Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 02:52 PM EDT

PDB ID	:	2I1W
Title	:	Crystal structure of NAD kinase 1 from Listeria monocytogenes
Authors	:	Poncet-Montange, G.; Assairi, L.; Arold, S.; Pochet, S.; Labesse, G.
Deposited on	:	2006-08-15
Resolution	:	2.34 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:

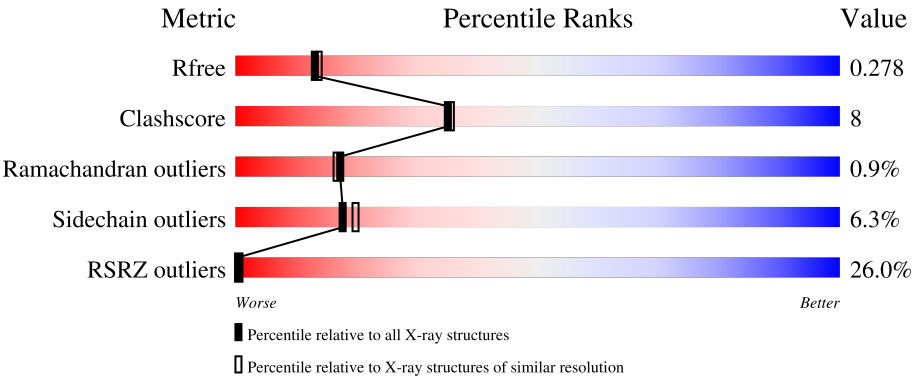
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	272	18% 71% 20% · 6%
1	B	272	25% 79% 14% ·· ·
1	C	272	31% 78% 14% · 5%
1	D	272	24% 70% 22% · · 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IOD	A	513	-	-	X	-
2	IOD	A	531	-	-	X	-
2	IOD	A	533	-	-	X	-
2	IOD	B	515	-	-	X	-
2	IOD	B	522	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8538 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 Probable inorganic polyphosphate/ATP-NAD kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2040	1309	341	381	9			
1	B	262	Total	C	N	O	S	0	0	0
			2069	1328	345	387	9			
1	C	258	Total	C	N	O	S	0	0	0
			2032	1305	341	377	9			
1	D	259	Total	C	N	O	S	0	0	0
			2016	1294	341	372	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	LEU	-	cloning artifact	UNP Q8Y8D7
A	266	GLU	-	cloning artifact	UNP Q8Y8D7
A	267	HIS	-	expression tag	UNP Q8Y8D7
A	268	HIS	-	expression tag	UNP Q8Y8D7
A	269	HIS	-	expression tag	UNP Q8Y8D7
A	270	HIS	-	expression tag	UNP Q8Y8D7
A	271	HIS	-	expression tag	UNP Q8Y8D7
A	272	HIS	-	expression tag	UNP Q8Y8D7
B	265	LEU	-	cloning artifact	UNP Q8Y8D7
B	266	GLU	-	cloning artifact	UNP Q8Y8D7
B	267	HIS	-	expression tag	UNP Q8Y8D7
B	268	HIS	-	expression tag	UNP Q8Y8D7
B	269	HIS	-	expression tag	UNP Q8Y8D7
B	270	HIS	-	expression tag	UNP Q8Y8D7
B	271	HIS	-	expression tag	UNP Q8Y8D7
B	272	HIS	-	expression tag	UNP Q8Y8D7
C	265	LEU	-	cloning artifact	UNP Q8Y8D7
C	266	GLU	-	cloning artifact	UNP Q8Y8D7
C	267	HIS	-	expression tag	UNP Q8Y8D7
C	268	HIS	-	expression tag	UNP Q8Y8D7
C	269	HIS	-	expression tag	UNP Q8Y8D7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	270	HIS	-	expression tag	UNP Q8Y8D7
C	271	HIS	-	expression tag	UNP Q8Y8D7
C	272	HIS	-	expression tag	UNP Q8Y8D7
D	265	LEU	-	cloning artifact	UNP Q8Y8D7
D	266	GLU	-	cloning artifact	UNP Q8Y8D7
D	267	HIS	-	expression tag	UNP Q8Y8D7
D	268	HIS	-	expression tag	UNP Q8Y8D7
D	269	HIS	-	expression tag	UNP Q8Y8D7
D	270	HIS	-	expression tag	UNP Q8Y8D7
D	271	HIS	-	expression tag	UNP Q8Y8D7
D	272	HIS	-	expression tag	UNP Q8Y8D7

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	8	Total I 9 9	0	1
2	B	5	Total I 6 6	0	1
2	C	2	Total I 3 3	0	1
2	D	3	Total I 4 4	0	1

- Molecule 3 is water.

