Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2023 – 02:07 PM JST

PDB ID	:	8I99
Title	:	N-carbamoyl-D-amino-acid hydrolase mutant - M4Th3
Authors	:	Hu, J.M.; Ni, Y.; Xu, G.C.
Deposited on	:	2023-02-06
Resolution	:	3.17 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:

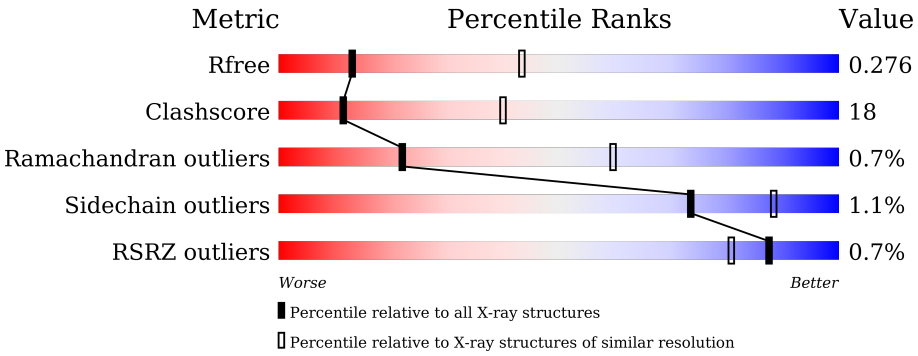
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 3.17 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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	307	65% 34%
1	B	307	61% 38%
1	C	307	61% 36%
1	D	307	64% 35%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9680 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-carbamoyl-D-amino-acid hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2410	1517	434	445	14			
1	B	307	Total	C	N	O	S	0	0	0
			2430	1529	437	450	14			
1	C	304	Total	C	N	O	S	0	0	0
			2410	1517	434	445	14			
1	D	307	Total	C	N	O	S	0	0	0
			2430	1529	437	450	14			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	ASN	ASP	conflict	UNP K2NMS4
A	200	ASN	ALA	conflict	UNP K2NMS4
A	202	PRO	SER	engineered mutation	UNP K2NMS4
A	207	ALA	SER	conflict	UNP K2NMS4
A	208	ASP	GLU	engineered mutation	UNP K2NMS4
A	211	GLY	ARG	conflict	UNP K2NMS4
A	277	LEU	ARG	engineered mutation	UNP K2NMS4
B	187	ASN	ASP	conflict	UNP K2NMS4
B	200	ASN	ALA	conflict	UNP K2NMS4
B	202	PRO	SER	engineered mutation	UNP K2NMS4
B	207	ALA	SER	conflict	UNP K2NMS4
B	208	ASP	GLU	engineered mutation	UNP K2NMS4
B	211	GLY	ARG	conflict	UNP K2NMS4
B	277	LEU	ARG	engineered mutation	UNP K2NMS4
C	187	ASN	ASP	conflict	UNP K2NMS4
C	200	ASN	ALA	conflict	UNP K2NMS4
C	202	PRO	SER	engineered mutation	UNP K2NMS4
C	207	ALA	SER	conflict	UNP K2NMS4
C	208	ASP	GLU	engineered mutation	UNP K2NMS4
C	211	GLY	ARG	conflict	UNP K2NMS4
C	277	LEU	ARG	engineered mutation	UNP K2NMS4

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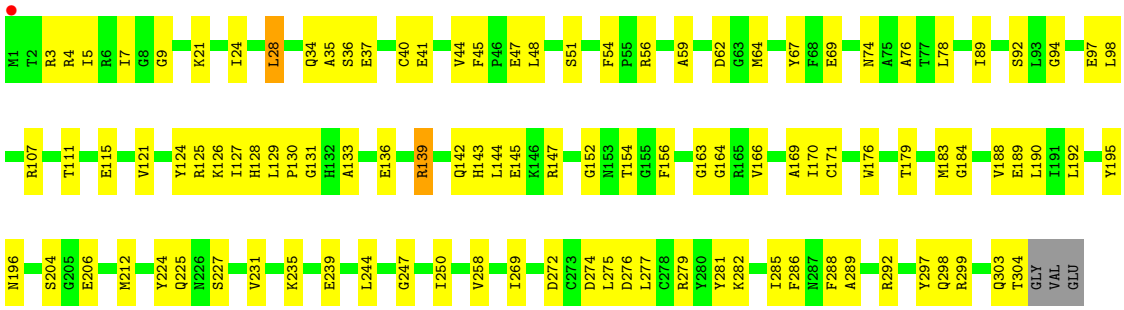
Chain	Residue	Modelled	Actual	Comment	Reference
D	187	ASN	ASP	conflict	UNP K2NMS4
D	200	ASN	ALA	conflict	UNP K2NMS4
D	202	PRO	SER	engineered mutation	UNP K2NMS4
D	207	ALA	SER	conflict	UNP K2NMS4
D	208	ASP	GLU	engineered mutation	UNP K2NMS4
D	211	GLY	ARG	conflict	UNP K2NMS4
D	277	LEU	ARG	engineered mutation	UNP K2NMS4

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.

