Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:18 AM GMT

PDB ID	:	2GGI
Title	:	The mutant E149C-A182C of Deinococcus Radiodurans N-acylamino acid racemase
Authors	:	Wang, W.C.; Chiu, W.C.
Deposited on	:	2006-03-24
Resolution	:	2.20 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:

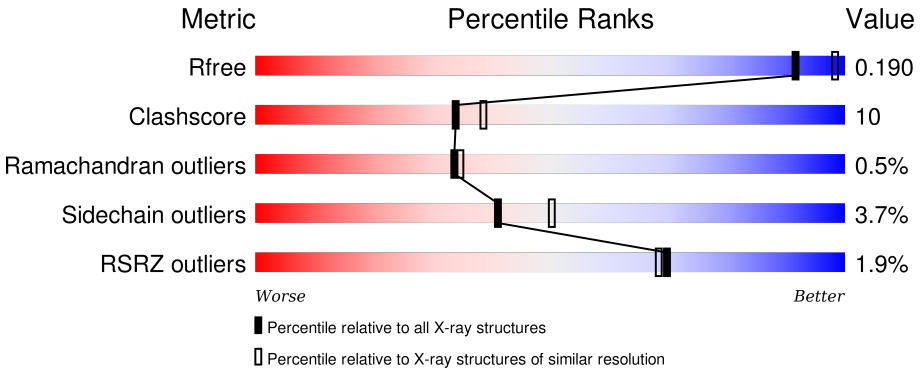
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	375	82% 13%
1	B	375	86% 9%
1	C	375	4% 74% 19%
1	D	375	3% 79% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12348 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
			2764	1731	507	514	12			
1	B	360	Total	C	N	O	S	0	0	0
			2764	1731	507	514	12			
1	C	360	Total	C	N	O	S	0	0	0
			2764	1731	507	514	12			
1	D	360	Total	C	N	O	S	0	0	0
			2764	1731	507	514	12			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	SER	ALA	SEE REMARK 999	UNP Q9RYA6
A	148	ASP	GLY	SEE REMARK 999	UNP Q9RYA6
A	149	CYS	GLU	ENGINEERED	UNP Q9RYA6
A	158	ARG	LYS	SEE REMARK 999	UNP Q9RYA6
A	182	CYS	ALA	ENGINEERED	UNP Q9RYA6
A	252	SER	ALA	SEE REMARK 999	UNP Q9RYA6
A	315	SER	PRO	SEE REMARK 999	UNP Q9RYA6
B	94	SER	ALA	SEE REMARK 999	UNP Q9RYA6
B	148	ASP	GLY	SEE REMARK 999	UNP Q9RYA6
B	149	CYS	GLU	ENGINEERED	UNP Q9RYA6
B	158	ARG	LYS	SEE REMARK 999	UNP Q9RYA6
B	182	CYS	ALA	ENGINEERED	UNP Q9RYA6
B	252	SER	ALA	SEE REMARK 999	UNP Q9RYA6
B	315	SER	PRO	SEE REMARK 999	UNP Q9RYA6
C	94	SER	ALA	SEE REMARK 999	UNP Q9RYA6
C	148	ASP	GLY	SEE REMARK 999	UNP Q9RYA6
C	149	CYS	GLU	ENGINEERED	UNP Q9RYA6
C	158	ARG	LYS	SEE REMARK 999	UNP Q9RYA6
C	182	CYS	ALA	ENGINEERED	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	94	SER	ALA	SEE REMARK 999	UNP Q9RYA6
D	148	ASP	GLY	SEE REMARK 999	UNP Q9RYA6
D	149	CYS	GLU	ENGINEERED	UNP Q9RYA6
D	158	ARG	LYS	SEE REMARK 999	UNP Q9RYA6
D	182	CYS	ALA	ENGINEERED	UNP Q9RYA6
D	252	SER	ALA	SEE REMARK 999	UNP Q9RYA6
D	315	SER	PRO	SEE REMARK 999	UNP Q9RYA6

- Molecule 2 is water.

