Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 12:25 AM EDT

PDB ID	:	2GGG
Title	:	The mutant A68C-D72C of Deinococcus Radiodurans N-acylamino acid racemase
Authors	:	Wang, W.C.; Chiu, W.C.
Deposited on	:	2006-03-24
Resolution	:	2.40 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:

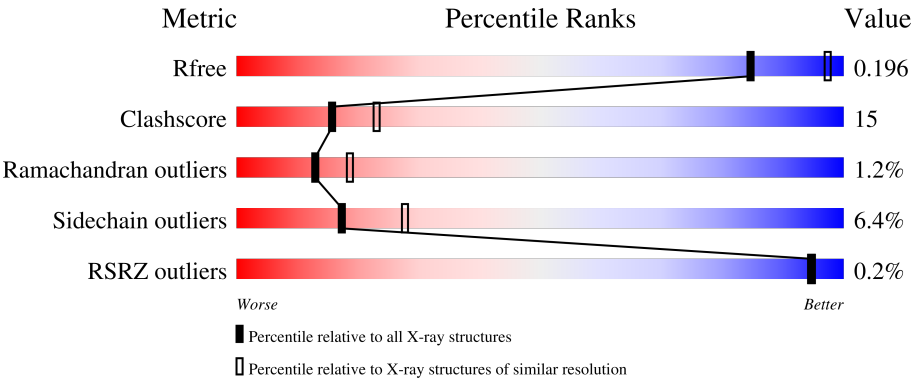
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	375	76% 18%
1	B	375	80% 15%
1	C	375	76% 18%
1	D	375	73% 19% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11909 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 N-acylamino acid racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2765	1732	507	514	12			
1	B	360	Total	C	N	O	S	0	0	0
			2765	1732	507	514	12			
1	C	370	Total	C	N	O	S	0	0	0
			2851	1789	521	529	12			
1	D	370	Total	C	N	O	S	0	0	0
			2851	1789	521	529	12			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	CYS	ALA	engineered mutation	UNP Q9RYA6
A	72	CYS	ASP	engineered mutation	UNP Q9RYA6
A	94	SER	ALA	SEE REMARK 999	UNP Q9RYA6
A	148	ASP	GLY	SEE REMARK 999	UNP Q9RYA6
A	158	ARG	LYS	SEE REMARK 999	UNP Q9RYA6
A	252	SER	ALA	SEE REMARK 999	UNP Q9RYA6
A	315	SER	PRO	SEE REMARK 999	UNP Q9RYA6
B	68	CYS	ALA	engineered mutation	UNP Q9RYA6
B	72	CYS	ASP	engineered mutation	UNP Q9RYA6
B	94	SER	ALA	SEE REMARK 999	UNP Q9RYA6
B	148	ASP	GLY	SEE REMARK 999	UNP Q9RYA6
B	158	ARG	LYS	SEE REMARK 999	UNP Q9RYA6
B	252	SER	ALA	SEE REMARK 999	UNP Q9RYA6
B	315	SER	PRO	SEE REMARK 999	UNP Q9RYA6
C	68	CYS	ALA	engineered mutation	UNP Q9RYA6
C	72	CYS	ASP	engineered mutation	UNP Q9RYA6
C	94	SER	ALA	SEE REMARK 999	UNP Q9RYA6
C	148	ASP	GLY	SEE REMARK 999	UNP Q9RYA6
C	158	ARG	LYS	SEE REMARK 999	UNP Q9RYA6
C	252	SER	ALA	SEE REMARK 999	UNP Q9RYA6
C	315	SER	PRO	SEE REMARK 999	UNP Q9RYA6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	68	CYS	ALA	engineered mutation	UNP Q9RYA6
D	72	CYS	ASP	engineered mutation	UNP Q9RYA6
D	94	SER	ALA	SEE REMARK 999	UNP Q9RYA6
D	148	ASP	GLY	SEE REMARK 999	UNP Q9RYA6
D	158	ARG	LYS	SEE REMARK 999	UNP Q9RYA6
D	252	SER	ALA	SEE REMARK 999	UNP Q9RYA6
D	315	SER	PRO	SEE REMARK 999	UNP Q9RYA6

- Molecule 2 is water.

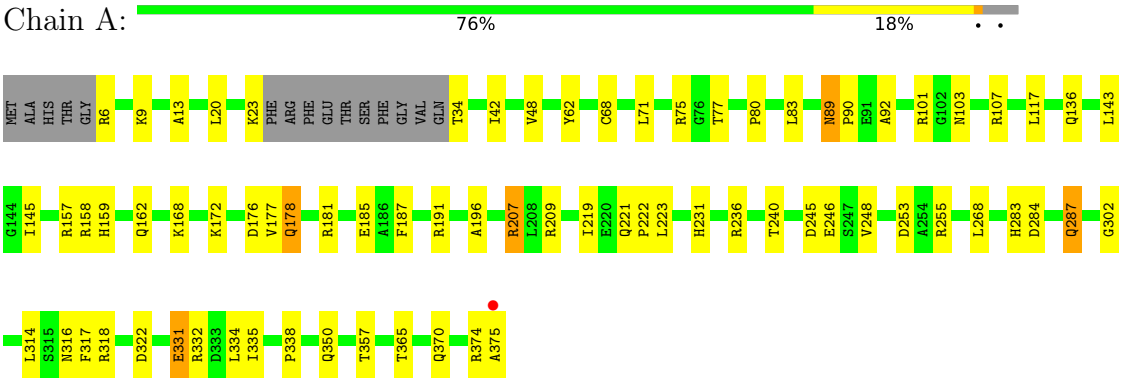
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	175	Total O 175 175	0	0
2	B	164	Total O 164 164	0	0
2	C	167	Total O 167 167	0	0
2	D	171	Total O 171 171	0	0

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.