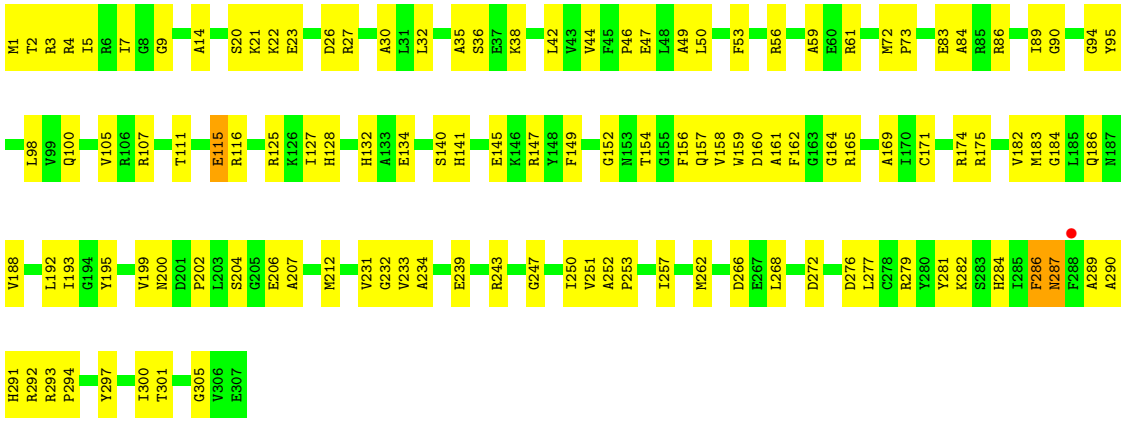
• Molecule 1: N-carbamoyl-D-amino-acid hydrolase

Chain A:



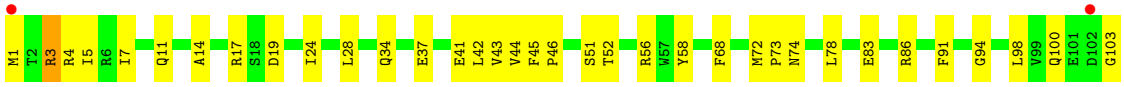
• Molecule 1: N-carbamoyl-D-amino-acid hydrolase

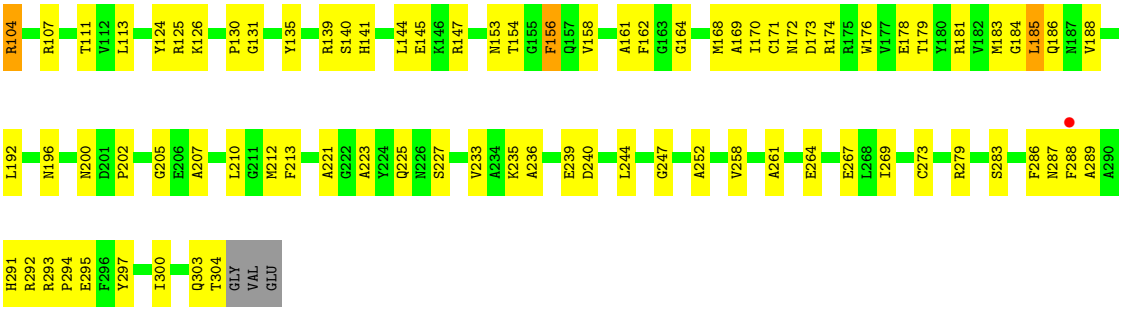
Chain B:



• Molecule 1: N-carbamoyl-D-amino-acid hydrolase

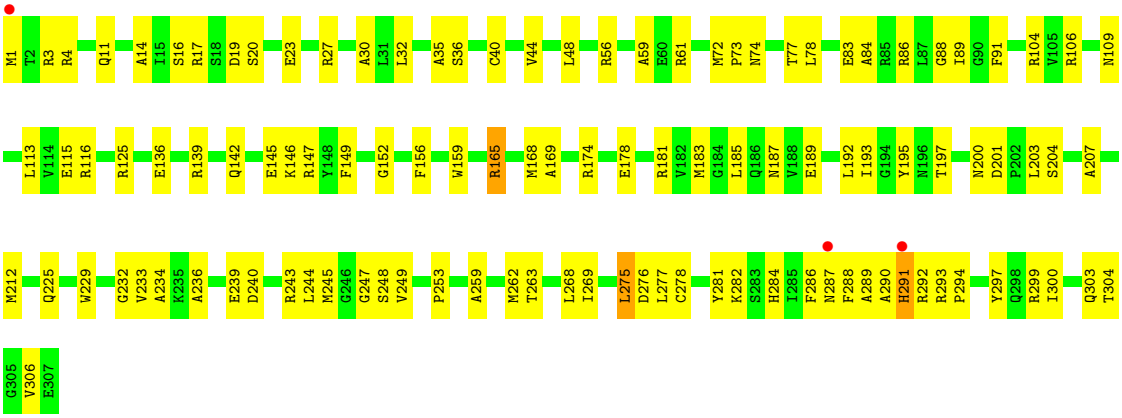
Chain C:





• Molecule 1: N-carbamoyl-D-amino-acid hydrolase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.14Å 73.55Å 77.71Å 84.08° 88.20° 89.73°	Depositor
Resolution (Å)	23.98 – 3.17 23.98 – 3.17	Depositor EDS
% Data completeness (in resolution range)	98.9 (23.98-3.17) 98.9 (23.98-3.17)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 3.17Å)	Xtriage
Refinement program	PHENIX v1.20	Depositor
R, R_{free}	0.201 , 0.278 0.202 , 0.276	Depositor DCC
R_{free} test set	1334 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 8.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.209 for h,-k,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	9680	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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	0.52	0/2462	0.76	0/3325
1	B	0.51	0/2482	0.76	0/3352
1	C	0.52	0/2462	0.75	0/3325
1	D	0.52	0/2482	0.77	0/3352
All	All	0.52	0/9888	0.76	0/13354

There are no bond length outliers.

