Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:42 am BST

PDB ID	:	2BE1
Title	:	Structure of the compact lumenal domain of yeast Ire1
Authors	:	Credle, J.J.; Finer-Moore, J.S.; Papa, F.R.; Stroud, R.M.; Walter, P.
Deposited on	:	2005-10-21
Resolution	:	2.98 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 following versions of software and data (see references ⓘ) were used in the production of this report:

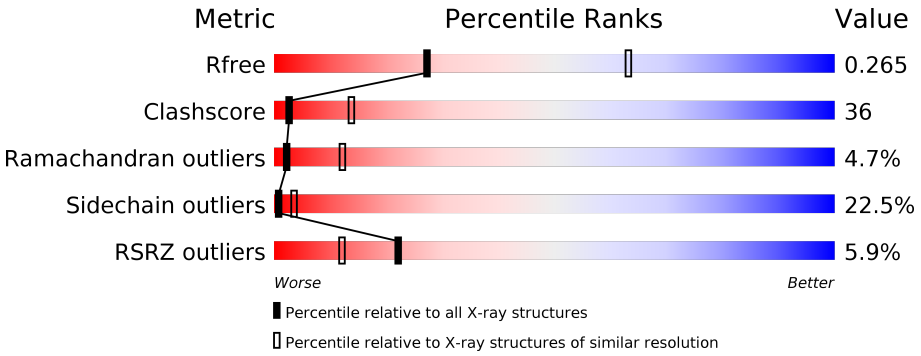
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.98 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}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 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 <=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	339	6% 33% 40% 14% • 11%
1	B	339	4% 36% 37% 14% • 11%
2	D	8	13% 25% 50% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4884 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 Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2401	1535	401	458	7			
1	B	301	Total	C	N	O	S	0	0	0
			2401	1535	401	458	7			

- Molecule 2 is a protein called peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	8	Total	C	N	O	0	0	0
			56	40	8	8			

- Molecule 3 is water.

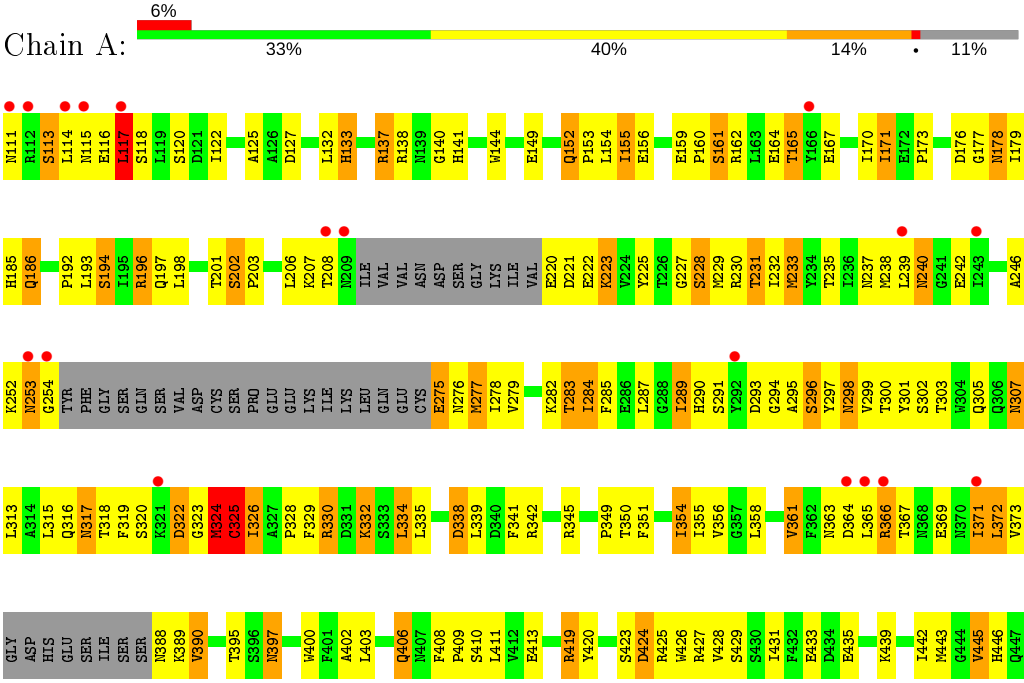
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	10	Total	O	0	0
			10	10		
3	D	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

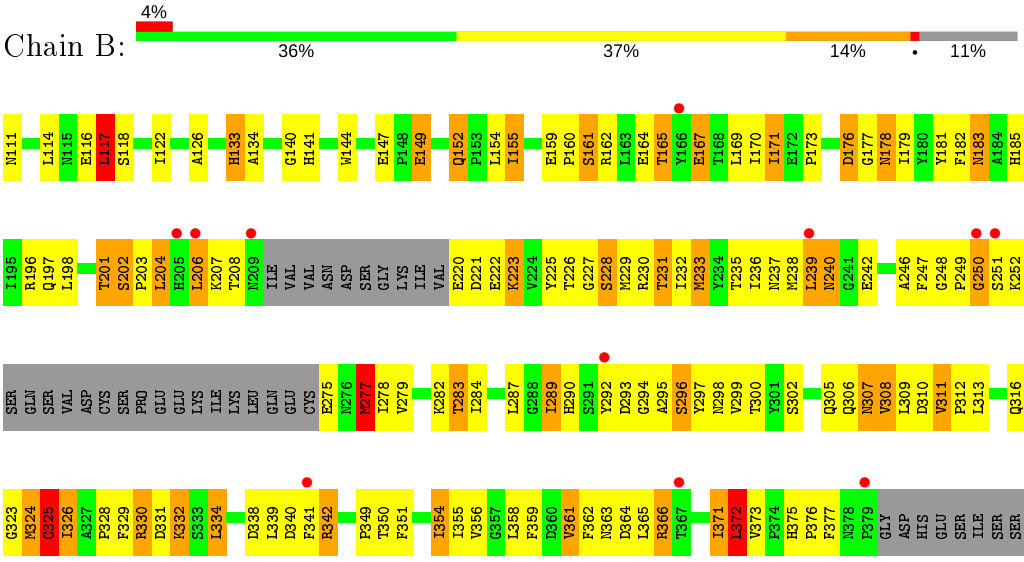
- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