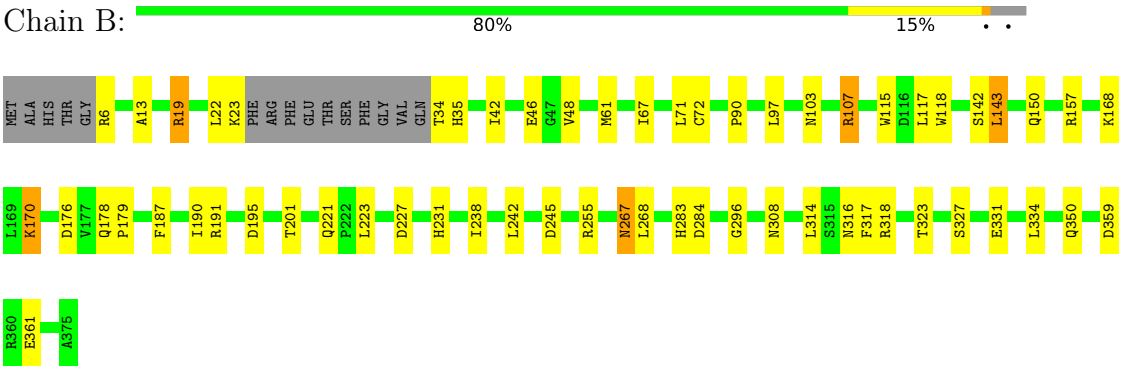
• Molecule 1: N-acylamino acid racemase

Chain A:



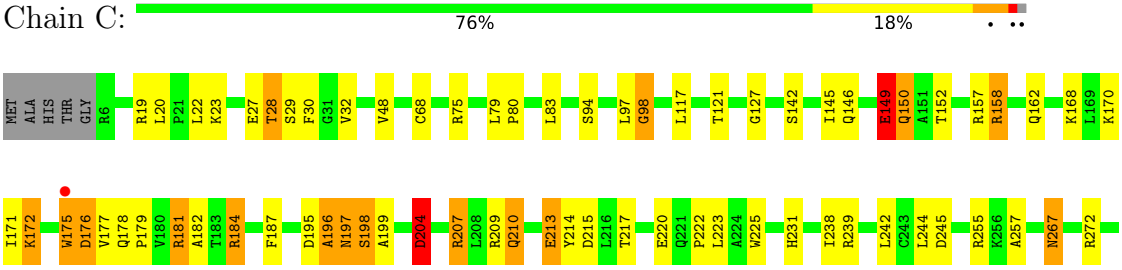
• Molecule 1: N-acylamino acid racemase

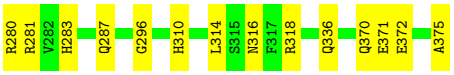
Chain B:



• Molecule 1: N-acylamino acid racemase

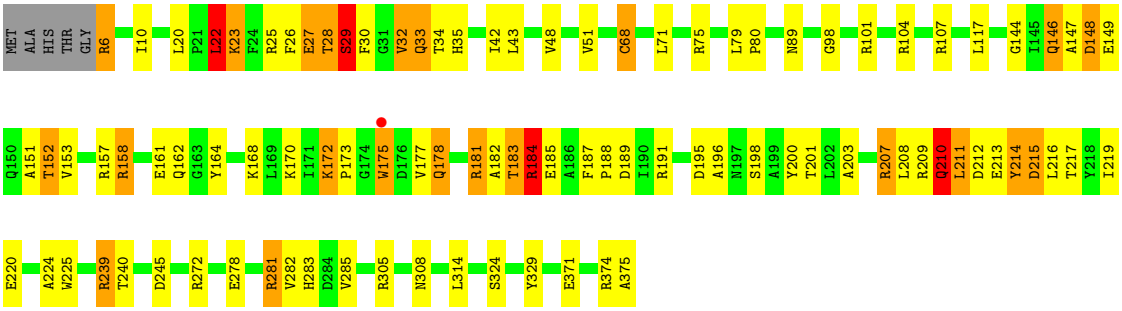
Chain C:





• Molecule 1: N-acylamino acid racemase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α, β, γ	115.64Å 115.64Å 120.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 27.07 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-2.40) 99.4 (27.07-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.170 , 0.207 0.171 , 0.196	Depositor DCC
R_{free} test set	3127 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 25.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.009 for -h,-l,-k 0.009 for -h,l,k 0.015 for l,-k,h 0.015 for -l,-k,-h 0.479 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11909	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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	0.56	0/2816	0.65	0/3820
1	B	0.55	0/2816	0.68	0/3820
1	C	0.52	0/2906	0.68	1/3942 (0.0%)
1	D	0.53	0/2906	0.70	1/3942 (0.0%)
All	All	0.54	0/11444	0.68	2/15524 (0.0%)

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	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	281	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	D	281	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	210	GLN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2765	0	2768	59	0
1	B	2765	0	2768	53	0
1	C	2851	0	2847	104	1
1	D	2851	0	2847	117	1
2	A	175	0	0	9	0
2	B	164	0	0	9	0
2	C	167	0	0	16	0
2	D	171	0	0	27	0
All	All	11909	0	11230	329	1

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 15.