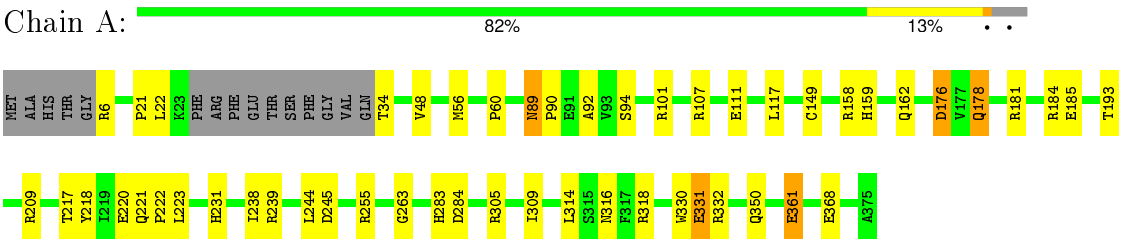
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	338	Total O 338 338	0	0
2	B	340	Total O 340 340	0	0
2	C	307	Total O 307 307	0	0
2	D	307	Total O 307 307	0	0

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.

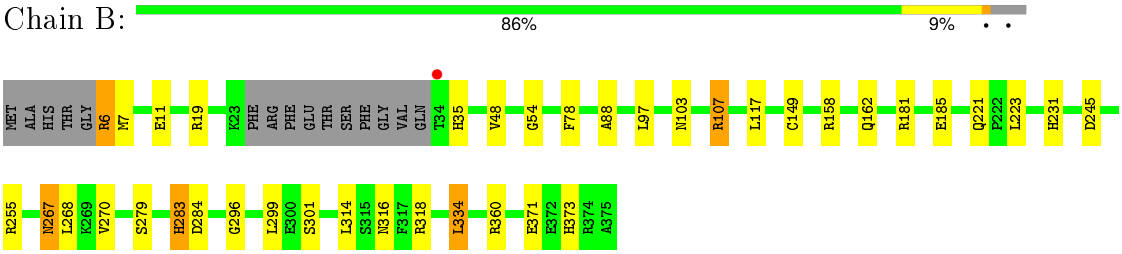
- Molecule 1: N-acylamino acid racemase

Chain A:



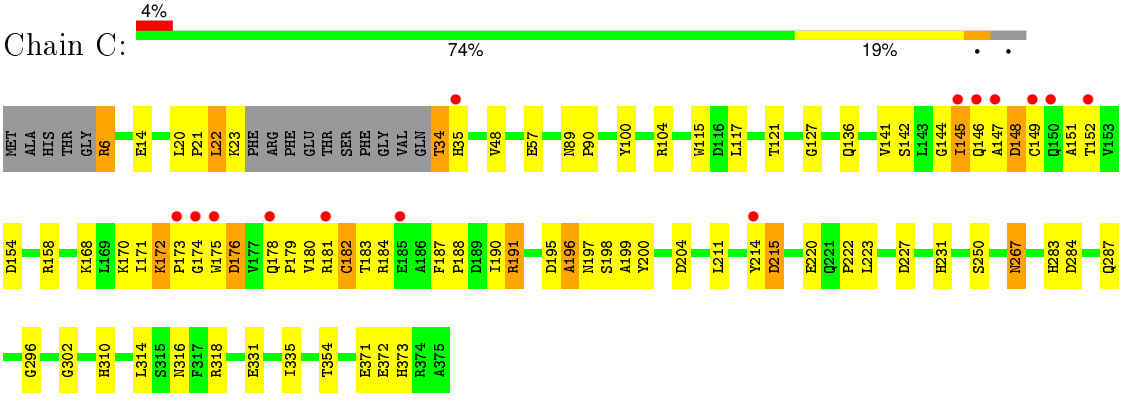
- Molecule 1: N-acylamino acid racemase

Chain B:



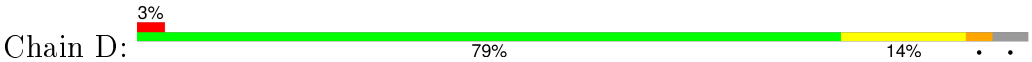
- Molecule 1: N-acylamino acid racemase

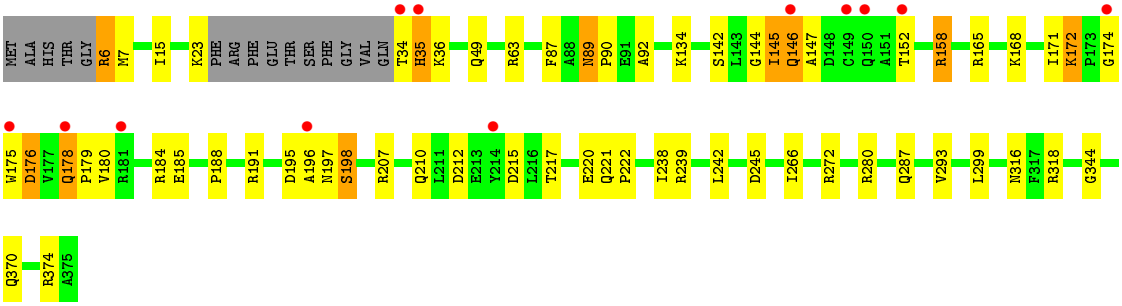
Chain C:



- Molecule 1: N-acylamino acid racemase

Chain D:




MET ALA HIS THR GLY R6 M7 I15 K23 PHE ARG PHE GLU THR SER PHE GLY VAL GLN T34 H35 K36 Q49 R63 F87 A88 N89 P90 E91 A92 K134 S142 L143 G144 I145 Q146 A147 D148 C149 Q150 A151 T152 R158 R165 K168 I171 K172 P173 G174
W175 D176 V177 Q178 P179 V180 R181 R184 E185 P188 R191 D195 A196 N197 S198 R207 Q210 L211 D212 E213 Y214 D215 L216 T217 E220 Q221 P222 I238 R239 L242 D245 I266 R272 R280 Q287 V293 L299 N316 F317 R318 G344
Q370 R374 A375

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α, β, γ	116.50Å 116.50Å 120.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.13 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-2.20) 99.1 (29.13-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.79 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.166 , 0.203 0.167 , 0.190	Depositor DCC
R_{free} test set	4064 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 26.5	EDS
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.005 for l,-k,h 0.006 for -l,-k,-h 0.487 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 80949 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12348	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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	0.54	0/2815	0.65	1/3819 (0.0%)
1	B	0.54	0/2815	0.64	0/3819
1	C	0.49	0/2815	0.65	0/3819
1	D	0.53	0/2815	0.65	0/3819
All	All	0.53	0/11260	0.65	1/15276 (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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	101	ARG	NE-CZ-NH1	5.26	122.93	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	97	LEU	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	2764	0	2766	51	0
1	B	2764	0	2766	35	0
1	C	2764	0	2766	81	0
1	D	2764	0	2766	58	0
2	A	338	0	0	7	0
2	B	340	0	0	5	1
2	C	307	0	0	13	0
2	D	307	0	0	18	0
All	All	12348	0	11064	223	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 10.