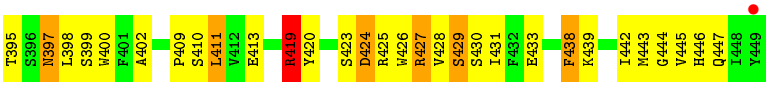
Chain A:



- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain B:





- Molecule 2: peptide

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	103.30Å 103.30Å 401.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.28 – 2.98 48.28 – 2.98	Depositor EDS
% Data completeness (in resolution range)	82.1 (48.28-2.98) 89.4 (48.28-2.98)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.240 , 0.279 0.225 , 0.265	Depositor DCC
R_{free} test set	2380 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å^2)	66.5	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 77.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4884	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	1.19	6/2457 (0.2%)	1.12	8/3337 (0.2%)
1	B	1.22	5/2457 (0.2%)	1.14	11/3337 (0.3%)
2	D	2.74	4/55 (7.3%)	1.81	2/77 (2.6%)
All	All	1.23	15/4969 (0.3%)	1.14	21/6751 (0.3%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	26	VAL	CA-CB	8.80	1.73	1.54
1	B	322	ASP	CB-CG	-8.78	1.33	1.51
2	D	26	VAL	CB-CG1	8.62	1.71	1.52
1	B	325	CYS	CB-SG	-8.56	1.67	1.82
1	B	181	TYR	CE2-CZ	7.58	1.48	1.38
1	A	181	TYR	CE2-CZ	6.85	1.47	1.38
1	B	126	ALA	CA-CB	-6.82	1.38	1.52
1	A	325	CYS	CB-SG	-6.69	1.70	1.82
1	A	435	GLU	CG-CD	6.50	1.61	1.51
1	B	181	TYR	CB-CG	-6.49	1.42	1.51
1	A	435	GLU	CD-OE1	6.13	1.32	1.25
1	A	322	ASP	CB-CG	-5.70	1.39	1.51
2	D	19	VAL	CB-CG2	5.67	1.64	1.52
2	D	19	VAL	CB-CG1	5.27	1.64	1.52
1	A	125	ALA	CA-CB	-5.10	1.41	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	419	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	B	322	ASP	CB-CG-OD1	-8.18	110.94	118.30
1	A	322	ASP	CB-CG-OD1	-7.47	111.58	118.30
1	B	239	LEU	CA-CB-CG	7.19	131.84	115.30
1	A	196	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	239	LEU	CA-CB-CG	6.74	130.79	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	26	VAL	CA-CB-CG1	6.67	120.91	110.90
1	B	204	LEU	CB-CG-CD2	-6.66	99.69	111.00
1	B	196	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	419	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	427	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	372	LEU	CB-CG-CD1	-5.54	101.58	111.00
1	A	277	MET	CB-CG-SD	-5.46	96.02	112.40
1	A	138	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	B	230	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	127	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	284	ILE	CB-CA-C	-5.23	101.13	111.60
2	D	22	VAL	CG1-CB-CG2	5.23	119.26	110.90
1	B	167	GLU	CB-CA-C	-5.19	100.02	110.40
1	B	372	LEU	CA-CB-CG	5.18	127.23	115.30
1	B	277	MET	CB-CG-SD	-5.04	97.28	112.40

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	2401	0	2343	185	0
1	B	2401	0	2343	174	0
2	D	56	0	71	13	0
3	A	14	0	0	2	0
3	B	10	0	0	6	0
3	D	2	0	0	4	0
All	All	4884	0	4757	348	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 36.

