Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2023 – 01:42 pm GMT

PDB ID	:	1OID
Title	:	5'-Nucleotidase (E. coli) with an Engineered Disulfide Bridge (S228C, P513C)
Authors	:	Schultz-Heienbrok, R.; Maier, T.; Straeter, N.
Deposited on	:	2003-06-13
Resolution	:	2.10 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:

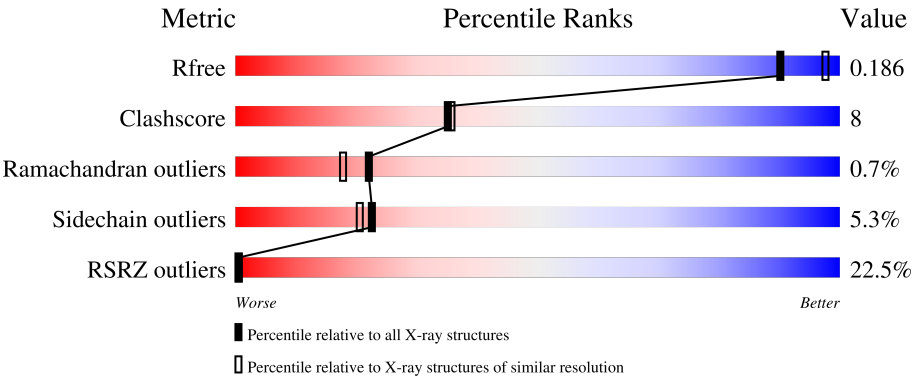
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	532	14% 77% 19%
1	B	532	31% 76% 19%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8920 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 PROTEIN USHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4098	2588	703	788	19			
1	B	523	Total	C	N	O	S	0	0	0
			4075	2572	699	785	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	CYS	SER	engineered mutation	UNP P07024
A	513	CYS	PRO	engineered mutation	UNP P07024
B	228	CYS	SER	engineered mutation	UNP P07024
B	513	CYS	PRO	engineered mutation	UNP P07024

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		

- Molecule 3 is water.

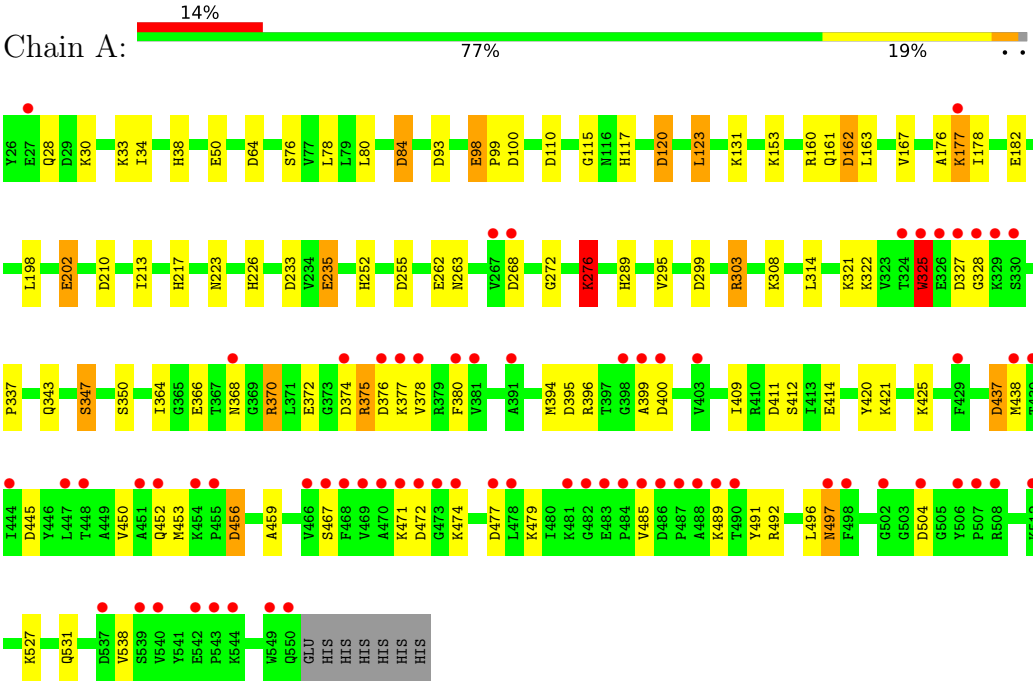
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	408	Total	O	0	0
			408	408		
3	B	338	Total	O	0	0
			338	338		

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.

