



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:46 AM UTC

PDB ID : 1OID / pdb_00001oid
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

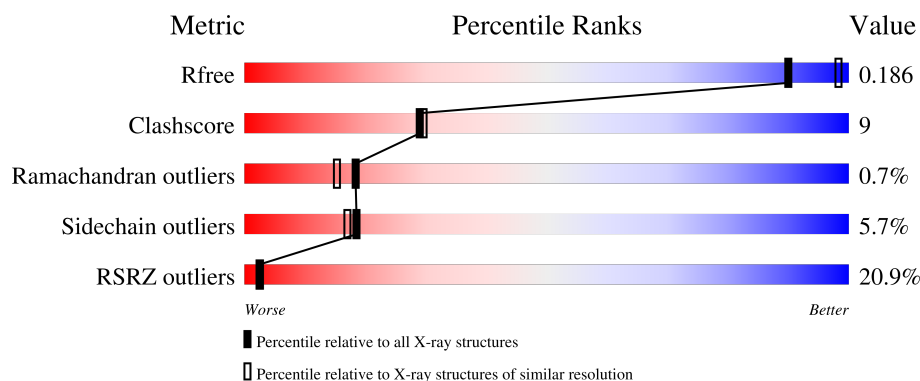
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	4% 72% 23% ..
1	B	532	38% 73% 22% ...

2 Entry composition

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 (CCD ID: NI) (formula: Ni).

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

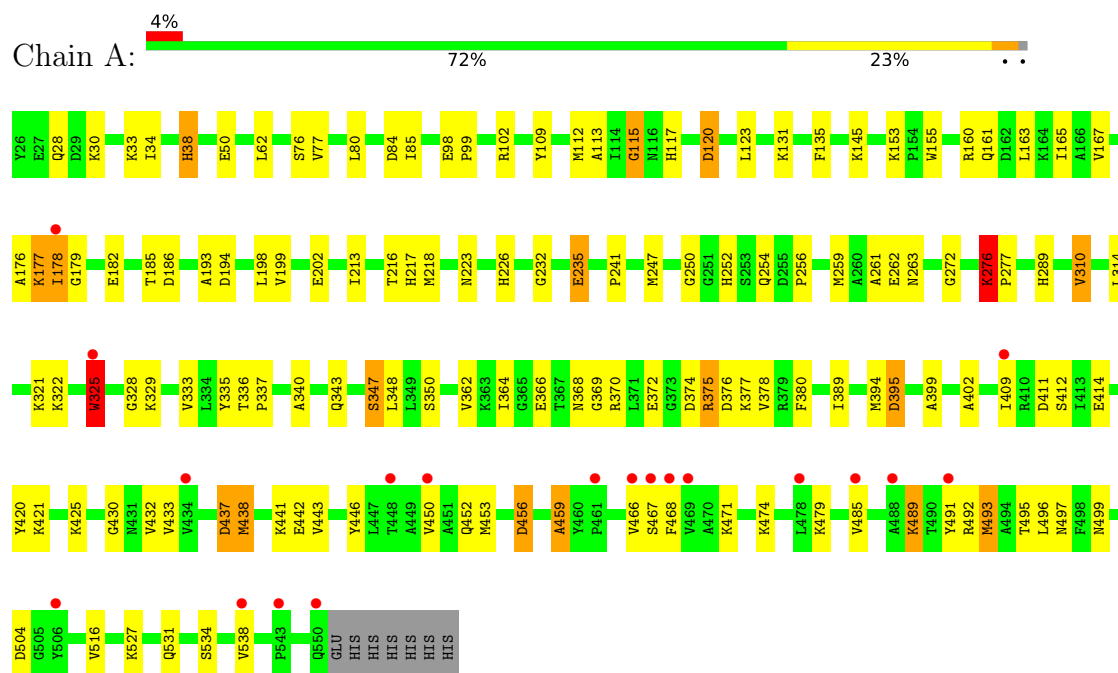
- Molecule 3 is water.