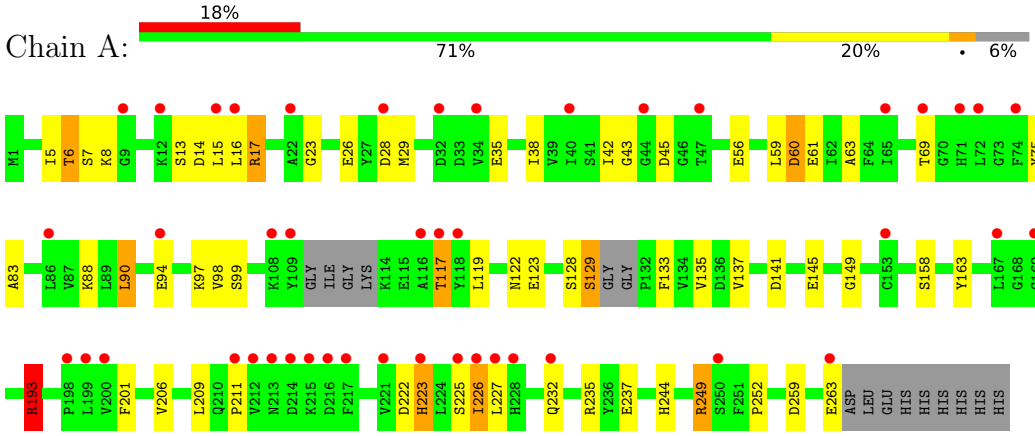
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	101	Total O 101 101	0	0
3	B	91	Total O 91 91	0	0
3	C	76	Total O 76 76	0	0
3	D	91	Total O 91 91	0	0

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.

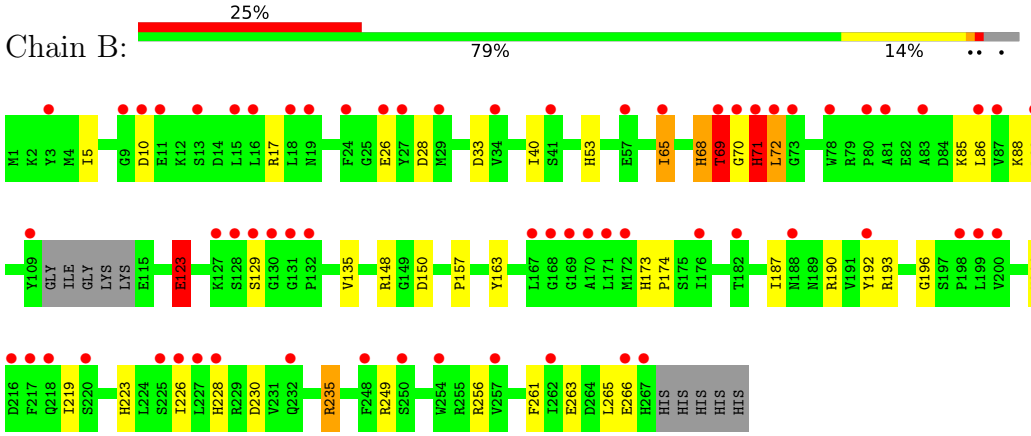
• Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase 1

Chain A:



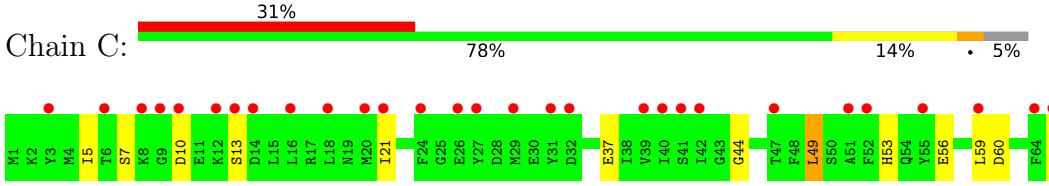
• Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase 1

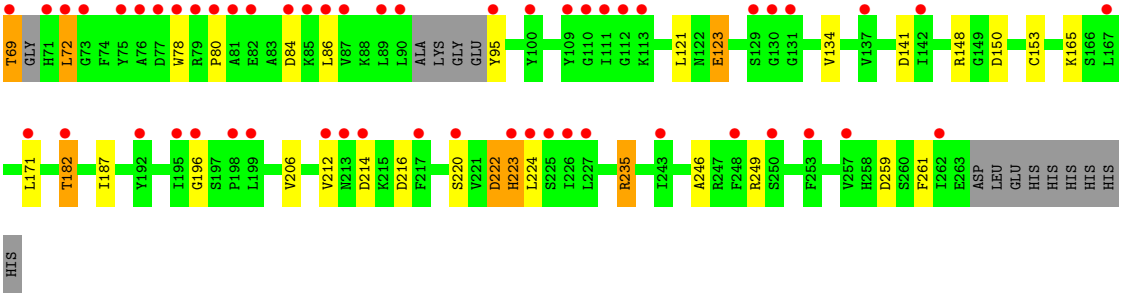
Chain B:



• Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase 1

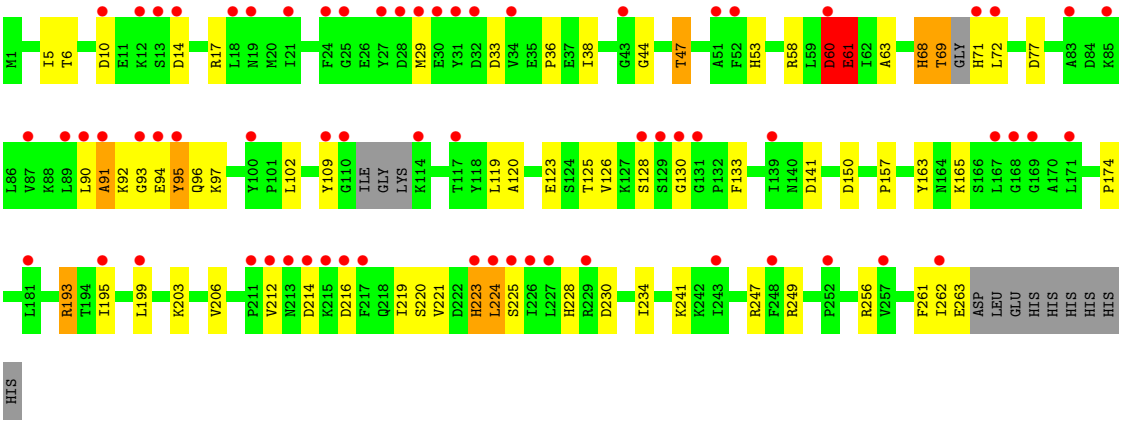
Chain C:





• Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.61Å 119.02Å 67.94Å 90.00° 102.08° 90.00°	Depositor
Resolution (Å)	34.37 – 2.34 34.47 – 2.34	Depositor EDS
% Data completeness (in resolution range)	97.5 (34.37-2.34) 97.5 (34.47-2.34)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.194 , 0.257 0.220 , 0.278	Depositor DCC
R_{free} test set	1330 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 72.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8538	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% 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

Bond lengths and bond angles in the following residue types are not validated in this section: IOD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.69	2/2088 (0.1%)	0.88	8/2820 (0.3%)
1	B	0.69	3/2120 (0.1%)	0.83	6/2870 (0.2%)
1	C	0.53	0/2081	0.80	8/2816 (0.3%)
1	D	0.58	1/2063 (0.0%)	0.83	10/2788 (0.4%)
All	All	0.62	6/8352 (0.1%)	0.84	32/11294 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	1	0
1	D	0	6
All	All	1	9

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	GLU	CD-OE2	9.35	1.35	1.25
1	B	26	GLU	CD-OE1	8.52	1.35	1.25
1	A	259	ASP	CB-CG	6.58	1.65	1.51
1	A	263	GLU	C-O	5.99	1.34	1.23
1	D	94	GLU	N-CA	5.14	1.56	1.46
1	B	266	GLU	CD-OE1	5.09	1.31	1.25

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	28	ASP	CB-CG-OD2	6.95	124.55	118.30
1	A	223	HIS	N-CA-C	6.40	128.27	111.00
1	A	60	ASP	CB-CG-OD2	6.37	124.03	118.30
1	B	10	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	15	LEU	CA-CB-CG	6.29	129.76	115.30
1	C	222	ASP	CB-CG-OD2	6.09	123.78	118.30
1	D	77	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	141	ASP	CB-CG-OD2	5.90	123.61	118.30
1	D	10	ASP	CB-CG-OD2	5.89	123.61	118.30
1	D	14	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	84	ASP	CB-CG-OD2	5.85	123.56	118.30
1	C	10	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	45	ASP	CB-CG-OD2	5.84	123.55	118.30
1	D	214	ASP	CB-CG-OD2	5.84	123.55	118.30
1	C	259	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	33	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	14	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	150	ASP	CB-CG-OD2	5.59	123.33	118.30
1	D	230	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	230	ASP	CB-CG-OD2	5.38	123.15	118.30
1	D	141	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	193	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	C	141	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	123	GLU	CB-CA-C	-5.27	99.86	110.40
1	B	214	ASP	CB-CG-OD2	5.24	123.01	118.30
1	C	60	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	216	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	94	GLU	N-CA-C	-5.21	96.94	111.00
1	D	33	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	216	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	214	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	17	ARG	NE-CZ-NH2	-5.04	117.78	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	95	TYR	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	ASP	Peptide
1	B	68	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	B	69	THR	Peptide
1	D	262	ILE	Peptide
1	D	60	ASP	Peptide
1	D	68	HIS	Peptide
1	D	92	LYS	Peptide
1	D	93	GLY	Peptide
1	D	95	TYR	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2040	0	1983	41	0
1	B	2069	0	1997	35	0
1	C	2032	0	1961	28	0
1	D	2016	0	1948	31	0
2	A	9	0	0	10	0
2	B	6	0	0	6	0
2	C	3	0	0	1	0
2	D	4	0	0	1	0
3	A	101	0	0	3	1
3	B	91	0	0	6	4
3	C	76	0	0	3	2
3	D	91	0	0	1	3
All	All	8538	0	7889	132	5

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 8.