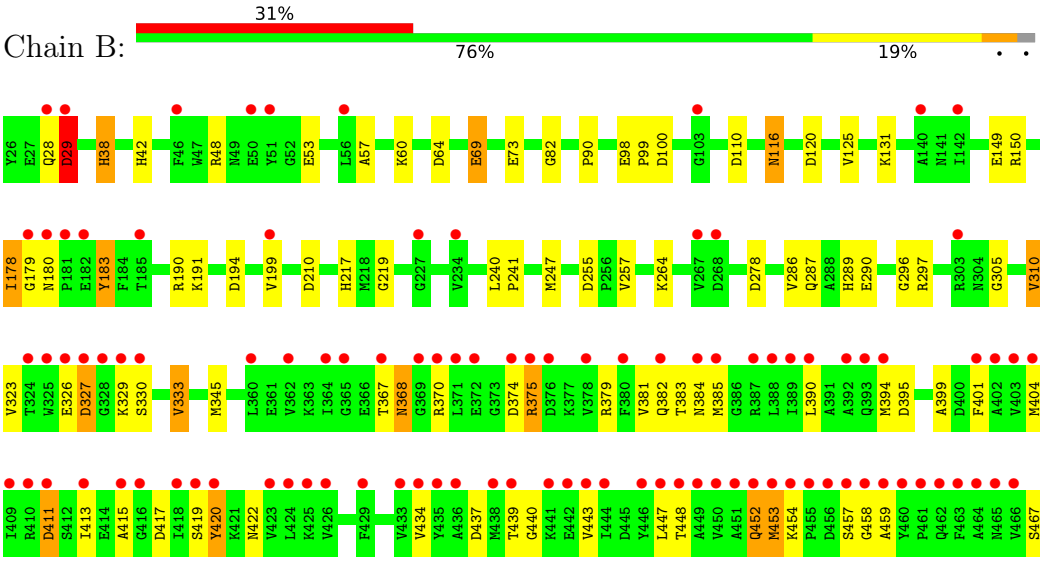
• Molecule 1: PROTEIN USHA

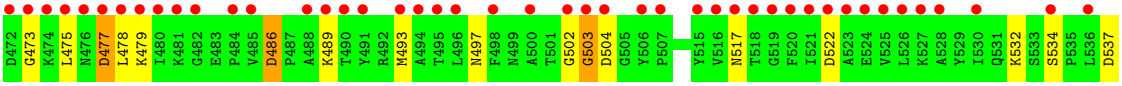
Chain A:



• Molecule 1: PROTEIN USHA

Chain B:




D472
G473
K474
L475
N476
D477
L478
K479
I480
K481
G482
E483
P484
V485
D486
P487
A488
K489
T490
Y491
R492
M493
A494
T495
L496
N497
F498
N499
A500
T501
G502
G503
D504
G505
Y506
P507
Y515
V516
N517
T518
G519
F520
I521
D522
A523
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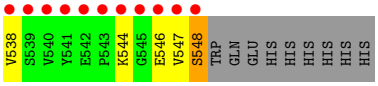
Y529
I530
Q531
K532
S533
S534
P535
L536
D537


V538
S539
V540
Y541
E542
P543
K544
G545
E546
V547
S548
TRP
GLN
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.50Å 93.71Å 82.90Å 90.00° 97.71° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 19.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.00-2.10) 98.4 (19.94-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.166 , 0.215 0.193 , 0.186	Depositor DCC
R_{free} test set	3530 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8920	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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 (i)

5.1 Standard geometry (i)

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

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	1.44	15/4185 (0.4%)	1.24	39/5662 (0.7%)
1	B	1.28	17/4160 (0.4%)	1.16	27/5627 (0.5%)
All	All	1.36	32/8345 (0.4%)	1.20	66/11289 (0.6%)

