



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:12 pm GMT

PDB ID : 1QW8  
Title : Crystal structure of a family 51 alpha-L-arabinofuranosidase in complex with Ara-alpha(1,3)-Xyl  
Authors : Hoevel, K.; Shallom, D.; Niefind, K.; Belakhov, V.; Shoham, G.; Bassov, T.; Shoham, Y.; Schomburg, D.  
Deposited on : 2003-09-01  
Resolution : 1.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

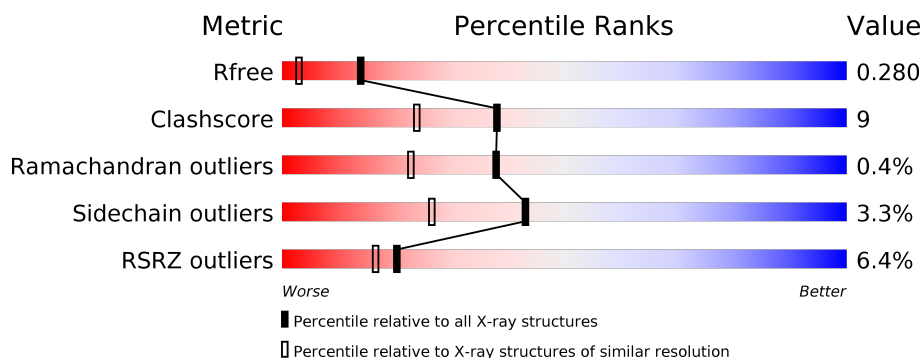
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	502	<div> <div>8%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	502	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>

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	KHO	A	950	-	-	-	X
2	KHO	B	951	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8940 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.

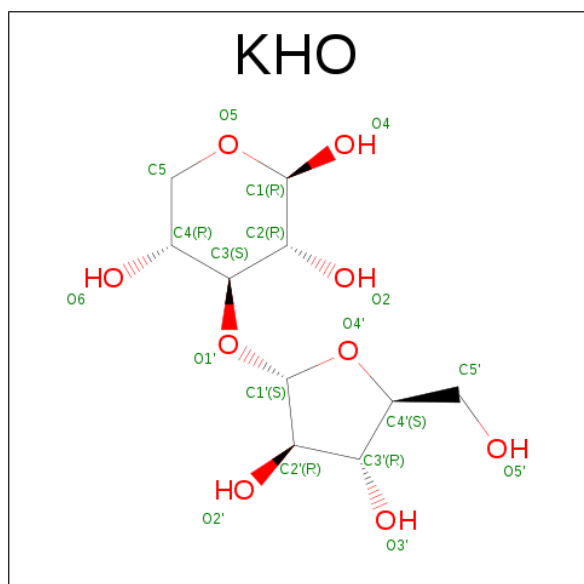
- Molecule 1 is a protein called Alpha-L-arabinofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3986	2540	680	746	20			
1	B	497	Total	C	N	O	S	0	0	0
			3986	2540	680	746	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	ALA	GLU	ENGINEERED	UNP Q9XBQ3
B	175	ALA	GLU	ENGINEERED	UNP Q9XBQ3

- Molecule 2 is 4-(3,4-DIHYDROXY-5-HYDROXYMETHYL-TETRAHYDRO-FURAN-2-YLOXY)-TETRAHYDRO-PYRAN-2,3,5-TRIOL (three-letter code: KHO) (formula: C<sub>10</sub>H<sub>18</sub>O<sub>9</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			19	10	9		
2	B	1	Total	C	O	0	0
			19	10	9		