All (348) 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:B:161:SER:OG	3:B:12:HOH:O	1.66	1.10
1:B:208:THR:HG22	1:B:221:ASP:O	1.51	1.09
1:A:152:GLN:NE2	1:A:282:LYS:HE2	1.75	1.00
1:A:231:THR:HG21	1:B:202:SER:CB	1.92	1.00
1:B:313:LEU:HD12	1:B:371:ILE:HD11	1.41	0.98
1:A:208:THR:HG22	1:A:221:ASP:O	1.65	0.95
1:A:313:LEU:HD12	1:A:371:ILE:HD11	1.48	0.93
1:A:231:THR:HG21	1:B:202:SER:HB2	1.48	0.92
1:A:283:THR:HG22	1:A:305:GLN:OE1	1.68	0.92
1:A:248:GLY:O	1:A:250:GLY:N	2.06	0.89
1:B:152:GLN:NE2	1:B:282:LYS:HE2	1.90	0.86
1:A:289:ILE:HG23	1:A:297:TYR:HB2	1.58	0.85
1:B:253:ASN:ND2	1:B:254:GLY:H	1.75	0.84
1:B:289:ILE:HG23	1:B:297:TYR:HB2	1.57	0.84
1:A:160:PRO:O	1:A:161:SER:HB2	1.77	0.82
1:A:423:SER:OG	1:A:425:ARG:HG2	1.79	0.82
1:A:395:THR:OG1	1:A:397:ASN:ND2	2.14	0.80
1:A:202:SER:CB	1:B:231:THR:HG21	2.13	0.79
1:B:283:THR:HG22	1:B:305:GLN:OE1	1.83	0.79
1:A:231:THR:HG21	1:B:202:SER:HB3	1.64	0.78
1:A:202:SER:HB2	1:B:231:THR:HG21	1.64	0.78
1:B:248:GLY:O	1:B:250:GLY:N	2.16	0.77
1:B:160:PRO:O	1:B:161:SER:HB2	1.82	0.77
1:A:442:ILE:O	1:A:446:HIS:HE1	1.67	0.76
1:B:183:ASN:OD1	1:B:183:ASN:C	2.25	0.74
1:B:197:GLN:O	1:B:201:THR:HG23	1.87	0.73
1:B:423:SER:OG	1:B:425:ARG:HG2	1.89	0.73
1:B:117:LEU:HD12	1:B:364:ASP:HA	1.71	0.72
1:B:442:ILE:O	1:B:446:HIS:HE1	1.72	0.72
1:A:409:PRO:HG2	1:A:410:SER:H	1.53	0.72
1:A:160:PRO:O	1:A:161:SER:CB	2.36	0.72
1:B:313:LEU:CD1	1:B:371:ILE:HD11	2.18	0.72
1:B:395:THR:OG1	1:B:397:ASN:ND2	2.24	0.71
1:A:253:ASN:ND2	1:A:254:GLY:H	1.88	0.71
1:A:223:LYS:HG2	1:A:289:ILE:HD11	1.72	0.69
1:B:160:PRO:O	1:B:161:SER:CB	2.40	0.68
1:A:439:LYS:HE3	1:A:443:MET:CE	2.23	0.68
1:A:313:LEU:CD1	1:A:371:ILE:HD11	2.23	0.68
1:A:203:PRO:HB2	1:B:233:MET:SD	2.33	0.68
1:A:354:ILE:HD12	1:A:411:LEU:HD11	1.76	0.68
1:A:114:LEU:H	1:A:316:GLN:HE22	1.40	0.68
1:A:117:LEU:HD12	1:A:364:ASP:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LYS:HA	1:A:222:GLU:HB3	1.77	0.67
1:A:203:PRO:O	1:B:308:VAL:HG12	1.93	0.66
1:B:207:LYS:HA	1:B:222:GLU:HB3	1.77	0.66
1:B:313:LEU:HD12	1:B:371:ILE:CD1	2.23	0.66
1:A:227:GLY:H	1:B:231:THR:CG2	2.09	0.66
1:A:419:ARG:HG2	1:A:426:TRP:CE2	2.31	0.65
1:A:313:LEU:HD12	1:A:371:ILE:CD1	2.23	0.65
1:A:318:THR:HG23	1:A:319:PHE:CD2	2.32	0.64
1:A:133:HIS:CD2	1:A:133:HIS:N	2.65	0.64
1:A:152:GLN:HE22	1:A:282:LYS:HE2	1.58	0.63
1:B:178:ASN:HD22	1:B:179:ILE:N	1.96	0.63
1:A:231:THR:CG2	1:B:202:SER:HB2	2.23	0.63
1:B:237:ASN:OD1	1:B:240:ASN:HB3	1.98	0.63
1:A:144:TRP:NE1	1:A:238:MET:O	2.30	0.63
1:B:354:ILE:HD12	1:B:411:LEU:HD11	1.81	0.63
1:A:183:ASN:OD1	1:A:185:HIS:N	2.29	0.63
1:B:420:TYR:CD1	1:B:427:ARG:HG2	2.34	0.62
1:A:409:PRO:HG2	1:A:410:SER:N	2.15	0.62
2:D:19:VAL:HG13	2:D:19:VAL:O	2.00	0.62
1:B:326:ILE:HD11	1:B:358:LEU:HD21	1.81	0.62
1:A:439:LYS:HE3	1:A:443:MET:HE3	1.82	0.62
1:A:308:VAL:O	1:A:311:VAL:HG12	2.00	0.61
1:A:170:ILE:HG12	1:A:400:TRP:HB3	1.82	0.61
1:B:206:LEU:HD12	1:B:207:LYS:N	2.16	0.61
1:B:167:GLU:HG2	1:B:183:ASN:HB2	1.82	0.61
1:A:183:ASN:OD1	1:A:183:ASN:C	2.39	0.61
1:A:164:GLU:HG3	1:A:165:THR:H	1.65	0.61
1:B:235:THR:HG22	1:B:279:VAL:HB	1.82	0.61
1:B:447:GLN:HG2	1:B:447:GLN:O	1.98	0.61
1:A:240:ASN:OD1	1:A:242:GLU:HG2	2.00	0.61
1:A:298:ASN:C	1:A:298:ASN:HD22	2.04	0.60
1:A:278:ILE:HD11	1:A:372:LEU:CD2	2.31	0.60
1:B:247:PHE:HD1	3:B:20:HOH:O	1.84	0.60
1:A:307:ASN:HD21	1:B:204:LEU:HD12	1.66	0.60
1:B:419:ARG:HG2	1:B:426:TRP:CE2	2.36	0.60
1:B:425:ARG:NH2	3:B:16:HOH:O	2.32	0.60
1:A:233:MET:SD	1:B:203:PRO:HB2	2.41	0.60
2:D:19:VAL:N	3:D:27:HOH:O	2.34	0.60
1:A:178:ASN:HD22	1:A:179:ILE:N	2.00	0.60
1:A:278:ILE:HD11	1:A:372:LEU:HD23	1.82	0.60
1:A:155:ILE:HD12	1:A:155:ILE:C	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:HIS:CD2	1:B:133:HIS:N	2.71	0.58
1:B:240:ASN:C	1:B:240:ASN:HD22	2.06	0.58
1:A:116:GLU:O	1:A:117:LEU:HB2	2.01	0.58
1:B:240:ASN:C	1:B:240:ASN:ND2	2.55	0.58
