	1.95	0.81
1:A:240:ASP:HB3	1:A:243:CYS:SG	2.22	0.79
2:B:211:LYS:HB3	2:B:212:PRO:HD2	1.64	0.78
2:B:24:ARG:O	2:B:26:PRO:HD3	1.85	0.77
1:A:92:GLU:CG	1:A:147:LYS:HE3	2.15	0.77
2:B:209:ARG:HE	2:B:260:VAL:CG1	1.97	0.76
2:B:262:PRO:CB	2:B:263:GLU:HA	2.15	0.75
2:B:257:VAL:C	2:B:258:GLN:HG3	2.05	0.75
1:A:170:GLU:OE2	1:A:223:PHE:HA	1.87	0.74
2:B:178:LEU:HD23	2:B:181:ARG:HD3	1.70	0.74
2:B:209:ARG:NH2	2:B:260:VAL:HG13	2.02	0.73
2:B:56:GLU:OE1	2:B:164:ILE:HG13	1.88	0.73
1:A:23:LEU:O	1:A:27:VAL:HG22	1.88	0.73
2:B:286:ALA:O	2:B:290:LEU:HB2	1.89	0.73
1:A:224:LEU:HA	1:A:226:TYR:HD1	1.53	0.73
2:B:102:THR:O	2:B:106:LYS:HG2	1.89	0.73
2:B:213:LEU:O	2:B:213:LEU:HD23	1.89	0.72
2:B:246:ARG:CB	2:B:247:GLY:HA3	2.17	0.72
1:A:192:ASP:OD2	1:A:254:LEU:HD11	1.89	0.72
2:B:264:MET:CE	2:B:269:ALA:HA	2.20	0.72
2:B:258:GLN:HA	2:B:261:VAL:N	2.04	0.72
2:B:193:THR:CG2	2:B:194:PRO:HD3	2.20	0.72
2:B:261:VAL:HG23	2:B:262:PRO:N	2.05	0.71
2:B:138:HIS:CD2	2:B:141:LEU:HD13	2.25	0.71
1:A:201:SER:C	1:A:237:ILE:HD11	2.11	0.71
2:B:205:ALA:CB	2:B:213:LEU:HD12	2.21	0.71
2:B:257:VAL:HB	2:B:258:GLN:HG3	1.72	0.70
1:A:155[B]:MET:HG2	1:A:160:PHE:CE1	2.27	0.70
2:B:261:VAL:HG21	2:B:264:MET:HB2	1.73	0.70
2:B:123:GLN:NE2	2:B:153:THR:O	2.25	0.69
2:B:83:THR:HG22	2:B:84:ASP:N	2.08	0.69
2:B:262:PRO:HB3	2:B:263:GLU:HA	1.73	0.69
2:B:213:LEU:HD21	2:B:229:LEU:CD1	2.22	0.69
2:B:112:LEU:HB2	2:B:113:PRO:CA	2.22	0.69
1:A:245:ARG:O	1:A:249:GLU:HG3	1.92	0.69
2:B:137:VAL:HG12	2:B:139:ARG:HG3	1.74	0.69
2:B:188:GLN:HG2	2:B:189:SER:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:THR:HG22	2:B:84:ASP:H	1.58	0.68
2:B:246:ARG:HB3	2:B:247:GLY:CA	2.24	0.68
2:B:146:ILE:C	2:B:147:LEU:HD23	2.14	0.68
2:B:116:THR:O	2:B:120:LEU:HB2	1.94	0.68
2:B:219:GLU:O	2:B:223:LEU:HG	1.94	0.67
1:A:120:THR:HA	2:B:44:GLU:OE2	1.94	0.67
2:B:176:VAL:HG13	2:B:177:THR:N	2.10	0.67
2:B:71:VAL:HG13	2:B:159:PHE:CZ	2.29	0.67
2:B:140:ASP:O	2:B:145:ASN:ND2	2.27	0.66
2:B:179:TRP:CE3	2:B:212:PRO:HG3	2.31	0.66
2:B:203:ILE:O	2:B:207:MET:HG3	1.96	0.66
2:B:292:HIS:CD2	2:B:293:SER:H	2.14	0.66
2:B:99:ASP:OD2	2:B:101:ARG:HB3	1.96	0.66
1:A:176:GLN:NE2	1:A:179:ARG:HH21	1.94	0.66