There are no bond angle outliers.

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	2410	0	2350	91	0
1	B	2430	0	2368	98	0
1	C	2410	0	2350	99	0
1	D	2430	0	2368	100	0
All	All	9680	0	9436	337	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 18.

All (337) 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:D:115:GLU:HG3	1:D:116:ARG:H	1.28	0.97
1:D:20:SER:HB3	1:D:23:GLU:HG3	1.51	0.92
1:B:20:SER:HB2	1:B:23:GLU:HG3	1.49	0.92
1:A:304:THR:HG21	1:B:292:ARG:HH11	1.40	0.86
1:D:115:GLU:HG3	1:D:116:ARG:N	1.88	0.86
1:B:184:GLY:HA2	1:B:188:VAL:HG12	1.61	0.83
1:A:196:ASN:HD21	1:A:235:LYS:HE2	1.43	0.81
1:A:196:ASN:ND2	1:A:235:LYS:HE2	1.95	0.81
1:A:3:ARG:HG3	1:A:276:ASP:OD2	1.86	0.74
1:C:176:TRP:HE1	1:D:288:PHE:HZ	1.36	0.73
1:A:304:THR:HB	1:B:292:ARG:HB3	1.71	0.72
1:A:166:VAL:HG22	1:A:190:LEU:HD23	1.70	0.72
1:A:59:ALA:O	1:A:147:ARG:NH1	2.25	0.70
1:A:4:ARG:HD3	1:A:274:ASP:OD1	1.91	0.70
1:C:303:GLN:HG2	1:D:185:LEU:HD22	1.74	0.70
1:D:277:LEU:HD22	1:D:281:TYR:CE2	2.27	0.70
1:B:284:HIS:O	1:B:287:ASN:HB2	1.92	0.69
1:C:7:ILE:HG12	1:C:42:LEU:HD23	1.75	0.69
1:B:115:GLU:HG3	1:B:116:ARG:H	1.58	0.69
1:A:156:PHE:HB3	1:A:183:MET:HG3	1.75	0.69
1:C:304:THR:HA	1:D:185:LEU:HD11	1.75	0.68
1:C:83:GLU:OE2	1:C:86:ARG:NH1	2.26	0.68
1:C:185:LEU:HA	1:D:306:VAL:HG23	1.75	0.67
1:D:35:ALA:HB1	1:D:40:CYS:HB2	1.77	0.67
1:D:201:ASP:HB3	1:D:204:SER:HB2	1.76	0.67
1:A:28:LEU:HD23	1:A:45:PHE:CD1	2.30	0.67
1:C:279:ARG:HG2	1:C:279:ARG:HH11	1.58	0.66
1:A:126:LYS:HD3	1:A:129:LEU:HD23	1.75	0.66
1:A:298:GLN:HE22	1:B:301:THR:HB	1.61	0.66
1:A:98:LEU:HD12	1:A:107:ARG:HG2	1.76	0.65
1:C:124:TYR:HA	1:C:154:THR:HG21	1.78	0.65
1:A:196:ASN:ND2	1:A:235:LYS:HB3	2.12	0.64
1:B:21:LYS:NZ	1:B:50:LEU:O	2.31	0.64
1:C:292:ARG:HH12	1:D:300:ILE:HA	1.63	0.64
1:C:289:ALA:HB3	1:D:146:LYS:NZ	2.13	0.63
1:B:174:ARG:HB3	1:B:193:ILE:HG21	1.79	0.63
1:D:17:ARG:HG2	1:D:240:ASP:OD2	1.99	0.63
1:A:125:ARG:HB2	1:A:152:GLY:HA3	1.81	0.62
1:A:54:PHE:HB2	1:A:64:MET:HE2	1.82	0.62
1:D:3:ARG:NH1	1:D:276:ASP:OD1	2.33	0.61
1:C:72:MET:HB3	1:C:73:PRO:HD3	1.82	0.61
1:D:59:ALA:O	1:D:147:ARG:NH1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HD21	1:B:84:ALA:HB2	1.81	0.61
1:C:292:ARG:O	1:D:304:THR:HG23	2.00	0.61
1:C:100:GLN:HE21	1:C:103:GLY:HA2	1.65	0.61
1:A:258:VAL:HG11	1:D:262:MET:HE1	1.81	0.61
1:C:139:ARG:HH21	1:D:286:PHE:HE2	1.48	0.61
1:A:35:ALA:HB1	1:A:40:CYS:HB2	1.83	0.60
1:A:225:GLN:O	1:A:286:PHE:HZ	1.84	0.60
1:A:298:GLN:NE2	1:B:301:THR:HB	2.16	0.60
1:B:195:TYR:CZ	1:B:234:ALA:HB2	2.36	0.60
1:C:7:ILE:HD12	1:C:273:CYS:SG	2.40	0.60
1:A:131:GLY:N	1:B:289:ALA:HA	2.16	0.60
1:B:115:GLU:OE2	1:B:116:ARG:NH1	2.35	0.60
1:A:97:GLU:OE2	1:A:125:ARG:NH1	2.34	0.60
1:D:284:HIS:HA	1:D:286:PHE:CD1	2.36	0.60
1:C:300:ILE:O	1:C:304:THR:OG1	2.20	0.59
1:A:125:ARG:HG3	1:A:154:THR:HG23	1.85	0.59
1:B:94:GLY:HA2	1:B:111:THR:HG22	1.84	0.59
1:B:47:GLU:OE1	1:B:171:CYS:HB2	2.02	0.59
1:D:284:HIS:HA	1:D:286:PHE:HD1	1.68	0.59
1:A:130:PRO:HA	1:B:289:ALA:O	2.03	0.59
1:D:32:LEU:HD21	1:D:84:ALA:HB2	1.84	0.58