1:A:178:ASN:HD22	1:A:179:ILE:H	1.51	0.58
1:B:223:LYS:HG2	1:B:289:ILE:HD11	1.86	0.58
1:A:334:LEU:HD22	1:A:351:PHE:CE1	2.39	0.57
1:B:340:ASP:OD2	2:D:22:VAL:HG13	2.04	0.57
1:B:284:ILE:HG12	1:B:302:SER:HB2	1.87	0.57
1:A:114:LEU:H	1:A:316:GLN:NE2	2.01	0.57
1:A:183:ASN:OD1	1:A:184:ALA:N	2.38	0.57
1:A:155:ILE:HD12	1:A:156:GLU:N	2.19	0.57
2:D:20:VAL:O	2:D:21:VAL:C	2.42	0.56
1:B:183:ASN:OD1	1:B:185:HIS:N	2.35	0.56
1:A:197:GLN:O	1:A:201:THR:HG23	2.06	0.56
1:A:354:ILE:HD12	1:A:411:LEU:CD1	2.36	0.56
1:B:149:GLU:H	1:B:149:GLU:CD	2.09	0.56
1:A:177:GLY:HA3	1:A:301:TYR:CE2	2.40	0.56
2:D:19:VAL:HB	3:D:28:HOH:O	2.06	0.55
1:B:178:ASN:HD22	1:B:179:ILE:H	1.52	0.55
1:A:118:SER:HB2	1:A:363:ASN:HB2	1.89	0.55
1:A:202:SER:HB3	1:B:231:THR:HG21	1.86	0.55
1:A:424:ASP:HA	1:A:427:ARG:HG3	1.88	0.55
1:B:198:LEU:HB3	1:B:287:LEU:HD13	1.89	0.55
1:B:186:GLN:HE21	1:B:186:GLN:H	1.55	0.54
1:B:238:MET:O	1:B:239:LEU:C	2.46	0.54
1:A:225:TYR:CZ	1:A:289:ILE:HD12	2.41	0.54
1:A:308:VAL:HG12	1:B:203:PRO:O	2.07	0.54
2:D:19:VAL:CG1	2:D:19:VAL:O	2.54	0.54
1:B:310:ASP:CG	1:B:371:ILE:HD12	2.27	0.54
1:A:155:ILE:HB	1:A:171:ILE:HD11	1.89	0.54
1:A:152:GLN:HE21	1:A:282:LYS:HE2	1.63	0.54
1:A:402:ALA:O	1:A:403:LEU:HD23	2.08	0.54
1:A:192:PRO:O	1:A:193:LEU:HD23	2.08	0.54
1:A:155:ILE:HD13	1:A:171:ILE:HD11	1.90	0.54
1:A:248:GLY:HA2	1:B:226:THR:OG1	2.07	0.54
1:A:439:LYS:HE3	1:A:443:MET:HE1	1.90	0.54
1:B:118:SER:HB2	1:B:363:ASN:HB2	1.90	0.54
1:B:162:ARG:N	3:B:12:HOH:O	2.39	0.54
1:A:183:ASN:HB3	1:A:186:GLN:NE2	2.23	0.53
1:B:253:ASN:ND2	1:B:254:GLY:N	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ILE:CD1	1:A:372:LEU:HD23	2.38	0.53
1:A:231:THR:CG2	1:B:227:GLY:H	2.21	0.53
1:B:439:LYS:HE3	1:B:443:MET:CE	2.38	0.53
1:A:114:LEU:N	1:A:316:GLN:HE22	2.05	0.53
1:A:332:LYS:HB2	1:A:350:THR:HG23	1.91	0.53
1:B:208:THR:O	1:B:220:GLU:HB3	2.08	0.53
1:B:159:GLU:HB2	1:B:160:PRO:CD	2.39	0.53
1:B:114:LEU:H	1:B:316:GLN:HE22	1.57	0.53
1:A:323:GLY:O	1:A:339:LEU:HB2	2.08	0.52
1:A:159:GLU:HB2	1:A:160:PRO:CD	2.40	0.52
1:A:235:THR:HG22	1:A:279:VAL:HB	1.90	0.52
1:A:283:THR:CG2	1:A:305:GLN:OE1	2.51	0.52
1:B:122:ILE:O	1:B:361:VAL:HG13	2.09	0.52
1:A:406:GLN:H	1:A:406:GLN:CD	2.13	0.52
1:B:202:SER:HB3	1:B:203:PRO:HA	1.92	0.52
1:B:116:GLU:O	1:B:117:LEU:HB2	2.08	0.52
1:B:439:LYS:HE3	1:B:443:MET:HE3	1.92	0.51
1:A:328:PRO:HB3	1:A:355:ILE:O	2.10	0.51
1:A:425:ARG:NH2	3:A:19:HOH:O	2.38	0.51
1:B:192:PRO:O	1:B:193:LEU:HD23	2.11	0.51
1:A:137:ARG:NE	1:A:322:ASP:OD2	2.36	0.51
1:B:359:PHE:HB3	1:B:372:LEU:HD13	1.92	0.51
1:B:283:THR:CG2	1:B:305:GLN:OE1	2.57	0.51
1:B:170:ILE:HG12	1:B:400:TRP:HB3	1.91	0.51
1:A:326:ILE:CD1	1:A:334:LEU:HG	2.41	0.51
1:A:350:THR:CG2	1:A:351:PHE:N	2.74	0.51
1:B:313:LEU:CD1	1:B:371:ILE:CD1	2.87	0.51
1:A:351:PHE:CD1	1:A:355:ILE:HD12	2.46	0.50
1:B:278:ILE:HD11	1:B:372:LEU:HD23	1.93	0.50
1:B:334:LEU:HD22	1:B:351:PHE:CE1	2.45	0.50
1:A:114:LEU:HB2	1:A:313:LEU:HD22	1.93	0.50
1:A:313:LEU:CD1	1:A:371:ILE:CD1	2.87	0.50
1:B:246:ALA:O	1:B:252:LYS:HA	2.10	0.50
1:A:428:VAL:CG2	1:A:429:SER:N	2.74	0.50
1:A:202:SER:HB3	1:A:203:PRO:HA	1.94	0.50
1:B:114:LEU:HB2	1:B:313:LEU:HD22	1.93	0.50
1:B:326:ILE:CD1	1:B:334:LEU:HG	2.42	0.50
1:A:315:LEU:HD12	1:A:315:LEU:N	2.26	0.49
1:B:134:ALA:HB2	1:B:144:TRP:CE2	2.47	0.49
1:B:350:THR:CG2	1:B:351:PHE:N	2.73	0.49
2:D:20:VAL:O	2:D:20:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:GLU:O	1:A:117:LEU:CB	2.60	0.49
1:A:227:GLY:H	1:B:231:THR:HG22	1.78	0.49
1:A:183:ASN:HB3	1:A:186:GLN:HE22	1.77	0.49
1:B:164:GLU:HG3	1:B:165:THR:H	1.77	0.49
1:B:426:TRP:HA	1:B:431:ILE:HD12	1.93	0.49
1:A:132:LEU:C	1:A:133:HIS:CD2	2.86	0.49
1:B:425:ARG:HG3	1:B:425:ARG:HH11	1.78	0.49
1:B:425:ARG:NH1	1:B:425:ARG:HG3	2.26	0.49
1:A:397:ASN:HD22	1:A:397:ASN:N	2.11	0.49
1:B:152:GLN:NE2	1:B:282:LYS:CE	2.70	0.49