All (132) 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)
2:A:530:IOD:I	3:A:596:HOH:O	2.29	1.19
2:A:531:IOD:I	3:A:535:HOH:O	2.43	1.06
1:C:196:GLY:O	2:C:523:IOD:I	2.56	0.94
1:D:69:THR:O	1:D:71:HIS:N	2.00	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ARG:HD3	3:B:559:HOH:O	1.70	0.91
1:A:128:SER:O	1:A:129:SER:HB3	1.71	0.88
1:B:196:GLY:O	2:B:528:IOD:I	2.63	0.87
1:A:6:THR:HG21	2:A:513:IOD:I	2.44	0.87
1:A:225:SER:C	1:A:226:ILE:HD13	1.97	0.84
1:B:265:LEU:HG	2:B:522:IOD:I	2.49	0.82
1:A:117:THR:CG2	2:A:531:IOD:I	3.01	0.79
1:C:235:ARG:HH11	1:C:235:ARG:HB2	1.47	0.78
1:D:58:ARG:O	1:D:61:GLU:HB3	1.89	0.73
1:C:153:CYS:HB3	1:C:182:THR:HG22	1.70	0.72
1:D:60:ASP:OD1	3:D:594:HOH:O	2.09	0.70
1:B:193:ARG:NH2	1:D:261:PHE:O	2.25	0.70
1:A:193:ARG:NH2	1:C:261:PHE:O	2.25	0.69
1:C:235:ARG:HH11	1:C:235:ARG:CG	2.06	0.68
1:D:38:ILE:HD13	1:D:90:LEU:HD22	1.75	0.68
1:C:235:ARG:HH11	1:C:235:ARG:CB	2.06	0.68
1:A:63:ALA:HB2	1:A:97:LYS:HE2	1.76	0.68
1:B:235:ARG:HH11	1:B:235:ARG:HG3	1.59	0.68
1:D:247:ARG:NH1	2:D:510:IOD:I	2.98	0.67
1:A:158:SER:O	3:A:586:HOH:O	2.14	0.65
1:C:53:HIS:HE1	1:C:222:ASP:OD2	1.80	0.64
1:B:190:ARG:CB	1:D:263:GLU:HB2	2.28	0.63
1:A:117:THR:HG22	2:A:531:IOD:I	2.69	0.63
1:A:7:SER:HB2	1:A:13:SER:HB3	1.81	0.62
1:C:69:THR:HA	1:C:80:PRO:HG3	1.83	0.61
1:A:226:ILE:HD13	1:A:226:ILE:N	2.16	0.60
1:C:235:ARG:HB2	1:C:235:ARG:NH1	2.15	0.60
1:B:88:LYS:HG3	1:B:89:LEU:N	2.18	0.59
1:B:123:GLU:CG	3:B:596:HOH:O	2.50	0.59
1:A:249:ARG:HH12	1:A:252:PRO:HD3	1.67	0.58
1:C:49:LEU:HD12	1:C:121:LEU:HD23	1.85	0.58
1:A:193:ARG:HH11	1:A:193:ARG:HG3	1.70	0.57
1:D:126:VAL:HG11	1:D:234:ILE:HD13	1.85	0.57
1:A:193:ARG:HH11	1:A:193:ARG:CG	2.17	0.57
1:B:261:PHE:O	1:D:193:ARG:NH2	2.35	0.57
1:D:126:VAL:HG12	1:D:219:ILE:HG13	1.86	0.56
1:D:128:SER:HB2	1:D:133:PHE:HB2	1.88	0.56
1:D:63:ALA:HB2	1:D:97:LYS:HE2	1.87	0.55
1:B:68:HIS:HB3	1:B:72:LEU:HA	1.88	0.55
1:C:235:ARG:HH11	1:C:235:ARG:HG3	1.71	0.55
1:A:99:SER:OG	1:A:244:HIS:ND1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:HH11	1:A:249:ARG:CG	2.20	0.54
1:C:134:VAL:HG22	1:C:148:ARG:HG3	1.88	0.54
1:A:128:SER:HB2	1:A:133:PHE:HB2	1.90	0.54
1:A:8:LYS:HG2	1:A:43:GLY:HA3	1.89	0.54
1:A:7:SER:HA	1:A:42:ILE:O	2.07	0.54
1:C:65:ILE:HG12	1:C:246:ALA:HB3	1.91	0.53
1:B:123:GLU:HG3	3:B:596:HOH:O	2.07	0.53
1:A:99:SER:OG	1:A:244:HIS:CE1	2.61	0.53
1:D:219:ILE:HD13	1:D:228:HIS:CD2	2.44	0.53
1:B:263:GLU:HG3	2:B:522:IOD:I	2.79	0.52
1:B:265:LEU:CG	2:B:522:IOD:I	3.27	0.52
1:B:235:ARG:HH11	1:B:235:ARG:CG	2.23	0.51
1:B:68:HIS:HD2	1:B:69:THR:H	1.59	0.51
1:A:28:ASP:O	1:A:29:MET:HG3	2.11	0.50
1:B:5:ILE:CG2	1:B:17:ARG:HG3	2.41	0.50
1:A:75:TYR:OH	1:A:122:ASN:ND2	2.44	0.50
1:A:117:THR:HG23	2:A:531:IOD:I	2.82	0.50
1:B:223:HIS:HB3	3:B:593:HOH:O	2.12	0.50
1:D:120:ALA:HB2	1:D:221:VAL:HG13	1.92	0.49
1:A:56:GLU:HA	1:A:59:LEU:HG	1.94	0.49
