Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:09 PM GMT

PDB ID	:	4NZS
Title	:	Crystal structure of beta-ketothiolase BktB B from Ralstonia eutropha H16
Authors	:	Kim, E.J.; Son, H.; Kim, S.; Kim, K.J.
Deposited on	:	2013-12-12
Resolution	:	2.29 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

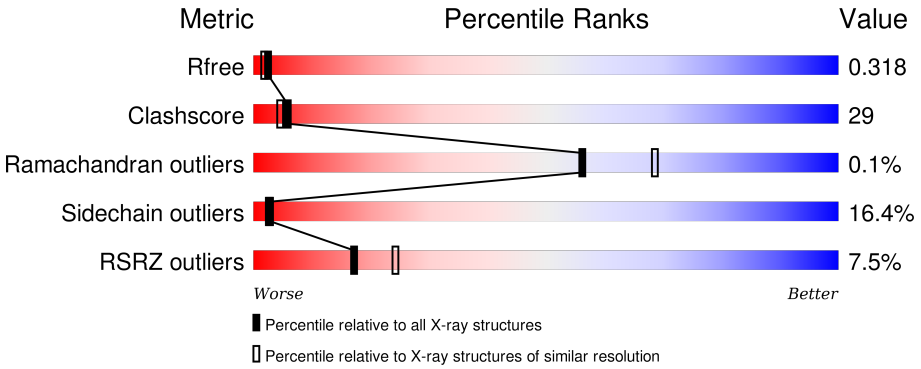
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.29 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	399	4% 57% 36% 6%
1	B	399	11% 51% 36% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5732 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 Beta-ketothiolase BktB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			2859	1777	526	542	14			
1	B	393	Total	C	N	O	S	0	0	0
			2859	1777	526	542	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP Q0KBP1
A	-3	HIS	-	EXPRESSION TAG	UNP Q0KBP1
A	-2	HIS	-	EXPRESSION TAG	UNP Q0KBP1
A	-1	HIS	-	EXPRESSION TAG	UNP Q0KBP1
A	0	HIS	-	EXPRESSION TAG	UNP Q0KBP1
A	1	HIS	-	EXPRESSION TAG	UNP Q0KBP1
B	-4	HIS	-	EXPRESSION TAG	UNP Q0KBP1
B	-3	HIS	-	EXPRESSION TAG	UNP Q0KBP1
B	-2	HIS	-	EXPRESSION TAG	UNP Q0KBP1
B	-1	HIS	-	EXPRESSION TAG	UNP Q0KBP1
B	0	HIS	-	EXPRESSION TAG	UNP Q0KBP1
B	1	HIS	-	EXPRESSION TAG	UNP Q0KBP1

- Molecule 2 is water.

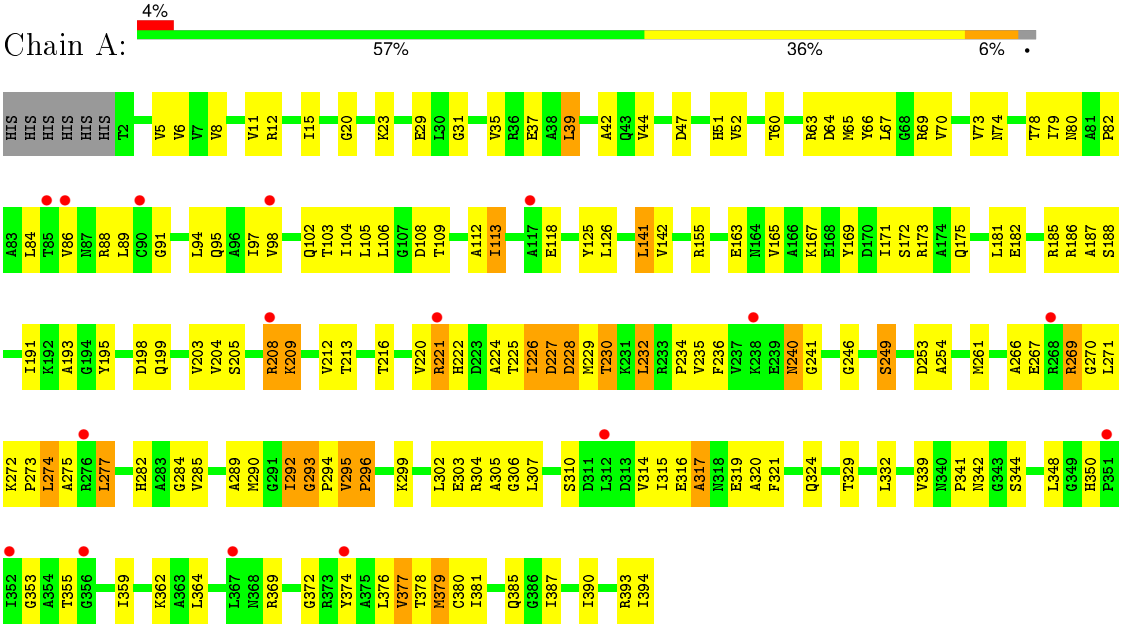
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	11	Total	O	0	0
			11	11		

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 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.