1:A:131:GLY:H	1:B:289:ALA:HA	1.67	0.58
1:B:59:ALA:O	1:B:147:ARG:NH1	2.37	0.58
1:C:286:PHE:O	1:D:139:ARG:NH2	2.37	0.58
1:D:3:ARG:NH2	1:D:189:GLU:OE1	2.36	0.57
1:D:44:VAL:HG21	1:D:192:LEU:HD22	1.86	0.57
1:D:56:ARG:HA	1:D:142:GLN:O	2.03	0.57
1:C:292:ARG:HH22	1:D:300:ILE:HG23	1.69	0.57
1:C:58:TYR:CE1	1:C:135:TYR:HB2	2.40	0.57
1:D:136:GLU:HB3	1:D:139:ARG:NH1	2.19	0.57
1:B:212:MET:SD	1:B:247:GLY:HA3	2.45	0.57
1:A:128:HIS:NE2	1:B:297:TYR:OH	2.29	0.56
1:B:277:LEU:HD22	1:B:281:TYR:CE2	2.41	0.56
1:C:130:PRO:HG3	1:C:172:ASN:ND2	2.20	0.56
1:A:3:ARG:NH1	1:A:163:GLY:O	2.38	0.56
1:A:3:ARG:NH2	1:A:189:GLU:OE2	2.35	0.56
1:B:141:HIS:CE1	1:B:202:PRO:HG3	2.40	0.56
1:C:104:ARG:HA	1:C:104:ARG:NE	2.19	0.56
1:A:44:VAL:HG21	1:A:192:LEU:HD22	1.88	0.56
1:D:88:GLY:O	1:D:116:ARG:HG2	2.06	0.56
1:A:21:LYS:NZ	1:A:69:GLU:OE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:GLY:HA2	1:C:111:THR:HG22	1.88	0.56
1:C:141:HIS:CE1	1:C:202:PRO:HB3	2.41	0.56
1:B:3:ARG:HH21	1:B:164:GLY:CA	2.18	0.56
1:B:200:ASN:HA	1:B:207:ALA:HA	1.88	0.56
1:B:287:ASN:HB3	1:B:289:ALA:H	1.70	0.56
1:C:5:ILE:HD11	1:C:41:GLU:HB2	1.87	0.56
1:D:200:ASN:HA	1:D:207:ALA:HA	1.87	0.56
1:A:292:ARG:HH22	1:B:300:ILE:HA	1.71	0.55
1:C:51:SER:OG	1:C:52:THR:O	2.24	0.55
1:A:131:GLY:HA3	1:A:143:HIS:HB3	1.89	0.55
1:A:144:LEU:HB3	1:A:147:ARG:HB3	1.89	0.55
1:C:17:ARG:HG3	1:C:240:ASP:CG	2.27	0.55
1:A:74:ASN:O	1:A:78:LEU:HB2	2.06	0.55
1:A:126:LYS:HE3	1:A:170:ILE:HG22	1.89	0.55
1:D:281:TYR:O	1:D:284:HIS:ND1	2.40	0.55
1:B:132:HIS:ND1	1:B:134:GLU:O	2.40	0.55
1:C:28:LEU:HD23	1:C:45:PHE:CD1	2.41	0.54
1:A:288:PHE:HB3	1:A:292:ARG:HG3	1.89	0.54
1:D:83:GLU:HG2	1:D:86:ARG:HH21	1.70	0.54
1:A:115:GLU:HB2	1:A:121:VAL:HG22	1.89	0.54
1:C:161:ALA:HB1	1:C:162:PHE:CD2	2.43	0.54
1:C:176:TRP:NE1	1:D:288:PHE:HZ	2.04	0.54
1:A:176:TRP:HZ3	1:B:292:ARG:HE	1.56	0.54
1:C:236:ALA:HB1	1:C:264:GLU:HG2	1.90	0.53
1:A:56:ARG:NH2	1:A:239:GLU:OE1	2.41	0.53
1:B:20:SER:HB2	1:B:23:GLU:CG	2.32	0.53
1:A:94:GLY:HA2	1:A:111:THR:HG22	1.90	0.53
1:B:44:VAL:HG21	1:B:192:LEU:HD22	1.91	0.53
1:B:94:GLY:CA	1:B:111:THR:HG22	2.39	0.53
1:B:160:ASP:OD1	1:B:165:ARG:HD2	2.07	0.53
1:C:304:THR:N	1:D:292:ARG:CZ	2.72	0.53
1:D:201:ASP:OD1	1:D:203:LEU:N	2.41	0.53
1:A:47:GLU:HG2	1:A:48:LEU:HG	1.91	0.52
1:A:184:GLY:HA2	1:A:188:VAL:HG12	1.90	0.52
1:B:20:SER:CB	1:B:23:GLU:HG3	2.30	0.52
1:D:236:ALA:HA	1:D:244:LEU:HB2	1.90	0.52
1:A:51:SER:HB2	1:A:67:TYR:CD1	2.44	0.52
1:A:304:THR:CB	1:B:292:ARG:HD2	2.39	0.52
1:D:195:TYR:CZ	1:D:234:ALA:HB2	2.45	0.52
1:C:74:ASN:O	1:C:78:LEU:HB2	2.09	0.52
1:C:176:TRP:HE3	1:D:181:ARG:NH2	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:THR:HA	1:B:294:PRO:HG3	1.92	0.51
1:A:166:VAL:CG2	1:A:190:LEU:HD23	2.40	0.51
1:D:1:MET:HA	1:D:4:ARG:HB3	1.92	0.51
1:A:24:ILE:O	1:A:28:LEU:HD12	2.11	0.51
1:A:235:LYS:HE3	1:A:239:GLU:OE2	2.10	0.51
1:C:34:GLN:O	1:C:37:GLU:HG2	2.11	0.51
1:A:304:THR:O	1:A:304:THR:OG1	2.16	0.51
1:A:196:ASN:HB3	1:A:244:LEU:HD22	1.93	0.51
1:D:14:ALA:HB1	1:D:239:GLU:HG2	1.92	0.51
1:D:299:ARG:HG2	1:D:303:GLN:HE21	1.76	0.51