All (223) 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:287:GLN:NE2	1:C:318:ARG:HH11	1.31	1.25
1:C:191:ARG:HG3	1:C:191:ARG:HH11	1.18	1.05
1:D:158:ARG:HH11	1:D:158:ARG:HG3	1.11	1.05
1:A:178:GLN:H	1:A:178:GLN:HE21	1.03	1.02
1:D:6:ARG:HG2	1:D:6:ARG:HH11	0.88	1.01
1:A:361:GLU:HG3	2:B:483:HOH:O	1.61	0.99
1:C:287:GLN:HE22	1:C:318:ARG:HH11	1.00	0.98
1:D:147:ALA:HB3	2:D:494:HOH:O	1.67	0.94
1:D:6:ARG:CG	1:D:6:ARG:HH11	1.79	0.94
1:C:287:GLN:HE22	1:C:318:ARG:NH1	1.67	0.93
1:C:287:GLN:NE2	1:C:318:ARG:NH1	2.15	0.92
1:D:6:ARG:HG2	1:D:6:ARG:NH1	1.65	0.91
1:B:316:ASN:HD22	1:B:318:ARG:HE	1.19	0.91
1:D:158:ARG:HH11	1:D:158:ARG:CG	1.88	0.86
1:A:21:PRO:O	1:A:331:GLU:OE2	1.93	0.86
1:A:107:ARG:HD2	2:A:454:HOH:O	1.74	0.85
1:A:316:ASN:HD22	1:A:318:ARG:HE	1.24	0.84
1:C:146:GLN:HG2	1:C:152:THR:HA	1.58	0.84
1:C:172:LYS:HB3	2:C:560:HOH:O	1.77	0.83
1:A:221:GLN:NE2	1:A:245:ASP:H	1.76	0.82
1:A:221:GLN:HE21	1:A:245:ASP:H	1.27	0.82
1:D:198:SER:HB3	2:D:427:HOH:O	1.80	0.80
1:B:48:VAL:HG23	1:B:117:LEU:HD12	1.64	0.78
1:C:191:ARG:CG	1:C:191:ARG:HH11	1.96	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ARG:HG3	1:C:191:ARG:NH1	1.85	0.78
1:A:283:HIS:HE1	1:A:316:ASN:H	1.31	0.78
1:A:283:HIS:CE1	1:A:316:ASN:H	2.02	0.78
1:D:34:THR:O	2:D:563:HOH:O	2.01	0.77
1:D:172:LYS:HB3	2:D:505:HOH:O	1.84	0.77
1:D:145:ILE:O	2:D:681:HOH:O	2.02	0.77
1:C:173:PRO:O	2:C:606:HOH:O	2.02	0.76
1:C:178:GLN:O	1:C:182:CYS:HB2	1.85	0.76
1:D:158:ARG:HG3	1:D:158:ARG:NH1	1.93	0.76
1:B:316:ASN:ND2	1:B:318:ARG:HE	1.83	0.76
1:C:34:THR:N	2:C:561:HOH:O	2.20	0.74
1:B:283:HIS:CE1	1:B:316:ASN:H	2.06	0.73
1:C:142:SER:HB2	1:C:168:LYS:HD2	1.69	0.73
1:C:283:HIS:CE1	1:C:316:ASN:H	2.05	0.73
1:C:287:GLN:HE21	1:C:318:ARG:HH11	1.31	0.73
1:A:331:GLU:OE2	1:A:331:GLU:N	2.22	0.73
1:C:104:ARG:NH2	1:C:250:SER:HB3	2.04	0.73
1:B:316:ASN:HD22	1:B:318:ARG:NE	1.86	0.72
1:B:221:GLN:NE2	1:B:245:ASP:H	1.87	0.72
1:B:283:HIS:HE1	1:B:316:ASN:H	1.37	0.72
1:D:23:LYS:HA	2:D:526:HOH:O	1.91	0.71
1:C:144:GLY:HA2	1:C:170:LYS:HE2	1.72	0.70
1:A:178:GLN:H	1:A:178:GLN:NE2	1.85	0.70
1:D:34:THR:O	1:D:35:HIS:HB2	1.90	0.70
1:D:198:SER:CB	2:D:427:HOH:O	2.38	0.69
1:C:283:HIS:CE1	1:C:314:LEU:HB3	2.28	0.69
1:C:331:GLU:HG2	2:C:465:HOH:O	1.93	0.69
1:C:142:SER:CB	1:C:168:LYS:HD2	2.23	0.68
1:D:207:ARG:O	1:D:210:GLN:HB2	1.94	0.68
1:B:267:ASN:C	1:B:267:ASN:HD22	1.95	0.68
1:C:283:HIS:HE1	1:C:316:ASN:H	1.41	0.68
1:D:146:GLN:NE2	1:D:146:GLN:HA	2.09	0.66
1:B:283:HIS:CE1	1:B:314:LEU:HB3	2.31	0.66
1:A:331:GLU:HG3	2:A:599:HOH:O	1.95	0.65
1:C:146:GLN:HG2	1:C:152:THR:CA	2.25	0.65
1:C:267:ASN:HD21	1:C:296:GLY:HA3	1.62	0.65
1:D:142:SER:HB3	1:D:168:LYS:HD3	1.78	0.65
1:B:181:ARG:O	1:B:185:GLU:HG3	1.97	0.64
1:C:144:GLY:HA2	1:C:170:LYS:CE	2.28	0.64
1:C:168:LYS:HG3	2:C:482:HOH:O	1.98	0.64
1:A:316:ASN:ND2	1:A:318:ARG:HE	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ARG:O	1:B:162:GLN:HG3	1.99	0.63
1:A:223:LEU:H	1:A:231:HIS:CE1	2.17	0.63
1:D:35:HIS:HD2	2:D:563:HOH:O	1.83	0.62
1:A:222:PRO:HD2	1:A:231:HIS:CE1	2.34	0.62
1:C:175:TRP:CE2	1:C:179:PRO:HG3	2.35	0.62
1:D:316:ASN:HD22	1:D:318:ARG:HE	1.46	0.62
1:C:174:GLY:N	2:C:569:HOH:O	2.32	0.61
1:C:184:ARG:O	1:C:188:PRO:HA	2.01	0.61
1:C:22:LEU:HB2	1:C:34:THR:O	2.01	0.60