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

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	VAL	CB-CG2	-10.24	1.31	1.52
1	B	333	VAL	CB-CG2	-9.18	1.33	1.52
1	A	347	SER	CB-OG	-8.95	1.30	1.42
1	A	235	GLU	CD-OE2	-8.45	1.16	1.25
1	B	69	GLU	CD-OE1	8.01	1.34	1.25
1	B	199	VAL	CB-CG1	-7.94	1.36	1.52
1	B	546	GLU	CD-OE1	7.42	1.33	1.25
1	A	98	GLU	CD-OE1	-7.21	1.17	1.25
1	B	69	GLU	CD-OE2	-6.82	1.18	1.25
1	A	343	GLN	CG-CD	6.77	1.66	1.51
1	A	347	SER	CA-CB	6.67	1.62	1.52
1	A	235	GLU	CG-CD	6.66	1.61	1.51
1	A	235	GLU	CD-OE1	-6.51	1.18	1.25
1	A	276	LYS	CD-CE	6.43	1.67	1.51
1	A	350	SER	CA-CB	6.21	1.62	1.52
1	A	202	GLU	CD-OE2	6.10	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	323	VAL	CB-CG2	-5.95	1.40	1.52
1	B	219	GLY	C-O	5.78	1.32	1.23
1	B	53	GLU	CD-OE1	-5.68	1.19	1.25
1	A	195	GLU	CD-OE2	-5.65	1.19	1.25
1	A	497	ASN	CB-CG	5.60	1.64	1.51
1	B	131	LYS	CD-CE	5.55	1.65	1.51
1	B	547	VAL	CA-CB	5.47	1.66	1.54
1	B	548	SER	CB-OG	5.45	1.49	1.42
1	B	247	MET	CG-SD	5.29	1.95	1.81
1	B	149	GLU	CD-OE1	-5.23	1.19	1.25
1	A	335	TYR	CE1-CZ	-5.17	1.31	1.38
1	A	272	GLY	C-O	-5.13	1.15	1.23
1	B	313	GLN	CB-CG	-5.09	1.38	1.52
1	B	497	ASN	CB-CG	5.09	1.62	1.51
1	B	125	VAL	CB-CG2	5.08	1.63	1.52
1	B	290	GLU	CG-CD	5.00	1.59	1.51

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	235	GLU	OE1-CD-OE2	-13.50	107.11	123.30
1	B	48	ARG	NE-CZ-NH1	13.28	126.94	120.30
1	B	64	ASP	CB-CG-OD1	11.16	128.34	118.30
1	B	210	ASP	CB-CG-OD2	10.76	127.99	118.30
1	A	162	ASP	CB-CG-OD2	10.71	127.94	118.30
1	B	48	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	B	255	ASP	CB-CG-OD2	8.69	126.12	118.30
1	A	347	SER	N-CA-CB	8.34	123.01	110.50
1	A	84	ASP	CB-CG-OD1	8.28	125.75	118.30
1	A	255	ASP	CB-CG-OD1	-8.14	110.97	118.30
1	A	303	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	B	255	ASP	CB-CG-OD1	-8.03	111.07	118.30
1	A	93	ASP	CB-CG-OD1	7.95	125.46	118.30
1	A	255	ASP	CB-CG-OD2	7.92	125.43	118.30
1	B	120	ASP	CB-CG-OD2	7.81	125.33	118.30
1	A	445	ASP	CB-CG-OD2	7.77	125.30	118.30
1	A	123	LEU	CB-CG-CD1	7.45	123.67	111.00
1	A	477	ASP	CB-CG-OD2	7.32	124.89	118.30
1	A	299	ASP	CB-CG-OD2	7.32	124.88	118.30
1	A	504	ASP	CB-CG-OD2	7.19	124.77	118.30
1	A	400	ASP	CB-CG-OD2	6.96	124.56	118.30
1	B	395	ASP	CB-CG-OD2	6.81	124.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	522	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	437	ASP	CB-CG-OD2	6.52	124.17	118.30
1	B	477	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	303	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	347	SER	CA-CB-OG	-6.43	93.83	111.20
1	A	162	ASP	CB-CG-OD1	-6.26	112.67	118.30
1	A	110	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	374	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	78	LEU	CB-CG-CD1	6.12	121.41	111.00
1	A	235	GLU	CG-CD-OE1	6.12	130.54	118.30
1	B	194	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	370	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	B	297	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	210	ASP	CB-CG-OD2	5.84	123.55	118.30
1	A	100	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	110	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	504	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	268	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	325	TRP	CA-CB-CG	5.68	124.49	113.70
1	A	233	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	472	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	537	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	186	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	185	THR	OG1-CB-CG2	-5.56	97.22	110.00
1	A	327	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	29	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	370	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	278	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	347	SER	CB-CA-C	-5.38	99.89	110.10
1	B	437	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	522	ASP	CB-CG-OD1	5.32	123.08	118.30
1	B	327	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	69	GLU	CG-CD-OE2	-5.28	107.74	118.30
1	B	60	LYS	CD-CE-NZ	-5.18	99.79	111.70
1	B	150	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	310	VAL	CG1-CB-CG2	5.16	119.16	110.90
1	A	295	VAL	CG1-CB-CG2	-5.13	102.69	110.90
1	B	411	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	396	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	B	486	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	417	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	210	ASP	CB-CG-OD1	-5.07	113.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	120	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	64	ASP	CB-CG-OD1	5.05	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	437	ASP	Mainchain