All (329) 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:C:172:LYS:HE2	1:C:175:TRP:CB	1.46	1.45
1:C:172:LYS:CE	1:C:175:TRP:HB3	1.58	1.34
1:C:172:LYS:HB2	2:C:530:HOH:O	1.27	1.30
1:C:162:GLN:HG3	2:C:539:HOH:O	1.26	1.25
1:D:146:GLN:HB3	2:D:396:HOH:O	1.09	1.23
1:A:191:ARG:HD3	2:A:539:HOH:O	1.38	1.21
1:B:191:ARG:HD3	2:B:510:HOH:O	1.42	1.18
1:A:287:GLN:HE22	1:A:318:ARG:NH2	1.39	1.18
1:D:149:GLU:HG3	1:D:182:ALA:HB2	1.19	1.17
1:D:28:THR:O	1:D:29:SER:HB3	1.45	1.15
1:D:212:ASP:HB3	2:D:484:HOH:O	1.44	1.14
1:D:162:GLN:HG3	2:D:537:HOH:O	0.97	1.12
1:D:175:TRP:CD1	2:D:441:HOH:O	2.00	1.11
1:D:149:GLU:O	1:D:182:ALA:HB1	1.51	1.11
1:C:158:ARG:HH21	1:C:158:ARG:HG3	1.08	1.10
1:A:287:GLN:NE2	1:A:318:ARG:HH21	1.50	1.09
1:D:210:GLN:HG3	1:D:212:ASP:HB2	1.13	1.09
1:D:149:GLU:O	1:D:182:ALA:CB	2.02	1.06
1:C:172:LYS:CB	2:C:530:HOH:O	1.90	1.03
1:B:170:LYS:HD3	2:B:480:HOH:O	1.60	1.01
1:D:152:THR:HA	2:D:438:HOH:O	1.57	1.01
1:C:28:THR:HG22	1:C:30:PHE:H	1.25	1.01
1:C:198:SER:N	2:C:531:HOH:O	1.97	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ARG:HG3	1:C:158:ARG:NH2	1.78	0.95
1:D:210:GLN:C	1:D:212:ASP:H	1.69	0.94
1:B:168:LYS:HG3	2:B:408:HOH:O	1.67	0.92
1:C:146:GLN:OE1	1:C:146:GLN:HA	1.70	0.92
1:C:197:ASN:O	1:C:199:ALA:N	2.04	0.91
1:C:150:GLN:NE2	2:C:534:HOH:O	1.99	0.91
1:A:236:ARG:HD2	2:A:549:HOH:O	1.73	0.89
1:C:283:HIS:HE1	1:C:316:ASN:H	1.21	0.88
1:B:142:SER:HB3	1:B:168:LYS:HE2	1.52	0.88
1:A:178:GLN:H	1:A:178:GLN:HE21	1.19	0.88
1:A:283:HIS:HE1	1:A:316:ASN:H	1.22	0.87
1:D:181:ARG:HD2	2:D:500:HOH:O	1.74	0.87
1:D:183:THR:O	1:D:185:GLU:N	2.06	0.87
1:A:221:GLN:NE2	1:A:245:ASP:H	1.73	0.86
1:C:29:SER:OG	1:C:197:ASN:HB2	1.75	0.85
1:C:287:GLN:HE22	1:C:318:ARG:HH11	1.23	0.85
1:D:210:GLN:CG	1:D:212:ASP:HB2	2.04	0.84
1:A:221:GLN:HE21	1:A:245:ASP:H	1.28	0.82
1:D:149:GLU:HG3	1:D:182:ALA:CB	2.05	0.82
1:B:221:GLN:HE21	1:B:245:ASP:H	1.22	0.82
1:C:172:LYS:HE2	1:C:175:TRP:CG	2.14	0.82
1:C:283:HIS:CE1	1:C:316:ASN:H	1.97	0.81
1:C:145:ILE:CD1	1:C:172:LYS:HD2	2.11	0.81
1:C:197:ASN:HA	2:C:531:HOH:O	1.82	0.79
1:D:210:GLN:C	1:D:212:ASP:N	2.36	0.79
1:D:27:GLU:HA	1:D:27:GLU:OE1	1.80	0.79
1:D:175:TRP:HA	1:D:175:TRP:CE3	2.17	0.79
1:B:19:ARG:HH11	1:B:19:ARG:HB3	1.48	0.78
1:C:28:THR:HG21	1:C:30:PHE:CE2	2.17	0.78
1:C:127:GLY:H	1:C:310:HIS:HD2	1.28	0.77
1:B:221:GLN:NE2	1:B:245:ASP:H	1.82	0.77
1:A:23:LYS:O	2:A:547:HOH:O	2.03	0.76
1:A:6:ARG:N	2:A:544:HOH:O	2.16	0.76
1:B:72:CYS:HB3	2:D:474:HOH:O	1.84	0.76
1:B:168:LYS:HD3	1:B:195:ASP:HB2	1.68	0.76
1:D:26:PHE:O	1:D:33:GLN:HB2	1.85	0.76
1:A:316:ASN:HD22	1:A:318:ARG:HE	1.33	0.76
1:A:287:GLN:HE22	1:A:318:ARG:HH21	0.77	0.75
1:B:103:ASN:O	1:B:107:ARG:HG2	1.84	0.75
1:A:283:HIS:CE1	1:A:316:ASN:H	2.04	0.75
1:C:145:ILE:HG12	1:C:172:LYS:HD2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:SER:CB	1:B:168:LYS:HE2	2.17	0.74
1:D:175:TRP:HA	1:D:175:TRP:HE3	1.52	0.74
1:B:48:VAL:HG23	1:B:117:LEU:HD12	1.70	0.73
1:D:27:GLU:H	1:D:32:VAL:HA	1.51	0.73
1:C:178:GLN:HB2	1:C:179:PRO:HD3	1.70	0.72
1:C:146:GLN:OE1	2:C:491:HOH:O	2.07	0.72
1:B:267:ASN:C	1:B:267:ASN:HD22	1.91	0.72
1:B:283:HIS:HE1	1:B:316:ASN:H	1.36	0.72
1:C:127:GLY:H	1:C:310:HIS:CD2	2.08	0.72
1:A:157:ARG:HG3	1:A:187:PHE:HZ	1.55	0.71
1:D:177:VAL:HG13	1:D:214:TYR:HE2	1.55	0.71
1:D:207:ARG:CD	2:D:536:HOH:O	2.39	0.71
1:D:147:ALA:HA	2:D:532:HOH:O	1.90	0.71
1:A:287:GLN:NE2	1:A:318:ARG:NH2	2.21	0.70
1:C:27:GLU:HG2	1:C:145:ILE:HB	1.72	0.70
1:D:375:ALA:HB3	2:D:487:HOH:O	1.92	0.70
1:D:157:ARG:O	1:D:161:GLU:HG3	1.93	0.69
1:B:283:HIS:CE1	1:B:316:ASN:H	2.10	0.68
