Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:38 PM GMT

PDB ID	:	1PZ2
Title	:	Crystal structure of a transient covalent reaction intermediate of a family 51 alpha-L-arabinofuranosidase
Authors	:	Hoevel, K.; Shallom, D.; Niefind, K.; Belakhov, V.; Shoham, G.; Baasov, T.; Shoham, Y.; Schomburg, D.
Deposited on	:	2003-07-09
Resolution	:	2.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

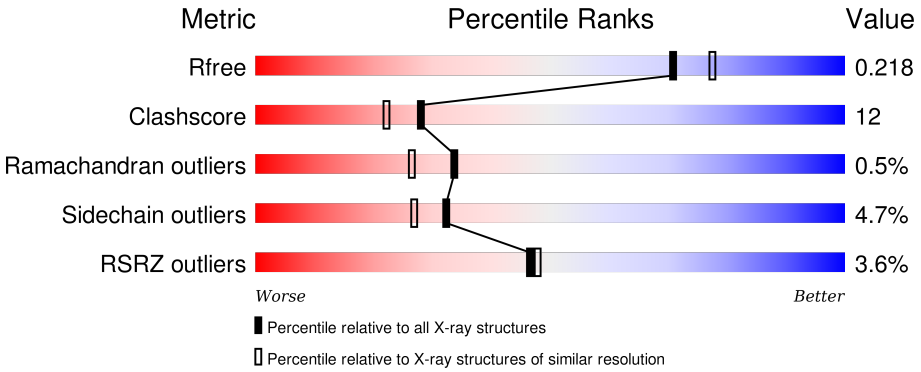
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 >=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 <=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	4% 79% 18%
1	B	502	3% 79% 19%

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	AHR	A	550	X	-	-	X
2	AHR	B	550	X	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8757 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.

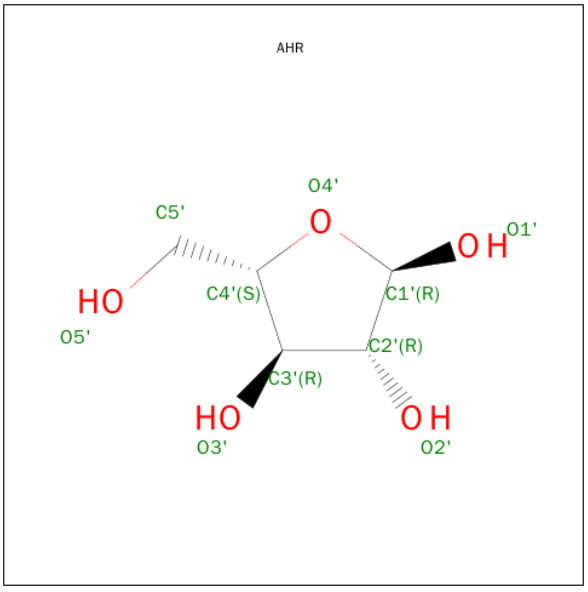
- Molecule 1 is a protein called Alpha-L-arabinofuranosidase.

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 ALPHA-L-ARABINOFURANOSE (three-letter code: AHR) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	5	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 9 5 4	0	0

- Molecule 3 is water.