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	4098	0	4015	58	1
1	B	4075	0	3997	74	0
2	A	1	0	0	0	0
3	A	408	0	0	13	1
3	B	338	0	0	9	0
All	All	8920	0	8012	132	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 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)
1:B:38:HIS:CE1	1:B:296:GLY:HA3	1.80	1.15
1:B:401:PHE:CE2	1:B:493:MET:HG3	1.83	1.14
1:B:73:GLU:HG2	3:B:2058:HOH:O	1.59	1.02
1:A:84:ASP:CG	1:A:217:HIS:HE1	1.67	0.98
1:B:217:HIS:HE1	3:B:2099:HOH:O	1.51	0.94
1:B:401:PHE:CZ	1:B:493:MET:HB2	2.05	0.92
1:B:38:HIS:HE1	1:B:296:GLY:HA3	1.37	0.88
1:A:217:HIS:CD2	1:A:252:HIS:HB2	2.10	0.87
1:A:115:GLY:CA	1:A:217:HIS:ND1	2.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:PHE:CE2	1:B:493:MET:CG	2.60	0.84
1:A:115:GLY:HA2	1:A:217:HIS:ND1	1.92	0.83
1:A:30:LYS:NZ	3:A:2006:HOH:O	2.13	0.82
1:A:153:LYS:HD2	3:A:2066:HOH:O	1.80	0.80
1:A:84:ASP:CG	1:A:217:HIS:CE1	2.55	0.79
1:B:38:HIS:CD2	1:B:286:VAL:CG2	2.67	0.77
1:B:38:HIS:ND1	1:B:296:GLY:HA3	2.01	0.75
1:B:38:HIS:CD2	1:B:286:VAL:HG21	2.22	0.75
1:B:217:HIS:CE1	3:B:2099:HOH:O	2.34	0.72
1:B:401:PHE:CZ	1:B:493:MET:CB	2.72	0.71
1:A:117:HIS:HD2	1:A:120:ASP:OD2	1.73	0.71
1:A:115:GLY:HA3	1:A:217:HIS:ND1	2.05	0.70
1:B:28:GLN:HG3	1:B:29:ASP:OD1	1.91	0.69
1:B:116:ASN:HD22	1:B:116:ASN:H	1.41	0.69
1:B:401:PHE:CD2	1:B:493:MET:HG3	2.29	0.68
1:A:467:SER:OG	1:A:479:LYS:HB2	1.93	0.67
1:B:401:PHE:CZ	1:B:493:MET:HG3	2.29	0.67
1:B:401:PHE:CZ	1:B:493:MET:CG	2.79	0.66
1:B:38:HIS:CD2	1:B:286:VAL:HG23	2.31	0.65
1:A:153:LYS:CD	3:A:2066:HOH:O	2.42	0.65
1:B:367:THR:HG23	1:B:415:ALA:HA	1.80	0.63
1:A:527:LYS:HE2	1:A:531:GLN:NE2	2.17	0.60
1:B:394:MET:HG2	1:B:399:ALA:HB3	1.84	0.60
1:A:276:LYS:HE2	3:A:2264:HOH:O	2.01	0.60
1:B:178:ILE:HG22	1:B:179:GLY:H	1.65	0.60
1:B:180:ASN:O	1:B:183:TYR:HB3	2.03	0.59
1:A:84:ASP:OD1	1:A:217:HIS:HE1	1.86	0.58
1:A:177:LYS:C	1:A:178:ILE:HD12	2.24	0.58
1:B:116:ASN:ND2	1:B:217:HIS:HE1	2.02	0.58
1:B:439:THR:O	1:B:443:VAL:HG23	2.04	0.57
1:B:116:ASN:ND2	1:B:217:HIS:CE1	2.72	0.57
1:B:38:HIS:HD2	1:B:286:VAL:CG2	2.16	0.57
1:B:448:THR:O	1:B:452:GLN:NE2	2.38	0.56
1:B:385:MET:HE1	1:B:413:ILE:HD12	1.86	0.56
1:A:198:LEU:O	1:A:202:GLU:HG3	2.05	0.55
1:A:84:ASP:CB	1:A:217:HIS:HE1	2.19	0.55
1:A:226:HIS:CD2	1:A:235:GLU:OE2	2.60	0.55
1:A:325:TRP:NE1	3:A:2302:HOH:O	2.39	0.55
1:A:117:HIS:CD2	1:A:120:ASP:OD2	2.58	0.54
1:A:527:LYS:HE2	1:A:531:GLN:HE22	1.72	0.54
1:A:178:ILE:HG13	1:A:516:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ASN:OD1	1:A:538:VAL:HG22	2.08	0.54
1:B:384:ASN:ND2	3:B:2311:HOH:O	2.39	0.54
1:B:544:LYS:NZ	3:B:2338:HOH:O	2.41	0.54
1:B:82:GLY:O	1:B:217:HIS:HD2	1.91	0.53
1:A:226:HIS:HD2	1:A:235:GLU:OE2	1.91	0.53
1:A:380:PHE:CZ	1:A:456:ASP:HB2	2.44	0.53
1:B:440:GLY:HA3	1:B:486:ASP:O	2.10	0.52
1:A:376:ASP:O	1:A:377:LYS:C	2.49	0.51
1:B:240:LEU:HB3	1:B:241:PRO:HD2	1.93	0.51
1:B:191:LYS:HE2	3:B:2173:HOH:O	2.10	0.51
1:A:115:GLY:HA3	1:A:217:HIS:CE1	2.45	0.50
1:A:489:LYS:HB3	1:A:491:TYR:CE2	2.45	0.50
1:A:421:LYS:HD2	1:A:425:LYS:NZ	2.27	0.50