1:D:207:ARG:HD3	2:D:536:HOH:O	1.91	0.68
1:D:177:VAL:HG13	1:D:214:TYR:CE2	2.28	0.68
1:D:6:ARG:HB3	1:D:6:ARG:CZ	2.22	0.68
1:C:28:THR:HG21	1:C:30:PHE:CD2	2.29	0.67
1:A:107:ARG:HD2	2:A:548:HOH:O	1.95	0.67
1:A:219:ILE:HG13	1:A:240:THR:HG21	1.76	0.67
1:C:267:ASN:C	1:C:267:ASN:HD22	1.97	0.67
1:A:159:HIS:HD2	1:A:162:GLN:OE1	1.77	0.66
1:C:145:ILE:CG1	1:C:172:LYS:HD2	2.23	0.66
1:C:283:HIS:HE1	1:C:316:ASN:N	1.92	0.66
1:D:28:THR:HB	2:D:542:HOH:O	1.94	0.66
1:C:182:ALA:HB1	2:C:534:HOH:O	1.96	0.66
1:C:283:HIS:CE1	1:C:316:ASN:HB3	2.32	0.65
1:C:117:LEU:O	1:C:121:THR:HG23	1.96	0.65
1:B:48:VAL:HG23	1:B:117:LEU:CD1	2.27	0.65
1:C:29:SER:OG	1:C:197:ASN:CB	2.44	0.65
1:C:48:VAL:HG23	1:C:117:LEU:HD12	1.79	0.65
1:C:267:ASN:HD21	1:C:296:GLY:HA3	1.61	0.65
1:D:148:ASP:OD1	1:D:151:ALA:HB3	1.97	0.64
1:D:28:THR:O	1:D:29:SER:CB	2.32	0.64
1:D:184:ARG:O	1:D:188:PRO:HA	1.97	0.64
1:A:48:VAL:HG23	1:A:117:LEU:HD12	1.80	0.64
1:B:359:ASP:OD2	1:B:361:GLU:HG2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ARG:N	2:B:517:HOH:O	2.31	0.63
1:A:178:GLN:H	1:A:178:GLN:NE2	1.95	0.63
1:C:172:LYS:CE	1:C:175:TRP:CB	2.39	0.63
1:A:283:HIS:HD2	1:A:284:ASP:OD1	1.81	0.62
1:D:153:VAL:HG13	1:D:187:PHE:HE1	1.63	0.62
1:D:210:GLN:CA	1:D:212:ASP:H	2.13	0.62
1:B:323:THR:HG22	2:B:537:HOH:O	1.98	0.62
1:A:89:ASN:ND2	1:A:92:ALA:H	1.97	0.62
1:D:224:ALA:HA	2:D:451:HOH:O	2.00	0.61
1:D:149:GLU:O	1:D:182:ALA:HB3	1.98	0.61
1:D:147:ALA:O	2:D:532:HOH:O	2.16	0.61
1:B:157:ARG:HG3	1:B:187:PHE:HZ	1.65	0.61
1:D:32:VAL:HG13	1:D:33:GLN:N	2.16	0.60
1:D:48:VAL:HG23	1:D:117:LEU:HD12	1.83	0.60
1:C:146:GLN:HG3	1:C:152:THR:HA	1.82	0.60
1:D:71:LEU:O	1:D:75:ARG:HG2	2.01	0.60
1:B:283:HIS:HD2	1:B:284:ASP:OD1	1.84	0.60
1:B:283:HIS:CE1	1:B:314:LEU:HB3	2.37	0.60
1:C:158:ARG:NH2	1:C:158:ARG:CG	2.57	0.60
1:D:210:GLN:HB2	2:D:463:HOH:O	2.01	0.60
1:B:316:ASN:HD22	1:B:318:ARG:HE	1.48	0.60
1:C:171:ILE:HD12	1:C:176:ASP:CB	2.32	0.60
1:C:172:LYS:HE2	1:C:175:TRP:HB3	0.67	0.59
1:C:29:SER:CB	1:C:197:ASN:HB2	2.32	0.59
1:B:267:ASN:HD21	1:B:296:GLY:HA3	1.67	0.59
1:D:172:LYS:NZ	1:D:172:LYS:HB3	2.18	0.59
1:D:48:VAL:HG23	1:D:117:LEU:CD1	2.33	0.58
1:C:28:THR:CG2	1:C:29:SER:N	2.67	0.58
1:C:142:SER:HB3	1:C:168:LYS:HD3	1.84	0.58
1:C:210:GLN:C	1:C:210:GLN:HE21	2.07	0.58
1:D:208:LEU:HA	1:D:211:LEU:HD23	1.86	0.58
1:B:316:ASN:HD22	1:B:318:ARG:NE	2.02	0.57
1:B:223:LEU:H	1:B:231:HIS:CE1	2.22	0.57
1:B:316:ASN:ND2	1:B:318:ARG:HE	2.03	0.57
1:C:157:ARG:NE	2:C:523:HOH:O	2.25	0.56
1:B:34:THR:OG1	1:B:35:HIS:HD2	1.89	0.56
1:D:278:GLU:O	1:D:282:VAL:HG23	2.04	0.56
1:C:172:LYS:CD	1:C:175:TRP:HB3	2.32	0.56
1:C:197:ASN:C	2:C:427:HOH:O	2.42	0.56
1:C:198:SER:HB3	1:C:223:LEU:O	2.06	0.56
1:B:67:ILE:O	1:B:71:LEU:HG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:PHE:HB3	1:B:190:ILE:HG12	1.87	0.56
1:D:146:GLN:HB2	1:D:152:THR:OG1	2.05	0.56
1:D:209:ARG:HG2	1:D:210:GLN:OE1	2.06	0.56
1:A:223:LEU:H	1:A:231:HIS:CE1	2.24	0.56
1:C:170:LYS:HD2	1:C:197:ASN:HD21	1.71	0.55
1:D:75:ARG:NH2	1:D:371:GLU:OE2	2.37	0.55
1:D:191:ARG:HG3	1:D:217:THR:OG1	2.07	0.55
1:A:255:ARG:HD2	1:A:255:ARG:C	2.27	0.54
1:D:219:ILE:HD12	1:D:240:THR:HB	1.89	0.54
1:D:151:ALA:HA	2:D:439:HOH:O	2.08	0.54
1:D:157:ARG:HA	1:D:187:PHE:CZ	2.43	0.54
1:A:101:ARG:HD2	1:C:225:TRP:CD1	2.41	0.54
1:B:143:LEU:HD12	1:B:143:LEU:N	2.23	0.54
1:C:146:GLN:OE1	1:C:146:GLN:CA	2.47	0.54
1:C:283:HIS:CE1	1:C:316:ASN:CB	2.90	0.54
1:A:89:ASN:HD22	1:A:92:ALA:H	1.53	0.54
1:C:157:ARG:HA	1:C:187:PHE:CZ	2.43	0.54
1:D:177:VAL:O	1:D:181:ARG:HB2	2.08	0.54