1:A:208:THR:O	1:A:220:GLU:HB3	2.13	0.48
1:B:149:GLU:CD	1:B:149:GLU:N	2.67	0.48
1:B:162:ARG:NH2	1:B:400:TRP:HE1	2.11	0.48
1:B:161:SER:O	1:B:165:THR:HG23	2.14	0.48
1:B:294:GLY:O	1:B:296:SER:N	2.47	0.48
1:B:326:ILE:HD12	1:B:334:LEU:HG	1.95	0.48
1:A:338:ASP:HB3	1:A:345:ARG:HE	1.79	0.48
1:A:350:THR:HG22	1:A:351:PHE:N	2.28	0.48
1:B:332:LYS:HB2	1:B:350:THR:HG23	1.95	0.48
1:B:152:GLN:HE22	1:B:282:LYS:HE2	1.77	0.48
1:B:118:SER:OG	1:B:365:LEU:HD11	2.14	0.48
1:B:397:ASN:O	1:B:398:LEU:HB2	2.14	0.48
1:B:173:PRO:HG2	1:B:356:VAL:HG21	1.96	0.48
1:A:167:GLU:HG2	1:A:183:ASN:HB2	1.96	0.47
1:A:173:PRO:HG2	1:A:356:VAL:HG21	1.96	0.47
1:A:426:TRP:HA	1:A:431:ILE:HD12	1.96	0.47
1:A:406:GLN:CD	1:A:406:GLN:N	2.68	0.47
1:B:114:LEU:HD11	1:B:362:PHE:CZ	2.50	0.47
1:A:152:GLN:HE22	1:A:282:LYS:CE	2.26	0.47
1:A:284:ILE:HG12	1:A:302:SER:HB2	1.97	0.47
1:B:409:PRO:HG2	1:B:410:SER:H	1.80	0.47
1:A:240:ASN:C	1:A:240:ASN:ND2	2.67	0.47
1:B:144:TRP:NE1	1:B:238:MET:O	2.47	0.47
1:B:311:VAL:N	1:B:312:PRO:HD2	2.29	0.47
1:A:309:LEU:HB2	1:B:204:LEU:CD1	2.45	0.47
1:B:155:ILE:HB	1:B:171:ILE:HD11	1.95	0.47
1:B:202:SER:CB	1:B:203:PRO:HA	2.44	0.47
1:A:206:LEU:HD12	1:A:207:LYS:N	2.30	0.47
1:B:232:ILE:CG2	1:B:233:MET:N	2.78	0.47
1:A:338:ASP:CG	1:A:345:ARG:HH21	2.19	0.46
1:A:232:ILE:HD11	1:A:250:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:VAL:HG21	3:D:28:HOH:O	2.15	0.46
1:A:397:ASN:H	1:A:397:ASN:HD22	1.64	0.46
1:B:233:MET:HE3	1:B:279:VAL:HG22	1.98	0.46
1:A:406:GLN:OE1	1:A:406:GLN:N	2.49	0.46
1:B:225:TYR:N	1:B:225:TYR:CD1	2.83	0.46
1:A:170:ILE:HG12	1:A:400:TRP:CB	2.46	0.46
1:A:276:ASN:OD1	1:A:276:ASN:N	2.49	0.46
1:B:225:TYR:CZ	1:B:289:ILE:HD12	2.51	0.46
1:B:308:VAL:CG2	1:B:308:VAL:O	2.63	0.46
1:B:329:PHE:CG	1:B:330:ARG:N	2.84	0.46
1:A:207:LYS:HG3	1:A:222:GLU:HB3	1.97	0.46
1:A:311:VAL:N	1:A:312:PRO:HD2	2.31	0.46
1:A:409:PRO:CG	1:A:410:SER:H	2.27	0.46
1:A:424:ASP:C	1:A:426:TRP:N	2.68	0.46
2:D:19:VAL:CG2	3:D:28:HOH:O	2.64	0.46
1:B:350:THR:HG22	1:B:351:PHE:N	2.31	0.46
1:B:371:ILE:HG13	1:B:372:LEU:N	2.27	0.46
1:B:424:ASP:C	1:B:426:TRP:H	2.18	0.46
1:B:328:PRO:HB3	1:B:355:ILE:O	2.16	0.46
1:A:246:ALA:O	1:A:252:LYS:HA	2.16	0.45
1:A:367:THR:OG1	1:A:369:GLU:HG3	2.16	0.45
1:A:310:ASP:CG	1:A:371:ILE:HD12	2.36	0.45
1:B:424:ASP:C	1:B:426:TRP:N	2.69	0.45
1:A:159:GLU:OE1	1:A:162:ARG:HD2	2.16	0.45
1:B:186:GLN:HE21	1:B:186:GLN:N	2.15	0.45
1:A:144:TRP:O	1:A:144:TRP:CE3	2.69	0.45
1:B:428:VAL:CG2	1:B:429:SER:N	2.79	0.45
1:A:252:LYS:HG2	1:B:290:HIS:NE2	2.32	0.45
1:B:116:GLU:O	1:B:117:LEU:CB	2.64	0.45
1:A:310:ASP:C	1:A:312:PRO:HD2	2.37	0.45
1:A:354:ILE:HG13	1:A:355:ILE:N	2.32	0.45
1:A:324:MET:CE	1:A:324:MET:HA	2.47	0.44
1:A:365:LEU:HD23	1:A:365:LEU:HA	1.71	0.44
1:A:237:ASN:OD1	1:A:240:ASN:HB3	2.17	0.44
1:A:248:GLY:C	1:A:250:GLY:N	2.71	0.44
1:B:409:PRO:HG2	1:B:410:SER:N	2.32	0.44
1:A:308:VAL:HG11	1:B:201:THR:O	2.17	0.44
1:A:428:VAL:HG22	1:A:429:SER:N	2.32	0.44
1:B:161:SER:C	3:B:12:HOH:O	2.55	0.44
1:B:114:LEU:N	1:B:316:GLN:HE22	2.15	0.44
1:B:240:ASN:OD1	1:B:242:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:VAL:HG22	1:B:429:SER:N	2.32	0.44
2:D:22:VAL:CG2	2:D:23:VAL:N	2.81	0.44
1:A:140:GLY:O	1:A:349:PRO:HD3	2.17	0.44
1:A:176:ASP:HB3	1:A:194:SER:OG	2.17	0.44
1:B:317:ASN:HD22	1:B:317:ASN:HA	1.61	0.44
1:B:330:ARG:O	1:B:331:ASP:HB2	2.18	0.44
1:B:152:GLN:HE22	1:B:282:LYS:CE	2.31	0.44
1:B:307:ASN:HD22	1:B:308:VAL:N	2.16	0.44
1:B:147:GLU:HB3	1:B:149:GLU:OE1	2.18	0.44
1:B:159:GLU:OE1	1:B:162:ARG:HD2	2.18	0.44
1:A:152:GLN:HA	1:A:153:PRO:HD2	1.74	0.43
1:B:167:GLU:HA	1:B:182:PHE:O	2.18	0.43
1:B:306:GLN:H	1:B:306:GLN:HG2	1.60	0.43
1:A:167:GLU:HA	1:A:182:PHE:O	2.18	0.43
1:A:278:ILE:HD11	1:A:372:LEU:HB3	2.00	0.43
1:A:290:HIS:NE2	1:B:252:LYS:HG2	2.34	0.43
1:A:449:TYR:HA	3:A:21:HOH:O	2.18	0.43
1:B:236:ILE:O	1:B:277:MET:HB3	2.18	0.43
