Full wwPDB X-ray Structure Validation Report ⓘ

Jul 17, 2023 – 12:07 PM JST

PDB ID	:	7YKC
Title	:	crystal structure of the Phenylalanine-regulated 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase (ARO3) from Saccharomyces cerevisiae
Authors	:	Liu, H.; Luo, Y.
Deposited on	:	2022-07-22
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

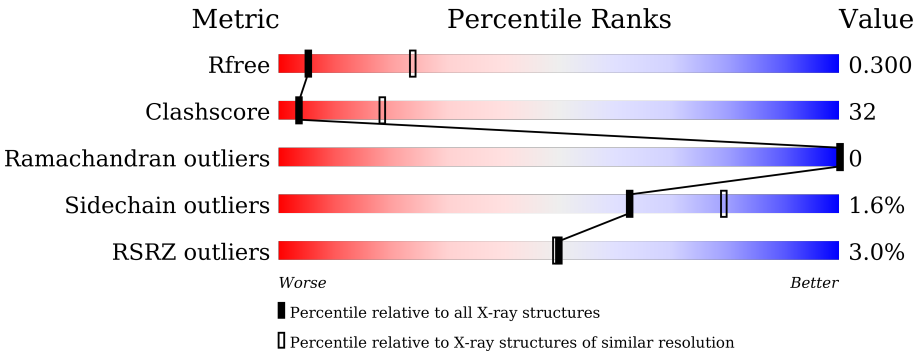
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	370	2% 46% 51% .
1	B	370	4% 51% 46% .

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5759 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 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase.

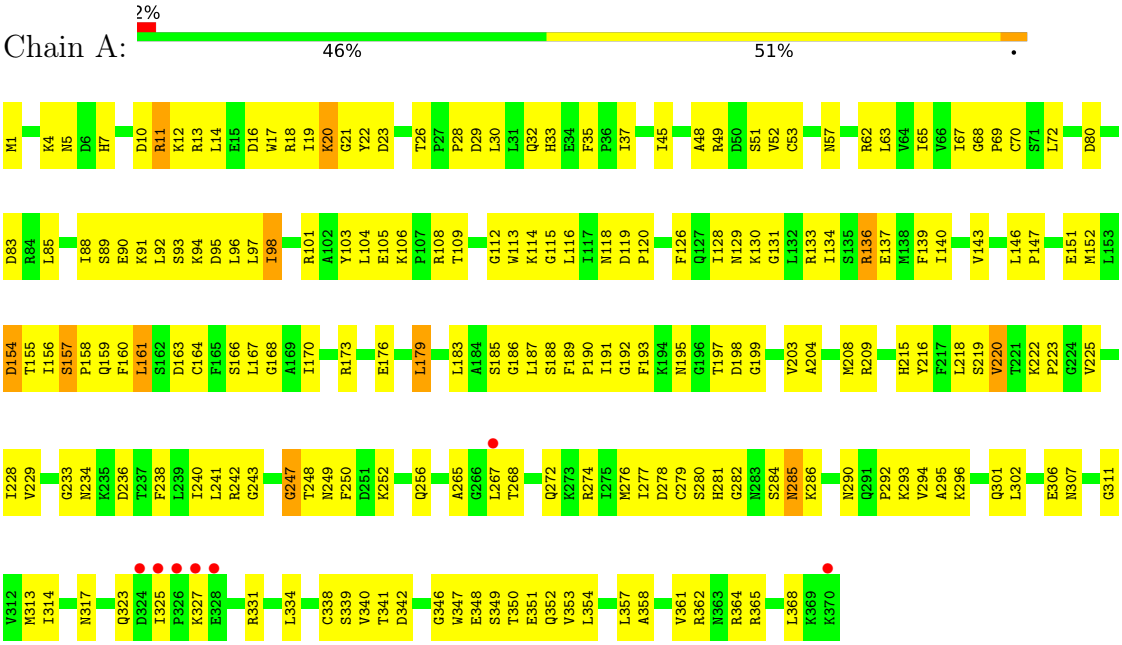
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2880	1799	511	554	16			
1	B	370	Total	C	N	O	S	0	0	0
			2879	1799	511	553	16			

3 Residue-property plots (i)

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

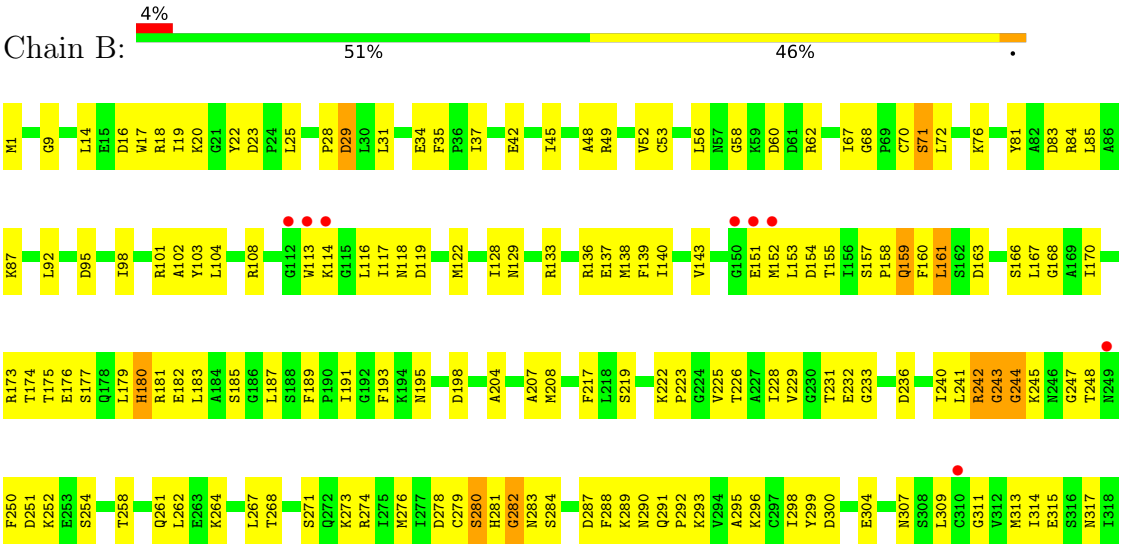
• Molecule 1: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase

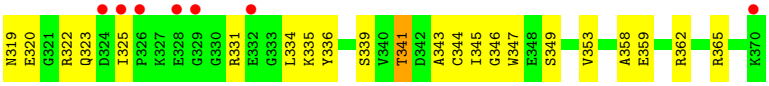
Chain A:



• Molecule 1: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase

Chain B:




N319
E320
G321
R322
Q323
D324
I325
P326
K327
E328
G329
G330
R331
E332
G333
L334
K335
Y336
S339
V340
T341
D342
A343
C344
I345
G346
W347
E348
S349
V353
A358
E359
R362
R365
K370

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.68Å 95.56Å 105.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.37 – 3.30 36.84 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.6 (34.37-3.30) 96.6 (36.84-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, R_{free}	0.252 , 0.295 0.255 , 0.300	Depositor DCC
R_{free} test set	1130 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å^2)	129.0	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 113.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5759	wwPDB-VP
Average B, all atoms (Å^2)	176.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% 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	0.69	0/2925	0.96	8/3931 (0.2%)
1	B	0.58	0/2924	0.88	10/3931 (0.3%)
All	All	0.64	0/5849	0.92	18/7862 (0.2%)

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	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	179	LEU	CB-CG-CD2	-8.87	95.92	111.00
1	B	243	GLY	N-CA-C	8.10	133.35	113.10
1	B	244	GLY	N-CA-C	7.33	131.43	113.10
1	B	282	GLY	N-CA-C	6.96	130.50	113.10
1	B	29	ASP	CB-CG-OD1	-6.43	112.52	118.30
1	A	20	LYS	CD-CE-NZ	6.21	125.97	111.70
1	B	161	LEU	N-CA-C	6.16	127.63	111.00
1	A	247	GLY	N-CA-C	6.15	128.47	113.10
1	A	161	LEU	N-CA-C	5.80	126.65	111.00
1	A	146	LEU	CA-CB-CG	5.59	128.17	115.30
1	B	242	ARG	N-CA-C	5.56	126.01	111.00
1	B	71	SER	N-CA-CB	5.54	118.81	110.50
1	B	280	SER	N-CA-C	-5.47	96.24	111.00
1	B	14	LEU	CB-CG-CD2	-5.40	101.83	111.00
1	A	11	ARG	N-CA-C	-5.37	96.51	111.00
1	A	146	LEU	CB-CG-CD1	-5.28	102.03	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	98	ILE	CG1-CB-CG2	-5.16	100.04	111.40
1	B	341	THR	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	ARG	Sidechain

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	2880	0	2905	196	0
1	B	2879	0	2905	199	0
All	All	5759	0	5810	366	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 32.