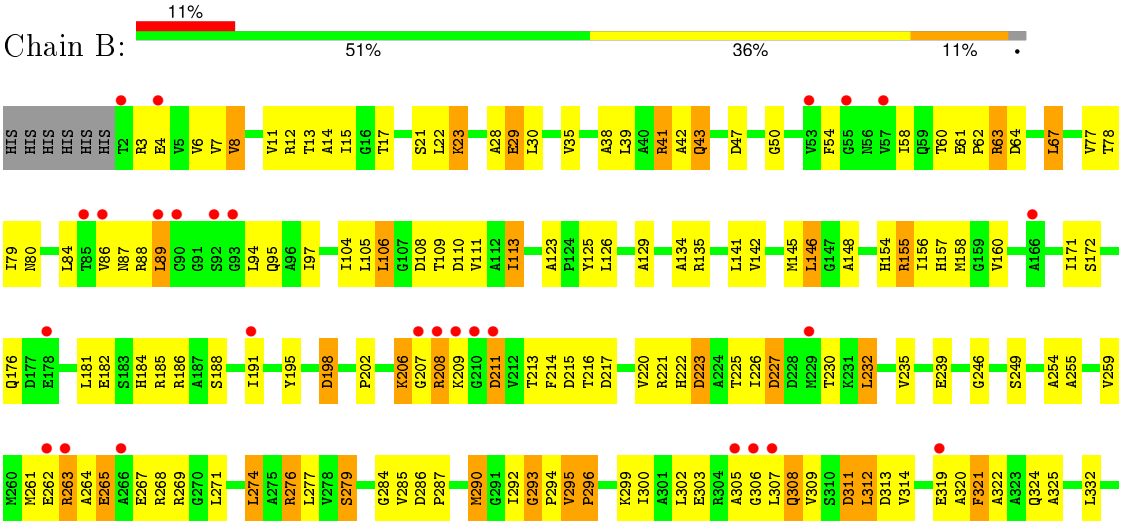
- Molecule 1: Beta-ketothiolase BktB

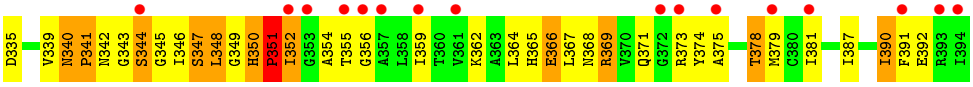
Chain A:



- Molecule 1: Beta-ketothiolase BktB

Chain B:




D335
V339
N340
P341
N342
G343
S344
G345
I346
S347
I348
G349
H350
P351
I352
G353
A354
T355
G356
A357
L358
I359
T360
V361
K362
A363
L364
H365
E366
L367
N368
R369
V370
Q371
G372
R373
Y374
A375
T378
M379
C380
I381
I387
I390
F391
E392
R393
I394

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	106.95Å 107.24Å 144.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.74 – 2.29 35.74 – 2.29	Depositor EDS
% Data completeness (in resolution range)	85.4 (35.74-2.29) 85.5 (35.74-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.253 , 0.319 0.251 , 0.318	Depositor DCC
R_{free} test set	1574 reflections (5.18%)	DCC
Wilson B-factor (Å^2)	41.7	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 53.0	EDS
Estimated twinning fraction	0.042 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 32063 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5732	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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, 0.375 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	0.74	0/2899	0.93	4/3930 (0.1%)
1	B	0.71	2/2899 (0.1%)	0.87	6/3930 (0.2%)
All	All	0.72	2/5798 (0.0%)	0.90	10/7860 (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
1	A	0	2
1	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	341	PRO	N-CD	5.29	1.55	1.47
1	B	351	PRO	N-CD	5.04	1.54	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	295	VAL	C-N-CD	6.99	143.09	128.40
1	B	63	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	296	PRO	CA-N-CD	-6.30	102.68	111.50
1	B	293	GLY	C-N-CD	6.17	141.35	128.40
1	A	293	GLY	C-N-CD	6.03	141.06	128.40
1	A	296	PRO	CA-N-CD	-5.81	103.36	111.50
1	A	63	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	350	HIS	C-N-CD	5.61	140.19	128.40
1	B	295	VAL	C-N-CD	5.55	140.06	128.40
1	B	340	ASN	C-N-CD	5.49	139.94	128.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	310	SER	Peptide
1	A	317	ALA	Peptide
1	B	351	PRO	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	2859	0	2896	145	0
1	B	2859	0	2896	207	0
2	A	3	0	0	0	0
2	B	11	0	0	2	0
All	All	5732	0	5792	332	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 29.