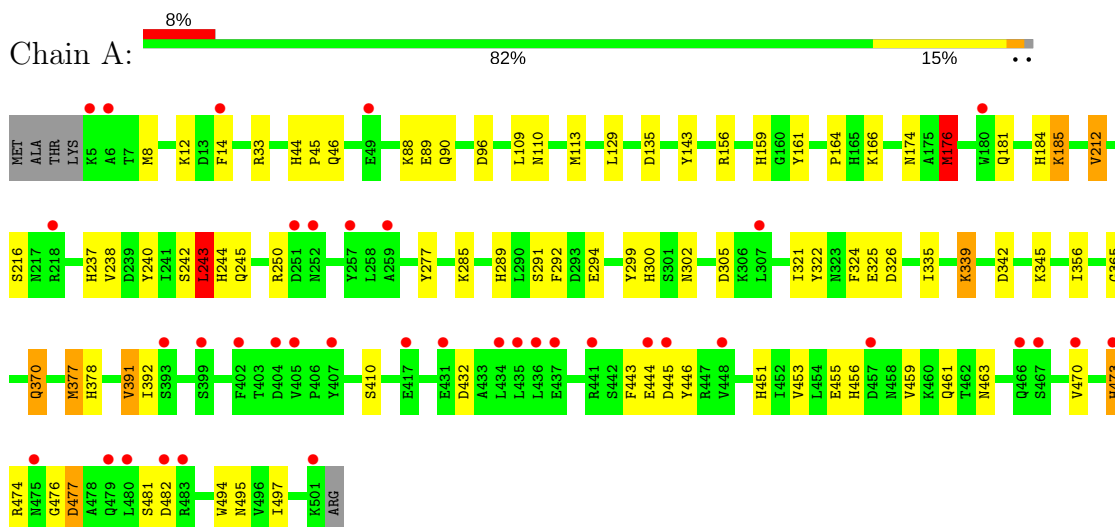
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	468	Total	O	0	0
			468	468		
3	B	462	Total	O	0	0
			462	462		

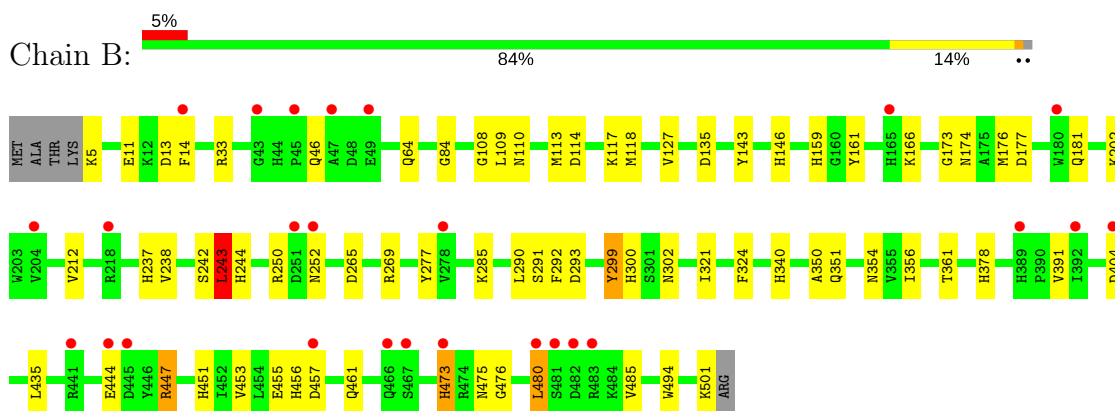
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Alpha-L-arabinofuranosidase



- Molecule 1: Alpha-L-arabinofuranosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.43Å 179.43Å 100.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.80 14.99 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-1.80) 96.4 (14.99-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.174 , 0.213 0.254 , 0.280	Depositor DCC
$R_{free}$ test set	5394 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8940	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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

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	0.62	0/4087	0.83	12/5553 (0.2%)
1	B	0.60	0/4087	0.81	10/5553 (0.2%)
All	All	0.61	0/8174	0.82	22/11106 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	LEU	CA-CB-CG	6.78	130.89	115.30
1	B	33	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	176	MET	CG-SD-CE	-6.25	90.21	100.20
1	B	457	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	135	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	33	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	33	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	185	LYS	CD-CE-NZ	-5.88	98.18	111.70
1	B	265	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	243	LEU	CA-CB-CG	5.68	128.36	115.30
1	A	445	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	177	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	477	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	432	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	342	ASP	CB-CG-OD1	5.27	123.05	118.30
1	B	135	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	33	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	B	13	ASP	CB-CG-OD2	5.12	122.90	118.30
1	B	114	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	305	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	404	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	96	ASP	CB-CG-OD2	5.02	122.81	118.30



There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3986	0	3890	81	0
1	B	3986	0	3890	59	0
2	A	19	0	18	0	0
2	B	19	0	18	0	0
3	A	468	0	0	33	3
3	B	462	0	0	17	1
All	All	8940	0	7816	138	3