All (366) 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:63:LEU:O	1:A:96:LEU:HB2	1.45	1.15
1:B:71:SER:CB	1:B:341:THR:HG21	1.91	0.99
1:A:69:PRO:HG2	1:A:72:LEU:HD13	1.46	0.98
1:B:71:SER:HB2	1:B:341:THR:HG21	1.45	0.97
1:B:280:SER:HB2	1:B:315:GLU:HB2	1.47	0.95
1:B:70:CYS:HA	1:B:101:ARG:HE	1.30	0.95
1:A:65:ILE:HD13	1:A:354:LEU:HD21	1.53	0.90
1:A:62:ARG:HB3	1:A:96:LEU:HA	1.52	0.90
1:B:117:ILE:O	1:B:128:ILE:HG23	1.72	0.89
1:A:26:THR:HG23	1:A:30:LEU:HD23	1.53	0.88
1:A:65:ILE:HD13	1:A:354:LEU:CD2	2.04	0.88
1:B:71:SER:HB3	1:B:341:THR:CG2	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:SER:CB	1:B:315:GLU:HB2	2.05	0.85
1:A:14:LEU:HD21	1:B:42:GLU:HG3	1.60	0.81
1:B:154:ASP:O	1:B:158:PRO:HD2	1.81	0.81
1:B:136:ARG:HG3	1:B:161:LEU:CD2	2.11	0.80
1:B:242:ARG:HE	1:B:281:HIS:CB	1.95	0.80
1:A:14:LEU:HD13	1:B:37:ILE:HD12	1.62	0.79
1:A:85:LEU:HD11	1:A:98:ILE:HG21	1.65	0.79
1:B:242:ARG:HE	1:B:281:HIS:HB3	1.48	0.79
1:B:280:SER:HB2	1:B:315:GLU:CB	2.13	0.79
1:A:35:PHE:HB3	1:A:140:ILE:HD13	1.65	0.78
1:B:242:ARG:NE	1:B:281:HIS:HB3	1.99	0.78
1:A:353:VAL:O	1:A:357:LEU:HD12	1.83	0.78
1:A:218:LEU:HD22	1:B:25:LEU:HD22	1.66	0.77
1:B:153:LEU:CD1	1:B:174:THR:HG21	2.15	0.76
1:B:71:SER:HB3	1:B:341:THR:HG21	1.65	0.76
1:B:254:SER:O	1:B:258:THR:HG23	1.85	0.76
1:A:225:VAL:HG12	1:B:225:VAL:HG12	1.66	0.75
1:A:302:LEU:HD22	1:A:364:ARG:HD2	1.68	0.75
1:A:5:ASN:ND2	1:A:16:ASP:O	2.20	0.75
1:A:116:LEU:O	1:A:120:PRO:HB3	1.86	0.75
1:B:83:ASP:O	1:B:87:LYS:HG2	1.87	0.74
1:B:315:GLU:OE2	1:B:344:CYS:SG	2.46	0.74
1:A:72:LEU:HD21	1:A:101:ARG:O	1.88	0.73
1:A:240:ILE:HG12	1:A:276:MET:HB3	1.68	0.73
1:B:136:ARG:HG3	1:B:161:LEU:HD23	1.69	0.73
1:B:279:CYS:SG	1:B:313:MET:O	2.47	0.72
1:A:95:ASP:OD2	1:A:362:ARG:NH2	2.23	0.72
1:A:317:ASN:HD22	1:A:339:SER:HB2	1.54	0.71
1:B:159:GLN:HA	1:B:159:GLN:OE1	1.90	0.71
1:A:29:ASP:OD1	1:A:222:LYS:HB3	1.90	0.71
1:A:105:GLU:HG3	1:A:114:LYS:O	1.91	0.71
1:A:95:ASP:OD2	1:A:362:ARG:NE	2.22	0.70
1:A:160:PHE:C	1:A:161:LEU:HD12	2.10	0.70
1:B:31:LEU:HG	1:B:136:ARG:HD3	1.74	0.70
1:A:286:LYS:N	1:A:286:LYS:HD2	2.06	0.70
1:A:170:ILE:HB	1:A:193:PHE:HD1	1.57	0.70
1:B:122:MET:SD	1:B:331:ARG:HB2	2.32	0.70
1:B:261:GLN:HA	1:B:264:LYS:HB3	1.74	0.70
1:B:153:LEU:HD13	1:B:174:THR:HG21	1.74	0.70
1:A:139:PHE:CE2	1:A:161:LEU:HD23	2.26	0.69
1:B:241:LEU:HD11	1:B:258:THR:HG21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:SER:HB3	1:B:341:THR:HG23	1.73	0.69
1:A:69:PRO:HG2	1:A:72:LEU:CD1	2.23	0.69
1:A:187:LEU:O	1:B:18:ARG:HD2	1.93	0.68
1:B:34:GLU:OE2	1:B:133:ARG:NH2	2.27	0.68
1:A:7:HIS:ND1	1:A:13:ARG:HD2	2.09	0.68
1:A:154:ASP:HB2	1:B:179:LEU:HD21	1.76	0.68
1:A:90:GLU:HA	1:A:93:SER:HB2	1.76	0.67
1:A:108:ARG:HH12	1:A:112:GLY:HA3	1.59	0.67
1:A:218:LEU:CD2	1:B:25:LEU:HD22	2.25	0.67
1:A:168:GLY:O	1:A:191:ILE:HA	1.96	0.66
1:A:185:SER:HB2	1:A:233:GLY:HA2	1.77	0.66
1:A:1:MET:O	1:A:4:LYS:HE2	1.95	0.66
1:B:258:THR:O	1:B:262:LEU:HD23	1.96	0.66
1:A:197:THR:HA	1:A:242:ARG:NH2	2.11	0.65
1:A:250:PHE:HD2	1:A:294:VAL:HG13	1.62	0.65
1:B:152:MET:HB2	1:B:170:ILE:CD1	2.26	0.65
1:A:37:ILE:HG12	1:A:140:ILE:HG22	1.79	0.65
1:A:208:MET:HE2	1:A:267:LEU:HD13	1.79	0.64
1:A:348:GLU:O	1:A:352:GLN:HG3	1.97	0.64
1:A:103:TYR:CE2	1:A:151:GLU:HB2	2.33	0.64