All (332) 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:181:LEU:CD2	1:B:226:ILE:HG13	1.74	1.18
1:B:181:LEU:HD23	1:B:226:ILE:HG13	1.24	1.09
1:B:308:GLN:OE1	1:B:309:VAL:N	1.90	1.04
1:B:314:VAL:CG1	1:B:367:LEU:HD13	1.91	1.00
1:B:295:VAL:HG13	1:B:332:LEU:HD21	1.42	0.97
1:B:176:GLN:HB2	1:B:322:ALA:CB	1.97	0.95
1:B:312:LEU:HD23	1:B:374:TYR:C	1.87	0.95
1:B:263:ARG:HD3	1:B:267:GLU:OE1	1.70	0.92
1:A:319:GLU:CD	1:A:344:SER:HB3	1.90	0.91
1:B:314:VAL:HG12	1:B:367:LEU:CD1	2.01	0.90
1:B:320:ALA:C	1:B:321:PHE:CD1	2.45	0.89
1:B:314:VAL:CG1	1:B:367:LEU:CD1	2.51	0.89
1:A:42:ALA:HB3	1:A:44:VAL:HG12	1.55	0.88
1:B:176:GLN:HB2	1:B:322:ALA:HB3	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ASP:O	1:B:230:THR:HG22	1.74	0.87
1:A:91:GLY:HA2	1:A:379:MET:CE	2.04	0.87
1:A:292:ILE:O	1:A:296:PRO:HD2	1.73	0.86
1:B:319:GLU:HG2	1:B:325:ALA:CB	2.07	0.84
1:B:319:GLU:OE2	1:B:346:ILE:HD12	1.77	0.84
1:B:292:ILE:O	1:B:296:PRO:HD2	1.77	0.84
1:B:206:LYS:HA	1:B:211:ASP:HB2	1.58	0.83
1:B:226:ILE:H	1:B:226:ILE:HD12	1.43	0.82
1:A:285:VAL:CG1	1:A:296:PRO:HG3	2.09	0.82
1:B:306:GLY:O	1:B:307:LEU:HD22	1.79	0.82
1:A:316:GLU:O	1:A:377:VAL:HA	1.81	0.81
1:B:263:ARG:O	1:B:267:GLU:HG2	1.81	0.81
1:B:373:ARG:O	1:B:392:GLU:HA	1.81	0.81
1:B:314:VAL:HG11	1:B:367:LEU:HD13	1.62	0.80
1:B:181:LEU:CD2	1:B:226:ILE:CG1	2.57	0.80
1:B:314:VAL:HG12	1:B:367:LEU:HD13	1.63	0.79
1:B:312:LEU:HD23	1:B:375:ALA:N	1.98	0.79
1:A:42:ALA:HB3	1:A:44:VAL:CG1	2.13	0.79
1:A:91:GLY:HA2	1:A:379:MET:HE2	1.63	0.79
1:A:369:ARG:HH21	1:A:369:ARG:HG2	1.48	0.78
1:B:188:SER:HB2	1:B:222:HIS:HD2	1.49	0.77
1:B:184:HIS:CD2	1:B:221:ARG:H	2.03	0.77
1:A:66:TYR:CE2	1:B:89:LEU:HD22	2.20	0.76
1:A:369:ARG:NH2	1:A:369:ARG:HG2	2.01	0.76
1:B:181:LEU:HD23	1:B:226:ILE:CG1	2.10	0.75
1:B:176:GLN:CB	1:B:322:ALA:HB1	2.17	0.74
1:B:176:GLN:CB	1:B:322:ALA:CB	2.65	0.74
1:A:182:GLU:OE2	1:A:186:ARG:NE	2.20	0.74
1:B:294:PRO:HB3	1:B:378:THR:OG1	1.87	0.73
1:B:4:GLU:HB3	1:B:263:ARG:HB2	1.71	0.71
1:B:171:ILE:HG22	1:B:176:GLN:HE21	1.55	0.70
1:B:312:LEU:HG	1:B:374:TYR:HB3	1.73	0.70
1:B:8:VAL:HG11	1:B:271:LEU:HD13	1.73	0.70
1:A:84:LEU:HD11	1:B:86:VAL:HG13	1.72	0.69
1:A:106:LEU:CD2	1:B:105:LEU:HD23	2.22	0.69
1:B:320:ALA:HB1	1:B:321:PHE:CE1	2.28	0.69
1:A:266:ALA:O	1:A:270:GLY:N	2.26	0.69
1:A:285:VAL:HG11	1:A:296:PRO:HG3	1.75	0.69
1:B:186:ARG:NH1	1:B:340:ASN:O	2.26	0.69
1:B:320:ALA:CB	1:B:321:PHE:HD1	2.06	0.68
1:B:41:ARG:NH1	1:B:198:ASP:O	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:HIS:HD2	1:B:221:ARG:H	1.39	0.68
1:A:91:GLY:HA2	1:A:379:MET:HE3	1.76	0.68
1:B:312:LEU:HD23	1:B:374:TYR:O	1.94	0.67
1:A:94:LEU:HB2	1:A:379:MET:HE1	1.76	0.67
1:A:381:ILE:HB	1:A:385:GLN:HB2	1.76	0.67
1:B:314:VAL:HG11	1:B:367:LEU:CD1	2.21	0.66
1:B:320:ALA:O	1:B:321:PHE:CD1	2.49	0.66
1:B:305:ALA:O	1:B:307:LEU:HD23	1.96	0.66
1:A:319:GLU:CG	1:A:344:SER:HB3	2.25	0.66
1:A:94:LEU:HD23	1:A:387:ILE:HG23	1.78	0.65
1:B:206:LYS:CA	1:B:211:ASP:HB2	2.26	0.65
1:B:312:LEU:CD2	1:B:375:ALA:N	2.59	0.65
1:B:320:ALA:C	1:B:321:PHE:HD1	1.99	0.64
1:A:226:ILE:O	1:A:230:THR:HG22	1.96	0.64
1:B:60:THR:HB	1:B:64:ASP:OD2	1.96	0.64
1:B:320:ALA:CB	1:B:321:PHE:CD1	2.80	0.64
1:B:342:ASN:HD21	1:B:366:GLU:HG3	1.63	0.64
1:B:320:ALA:HB1	1:B:321:PHE:CD1	2.34	0.63
1:A:195:TYR:CE2	1:A:369:ARG:NE	2.66	0.63
1:B:319:GLU:HG2	1:B:325:ALA:HB1	1.78	0.62
1:B:350:HIS:CE1	1:B:352:ILE:HG22	2.35	0.62
1:B:311:ASP:N	1:B:311:ASP:OD1	2.30	0.62
1:B:306:GLY:C	1:B:307:LEU:HD22	2.19	0.62
1:B:182:GLU:O	1:B:186:ARG:HG3	2.00	0.62
1:A:191:ILE:CD1	1:A:220:VAL:HG11	2.29	0.62
1:B:302:LEU:O	1:B:306:GLY:N	2.33	0.62
1:B:319:GLU:HB2	1:B:344:SER:HB3	1.82	0.62
1:B:279:SER:OG	1:B:390:ILE:HD11	1.99	0.62
1:B:64:ASP:O	1:B:67:LEU:HB2	2.00	0.62