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

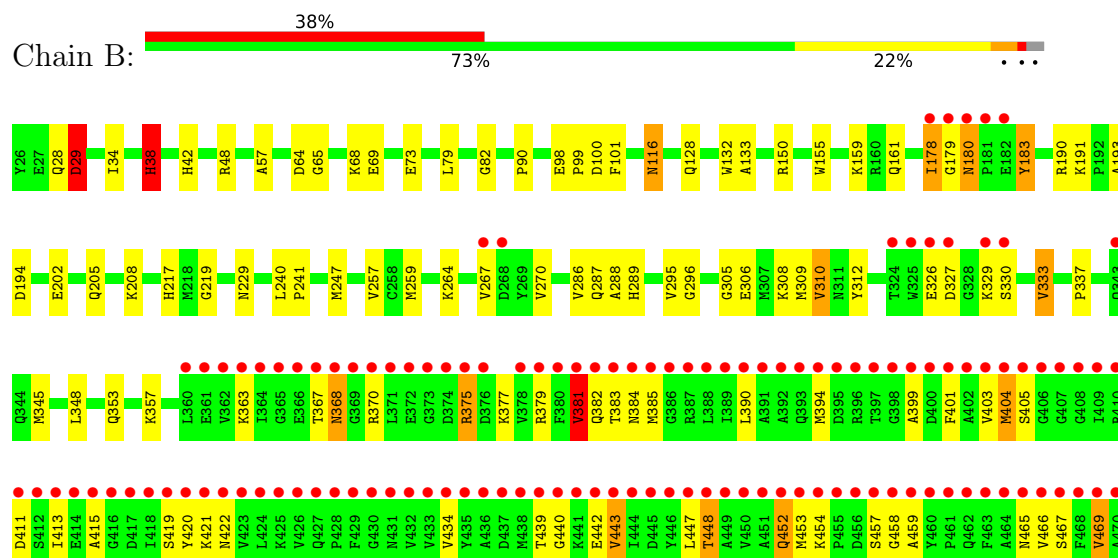
3 Residue-property plots

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



• Molecule 1: PROTEIN USHA





4 Data and refinement statistics

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 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.00-2.10) 98.3 (30.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.35 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	1.77	56/4185 (1.3%)	1.36	13/5662 (0.2%)
1	B	1.59	36/4160 (0.9%)	1.32	17/5627 (0.3%)
All	All	1.68	92/8345 (1.1%)	1.34	30/11289 (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