1:B:257:VAL:HG23	1:B:287:GLN:HB3	1.94	0.49
1:A:262:GLU:OE1	3:A:2244:HOH:O	2.20	0.49
1:A:372:GLU:OE2	1:A:374:ASP:HB3	2.12	0.49
1:A:153:LYS:CE	3:A:2066:HOH:O	2.60	0.49
1:B:116:ASN:HD21	1:B:217:HIS:HE1	1.59	0.49
1:B:405:SER:HB3	1:B:458:GLY:O	2.13	0.49
1:B:38:HIS:NE2	1:B:286:VAL:CG2	2.75	0.49
1:A:527:LYS:CE	3:A:2398:HOH:O	2.60	0.48
1:B:326:GLU:HG3	1:B:327:ASP:N	2.27	0.48
1:B:419:SER:H	1:B:422:ASN:ND2	2.11	0.48
1:B:190:ARG:HD3	3:B:2170:HOH:O	2.14	0.48
1:B:401:PHE:CE1	1:B:493:MET:HB2	2.49	0.48
1:A:84:ASP:OD1	1:A:217:HIS:CE1	2.66	0.48
1:B:38:HIS:HD2	1:B:286:VAL:HG23	1.78	0.48
1:B:486:ASP:OD1	1:B:489:LYS:HE3	2.13	0.48
1:A:176:ALA:HB3	3:A:2175:HOH:O	2.14	0.47
1:A:76:SER:HB2	1:A:160:ARG:HD2	1.97	0.47
1:B:401:PHE:CE2	1:B:493:MET:SD	3.08	0.47
1:A:399:ALA:HA	1:A:492:ARG:HB3	1.97	0.47
1:B:183:TYR:C	1:B:183:TYR:CD1	2.88	0.47
1:B:368:ASN:O	1:B:538:VAL:HG22	2.14	0.47
1:A:33:LYS:HE2	3:A:2007:HOH:O	2.15	0.46
1:A:34:ILE:HD11	1:A:163:LEU:HD12	1.97	0.46
1:B:90:PRO:HB3	1:B:420:TYR:CE2	2.50	0.46
1:B:379:ARG:NH1	1:B:458:GLY:N	2.64	0.46
1:B:467:SER:O	1:B:478:LEU:HA	2.15	0.46
1:B:98:GLU:N	1:B:99:PRO:HD2	2.30	0.46
1:A:84:ASP:CB	1:A:217:HIS:CE1	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ALA:HA	1:B:345:MET:HG2	1.98	0.46
1:B:42:HIS:HE1	1:B:100:ASP:OD2	1.98	0.45
1:A:453:MET:HE2	1:A:459:ALA:HB1	1.98	0.45
1:B:453:MET:HG2	1:B:459:ALA:HB1	1.99	0.45
1:A:223:ASN:HB2	1:A:263:ASN:HB3	1.99	0.44
1:B:116:ASN:HD22	1:B:217:HIS:CE1	2.35	0.44
1:B:434:VAL:HG12	1:B:517:ASN:HA	1.99	0.44
1:A:38:HIS:HA	1:A:80:LEU:O	2.17	0.44
1:B:38:HIS:CE1	1:B:312:TYR:OH	2.70	0.44
1:B:447:LEU:HD13	1:B:478:LEU:HD11	2.00	0.44
1:B:448:THR:HG23	1:B:473:GLY:O	2.18	0.44
1:B:161:GLN:NE2	3:B:2152:HOH:O	2.11	0.44
1:B:448:THR:OG1	1:B:475:LEU:CD1	2.66	0.44
1:A:325:TRP:CE2	3:A:2302:HOH:O	2.57	0.43
1:B:116:ASN:H	1:B:116:ASN:ND2	2.12	0.43
1:B:38:HIS:CE1	1:B:296:GLY:CA	2.75	0.43
1:B:305:GLY:HA2	3:B:2193:HOH:O	2.18	0.43
1:A:364:ILE:HD13	1:A:527:LYS:HG2	2.01	0.42
1:A:497:ASN:HA	3:A:2390:HOH:O	2.19	0.42
1:A:375:ARG:CG	1:A:376:ASP:N	2.83	0.42
1:B:183:TYR:CD1	1:B:183:TYR:O	2.73	0.42
1:A:321:LYS:HB2	1:A:335:TYR:CZ	2.55	0.41
1:B:502:GLY:O	1:B:503:GLY:C	2.58	0.41
1:B:69:GLU:OE2	1:B:73:GLU:OE2	2.38	0.41
1:B:379:ARG:HD3	1:B:457:SER:C	2.41	0.41
1:A:98:GLU:N	1:A:99:PRO:HD2	2.35	0.41
1:B:390:LEU:HD21	1:B:404:MET:HG2	2.02	0.41
1:A:453:MET:HE3	3:A:2380:HOH:O	2.21	0.41
1:A:160:ARG:O	1:A:161:GLN:HB2	2.20	0.41
1:A:167:VAL:HA	1:A:213:ILE:O	2.21	0.41
1:A:378:VAL:HG11	1:A:409:ILE:HG21	2.03	0.41
1:A:394:MET:O	1:A:395:ASP:C	2.55	0.41
1:B:375:ARG:H	1:B:375:ARG:HG3	1.71	0.41
1:B:447:LEU:CD1	1:B:478:LEU:HD11	2.51	0.41
1:B:469:VAL:HG13	1:B:548:SER:OG	2.20	0.41
1:B:381:VAL:HG12	1:B:382:GLN:N	2.36	0.41
1:A:336:THR:HB	1:A:337:PRO:HD2	2.03	0.40
1:A:370:ARG:NH1	1:A:372:GLU:OE1	2.42	0.40
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.97	0.40
1:A:411:ASP:OD2	1:A:412:SER:N	2.45	0.40
1:B:453:MET:CG	1:B:459:ALA:HB1	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLU:OE2	3:A:2286:HOH:O[2_945]	1.99	0.21