1:B:186:ARG:NH1	1:B:341:PRO:HA	2.14	0.61
1:B:186:ARG:HH11	1:B:341:PRO:HA	1.66	0.61
1:B:335:ASP:O	1:B:339:VAL:HG23	2.00	0.60
1:B:292:ILE:C	1:B:292:ILE:HD12	2.22	0.60
1:A:193:ALA:HB1	1:A:195:TYR:CE1	2.37	0.60
1:B:11:VAL:HG12	1:B:38:ALA:HB2	1.84	0.60
1:A:188:SER:HB2	1:A:222:HIS:ND1	2.17	0.59
1:A:42:ALA:CB	1:A:44:VAL:HG12	2.32	0.59
1:A:225:THR:HB	1:A:228:ASP:HB2	1.84	0.59
1:B:345:GLY:HA2	1:B:349:GLY:O	2.02	0.59
1:A:249:SER:HB2	1:A:320:ALA:O	2.03	0.58
1:B:249:SER:HB2	1:B:320:ALA:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:HIS:O	1:B:155:ARG:HG2	2.04	0.57
1:B:207:GLY:HA3	2:B:408:HOH:O	2.04	0.57
1:B:312:LEU:HD23	1:B:375:ALA:CA	2.35	0.57
1:A:5:VAL:HG23	1:A:277:LEU:HB2	1.85	0.57
1:A:285:VAL:HG12	1:A:296:PRO:HG3	1.86	0.56
1:B:176:GLN:CB	1:B:322:ALA:HB3	2.32	0.56
1:B:350:HIS:HD2	1:B:355:THR:OG1	1.88	0.56
1:B:184:HIS:HA	1:B:347:SER:OG	2.05	0.56
1:B:302:LEU:HB3	1:B:307:LEU:O	2.05	0.56
1:A:305:ALA:HB2	1:A:390:ILE:HD11	1.85	0.56
1:B:7:VAL:HG21	1:B:364:LEU:HD21	1.88	0.56
1:B:191:ILE:HD11	1:B:220:VAL:HG21	1.88	0.56
1:B:188:SER:CB	1:B:222:HIS:HD2	2.19	0.55
1:A:284:GLY:O	1:B:80:ASN:HA	2.05	0.55
1:B:321:PHE:N	1:B:321:PHE:CD1	2.74	0.55
1:B:321:PHE:H	1:B:324:GLN:HE21	1.53	0.55
1:A:369:ARG:HH21	1:A:369:ARG:CG	2.14	0.55
1:B:274:LEU:H	1:B:274:LEU:HD12	1.72	0.55
1:B:312:LEU:CD2	1:B:375:ALA:CA	2.84	0.55
1:B:172:SER:O	1:B:176:GLN:HG2	2.07	0.55
1:B:94:LEU:HB2	1:B:379:MET:CE	2.37	0.55
1:B:181:LEU:HD21	1:B:226:ILE:N	2.21	0.55
1:B:319:GLU:HG2	1:B:325:ALA:HB2	1.90	0.54
1:A:294:PRO:HD3	1:A:380:CYS:HB3	1.90	0.54
1:B:14:ALA:HB3	1:B:214:PHE:CE2	2.43	0.54
1:A:306:GLY:C	1:A:307:LEU:HD23	2.28	0.54
1:A:321:PHE:O	1:A:324:GLN:HG3	2.07	0.54
1:B:202:PRO:HB3	1:B:215:ASP:HB3	1.90	0.54
1:A:66:TYR:CE2	1:B:89:LEU:CD2	2.91	0.54
1:B:104:ILE:HA	1:B:109:THR:O	2.08	0.53
1:A:126:LEU:HD23	1:B:126:LEU:HD22	1.88	0.53
1:A:69:ARG:O	1:A:73:VAL:HG23	2.08	0.53
1:B:232:LEU:HD13	1:B:246:GLY:HA3	1.89	0.53
1:A:296:PRO:HA	1:A:299:LYS:HE3	1.91	0.53
1:B:171:ILE:CG2	1:B:176:GLN:HE21	2.20	0.53
1:B:254:ALA:HB3	1:B:351:PRO:HG3	1.89	0.53
1:A:209:LYS:HD2	1:A:209:LYS:O	2.09	0.53
1:A:186:ARG:NH1	1:A:339:VAL:O	2.42	0.53
1:A:66:TYR:CZ	1:B:89:LEU:HD22	2.44	0.52
1:A:86:VAL:HG13	1:B:84:LEU:HD11	1.90	0.52
1:A:88:ARG:O	1:A:381:ILE:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:OE1	1:A:163:GLU:HA	2.08	0.52
1:B:249:SER:OG	1:B:350:HIS:HB2	2.09	0.52
1:B:350:HIS:NE2	1:B:352:ILE:HG22	2.24	0.52
1:B:186:ARG:HD2	1:B:341:PRO:O	2.10	0.52
1:B:351:PRO:HG2	1:B:351:PRO:O	2.10	0.52
1:A:118:GLU:OE2	1:A:353:GLY:N	2.42	0.52
1:A:47:ASP:HA	1:A:78:THR:HG23	1.92	0.52
1:B:12:ARG:NH1	1:B:13:THR:O	2.43	0.52
1:B:181:LEU:CD2	1:B:226:ILE:N	2.73	0.52
1:A:293:GLY:N	1:A:294:PRO:CD	2.73	0.52
1:A:52:VAL:HG13	1:A:113:ILE:HG22	1.92	0.51
1:B:295:VAL:HG12	1:B:299:LYS:HE2	1.92	0.51
1:B:195:TYR:CE1	1:B:369:ARG:HD2	2.44	0.51
1:A:267:GLU:O	1:A:270:GLY:N	2.43	0.51
1:A:104:ILE:HD11	1:A:112:ALA:HB3	1.90	0.51
1:B:15:ILE:CD1	1:B:348:LEU:HB3	2.41	0.51
1:B:217:ASP:O	1:B:220:VAL:HG23	2.10	0.51
1:B:232:LEU:CD1	1:B:246:GLY:HA3	2.40	0.51
1:A:227:ASP:HA	1:A:230:THR:HG23	1.93	0.51
1:B:188:SER:HB2	1:B:222:HIS:CD2	2.38	0.51
1:B:355:THR:O	1:B:359:ILE:HG12	2.10	0.51
1:B:188:SER:CB	1:B:222:HIS:CD2	2.94	0.51
1:A:82:PRO:HD3	1:B:284:GLY:N	2.26	0.51
1:A:8:VAL:O	1:A:274:LEU:HD21	2.11	0.51
1:B:296:PRO:O	1:B:300:ILE:HD12	2.11	0.51
1:B:22:LEU:O	1:B:23:LYS:C	2.49	0.51
1:A:274:LEU:HD23	1:A:274:LEU:N	2.26	0.50
1:A:94:LEU:CB	1:A:379:MET:HE1	2.41	0.50
1:A:285:VAL:HG11	1:A:296:PRO:CG	2.41	0.50
1:A:125:TYR:HA	1:A:142:VAL:O	2.11	0.50
1:B:217:ASP:CB	1:B:348:LEU:HD23	2.42	0.50
1:A:359:ILE:HA	1:A:362:LYS:HD3	1.93	0.50
1:B:262:GLU:O	1:B:263:ARG:C	2.49	0.50
