Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 09:21 AM EDT

PDB ID	:	2FKP
Title	:	The mutant G127C-T313C of Deinococcus Radiodurans N-acylamino acid racemase
Authors	:	Wang, W.C.; Chiu, W.C.
Deposited on	:	2006-01-05
Resolution	:	2.00 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:

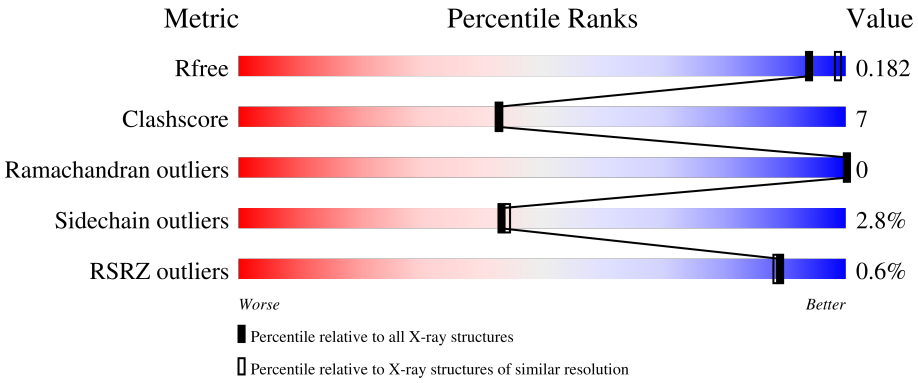
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	86% 9%
1	B	375	85% 10%
1	C	375	% 81% 14%
1	D	375	% 86% 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11959 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
			2767	1733	507	515	12			
1	B	360	Total	C	N	O	S	0	0	0
			2767	1733	507	515	12			
1	C	360	Total	C	N	O	S	0	0	0
			2767	1733	507	515	12			
1	D	360	Total	C	N	O	S	0	0	0
			2767	1733	507	515	12			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	SER	ALA	SEE REMARK 999	GB 15805085
A	127	CYS	GLY	engineered mutation	GB 15805085
A	148	ASP	GLY	SEE REMARK 999	GB 15805085
A	158	ARG	LYS	SEE REMARK 999	GB 15805085
A	252	SER	ALA	SEE REMARK 999	GB 15805085
A	313	CYS	THR	engineered mutation	GB 15805085
A	315	SER	PRO	SEE REMARK 999	GB 15805085
B	94	SER	ALA	SEE REMARK 999	GB 15805085
B	127	CYS	GLY	engineered mutation	GB 15805085
B	148	ASP	GLY	SEE REMARK 999	GB 15805085
B	158	ARG	LYS	SEE REMARK 999	GB 15805085
B	252	SER	ALA	SEE REMARK 999	GB 15805085
B	313	CYS	THR	engineered mutation	GB 15805085
B	315	SER	PRO	SEE REMARK 999	GB 15805085
C	94	SER	ALA	SEE REMARK 999	GB 15805085
C	127	CYS	GLY	engineered mutation	GB 15805085
C	148	ASP	GLY	SEE REMARK 999	GB 15805085
C	158	ARG	LYS	SEE REMARK 999	GB 15805085
C	252	SER	ALA	SEE REMARK 999	GB 15805085
C	313	CYS	THR	engineered mutation	GB 15805085
C	315	SER	PRO	SEE REMARK 999	GB 15805085

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Chain	Residue	Modelled	Actual	Comment	Reference
D	94	SER	ALA	SEE REMARK 999	GB 15805085
D	127	CYS	GLY	engineered mutation	GB 15805085
D	148	ASP	GLY	SEE REMARK 999	GB 15805085
D	158	ARG	LYS	SEE REMARK 999	GB 15805085
D	252	SER	ALA	SEE REMARK 999	GB 15805085
D	313	CYS	THR	engineered mutation	GB 15805085
D	315	SER	PRO	SEE REMARK 999	GB 15805085

- Molecule 2 is water.