1:C:287:ASN:HD22	1:C:288:PHE:HD1	1.59	0.51
1:A:5:ILE:HD11	1:A:41:GLU:HB2	1.93	0.50
1:B:61:ARG:HG2	1:B:147:ARG:HG3	1.92	0.50
1:C:14:ALA:HB1	1:C:239:GLU:HG2	1.93	0.50
1:A:225:GLN:C	1:A:286:PHE:HZ	2.13	0.50
1:C:303:GLN:O	1:C:304:THR:OG1	2.28	0.50
1:A:304:THR:HB	1:B:292:ARG:HD2	1.94	0.50
1:B:286:PHE:CE2	1:B:292:ARG:HG3	2.46	0.50
1:C:293:ARG:NE	1:C:295:GLU:OE1	2.45	0.50
1:A:196:ASN:HD21	1:A:235:LYS:HB3	1.76	0.50
1:D:169:ALA:O	1:D:193:ILE:HA	2.12	0.50
1:D:294:PRO:HA	1:D:297:TYR:CD2	2.47	0.50
1:D:125:ARG:O	1:D:152:GLY:HA3	2.12	0.49
1:C:300:ILE:HG21	1:D:300:ILE:HD13	1.94	0.49
1:C:289:ALA:HB3	1:D:146:LYS:HZ2	1.78	0.49
1:B:282:LYS:O	1:B:286:PHE:HB3	2.12	0.49
1:A:44:VAL:HG13	1:A:92:SER:OG	2.12	0.49
1:A:136:GLU:H	1:A:142:GLN:HE22	1.59	0.49
1:A:156:PHE:CE1	1:A:179:THR:HG23	2.48	0.49
1:B:158:VAL:HG22	1:B:183:MET:HG2	1.95	0.49
1:C:68:PHE:CE2	1:C:107:ARG:HB3	2.48	0.49
1:C:56:ARG:HH12	1:C:239:GLU:HB2	1.78	0.49
1:A:34:GLN:HA	1:A:37:GLU:HG2	1.94	0.48
1:C:210:LEU:HD22	1:C:213:PHE:CD2	2.48	0.48
1:D:268:LEU:HD23	1:D:269:ILE:N	2.29	0.48
1:A:36:SER:HB2	1:A:89:ILE:HD11	1.94	0.48
1:A:224:TYR:OH	1:B:175:ARG:NH2	2.36	0.48
1:B:251:VAL:HG22	1:B:257:ILE:HG12	1.94	0.48
1:C:303:GLN:CG	1:D:185:LEU:HD22	2.43	0.48
1:D:74:ASN:OD1	1:D:77:THR:OG1	2.31	0.48
1:B:115:GLU:CG	1:B:116:ARG:H	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:MET:SD	1:C:247:GLY:HA3	2.54	0.48
1:B:157:GLN:HB2	1:B:159:TRP:CH2	2.48	0.48
1:A:171:CYS:HA	1:A:195:TYR:CB	2.44	0.48
1:D:104:ARG:HH21	1:D:106:ARG:NE	2.12	0.48
1:D:247:GLY:O	1:D:249:VAL:HG13	2.13	0.48
1:A:127:ILE:HG22	1:B:293:ARG:HG3	1.95	0.48
1:B:72:MET:HB3	1:B:73:PRO:HD3	1.95	0.48
1:B:89:ILE:HG22	1:B:90:GLY:O	2.14	0.48
1:B:262:MET:HE1	1:C:258:VAL:HG11	1.95	0.48
1:A:54:PHE:HB2	1:A:64:MET:CE	2.44	0.48
1:B:127:ILE:HD12	1:B:156:PHE:CZ	2.49	0.48
1:A:258:VAL:CG1	1:D:262:MET:HE1	2.43	0.47
1:C:173:ASP:O	1:C:179:THR:HG21	2.13	0.47
1:A:289:ALA:HB2	1:B:305:GLY:HA3	1.97	0.47
1:B:3:ARG:HH21	1:B:164:GLY:HA3	1.79	0.47
1:B:169:ALA:O	1:B:193:ILE:HA	2.14	0.47
1:C:43:VAL:O	1:C:91:PHE:HA	2.14	0.47
1:D:165:ARG:HE	1:D:165:ARG:HB3	1.52	0.47
1:A:21:LYS:HG2	1:A:76:ALA:HB1	1.95	0.47
1:B:115:GLU:HG3	1:B:116:ARG:N	2.28	0.47
1:C:185:LEU:CA	1:D:306:VAL:HG23	2.43	0.47
1:B:100:GLN:HG3	1:B:105:VAL:HG22	1.96	0.47
1:C:158:VAL:HG23	1:C:183:MET:HG2	1.96	0.47
1:C:283:SER:HB3	1:C:286:PHE:CZ	2.50	0.47
1:C:304:THR:H	1:D:292:ARG:CZ	2.26	0.47
1:A:225:GLN:O	1:A:286:PHE:CZ	2.67	0.47
1:B:27:ARG:NH2	1:B:266:ASP:OD1	2.48	0.47
1:C:100:GLN:NE2	1:C:103:GLY:HA2	2.29	0.47
1:C:181:ARG:NH1	1:D:178:GLU:OE2	2.48	0.47
1:A:304:THR:HB	1:B:292:ARG:CB	2.44	0.47
1:B:1:MET:HB2	1:B:4:ARG:CZ	2.45	0.47
1:B:276:ASP:O	1:B:279:ARG:HG2	2.15	0.47
1:B:286:PHE:HE2	1:B:292:ARG:CZ	2.28	0.47
1:D:193:ILE:O	1:D:232:GLY:HA2	2.14	0.47
1:C:140:SER:OG	1:C:205:GLY:HA2	2.15	0.47
1:C:184:GLY:C	1:C:186:GLN:H	2.18	0.47
1:D:249:VAL:HA	1:D:259:ALA:O	2.14	0.47
1:A:279:ARG:HA	1:A:282:LYS:HB2	1.97	0.47
1:A:299:ARG:HD3	1:A:303:GLN:NE2	2.30	0.47
1:D:291:HIS:O	1:D:293:ARG:HD3	2.15	0.47