1:A:64:ASP:HA	1:A:67:LEU:HB2	1.94	0.50
1:B:308:GLN:OE1	1:B:309:VAL:HG23	2.12	0.50
1:B:308:GLN:CD	1:B:309:VAL:H	2.01	0.50
1:B:249:SER:OG	1:B:350:HIS:CB	2.60	0.50
1:A:69:ARG:NH2	1:B:285:VAL:O	2.45	0.50
1:A:70:VAL:O	1:A:74:ASN:HB2	2.12	0.49
1:B:42:ALA:O	1:B:43:GLN:HB2	2.12	0.49
1:B:345:GLY:O	1:B:349:GLY:HA2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:GLY:HA2	1:B:349:GLY:C	2.32	0.49
1:A:204:VAL:O	1:A:204:VAL:HG23	2.12	0.49
1:A:169:TYR:HB2	1:A:171:ILE:CD1	2.41	0.49
1:B:157:HIS:ND1	1:B:158:MET:N	2.60	0.49
1:B:50:GLY:N	1:B:111:VAL:O	2.34	0.49
1:B:362:LYS:O	1:B:366:GLU:HB2	2.11	0.49
1:A:78:THR:HB	1:A:80:ASN:H	1.77	0.49
1:B:367:LEU:HD13	1:B:375:ALA:HB2	1.94	0.49
1:B:7:VAL:O	1:B:274:LEU:HD12	2.11	0.49
1:B:176:GLN:CA	1:B:322:ALA:HB1	2.43	0.49
1:B:290:MET:HB2	1:B:381:ILE:O	2.13	0.49
1:B:94:LEU:HB2	1:B:379:MET:HE1	1.96	0.48
1:B:123:ALA:CB	1:B:145:MET:HB2	2.44	0.48
1:A:229:MET:HA	1:A:232:LEU:HD22	1.95	0.48
1:A:8:VAL:HG11	1:A:271:LEU:HD13	1.96	0.48
1:A:216:THR:HG23	1:A:216:THR:O	2.14	0.48
1:B:181:LEU:HD22	1:B:226:ILE:HA	1.96	0.48
1:A:66:TYR:OH	1:B:148:ALA:O	2.20	0.48
1:A:186:ARG:HD3	1:A:341:PRO:HA	1.96	0.48
1:B:186:ARG:HH11	1:B:341:PRO:CA	2.26	0.48
1:A:60:THR:HB	1:A:64:ASP:OD2	2.14	0.48
1:B:320:ALA:HB1	1:B:321:PHE:HE1	1.77	0.48
1:B:293:GLY:N	1:B:294:PRO:CD	2.77	0.48
1:A:350:HIS:HD2	1:A:355:THR:OG1	1.97	0.48
1:B:6:VAL:HG12	1:B:276:ARG:CB	2.43	0.48
1:A:181:LEU:CD1	1:A:224:ALA:HB1	2.44	0.47
1:A:307:LEU:HD13	1:A:374:TYR:CE2	2.48	0.47
1:A:6:VAL:HG22	1:A:261:MET:O	2.14	0.47
1:B:176:GLN:HB2	1:B:322:ALA:HB1	1.77	0.47
1:A:39:LEU:HD12	1:A:44:VAL:HG13	1.95	0.47
1:B:312:LEU:CD2	1:B:374:TYR:C	2.73	0.47
1:B:222:HIS:HB3	1:B:223:ASP:OD1	2.14	0.47
1:B:223:ASP:OD1	1:B:223:ASP:N	2.47	0.47
1:A:187:ALA:HA	1:A:342:ASN:O	2.14	0.47
1:A:169:TYR:N	1:A:169:TYR:CD1	2.82	0.47
1:B:125:TYR:HA	1:B:142:VAL:O	2.15	0.47
1:A:304:ARG:NH1	1:B:108:ASP:OD1	2.48	0.47
1:B:35:VAL:HG22	1:B:113:ILE:HD11	1.97	0.47
1:B:86:VAL:HG11	1:B:95:GLN:HG2	1.97	0.47
1:A:31:GLY:O	1:A:35:VAL:HG23	2.15	0.47
1:A:274:LEU:O	1:A:275:ALA:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ILE:HD12	1:B:160:VAL:HB	1.96	0.47
1:A:103:THR:HB	1:A:108:ASP:HB2	1.95	0.46
1:B:181:LEU:CD2	1:B:226:ILE:CD1	2.93	0.46
1:A:91:GLY:CA	1:A:379:MET:HE2	2.39	0.46
1:B:351:PRO:HG2	1:B:354:ALA:HB3	1.96	0.46
1:A:88:ARG:O	1:A:381:ILE:CG2	2.64	0.46
1:B:176:GLN:HA	1:B:322:ALA:HB1	1.98	0.46
1:A:5:VAL:HG13	1:A:105:LEU:CD1	2.46	0.46
1:A:20:GLY:O	1:A:23:LYS:HB2	2.15	0.46
1:A:88:ARG:CD	1:A:381:ILE:HD13	2.45	0.46
1:B:181:LEU:HD21	1:B:226:ILE:HD12	1.98	0.46
1:B:181:LEU:HD22	1:B:226:ILE:HG13	1.81	0.46
1:A:195:TYR:CE2	1:A:369:ARG:CD	2.98	0.46
1:B:261:MET:CE	1:B:265:GLU:HB3	2.46	0.46
1:B:110:ASP:O	1:B:261:MET:HA	2.15	0.46
1:A:240:ASN:O	1:A:240:ASN:ND2	2.40	0.46
1:A:235:VAL:HG23	1:A:236:PHE:CE2	2.50	0.46
1:B:181:LEU:HD21	1:B:226:ILE:CD1	2.45	0.46
1:A:182:GLU:O	1:A:185:ARG:N	2.48	0.46
1:B:186:ARG:CD	1:B:341:PRO:O	2.64	0.46
1:A:106:LEU:HD11	1:B:106:LEU:HD21	1.97	0.45
1:B:206:LYS:HB3	1:B:211:ASP:HB2	1.98	0.45
1:B:339:VAL:O	1:B:340:ASN:HB2	2.16	0.45
1:A:37:GLU:OE1	1:A:37:GLU:HA	2.15	0.45
1:B:365:HIS:O	1:B:368:ASN:HB2	2.16	0.45
1:A:187:ALA:O	1:A:191:ILE:HG13	2.17	0.45
1:B:276:ARG:O	1:B:391:PHE:HB3	2.17	0.45
1:B:374:TYR:CD1	1:B:392:GLU:HG3	2.52	0.45
1:A:292:ILE:H	1:A:292:ILE:HG13	1.56	0.45
1:B:207:GLY:H	1:B:211:ASP:HA	1.81	0.45
1:B:314:VAL:CG1	1:B:367:LEU:HD12	2.41	0.45
1:A:172:SER:O	1:A:173:ARG:C	2.54	0.45
1:B:344:SER:O	1:B:347:SER:N	2.48	0.45
1:B:269:ARG:HB3	1:B:271:LEU:HD12	1.99	0.45
1:B:111:VAL:HG23	2:B:406:HOH:O	2.17	0.45
1:A:66:TYR:CD2	1:B:89:LEU:HD21	2.52	0.44
1:A:261:MET:HE1	1:A:269:ARG:HD2	1.99	0.44