1:B:70:CYS:HB2	1:B:315:GLU:CD	2.18	0.64
1:A:130:LYS:O	1:A:134:ILE:HG12	1.97	0.64
1:A:279:CYS:O	1:A:284:SER:HB3	1.96	0.64
1:A:268:THR:HA	1:A:272:GLN:OE1	1.98	0.63
1:B:293:LYS:O	1:B:296:LYS:HB3	1.98	0.63
1:B:70:CYS:HB2	1:B:315:GLU:OE2	1.98	0.63
1:A:173:ARG:HB3	1:B:176:GLU:HB3	1.82	0.62
1:B:182:GLU:HB3	1:B:217:PHE:CE2	2.34	0.62
1:A:65:ILE:HG23	1:A:65:ILE:O	1.99	0.62
1:A:65:ILE:CD1	1:A:354:LEU:HD21	2.29	0.61
1:A:134:ILE:O	1:A:137:GLU:HB3	1.99	0.61
1:A:26:THR:CG2	1:A:30:LEU:HD23	2.25	0.61
1:A:278:ASP:OD2	1:A:281:HIS:ND1	2.33	0.61
1:B:181:ARG:HD3	1:B:207:ALA:HA	1.82	0.61
1:A:20:LYS:HE3	1:B:232:GLU:HA	1.82	0.61
1:A:250:PHE:CG	1:A:250:PHE:O	2.54	0.61
1:B:154:ASP:O	1:B:155:THR:C	2.37	0.61
1:B:323:GLN:HE22	1:B:335:LYS:H	1.46	0.61
1:B:176:GLU:HA	1:B:181:ARG:NH2	2.16	0.60
1:A:22:TYR:HD1	1:B:229:VAL:HG22	1.65	0.60
1:B:183:LEU:O	1:B:187:LEU:HG	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LYS:NZ	1:B:304:GLU:OE1	2.35	0.60
1:A:14:LEU:CD2	1:B:42:GLU:HG3	2.32	0.60
1:A:250:PHE:CD2	1:A:294:VAL:HG13	2.36	0.60
1:A:323:GLN:NE2	1:A:338:CYS:HB3	2.17	0.60
1:B:280:SER:O	1:B:281:HIS:HB2	2.01	0.60
1:B:292:PRO:O	1:B:295:ALA:HB3	2.01	0.60
1:B:92:LEU:HD11	1:B:358:ALA:HB2	1.83	0.59
1:A:218:LEU:HD22	1:B:25:LEU:CD2	2.33	0.59
1:A:155:THR:HG21	1:A:179:LEU:HG	1.84	0.58
1:A:247:GLY:O	1:A:248:THR:C	2.41	0.58
1:B:262:LEU:HB3	1:B:268:THR:HG22	1.85	0.58
1:A:95:ASP:HA	1:A:365:ARG:HH22	1.68	0.58
1:A:285:ASN:C	1:A:286:LYS:HD2	2.24	0.58
1:B:219:SER:HB3	1:B:229:VAL:HG21	1.86	0.58
1:A:163:ASP:N	1:A:163:ASP:OD1	2.34	0.58
1:B:240:ILE:HG21	1:B:313:MET:SD	2.44	0.58
1:A:118:ASN:HA	1:A:128:ILE:HG12	1.85	0.58
1:A:19:ILE:HG22	1:A:21:GLY:H	1.68	0.58
1:A:139:PHE:HB3	1:A:164:CYS:SG	2.44	0.58
1:B:208:MET:HE2	1:B:267:LEU:HD22	1.86	0.57
1:B:17:TRP:CH2	1:B:18:ARG:CZ	2.88	0.57
1:A:89:SER:HA	1:A:98:ILE:HD12	1.87	0.57
1:B:243:GLY:O	1:B:247:GLY:O	2.22	0.57
1:B:136:ARG:HG3	1:B:161:LEU:HD21	1.86	0.57
1:A:18:ARG:HD2	1:B:187:LEU:O	2.05	0.56
1:B:31:LEU:HG	1:B:136:ARG:CD	2.35	0.56
1:B:16:ASP:HA	1:B:19:ILE:HG12	1.88	0.56
1:B:103:TYR:CZ	1:B:151:GLU:HB2	2.41	0.56
1:B:242:ARG:HE	1:B:281:HIS:CG	2.24	0.56
1:B:280:SER:HB2	1:B:291:GLN:OE1	2.05	0.56
1:A:290:ASN:O	1:A:294:VAL:HG23	2.05	0.56
1:B:108:ARG:NH2	1:B:113:TRP:O	2.38	0.56
1:A:250:PHE:CE2	1:A:294:VAL:HG22	2.40	0.56
1:A:186:GLY:O	1:B:18:ARG:HB2	2.04	0.56
1:B:289:LYS:O	1:B:292:PRO:HD2	2.06	0.56
1:A:108:ARG:HH12	1:A:112:GLY:CA	2.19	0.56
1:B:153:LEU:HD12	1:B:180:HIS:NE2	2.22	0.55
1:B:240:ILE:HA	1:B:276:MET:O	2.06	0.55
1:B:242:ARG:O	1:B:283:ASN:ND2	2.39	0.55
1:A:65:ILE:CD1	1:A:354:LEU:CD2	2.82	0.55
1:B:71:SER:CB	1:B:341:THR:CG2	2.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ILE:HG12	1:B:276:MET:HB3	1.88	0.55
1:A:272:GLN:NE2	1:A:274:ARG:HH21	2.04	0.55
1:B:320:GLU:HB3	1:B:346:GLY:N	2.21	0.55
1:B:322:ARG:HD2	1:B:343:ALA:HB2	1.87	0.55
1:B:168:GLY:O	1:B:191:ILE:HA	2.06	0.55
1:A:156:ILE:HG12	1:A:220:VAL:HG21	1.88	0.55
1:A:52:VAL:HG11	1:A:167:LEU:HD12	1.87	0.55
1:A:113:TRP:NE1	1:A:119:ASP:O	2.35	0.55
1:A:220:VAL:HG11	1:B:226:THR:HG21	1.89	0.55
1:A:241:LEU:HD22	1:A:249:ASN:ND2	2.22	0.54
1:B:70:CYS:HB2	1:B:315:GLU:OE1	2.06	0.54
1:B:287:ASP:HB3	1:B:290:ASN:ND2	2.21	0.54
1:A:95:ASP:OD2	1:A:362:ARG:CZ	2.55	0.54