1:B:145:GLU:HG3	1:B:149:PHE:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:VAL:HG21	1:C:192:LEU:HD22	1.96	0.46
1:C:297:TYR:HB3	1:C:300:ILE:HD12	1.97	0.46
1:D:290:ALA:C	1:D:292:ARG:N	2.69	0.46
1:B:204:SER:HB2	1:B:206:GLU:HG3	1.96	0.46
1:C:196:ASN:OD1	1:C:235:LYS:HE2	2.15	0.46
1:C:17:ARG:HG3	1:C:240:ASP:OD2	2.15	0.46
1:D:287:ASN:OD1	1:D:288:PHE:N	2.48	0.46
1:A:133:ALA:O	1:A:147:ARG:HB2	2.15	0.46
1:B:262:MET:HE1	1:C:252:ALA:HB2	1.98	0.46
1:B:140:SER:N	1:B:202:PRO:O	2.33	0.46
1:A:9:GLY:N	1:A:269:ILE:O	2.46	0.45
1:A:297:TYR:OH	1:B:128:HIS:NE2	2.25	0.45
1:A:64:MET:HE2	1:A:64:MET:HB3	1.76	0.45
1:B:286:PHE:HE2	1:B:292:ARG:NH1	2.14	0.45
1:D:44:VAL:CG2	1:D:192:LEU:HD22	2.46	0.45
1:B:53:PHE:O	1:B:56:ARG:HG2	2.16	0.45
1:C:158:VAL:HG21	1:C:188:VAL:HB	1.98	0.45
1:C:176:TRP:CZ2	1:D:288:PHE:CE2	3.05	0.45
1:D:44:VAL:O	1:D:233:VAL:HG21	2.17	0.45
1:D:292:ARG:HH22	1:D:294:PRO:HB3	1.82	0.45
1:A:5:ILE:CD1	1:A:41:GLU:HB2	2.47	0.45
1:C:169:ALA:HB2	1:C:183:MET:HE1	1.98	0.45
1:C:289:ALA:HB3	1:D:146:LYS:HZ1	1.79	0.45
1:C:304:THR:C	1:D:292:ARG:CD	2.85	0.45
1:B:252:ALA:HB1	1:B:253:PRO:HD2	1.99	0.44
1:C:196:ASN:HB3	1:C:244:LEU:HD13	1.99	0.44
1:D:197:THR:HB	1:D:245:MET:HG2	1.99	0.44
1:B:158:VAL:HG21	1:B:186:GLN:HB2	1.98	0.44
1:D:3:ARG:NH2	1:D:275:LEU:HB3	2.32	0.44
1:D:48:LEU:HD11	1:D:109:ASN:ND2	2.33	0.44
1:A:212:MET:SD	1:A:247:GLY:HA3	2.57	0.44
1:D:16:SER:HB3	1:D:19:ASP:OD1	2.18	0.44
1:B:115:GLU:CG	1:B:116:ARG:N	2.80	0.44
1:C:126:LYS:HZ3	1:C:145:GLU:CD	2.21	0.44
1:D:91:PHE:O	1:D:113:LEU:HD12	2.17	0.44
1:B:46:PRO:HD2	1:B:49:ALA:HB2	2.00	0.44
1:D:201:ASP:CB	1:D:204:SER:HB2	2.47	0.44
1:C:221:ALA:O	1:C:225:GLN:HB2	2.17	0.44
1:D:181:ARG:NH1	1:D:225:GLN:O	2.51	0.44
1:A:62:ASP:OD1	1:A:62:ASP:N	2.51	0.44
1:B:35:ALA:HB2	1:B:268:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ARG:HB3	1:C:4:ARG:H	1.63	0.44
1:B:98:LEU:HD13	1:B:107:ARG:HG2	2.00	0.43
1:C:11:GLN:N	1:C:267:GLU:O	2.50	0.43
1:C:94:GLY:CA	1:C:111:THR:HG22	2.48	0.43
1:C:304:THR:HB	1:D:292:ARG:HE	1.83	0.43
1:B:26:ASP:O	1:B:30:ALA:N	2.39	0.43
1:B:89:ILE:HD13	1:B:89:ILE:HG21	1.84	0.43
1:C:144:LEU:HB3	1:C:147:ARG:HB3	2.01	0.43
1:C:292:ARG:C	1:C:294:PRO:HD3	2.38	0.43
1:C:176:TRP:NE1	1:D:288:PHE:CZ	2.84	0.43
1:D:145:GLU:HG2	1:D:149:PHE:HD2	1.84	0.43
1:D:72:MET:HB3	1:D:73:PRO:HD3	2.00	0.43
1:D:229:TRP:CE2	1:D:253:PRO:HD3	2.54	0.43
1:C:98:LEU:HD12	1:C:98:LEU:HA	1.66	0.43
1:D:278:CYS:O	1:D:282:LYS:HG3	2.18	0.43
1:B:3:ARG:HH21	1:B:164:GLY:HA2	1.83	0.43
1:B:125:ARG:O	1:B:152:GLY:HA3	2.18	0.43
1:C:24:ILE:O	1:C:28:LEU:HD12	2.18	0.43
1:C:261:ALA:HB2	1:C:269:ILE:CG2	2.49	0.43
1:A:94:GLY:CA	1:A:111:THR:HG22	2.49	0.43
1:B:161:ALA:HB1	1:B:162:PHE:CD1	2.54	0.43
1:D:281:TYR:C	1:D:284:HIS:HD1	2.22	0.43
1:B:44:VAL:O	1:B:233:VAL:HG21	2.18	0.42
1:D:187:ASN:OD1	1:D:282:LYS:HE3	2.19	0.42
1:A:126:LYS:NZ	1:A:145:GLU:OE1	2.44	0.42
1:B:1:MET:HB3	1:B:2:THR:H	1.49	0.42
1:C:46:PRO:HG3	1:C:233:VAL:HG12	2.01	0.42
1:C:171:CYS:O	1:C:174:ARG:HD3	2.20	0.42
1:C:124:TYR:CD2	1:C:170:ILE:HG13	2.54	0.42
1:C:131:GLY:N	1:D:287:ASN:O	2.52	0.42