1:A:235:VAL:HG23	1:A:236:PHE:CD2	2.52	0.44
1:A:102:GLN:O	1:A:106:LEU:HD12	2.17	0.44
1:B:356:GLY:HA3	1:B:379:MET:CE	2.48	0.44
1:B:208:ARG:HG3	1:B:209:LYS:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ALA:HA	1:A:378:THR:O	2.18	0.44
1:B:263:ARG:CG	1:B:263:ARG:HH11	2.30	0.44
1:A:227:ASP:N	1:A:227:ASP:OD1	2.51	0.44
1:B:77:VAL:HG12	1:B:78:THR:N	2.33	0.44
1:A:65:MET:CE	1:B:58:ILE:HG12	2.48	0.44
1:B:295:VAL:HG13	1:B:332:LEU:CD2	2.29	0.44
1:A:285:VAL:CG1	1:A:296:PRO:CG	2.90	0.44
1:B:343:GLY:O	1:B:362:LYS:NZ	2.51	0.44
1:B:181:LEU:HD22	1:B:226:ILE:CA	2.47	0.44
1:A:305:ALA:CB	1:A:390:ILE:HD11	2.46	0.43
1:B:227:ASP:HA	1:B:230:THR:HG22	1.98	0.43
1:B:306:GLY:C	1:B:307:LEU:CD2	2.87	0.43
1:A:193:ALA:CB	1:A:195:TYR:CD1	3.01	0.43
1:B:89:LEU:HB2	1:B:381:ILE:HG23	1.99	0.43
1:B:286:ASP:O	1:B:287:PRO:C	2.55	0.43
1:A:221:ARG:HB2	1:A:221:ARG:HH11	1.82	0.43
1:A:165:VAL:CG2	1:A:289:ALA:HB1	2.49	0.43
1:B:94:LEU:HB3	1:B:387:ILE:HD13	2.00	0.43
1:A:169:TYR:HB2	1:A:171:ILE:HD12	2.01	0.43
1:A:285:VAL:HG11	1:A:293:GLY:HA2	2.01	0.43
1:A:65:MET:O	1:B:87:ASN:ND2	2.52	0.43
1:A:221:ARG:CB	1:A:221:ARG:HH11	2.31	0.43
1:A:141:LEU:HD12	1:A:141:LEU:HA	1.82	0.43
1:A:253:ASP:O	1:A:254:ALA:HB2	2.19	0.43
1:B:262:GLU:O	1:B:264:ALA:N	2.51	0.43
1:B:261:MET:HE2	1:B:265:GLU:HB3	2.01	0.43
1:B:227:ASP:HA	1:B:230:THR:CG2	2.48	0.43
1:A:89:LEU:HB2	1:A:381:ILE:CG2	2.48	0.43
1:A:225:THR:HG22	1:A:227:ASP:H	1.84	0.43
1:B:362:LYS:HE3	1:B:362:LYS:HB2	1.95	0.42
1:B:29:GLU:CD	1:B:63:ARG:HH22	2.22	0.42
1:A:66:TYR:CD2	1:B:89:LEU:CD2	3.02	0.42
1:B:30:LEU:HB3	1:B:255:ALA:HB2	2.00	0.42
1:A:393:ARG:O	1:A:394:ILE:O	2.37	0.42
1:B:312:LEU:CD2	1:B:375:ALA:C	2.87	0.42
1:B:104:ILE:HG23	1:B:110:ASP:HA	2.00	0.42
1:A:126:LEU:HD23	1:B:126:LEU:CD2	2.50	0.42
1:A:269:ARG:HB3	1:A:271:LEU:HG	2.02	0.42
1:A:319:GLU:CD	1:A:344:SER:CB	2.74	0.42
1:A:193:ALA:HB3	1:A:195:TYR:CD1	2.54	0.42
1:A:97:ILE:HG22	1:A:98:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ARG:HE	1:A:199:GLN:HE21	1.67	0.42
1:B:39:LEU:HD12	1:B:259:VAL:HG21	2.02	0.42
1:A:5:VAL:HG13	1:A:105:LEU:HD12	2.02	0.41
1:A:232:LEU:HD23	1:A:246:GLY:HA3	2.01	0.41
1:A:372:GLY:O	1:A:393:ARG:HD3	2.20	0.41
1:A:106:LEU:HD11	1:B:106:LEU:CD2	2.50	0.41
1:A:208:ARG:HG2	1:A:209:LYS:N	2.33	0.41
1:A:315:ILE:HG12	1:A:376:LEU:HB3	2.02	0.41
1:B:320:ALA:HB3	1:B:321:PHE:HD1	1.81	0.41
1:B:146:LEU:HA	1:B:146:LEU:HD13	1.90	0.41
1:A:95:GLN:O	1:A:95:GLN:NE2	2.51	0.41
1:B:129:ALA:HB1	1:B:134:ALA:HB2	2.02	0.41
1:A:5:VAL:HG11	1:A:104:ILE:HB	2.02	0.41
1:B:367:LEU:O	1:B:371:GLN:N	2.53	0.41
1:A:181:LEU:HD12	1:A:224:ALA:HB1	2.02	0.41
1:A:193:ALA:CB	1:A:195:TYR:CE1	3.04	0.41
1:B:254:ALA:O	1:B:354:ALA:HB2	2.21	0.41
1:A:234:PRO:CB	1:A:241:GLY:HA3	2.51	0.41
1:A:191:ILE:HD11	1:A:220:VAL:HG11	2.01	0.41
1:B:206:LYS:CB	1:B:211:ASP:HB2	2.51	0.41
1:A:295:VAL:HG22	1:A:332:LEU:HG	2.04	0.41
1:A:88:ARG:HD2	1:A:381:ILE:HD13	2.02	0.40
1:B:61:GLU:OE1	1:B:63:ARG:HD3	2.21	0.40
1:B:94:LEU:O	1:B:97:ILE:N	2.54	0.40
1:B:28:ALA:CB	1:B:63:ARG:NH2	2.84	0.40
1:A:302:LEU:O	1:A:303:GLU:C	2.60	0.40
1:A:267:GLU:C	1:A:270:GLY:H	2.24	0.40
1:B:47:ASP:HA	1:B:78:THR:HB	2.04	0.40
1:A:15:ILE:HD12	1:A:348:LEU:HB3	2.02	0.40
1:A:5:VAL:HG22	1:A:105:LEU:HD11	2.02	0.40
1:A:126:LEU:CD2	1:B:126:LEU:CD2	3.00	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	391/399 (98%)	356 (91%)	34 (9%)	1 (0%)	46 57
1	B	391/399 (98%)	363 (93%)	28 (7%)	0	100 100
All	All	782/798 (98%)	719 (92%)	62 (8%)	1 (0%)	56 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	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	287/293 (98%)	249 (87%)	38 (13%)	5 5
1	B	287/293 (98%)	231 (80%)	56 (20%)	2 1
All	All	574/586 (98%)	480 (84%)	94 (16%)	3 2