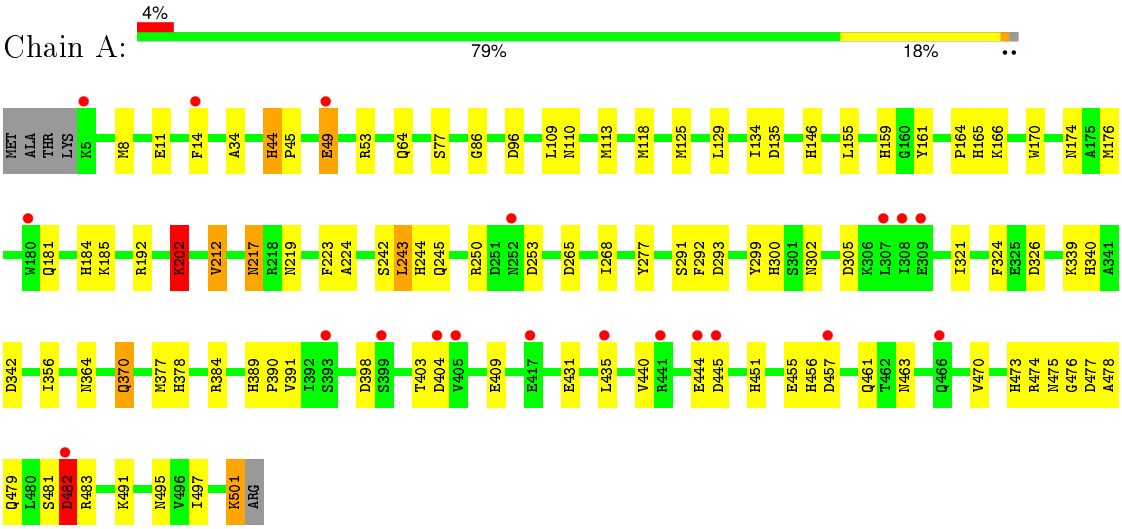
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	399	Total O 399 399	0	0
3	B	368	Total O 368 368	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

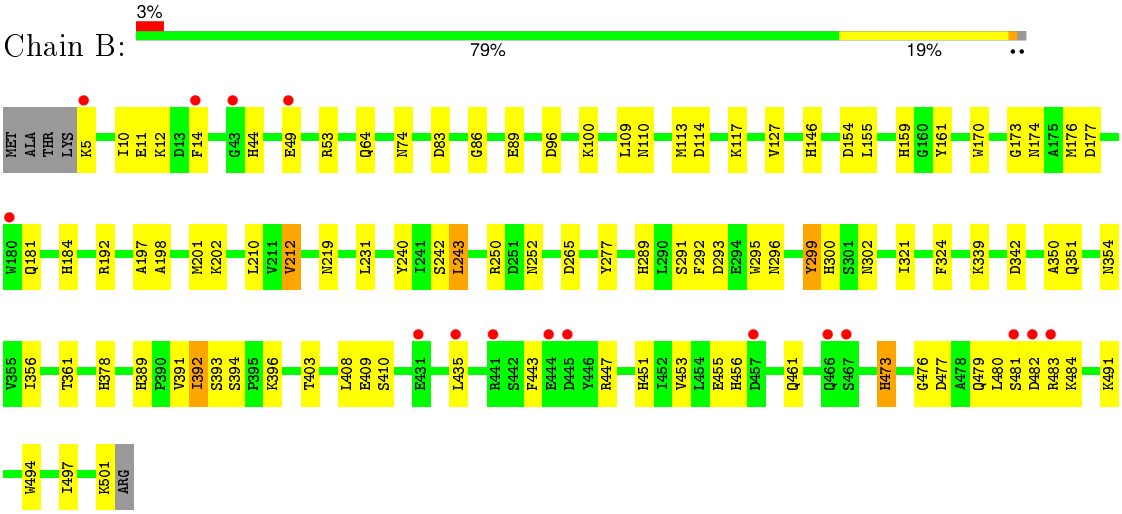
- Molecule 1: Alpha-L-arabinofuranosidase

Chain A:



- Molecule 1: Alpha-L-arabinofuranosidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	179.43Å 179.43Å 100.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00 14.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-2.00) 93.3 (14.99-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.169 , 0.215 0.179 , 0.218	Depositor DCC
R_{free} test set	3815 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.3	EDS
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 75720 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8757	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 4.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: AHR