1:A:115:GLU:HB2	1:A:121:VAL:CG2	2.50	0.42
1:A:164:GLY:HA3	1:A:275:LEU:HD12	2.01	0.42
1:B:193:ILE:O	1:B:232:GLY:HA2	2.20	0.42
1:D:281:TYR:HA	1:D:284:HIS:HD1	1.83	0.42
1:B:83:GLU:HG2	1:B:86:ARG:NH1	2.34	0.42
1:D:116:ARG:HE	1:D:116:ARG:HB2	1.74	0.42
1:B:44:VAL:CG2	1:B:192:LEU:HD22	2.49	0.42
1:B:231:VAL:HG22	1:B:250:ILE:HG12	2.01	0.42
1:C:223:ALA:HB1	1:C:252:ALA:O	2.20	0.42
1:D:11:GLN:HB2	1:D:248:SER:OG	2.20	0.42
1:A:250:ILE:HG13	1:A:269:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LYS:HD3	1:B:26:ASP:OD2	2.20	0.42
1:C:304:THR:O	1:D:292:ARG:HD2	2.20	0.42
1:A:124:TYR:OH	1:A:127:ILE:HD12	2.20	0.42
1:A:136:GLU:HB3	1:A:139:ARG:HH11	1.85	0.42
1:A:277:LEU:HG	1:A:281:TYR:CE2	2.55	0.42
1:C:1:MET:HG3	1:C:164:GLY:CA	2.49	0.42
1:C:7:ILE:HG23	1:C:42:LEU:HD23	2.02	0.41
1:C:113:LEU:HB2	1:C:168:MET:SD	2.60	0.41
1:C:125:ARG:NH1	1:C:153:ASN:OD1	2.53	0.41
1:D:74:ASN:O	1:D:78:LEU:HB2	2.19	0.41
1:D:195:TYR:CE1	1:D:234:ALA:HB2	2.54	0.41
1:A:7:ILE:HD13	1:A:231:VAL:HG21	2.01	0.41
1:B:14:ALA:HB1	1:B:239:GLU:HG2	2.01	0.41
1:B:4:ARG:HD3	1:B:272:ASP:HB3	2.02	0.41
1:B:199:VAL:HG12	1:B:243:ARG:O	2.20	0.41
1:D:277:LEU:HD22	1:D:281:TYR:CZ	2.55	0.41
1:B:7:ILE:HG23	1:B:42:LEU:HD23	2.02	0.41
1:B:9:GLY:O	1:B:268:LEU:HA	2.21	0.41
1:C:68:PHE:HE2	1:C:107:ARG:HB3	1.85	0.41
1:A:292:ARG:HD2	1:A:297:TYR:HE2	1.85	0.41
1:B:125:ARG:HD2	1:B:154:THR:HG23	2.01	0.41
1:B:38:LYS:HE2	1:B:38:LYS:HB3	1.89	0.41
1:B:251:VAL:HG22	1:B:257:ILE:CG1	2.51	0.41
1:B:286:PHE:CD1	1:B:290:ALA:HB3	2.55	0.41
1:C:156:PHE:CE2	1:C:179:THR:HG22	2.55	0.41
1:D:61:ARG:HG2	1:D:147:ARG:HG3	2.02	0.41
1:D:156:PHE:HB3	1:D:183:MET:HG3	2.02	0.41
1:C:200:ASN:HA	1:C:207:ALA:HA	2.03	0.41
1:A:169:ALA:HB2	1:A:183:MET:HE1	2.03	0.41
1:C:19:ASP:OD1	1:C:19:ASP:N	2.53	0.41
1:D:3:ARG:O	1:D:275:LEU:N	2.54	0.41
1:B:50:LEU:HD12	1:B:95:TYR:HB3	2.03	0.41
1:D:174:ARG:HB3	1:D:193:ILE:HG21	2.03	0.41
1:C:178:GLU:OE2	1:D:181:ARG:NE	2.55	0.40
1:C:223:ALA:O	1:C:227:SER:N	2.54	0.40
1:D:11:GLN:NE2	1:D:263:THR:O	2.54	0.40
1:D:27:ARG:O	1:D:30:ALA:HB3	2.21	0.40
1:A:35:ALA:HB1	1:A:40:CYS:CB	2.50	0.40
1:A:292:ARG:HH12	1:B:300:ILE:HG23	1.86	0.40
1:B:36:SER:HB2	1:B:89:ILE:HD11	2.04	0.40
1:C:300:ILE:HG21	1:D:300:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:SER:OG	1:A:206:GLU:HB2	2.21	0.40
1:C:289:ALA:HB1	1:C:291:HIS:CD2	2.55	0.40
1:D:212:MET:SD	1:D:247:GLY:HA3	2.61	0.40
1:C:297:TYR:N	1:C:297:TYR:CD1	2.88	0.40
1:D:36:SER:HB2	1:D:89:ILE:HD11	2.03	0.40
1:B:5:ILE:HD13	1:B:162:PHE:HB3	2.03	0.40
1:C:293:ARG:HA	1:C:293:ARG:HD2	1.88	0.40
1:D:159:TRP:HZ3	1:D:168:MET:HG3	1.87	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	302/307 (98%)	285 (94%)	16 (5%)	1 (0%)	41	73
1	B	305/307 (99%)	279 (92%)	24 (8%)	2 (1%)	22	60
1	C	302/307 (98%)	280 (93%)	20 (7%)	2 (1%)	22	60
1	D	305/307 (99%)	275 (90%)	27 (9%)	3 (1%)	15	52
All	All	1214/1228 (99%)	1119 (92%)	87 (7%)	8 (1%)	22	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3	ARG
1	A	285	ILE
1	D	275	LEU
1	D	291	HIS
1	B	287	ASN
1	D	289	ALA
1	C	185	LEU