1:D:6:ARG:N	2:D:680:HOH:O	2.34	0.60
1:D:212:ASP:OD2	1:D:239:ARG:HB2	2.01	0.59
1:C:144:GLY:HA3	2:C:545:HOH:O	2.02	0.59
1:C:267:ASN:HD22	1:C:267:ASN:C	2.05	0.59
1:C:145:ILE:HD13	1:C:146:GLN:H	1.68	0.59
1:B:223:LEU:H	1:B:231:HIS:CE1	2.20	0.59
1:B:221:GLN:HE21	1:B:245:ASP:H	1.49	0.58
1:A:331:GLU:CD	1:A:332:ARG:H	2.07	0.57
1:C:147:ALA:O	1:C:148:ASP:HB3	2.04	0.57
1:C:154:ASP:HB3	2:C:562:HOH:O	2.04	0.57
1:A:209:ARG:HB2	1:A:238:ILE:HG22	1.86	0.57
1:B:267:ASN:HD21	1:B:296:GLY:HA3	1.68	0.56
1:D:185:GLU:O	1:D:188:PRO:HD3	2.06	0.56
1:C:127:GLY:H	1:C:310:HIS:CD2	2.23	0.56
1:C:21:PRO:HA	1:C:35:HIS:HD2	1.71	0.55
1:D:172:LYS:HG2	1:D:175:TRP:HB3	1.87	0.55
1:A:283:HIS:CE1	1:A:314:LEU:HB3	2.40	0.55
1:D:158:ARG:NH1	1:D:158:ARG:CG	2.56	0.55
1:C:168:LYS:HD3	1:C:195:ASP:HB2	1.89	0.55
1:D:207:ARG:HD2	2:D:464:HOH:O	2.07	0.55
1:C:145:ILE:HD11	1:C:175:TRP:HD1	1.73	0.54
1:A:158:ARG:O	1:A:162:GLN:HG3	2.07	0.54
1:D:239:ARG:CD	2:D:624:HOH:O	2.56	0.54
1:B:283:HIS:HD2	1:B:284:ASP:OD1	1.90	0.54
1:C:283:HIS:HD2	1:C:284:ASP:OD1	1.91	0.54
1:C:171:ILE:CG1	1:C:196:ALA:HA	2.39	0.53
1:C:178:GLN:N	1:C:179:PRO:HD2	2.22	0.53
1:D:171:ILE:CG1	1:D:196:ALA:HA	2.39	0.53
1:C:195:ASP:HA	1:C:220:GLU:HB3	1.90	0.53
1:D:184:ARG:O	1:D:188:PRO:HA	2.08	0.53
1:C:117:LEU:O	1:C:121:THR:HG23	2.09	0.53
1:C:175:TRP:N	2:C:569:HOH:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ILE:HB	1:C:176:ASP:HB3	1.91	0.53
1:C:223:LEU:H	1:C:231:HIS:CE1	2.26	0.53
1:D:147:ALA:CB	2:D:494:HOH:O	2.39	0.52
1:A:22:LEU:HD23	1:A:330:TRP:CZ3	2.45	0.52
1:A:178:GLN:N	1:A:178:GLN:HE21	1.88	0.52
1:C:34:THR:HG22	2:C:535:HOH:O	2.09	0.52
1:B:103:ASN:O	1:B:107:ARG:HG2	2.09	0.52
1:A:159:HIS:HD2	1:A:162:GLN:OE1	1.93	0.51
1:C:179:PRO:O	1:C:182:CYS:HB3	2.09	0.51
1:A:316:ASN:HD22	1:A:318:ARG:NE	2.01	0.51
1:A:89:ASN:HB2	1:A:90:PRO:CD	2.41	0.51
1:A:283:HIS:HD2	1:A:284:ASP:OD1	1.93	0.51
1:C:181:ARG:HB2	1:C:214:TYR:CZ	2.46	0.51
1:A:244:LEU:CD2	1:A:263:GLY:HA3	2.40	0.51
1:A:244:LEU:HD21	1:A:263:GLY:HA3	1.92	0.50
1:B:48:VAL:HG23	1:B:117:LEU:CD1	2.37	0.50
1:D:195:ASP:C	1:D:197:ASN:H	2.15	0.50
1:B:301:SER:OG	1:B:334:LEU:HD11	2.11	0.50
1:C:200:TYR:HA	1:C:204:ASP:OD2	2.12	0.50
1:A:222:PRO:HD2	1:A:231:HIS:HE1	1.75	0.49
1:D:195:ASP:HA	1:D:220:GLU:HB3	1.94	0.49
1:C:151:ALA:HB1	2:C:574:HOH:O	2.10	0.49
1:A:6:ARG:N	2:A:509:HOH:O	2.45	0.49
1:B:6:ARG:N	2:B:429:HOH:O	2.45	0.49
1:C:48:VAL:HG23	1:C:117:LEU:HD12	1.95	0.49
1:A:181:ARG:O	1:A:185:GLU:HG3	2.13	0.49
1:C:227:ASP:OD2	1:C:231:HIS:HD2	1.95	0.48
1:B:267:ASN:C	1:B:267:ASN:ND2	2.64	0.48
1:D:196:ALA:HB3	1:D:222:PRO:HA	1.96	0.48
1:D:172:LYS:O	1:D:176:ASP:OD2	2.30	0.48
1:A:48:VAL:HG23	1:A:117:LEU:HD12	1.94	0.48
1:D:239:ARG:HD2	2:D:624:HOH:O	2.12	0.48
1:A:89:ASN:ND2	1:A:92:ALA:H	2.12	0.48
1:D:146:GLN:CG	1:D:152:THR:HA	2.44	0.47
1:D:178:GLN:N	1:D:179:PRO:HD2	2.30	0.47
1:C:89:ASN:HB2	1:C:90:PRO:CD	2.45	0.47
1:B:78:PHE:CZ	1:B:107:ARG:HD2	2.49	0.47
1:A:331:GLU:HG2	2:A:421:HOH:O	2.14	0.47
1:D:178:GLN:HE21	1:D:178:GLN:HB2	1.60	0.46
1:C:145:ILE:HD13	1:C:146:GLN:N	2.29	0.46
1:C:180:VAL:HG21	1:C:211:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:MET:HB3	1:D:87:PHE:O	2.16	0.46
1:A:89:ASN:HD22	1:A:92:ALA:H	1.63	0.45