1:D:210:GLN:HG3	1:D:212:ASP:CB	2.08	0.54
1:D:181:ARG:HG2	1:D:214:TYR:CE1	2.42	0.53
1:D:153:VAL:HG13	1:D:187:PHE:CE1	2.43	0.53
1:A:316:ASN:ND2	1:A:318:ARG:HE	2.05	0.53
1:C:97:LEU:O	1:C:98:GLY:O	2.27	0.53
1:C:178:GLN:OE1	1:C:179:PRO:HD3	2.08	0.53
1:C:204:ASP:OD1	1:C:204:ASP:N	2.41	0.53
1:A:268:LEU:HD23	1:A:317:PHE:CZ	2.44	0.53
1:B:90:PRO:HD3	1:B:118:TRP:CD1	2.44	0.52
1:D:148:ASP:O	1:D:152:THR:HB	2.10	0.52
1:B:267:ASN:C	1:B:267:ASN:ND2	2.62	0.52
1:D:195:ASP:HA	1:D:220:GLU:HB3	1.92	0.52
1:C:146:GLN:HG3	1:C:152:THR:OG1	2.09	0.52
1:C:287:GLN:HG2	2:C:440:HOH:O	2.09	0.52
1:C:28:THR:HG22	1:C:30:PHE:N	2.08	0.52
1:C:145:ILE:HD13	1:C:172:LYS:HD2	1.92	0.52
1:C:146:GLN:HG3	1:C:152:THR:CA	2.39	0.52
1:A:331:GLU:CD	1:A:332:ARG:H	2.12	0.52
1:D:175:TRP:CZ3	1:D:178:GLN:HB2	2.44	0.52
1:C:171:ILE:HD12	1:C:176:ASP:HB3	1.91	0.52
1:D:22:LEU:HB2	1:D:34:THR:O	2.10	0.52
1:D:245:ASP:OD2	1:D:272:ARG:NH2	2.43	0.52
1:C:171:ILE:HD12	1:C:176:ASP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:VAL:HG13	1:D:33:GLN:H	1.75	0.51
1:D:79:LEU:HB2	1:D:80:PRO:HD3	1.91	0.51
1:D:98:GLY:O	1:D:107:ARG:NH2	2.43	0.51
1:D:210:GLN:HA	1:D:212:ASP:H	1.74	0.51
1:D:25:ARG:NH2	1:D:27:GLU:HG3	2.26	0.51
1:D:213:GLU:C	1:D:215:ASP:H	2.14	0.51
1:C:195:ASP:HA	1:C:220:GLU:HB3	1.92	0.51
1:C:196:ALA:O	1:C:197:ASN:C	2.49	0.51
1:D:175:TRP:CZ3	1:D:178:GLN:CB	2.93	0.51
1:C:158:ARG:HH21	1:C:158:ARG:CG	1.94	0.51
1:D:147:ALA:HB1	2:D:386:HOH:O	2.11	0.51
1:C:197:ASN:HB3	2:C:427:HOH:O	2.10	0.50
1:D:6:ARG:CZ	1:D:6:ARG:CB	2.89	0.50
1:D:28:THR:HG21	1:D:30:PHE:CZ	2.47	0.50
1:A:375:ALA:HA	2:A:485:HOH:O	2.10	0.50
1:B:97:LEU:C	2:B:452:HOH:O	2.50	0.50
1:C:79:LEU:HB2	1:C:80:PRO:HD3	1.92	0.50
1:D:239:ARG:HB3	2:D:484:HOH:O	2.12	0.50
1:A:283:HIS:CE1	1:A:314:LEU:HB3	2.47	0.49
1:B:268:LEU:HD23	1:B:317:PHE:CZ	2.47	0.49
1:C:168:LYS:HE3	1:C:195:ASP:HB2	1.93	0.49
1:A:176:ASP:OD2	1:A:177:VAL:N	2.45	0.49
1:C:177:VAL:O	1:C:181:ARG:HB2	2.12	0.49
1:D:158:ARG:O	1:D:162:GLN:HG2	2.12	0.49
1:B:238:ILE:HD11	1:B:242:LEU:HD21	1.95	0.49
1:C:162:GLN:NE2	2:C:496:HOH:O	2.21	0.49
1:C:245:ASP:OD1	1:C:272:ARG:NH2	2.46	0.49
1:D:185:GLU:HB2	2:D:459:HOH:O	2.11	0.49
1:C:267:ASN:C	1:C:267:ASN:ND2	2.66	0.49
1:C:28:THR:CG2	1:C:30:PHE:CD2	2.96	0.48
1:D:104:ARG:HD3	2:D:436:HOH:O	2.11	0.48
1:D:149:GLU:CG	1:D:182:ALA:HB2	2.13	0.48
1:B:22:LEU:HD12	1:B:22:LEU:N	2.28	0.48
1:D:32:VAL:O	1:D:33:GLN:CB	2.62	0.48
1:B:150:GLN:HG2	2:B:515:HOH:O	2.13	0.48
1:D:149:GLU:C	1:D:182:ALA:CB	2.79	0.48
1:A:158:ARG:O	1:A:162:GLN:HG3	2.13	0.48
1:C:223:LEU:H	1:C:231:HIS:CE1	2.32	0.48
1:D:32:VAL:HG22	1:D:33:GLN:H	1.79	0.47
1:B:90:PRO:HG2	1:B:115:TRP:CD2	2.49	0.47
1:D:75:ARG:HH21	1:D:371:GLU:CD	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:HD13	1:A:334:LEU:HD21	1.96	0.47
1:C:172:LYS:CE	1:C:175:TRP:CG	2.93	0.47
1:D:184:ARG:NH2	1:D:214:TYR:O	2.46	0.47
1:A:168:LYS:HE2	2:A:388:HOH:O	2.13	0.47
1:C:48:VAL:HG23	1:C:117:LEU:CD1	2.44	0.47
1:C:222:PRO:HD2	1:C:231:HIS:CE1	2.50	0.46
1:D:201:THR:OG1	1:D:203:ALA:HB3	2.15	0.46
1:C:149:GLU:OE1	1:C:149:GLU:O	2.33	0.46
1:D:144:GLY:O	1:D:146:GLN:HG3	2.15	0.46
1:C:222:PRO:HD2	1:C:231:HIS:HE1	1.81	0.46
1:B:13:ALA:HA	1:B:42:ILE:O	2.16	0.46
1:C:75:ARG:NH1	1:C:371:GLU:OE2	2.32	0.46
1:D:198:SER:HB2	1:D:225:TRP:N	2.30	0.46
1:A:178:GLN:HE21	1:A:178:GLN:N	2.00	0.46
1:C:171:ILE:HG12	1:C:195:ASP:O	2.15	0.46
1:B:255:ARG:C	1:B:255:ARG:HD2	2.37	0.46
1:D:172:LYS:HG3	1:D:173:PRO:HD2	1.98	0.46
1:A:168:LYS:NZ	1:A:322:ASP:OD2	2.48	0.45
1:C:210:GLN:HE21	1:C:210:GLN:CA	2.29	0.45
1:D:207:ARG:HB3	2:D:425:HOH:O	2.15	0.45