1:A:135:VAL:HG21	1:A:209:LEU:HB3	1.94	0.49
1:D:72:LEU:HD13	1:D:256:ARG:NH2	2.28	0.49
1:C:148:ARG:HD3	1:C:187:ILE:HD12	1.94	0.49
1:D:36:PRO:O	1:D:58:ARG:NH1	2.45	0.49
1:C:7:SER:HB2	1:C:13:SER:HB3	1.95	0.48
1:A:133:PHE:HB3	1:A:149:GLY:O	2.14	0.48
1:B:53:HIS:CD2	1:B:223:HIS:HE1	2.32	0.48
1:C:44:GLY:HA2	1:C:68:HIS:CD2	2.49	0.47
1:A:23:GLY:O	1:A:26:GLU:HG3	2.14	0.47
1:A:60:ASP:HB3	1:A:61:GLU:HG2	1.96	0.47
1:C:78:TRP:CE2	1:C:86:LEU:HD13	2.49	0.47
1:A:163:TYR:OH	1:C:150:ASP:OD2	2.32	0.47
1:D:44:GLY:H	1:D:47:THR:HG23	1.81	0.46
1:B:65:ILE:CD1	1:B:86:LEU:HD21	2.46	0.46
1:A:193:ARG:CG	1:A:193:ARG:NH1	2.77	0.46
1:B:68:HIS:CB	1:B:72:LEU:HA	2.44	0.46
1:B:70:GLY:O	1:B:71:HIS:O	2.33	0.46
2:B:515:IOD:I	1:D:165:LYS:HD3	2.85	0.46
1:A:29:MET:HE1	1:A:90:LEU:HD13	1.97	0.46
1:A:211:PRO:HD2	1:A:232:GLN:O	2.15	0.46
1:C:49:LEU:HB3	1:C:223:HIS:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:GLU:CG	3:C:526:HOH:O	2.65	0.45
2:A:533:IOD:I	2:A:534:IOD:I	3.75	0.45
1:D:53:HIS:CD2	1:D:223:HIS:CE1	3.04	0.45
1:D:125:THR:OG1	1:D:220:SER:OG	2.35	0.45
1:D:58:ARG:HG2	1:D:61:GLU:HG2	1.98	0.45
1:B:148:ARG:HD3	1:B:192:TYR:CE2	2.52	0.45
1:B:68:HIS:CG	1:B:72:LEU:HA	2.52	0.45
1:C:165:LYS:HG3	1:C:171:LEU:HD21	1.98	0.45
1:D:95:TYR:CD1	1:D:95:TYR:O	2.70	0.45
1:A:235:ARG:NH1	1:A:237:GLU:OE1	2.49	0.45
1:B:150:ASP:OD2	1:D:163:TYR:OH	2.31	0.45
1:B:88:LYS:HG3	1:B:89:LEU:H	1.81	0.45
1:B:173:HIS:HE1	3:B:573:HOH:O	2.00	0.45
1:C:5:ILE:HD12	1:C:21:ILE:HG13	2.00	0.44
1:B:71:HIS:HB2	1:B:72:LEU:H	1.67	0.44
1:C:123:GLU:HG2	3:C:526:HOH:O	2.17	0.44
1:C:78:TRP:CZ2	1:C:86:LEU:HD13	2.52	0.43
1:D:157:PRO:HB2	1:D:174:PRO:HA	1.99	0.43
1:B:173:HIS:CE1	3:B:573:HOH:O	2.71	0.43
1:D:195:ILE:HG21	1:D:199:LEU:HD21	1.99	0.43
1:C:235:ARG:CG	1:C:235:ARG:NH1	2.75	0.43
1:C:56:GLU:HA	1:C:59:LEU:HG	2.01	0.42
1:A:137:VAL:HB	1:A:145:GLU:HG2	2.01	0.42
1:B:40:ILE:HG12	1:B:65:ILE:HG23	2.01	0.42
1:D:109:TYR:HH	1:D:228:HIS:CE1	2.35	0.42
1:A:16:LEU:HD11	1:A:83:ALA:CB	2.49	0.42
1:C:53:HIS:CE1	1:C:222:ASP:OD2	2.67	0.42
1:B:5:ILE:HG21	1:B:17:ARG:HG3	2.02	0.42
1:B:85:LYS:HG2	1:B:88:LYS:HE2	2.01	0.41
1:D:5:ILE:O	1:D:17:ARG:HD2	2.20	0.41
1:D:95:TYR:CD1	1:D:95:TYR:C	2.93	0.41
1:B:219:ILE:HB	1:B:228:HIS:CD2	2.54	0.41
1:A:178:ALA:HA	1:A:201:PHE:O	2.21	0.41
1:A:225:SER:O	1:A:226:ILE:HD13	2.17	0.41
1:D:220:SER:HA	1:D:224:LEU:O	2.20	0.41
1:D:119:LEU:HD11	1:D:241:LYS:HD3	2.03	0.41
1:A:119:LEU:HG	2:A:531:IOD:I	2.91	0.41
1:B:187:ILE:HA	2:B:515:IOD:I	2.91	0.41
1:A:5:ILE:HB	1:A:17:ARG:HG3	2.03	0.40
1:A:38:ILE:HG21	1:A:90:LEU:HD11	2.02	0.40
1:A:98:VAL:HG11	2:A:533:IOD:I	2.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:PRO:HB2	1:B:174:PRO:HA	2.02	0.40
1:A:6:THR:CG2	2:A:513:IOD:I	3.30	0.40
1:B:68:HIS:HD2	1:B:69:THR:N	2.20	0.40
1:C:182:THR:HB	3:C:533:HOH:O	2.21	0.40
1:D:90:LEU:O	1:D:91:ALA:C	2.60	0.40