2:B:50:PRO:O	2:B:54:VAL:HG12	1.96	0.66
2:B:184:GLU:OE2	2:B:283:ARG:NH1	2.26	0.66
2:B:3:THR:HG23	3:B:2002:HOH:O	1.96	0.66
2:B:211:LYS:CB	2:B:212:PRO:HD2	2.26	0.65
2:B:214:PHE:CE1	2:B:226:ILE:HA	2.31	0.65
1:A:162:GLU:OE1	1:A:179:ARG:NH1	2.30	0.65
1:A:156:THR:O	1:A:159:ASP:HB2	1.97	0.65
2:B:190:THR:O	2:B:192:ALA:N	2.29	0.65
1:A:98:ARG:NH1	1:A:98:ARG:HG2	2.12	0.65
2:B:25:ASP:O	2:B:29:GLY:N	2.31	0.64
2:B:68:HIS:CG	2:B:69:PRO:HD2	2.33	0.64
2:B:264:MET:HE1	2:B:269:ALA:HA	1.79	0.63
2:B:175:VAL:O	2:B:176:VAL:HB	1.98	0.63
2:B:205:ALA:HB1	2:B:213:LEU:HD12	1.80	0.63
2:B:139:ARG:HD2	2:B:191:TYR:CD1	2.33	0.63
2:B:177:THR:O	2:B:179:TRP:N	2.31	0.63
2:B:271:LEU:HB2	2:B:292:HIS:ND1	2.13	0.63
2:B:236:ASP:O	2:B:238:TRP:N	2.30	0.63
2:B:153:THR:O	2:B:154:VAL:HG22	1.99	0.63
2:B:112:LEU:CB	2:B:113:PRO:HA	2.26	0.63
2:B:263:GLU:HG2	2:B:263:GLU:O	1.97	0.63
2:B:250:PRO:HB2	2:B:252:ARG:HH21	1.64	0.63
2:B:96:VAL:HG21	2:B:155:LYS:HG3	1.81	0.63
2:B:183:PRO:O	2:B:187:LEU:HD22	1.99	0.62
2:B:257:VAL:HG21	2:B:269:ALA:HB1	1.82	0.62
2:B:187:LEU:HD21	2:B:278:PHE:HZ	1.63	0.62
2:B:51:ILE:HD13	2:B:51:ILE:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:ARG:O	2:B:126:ARG:HG3	2.00	0.62
1:A:237:ILE:HG23	1:A:239:CYS:HB3	1.81	0.61
2:B:108:PRO:N	2:B:109:PRO:HD2	2.15	0.61
1:A:263:GLN:O	1:A:265:ASN:N	2.30	0.61
2:B:147:LEU:O	2:B:154:VAL:HA	2.00	0.61
1:A:145:VAL:HG22	1:A:152:LEU:HD11	1.84	0.60
1:A:173:GLU:H	1:A:173:GLU:CD	2.04	0.60
2:B:123:GLN:HB3	2:B:154:VAL:CG2	2.32	0.60
1:A:88:PHE:CE1	1:A:147:LYS:HG3	2.36	0.60
1:A:162:GLU:OE2	1:A:179:ARG:HD3	2.01	0.60
1:A:35:GLU:OE2	1:A:200:PRO:HD2	2.02	0.59
2:B:125:LEU:HB2	2:B:290:LEU:HG	1.84	0.59
1:A:26:ARG:HB2	1:A:26:ARG:NH1	2.17	0.59
2:B:257:VAL:HB	2:B:258:GLN:CG	2.32	0.59
2:B:125:LEU:CB	2:B:290:LEU:HG	2.33	0.59
2:B:209:ARG:HE	2:B:260:VAL:HG12	1.67	0.59
2:B:105:ASP:O	2:B:107:ALA:N	2.30	0.59
2:B:142:LYS:O	2:B:146:ILE:HG13	2.03	0.59
2:B:25:ASP:CG	2:B:28:SER:HB3	2.22	0.59
2:B:71:VAL:HG13	2:B:159:PHE:HE1	1.67	0.58
2:B:103:TYR:HD2	2:B:104:LEU:HD23	1.69	0.58
2:B:126:ARG:HG3	2:B:290:LEU:HD11	1.85	0.58
2:B:139:ARG:HH11	2:B:191:TYR:HE1	1.49	0.58
1:A:224:LEU:HA	1:A:226:TYR:CD1	2.38	0.57