1:D:27:GLU:OE1	1:D:27:GLU:CA	2.59	0.45
1:C:172:LYS:HB3	2:C:530:HOH:O	1.86	0.45
1:C:238:ILE:HD11	1:C:242:LEU:HD21	1.98	0.45
1:D:200:TYR:CD2	1:D:208:LEU:HD23	2.51	0.45
1:A:181:ARG:O	1:A:185:GLU:HB2	2.18	0.44
1:C:255:ARG:HD2	1:C:255:ARG:C	2.38	0.44
1:C:283:HIS:CE1	1:C:316:ASN:N	2.73	0.44
1:D:216:LEU:HB2	1:D:240:THR:HG21	1.99	0.44
1:A:248:VAL:HA	1:A:253:ASP:HB3	2.00	0.44
1:B:201:THR:HB	2:B:536:HOH:O	2.17	0.44
1:A:103:ASN:O	1:A:107:ARG:HG3	2.17	0.44
1:B:61:MET:O	1:D:101:ARG:HD2	2.17	0.44
1:B:178:GLN:HB2	1:B:179:PRO:CD	2.47	0.44
1:B:267:ASN:HD22	1:B:268:LEU:N	2.15	0.44
1:C:28:THR:HG23	1:C:29:SER:N	2.31	0.44
1:A:13:ALA:HA	1:A:42:ILE:O	2.17	0.44
1:D:181:ARG:HG3	1:D:214:TYR:OH	2.18	0.44
1:D:153:VAL:CG1	1:D:187:PHE:HE1	2.31	0.43
1:A:158:ARG:NH1	1:B:331:GLU:O	2.51	0.43
1:A:196:ALA:HB3	1:A:222:PRO:HA	1.99	0.43
1:D:25:ARG:NH1	1:D:27:GLU:HG2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:LEU:HA	1:D:211:LEU:CD2	2.48	0.43
1:D:68:CYS:HB3	2:D:474:HOH:O	2.19	0.43
1:D:146:GLN:CB	1:D:152:THR:OG1	2.66	0.43
1:D:172:LYS:HB3	1:D:172:LYS:HZ2	1.83	0.43
1:C:150:GLN:HG2	2:C:392:HOH:O	2.19	0.43
1:C:172:LYS:HG2	1:C:175:TRP:HB2	2.01	0.43
1:D:172:LYS:CG	1:D:173:PRO:HD2	2.49	0.43
1:B:23:LYS:HE3	1:B:327:SER:O	2.19	0.42
1:D:173:PRO:HA	1:D:200:TYR:HE1	1.83	0.42
1:A:338:PRO:HD3	1:B:157:ARG:HD2	2.01	0.42
1:A:77:THR:C	1:A:80:PRO:HD2	2.40	0.42
1:C:83:LEU:HB3	1:C:375:ALA:HA	2.02	0.42
1:C:244:LEU:CD1	1:C:257:ALA:HB1	2.49	0.42
1:C:287:GLN:NE2	1:C:318:ARG:HH11	2.03	0.42
1:D:164:TYR:OH	1:D:324:SER:HB2	2.19	0.42
1:A:83:LEU:HD23	1:A:83:LEU:HA	1.87	0.42
1:A:283:HIS:CE1	1:A:316:ASN:HB3	2.55	0.42
1:C:280:ARG:HG3	1:C:314:LEU:HD21	2.02	0.42
1:D:23:LYS:HB2	1:D:329:TYR:O	2.20	0.42
1:D:32:VAL:O	1:D:33:GLN:HG3	2.19	0.42
1:D:144:GLY:HA2	1:D:170:LYS:HG3	2.00	0.42
1:D:281:ARG:O	1:D:285:VAL:HG23	2.19	0.42
1:B:19:ARG:HD2	1:B:35:HIS:CB	2.50	0.42
1:B:23:LYS:HA	1:B:331:GLU:HG2	2.02	0.42
1:C:150:GLN:CG	2:C:392:HOH:O	2.68	0.42
1:A:223:LEU:H	1:A:231:HIS:HE1	1.68	0.41
1:C:283:HIS:CE1	1:C:314:LEU:HB3	2.55	0.41
1:C:157:ARG:CB	1:C:187:PHE:HZ	2.33	0.41
1:C:175:TRP:HA	1:C:178:GLN:OE1	2.20	0.41
1:C:210:GLN:O	1:C:213:GLU:HB3	2.20	0.41
1:A:34:THR:HG23	1:A:34:THR:O	2.21	0.41
1:A:71:LEU:O	1:A:75:ARG:HG2	2.19	0.41
1:D:168:LYS:HD2	2:D:430:HOH:O	2.20	0.41
1:A:62:TYR:CE1	1:A:246:GLU:HG3	2.56	0.41
1:B:107:ARG:HE	1:B:107:ARG:HB3	1.52	0.41
1:D:283:HIS:NE2	1:D:314:LEU:HB3	2.35	0.41
1:A:374:ARG:O	1:A:375:ALA:C	2.59	0.41
1:C:172:LYS:HG2	1:C:175:TRP:CB	2.50	0.41
1:C:287:GLN:HE22	1:C:318:ARG:NH1	2.03	0.41
1:D:10:ILE:HD13	1:D:43:LEU:HD13	2.02	0.41
1:D:27:GLU:HB3	2:D:465:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:HD13	1:A:172:LYS:HD3	2.03	0.41
1:A:168:LYS:CE	2:A:388:HOH:O	2.68	0.41
1:B:19:ARG:HD2	1:B:35:HIS:HB3	2.01	0.41
1:D:29:SER:HB3	2:D:543:HOH:O	2.20	0.41
1:A:89:ASN:HD22	1:A:89:ASN:C	2.24	0.41
1:A:89:ASN:HB2	1:A:90:PRO:CD	2.51	0.41
1:A:207:ARG:HG3	2:A:504:HOH:O	2.21	0.41
1:B:308:ASN:ND2	2:B:537:HOH:O	2.53	0.41
1:D:22:LEU:HB3	1:D:23:LYS:H	1.69	0.41
1:D:35:HIS:CE1	2:D:486:HOH:O	2.73	0.41
1:D:375:ALA:CB	2:D:487:HOH:O	2.60	0.41
1:A:302:GLY:HA3	1:A:335:ILE:HG12	2.03	0.40
1:D:207:ARG:H	1:D:207:ARG:HG2	1.54	0.40
1:D:32:VAL:O	1:D:33:GLN:HB2	2.19	0.40
1:A:48:VAL:HG23	1:A:117:LEU:CD1	2.48	0.40
1:C:176:ASP:OD1	1:C:207:ARG:NE	2.55	0.40
1:C:184:ARG:HD2	1:C:184:ARG:HA	1.70	0.40
1:D:42:ILE:HG12	1:D:51:VAL:HG13	2.03	0.40
1:D:305:ARG:O	1:D:308:ASN:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:GLN:OE1	1:D:158:ARG:NH2[2_656]	2.12	0.08