1:B:70:CYS:CB	1:B:315:GLU:OE2	2.55	0.54
1:B:104:LEU:HD22	1:B:116:LEU:HD23	1.89	0.54
1:B:152:MET:HB2	1:B:170:ILE:HD13	1.88	0.54
1:B:152:MET:SD	1:B:158:PRO:HG3	2.48	0.54
1:B:174:THR:HB	1:B:180:HIS:CD2	2.43	0.54
1:A:192:GLY:HA3	1:A:238:PHE:CZ	2.43	0.54
1:A:229:VAL:HG22	1:B:22:TYR:CE1	2.42	0.53
1:A:292:PRO:O	1:A:295:ALA:HB3	2.08	0.53
1:B:48:ALA:O	1:B:52:VAL:HG23	2.09	0.53
1:B:68:GLY:HA2	1:B:81:TYR:OH	2.09	0.53
1:A:155:THR:HG21	1:A:179:LEU:CG	2.38	0.53
1:A:242:ARG:HD2	1:A:242:ARG:C	2.29	0.53
1:A:347:TRP:O	1:A:351:GLU:HG3	2.08	0.53
1:A:103:TYR:CZ	1:A:151:GLU:HB2	2.44	0.53
1:A:29:ASP:OD1	1:A:222:LYS:CB	2.55	0.52
1:B:276:MET:HA	1:B:311:GLY:O	2.09	0.52
1:A:35:PHE:HB3	1:A:140:ILE:CD1	2.37	0.52
1:B:49:ARG:HE	1:B:189:PHE:HB3	1.75	0.52
1:B:319:ASN:ND2	1:B:336:TYR:O	2.43	0.52
1:B:325:ILE:HG23	1:B:334:LEU:HD21	1.90	0.52
1:A:29:ASP:OD2	1:A:223:PRO:HA	2.08	0.52
1:B:84:ARG:HG2	1:B:347:TRP:CZ2	2.45	0.52
1:B:358:ALA:HB1	1:B:362:ARG:NH2	2.25	0.52
1:A:348:GLU:OE1	1:A:348:GLU:N	2.29	0.52
1:B:278:ASP:HB2	1:B:313:MET:SD	2.50	0.52
1:A:11:ARG:O	1:A:11:ARG:CG	2.57	0.51
1:A:361:VAL:O	1:A:364:ARG:HG2	2.11	0.51
1:B:291:GLN:NE2	1:B:315:GLU:HB3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:THR:HG22	1:B:181:ARG:HH12	1.76	0.51
1:B:288:PHE:CD1	1:B:288:PHE:N	2.78	0.51
1:A:48:ALA:HB2	1:A:147:PRO:HG3	1.91	0.51
1:A:349:SER:O	1:A:353:VAL:HG23	2.09	0.51
1:B:175:THR:O	1:B:181:ARG:NE	2.40	0.51
1:B:248:THR:HB	1:B:250:PHE:CE2	2.46	0.51
1:B:315:GLU:HG3	1:B:344:CYS:SG	2.50	0.51
1:B:362:ARG:O	1:B:365:ARG:HB2	2.10	0.50
1:B:29:ASP:OD1	1:B:223:PRO:HA	2.11	0.50
1:A:242:ARG:HD2	1:A:243:GLY:N	2.26	0.50
1:A:92:LEU:HD22	1:A:358:ALA:CB	2.42	0.50
1:A:112:GLY:HA2	1:A:327:LYS:NZ	2.26	0.50
1:B:288:PHE:H	1:B:288:PHE:HD1	1.58	0.49
1:B:182:GLU:HB3	1:B:217:PHE:CD2	2.47	0.49
1:A:313:MET:C	1:A:314:ILE:HG13	2.32	0.49
1:B:72:LEU:HD11	1:B:102:ALA:HA	1.94	0.49
1:A:62:ARG:HD3	1:A:94:LYS:O	2.12	0.49
1:B:217:PHE:HE1	1:B:219:SER:HB2	1.78	0.49
1:A:192:GLY:HA3	1:A:238:PHE:CE2	2.48	0.49
1:A:268:THR:HB	1:A:274:ARG:HG3	1.95	0.49
1:B:278:ASP:HA	1:B:313:MET:HB2	1.95	0.49
1:B:28:PRO:HD3	1:B:160:PHE:CZ	2.48	0.49
1:A:216:TYR:HA	1:A:229:VAL:O	2.13	0.48
1:A:65:ILE:HD13	1:A:354:LEU:HD23	1.88	0.48
1:A:112:GLY:HA2	1:A:327:LYS:HZ2	1.78	0.48
1:B:122:MET:CE	1:B:331:ARG:HB2	2.43	0.48
1:B:154:ASP:O	1:B:157:SER:N	2.47	0.48
1:B:113:TRP:CD1	1:B:119:ASP:HB3	2.48	0.48
1:A:228:ILE:HB	1:B:23:ASP:HB2	1.95	0.48
1:A:218:LEU:CD2	1:B:25:LEU:CD2	2.92	0.48
1:B:251:ASP:OD1	1:B:252:LYS:N	2.47	0.48
1:B:298:ILE:O	1:B:299:TYR:C	2.49	0.48
1:A:268:THR:OG1	1:A:272:GLN:HB2	2.14	0.48
1:B:9:GLY:N	1:B:17:TRP:O	2.46	0.48
1:A:276:MET:HA	1:A:311:GLY:O	2.14	0.48
1:A:286:LYS:N	1:A:286:LYS:CD	2.73	0.47
1:A:92:LEU:O	1:A:95:ASP:N	2.47	0.47
1:B:154:ASP:HB3	1:B:157:SER:H	1.79	0.47
1:A:276:MET:HG3	1:A:311:GLY:C	2.34	0.47
1:A:325:ILE:O	1:A:325:ILE:HG13	2.13	0.47
1:B:28:PRO:HA	1:B:160:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:HB3	1:B:274:ARG:NH1	2.30	0.47
1:B:244:GLY:HA2	1:B:247:GLY:O	2.14	0.47
1:B:317:ASN:HD22	1:B:339:SER:HB2	1.79	0.47
1:A:49:ARG:HG2	1:A:166:SER:O	2.14	0.47
1:A:45:ILE:HD11	1:A:143:VAL:HG11	1.94	0.47
1:A:229:VAL:HG22	1:B:22:TYR:CD1	2.49	0.47