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	0.85	1/4087 (0.0%)	0.92	14/5553 (0.3%)
1	B	0.79	1/4087 (0.0%)	0.87	12/5553 (0.2%)
All	All	0.82	2/8174 (0.0%)	0.90	26/11106 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	VAL	CB-CG1	-6.07	1.40	1.52
1	A	202	LYS	CD-CE	5.06	1.64	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	96	ASP	CB-CG-OD2	7.37	124.93	118.30
1	A	212	VAL	CB-CA-C	-6.95	98.19	111.40
1	A	445	ASP	CB-CG-OD2	6.59	124.23	118.30
1	B	293	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	398	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	265	ASP	CB-CG-OD2	6.41	124.06	118.30
1	A	96	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	243	LEU	CA-CB-CG	6.35	129.91	115.30
1	A	342	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	404	ASP	CB-CG-OD2	6.03	123.73	118.30
1	B	154	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	243	LEU	CA-CB-CG	5.88	128.84	115.30
1	B	482	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	482	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	192	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	253	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	177	ASP	CB-CG-OD2	5.43	123.18	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	384	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	192	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	477	ASP	CB-CG-OD2	5.30	123.08	118.30
1	A	265	ASP	CB-CG-OD2	5.28	123.06	118.30
1	A	305	ASP	CB-CG-OD2	5.28	123.06	118.30
1	B	114	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	135	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	83	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	342	ASP	CB-CG-OD1	5.00	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3986	0	3890	104	0
1	B	3986	0	3890	91	0
2	A	9	0	7	0	0
2	B	9	0	7	0	0
3	A	399	0	0	33	1
3	B	368	0	0	23	1
All	All	8757	0	7794	185	2

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 12.