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	547	VAL	CA-CB	9.21	1.66	1.54
1	B	208	LYS	CA-C	8.04	1.58	1.53
1	A	495	THR	CA-CB	-7.75	1.44	1.54
1	A	389	ILE	CA-CB	7.29	1.63	1.54
1	B	353	GLN	C-O	7.24	1.32	1.24
1	A	277	PRO	CA-C	7.19	1.61	1.52
1	A	362	VAL	CA-CB	7.19	1.62	1.54
1	B	348	LEU	C-O	-7.17	1.15	1.24
1	A	115	GLY	N-CA	7.13	1.52	1.44
1	B	357	LYS	C-O	-7.11	1.15	1.24
1	A	443	VAL	CA-CB	7.00	1.62	1.54
1	B	101	PHE	N-CA	-6.86	1.38	1.46
1	B	443	VAL	CA-CB	6.79	1.63	1.54
1	B	259	MET	SD-CE	6.75	1.96	1.79
1	A	216	THR	CA-C	-6.70	1.44	1.52
1	B	219	GLY	C-O	6.65	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	493	MET	CA-C	6.63	1.61	1.52
1	A	62	LEU	C-O	6.55	1.31	1.24
1	A	310	VAL	C-O	-6.49	1.17	1.24
1	A	333	VAL	CB-CG2	-6.42	1.31	1.52
1	A	109	TYR	C-O	6.37	1.31	1.23
1	B	542	GLU	CA-C	6.25	1.60	1.52
1	A	272	GLY	C-O	-6.19	1.15	1.24
1	A	199	VAL	C-O	-6.19	1.17	1.24
1	A	347	SER	CA-CB	6.18	1.62	1.53
1	A	232	GLY	C-O	6.14	1.29	1.24
1	A	350	SER	CA-CB	6.12	1.62	1.53
1	B	270	VAL	CA-C	6.12	1.57	1.53
1	A	261	ALA	C-O	6.08	1.30	1.23
1	B	38	HIS	CE1-NE2	-6.00	1.26	1.32
1	A	495	THR	C-O	5.98	1.28	1.24
1	A	186	ASP	CA-CB	5.93	1.61	1.53
1	A	120	ASP	C-O	-5.92	1.16	1.24
1	A	38	HIS	C-O	5.92	1.31	1.23
1	A	433	VAL	CA-CB	-5.91	1.46	1.54
1	A	499	ASN	C-O	5.90	1.31	1.24
1	B	68	LYS	C-O	-5.89	1.17	1.24
1	A	135	PHE	CA-C	5.86	1.58	1.52
1	A	343	GLN	CG-CD	5.83	1.66	1.52
1	B	466	VAL	CA-CB	5.81	1.61	1.54
1	B	193	ALA	C-O	-5.78	1.17	1.24
1	B	205	GLN	C-O	-5.77	1.17	1.24
1	A	347	SER	CB-OG	-5.77	1.30	1.42
1	A	113	ALA	CA-CB	-5.75	1.44	1.53
1	B	333	VAL	CB-CG2	-5.75	1.33	1.52
1	A	179	GLY	N-CA	5.70	1.49	1.44
1	A	218	MET	SD-CE	-5.66	1.65	1.79
1	B	247	MET	CG-SD	5.66	1.95	1.80
1	B	465	ASN	CA-C	5.61	1.60	1.52
1	A	459	ALA	CA-CB	-5.61	1.43	1.53
1	B	64	ASP	C-O	-5.61	1.17	1.24
1	A	369	GLY	C-O	5.54	1.29	1.23
1	A	466	VAL	CA-C	5.52	1.59	1.52
1	A	432	VAL	C-O	-5.49	1.18	1.24
1	A	340	ALA	C-O	-5.47	1.17	1.23
1	A	347	SER	C-O	-5.46	1.17	1.24
1	B	295	VAL	CA-CB	-5.45	1.47	1.54
1	A	85	ILE	C-O	5.44	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	GLU	C-O	-5.43	1.17	1.24
1	A	250	GLY	N-CA	-5.43	1.40	1.44
1	A	259	MET	CA-C	5.40	1.59	1.52
1	B	404	MET	SD-CE	5.38	1.93	1.79
1	A	77	VAL	C-O	-5.38	1.18	1.24
1	A	402	ALA	CA-CB	5.33	1.62	1.53