1:B:420:TYR:O	1:B:427:ARG:HD3	2.18	0.43
1:A:186:GLN:H	1:A:186:GLN:HE21	1.66	0.43
1:B:326:ILE:HG13	1:B:326:ILE:O	2.10	0.43
1:B:419:ARG:HB2	3:B:7:HOH:O	2.17	0.43
1:A:202:SER:HB2	1:B:231:THR:CG2	2.43	0.43
1:A:317:ASN:HD22	1:A:317:ASN:HA	1.61	0.43
1:A:351:PHE:CD1	1:A:355:ILE:CD1	3.01	0.43
1:B:390:VAL:CG2	1:B:391:TYR:N	2.80	0.43
1:B:176:ASP:HB3	1:B:194:SER:OG	2.19	0.43
1:A:120:SER:HB3	1:A:361:VAL:O	2.19	0.43
1:A:198:LEU:HB3	1:A:287:LEU:HD13	1.99	0.43
1:A:253:ASN:ND2	1:A:254:GLY:N	2.61	0.43
1:A:445:VAL:HG23	1:A:446:HIS:O	2.19	0.43
1:A:298:ASN:C	1:A:298:ASN:ND2	2.72	0.43
1:A:310:ASP:O	1:A:313:LEU:HB2	2.18	0.43
1:A:389:LYS:HG2	1:A:389:LYS:H	1.66	0.43
1:A:356:VAL:HG23	1:A:408:PHE:CZ	2.53	0.43
1:B:164:GLU:HG3	1:B:165:THR:N	2.34	0.43
1:B:351:PHE:CD1	1:B:355:ILE:HD12	2.54	0.43
1:B:390:VAL:HG21	1:B:402:ALA:HB1	2.01	0.42
1:A:358:LEU:HA	1:A:358:LEU:HD12	1.64	0.42
1:B:310:ASP:O	1:B:313:LEU:HB2	2.19	0.42
1:B:397:ASN:HD22	1:B:397:ASN:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:VAL:HG13	2:D:21:VAL:O	2.19	0.42
1:A:448:ILE:HG13	1:A:448:ILE:O	2.18	0.42
1:B:323:GLY:O	1:B:339:LEU:HB2	2.20	0.42
1:A:152:GLN:NE2	1:A:152:GLN:N	2.67	0.42
2:D:20:VAL:HG22	2:D:20:VAL:O	2.19	0.42
1:A:155:ILE:HD13	1:A:171:ILE:CD1	2.50	0.42
1:A:420:TYR:CD1	1:A:427:ARG:HG2	2.55	0.42
1:B:194:SER:HB3	1:B:197:GLN:HB3	2.02	0.42
1:A:202:SER:CB	1:A:203:PRO:HA	2.49	0.42
1:A:326:ILE:HD12	1:A:334:LEU:HG	2.01	0.42
1:B:278:ILE:CD1	1:B:372:LEU:HD23	2.49	0.42
1:B:438:PHE:HE1	1:B:442:ILE:HD13	1.85	0.42
1:A:122:ILE:O	1:A:361:VAL:HG13	2.19	0.42
1:B:308:VAL:O	1:B:311:VAL:HG12	2.20	0.41
1:B:354:ILE:HD12	1:B:411:LEU:CD1	2.49	0.41
1:A:230:ARG:HH21	1:A:230:ARG:HG3	1.85	0.41
1:B:390:VAL:HG23	1:B:391:TYR:N	2.35	0.41
1:B:311:VAL:H	1:B:311:VAL:HG12	1.43	0.41
1:A:240:ASN:HD22	1:A:240:ASN:C	2.23	0.41
1:A:420:TYR:CZ	1:A:427:ARG:HD2	2.54	0.41
1:A:149:GLU:H	1:A:149:GLU:CD	2.24	0.41
1:A:294:GLY:O	1:A:296:SER:N	2.49	0.41
1:A:313:LEU:HD23	1:A:313:LEU:HA	1.87	0.41
1:A:278:ILE:CG1	1:A:372:LEU:HD23	2.51	0.41
1:A:409:PRO:CG	1:A:410:SER:N	2.77	0.41
1:A:196:ARG:HA	1:A:285:PHE:CE2	2.56	0.41
1:B:170:ILE:HG12	1:B:400:TRP:CB	2.51	0.41
1:B:307:ASN:ND2	1:B:307:ASN:C	2.74	0.41
1:B:342:ARG:HD2	1:B:342:ARG:HA	1.92	0.41
1:B:443:MET:HG2	1:B:444:GLY:N	2.34	0.41
1:B:207:LYS:HG3	1:B:222:GLU:HB3	2.03	0.41
1:B:140:GLY:O	1:B:349:PRO:HD3	2.20	0.41
1:A:231:THR:HG22	1:B:226:THR:HA	2.02	0.41
1:A:351:PHE:CG	1:A:355:ILE:HD11	2.56	0.41
1:B:324:MET:O	1:B:325:CYS:HB2	2.20	0.41
1:A:232:ILE:CG2	1:A:233:MET:N	2.83	0.41
1:B:169:LEU:C	1:B:170:ILE:HG13	2.40	0.41
1:A:247:PHE:CZ	1:A:253:ASN:O	2.74	0.41
1:A:329:PHE:CG	1:A:330:ARG:N	2.89	0.41
1:A:317:ASN:O	1:A:376:PRO:HB3	2.20	0.41
1:A:247:PHE:HE1	1:B:292:TYR:HH	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:TYR:CE2	1:A:289:ILE:HD12	2.55	0.41
1:A:326:ILE:CG1	1:A:358:LEU:HD21	2.51	0.41
1:B:420:TYR:CZ	1:B:427:ARG:HD2	2.56	0.41
1:B:309:LEU:O	1:B:312:PRO:HD2	2.20	0.40
1:B:375:HIS:ND1	1:B:376:PRO:HD2	2.36	0.40
1:A:275:GLU:HB3	1:A:276:ASN:H	1.70	0.40
1:B:365:LEU:HD23	1:B:365:LEU:HA	1.71	0.40
1:A:113:SER:C	1:A:115:ASN:N	2.73	0.40
1:A:223:LYS:HE3	1:A:291:SER:OG	2.22	0.40
1:A:390:VAL:HG21	1:A:402:ALA:HB1	2.03	0.40
1:B:144:TRP:O	1:B:144:TRP:CE3	2.74	0.40
1:B:278:ILE:HD11	1:B:372:LEU:HB3	2.03	0.40
1:B:233:MET:CE	1:B:279:VAL:HG22	2.51	0.40
2:D:22:VAL:HG22	2:D:23:VAL:N	2.36	0.40
1:A:315:LEU:H	1:A:315:LEU:CD1	2.34	0.40
1:A:311:VAL:HG13	1:A:312:PRO:HD3	2.02	0.40
1:A:329:PHE:HB2	1:A:335:LEU:HB3	2.03	0.40
1:B:152:GLN:NE2	1:B:152:GLN:N	2.70	0.40
1:B:372:LEU:HD12	1:B:372:LEU:C	2.42	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	293/339 (86%)	243 (83%)	38 (13%)	12 (4%)	3 14
1	B	293/339 (86%)	245 (84%)	34 (12%)	14 (5%)	2 12
2	D	6/8 (75%)	1 (17%)	3 (50%)	2 (33%)	0 0
All	All	592/686 (86%)	489 (83%)	75 (13%)	28 (5%)	2 12