All (5) 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)
3:B:611:HOH:O	3:C:584:HOH:O[1_556]	1.34	0.86
3:B:604:HOH:O	3:D:589:HOH:O[1_556]	1.63	0.57
3:B:613:HOH:O	3:D:586:HOH:O[1_556]	2.05	0.15
3:A:588:HOH:O	3:C:580:HOH:O[1_556]	2.11	0.09
3:B:612:HOH:O	3:D:587:HOH:O[1_556]	2.17	0.03

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	251/272 (92%)	238 (95%)	12 (5%)	1 (0%)	34	38
1	B	258/272 (95%)	243 (94%)	13 (5%)	2 (1%)	19	20
1	C	252/272 (93%)	240 (95%)	11 (4%)	1 (0%)	34	38
1	D	253/272 (93%)	231 (91%)	17 (7%)	5 (2%)	7	4
All	All	1014/1088 (93%)	952 (94%)	53 (5%)	9 (1%)	17	17

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	HIS

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Mol	Chain	Res	Type
1	B	71	HIS
1	C	72	LEU
1	D	61	GLU
1	D	68	HIS
1	D	91	ALA
1	D	96	GLN
1	B	129	SER
1	D	130	GLY

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	219/237 (92%)	205 (94%)	14 (6%)	17	19
1	B	221/237 (93%)	210 (95%)	11 (5%)	24	30
1	C	216/237 (91%)	202 (94%)	14 (6%)	17	19
1	D	212/237 (90%)	196 (92%)	16 (8%)	13	14
All	All	868/948 (92%)	813 (94%)	55 (6%)	18	20

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	35	GLU
1	A	69	THR
1	A	88	LYS
1	A	90	LEU
1	A	94	GLU
1	A	117	THR
1	A	123	GLU
1	A	129	SER
1	A	193	ARG
1	A	206	VAL
1	A	226	ILE
1	A	227	LEU

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Mol	Chain	Res	Type
1	A	249	ARG
1	B	65	ILE
1	B	69	THR
1	B	71	HIS
1	B	72	LEU
1	B	123	GLU
1	B	135	VAL
1	B	163	TYR
1	B	206	VAL
1	B	226	ILE
1	B	235	ARG
1	B	249	ARG
1	C	37	GLU
1	C	49	LEU
1	C	69	THR
1	C	72	LEU
1	C	95	TYR
1	C	123	GLU
1	C	182	THR
1	C	206	VAL
1	C	212	VAL
1	C	220	SER
1	C	223	HIS
1	C	224	LEU
1	C	235	ARG
1	C	249	ARG
1	D	6	THR
1	D	29	MET
1	D	47	THR
1	D	60	ASP
1	D	61	GLU
1	D	69	THR
1	D	102	LEU
1	D	123	GLU
1	D	193	ARG
1	D	203	LYS
1	D	206	VAL
1	D	212	VAL
1	D	223	HIS
1	D	224	LEU
1	D	225	SER
1	D	249	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	122	ASN
1	A	210	GLN
1	A	218	GLN
1	B	68	HIS
1	B	173	HIS
1	B	223	HIS
1	C	53	HIS
1	C	173	HIS
1	C	223	HIS
1	D	143	HIS
1	D	188	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

Of 22 ligands modelled in this entry, 22 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	257/272 (94%)	1.37	49 (19%)	1 2	33, 40, 51, 55	14 (5%)
1	B	262/272 (96%)	1.59	69 (26%)	0 0	31, 40, 48, 55	13 (4%)
1	C	258/272 (94%)	1.65	85 (32%)	0 0	35, 41, 47, 50	8 (3%)
1	D	259/272 (95%)	1.51	66 (25%)	0 1	35, 40, 47, 50	10 (3%)
All	All	1036/1088 (95%)	1.53	269 (25%)	0 1	31, 40, 48, 55	45 (4%)