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	523/532 (98%)	495 (95%)	25 (5%)	3 (1%)	25	21
1	B	521/532 (98%)	496 (95%)	21 (4%)	4 (1%)	19	15
All	All	1044/1064 (98%)	991 (95%)	46 (4%)	7 (1%)	22	18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	GLY
1	B	183	TYR
1	B	503	GLY
1	A	289	HIS
1	B	29	ASP
1	B	289	HIS
1	A	456	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	433/440 (98%)	409 (94%)	24 (6%)	21 19
1	B	431/440 (98%)	409 (95%)	22 (5%)	24 22
All	All	864/880 (98%)	818 (95%)	46 (5%)	22 20

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	50	GLU
1	A	123	LEU
1	A	131	LYS
1	A	162	ASP
1	A	177	LYS
1	A	182	GLU
1	A	276	LYS
1	A	303	ARG
1	A	308	LYS
1	A	322	LYS
1	A	325	TRP
1	A	347	SER
1	A	366	GLU
1	A	375	ARG
1	A	420	TYR
1	A	438	MET
1	A	441	LYS
1	A	450	VAL
1	A	452	GLN
1	A	471	LYS
1	A	474	LYS
1	A	485	VAL
1	A	496	LEU
1	B	38	HIS
1	B	116	ASN
1	B	178	ILE
1	B	264	LYS
1	B	310	VAL
1	B	329	LYS
1	B	330	SER
1	B	333	VAL
1	B	368	ASN
1	B	370	ARG
1	B	375	ARG