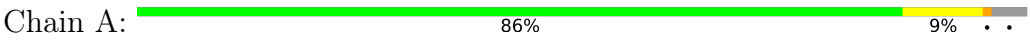
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	266	Total O 266 266	0	0
2	B	253	Total O 253 253	0	0
2	C	191	Total O 191 191	0	0
2	D	181	Total O 181 181	0	0

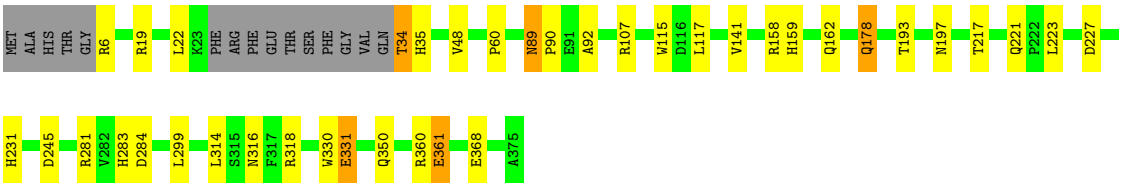
3 Residue-property plots (i)

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

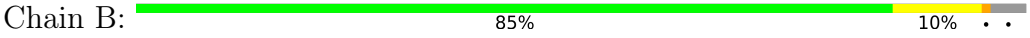
Chain A:

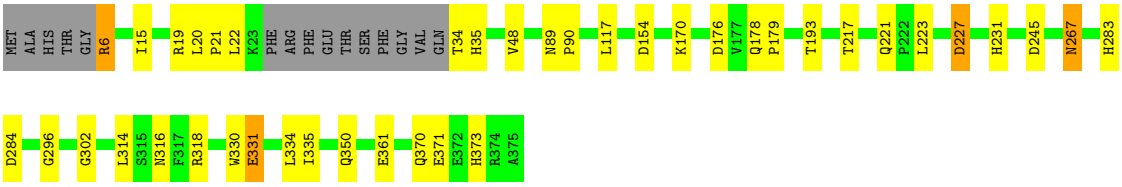




• Molecule 1: N-acylamino acid racemase

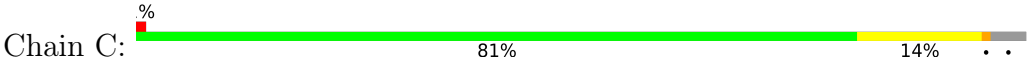
Chain B:

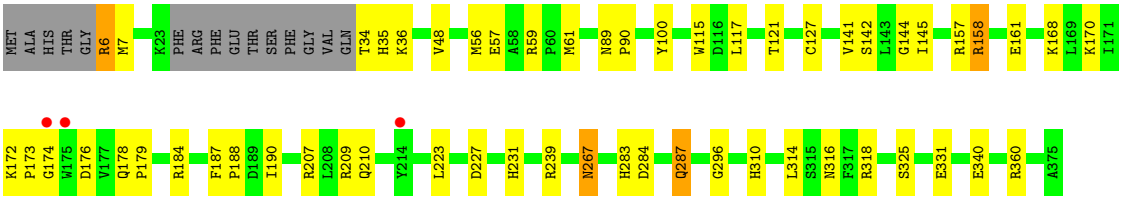




• Molecule 1: N-acylamino acid racemase

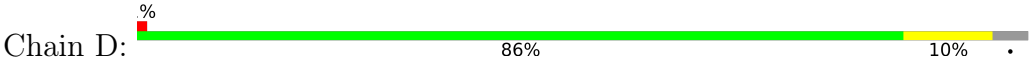
Chain C:

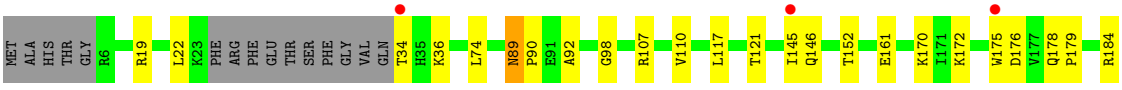


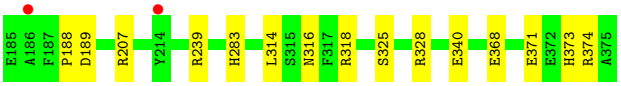


• Molecule 1: N-acylamino acid racemase

Chain D:






E185
A186
F187
P188
D189
R207
Y214
R239
H283
L314
S315
N316
F317
R318
S325
R328
E340
E368
E371
E372
H373
R374
A375

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α, β, γ	116.13Å 116.13Å 120.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 23.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (30.00-2.00) 97.1 (23.60-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.182 , 0.227 0.186 , 0.182	Depositor DCC
R_{free} test set	5255 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 28.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.006 for -h,-l,-k 0.005 for -h,l,k 0.009 for l,-k,h 0.008 for -l,-k,-h 0.487 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11959	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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	0.63	2/2818 (0.1%)	0.68	1/3823 (0.0%)
1	B	0.61	0/2818	0.67	0/3823
1	C	0.58	0/2818	0.66	0/3823
1	D	0.58	0/2818	0.64	0/3823
All	All	0.60	2/11272 (0.0%)	0.66	1/15292 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	GLU	CG-CD	6.22	1.61	1.51
1	A	361	GLU	CB-CG	5.47	1.62	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	281	ARG	NE-CZ-NH2	-6.07	117.27	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2767	0	2768	35	0
1	B	2767	0	2769	30	0
1	C	2767	0	2769	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2767	0	2769	25	0
2	A	266	0	0	3	0
2	B	253	0	0	3	0
2	C	191	0	0	8	0
2	D	181	0	0	2	0
All	All	11959	0	11075	150	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 7.