1:A:63:TRP:O	1:A:67:VAL:HG23	2.04	0.57
1:A:108:PHE:O	1:A:112:LYS:HG3	2.04	0.57
2:B:128:LEU:HD13	2:B:132:HIS:CE1	2.39	0.57
1:A:216:ASN:HB2	1:A:223:PHE:HB2	1.85	0.57
2:B:147:LEU:HD23	2:B:147:LEU:N	2.19	0.57
2:B:208:PHE:CZ	2:B:264:MET:HG2	2.40	0.57
2:B:196:ASP:O	2:B:200:VAL:HG23	2.03	0.57
2:B:227:PHE:HD1	2:B:232:LEU:HA	1.69	0.57
2:B:184:GLU:HG2	2:B:280:PRO:HG3	1.87	0.57
2:B:218:SER:CA	2:B:221:ASP:HB2	2.35	0.56
2:B:138:HIS:O	2:B:139:ARG:HB2	2.05	0.56
2:B:124:PHE:CE2	2:B:200:VAL:HG22	2.40	0.56
2:B:28:SER:OG	2:B:30:HIS:HD2	1.89	0.56
1:A:98:ARG:HH11	1:A:98:ARG:CG	2.13	0.56
2:B:188:GLN:HG2	2:B:189:SER:H	1.71	0.56
2:B:137:VAL:CG1	2:B:139:ARG:HG3	2.35	0.56
2:B:261:VAL:CG2	2:B:262:PRO:HA	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:ASP:C	2:B:238:TRP:H	2.10	0.55
2:B:72:VAL:HG13	2:B:155:LYS:HB3	1.88	0.55
2:B:123:GLN:HB3	2:B:154:VAL:HG21	1.89	0.55
2:B:188:GLN:O	2:B:189:SER:HB2	2.06	0.55
2:B:250:PRO:HB2	2:B:252:ARG:NH2	2.21	0.55
2:B:176:VAL:HG22	2:B:177:THR:H	1.72	0.55
2:B:124:PHE:HE2	2:B:200:VAL:HG13	1.68	0.55
2:B:208:PHE:CD2	2:B:208:PHE:N	2.73	0.55
2:B:178:LEU:CD2	2:B:181:ARG:HH11	2.20	0.54
2:B:35:LYS:HE3	2:B:158:ASP:OD1	2.08	0.54
1:A:29:ARG:O	1:A:33:LYS:HG3	2.07	0.54
1:A:189:CYS:SG	1:A:251:ILE:HG12	2.46	0.54
2:B:258:GLN:CA	2:B:261:VAL:HG22	2.37	0.54
1:A:25[A]:ASP:OD2	1:A:26:ARG:N	2.41	0.54
2:B:14:VAL:HG12	2:B:19:THR:OG1	2.07	0.54
2:B:123:GLN:CB	2:B:154:VAL:HG21	2.37	0.54
2:B:178:LEU:HA	2:B:181:ARG:HD3	1.88	0.54
2:B:262:PRO:CB	2:B:263:GLU:CA	2.84	0.54
2:B:187:LEU:CD2	2:B:278:PHE:HZ	2.21	0.54
1:A:263:GLN:C	1:A:265:ASN:H	2.11	0.53
2:B:198:TRP:CZ3	2:B:276:LEU:HA	2.43	0.53
2:B:126:ARG:CG	2:B:290:LEU:HD11	2.38	0.53
1:A:237:ILE:CG2	1:A:239:CYS:HB3	2.38	0.53
2:B:12:ILE:O	2:B:12:ILE:HG13	2.06	0.53
2:B:175:VAL:HG12	2:B:176:VAL:N	2.11	0.53
2:B:144:GLU:OE1	2:B:144:GLU:N	2.41	0.53
1:A:266:MET:HG3	1:A:267:ASP:N	2.24	0.53
2:B:205:ALA:HB2	2:B:272:LEU:CD2	2.33	0.53
2:B:187:LEU:CD1	2:B:223:LEU:HD11	2.39	0.53
2:B:139:ARG:NH1	2:B:191:TYR:CE1	2.77	0.52
1:A:78:PHE:HB3	1:A:79:PRO:HD3	1.91	0.52
1:A:92:GLU:HG2	1:A:147:LYS:HE3	1.87	0.52
2:B:290:LEU:O	2:B:291:GLN:HG3	2.10	0.52