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 (138) 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:244:HIS:CE1	3:B:1364:HOH:O	1.65	1.28
1:A:216:SER:CB	3:A:1370:HOH:O	1.82	1.25
1:A:377:MET:SD	3:A:1369:HOH:O	2.08	1.08
1:A:216:SER:HB3	3:A:1370:HOH:O	1.42	1.07
1:B:118:MET:HG3	3:B:1373:HOH:O	1.57	1.03
1:A:451:HIS:ND1	1:A:476:GLY:HA3	1.81	0.95
1:A:129:LEU:O	1:A:176:MET:HE1	1.72	0.90
1:A:244:HIS:CE1	3:A:1404:HOH:O	2.25	0.89
1:B:354:ASN:HD21	1:B:361:THR:H	1.22	0.87
1:A:473:HIS:CE1	3:A:1374:HOH:O	2.27	0.86
1:A:377:MET:CG	3:A:1369:HOH:O	2.22	0.85
1:B:244:HIS:NE2	1:B:293:ASP:OD1	2.13	0.81
1:B:244:HIS:ND1	3:B:1364:HOH:O	1.81	0.81
1:A:174:ASN:O	1:A:176:MET:HG2	1.82	0.80
1:A:8:MET:SD	3:A:1410:HOH:O	2.39	0.80
1:A:250:ARG:HH21	1:A:302:ASN:HD21	1.31	0.78
1:B:300:HIS:HD2	1:B:321:ILE:O	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:HIS:HD2	1:B:494:TRP:HE1	1.33	0.74
1:A:44:HIS:HD2	1:A:46:GLN:H	1.33	0.74
1:B:456:HIS:CE1	1:B:461:GLN:HG2	2.22	0.74
1:B:243:LEU:O	1:B:244:HIS:HD2	1.72	0.73
1:B:480:LEU:HD22	1:B:485:VAL:HG22	1.73	0.71
1:A:463:ASN:HD21	1:A:470:VAL:H	1.39	0.70
1:B:244:HIS:HE1	3:B:1364:HOH:O	1.31	0.70
1:A:473:HIS:ND1	3:A:1374:HOH:O	2.21	0.70
1:A:451:HIS:CD2	1:A:497:ILE:HG12	2.27	0.70
1:A:174:ASN:C	3:A:1397:HOH:O	2.30	0.68
1:A:377:MET:HG2	3:A:1369:HOH:O	1.87	0.68
1:B:456:HIS:HE1	1:B:461:GLN:HG2	1.58	0.67
1:A:216:SER:OG	3:A:1370:HOH:O	1.69	0.66
1:A:473:HIS:CG	3:A:1374:HOH:O	2.49	0.66
1:B:118:MET:SD	3:B:1373:HOH:O	2.54	0.65
1:B:202:LYS:HD2	3:B:1293:HOH:O	1.97	0.65
1:A:451:HIS:CE1	1:A:495:ASN:HD22	2.15	0.64
1:B:176:MET:HE3	3:B:1370:HOH:O	1.97	0.64
1:B:300:HIS:CD2	1:B:321:ILE:O	2.49	0.63
1:A:300:HIS:HE1	1:A:326:ASP:OD2	1.81	0.63
1:B:176:MET:HG2	1:B:181:GLN:HG2	1.81	0.63
1:B:174:ASN:HD22	1:B:181:GLN:HE22	1.48	0.61
1:A:174:ASN:O	3:A:1397:HOH:O	2.16	0.61
1:B:212:VAL:HG13	1:B:238:VAL:HG11	1.83	0.61
1:A:245:GLN:NE2	3:A:1122:HOH:O	2.35	0.60
1:B:250:ARG:HH21	1:B:302:ASN:HD21	1.48	0.59
1:B:299:TYR:CE1	1:B:300:HIS:CE1	2.90	0.59
1:B:143:TYR:OH	1:B:159:HIS:HD2	1.84	0.59
1:A:289:HIS:ND1	1:A:345:LYS:HE2	2.18	0.59
1:A:44:HIS:CD2	1:A:46:GLN:H	2.20	0.59
1:A:391:VAL:HB	1:B:14:PHE:CZ	2.38	0.59
1:A:174:ASN:HD22	1:A:181:GLN:HE22	1.50	0.58
1:A:143:TYR:OH	1:A:159:HIS:HD2	1.87	0.57
1:B:118:MET:CG	3:B:1373:HOH:O	2.26	0.57
1:A:377:MET:CE	3:A:1369:HOH:O	2.46	0.57
1:B:456:HIS:HD2	3:B:1286:HOH:O	1.89	0.56
1:B:243:LEU:C	1:B:244:HIS:CD2	2.79	0.55
1:B:243:LEU:C	1:B:244:HIS:HD2	2.10	0.55
1:B:299:TYR:CZ	1:B:300:HIS:CE1	2.94	0.55
1:A:456:HIS:CE1	1:A:461:GLN:HG2	2.42	0.55
1:B:237:HIS:HE1	3:B:1306:HOH:O	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:HG2	3:A:1342:HOH:O	2.06	0.54
1:A:244:HIS:CE1	3:A:1382:HOH:O	2.61	0.54
1:A:237:HIS:HE1	3:A:1320:HOH:O	1.91	0.53
1:A:473:HIS:CE1	3:A:1403:HOH:O	2.60	0.53
1:A:244:HIS:HE1	3:A:1047:HOH:O	1.91	0.52
1:B:146:HIS:HD2	3:B:1058:HOH:O	1.92	0.52
1:B:378:HIS:HE1	3:B:1163:HOH:O	1.94	0.51
1:B:354:ASN:ND2	1:B:361:THR:H	2.01	0.51
1:A:392:ILE:HD11	3:A:1410:HOH:O	2.10	0.50