1:B:129:ASN:O	1:B:133:ARG:HG3	2.14	0.47
1:A:22:TYR:CD1	1:B:229:VAL:HG22	2.47	0.47
1:A:133:ARG:O	1:A:134:ILE:C	2.52	0.47
1:B:242:ARG:HH21	1:B:281:HIS:HD1	1.60	0.47
1:A:18:ARG:HD3	1:B:233:GLY:O	2.13	0.47
1:A:32:GLN:NE2	1:A:222:LYS:HD2	2.30	0.47
1:B:101:ARG:NH2	1:B:281:HIS:NE2	2.63	0.47
1:A:89:SER:HA	1:A:98:ILE:CD1	2.45	0.47
1:A:234:ASN:OD1	1:A:236:ASP:HB2	2.15	0.47
1:A:161:LEU:HD12	1:A:161:LEU:N	2.30	0.47
1:A:331:ARG:HA	1:A:334:LEU:HD12	1.97	0.47
1:A:278:ASP:HA	1:A:313:MET:HB2	1.97	0.46
1:B:53:CYS:SG	1:B:236:ASP:OD2	2.74	0.46
1:A:129:ASN:OD1	1:A:130:LYS:N	2.46	0.46
1:A:280:SER:HA	1:A:284:SER:OG	2.15	0.46
1:B:242:ARG:CZ	1:B:281:HIS:HB3	2.46	0.46
1:B:359:GLU:HA	1:B:362:ARG:HD2	1.98	0.46
1:A:256:GLN:NE2	1:A:306:GLU:OE1	2.47	0.46
1:B:114:LYS:HB3	1:B:118:ASN:HD22	1.80	0.46
1:A:51:SER:HB3	1:A:97:LEU:HD22	1.97	0.46
1:B:291:GLN:NE2	1:B:315:GLU:O	2.48	0.46
1:B:288:PHE:CD1	1:B:343:ALA:HB1	2.51	0.46
1:A:293:LYS:O	1:A:296:LYS:HB3	2.15	0.46
1:B:251:ASP:O	1:B:254:SER:OG	2.34	0.46
1:A:28:PRO:HD3	1:A:160:PHE:CZ	2.51	0.46
1:A:65:ILE:CG2	1:A:98:ILE:HG12	2.46	0.46
1:A:252:LYS:HA	1:A:301:GLN:OE1	2.16	0.46
1:A:35:PHE:CE2	1:A:137:GLU:HB2	2.50	0.46
1:A:104:LEU:HD22	1:A:116:LEU:HD23	1.98	0.46
1:B:70:CYS:O	1:B:103:TYR:HB2	2.15	0.46
1:B:28:PRO:N	1:B:160:PHE:CE1	2.84	0.45
1:A:152:MET:HB2	1:A:170:ILE:HD13	1.98	0.45
1:A:166:SER:O	1:A:189:PHE:HB2	2.15	0.45
1:B:20:LYS:HB3	1:B:20:LYS:HE3	1.83	0.45
1:B:187:LEU:HD23	1:B:187:LEU:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:PRO:CA	1:B:160:PHE:CE1	3.00	0.45
1:B:296:LYS:O	1:B:300:ASP:OD2	2.34	0.45
1:A:65:ILE:HD11	1:A:314:ILE:CD1	2.46	0.45
1:A:282:GLY:O	1:A:285:ASN:ND2	2.47	0.45
1:B:60:ASP:OD1	1:B:62:ARG:HG3	2.16	0.45
1:A:65:ILE:O	1:A:65:ILE:CG2	2.65	0.45
1:A:67:ILE:HD11	1:A:350:THR:HG23	1.98	0.45
1:A:189:PHE:HB2	1:A:190:PRO:CD	2.47	0.45
1:B:280:SER:O	1:B:281:HIS:CB	2.65	0.45
1:A:65:ILE:HG21	1:A:98:ILE:HG12	1.99	0.45
1:B:241:LEU:HD21	1:B:258:THR:HG21	1.99	0.45
1:A:189:PHE:O	1:A:234:ASN:ND2	2.50	0.44
1:A:85:LEU:O	1:A:89:SER:HB3	2.17	0.44
1:A:108:ARG:NH2	1:A:113:TRP:O	2.50	0.44
1:B:315:GLU:HG3	1:B:344:CYS:HA	1.98	0.44
1:A:285:ASN:C	1:A:286:LYS:CD	2.85	0.44
1:A:358:ALA:HB1	1:A:362:ARG:NH2	2.32	0.44
1:B:76:LYS:H	1:B:76:LYS:HG3	1.37	0.44
1:B:136:ARG:CB	1:B:161:LEU:HD21	2.47	0.44
1:B:155:THR:HA	1:B:183:LEU:HD22	1.98	0.44
1:A:105:GLU:CG	1:A:115:GLY:HA3	2.48	0.44
1:A:113:TRP:CZ2	1:A:116:LEU:HA	2.51	0.44
1:B:185:SER:O	1:B:231:THR:HB	2.17	0.44
1:A:68:GLY:HA3	1:A:101:ARG:HB3	2.00	0.44
1:B:1:MET:N	1:B:1:MET:SD	2.88	0.44
1:B:198:ASP:HA	1:B:245:LYS:HE2	1.97	0.44
1:A:96:LEU:HD12	1:A:96:LEU:C	2.38	0.44
1:A:197:THR:HA	1:A:242:ARG:HH22	1.82	0.44
1:A:188:SER:HB3	1:B:17:TRP:NE1	2.33	0.44
1:A:198:ASP:OD2	1:B:245:LYS:NZ	2.50	0.44
1:A:368:LEU:HA	1:A:368:LEU:HD23	1.66	0.44
1:B:323:GLN:HE22	1:B:335:LYS:N	2.16	0.43
1:B:95:ASP:OD1	1:B:365:ARG:NH1	2.37	0.43
1:B:315:GLU:O	1:B:345:ILE:HG12	2.19	0.43
1:A:159:GLN:NE2	1:A:220:VAL:O	2.51	0.43
1:B:273:LYS:HD3	1:B:309:LEU:O	2.19	0.43
1:A:139:PHE:N	1:A:139:PHE:CD1	2.85	0.43
1:A:307:ASN:OD1	1:A:364:ARG:NH2	2.51	0.43
1:B:349:SER:O	1:B:353:VAL:HG23	2.19	0.43
1:B:71:SER:N	1:B:341:THR:OG1	2.52	0.43
1:B:104:LEU:HD22	1:B:116:LEU:CD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:GLU:O	1:B:140:ILE:HG12	2.19	0.43