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Mol	Chain	Res	Type
1	B	383	THR
1	B	411	ASP
1	B	420	TYR
1	B	452	GLN
1	B	453	MET
1	B	454	LYS
1	B	469	VAL
1	B	477	ASP
1	B	479	LYS
1	B	532	LYS
1	B	534	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	117	HIS
1	A	204	GLN
1	A	217	HIS
1	A	226	HIS
1	A	266	GLN
1	A	289	HIS
1	A	531	GLN
1	B	38	HIS
1	B	42	HIS
1	B	116	ASN
1	B	217	HIS
1	B	279	GLN
1	B	353	GLN
1	B	422	ASN
1	B	431	ASN
1	B	452	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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	525/532 (98%)	0.53	72 (13%)	3 4	18, 32, 63, 82	0
1	B	523/532 (98%)	1.51	164 (31%)	0 0	22, 38, 80, 94	0
All	All	1048/1064 (98%)	1.02	236 (22%)	0 0	18, 35, 75, 94	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	401	PHE	9.7
1	B	463	PHE	9.3
1	B	454	LYS	9.0
1	B	491	TYR	8.9
1	B	389	ILE	8.7
1	B	403	VAL	8.6
1	A	325	TRP	8.2
1	B	402	ALA	8.2
1	B	490	THR	8.0
1	B	530	ILE	7.9
1	B	526	LEU	7.6
1	B	494	ALA	7.6
1	B	464	ALA	7.5
1	B	547	VAL	7.0
1	B	523	ALA	6.9
1	B	543	PRO	6.9
1	B	458	GLY	6.7
1	B	443	VAL	6.7
1	B	482	GLY	6.7
1	A	490	THR	6.5
1	B	466	VAL	6.5
1	A	473	GLY	6.5
1	B	478	LEU	6.5
1	B	404	MET	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	493	MET	6.2
1	B	502	GLY	6.2
1	B	469	VAL	6.2
1	B	434	VAL	6.1
1	A	484	PRO	6.1
1	B	495	THR	6.0
1	A	482	GLY	6.0
1	B	520	PHE	6.0
1	A	488	ALA	6.0
1	B	423	VAL	5.9
1	A	326	GLU	5.9
1	B	480	ILE	5.8
1	B	447	LEU	5.7
1	B	436	ALA	5.7
1	B	473	GLY	5.6
1	B	388	LEU	5.6
1	B	420	TYR	5.6
1	B	324	THR	5.6
1	B	470	ALA	5.5
1	B	329	LYS	5.4
1	B	390	LEU	5.4
1	B	327	ASP	5.4
1	B	539	SER	5.3
1	B	376	ASP	5.2
1	B	468	PHE	5.2
1	B	472	ASP	5.2
1	B	446	TYR	5.2
1	B	527	LYS	5.2
1	B	180	ASN	5.0
1	B	409	ILE	5.0
1	A	448	THR	4.9
1	B	485	VAL	4.9
1	B	459	ALA	4.9
1	B	378	VAL	4.8
1	B	433	VAL	4.8
1	B	484	PRO	4.8
1	B	471	LYS	4.8
1	B	393	GLN	4.7
1	A	454	LYS	4.6
1	B	435	TYR	4.6
1	A	328	GLY	4.6
1	B	182	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	367	THR	4.5
1	B	521	ILE	4.5
1	B	516	VAL	4.5
1	B	450	VAL	4.4
1	B	525	VAL	4.4
1	A	327	ASP	4.4
1	B	416	GLY	4.4
1	B	438	MET	4.4
1	A	486	ASP	4.4
1	A	485	VAL	4.3
1	B	418	ILE	4.3
1	B	536	LEU	4.3
1	B	267	VAL	4.3
1	B	456	ASP	4.2
1	B	326	GLU	4.1
1	B	462	GLN	4.1
1	A	451	ALA	4.1
1	B	475	LEU	4.1
1	B	489	LYS	4.0
1	A	483	GLU	4.0
1	B	56	LEU	4.0
1	A	477	ASP	4.0
1	B	515	TYR	4.0
1	A	469	VAL	4.0
1	B	375	ARG	3.9
1	A	489	LYS	3.8
1	A	439	THR	3.8
1	B	360	LEU	3.8
1	A	452	GLN	3.8
1	A	470	ALA	3.8
1	A	467	SER	3.7
1	B	519	GLY	3.7
1	B	424	LEU	3.7
1	B	268	ASP	3.6
1	B	429	PHE	3.6
1	B	518	THR	3.6