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	356/375 (95%)	340 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	356/375 (95%)	343 (96%)	13 (4%)	0	100 100
1	C	368/375 (98%)	344 (94%)	17 (5%)	7 (2%)	8 10
1	D	368/375 (98%)	335 (91%)	23 (6%)	10 (3%)	5 5
All	All	1448/1500 (96%)	1362 (94%)	69 (5%)	17 (1%)	13 19

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	98	GLY
1	C	196	ALA
1	C	197	ASN
1	C	198	SER
1	D	33	GLN
1	D	183	THR
1	D	184	ARG
1	D	196	ALA
1	D	22	LEU
1	D	23	LYS
1	D	29	SER
1	D	32	VAL
1	C	214	TYR
1	D	214	TYR
1	C	149	GLU
1	D	211	LEU
1	C	204	ASP

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	285/297 (96%)	271 (95%)	14 (5%)	25 40
1	B	285/297 (96%)	275 (96%)	10 (4%)	36 55
1	C	294/297 (99%)	267 (91%)	27 (9%)	9 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	294/297 (99%)	271 (92%)	23 (8%)	12 19
All	All	1158/1188 (98%)	1084 (94%)	74 (6%)	17 28

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	68	CYS
1	A	89	ASN
1	A	136	GLN
1	A	143	LEU
1	A	178	GLN
1	A	207	ARG
1	A	209	ARG
1	A	287	GLN
1	A	331	GLU
1	A	350	GLN
1	A	357	THR
1	A	365	THR
1	A	370	GLN
1	B	19	ARG
1	B	46	GLU
1	B	107	ARG
1	B	143	LEU
1	B	170	LYS
1	B	176	ASP
1	B	227	ASP
1	B	267	ASN
1	B	334	LEU
1	B	350	GLN
1	C	19	ARG
1	C	20	LEU
1	C	22	LEU
1	C	23	LYS
1	C	28	THR
1	C	32	VAL
1	C	68	CYS
1	C	94	SER
1	C	149	GLU
1	C	150	GLN
1	C	158	ARG
1	C	172	LYS