1:C:57:GLU:HG2	2:C:642:HOH:O	2.16	0.45
1:B:107:ARG:HE	1:B:107:ARG:HB3	1.65	0.45
1:C:6:ARG:HB2	1:C:6:ARG:CZ	2.45	0.45
1:C:183:THR:O	1:C:187:PHE:N	2.50	0.44
1:A:220:GLU:OE1	2:A:711:HOH:O	2.21	0.44
1:B:371:GLU:HG3	1:B:373:HIS:CE1	2.52	0.44
1:C:154:ASP:CB	2:C:562:HOH:O	2.63	0.44
1:C:371:GLU:OE1	1:C:373:HIS:NE2	2.36	0.44
1:C:171:ILE:HG13	1:C:196:ALA:HA	1.98	0.44
1:B:11:GLU:HG2	2:B:557:HOH:O	2.17	0.44
1:C:267:ASN:ND2	1:C:267:ASN:C	2.71	0.44
1:B:223:LEU:H	1:B:231:HIS:HE1	1.65	0.44
1:D:198:SER:N	1:D:221:GLN:O	2.50	0.43
1:D:35:HIS:CD2	2:D:563:HOH:O	2.65	0.43
1:D:165:ARG:HG3	1:D:344:GLY:HA3	2.00	0.43
1:C:142:SER:HB3	1:C:168:LYS:HD2	1.99	0.43
1:A:60:PRO:HG2	1:C:100:TYR:HB3	2.00	0.43
1:D:191:ARG:HG3	1:D:217:THR:OG1	2.18	0.43
1:C:197:ASN:O	1:C:199:ALA:N	2.52	0.43
1:A:244:LEU:N	1:A:244:LEU:HD22	2.33	0.43
1:D:144:GLY:HA3	2:D:474:HOH:O	2.18	0.43
1:A:331:GLU:CG	2:A:421:HOH:O	2.66	0.43
1:D:36:LYS:HE3	1:D:299:LEU:HB2	1.99	0.43
1:A:331:GLU:N	1:A:331:GLU:CD	2.71	0.43
1:D:316:ASN:HD22	1:D:318:ARG:NE	2.14	0.43
1:D:195:ASP:C	1:D:197:ASN:N	2.72	0.43
1:C:302:GLY:HA3	1:C:335:ILE:HD13	2.01	0.43
1:A:283:HIS:CE1	1:A:316:ASN:HB3	2.54	0.43
1:C:227:ASP:OD2	1:C:231:HIS:CD2	2.72	0.43
1:D:15:ILE:O	1:D:370:GLN:HA	2.19	0.43
1:A:94:SER:OG	1:A:111:GLU:HG3	2.19	0.42
1:A:89:ASN:HB2	1:A:90:PRO:HD2	2.00	0.42
1:D:89:ASN:HD22	1:D:92:ALA:H	1.67	0.42
1:C:196:ALA:HB3	1:C:222:PRO:HA	2.01	0.42
1:D:178:GLN:H	1:D:179:PRO:HD2	1.84	0.42
1:A:239:ARG:NH1	2:A:422:HOH:O	2.15	0.42
1:B:255:ARG:C	1:B:255:ARG:HD2	2.40	0.42
1:C:195:ASP:O	1:C:197:ASN:N	2.53	0.42
1:C:21:PRO:HA	1:C:35:HIS:CD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:THR:HG21	1:A:218:TYR:CZ	2.55	0.42
1:A:193:THR:HG22	1:A:217:THR:HB	2.01	0.42
1:A:255:ARG:HD2	1:A:255:ARG:C	2.39	0.42
1:A:331:GLU:O	1:B:158:ARG:NH2	2.53	0.42
1:D:176:ASP:O	1:D:180:VAL:HG23	2.19	0.42
1:C:90:PRO:HG2	1:C:115:TRP:CD2	2.54	0.42
1:D:238:ILE:HD11	1:D:242:LEU:HD21	2.01	0.42
1:B:360:ARG:HD2	1:B:360:ARG:HA	1.82	0.42
1:A:176:ASP:H	1:A:178:GLN:HE22	1.67	0.42
1:B:299:LEU:HD13	2:B:624:HOH:O	2.20	0.42
1:C:14:GLU:HG2	1:C:372:GLU:HG3	2.01	0.42
1:C:184:ARG:NH2	1:C:190:ILE:O	2.48	0.41
1:D:266:ILE:HB	1:D:293:VAL:HG12	2.02	0.41
1:A:222:PRO:CD	1:A:231:HIS:HE1	2.32	0.41
1:C:89:ASN:HB2	1:C:90:PRO:HD2	2.01	0.41
1:C:145:ILE:CD1	1:C:175:TRP:HD1	2.32	0.41
1:C:158:ARG:HB3	1:C:158:ARG:HE	1.69	0.41
1:B:371:GLU:HG3	1:B:373:HIS:HE1	1.85	0.41
1:D:89:ASN:HB2	1:D:90:PRO:CD	2.50	0.41
1:B:270:VAL:HA	1:B:279:SER:OG	2.21	0.41
1:A:305:ARG:O	1:A:309:ILE:HG13	2.20	0.41
1:C:310:HIS:HE1	1:C:354:THR:O	2.04	0.41
1:D:172:LYS:CB	2:D:505:HOH:O	2.57	0.41
1:B:267:ASN:HD22	1:B:268:LEU:N	2.18	0.41
1:C:172:LYS:HD2	1:C:175:TRP:HB3	2.02	0.41
1:D:63:ARG:HB3	2:D:419:HOH:O	2.21	0.41
1:B:7:MET:HG2	1:B:88:ALA:HA	2.02	0.41
1:A:184:ARG:HA	1:A:184:ARG:HD3	1.79	0.41
1:D:174:GLY:HA2	2:D:547:HOH:O	2.21	0.41
1:D:287:GLN:HE21	1:D:318:ARG:HH21	1.69	0.40
1:B:19:ARG:HG2	1:B:35:HIS:HB3	2.03	0.40
1:B:54:GLY:HA2	2:B:377:HOH:O	2.21	0.40
1:C:22:LEU:HB3	1:C:23:LYS:H	1.70	0.40
1:C:187:PHE:N	1:C:188:PRO:HD3	2.36	0.40
1:D:245:ASP:OD2	1:D:272:ARG:NH2	2.55	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)
2:B:715:HOH:O	2:B:715:HOH:O[4_555]	2.01	0.19