1:A:245:GLN:NE2	3:A:1314:HOH:O	2.45	0.50
1:B:146:HIS:HE1	3:B:1131:HOH:O	1.93	0.50
1:B:453:VAL:HB	1:B:473:HIS:CD2	2.47	0.50
1:B:378:HIS:CD2	1:B:494:TRP:HE1	2.22	0.50
1:A:44:HIS:HE1	1:A:365:GLY:O	1.94	0.49
1:A:250:ARG:HH21	1:A:302:ASN:ND2	2.07	0.48
1:A:324:PHE:CZ	1:A:455:GLU:HA	2.48	0.48
1:B:64:GLN:NE2	3:B:1047:HOH:O	2.46	0.48
1:B:269:ARG:HG3	1:B:340:HIS:HE1	1.78	0.48
1:A:176:MET:O	1:A:184:HIS:HD2	1.96	0.48
1:A:243:LEU:N	1:A:243:LEU:HD12	2.28	0.48
1:B:174:ASN:HD22	1:B:181:GLN:NE2	2.11	0.48
1:A:322:TYR:H	1:A:370:GLN:NE2	2.11	0.47
1:A:453:VAL:HB	1:A:473:HIS:CE1	2.50	0.47
1:B:110:ASN:HB3	1:B:161:TYR:CZ	2.49	0.47
1:B:447:ARG:NH2	3:B:1304:HOH:O	2.47	0.47
1:B:242:SER:HA	1:B:291:SER:O	2.14	0.47
1:B:127:VAL:O	1:B:173:GLY:HA2	2.16	0.46
1:A:212:VAL:HG13	1:A:238:VAL:HG11	1.97	0.46
1:A:129:LEU:O	1:A:185:LYS:HE3	2.16	0.46
1:B:451:HIS:CG	1:B:476:GLY:HA3	2.51	0.46
1:A:242:SER:C	1:A:243:LEU:HD12	2.36	0.46
1:A:451:HIS:HD2	1:A:497:ILE:HG12	1.76	0.46
1:B:117:LYS:HB3	1:B:117:LYS:HZ3	1.81	0.46
1:A:242:SER:HA	1:A:291:SER:O	2.16	0.46
1:A:322:TYR:H	1:A:370:GLN:HE22	1.64	0.46
1:A:181:GLN:NE2	3:A:1397:HOH:O	2.49	0.45
1:A:176:MET:O	1:A:184:HIS:CD2	2.70	0.45
1:B:174:ASN:O	1:B:176:MET:HG3	2.16	0.45
1:B:480:LEU:HD22	1:B:485:VAL:CG2	2.43	0.45
1:A:377:MET:HE3	1:A:377:MET:HB3	1.78	0.45
1:A:240:TYR:HA	1:A:289:HIS:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:PHE:CZ	1:B:455:GLU:HA	2.51	0.45
1:A:159:HIS:HE1	3:A:1022:HOH:O	1.98	0.44
1:A:378:HIS:CD2	1:A:494:TRP:HE1	2.36	0.44
1:B:109:LEU:O	1:B:113:MET:HG2	2.17	0.44
1:B:11:GLU:CG	1:B:14:PHE:HD1	2.31	0.44
1:A:164:PRO:HG2	1:A:166:LYS:HE2	1.99	0.44
1:A:473:HIS:CD2	3:A:1374:HOH:O	2.69	0.44
1:A:244:HIS:CE1	3:A:1047:HOH:O	2.69	0.44
1:A:446:TYR:OH	3:A:1386:HOH:O	2.21	0.43
1:A:325:GLU:HB3	1:A:459:VAL:HB	2.01	0.43
1:B:243:LEU:HD12	1:B:243:LEU:N	2.33	0.43
1:B:166:LYS:HG3	3:B:1209:HOH:O	2.18	0.43
1:B:473:HIS:CE1	1:B:475:ASN:HB2	2.54	0.43
1:A:89:GLU:HG2	1:A:90:GLN:NE2	2.33	0.43
1:A:289:HIS:CE1	1:A:345:LYS:HE2	2.54	0.43
1:A:110:ASN:HB3	1:A:161:TYR:CZ	2.54	0.42
1:A:321:ILE:HA	1:A:370:GLN:HE22	1.85	0.42
1:A:378:HIS:HE1	3:A:1162:HOH:O	2.02	0.42
1:A:451:HIS:CG	1:A:476:GLY:HA3	2.51	0.42
1:A:335:ILE:O	1:A:339:LYS:HG2	2.19	0.42
1:A:477:ASP:OD1	1:A:477:ASP:C	2.57	0.42
1:B:299:TYR:CZ	1:B:300:HIS:HE1	2.37	0.42
1:B:456:HIS:CD2	3:B:1286:HOH:O	2.68	0.42
1:A:184:HIS:HE1	3:A:1409:HOH:O	2.03	0.41
1:B:11:GLU:HG2	1:B:14:PHE:HD1	1.85	0.41
1:A:14:PHE:CE2	1:B:391:VAL:CG2	3.03	0.41
1:A:166:LYS:HG3	3:A:1108:HOH:O	2.20	0.41
1:A:174:ASN:HD22	1:A:181:GLN:NE2	2.16	0.41
1:A:88:LYS:NZ	3:A:1283:HOH:O	2.47	0.41
1:A:109:LEU:O	1:A:113:MET:HG2	2.21	0.41
1:A:44:HIS:CD2	1:A:45:PRO:HD2	2.56	0.41
1:B:84:GLY:O	1:B:108:GLY:HA3	2.20	0.41
1:A:245:GLN:CD	3:A:1314:HOH:O	2.60	0.41
1:A:143:TYR:O	1:A:156:ARG:HD3	2.21	0.41
1:B:350:ALA:HA	1:B:351:GLN:HA	1.86	0.41
1:A:410:SER:HB3	3:A:1410:HOH:O	2.21	0.40
1:A:244:HIS:CD2	1:A:294:GLU:HB2	2.56	0.40
1:A:12:LYS:HE2	1:A:443:PHE:CE2	2.57	0.40
1:B:243:LEU:HD11	1:B:290:LEU:HD23	2.02	0.40