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	LEU	7.3
1	B	91	ALA	6.6
1	B	130	GLY	6.3
1	C	9	GLY	6.1
1	A	217	PHE	6.0
1	C	68	HIS	6.0
1	A	214	ASP	6.0
1	A	71	HIS	5.9
1	D	131	GLY	5.9
1	D	34	VAL	5.8
1	A	228	HIS	5.6
1	B	227	LEU	5.6
1	C	78	TRP	5.6
1	D	214	ASP	5.6
1	A	69	THR	5.5
1	C	71	HIS	5.5
1	D	129	SER	5.5
1	B	87	VAL	5.5
1	B	71	HIS	5.5
1	B	217	PHE	5.3
1	C	16	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	D	71	HIS	5.2
1	B	72	LEU	5.1
1	C	69	THR	5.1
1	A	216	ASP	5.0
1	B	73	GLY	4.8
1	A	226	ILE	4.7
1	D	227	LEU	4.7
1	C	24	PHE	4.6
1	D	223	HIS	4.4
1	A	94	GLU	4.4
1	C	112	GLY	4.4
1	B	226	ILE	4.3
1	C	86	LEU	4.3
1	D	217	PHE	4.3
1	C	82	GLU	4.2
1	B	13	SER	4.2
1	D	95	TYR	4.2
1	B	131	GLY	4.2
1	B	69	THR	4.2
1	B	109	TYR	4.2
1	B	80	PRO	4.1
1	D	229	ARG	4.1
1	C	42	ILE	4.1
1	B	9	GLY	4.1
1	C	90	LEU	4.1
1	D	130	GLY	4.0
1	D	72	LEU	4.0
1	C	111	ILE	4.0
1	B	129	SER	4.0
1	B	19	ASN	3.9
1	C	84	ASP	3.9
1	C	10	ASP	3.9
1	C	212	VAL	3.8
1	A	44	GLY	3.8
1	C	77	ASP	3.8
1	A	109	TYR	3.8
1	B	18	LEU	3.8
1	C	65	ILE	3.7
1	A	116	ALA	3.7
1	B	34	VAL	3.7
1	C	89	LEU	3.7
1	B	83	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	3	TYR	3.6
1	B	213	ASN	3.6
1	C	130	GLY	3.6
1	B	220	SER	3.6
1	D	13	SER	3.6
1	C	14	ASP	3.5
1	D	60	ASP	3.4
1	C	6	THR	3.4
1	D	248	PHE	3.4
1	C	41	SER	3.4
1	C	72	LEU	3.4
1	D	199	LEU	3.4
1	D	213	ASN	3.4
1	A	221	VAL	3.3
1	C	75	TYR	3.3
1	B	216	ASP	3.3
1	C	13	SER	3.3
1	B	188	ASN	3.3
1	B	128	SER	3.3
1	C	223	HIS	3.3
1	C	18	LEU	3.2
1	C	171	LEU	3.2
1	D	224	LEU	3.2
1	A	9	GLY	3.2
1	B	171	LEU	3.2
1	B	199	LEU	3.2
1	B	89	LEU	3.2
1	C	224	LEU	3.2
1	D	181	LEU	3.2
1	D	226	ILE	3.2
1	D	109	TYR	3.2
1	D	128	SER	3.2
1	A	171	LEU	3.2
1	D	212	VAL	3.1
1	C	12	LYS	3.1
1	C	213	ASN	3.1
1	C	73	GLY	3.1
1	A	213	ASN	3.1
1	B	170	ALA	3.1
1	D	171	LEU	3.0
1	B	81	ALA	3.0
1	C	64	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	34	VAL	3.0
1	C	81	ALA	3.0
1	B	10	ASP	3.0
1	A	198	PRO	3.0
1	B	267	HIS	3.0
1	C	79	ARG	2.9
1	C	29	MET	2.9
1	D	216	ASP	2.9
1	B	24	PHE	2.9
1	D	28	ASP	2.9
1	D	14	ASP	2.9
1	A	250	SER	2.9
1	C	199	LEU	2.9
1	C	100	TYR	2.9
1	D	27	TYR	2.9
1	B	16	LEU	2.8
1	C	248	PHE	2.8
1	B	70	GLY	2.8
1	C	27	TYR	2.8
1	A	28	ASP	2.8
1	C	95	TYR	2.8
1	B	132	PRO	2.8
1	B	192	TYR	2.8
1	B	26	GLU	2.8
1	A	212	VAL	2.7
1	C	87	VAL	2.7
1	A	40	ILE	2.7
1	C	195	ILE	2.7
1	C	262	ILE	2.7
1	B	78	TRP	2.7
1	A	117	THR	2.7
1	C	26	GLU	2.7
1	D	225	SER	2.7
1	C	8	LYS	2.7
1	B	15	LEU	2.7
1	B	90	LEU	2.7
1	B	228	HIS	2.7
1	C	257	VAL	2.7
1	D	83	ALA	2.7
1	C	21	ILE	2.7
1	B	94	GLU	2.7
1	B	248	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	20	MET	2.7
1	C	167	LEU	2.6
1	D	10	ASP	2.6
1	C	3	TYR	2.6
1	D	29	MET	2.6
1	B	168	GLY	2.6
1	D	110	GLY	2.6
1	B	257	VAL	2.6
1	D	167	LEU	2.6
1	D	21	ILE	2.6
1	A	211	PRO	2.6
1	D	31	TYR	2.6
1	A	22	ALA	2.6
1	C	51	ALA	2.6
1	D	12	LYS	2.6
1	C	198	PRO	2.6
1	C	32	ASP	2.6