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%)	343 (96%)	13 (4%)	0	100	100
1	B	356/375 (95%)	346 (97%)	10 (3%)	0	100	100
1	C	356/375 (95%)	337 (95%)	15 (4%)	4 (1%)	17	14
1	D	356/375 (95%)	338 (95%)	15 (4%)	3 (1%)	24	22
All	All	1424/1500 (95%)	1364 (96%)	53 (4%)	7 (0%)	34	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	182	CYS
1	C	198	SER
1	D	35	HIS
1	C	196	ALA
1	C	215	ASP
1	D	198	SER
1	D	215	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%)	275 (96%)	10 (4%)	43	53
1	B	285/297 (96%)	279 (98%)	6 (2%)	61	74
1	C	285/297 (96%)	271 (95%)	14 (5%)	31	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	285/297 (96%)	273 (96%)	12 (4%)	36 44
All	All	1140/1188 (96%)	1098 (96%)	42 (4%)	41 50

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	56	MET
1	A	89	ASN
1	A	149	CYS
1	A	176	ASP
1	A	178	GLN
1	A	331	GLU
1	A	350	GLN
1	A	361	GLU
1	A	368	GLU
1	B	6	ARG
1	B	107	ARG
1	B	149	CYS
1	B	267	ASN
1	B	283	HIS
1	B	334	LEU
1	C	6	ARG
1	C	20	LEU
1	C	22	LEU
1	C	34	THR
1	C	136	GLN
1	C	141	VAL
1	C	145	ILE
1	C	148	ASP
1	C	149	CYS
1	C	172	LYS
1	C	176	ASP
1	C	191	ARG
1	C	215	ASP
1	C	267	ASN
1	D	6	ARG
1	D	49	GLN
1	D	89	ASN
1	D	134	LYS
1	D	145	ILE
1	D	146	GLN