All (150) 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:HE22	1:C:318:ARG:HH11	1.03	0.99
1:A:178:GLN:HE21	1:A:178:GLN:H	1.07	0.94
1:A:107:ARG:HD2	2:A:606:HOH:O	1.72	0.89
1:C:331:GLU:HG2	2:C:412:HOH:O	1.75	0.86
1:A:283:HIS:HE1	1:A:316:ASN:H	1.24	0.85
1:B:283:HIS:HE1	1:B:316:ASN:H	1.25	0.85
1:B:316:ASN:HD22	1:B:318:ARG:HE	1.23	0.85
1:A:283:HIS:CE1	1:A:316:ASN:H	1.97	0.83
1:A:221:GLN:NE2	1:A:245:ASP:H	1.77	0.82
1:C:127:CYS:H	1:C:310:HIS:HD2	1.26	0.81
1:B:154:ASP:HB2	2:B:609:HOH:O	1.81	0.80
1:C:207:ARG:HG2	2:C:468:HOH:O	1.87	0.74
1:C:283:HIS:CE1	1:C:316:ASN:H	2.05	0.74
1:B:221:GLN:NE2	1:B:245:ASP:H	1.86	0.74
1:C:287:GLN:NE2	1:C:318:ARG:HH11	1.83	0.74
1:C:283:HIS:HE1	1:C:316:ASN:H	1.34	0.73
1:A:316:ASN:HD22	1:A:318:ARG:HE	1.37	0.72
1:B:221:GLN:HE21	1:B:245:ASP:H	1.38	0.72
1:B:283:HIS:CE1	1:B:316:ASN:H	2.06	0.72
1:C:144:GLY:HA2	1:C:170:LYS:HE3	1.70	0.71
1:A:221:GLN:HE21	1:A:245:ASP:H	1.36	0.71
1:A:48:VAL:HG23	1:A:117:LEU:HD12	1.73	0.71
1:D:316:ASN:HD22	1:D:318:ARG:HE	1.38	0.71
1:B:267:ASN:HD21	1:B:296:GLY:HA3	1.55	0.71
1:C:145:ILE:H	1:C:170:LYS:NZ	1.89	0.71
1:C:173:PRO:O	2:C:479:HOH:O	2.10	0.70
1:A:283:HIS:CE1	1:A:314:LEU:HB3	2.26	0.70
1:D:188:PRO:HG2	1:D:189:ASP:OD2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:ASN:C	1:B:267:ASN:HD22	1.95	0.68
1:C:283:HIS:CE1	1:C:314:LEU:HB3	2.29	0.68
1:A:178:GLN:H	1:A:178:GLN:NE2	1.88	0.67
1:C:178:GLN:HB2	1:C:179:PRO:CD	2.24	0.67
1:B:48:VAL:HG23	1:B:117:LEU:HD12	1.77	0.66
1:C:127:CYS:H	1:C:310:HIS:CD2	2.12	0.66
1:B:316:ASN:ND2	1:B:318:ARG:HE	1.94	0.66
1:B:6:ARG:N	2:B:538:HOH:O	2.29	0.64
1:B:283:HIS:CE1	1:B:314:LEU:HB3	2.33	0.63
1:D:98:GLY:O	1:D:107:ARG:NH2	2.32	0.61
1:C:6:ARG:HB2	1:C:6:ARG:CZ	2.29	0.61
1:C:157:ARG:O	1:C:161:GLU:HG3	1.99	0.61
1:B:316:ASN:HD22	1:B:318:ARG:NE	1.98	0.61
1:B:361:GLU:HG3	2:B:533:HOH:O	2.01	0.60
1:C:267:ASN:C	1:C:267:ASN:HD22	2.05	0.60
1:B:283:HIS:HD2	1:B:284:ASP:OD1	1.85	0.60
1:C:267:ASN:HD21	1:C:296:GLY:HA3	1.65	0.59
1:A:19:ARG:HD3	1:A:368:GLU:OE2	2.03	0.59
1:A:34:THR:OG1	1:A:35:HIS:N	2.37	0.57
1:C:158:ARG:HH21	1:C:158:ARG:HG3	1.70	0.57
1:B:371:GLU:OE2	1:B:373:HIS:HE1	1.88	0.56
1:A:223:LEU:H	1:A:231:HIS:CE1	2.24	0.56
1:C:209:ARG:NH2	1:C:239:ARG:NH1	2.54	0.55
1:A:159:HIS:HD2	1:A:162:GLN:OE1	1.89	0.55
1:C:6:ARG:CG	1:C:6:ARG:HH21	2.18	0.55
1:C:227:ASP:OD2	1:C:231:HIS:HD2	1.90	0.54
1:B:223:LEU:H	1:B:231:HIS:CE1	2.25	0.54
1:C:283:HIS:HD2	1:C:284:ASP:OD1	1.90	0.53
1:C:7:MET:HE2	2:C:510:HOH:O	2.08	0.53
1:C:207:ARG:NH1	1:C:210:GLN:OE1	2.39	0.53
1:C:158:ARG:HG3	1:C:158:ARG:NH2	2.23	0.53
1:C:34:THR:HB	1:C:35:HIS:HD2	1.74	0.53
1:A:197:ASN:ND2	2:A:631:HOH:O	2.42	0.52
1:B:227:ASP:OD1	1:B:231:HIS:HD2	1.93	0.52
1:C:61:MET:HE1	2:C:532:HOH:O	2.10	0.51
1:C:6:ARG:HH21	1:C:6:ARG:HG2	1.76	0.51
1:C:34:THR:N	2:C:513:HOH:O	2.43	0.51
1:D:316:ASN:ND2	1:D:318:ARG:HE	2.09	0.50
1:A:283:HIS:HD2	1:A:284:ASP:OD1	1.94	0.50
1:A:159:HIS:HE1	2:A:596:HOH:O	1.95	0.50
1:C:178:GLN:HB2	1:C:179:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ARG:NH2	1:C:6:ARG:CB	2.76	0.49
1:D:184:ARG:HD2	1:D:188:PRO:HA	1.93	0.49
1:A:22:LEU:HD12	1:A:34:THR:N	2.27	0.49
1:C:223:LEU:H	1:C:231:HIS:CE1	2.29	0.49
1:D:117:LEU:O	1:D:121:THR:HG23	2.11	0.49
1:D:19:ARG:HD3	1:D:368:GLU:OE1	2.12	0.49
1:C:48:VAL:HG23	1:C:117:LEU:HD12	1.95	0.49
1:C:227:ASP:OD2	1:C:231:HIS:CD2	2.66	0.49
1:A:158:ARG:NH1	1:B:331:GLU:O	2.46	0.49
1:D:178:GLN:HB2	1:D:179:PRO:CD	2.43	0.48
1:B:193:THR:HG22	1:B:217:THR:HB	1.95	0.48
1:A:89:ASN:ND2	1:A:92:ALA:H	2.12	0.48