All (185) 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:A:244:HIS:CE1	3:A:921:HOH:O	1.89	1.20
1:A:44:HIS:ND1	1:A:45:PRO:HD2	1.67	1.07
1:A:391:VAL:HG21	1:B:14:PHE:CZ	1.88	1.07
1:B:451:HIS:ND1	1:B:476:GLY:HA3	1.75	1.01
1:A:340:HIS:CD2	3:A:922:HOH:O	2.13	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:HIS:CG	3:A:922:HOH:O	2.19	0.94
1:A:14:PHE:CE2	1:B:391:VAL:HG21	2.04	0.92
1:A:113:MET:HG3	1:A:165:HIS:ND1	1.89	0.87
1:A:451:HIS:CE1	1:A:495:ASN:HD22	1.96	0.84
1:A:155:LEU:O	1:A:159:HIS:HD2	1.61	0.83
1:A:451:HIS:HE1	1:A:495:ASN:HD22	1.26	0.83
1:A:391:VAL:CG2	1:B:14:PHE:CZ	2.62	0.82
1:A:391:VAL:CG2	1:B:14:PHE:CE2	2.64	0.80
1:B:299:TYR:CE1	1:B:300:HIS:CE1	2.68	0.80
1:A:86:GLY:HA2	1:A:159:HIS:ND1	1.97	0.79
1:A:377:MET:SD	3:A:920:HOH:O	2.41	0.79
1:B:410:SER:HB3	3:B:778:HOH:O	1.82	0.78
1:B:456:HIS:CE1	1:B:461:GLN:HG2	2.19	0.78
1:B:86:GLY:N	1:B:159:HIS:HD2	1.83	0.77
1:B:250:ARG:HH21	1:B:302:ASN:HD21	1.33	0.76
1:B:86:GLY:N	1:B:159:HIS:CD2	2.54	0.76
1:A:268:ILE:CG2	1:A:340:HIS:HD2	1.98	0.75
1:A:250:ARG:HH21	1:A:302:ASN:HD21	1.31	0.75
1:A:14:PHE:CZ	1:B:391:VAL:HG21	2.20	0.75
1:A:14:PHE:CE2	1:B:391:VAL:CG2	2.68	0.75
1:B:451:HIS:ND1	1:B:476:GLY:CA	2.49	0.75
1:A:217:ASN:HD21	1:A:219:ASN:HB2	1.51	0.75
1:A:86:GLY:CA	1:A:159:HIS:ND1	2.50	0.74
1:B:86:GLY:CA	1:B:159:HIS:CD2	2.71	0.74
1:B:354:ASN:HD21	1:B:361:THR:H	1.32	0.74
1:A:391:VAL:HG21	1:B:14:PHE:CE2	2.23	0.73
1:A:268:ILE:HG21	1:A:340:HIS:HD2	1.54	0.71
1:B:86:GLY:HA2	1:B:159:HIS:CD2	2.25	0.71
1:B:174:ASN:C	3:B:911:HOH:O	2.29	0.70
1:A:456:HIS:CE1	1:A:461:GLN:HG2	2.28	0.69
1:A:300:HIS:HE1	1:A:326:ASP:OD2	1.76	0.68
1:B:451:HIS:CD2	1:B:497:ILE:HG12	2.28	0.67
1:B:299:TYR:CE1	1:B:300:HIS:HE1	2.10	0.67
1:A:11:GLU:HG2	1:A:14:PHE:CD1	2.30	0.67
1:A:245:GLN:NE2	3:A:789:HOH:O	2.28	0.66
1:B:456:HIS:HE1	1:B:461:GLN:HG2	1.59	0.66
1:B:11:GLU:CG	1:B:14:PHE:HD1	2.08	0.65
1:B:378:HIS:HD2	1:B:494:TRP:HE1	1.45	0.65
1:A:174:ASN:HD22	1:A:181:GLN:HE22	1.45	0.65
1:B:403:THR:HG23	3:B:916:HOH:O	1.97	0.64
1:B:389:HIS:HD2	3:B:773:HOH:O	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LEU:O	1:A:159:HIS:CD2	2.49	0.64
1:A:268:ILE:HG21	1:A:340:HIS:CD2	2.34	0.63
1:A:11:GLU:HG2	1:A:14:PHE:HD1	1.64	0.62
1:B:299:TYR:CZ	1:B:300:HIS:CE1	2.88	0.61
1:B:339:LYS:NZ	1:B:409:GLU:OE2	2.31	0.61
1:B:11:GLU:HG2	1:B:14:PHE:HD1	1.64	0.61
1:B:86:GLY:H	1:B:159:HIS:HD2	1.49	0.61
1:A:451:HIS:HD2	1:A:478:ALA:HB2	1.65	0.60
1:A:377:MET:HE2	3:A:920:HOH:O	2.00	0.60
1:B:74:ASN:HA	1:B:181:GLN:HE22	1.65	0.60
1:A:155:LEU:HD11	1:A:159:HIS:HE2	1.66	0.60
1:A:44:HIS:ND1	1:A:45:PRO:CD	2.56	0.60
1:B:146:HIS:HD2	3:B:646:HOH:O	1.86	0.59
1:A:44:HIS:HE1	3:A:657:HOH:O	1.86	0.59