1:B:195:ASN:OD1	1:B:242:ARG:N	2.46	0.43
1:A:106:LYS:HE2	1:A:342:ASP:OD2	2.19	0.43
1:A:152:MET:HB2	1:A:170:ILE:CD1	2.49	0.43
1:A:362:ARG:O	1:A:365:ARG:HB2	2.19	0.43
1:B:104:LEU:O	1:B:116:LEU:N	2.40	0.43
1:A:10:ASP:CG	1:A:12:LYS:HB2	2.40	0.42
1:A:53:CYS:O	1:A:57:ASN:ND2	2.52	0.42
1:B:217:PHE:CE1	1:B:219:SER:HB2	2.54	0.42
1:A:70:CYS:CB	1:A:341:THR:HG1	2.32	0.42
1:B:68:GLY:HA3	1:B:101:ARG:HB3	2.01	0.42
1:B:175:THR:O	1:B:181:ARG:NH2	2.51	0.42
1:B:177:SER:O	1:B:181:ARG:HG3	2.19	0.42
1:B:138:MET:HG2	1:B:139:PHE:HD1	1.84	0.42
1:B:52:VAL:HG11	1:B:167:LEU:HD12	2.00	0.42
1:A:346:GLY:O	1:A:350:THR:OG1	2.28	0.42
1:B:193:PHE:CE1	1:B:207:ALA:HB1	2.55	0.42
1:B:284:SER:O	1:B:290:ASN:ND2	2.26	0.42
1:B:290:ASN:HA	1:B:293:LYS:HD2	2.01	0.42
1:B:53:CYS:SG	1:B:236:ASP:CG	2.98	0.42
1:B:139:PHE:N	1:B:139:PHE:CD1	2.87	0.42
1:B:204:ALA:O	1:B:208:MET:HG3	2.20	0.42
1:A:109:THR:HG22	1:B:181:ARG:NH1	2.34	0.42
1:A:118:ASN:O	1:A:126:PHE:HA	2.19	0.42
1:B:163:ASP:OD1	1:B:163:ASP:N	2.53	0.42
1:B:322:ARG:CD	1:B:343:ALA:HB2	2.50	0.42
1:A:80:ASP:O	1:A:83:ASP:HB2	2.20	0.42
1:B:276:MET:HG3	1:B:311:GLY:C	2.39	0.42
1:A:120:PRO:HG3	1:A:131:GLY:CA	2.50	0.41
1:A:23:ASP:HB2	1:B:228:ILE:HB	2.02	0.41
1:A:209:ARG:HH21	1:A:265:ALA:HA	1.85	0.41
1:A:240:ILE:HA	1:A:276:MET:O	2.20	0.41
1:B:139:PHE:O	1:B:143:VAL:HG22	2.19	0.41
1:A:72:LEU:HD23	1:A:103:TYR:H	1.84	0.41
1:A:136:ARG:O	1:A:140:ILE:HG12	2.20	0.41
1:A:154:ASP:OD1	1:A:157:SER:HB3	2.20	0.41
1:A:17:TRP:HE3	1:A:17:TRP:O	2.03	0.41
1:A:88:ILE:O	1:A:91:LYS:HB3	2.20	0.41
1:A:195:ASN:ND2	1:A:199:GLY:HA2	2.35	0.41
1:A:10:ASP:C	1:A:12:LYS:N	2.73	0.41
1:A:70:CYS:HB3	1:A:341:THR:HG1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LEU:N	1:A:161:LEU:CD1	2.84	0.41
1:A:188:SER:HA	1:B:18:ARG:HH11	1.85	0.41
1:B:85:LEU:HD11	1:B:98:ILE:HG21	2.02	0.41
1:B:45:ILE:HA	1:B:166:SER:OG	2.20	0.41
1:B:180:HIS:HD1	1:B:180:HIS:N	2.18	0.41
1:A:12:LYS:HA	1:A:12:LYS:HD3	1.93	0.41
1:A:277:ILE:O	1:A:313:MET:N	2.37	0.41
1:B:34:GLU:HG2	1:B:35:PHE:CD1	2.56	0.41
1:B:122:MET:HE1	1:B:331:ARG:HB2	2.01	0.41
1:A:10:ASP:C	1:A:12:LYS:H	2.24	0.41
1:A:139:PHE:N	1:A:139:PHE:HD1	2.18	0.41
1:A:154:ASP:O	1:A:158:PRO:HD3	2.20	0.41
1:A:203:VAL:HG23	1:A:204:ALA:N	2.36	0.41
1:B:243:GLY:HA2	1:B:282:GLY:HA3	2.03	0.41
1:A:65:ILE:HD11	1:A:314:ILE:HD12	2.03	0.41
1:B:28:PRO:HA	1:B:160:PHE:CD1	2.56	0.41
1:B:273:LYS:HG2	1:B:307:ASN:O	2.21	0.41
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.74	0.40
1:A:176:GLU:HB3	1:B:173:ARG:HG2	2.03	0.40
1:B:67:ILE:HG13	1:B:314:ILE:HB	2.04	0.40
1:B:241:LEU:HD21	1:B:258:THR:CG2	2.50	0.40
1:B:58:GLY:HA3	1:B:271:SER:O	2.22	0.40
1:B:222:LYS:HB2	1:B:223:PRO:HD3	2.03	0.40
1:A:325:ILE:HG23	1:A:340:VAL:HB	2.03	0.40
1:A:128:ILE:HD13	1:A:128:ILE:HG21	1.91	0.40
1:A:220:VAL:HG11	1:B:226:THR:CG2	2.51	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	368/370 (100%)	347 (94%)	21 (6%)	0	100	100
1	B	368/370 (100%)	352 (96%)	16 (4%)	0	100	100
All	All	736/740 (100%)	699 (95%)	37 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	314/314 (100%)	306 (98%)	8 (2%)	47	72
1	B	314/314 (100%)	312 (99%)	2 (1%)	86	91
All	All	628/628 (100%)	618 (98%)	10 (2%)	62	79