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	161	SER
1	A	249	PRO
1	A	295	ALA
1	A	325	CYS
1	B	117	LEU
1	B	161	SER
1	B	249	PRO
1	B	295	ALA
1	B	325	CYS
2	D	21	VAL
1	A	137	ARG
1	A	324	MET
1	A	366	ARG
1	B	366	ARG
2	D	24	VAL
1	A	228	SER
1	A	303	THR
1	A	342	ARG
1	B	228	SER
1	B	342	ARG
1	B	430	SER
1	B	250	GLY
1	B	322	ASP
1	B	176	ASP
1	B	251	SER
1	B	177	GLY
1	A	250	GLY

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	269/304 (88%)	211 (78%)	58 (22%)	1 4
1	B	269/304 (88%)	207 (77%)	62 (23%)	1 3
2	D	8/8 (100%)	5 (62%)	3 (38%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	546/616 (89%)	423 (78%)	123 (22%)	1 3

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	113	SER
1	A	117	LEU
1	A	133	HIS
1	A	141	HIS
1	A	152	GLN
1	A	154	LEU
1	A	155	ILE
1	A	165	THR
1	A	171	ILE
1	A	178	ASN
1	A	186	GLN
1	A	194	SER
1	A	202	SER
1	A	223	LYS
1	A	228	SER
1	A	229	MET
1	A	231	THR
1	A	233	MET
1	A	240	ASN
1	A	249	PRO
1	A	253	ASN
1	A	275	GLU
1	A	277	MET
1	A	283	THR
1	A	289	ILE
1	A	293	ASP
1	A	296	SER
1	A	298	ASN
1	A	299	VAL
1	A	300	THR
1	A	307	ASN
1	A	308	VAL
1	A	317	ASN
1	A	320	SER
1	A	324	MET
1	A	325	CYS