All (3) 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:A:1237:HOH:O	3:A:1390:HOH:O[3_665]	1.92	0.28
3:A:1044:HOH:O	3:B:1301:HOH:O[1_554]	2.10	0.10
3:A:1116:HOH:O	3:A:1409:HOH:O[3_665]	2.15	0.05

## 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	495/502 (99%)	479 (97%)	14 (3%)	2 (0%)	38	23
1	B	495/502 (99%)	473 (96%)	20 (4%)	2 (0%)	38	23
All	All	990/1004 (99%)	952 (96%)	34 (3%)	4 (0%)	38	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	299	TYR
1	A	299	TYR
1	B	356	ILE
1	A	356	ILE

### 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	429/433 (99%)	414 (96%)	15 (4%)	41	24
1	B	429/433 (99%)	416 (97%)	13 (3%)	46	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	858/866 (99%)	830 (97%)	28 (3%)	43 26

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	MET
1	A	212	VAL
1	A	243	LEU
1	A	277	TYR
1	A	285	LYS
1	A	292	PHE
1	A	339	LYS
1	A	370	GLN
1	A	377	MET
1	A	391	VAL
1	A	444	GLU
1	A	473	HIS
1	A	474	ARG
1	A	481	SER
1	A	482	ASP
1	B	5	LYS
1	B	46	GLN
1	B	243	LEU
1	B	252	ASN
1	B	277	TYR
1	B	285	LYS
1	B	292	PHE
1	B	435	LEU
1	B	444	GLU
1	B	447	ARG
1	B	473	HIS
1	B	480	LEU
1	B	501	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	159	HIS
1	A	181	GLN
1	A	184	HIS