1:A:316:ASN:HD22	1:A:318:ARG:NE	2.10	0.48
1:C:145:ILE:HD13	1:C:172:LYS:HE2	1.96	0.48
1:C:184:ARG:HD2	1:C:188:PRO:HA	1.96	0.48
1:D:325:SER:HB3	1:D:340:GLU:OE2	2.14	0.48
1:A:193:THR:HG22	1:A:217:THR:HB	1.95	0.48
1:C:61:MET:CE	2:C:532:HOH:O	2.62	0.48
1:C:7:MET:CE	2:C:510:HOH:O	2.61	0.47
1:D:89:ASN:ND2	1:D:92:ALA:H	2.12	0.47
1:C:287:GLN:HE22	1:C:318:ARG:NH1	1.88	0.47
1:C:360:ARG:HA	1:C:360:ARG:HD2	1.70	0.47
1:D:283:HIS:NE2	1:D:314:LEU:HB3	2.29	0.47
1:C:90:PRO:HG2	1:C:115:TRP:CD2	2.50	0.47
1:A:22:LEU:HD23	1:A:330:TRP:CZ3	2.51	0.46
1:A:227:ASP:OD2	1:A:231:HIS:HD2	1.97	0.46
1:C:142:SER:HB3	1:C:168:LYS:HE3	1.97	0.46
1:D:89:ASN:HD22	1:D:92:ALA:H	1.64	0.46
1:D:316:ASN:HD22	1:D:318:ARG:NE	2.09	0.46
1:B:302:GLY:HA3	1:B:335:ILE:HD13	1.98	0.46
1:A:19:ARG:HG2	1:A:35:HIS:HB3	1.98	0.46
1:B:267:ASN:C	1:B:267:ASN:ND2	2.67	0.45
1:A:90:PRO:HG2	1:A:115:TRP:CD2	2.51	0.45
1:A:331:GLU:N	1:A:331:GLU:OE2	2.48	0.45
1:B:178:GLN:N	1:B:179:PRO:HD2	2.31	0.45
1:C:178:GLN:HB2	1:C:179:PRO:HD2	1.98	0.45
1:D:161:GLU:HG3	2:D:418:HOH:O	2.16	0.45
1:A:141:VAL:HG11	1:A:159:HIS:HB3	1.98	0.45
1:C:145:ILE:H	1:C:170:LYS:HZ2	1.62	0.45
1:D:325:SER:O	1:D:328:ARG:HB2	2.16	0.44
1:D:175:TRP:CE2	1:D:179:PRO:HD3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLN:HE21	1:A:178:GLN:N	1.91	0.44
1:D:74:LEU:HD21	1:D:110:VAL:HG23	1.98	0.44
1:B:34:THR:OG1	1:B:35:HIS:HD2	2.01	0.44
1:A:60:PRO:HG2	1:C:100:TYR:HB3	2.00	0.44
1:B:22:LEU:HD23	1:B:330:TRP:CZ3	2.53	0.44
1:C:6:ARG:HB2	1:C:6:ARG:NH2	2.32	0.44
1:C:267:ASN:C	1:C:267:ASN:ND2	2.71	0.44
1:D:184:ARG:HA	1:D:184:ARG:HD3	1.76	0.44
1:C:89:ASN:HB2	1:C:90:PRO:CD	2.47	0.43
1:C:207:ARG:O	1:C:210:GLN:HB2	2.17	0.43
1:C:145:ILE:H	1:C:170:LYS:HZ1	1.61	0.43
1:C:283:HIS:HE1	1:C:316:ASN:N	2.11	0.43
1:A:89:ASN:HD22	1:A:92:ALA:H	1.65	0.43
1:A:360:ARG:HA	1:A:360:ARG:HD2	1.84	0.43
1:B:170:LYS:HB2	1:B:170:LYS:HE3	1.87	0.43
1:C:34:THR:HB	1:C:35:HIS:CD2	2.52	0.43
1:B:283:HIS:CE1	1:B:316:ASN:HB3	2.54	0.43
1:C:178:GLN:CB	1:C:179:PRO:CD	2.94	0.43
1:D:161:GLU:CG	2:D:418:HOH:O	2.66	0.43
1:A:48:VAL:HG23	1:A:117:LEU:CD1	2.44	0.43
1:C:158:ARG:HH21	1:C:158:ARG:CG	2.32	0.43
1:B:15:ILE:O	1:B:370:GLN:HA	2.19	0.42
1:C:283:HIS:CE1	1:C:316:ASN:HB3	2.54	0.42
1:B:89:ASN:HB2	1:B:90:PRO:CD	2.50	0.42
1:C:117:LEU:O	1:C:121:THR:HG23	2.20	0.42
1:C:325:SER:HB3	1:C:340:GLU:OE2	2.19	0.42
1:D:145:ILE:CD1	1:D:172:LYS:HG2	2.49	0.42
1:B:20:LEU:HA	1:B:21:PRO:HD3	1.92	0.42
1:C:184:ARG:HD3	1:C:184:ARG:HA	1.69	0.42
1:D:146:GLN:HB2	1:D:152:THR:OG1	2.20	0.42
1:A:89:ASN:HD22	1:A:89:ASN:C	2.24	0.41
1:D:89:ASN:HB2	1:D:90:PRO:CD	2.49	0.41
1:A:316:ASN:ND2	1:A:318:ARG:HE	2.11	0.41
1:C:173:PRO:HA	1:C:174:GLY:HA2	1.79	0.41
1:D:74:LEU:HA	1:D:74:LEU:HD23	1.78	0.41
1:D:371:GLU:OE1	1:D:373:HIS:NE2	2.49	0.41
1:D:170:LYS:HE2	1:D:170:LYS:HB2	1.83	0.40
1:C:6:ARG:CG	1:C:6:ARG:NH2	2.82	0.40
1:C:187:PHE:HB3	1:C:190:ILE:HG23	2.03	0.40
1:C:57:GLU:HB2	1:C:59:ARG:O	2.22	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	356/375 (95%)	342 (96%)	14 (4%)	0	100	100
1	B	356/375 (95%)	345 (97%)	11 (3%)	0	100	100
1	C	356/375 (95%)	344 (97%)	12 (3%)	0	100	100
1	D	356/375 (95%)	341 (96%)	15 (4%)	0	100	100
All	All	1424/1500 (95%)	1372 (96%)	52 (4%)	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	285/297 (96%)	277 (97%)	8 (3%)	43	44
1	B	285/297 (96%)	277 (97%)	8 (3%)	43	44
1	C	285/297 (96%)	277 (97%)	8 (3%)	43	44
1	D	285/297 (96%)	277 (97%)	8 (3%)	43	44
All	All	1140/1188 (96%)	1108 (97%)	32 (3%)	43	44