1:B:11:GLU:HG2	1:B:14:PHE:CD1	2.38	0.59
1:B:451:HIS:HD2	1:B:497:ILE:HG12	1.68	0.58
1:B:219:ASN:ND2	3:B:886:HOH:O	2.36	0.58
1:B:155:LEU:HG	1:B:159:HIS:CE1	2.38	0.58
1:B:174:ASN:HD22	1:B:181:GLN:NE2	2.02	0.58
1:A:244:HIS:ND1	3:A:921:HOH:O	2.12	0.57
1:A:474:ARG:HD3	3:A:841:HOH:O	2.05	0.57
1:B:174:ASN:HD22	1:B:181:GLN:HE22	1.52	0.57
1:A:244:HIS:NE2	1:A:293:ASP:OD1	2.39	0.56
1:B:378:HIS:HE1	3:B:707:HOH:O	1.88	0.55
1:A:389:HIS:CD2	3:A:791:HOH:O	2.60	0.55
1:A:11:GLU:CG	1:A:14:PHE:HD1	2.18	0.55
1:A:377:MET:CE	3:A:920:HOH:O	2.54	0.55
1:A:455:GLU:OE2	1:A:473:HIS:HE1	1.90	0.55
1:A:245:GLN:NE2	3:A:773:HOH:O	2.39	0.55
1:A:268:ILE:CG2	1:A:340:HIS:CD2	2.86	0.55
1:B:202:LYS:HD2	3:B:764:HOH:O	2.06	0.55
1:A:390:PRO:HG3	3:A:887:HOH:O	2.06	0.54
1:A:391:VAL:HG22	1:B:14:PHE:CE2	2.42	0.54
1:A:49:GLU:HG2	3:A:822:HOH:O	2.06	0.54
1:A:391:VAL:HG21	1:B:14:PHE:CE1	2.41	0.54
1:A:86:GLY:CA	1:A:159:HIS:CE1	2.91	0.54
1:A:390:PRO:HA	3:A:855:HOH:O	2.07	0.54
1:B:455:GLU:OE2	1:B:473:HIS:HE1	1.91	0.53
1:A:185:LYS:HE2	3:A:571:HOH:O	2.09	0.53
1:B:300:HIS:HD2	1:B:321:ILE:O	1.91	0.53
1:B:146:HIS:HE1	3:B:691:HOH:O	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:MET:HG3	3:A:920:HOH:O	2.09	0.52
1:B:453:VAL:HB	1:B:473:HIS:NE2	2.25	0.52
1:A:440:VAL:O	1:A:440:VAL:HG23	2.10	0.52
1:A:340:HIS:CE1	3:A:922:HOH:O	2.61	0.51
1:B:197:ALA:O	1:B:201:MET:HG3	2.10	0.51
1:A:146:HIS:HE1	3:A:687:HOH:O	1.92	0.51
1:A:34:ALA:HB1	3:A:943:HOH:O	2.11	0.51
1:A:501:LYS:NZ	1:A:501:LYS:HB3	2.25	0.51
1:A:321:ILE:HA	1:A:370:GLN:HE22	1.75	0.51
1:B:64:GLN:NE2	3:B:902:HOH:O	2.28	0.51
1:A:451:HIS:HE1	1:A:495:ASN:ND2	2.03	0.50
1:A:86:GLY:HA3	1:A:159:HIS:CE1	2.46	0.50
1:B:392:ILE:HD13	1:B:408:LEU:HD23	1.92	0.50
1:A:109:LEU:O	1:A:113:MET:HG2	2.12	0.50
1:A:155:LEU:CD1	1:A:159:HIS:HE2	2.24	0.50
1:A:477:ASP:OD1	1:A:477:ASP:C	2.50	0.50
1:B:176:MET:HE2	3:B:756:HOH:O	2.11	0.50
1:B:453:VAL:HB	1:B:473:HIS:CD2	2.47	0.50
1:A:324:PHE:CZ	1:A:455:GLU:HA	2.46	0.49
1:A:451:HIS:ND1	1:A:476:GLY:HA3	2.27	0.49
1:A:451:HIS:CD2	1:A:497:ILE:HG12	2.48	0.49
1:B:110:ASN:HB3	1:B:161:TYR:CZ	2.48	0.49
1:A:463:ASN:HD21	1:A:470:VAL:H	1.58	0.49
1:B:392:ILE:CD1	1:B:394:SER:HB2	2.42	0.49
1:B:109:LEU:O	1:B:113:MET:HG2	2.13	0.49
1:B:295:TRP:O	1:B:296:ASN:HB2	2.11	0.49
1:A:113:MET:HG3	1:A:165:HIS:CE1	2.47	0.49
1:B:378:HIS:CD2	1:B:494:TRP:HE1	2.27	0.48
1:B:110:ASN:HB3	1:B:161:TYR:CE1	2.48	0.48
1:A:176:MET:HG2	1:A:181:GLN:HG2	1.95	0.48
1:A:473:HIS:HD2	1:A:475:ASN:H	1.61	0.48
1:B:100:LYS:NZ	3:B:727:HOH:O	2.47	0.48
1:A:244:HIS:HE1	3:A:643:HOH:O	1.96	0.47
1:B:174:ASN:HB3	3:B:911:HOH:O	2.14	0.47
1:B:455:GLU:OE2	1:B:473:HIS:CE1	2.68	0.47