1	A	347	SER	N-CA	5.31	1.52	1.46
1	B	259	MET	CA-C	5.30	1.59	1.52
1	A	256	PRO	C-O	-5.29	1.18	1.23
1	B	288	ALA	CA-CB	-5.27	1.45	1.53
1	A	165	ILE	CA-CB	5.26	1.60	1.54
1	B	155	TRP	N-CA	-5.26	1.39	1.45
1	A	241	PRO	C-O	5.24	1.29	1.23
1	A	112	MET	C-O	5.24	1.30	1.23
1	B	38	HIS	CA-C	-5.24	1.46	1.52
1	A	193	ALA	CA-CB	5.23	1.61	1.53
1	A	102	ARG	CA-C	-5.20	1.46	1.52
1	A	340	ALA	CA-CB	5.17	1.61	1.53
1	B	79	LEU	CA-CB	5.16	1.60	1.53
1	B	180	ASN	CA-C	5.15	1.59	1.52
1	A	145	LYS	C-O	-5.14	1.18	1.24
1	A	499	ASN	CA-C	5.12	1.59	1.52
1	A	395	ASP	CA-C	5.12	1.59	1.52
1	B	229	ASN	CG-ND2	-5.08	1.22	1.33
1	B	309	MET	SD-CE	-5.07	1.66	1.79
1	A	276	LYS	C-O	-5.07	1.18	1.24
1	B	150	ARG	NE-CZ	5.06	1.38	1.33
1	A	254	GLN	C-O	-5.05	1.17	1.24
1	B	442	GLU	CA-C	5.04	1.59	1.52
1	A	348	LEU	CA-C	-5.04	1.46	1.52
1	B	308	LYS	CG-CD	5.04	1.67	1.52
1	A	430	GLY	C-O	-5.03	1.17	1.24
1	B	34	ILE	CA-CB	-5.03	1.48	1.54
1	B	448	THR	CB-OG1	5.03	1.51	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	SER	N-CA-CB	8.77	123.01	110.12
1	A	347	SER	CA-CB-OG	-8.64	93.83	111.10
1	B	310	VAL	N-CA-CB	-7.58	101.89	112.12
1	A	178	ILE	N-CA-CB	-7.10	103.10	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	VAL	N-CA-C	-7.05	98.15	108.87
1	A	235	GLU	OE1-CD-OE2	-6.58	107.11	122.90
1	A	347	SER	CB-CA-C	-6.57	99.89	110.79
1	A	420	TYR	N-CA-C	-6.51	104.19	111.28
1	A	437	ASP	O-C-N	-6.42	115.72	123.16
1	A	235	GLU	CB-CG-CD	6.23	123.18	112.60
1	A	185	THR	OG1-CB-CG2	-6.04	97.22	109.30
1	A	534	SER	N-CA-C	6.03	117.48	109.83
1	B	65	GLY	N-CA-C	-5.83	105.30	112.77
1	B	306	GLU	N-CA-C	5.76	119.64	109.96
1	A	325	TRP	CA-CB-CG	5.73	124.49	113.60
1	B	194	ASP	N-CA-C	-5.66	105.20	111.36
1	B	381	VAL	N-CA-C	5.65	117.55	108.85
1	B	485	VAL	CB-CA-C	-5.64	104.13	110.96
1	B	542	GLU	N-CA-C	5.58	119.54	109.44
1	B	48	ARG	NE-CZ-NH1	5.44	126.94	121.50
1	B	133	ALA	CA-C-N	-5.32	113.42	122.56
1	B	133	ALA	C-N-CA	-5.32	113.42	122.56
1	B	403	VAL	N-CA-C	5.29	115.98	108.42
1	A	235	GLU	CG-CD-OE1	5.28	130.54	118.40
1	A	194	ASP	N-CA-C	-5.18	105.71	111.36
1	B	310	VAL	CB-CA-C	5.17	115.72	110.65
1	B	159	LYS	CA-CB-CG	-5.08	103.94	114.10
1	B	485	VAL	N-CA-C	5.08	115.99	108.23
1	B	29	ASP	N-CA-C	5.02	121.50	110.80
1	B	337	PRO	CA-C-O	5.00	127.36	121.56