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	34	THR

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Mol	Chain	Res	Type
1	A	89	ASN
1	A	178	GLN
1	A	299	LEU
1	A	331	GLU
1	A	350	GLN
1	A	361	GLU
1	B	6	ARG
1	B	19	ARG
1	B	176	ASP
1	B	227	ASP
1	B	267	ASN
1	B	331	GLU
1	B	334	LEU
1	B	350	GLN
1	C	6	ARG
1	C	36	LYS
1	C	56	MET
1	C	141	VAL
1	C	158	ARG
1	C	176	ASP
1	C	267	ASN
1	C	287	GLN
1	D	22	LEU
1	D	34	THR
1	D	36	LYS
1	D	89	ASN
1	D	176	ASP
1	D	207	ARG
1	D	239	ARG
1	D	374	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	89	ASN
1	A	103	ASN
1	A	136	GLN
1	A	159	HIS
1	A	178	GLN
1	A	197	ASN
1	A	221	GLN

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Mol	Chain	Res	Type
1	A	231	HIS
1	A	283	HIS
1	A	316	ASN
1	B	35	HIS
1	B	85	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	35	HIS
1	C	136	GLN
1	C	150	GLN
1	C	231	HIS
1	C	267	ASN
1	C	283	HIS
1	C	287	GLN
1	C	310	HIS
1	D	35	HIS
1	D	85	GLN
1	D	89	ASN
1	D	103	ASN
1	D	146	GLN
1	D	150	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 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	360/375 (96%)	-0.77	0	100	100	11, 16, 28, 42	0
1	B	360/375 (96%)	-0.77	0	100	100	11, 16, 29, 41	0
1	C	360/375 (96%)	-0.48	3 (0%)	86	85	10, 19, 40, 44	0
1	D	360/375 (96%)	-0.49	5 (1%)	75	74	10, 19, 39, 45	0
All	All	1440/1500 (96%)	-0.63	8 (0%)	89	88	10, 17, 38, 45	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	175	TRP	3.3
1	C	214	TYR	3.3
1	D	34	THR	3.2
1	D	175	TRP	2.7
1	D	214	TYR	2.7
1	D	186	ALA	2.7
1	D	145	ILE	2.5
1	C	174	GLY	2.2

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.