1:A:42:VAL:HG23	1:A:197:SER:HB3	1.90	0.52
2:B:32:VAL:CG1	2:B:92:VAL:HG13	2.40	0.52
2:B:68:HIS:ND1	2:B:69:PRO:HD2	2.25	0.52
2:B:190:THR:C	2:B:192:ALA:H	2.13	0.52
2:B:227:PHE:CD1	2:B:232:LEU:HA	2.45	0.52
2:B:213:LEU:C	2:B:213:LEU:HD23	2.29	0.52
2:B:278:PHE:O	2:B:280:PRO:HD3	2.10	0.52
2:B:177:THR:C	2:B:179:TRP:H	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:PRO:N	2:B:109:PRO:CD	2.72	0.51
1:A:202:MET:N	1:A:237:ILE:HD11	2.25	0.51
2:B:6:TYR:CE1	2:B:32:VAL:HG21	2.46	0.51
2:B:227:PHE:CE1	2:B:233:PRO:HD2	2.46	0.51
2:B:182:ALA:HA	2:B:198:TRP:CD1	2.44	0.51
2:B:105:ASP:C	2:B:107:ALA:H	2.13	0.51
2:B:139:ARG:CD	2:B:191:TYR:CD1	2.94	0.51
1:A:145:VAL:CG1	1:A:150:TRP:CE2	2.94	0.51
2:B:218:SER:HB3	2:B:221:ASP:CB	2.17	0.51
2:B:209:ARG:HE	2:B:260:VAL:HG13	1.73	0.51
2:B:147:LEU:C	2:B:148:VAL:HG12	2.31	0.51
2:B:262:PRO:HB3	2:B:263:GLU:CA	2.40	0.51
2:B:193:THR:N	2:B:194:PRO:CD	2.74	0.50
2:B:198:TRP:CE3	2:B:276:LEU:HA	2.46	0.50
1:A:237:ILE:HG21	1:A:239:CYS:SG	2.51	0.50
2:B:59:LEU:O	2:B:62:ARG:O	2.29	0.50
1:A:238:LYS:N	1:A:238:LYS:HD2	2.26	0.50
2:B:235:GLU:CD	2:B:235:GLU:H	2.14	0.50
1:A:27:VAL:O	1:A:31:MET:HG2	2.11	0.50
2:B:83:THR:O	2:B:84:ASP:OD1	2.30	0.50
1:A:199:PRO:HD2	1:A:202:MET:HE3	1.93	0.50
2:B:289:ALA:C	2:B:291:GLN:H	2.15	0.50
2:B:208:PHE:CZ	2:B:264:MET:CG	2.94	0.50
2:B:210:ARG:O	2:B:211:LYS:HG3	2.11	0.50
1:A:155[B]:MET:HG2	1:A:160:PHE:CZ	2.47	0.50
2:B:238:TRP:HZ2	2:B:246:ARG:O	1.94	0.50
2:B:106:LYS:HG3	2:B:106:LYS:O	2.12	0.50
2:B:101:ARG:HH12	2:B:144:GLU:CD	2.16	0.49
1:A:250:GLN:NE2	3:A:2151:HOH:O	2.44	0.49
1:A:50:LYS:N	1:A:50:LYS:HD2	2.27	0.49
2:B:271:LEU:HB2	2:B:292:HIS:CE1	2.48	0.49
1:A:133:ARG:HD3	1:A:135:GLU:OE1	2.12	0.49
2:B:38:ARG:HG2	2:B:168:GLN:HE21	1.78	0.49
2:B:184:GLU:CG	2:B:280:PRO:HG3	2.42	0.48
2:B:204:PHE:O	2:B:207:MET:HB2	2.13	0.48
2:B:51:ILE:HD13	2:B:51:ILE:H	1.77	0.48
2:B:262:PRO:HA	2:B:264:MET:N	2.29	0.48
2:B:139:ARG:NH1	2:B:191:TYR:CD1	2.81	0.48
1:A:201:SER:O	1:A:237:ILE:HD11	2.14	0.48
2:B:176:VAL:O	2:B:177:THR:HB	2.13	0.48
2:B:248:ALA:O	2:B:249:PHE:HD1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLU:HG3	1:A:147:LYS:HE3	1.91	0.48
2:B:24:ARG:HH21	2:B:29:GLY:HA2	1.79	0.48