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	29	GLU
1	A	39	LEU
1	A	51	HIS
1	A	79	ILE
1	A	109	THR
1	A	113	ILE
1	A	141	LEU
1	A	155	ARG
1	A	167	LYS
1	A	175	GLN
1	A	198	ASP

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Mol	Chain	Res	Type
1	A	203	VAL
1	A	205	SER
1	A	208	ARG
1	A	209	LYS
1	A	212	VAL
1	A	213	THR
1	A	221	ARG
1	A	226	ILE
1	A	227	ASP
1	A	228	ASP
1	A	230	THR
1	A	232	LEU
1	A	240	ASN
1	A	249	SER
1	A	269	ARG
1	A	272	LYS
1	A	274	LEU
1	A	277	LEU
1	A	282	HIS
1	A	290	MET
1	A	292	ILE
1	A	314	VAL
1	A	329	THR
1	A	364	LEU
1	A	377	VAL
1	A	379	MET
1	B	3	ARG
1	B	8	VAL
1	B	17	THR
1	B	21	SER
1	B	23	LYS
1	B	29	GLU
1	B	41	ARG
1	B	43	GLN
1	B	54	PHE
1	B	62	PRO
1	B	67	LEU
1	B	79	ILE
1	B	88	ARG
1	B	89	LEU
1	B	106	LEU
1	B	113	ILE