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Mol	Chain	Res	Type
1	A	326	ILE
1	A	330	ARG
1	A	332	LYS
1	A	334	LEU
1	A	338	ASP
1	A	341	PHE
1	A	354	ILE
1	A	361	VAL
1	A	366	ARG
1	A	371	ILE
1	A	373	VAL
1	A	377	PHE
1	A	388	ASN
1	A	390	VAL
1	A	397	ASN
1	A	406	GLN
1	A	413	GLU
1	A	419	ARG
1	A	424	ASP
1	A	433	GLU
1	A	445	VAL
1	B	111	ASN
1	B	117	LEU
1	B	133	HIS
1	B	141	HIS
1	B	149	GLU
1	B	152	GLN
1	B	154	LEU
1	B	155	ILE
1	B	165	THR
1	B	171	ILE
1	B	178	ASN
1	B	183	ASN
1	B	186	GLN
1	B	201	THR
1	B	202	SER
1	B	206	LEU
1	B	223	LYS
1	B	228	SER
1	B	229	MET
1	B	231	THR
1	B	233	MET

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Mol	Chain	Res	Type
1	B	240	ASN
1	B	275	GLU
1	B	277	MET
1	B	283	THR
1	B	289	ILE
1	B	293	ASP
1	B	296	SER
1	B	298	ASN
1	B	299	VAL
1	B	300	THR
1	B	307	ASN
1	B	308	VAL
1	B	311	VAL
1	B	317	ASN
1	B	320	SER
1	B	324	MET
1	B	326	ILE
1	B	330	ARG
1	B	332	LYS
1	B	334	LEU
1	B	338	ASP
1	B	341	PHE
1	B	354	ILE
1	B	361	VAL
1	B	366	ARG
1	B	371	ILE
1	B	372	LEU
1	B	373	VAL
1	B	377	PHE
1	B	388	ASN
1	B	390	VAL
1	B	397	ASN
1	B	399	SER
1	B	411	LEU
1	B	413	GLU
1	B	419	ARG
1	B	424	ASP
1	B	429	SER
1	B	433	GLU
1	B	438	PHE
1	B	445	VAL
2	D	20	VAL

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Mol	Chain	Res	Type
2	D	22	VAL
2	D	24	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	152	GLN
1	A	158	GLN
1	A	178	ASN
1	A	186	GLN
1	A	253	ASN
1	A	298	ASN
1	A	307	ASN
1	A	316	GLN
1	A	317	ASN
1	A	363	ASN
1	A	388	ASN
1	A	394	GLN
1	A	397	ASN
1	A	446	HIS
1	B	150	ASN
1	B	152	GLN
1	B	158	GLN
1	B	178	ASN
1	B	186	GLN
1	B	189	GLN
1	B	253	ASN
1	B	298	ASN
1	B	307	ASN
1	B	316	GLN
1	B	317	ASN
1	B	363	ASN
1	B	388	ASN
1	B	394	GLN
1	B	397	ASN
1	B	446	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	301/339 (88%)	0.35	22 (7%) 15 7	13, 37, 75, 94	0
1	B	301/339 (88%)	0.33	14 (4%) 31 18	13, 37, 75, 94	0
2	D	8/8 (100%)	0.59	0 100 100	48, 50, 52, 52	0
All	All	610/686 (88%)	0.34	36 (5%) 22 12	13, 37, 77, 94	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	ASN	6.8
1	B	250	GLY	5.3
1	A	114	LEU	4.9
1	B	254	GLY	4.7
1	A	292	TYR	4.3
1	A	209	ASN	4.3
1	A	253	ASN	4.0
1	B	253	ASN	3.9
1	A	365	LEU	3.8
1	A	111	ASN	3.8
1	A	251	SER	3.8
1	B	292	TYR	3.7
1	B	239	LEU	3.7
1	A	449	TYR	3.5
1	A	239	LEU	3.4
1	A	117	LEU	3.3
1	A	208	THR	3.3
1	B	251	SER	3.1
1	A	112	ARG	3.1
1	A	379	PRO	3.1
1	A	247	PHE	3.0
1	A	366	ARG	3.0
1	A	166	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	379	PRO	2.8
1	A	364	ASP	2.8
1	B	367	THR	2.7
1	B	206	LEU	2.7
1	A	254	GLY	2.7
1	B	341	PHE	2.6
1	A	371	ILE	2.6
1	B	449	TYR	2.4
1	A	115	ASN	2.3
1	B	205	HIS	2.2
1	A	321	LYS	2.2
1	B	166	TYR	2.1
1	A	243	ILE	2.1

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.