2:B:227:PHE:HE1	2:B:233:PRO:HD2	1.77	0.47
2:B:98:GLN:OE1	2:B:103:TYR:HD1	1.96	0.47
2:B:101:ARG:O	2:B:104:LEU:N	2.45	0.47
2:B:257:VAL:HG12	2:B:258:GLN:H	1.79	0.47
1:A:112:LYS:O	2:B:55:ARG:NH1	2.47	0.47
2:B:14:VAL:HG23	2:B:14:VAL:O	2.13	0.47
1:A:220:PRO:O	1:A:221:ASN:HB2	2.14	0.47
1:A:193:VAL:O	1:A:196:ILE:HG13	2.14	0.47
2:B:174:VAL:CB	2:B:175:VAL:HG23	2.41	0.47
2:B:197:MET:HE1	2:B:286:ALA:HA	1.97	0.47
2:B:154:VAL:HG23	2:B:154:VAL:O	2.14	0.47
2:B:227:PHE:CE1	2:B:233:PRO:CD	2.98	0.47
2:B:20:VAL:HG22	2:B:35:LYS:HG2	1.97	0.47
2:B:250:PRO:O	2:B:252:ARG:HG2	2.15	0.47
2:B:258:GLN:HA	2:B:261:VAL:CA	2.44	0.47
2:B:238:TRP:HA	2:B:239:PRO:HD2	1.72	0.47
1:A:190:ALA:HA	1:A:195:PHE:CG	2.50	0.47
2:B:265:GLU:HG3	2:B:266:GLU:N	2.30	0.47
2:B:148:VAL:HB	2:B:154:VAL:H	1.81	0.46
2:B:223:LEU:O	2:B:226:ILE:N	2.45	0.46
1:A:134:PRO:O	1:A:138:LEU:HG	2.14	0.46
2:B:235:GLU:CB	2:B:236:ASP:HA	2.23	0.46
2:B:289:ALA:O	2:B:291:GLN:N	2.48	0.46
1:A:237:ILE:CG2	1:A:239:CYS:SG	3.03	0.46
1:A:56:MET:O	1:A:60:VAL:HG23	2.16	0.46
2:B:262:PRO:HB3	2:B:263:GLU:C	2.35	0.46
1:A:98:ARG:NH1	1:A:98:ARG:CG	2.73	0.46
2:B:138:HIS:NE2	2:B:157:ALA:O	2.43	0.46
1:A:171:ALA:HB1	1:A:173:GLU:OE1	2.15	0.46
2:B:142:LYS:HE2	2:B:177:THR:CG2	2.46	0.46
2:B:19:THR:CG2	2:B:21:TYR:CE1	2.99	0.46
2:B:233:PRO:HG2	2:B:278:PHE:CD2	2.51	0.46
1:A:155[A]:MET:CE	1:A:159:ASP:HB3	2.44	0.46
1:A:60:VAL:HG21	1:A:99:LEU:CD2	2.46	0.46
2:B:139:ARG:CD	2:B:191:TYR:CE1	2.99	0.46
2:B:7:GLU:O	2:B:9:VAL:HG23	2.16	0.46
2:B:108:PRO:O	2:B:110:PRO:HD2	2.16	0.46
2:B:128:LEU:CD1	2:B:132:HIS:CE1	2.99	0.46
2:B:249:PHE:HB3	2:B:250:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:THR:HG22	2:B:279:ASN:H	1.82	0.45
2:B:32:VAL:CG1	2:B:33:ALA:N	2.78	0.45
2:B:264:MET:HE3	2:B:268:GLY:C	2.36	0.45
1:A:132:ILE:HB	1:A:136:GLU:OE1	2.16	0.45
2:B:261:VAL:CG2	2:B:262:PRO:N	2.75	0.45
2:B:221:ASP:O	2:B:225:LYS:HB2	2.16	0.45
2:B:187:LEU:CD2	2:B:278:PHE:CZ	2.99	0.45
2:B:219:GLU:N	2:B:219:GLU:OE1	2.35	0.45
1:A:236:VAL:HG22	3:A:2142:HOH:O	2.17	0.45
1:A:199:PRO:HD2	1:A:202:MET:HB3	1.99	0.45
2:B:188:GLN:CG	2:B:189:SER:H	2.29	0.45
2:B:187:LEU:HD21	2:B:278:PHE:CZ	2.47	0.45