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	154	ASP
1	A	157	SER
1	A	183	LEU
1	A	215	HIS
1	A	219	SER
1	A	220	VAL
1	A	285	ASN
1	B	159	GLN
1	B	180	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	B	323	GLN

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 monosaccharides 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	370/370 (100%)	-0.16	7 (1%)	66	65	86, 155, 254, 308	0
1	B	370/370 (100%)	0.06	15 (4%)	37	35	86, 187, 265, 304	0
All	All	740/740 (100%)	-0.05	22 (2%)	50	49	86, 174, 262, 308	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	370	LYS	7.7
1	B	370	LYS	4.6
1	B	249	ASN	4.4
1	B	329	GLY	4.0
1	B	325	ILE	4.0
1	B	332	GLU	3.6
1	A	327	LYS	3.2
1	A	324	ASP	3.2
1	B	150	GLY	2.9
1	B	326	PRO	2.8
1	A	326	PRO	2.7
1	B	114	LYS	2.6
1	B	324	ASP	2.6
1	B	152	MET	2.5
1	A	325	ILE	2.5
1	A	328	GLU	2.5
1	A	267	LEU	2.3
1	B	113	TRP	2.3
1	B	328	GLU	2.3
1	B	151	GLU	2.1
1	B	310	CYS	2.1
1	B	112	GLY	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 monosaccharides 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.