1:A:364:ASN:HB3	3:A:809:HOH:O	2.14	0.47
1:B:176:MET:O	1:B:184:HIS:CD2	2.68	0.47
1:B:392:ILE:HG21	3:B:778:HOH:O	2.13	0.47
1:A:176:MET:O	1:A:184:HIS:HD2	1.98	0.47
1:A:364:ASN:CG	3:A:809:HOH:O	2.53	0.47
1:B:117:LYS:HD3	3:B:819:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ARG:HH21	1:B:302:ASN:ND2	2.07	0.47
1:B:202:LYS:HE3	1:B:210:LEU:HD12	1.97	0.47
1:B:389:HIS:CD2	3:B:773:HOH:O	2.62	0.47
1:B:451:HIS:CG	1:B:476:GLY:HA3	2.49	0.46
1:A:364:ASN:ND2	3:A:842:HOH:O	2.47	0.46
1:B:181:GLN:NE2	3:B:911:HOH:O	2.48	0.46
1:B:392:ILE:HD12	1:B:393:SER:N	2.31	0.46
1:B:127:VAL:O	1:B:173:GLY:HA2	2.16	0.46
1:A:110:ASN:HB3	1:A:161:TYR:CZ	2.51	0.46
1:B:89:GLU:HB3	3:B:887:HOH:O	2.15	0.45
1:B:44:HIS:CD2	1:B:53:ARG:CZ	2.99	0.45
1:A:146:HIS:HD2	3:A:584:HOH:O	1.99	0.45
1:B:174:ASN:O	3:B:911:HOH:O	2.21	0.45
1:A:118:MET:HE2	3:A:816:HOH:O	2.16	0.45
1:B:202:LYS:HG2	3:B:737:HOH:O	2.15	0.45
1:A:223:PHE:O	1:A:224:ALA:HB3	2.17	0.45
1:B:12:LYS:HB2	1:B:443:PHE:CZ	2.52	0.44
1:A:164:PRO:HG2	1:A:166:LYS:HE2	1.99	0.44
1:B:299:TYR:CE1	1:B:300:HIS:ND1	2.85	0.44
1:B:176:MET:HG2	1:B:181:GLN:HG2	2.00	0.44
1:B:350:ALA:HA	1:B:351:GLN:HA	1.85	0.44
1:A:184:HIS:HE1	3:A:793:HOH:O	2.01	0.43
1:A:166:LYS:HG2	3:A:810:HOH:O	2.17	0.43
1:A:501:LYS:HB3	1:A:501:LYS:HZ3	1.83	0.43
1:B:202:LYS:CD	3:B:737:HOH:O	2.67	0.43
1:B:176:MET:HG3	3:B:911:HOH:O	2.18	0.43
1:A:456:HIS:HD2	1:A:457:ASP:H	1.65	0.43
1:A:176:MET:HE2	3:A:837:HOH:O	2.17	0.43
1:A:155:LEU:HG	1:A:159:HIS:CD2	2.53	0.43
1:A:110:ASN:HB3	1:A:161:TYR:CE1	2.53	0.43
1:A:44:HIS:CD2	1:A:53:ARG:CZ	3.01	0.43
1:A:174:ASN:HD22	1:A:181:GLN:NE2	2.14	0.43
1:B:242:SER:HA	1:B:291:SER:O	2.19	0.43
1:A:64:GLN:NE2	3:A:854:HOH:O	2.52	0.42
1:A:77:SER:OG	1:A:181:GLN:NE2	2.52	0.42
1:A:339:LYS:NZ	3:A:828:HOH:O	2.52	0.42
1:B:324:PHE:CZ	1:B:455:GLU:HA	2.54	0.42
1:B:240:TYR:HA	1:B:289:HIS:O	2.20	0.42
1:A:339:LYS:NZ	1:A:409:GLU:OE2	2.38	0.42
1:A:125:MET:O	1:A:170:TRP:HA	2.20	0.41
1:B:354:ASN:ND2	1:B:361:THR:H	2.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLY:N	1:A:159:HIS:ND1	2.68	0.41
1:A:217:ASN:ND2	3:A:926:HOH:O	2.53	0.41
1:A:242:SER:HA	1:A:291:SER:O	2.21	0.41
1:B:479:GLN:HG3	3:B:831:HOH:O	2.19	0.41
1:A:245:GLN:CD	3:A:773:HOH:O	2.58	0.41
1:B:198:ALA:HB1	1:B:210:LEU:HD13	2.02	0.41
1:A:129:LEU:O	1:A:185:LYS:HE3	2.21	0.41
1:A:501:LYS:CB	1:A:501:LYS:NZ	2.84	0.41
1:A:134:ILE:HG21	1:A:134:ILE:HD13	1.81	0.41
1:B:170:TRP:CD1	1:B:170:TRP:N	2.89	0.41
1:A:14:PHE:CD2	1:B:14:PHE:CE2	3.08	0.41
1:B:300:HIS:CD2	1:B:321:ILE:O	2.72	0.41
1:B:231:LEU:HD23	1:B:231:LEU:HA	1.93	0.41
1:A:202:LYS:HB2	1:A:202:LYS:HE3	1.94	0.40
1:A:451:HIS:CG	1:A:476:GLY:HA3	2.56	0.40
1:B:473:HIS:CD2	1:B:473:HIS:C	2.94	0.40