2:B:131:LEU:HD21	2:B:159:PHE:CD1	2.52	0.45
1:A:92:GLU:HG2	1:A:147:LYS:CE	2.47	0.45
2:B:100:LEU:O	2:B:104:LEU:HG	2.17	0.45
2:B:32:VAL:HG11	2:B:34:LEU:HD21	1.98	0.45
2:B:209:ARG:O	2:B:210:ARG:HG3	2.17	0.45
2:B:260:VAL:HG12	2:B:260:VAL:O	2.17	0.45
1:A:145:VAL:CG1	1:A:150:TRP:NE1	2.79	0.45
1:A:155[B]:MET:CG	1:A:160:PHE:CZ	3.00	0.44
2:B:183:PRO:HB2	2:B:278:PHE:CD1	2.49	0.44
2:B:51:ILE:CD1	2:B:51:ILE:H	2.26	0.44
2:B:32:VAL:HG11	2:B:92:VAL:HG13	1.99	0.44
2:B:292:HIS:CD2	2:B:293:SER:N	2.84	0.44
1:A:26:ARG:CZ	1:A:26:ARG:HB2	2.48	0.44
1:A:62:THR:O	1:A:66:GLU:HG3	2.17	0.44
2:B:265:GLU:CG	2:B:266:GLU:N	2.78	0.44
2:B:227:PHE:HE1	2:B:233:PRO:CD	2.30	0.44
1:A:202:MET:HE2	1:A:202:MET:HB2	1.87	0.44
2:B:209:ARG:HH21	2:B:260:VAL:CG1	2.16	0.44
2:B:212:PRO:HB2	2:B:215:CYS:HB2	1.99	0.44
2:B:120:LEU:HD23	2:B:207:MET:HE3	1.99	0.44
2:B:232:LEU:HA	2:B:233:PRO:HD3	1.75	0.43
2:B:125:LEU:HB3	2:B:290:LEU:HG	2.00	0.43
1:A:202:MET:HA	1:A:237:ILE:HD11	2.00	0.43
2:B:83:THR:CG2	2:B:84:ASP:H	2.23	0.43
2:B:179:TRP:CE3	2:B:212:PRO:CG	3.01	0.43
2:B:139:ARG:HD2	2:B:191:TYR:CE1	2.54	0.43
2:B:227:PHE:CD1	2:B:233:PRO:HD3	2.53	0.43
2:B:171:LEU:HD12	3:B:2040:HOH:O	2.18	0.43
2:B:63:LEU:HA	2:B:63:LEU:HD22	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:ALA:C	2:B:109:PRO:HD2	2.39	0.43
1:A:194:LYS:CG	1:A:195:PHE:N	2.80	0.43
2:B:26:PRO:HD2	3:B:2005:HOH:O	2.19	0.43
2:B:248:ALA:C	2:B:249:PHE:HD1	2.22	0.43
2:B:232:LEU:HD23	2:B:232:LEU:C	2.39	0.43
1:A:256:GLU:O	1:A:259:LEU:HG	2.19	0.43
2:B:140:ASP:OD1	2:B:142:LYS:HE3	2.20	0.42
1:A:138:LEU:HB2	2:B:82:ARG:HH22	1.83	0.42
2:B:71:VAL:HG21	2:B:131:LEU:CD1	2.49	0.42
2:B:124:PHE:CD2	2:B:200:VAL:HG13	2.53	0.42
1:A:224:LEU:HG	1:A:224:LEU:H	1.74	0.42
1:A:123:LYS:HE3	1:A:123:LYS:HB2	1.87	0.42
2:B:213:LEU:HG	2:B:260:VAL:HG11	2.00	0.42
1:A:139:GLN:HG3	2:B:82:ARG:HH12	1.84	0.42
2:B:262:PRO:HA	2:B:264:MET:H	1.84	0.42
2:B:149:THR:HG23	2:B:150:SER:N	2.35	0.42
2:B:148:VAL:HG23	2:B:153:THR:H	1.85	0.42
2:B:142:LYS:HE2	2:B:177:THR:HG21	2.01	0.42
2:B:211:LYS:HB3	2:B:212:PRO:CD	2.43	0.42
1:A:44:TYR:CE2	1:A:89:LEU:HB3	2.55	0.42
1:A:165:LEU:HA	1:A:165:LEU:HD12	1.79	0.42
2:B:123:GLN:HB2	2:B:154:VAL:HG21	2.02	0.42