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

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	64	1
1	B	4075	0	3997	76	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	140	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 9.

All (140) 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:A:84:ASP:CG	1:A:217:HIS:HE1	1.67	1.03
1:B:73:GLU:HG2	3:B:2058:HOH:O	1.59	1.02
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
1:B:401:PHE:CE2	1:B:493:MET:CG	2.60	0.84
1:A:84:ASP:CG	1:A:217:HIS:CE1	2.55	0.83
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:THR:HG23	1:B:415:ALA:HA	1.80	0.63
1:A:177:LYS:C	1:A:178:ILE:HD12	2.24	0.62
1:A:438:MET:HE2	1:A:442:GLU:HB3	1.82	0.62
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: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:A:527:LYS:NZ	3:A:2398:HOH:O	2.37	0.57
1:B:448:THR:O	1:B:452:GLN:NE2	2.38	0.56
1:A:376:ASP:O	1:A:377:LYS:C	2.49	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
1:B:385:MET:HE1	1:B:413:ILE:HD12	1.90	0.54
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:B:183:TYR:C	1:B:183:TYR:CD1	2.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ASN:HD21	1:B:217:HIS:HE1	1.59	0.49
1:A:453:MET:HE2	1:A:504:ASP:O	2.13	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:A:453:MET:HE3	1:A:459:ALA:CB	2.44	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: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:A:421:LYS:HD2	1:A:425:LYS:HZ3	1.80	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:502:GLY:O	1:B:503:GLY:C	2.58	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
1:B:57:ALA:HA	1:B:345:MET:HG2	1.98	0.46
1:B:379:ARG:HD3	1:B:457:SER:C	2.41	0.46
1:B:42:HIS:HE1	1:B:100:ASP:OD2	1.98	0.45
1:A:394:MET:O	1:A:395:ASP:C	2.55	0.45
1:B:453:MET:HG2	1:B:459:ALA:HB1	1.99	0.45
1:A:84:ASP:OD1	1:A:217:HIS:CE1	2.66	0.44
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:A:468:PHE:C	1:A:468:PHE:CD1	2.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:128:GLN:HE21	1:B:132:TRP:CD1	2.38	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:69:GLU:OE2	1:B:73:GLU:OE2	2.38	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:446:TYR:CZ	1:A:493:MET:HE1	2.55	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:155:TRP:CD1	1:A:155:TRP:C	2.99	0.41
1:A:378:VAL:HG11	1:A:409:ILE:HG21	2.03	0.41
1:B:128:GLN:HE21	1:B:132:TRP:NE1	2.19	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%)	21	18
1	B	521/532 (98%)	496 (95%)	21 (4%)	4 (1%)	16	12
All	All	1044/1064 (98%)	991 (95%)	46 (4%)	7 (1%)	18	15

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%)	19	18
1	B	431/440 (98%)	406 (94%)	25 (6%)	18	16
All	All	864/880 (98%)	815 (94%)	49 (6%)	18	17

All (49) 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	177	LYS
1	A	182	GLU
1	A	247	MET
1	A	276	LYS
1	A	310	VAL
1	A	322	LYS
1	A	325	TRP
1	A	329	LYS
1	A	347	SER
1	A	366	GLU
1	A	375	ARG
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	489	LYS
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	363	LYS
1	B	368	ASN
1	B	370	ARG
1	B	375	ARG
1	B	377	LYS
1	B	381	VAL
1	B	383	THR
1	B	411	ASP
1	B	421	LYS
1	B	452	GLN
1	B	454	LYS