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Mol	Chain	Res	Type
1	D	158	ARG
1	D	172	LYS
1	D	176	ASP
1	D	178	GLN
1	D	280	ARG
1	D	374	ARG

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	89	ASN
1	A	103	ASN
1	A	159	HIS
1	A	178	GLN
1	A	197	ASN
1	A	221	GLN
1	A	231	HIS
1	A	283	HIS
1	A	316	ASN
1	B	35	HIS
1	B	49	GLN
1	B	221	GLN
1	B	231	HIS
1	B	267	ASN
1	B	283	HIS
1	B	316	ASN
1	B	373	HIS
1	C	85	GLN
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	49	GLN
1	D	89	ASN
1	D	146	GLN
1	D	178	GLN
1	D	287	GLN
1	D	316	ASN

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	360/375 (96%)	-0.85	0 100 100	8, 16, 31, 55	0
1	B	360/375 (96%)	-0.85	1 (0%) 94 94	9, 16, 31, 52	0
1	C	360/375 (96%)	-0.47	14 (3%) 43 42	9, 19, 53, 68	0
1	D	360/375 (96%)	-0.46	12 (3%) 50 49	9, 19, 53, 67	0
All	All	1440/1500 (96%)	-0.66	27 (1%) 70 68	8, 17, 47, 68	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	175	TRP	8.8
1	D	175	TRP	6.7
1	C	174	GLY	3.7
1	D	174	GLY	3.7
1	D	152	THR	3.5
1	C	185	GLU	3.4
1	D	178	GLN	3.4
1	C	178	GLN	3.2
1	C	149	CYS	3.1
1	D	34	THR	3.1
1	D	35	HIS	3.0
1	D	149	CYS	3.0
1	C	152	THR	2.9
1	D	214	TYR	2.9
1	D	146	GLN	2.7
1	C	150	GLN	2.6
1	C	181	ARG	2.5
1	C	214	TYR	2.5
1	C	146	GLN	2.5
1	C	145	ILE	2.5
1	D	150	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	181	ARG	2.4
1	C	147	ALA	2.4
1	D	196	ALA	2.4
1	B	34	THR	2.2
1	C	173	PRO	2.2
1	C	35	HIS	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.