2:B:167:TYR:HB3	3:B:2014:HOH:O	2.19	0.42
1:A:112:LYS:HD2	2:B:51:ILE:HD12	2.02	0.42
1:A:112:LYS:HB3	2:B:51:ILE:HG23	2.02	0.42
1:A:189:CYS:SG	1:A:194:LYS:HD3	2.60	0.42
2:B:205:ALA:HB3	2:B:213:LEU:HD12	1.98	0.41
1:A:26:ARG:HD3	3:A:2003:HOH:O	2.19	0.41
2:B:38:ARG:H	2:B:168:GLN:HE21	1.68	0.41
2:B:114:ALA:O	2:B:118:LYS:HG3	2.21	0.41
2:B:264:MET:CE	2:B:269:ALA:CA	2.96	0.41
2:B:184:GLU:HG2	2:B:280:PRO:CG	2.48	0.41
1:A:198:ASN:HA	1:A:199:PRO:HD3	1.82	0.41
2:B:274:GLU:HB3	2:B:284:ILE:HB	2.01	0.41
2:B:245:PRO:O	2:B:245:PRO:HG2	2.20	0.41
2:B:178:LEU:CD2	2:B:181:ARG:HD3	2.45	0.41
2:B:141:LEU:HD12	2:B:141:LEU:HA	1.80	0.41
1:A:202:MET:CA	1:A:237:ILE:HD11	2.50	0.41
2:B:98:GLN:OE1	2:B:103:TYR:HB2	2.21	0.41
2:B:218:SER:N	2:B:221:ASP:HB2	2.34	0.41
2:B:209:ARG:NE	2:B:260:VAL:CG1	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:SER:O	1:A:229:LEU:HD13	2.20	0.41
2:B:209:ARG:NE	2:B:260:VAL:HG13	2.34	0.41
1:A:23:LEU:HD23	1:A:23:LEU:HA	1.85	0.41
2:B:139:ARG:CZ	2:B:191:TYR:HD1	2.34	0.41
1:A:42:VAL:CG2	1:A:197:SER:HB3	2.51	0.41
1:A:170:GLU:O	1:A:175:LYS:HE3	2.21	0.41
2:B:292:HIS:CG	2:B:293:SER:N	2.88	0.41
2:B:218:SER:N	2:B:221:ASP:CB	2.84	0.41
2:B:249:PHE:CB	2:B:250:PRO:HD2	2.51	0.41
1:A:145:VAL:HG13	1:A:150:TRP:CD1	2.56	0.41
2:B:9:VAL:N	2:B:22:LYS:O	2.53	0.41
2:B:71:VAL:CG1	2:B:159:PHE:CZ	3.02	0.41
2:B:32:VAL:HG11	2:B:34:LEU:CD2	2.50	0.41
2:B:261:VAL:CG2	2:B:262:PRO:CA	2.92	0.40
2:B:32:VAL:CG1	2:B:34:LEU:CD2	2.99	0.40
2:B:177:THR:C	2:B:179:TRP:N	2.73	0.40
2:B:249:PHE:HB3	2:B:250:PRO:CD	2.51	0.40
2:B:32:VAL:CG1	2:B:34:LEU:HD23	2.51	0.40
1:A:63:TRP:CZ3	1:A:107:MET:HE1	2.57	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	246/257 (96%)	232 (94%)	13 (5%)	1 (0%)	39	49
2	B	283/306 (92%)	216 (76%)	46 (16%)	21 (7%)	1	0
All	All	529/563 (94%)	448 (85%)	59 (11%)	22 (4%)	3	1

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
2	B	63	LEU
2	B	148	VAL
2	B	176	VAL
2	B	177	THR
2	B	189	SER
2	B	191	TYR
2	B	237	ASP
2	B	239	PRO
2	B	102	THR
2	B	106	LYS
2	B	175	VAL
2	B	178	LEU
2	B	257	VAL
2	B	266	GLU
2	B	249	PHE
2	B	290	LEU
2	B	154	VAL
2	B	212	PRO
2	B	251	PRO
2	B	26	PRO
2	B	108	PRO