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Mol	Chain	Res	Type
1	B	135	ARG
1	B	141	LEU
1	B	146	LEU
1	B	155	ARG
1	B	185	ARG
1	B	198	ASP
1	B	206	LYS
1	B	208	ARG
1	B	211	ASP
1	B	213	THR
1	B	216	THR
1	B	223	ASP
1	B	225	THR
1	B	227	ASP
1	B	232	LEU
1	B	235	VAL
1	B	239	GLU
1	B	263	ARG
1	B	265	GLU
1	B	268	ARG
1	B	274	LEU
1	B	276	ARG
1	B	277	LEU
1	B	279	SER
1	B	290	MET
1	B	303	GLU
1	B	308	GLN
1	B	311	ASP
1	B	312	LEU
1	B	313	ASP
1	B	321	PHE
1	B	344	SER
1	B	347	SER
1	B	348	LEU
1	B	351	PRO
1	B	352	ILE
1	B	366	GLU
1	B	369	ARG
1	B	378	THR
1	B	390	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	59	GLN
1	A	102	GLN
1	A	175	GLN
1	A	199	GLN
1	A	252	ASN
1	A	308	GLN
1	A	350	HIS
1	B	56	ASN
1	B	59	GLN
1	B	176	GLN
1	B	184	HIS
1	B	222	HIS
1	B	252	ASN
1	B	324	GLN
1	B	342	ASN
1	B	350	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	393/399 (98%)	0.25	16 (4%) 41 50	21, 52, 80, 116	0
1	B	393/399 (98%)	0.55	43 (10%) 7 11	20, 62, 93, 110	0
All	All	786/798 (98%)	0.40	59 (7%) 17 24	20, 57, 89, 116	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	394	ILE	6.6
1	B	375	ALA	5.0
1	B	210	GLY	5.0
1	B	2	THR	4.3
1	B	166	ALA	4.3
1	B	319	GLU	3.8
1	B	209	LYS	3.7
1	B	306	GLY	3.7
1	B	4	GLU	3.7
1	A	312	LEU	3.6
1	A	86	VAL	3.5
1	B	361	VAL	3.3
1	B	357	ALA	3.3
1	A	208	ARG	3.3
1	B	355	THR	3.3
1	B	178	GLU	3.2
1	B	229	MET	3.1
1	B	373	ARG	3.0
1	B	208	ARG	3.0
1	B	92	SER	2.9
1	B	266	ALA	2.9
1	B	353	GLY	2.8
1	B	352	ILE	2.8
1	B	263	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	238	LYS	2.7
1	B	90	CYS	2.7
1	B	55	GLY	2.7
1	B	356	GLY	2.6
1	B	207	GLY	2.6
1	B	381	ILE	2.6
1	B	379	MET	2.5
1	B	372	GLY	2.5
1	A	374	TYR	2.5
1	B	344	SER	2.5
1	A	221	ARG	2.5
1	B	89	LEU	2.4
1	A	356	GLY	2.4
1	B	93	GLY	2.4
1	B	391	PHE	2.4
1	A	85	THR	2.4
1	A	367	LEU	2.4
1	B	86	VAL	2.3
1	B	262	GLU	2.3
1	B	53	VAL	2.3
1	A	90	CYS	2.3
1	B	211	ASP	2.2
1	A	351	PRO	2.2
1	B	57	VAL	2.2
1	B	85	THR	2.2
1	B	305	ALA	2.2
1	B	307	LEU	2.2
1	A	276	ARG	2.1
1	B	393	ARG	2.1
1	A	117	ALA	2.1
1	A	352	ILE	2.1
1	A	98	VAL	2.1
1	B	359	ILE	2.0
1	A	268	ARG	2.0
1	B	191	ILE	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.