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Mol	Chain	Res	Type
1	B	182	VAL

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	249/251 (99%)	245 (98%)	4 (2%)	62 83
1	B	251/251 (100%)	248 (99%)	3 (1%)	71 87
1	C	249/251 (99%)	247 (99%)	2 (1%)	81 92
1	D	251/251 (100%)	249 (99%)	2 (1%)	81 92
All	All	1000/1004 (100%)	989 (99%)	11 (1%)	73 88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	139	ARG
1	A	227	SER
1	A	272	ASP
1	B	115	GLU
1	B	286	PHE
1	B	291	HIS
1	C	104	ARG
1	C	156	PHE
1	D	165	ARG
1	D	243	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	196	ASN
1	A	298	GLN
1	B	141	HIS

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Mol	Chain	Res	Type
1	B	215	ASN
1	C	100	GLN
1	C	172	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	304/307 (99%)	-0.63	1 (0%)	94	92	5, 15, 45, 70	0
1	B	307/307 (100%)	-0.60	1 (0%)	94	92	6, 16, 47, 75	0
1	C	304/307 (99%)	-0.63	3 (0%)	82	72	6, 16, 48, 76	0
1	D	307/307 (100%)	-0.59	3 (0%)	82	72	6, 16, 46, 82	0
All	All	1222/1228 (99%)	-0.61	8 (0%)	87	81	5, 16, 47, 82	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	287	ASN	3.5
1	C	1	MET	2.7
1	A	1	MET	2.6
1	D	291	HIS	2.5
1	D	1	MET	2.5
1	B	288	PHE	2.2
1	C	288	PHE	2.1
1	C	102	ASP	2.0

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.