5.3.2 Protein sidechains (i)

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	224/229 (98%)	211 (94%)	13 (6%)	25	34
2	B	246/264 (93%)	222 (90%)	24 (10%)	10	11
All	All	470/493 (95%)	433 (92%)	37 (8%)	15	20

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

Mol	Chain	Res	Type
1	A	44	TYR
1	A	50	LYS

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Mol	Chain	Res	Type
1	A	89	LEU
1	A	98	ARG
1	A	132	ILE
1	A	145	VAL
1	A	165	LEU
1	A	170	GLU
1	A	188	LEU
1	A	193	VAL
1	A	202	MET
1	A	224	LEU
1	A	237	ILE
2	B	5	ARG
2	B	12	ILE
2	B	36	SER
2	B	43	GLU
2	B	51	ILE
2	B	54	VAL
2	B	63	LEU
2	B	112	LEU
2	B	128	LEU
2	B	148	VAL
2	B	149	THR
2	B	153	THR
2	B	166	SER
2	B	181	ARG
2	B	187	LEU
2	B	208	PHE
2	B	215	CYS
2	B	229	LEU
2	B	245	PRO
2	B	249	PHE
2	B	258	GLN
2	B	259	SER
2	B	261	VAL
2	B	290	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	176	GLN
1	A	248	GLN

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Mol	Chain	Res	Type
2	B	30	HIS
2	B	70	ASN
2	B	123	GLN
2	B	168	GLN
2	B	222	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	246/257 (95%)	0.18	12 (4%)	33	36	19, 39, 95, 193	0
2	B	287/306 (93%)	0.86	36 (12%)	5	5	34, 74, 134, 189	0
All	All	533/563 (94%)	0.55	48 (9%)	12	12	19, 55, 127, 193	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	111	GLY	9.3
2	B	112	LEU	8.1
2	B	3	THR	7.8
2	B	2	ALA	7.6
1	A	266	MET	7.0
1	A	259	LEU	6.5
1	A	265	ASN	5.3
2	B	255	ARG	5.3
1	A	261	GLN	4.6
1	A	267	ASP	4.6
2	B	191	TYR	4.4
2	B	240	ARG	4.4
2	B	252	ARG	4.2
2	B	27	HIS	3.7
2	B	108	PRO	3.7
2	B	236	ASP	3.4
2	B	26	PRO	3.2
2	B	230	ILE	3.2
2	B	205	ALA	3.2
2	B	254	PRO	3.2
1	A	222	ASN	3.1
1	A	260	ARG	3.0
1	A	262	ALA	2.7
1	A	23	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	7	GLU	2.7
2	B	16	ALA	2.7
2	B	227	PHE	2.7
2	B	232	LEU	2.6
2	B	263	GLU	2.6
1	A	26	ARG	2.5
2	B	5	ARG	2.5
1	A	264	GLN	2.5
2	B	245	PRO	2.5
2	B	103	TYR	2.4
2	B	234	PRO	2.4
2	B	178	LEU	2.4
2	B	238	TRP	2.4
2	B	154	VAL	2.4
2	B	214	PHE	2.3
2	B	264	MET	2.2
2	B	153	THR	2.2
2	B	113	PRO	2.2
2	B	201	GLY	2.2
1	A	195	PHE	2.2
2	B	197	MET	2.1
2	B	231	GLY	2.1
2	B	291	GLN	2.1
2	B	187	LEU	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.