1	B	11	GLU	2.5
1	B	266	GLU	2.5
1	B	65	ILE	2.5
1	D	168	GLY	2.5
1	C	39	VAL	2.5
1	A	108	LYS	2.5
1	C	220	SER	2.5
1	C	250	SER	2.4
1	C	52	PHE	2.4
1	C	109	TYR	2.4
1	B	262	ILE	2.4
1	B	176	ILE	2.4
1	D	52	PHE	2.4
1	D	94	GLU	2.4
1	A	118	TYR	2.4
1	A	86	LEU	2.4
1	B	169	GLY	2.4
1	A	74	PHE	2.4
1	D	25	GLY	2.4
1	D	93	GLY	2.4
1	A	225	SER	2.4
1	A	65	ILE	2.4
1	B	254	TRP	2.4
1	C	214	ASP	2.4
1	D	169	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	80	PRO	2.4
1	C	66	GLY	2.3
1	D	51	ALA	2.3
1	C	253	PHE	2.3
1	D	32	ASP	2.3
1	C	182	THR	2.3
1	D	43	GLY	2.3
1	A	16	LEU	2.3
1	B	86	LEU	2.3
1	C	55	TYR	2.3
1	D	100	TYR	2.3
1	A	153	CYS	2.3
1	B	167	LEU	2.3
1	C	192	TYR	2.3
1	C	85	LYS	2.3
1	C	110	GLY	2.3
1	D	85	LYS	2.3
1	D	114	LYS	2.3
1	B	225	SER	2.3
1	C	137	VAL	2.3
1	C	113	LYS	2.3
1	B	218	GLN	2.3
1	C	142	ILE	2.3
1	D	243	ILE	2.3
1	B	27	TYR	2.2
1	A	47	THR	2.2
1	C	227	LEU	2.2
1	D	18	LEU	2.2
1	B	232	GLN	2.2
1	C	217	PHE	2.2
1	A	232	GLN	2.2
1	C	31	TYR	2.2
1	C	131	GLY	2.2
1	A	223	HIS	2.2
1	B	198	PRO	2.2
1	D	139	ILE	2.2
1	A	15	LEU	2.2
1	A	199	LEU	2.2
1	D	252	PRO	2.2
1	B	250	SER	2.2
1	A	32	ASP	2.2
1	B	200	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	195	ILE	2.2
1	A	263	GLU	2.2
1	B	41	SER	2.2
1	A	169	GLY	2.2
1	A	200	VAL	2.1
1	D	24	PHE	2.1
1	A	12	LYS	2.1
1	A	167	LEU	2.1
1	B	182	THR	2.1
1	C	40	ILE	2.1
1	C	225	SER	2.1
1	A	72	LEU	2.1
1	D	262	ILE	2.1
1	B	57	GLU	2.1
1	C	76	ALA	2.1
1	D	87	VAL	2.1
1	D	257	VAL	2.1
1	B	127	LYS	2.1
1	D	215	LYS	2.1
1	A	79	ARG	2.1
1	A	170	ALA	2.1
1	D	211	PRO	2.1
1	C	59	LEU	2.0
1	C	226	ILE	2.0
1	C	243	ILE	2.0
1	B	172	MET	2.0
1	D	19	ASN	2.0
1	D	30	GLU	2.0
1	D	89	LEU	2.0
1	D	90	LEU	2.0
1	D	117	THR	2.0
1	C	129	SER	2.0
1	D	91	ALA	2.0
1	A	80	PRO	2.0
1	A	215	LYS	2.0
1	B	29	MET	2.0
1	C	196	GLY	2.0
1	C	47	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	IOD	A	534	1/1	0.93	0.42	39,39,39,39	1
2	IOD	B	515	1/1	0.93	0.15	49,49,49,49	1
2	IOD	A	530	1/1	0.94	0.48	45,45,45,45	1
2	IOD	A	531	1/1	0.96	0.21	46,46,46,46	1
2	IOD	B	522	1/1	0.96	0.06	40,40,40,40	1
2	IOD	C	523	1/1	0.96	0.15	40,40,40,40	1
2	IOD	A	533	1/1	0.97	0.38	48,48,48,48	1
2	IOD	A	513	1/1	0.97	0.17	49,49,49,49	1
2	IOD	B	535	1/1	0.97	0.09	33,33,33,33	1
2	IOD	A	532	1/1	0.97	0.28	41,41,41,41	1
2	IOD	B	528	1/1	0.98	0.25	31,31,31,31	1
2	IOD	A	502[A]	1/1	0.98	0.24	43,43,43,43	1
2	IOD	C	504[A]	1/1	0.98	0.06	33,33,33,33	1
2	IOD	C	504[B]	1/1	0.98	0.06	35,35,35,35	1
2	IOD	A	502[B]	1/1	0.98	0.24	35,35,35,35	1
2	IOD	D	506[A]	1/1	0.98	0.06	33,33,33,33	1
2	IOD	D	506[B]	1/1	0.98	0.06	39,39,39,39	1
2	IOD	D	520	1/1	0.98	0.05	41,41,41,41	1
2	IOD	B	508[A]	1/1	0.99	0.06	37,37,37,37	1
2	IOD	B	508[B]	1/1	0.99	0.06	41,41,41,41	1
2	IOD	D	510	1/1	0.99	0.07	40,40,40,40	1
2	IOD	A	501	1/1	0.99	0.23	36,36,36,36	1

6.5 Other polymers (i)

There are no such residues in this entry.