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Mol	Chain	Res	Type
1	B	469	VAL
1	B	477	ASP
1	B	479	LYS
1	B	532	LYS
1	B	534	SER
1	B	547	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	43	HIS
1	A	117	HIS
1	A	128	GLN
1	A	204	GLN
1	A	217	HIS
1	A	226	HIS
1	A	266	GLN
1	A	279	GLN
1	A	313	GLN
1	A	531	GLN
1	B	42	HIS
1	B	95	GLN
1	B	116	ASN
1	B	128	GLN
1	B	180	ASN
1	B	217	HIS
1	B	229	ASN
1	B	279	GLN
1	B	344	GLN
1	B	353	GLN
1	B	368	ASN
1	B	422	ASN
1	B	431	ASN
1	B	531	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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, 95th 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%)	0.06	19 (3%) 46 48	18, 32, 63, 82	0
1	B	523/532 (98%)	1.71	200 (38%) 1 1	22, 38, 80, 94	0
All	All	1048/1064 (98%)	0.88	219 (20%) 2 2	18, 35, 75, 94	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	520	PHE	9.4
1	B	523	ALA	9.2
1	B	513	CYS	9.0
1	B	530	ILE	8.3
1	B	521	ILE	8.2
1	B	420	TYR	8.0
1	B	463	PHE	7.9
1	B	490	THR	7.6
1	B	538	VAL	7.5
1	B	435	TYR	7.3
1	B	464	ALA	7.3
1	B	469	VAL	7.1
1	B	485	VAL	7.1
1	B	541	TYR	7.0
1	B	371	LEU	7.0
1	B	519	GLY	7.0
1	B	378	VAL	6.9
1	B	540	VAL	6.9
1	B	515	TYR	6.9
1	B	480	ILE	6.9
1	B	393	GLN	6.8
1	B	360	LEU	6.8
1	B	514	GLY	6.7
1	B	434	VAL	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	516	VAL	6.4
1	B	364	ILE	6.4
1	B	401	PHE	6.4
1	B	390	LEU	6.4
1	B	543	PRO	6.3
1	B	475	LEU	6.3
1	B	466	VAL	6.2
1	B	454	LYS	6.2
1	B	517	ASN	6.2
1	B	491	TYR	6.1
1	B	398	GLY	6.1
1	B	424	LEU	6.0
1	B	465	ASN	6.0
1	B	433	VAL	5.9
1	B	362	VAL	5.8
1	B	443	VAL	5.8
1	B	436	ALA	5.7
1	B	370	ARG	5.7
1	B	518	THR	5.6
1	B	525	VAL	5.6
1	B	369	GLY	5.6
1	B	397	THR	5.6
1	B	460	TYR	5.5
1	B	395	ASP	5.5
1	B	431	ASN	5.5
1	B	444	ILE	5.5
1	B	382	GLN	5.5
1	B	402	ALA	5.5
1	B	458	GLY	5.4
1	B	535	PRO	5.4
1	B	388	LEU	5.4
1	B	547	VAL	5.4
1	B	423	VAL	5.3
1	B	500	ALA	5.3
1	B	526	LEU	5.3
1	B	524	GLU	5.3
1	B	484	PRO	5.3
1	B	389	ILE	5.3
1	B	399	ALA	5.2
1	B	462	GLN	5.2
1	B	488	ALA	5.2
1	B	528	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	438	MET	5.1
1	B	430	GLY	5.1
1	B	494	ALA	5.1
1	B	522	ASP	5.1
1	B	447	LEU	5.1
1	B	403	VAL	5.1
1	B	468	PHE	5.0
1	B	392	ALA	5.0
1	B	470	ALA	5.0
1	B	536	LEU	5.0
1	B	446	TYR	5.0
1	B	394	MET	4.9
1	B	495	THR	4.9
1	B	418	ILE	4.8
1	B	509	LEU	4.8
1	B	406	GLY	4.7
1	B	384	ASN	4.7
1	B	505	GLY	4.7
1	B	545	GLY	4.7
1	B	527	LYS	4.6
1	B	376	ASP	4.6
1	B	492	ARG	4.6
1	B	450	VAL	4.6
1	B	437	ASP	4.6