1	B	364	ILE	3.5
1	B	524	GLU	3.5
1	B	451	ALA	3.5
1	A	398	GLY	3.5
1	B	460	TYR	3.5
1	B	380	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	544	LYS	3.4
1	A	268	ASP	3.4
1	A	487	PRO	3.4
1	B	541	TYR	3.4
1	A	502	GLY	3.4
1	B	465	ASN	3.4
1	A	540	VAL	3.4
1	B	382	GLN	3.3
1	B	534	SER	3.3
1	B	453	MET	3.3
1	A	471	LYS	3.3
1	B	528	ALA	3.3
1	B	405	SER	3.3
1	A	329	LYS	3.3
1	A	466	VAL	3.3
1	B	29	ASP	3.2
1	B	457	SER	3.2
1	B	548	SER	3.2
1	B	517	ASN	3.2
1	A	429	PHE	3.2
1	B	330	SER	3.2
1	B	461	PRO	3.2
1	A	481	LYS	3.2
1	B	488	ALA	3.2
1	A	504	ASP	3.2
1	A	507	PRO	3.1
1	A	472	ASP	3.1
1	A	324	THR	3.1
1	B	542	GLU	3.1
1	B	439	THR	3.1
1	B	498	PHE	3.1
1	B	385	MET	3.1
1	B	481	LYS	3.1
1	B	476	ASN	3.1
1	B	181	PRO	3.1
1	A	438	MET	3.1
1	A	399	ALA	3.0
1	A	512	LYS	3.0
1	B	452	GLN	3.0
1	A	539	SER	3.0
1	B	479	LYS	3.0
1	B	503	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	368	ASN	3.0
1	B	328	GLY	3.0
1	B	444	ILE	2.9
1	A	508	ARG	2.9
1	A	377	LYS	2.9
1	B	474	LYS	2.9
1	B	411	ASP	2.9
1	B	413	ILE	2.9
1	B	51	TYR	2.9
1	A	550	GLN	2.8
1	B	142	ILE	2.8
1	A	537	ASP	2.8
1	A	267	VAL	2.8
1	A	544	LYS	2.8
1	A	498	PHE	2.8
1	B	426	VAL	2.8
1	B	496	LEU	2.8
1	B	392	ALA	2.8
1	B	46	PHE	2.8
1	B	371	LEU	2.8
1	A	380	PHE	2.7
1	A	391	ALA	2.7
1	A	455	PRO	2.7
1	B	545	GLY	2.7
1	B	384	ASN	2.7
1	A	443	VAL	2.6
1	A	542	GLU	2.6
1	B	415	ALA	2.6
1	A	474	LYS	2.6
1	B	372	GLU	2.6
1	B	500	ALA	2.6
1	B	448	THR	2.6
1	B	28	GLN	2.6
1	B	504	ASP	2.6
1	B	325	TRP	2.6
1	B	477	ASP	2.6
1	B	506	TYR	2.6
1	A	378	VAL	2.5
1	B	362	VAL	2.5
1	A	376	ASP	2.5
1	B	50	GLU	2.5
1	B	441	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	447	LEU	2.5
1	B	455	PRO	2.4
1	B	419	SER	2.4
1	B	387	ARG	2.4
1	B	394	MET	2.4
1	A	441	LYS	2.4
1	A	468	PHE	2.4
1	B	425	LYS	2.4
1	A	400	ASP	2.4
1	A	381	VAL	2.4
1	B	410	ARG	2.4
1	B	507	PRO	2.3
1	B	370	ARG	2.3
1	B	103	GLY	2.3
1	B	374	ASP	2.3
1	A	403	VAL	2.3
1	A	549	TRP	2.3
1	A	497	ASN	2.3
1	A	506	TYR	2.2
1	B	449	ALA	2.2
1	B	227	GLY	2.2
1	B	406	GLY	2.2
1	B	546	GLU	2.2
1	A	543	PRO	2.2
1	A	374	ASP	2.2
1	B	199	VAL	2.2
1	A	330	SER	2.2
1	B	540	VAL	2.2
1	B	165	ILE	2.1
1	A	478	LEU	2.1
1	A	177	LYS	2.1
1	B	407	GLY	2.1
1	B	185	THR	2.1
1	A	444	ILE	2.1
1	B	442	GLU	2.1
1	B	303	ARG	2.1
1	B	179	GLY	2.1
1	B	369	GLY	2.1
1	A	27	GLU	2.1
1	B	365	GLY	2.1
1	B	140	ALA	2.1
1	B	522	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	234	VAL	2.0
1	B	538	VAL	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	NI	A	1551	1/1	0.97	0.11	66,66,66,66	0

6.5 Other polymers (i)

There are no such residues in this entry.