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Mol	Chain	Res	Type
1	A	237	HIS
1	A	244	HIS
1	A	300	HIS
1	A	302	ASN
1	A	370	GLN
1	A	378	HIS
1	A	451	HIS
1	A	456	HIS
1	A	463	ASN
1	A	495	ASN
1	B	64	GLN
1	B	146	HIS
1	B	159	HIS
1	B	181	GLN
1	B	184	HIS
1	B	252	ASN
1	B	300	HIS
1	B	302	ASN
1	B	354	ASN
1	B	364	ASN
1	B	378	HIS
1	B	475	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	KHO	A	950	-	20,20,20	0.95	0	27,29,29	1.51	7 (25%)
2	KHO	B	951	-	20,20,20	1.09	1 (5%)	27,29,29	1.74	4 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KHO	A	950	-	-	0/6/39/39	0/2/2/2
2	KHO	B	951	-	-	0/6/39/39	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	951	KHO	C1'-C2'	2.77	1.56	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	951	KHO	O1'-C1'-O4'	-5.29	105.70	111.43
2	A	950	KHO	O1'-C1'-O4'	-2.90	108.29	111.43
2	A	950	KHO	O5-C1-C2	-2.17	106.40	109.31
2	A	950	KHO	C1-C2-C3	-2.00	107.05	110.66
2	A	950	KHO	O2-C2-C3	2.13	114.71	109.87
2	B	951	KHO	C5-C4-C3	2.14	111.75	109.17
2	B	951	KHO	O5-C5-C4	2.30	114.39	110.79
2	A	950	KHO	O5-C5-C4	2.55	114.79	110.79
2	A	950	KHO	C5-C4-C3	2.67	112.40	109.17
2	A	950	KHO	C1'-O1'-C3	3.30	126.02	118.00
2	B	951	KHO	C1'-O1'-C3	4.38	128.67	118.00

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

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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	497/502 (99%)	0.92	38 (7%)	15 12	17, 28, 48, 61	0
1	B	497/502 (99%)	0.65	26 (5%)	28 23	19, 27, 43, 57	0
All	All	994/1004 (99%)	0.79	64 (6%)	20 16	17, 28, 46, 61	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	482	ASP	8.2
1	A	441	ARG	5.9
1	B	482	ASP	5.4
1	A	435	LEU	5.1
1	A	444	GLU	5.1
1	A	457	ASP	5.0
1	A	417	GLU	4.8
1	B	466	GLN	4.5
1	A	445	ASP	4.3
1	B	441	ARG	4.0
1	B	43	GLY	4.0
1	A	14	PHE	3.8
1	A	466	GLN	3.7
1	B	481	SER	3.7
1	A	483	ARG	3.5
1	B	444	GLU	3.5
1	A	5	LYS	3.5
1	A	259	ALA	3.3
1	A	251	ASP	3.3
1	B	480	LEU	3.3
1	B	483	ARG	3.2
1	A	407	TYR	3.2
1	A	402	PHE	3.1
1	A	252	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	501	LYS	3.0
1	A	393	SER	2.9
1	A	180	TRP	2.9
1	B	180	TRP	2.9
1	A	431	GLU	2.9
1	A	405	VAL	2.8
1	B	49	GLU	2.8
1	B	14	PHE	2.8
1	A	473	HIS	2.7
1	A	470	VAL	2.6
1	B	392	ILE	2.6
1	A	467	SER	2.6
1	B	457	ASP	2.6
1	A	480	LEU	2.5
1	B	445	ASP	2.5
1	A	307	LEU	2.5
1	A	434	LEU	2.5
1	B	45	PRO	2.4
1	A	257	TYR	2.4
1	B	404	ASP	2.4
1	B	473	HIS	2.4
1	B	252	ASN	2.4
1	A	49	GLU	2.4
1	A	6	ALA	2.3
1	A	404	ASP	2.2
1	B	47	ALA	2.2
1	B	251	ASP	2.2
1	A	436	LEU	2.1
1	A	437	GLU	2.1
1	B	467	SER	2.1
1	B	389	HIS	2.1
1	A	448	VAL	2.1
1	A	479	GLN	2.1
1	A	475	ASN	2.1
1	A	399	SER	2.1
1	B	278	VAL	2.0
1	B	204	VAL	2.0
1	B	165	HIS	2.0
1	A	218	ARG	2.0
1	B	218	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	KHO	A	950	19/19	0.68	0.24	3.37	25,37,55,57	0
2	KHO	B	951	19/19	0.72	0.26	3.32	27,39,56,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.