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Mol	Chain	Res	Type
1	C	175	TRP
1	C	176	ASP
1	C	181	ARG
1	C	184	ARG
1	C	204	ASP
1	C	207	ARG
1	C	209	ARG
1	C	210	GLN
1	C	213	GLU
1	C	215	ASP
1	C	217	THR
1	C	239	ARG
1	C	267	ASN
1	C	370	GLN
1	C	372	GLU
1	D	6	ARG
1	D	20	LEU
1	D	22	LEU
1	D	27	GLU
1	D	28	THR
1	D	29	SER
1	D	68	CYS
1	D	89	ASN
1	D	146	GLN
1	D	148	ASP
1	D	152	THR
1	D	158	ARG
1	D	172	LYS
1	D	175	TRP
1	D	178	GLN
1	D	181	ARG
1	D	184	ARG
1	D	189	ASP
1	D	207	ARG
1	D	210	GLN
1	D	215	ASP
1	D	239	ARG
1	D	374	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	159	HIS
1	A	178	GLN
1	A	221	GLN
1	A	231	HIS
1	A	283	HIS
1	A	287	GLN
1	A	316	ASN
1	B	35	HIS
1	B	85	GLN
1	B	146	GLN
1	B	221	GLN
1	B	231	HIS
1	B	267	ASN
1	B	283	HIS
1	B	287	GLN
1	B	316	ASN
1	B	370	GLN
1	B	373	HIS
1	C	33	GLN
1	C	85	GLN
1	C	136	GLN
1	C	150	GLN
1	C	197	ASN
1	C	210	GLN
1	C	231	HIS
1	C	267	ASN
1	C	283	HIS
1	C	287	GLN
1	C	310	HIS
1	C	370	GLN
1	D	35	HIS
1	D	49	GLN
1	D	89	ASN
1	D	103	ASN
1	D	178	GLN
1	D	316	ASN
1	D	350	GLN

5.3.3 RNA

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 monosaccharides 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

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	360/375 (96%)	-0.96	1 (0%) 94 93	10, 23, 42, 59	0
1	B	360/375 (96%)	-0.97	0 100 100	13, 24, 41, 61	0
1	C	370/375 (98%)	-0.76	1 (0%) 94 93	12, 26, 57, 72	0
1	D	370/375 (98%)	-0.73	1 (0%) 94 93	12, 26, 61, 78	0
All	All	1460/1500 (97%)	-0.85	3 (0%) 95 94	10, 25, 56, 78	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	175	TRP	4.2
1	A	375	ALA	2.8
1	C	175	TRP	2.4

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

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

6.3 Carbohydrates

There are no monosaccharides 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.