1	B	461	PRO	4.6
1	B	478	LEU	4.6
1	B	512	LYS	4.5
1	B	391	ALA	4.5
1	B	539	SER	4.5
1	B	432	VAL	4.5
1	B	548	SER	4.5
1	B	506	TYR	4.4
1	B	324	THR	4.4
1	B	367	THR	4.4
1	B	501	THR	4.4
1	B	498	PHE	4.4
1	B	493	MET	4.4
1	B	496	LEU	4.4
1	B	413	ILE	4.4
1	B	449	ALA	4.2
1	B	404	MET	4.2
1	B	459	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	532	LYS	4.2
1	B	487	PRO	4.2
1	B	510	ASP	4.2
1	B	400	ASP	4.1
1	B	467	SER	4.1
1	B	489	LYS	4.1
1	B	546	GLU	4.1
1	B	451	ALA	4.0
1	B	419	SER	3.9
1	B	407	GLY	3.9
1	B	439	THR	3.9
1	B	409	ILE	3.9
1	B	361	GLU	3.9
1	B	537	ASP	3.8
1	B	529	TYR	3.8
1	B	486	ASP	3.8
1	B	429	PHE	3.8
1	B	544	LYS	3.8
1	B	365	GLY	3.8
1	B	416	GLY	3.7
1	B	533	SER	3.7
1	B	363	LYS	3.7
1	B	481	LYS	3.7
1	B	373	GLY	3.7
1	B	456	ASP	3.7
1	B	375	ARG	3.7
1	B	455	PRO	3.7
1	B	405	SER	3.7
1	B	396	ARG	3.7
1	B	482	GLY	3.6
1	B	383	THR	3.6
1	B	421	LYS	3.6
1	B	534	SER	3.6
1	B	179	GLY	3.6
1	B	417	ASP	3.5
1	B	426	VAL	3.5
1	B	511	ASN	3.5
1	B	415	ALA	3.4
1	B	483	GLU	3.4
1	B	542	GLU	3.4
1	B	422	ASN	3.4
1	B	497	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	182	GLU	3.4
1	B	366	GLU	3.4
1	B	507	PRO	3.4
1	B	442	GLU	3.3
1	B	453	MET	3.3
1	B	499	ASN	3.3
1	B	372	GLU	3.3
1	B	385	MET	3.3
1	A	325	TRP	3.3
1	A	485	VAL	3.3
1	B	268	ASP	3.3
1	B	448	THR	3.2
1	B	476	ASN	3.2
1	B	445	ASP	3.1
1	A	538	VAL	3.1
1	B	412	SER	3.1
1	A	543	PRO	3.1
1	B	427	GLN	3.1
1	B	408	GLY	3.0
1	B	368	ASN	3.0
1	B	326	GLU	3.0
1	B	386	GLY	3.0
1	B	414	GLU	3.0
1	A	178	ILE	3.0
1	B	441	LYS	3.0
1	B	440	GLY	2.9
1	B	411	ASP	2.9
1	B	425	LYS	2.9
1	A	469	VAL	2.9
1	B	329	LYS	2.8
1	B	379	ARG	2.8
1	B	474	LYS	2.8
1	B	479	LYS	2.8
1	B	387	ARG	2.8
1	B	428	PRO	2.8
1	B	380	PHE	2.8
1	B	410	ARG	2.7
1	B	327	ASP	2.7
1	A	468	PHE	2.7
1	B	471	LYS	2.7
1	B	502	GLY	2.7
1	B	452	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	330	SER	2.7
1	B	178	ILE	2.7
1	B	381	VAL	2.6
1	A	466	VAL	2.6
1	B	531	GLN	2.5
1	A	450	VAL	2.5
1	B	180	ASN	2.5
1	A	434	VAL	2.4
1	B	477	ASP	2.4
1	B	457	SER	2.4
1	A	478	LEU	2.4
1	A	550	GLN	2.4
1	A	488	ALA	2.4
1	B	343	GLN	2.3
1	A	491	TYR	2.3
1	A	448	THR	2.3
1	B	181	PRO	2.2
1	B	508	ARG	2.2
1	A	467	SER	2.2
1	A	461	PRO	2.1
1	B	374	ASP	2.1
1	B	325	TRP	2.1
1	B	473	GLY	2.1
1	B	267	VAL	2.1
1	A	506	TYR	2.0
1	A	409	ILE	2.0
1	B	472	ASP	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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
2	NI	A	1551	1/1	0.96	0.06	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.