All (2) 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:667:HOH:O	3:A:924:HOH:O[3_665]	2.13	0.07
3:B:791:HOH:O	3:B:914:HOH:O[3_665]	2.19	0.01

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%)	476 (96%)	16 (3%)	3 (1%)	30	22
1	B	495/502 (99%)	473 (96%)	20 (4%)	2 (0%)	39	33
All	All	990/1004 (99%)	949 (96%)	36 (4%)	5 (0%)	34	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	TYR
1	B	299	TYR
1	A	482	ASP
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%)	408 (95%)	21 (5%)	31	25
1	B	429/433 (99%)	410 (96%)	19 (4%)	35	30
All	All	858/866 (99%)	818 (95%)	40 (5%)	32	27

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	MET
1	A	44	HIS
1	A	49	GLU
1	A	202	LYS
1	A	212	VAL
1	A	217	ASN
1	A	243	LEU
1	A	277	TYR
1	A	292	PHE
1	A	370	GLN
1	A	378	HIS
1	A	403	THR
1	A	431	GLU
1	A	435	LEU
1	A	444	GLU
1	A	479	GLN
1	A	481	SER
1	A	482	ASP

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Mol	Chain	Res	Type
1	A	483	ARG
1	A	491	LYS
1	A	501	LYS
1	B	5	LYS
1	B	10	ILE
1	B	49	GLU
1	B	212	VAL
1	B	243	LEU
1	B	252	ASN
1	B	277	TYR
1	B	292	PHE
1	B	392	ILE
1	B	396	LYS
1	B	435	LEU
1	B	447	ARG
1	B	473	HIS
1	B	480	LEU
1	B	481	SER
1	B	483	ARG
1	B	484	LYS
1	B	491	LYS
1	B	501	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	HIS
1	A	159	HIS
1	A	181	GLN
1	A	184	HIS
1	A	217	ASN
1	A	237	HIS
1	A	300	HIS
1	A	302	ASN
1	A	340	HIS
1	A	370	GLN
1	A	378	HIS
1	A	451	HIS
1	A	456	HIS
1	A	463	ASN
1	A	473	HIS
1	A	479	GLN

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Mol	Chain	Res	Type
1	A	495	ASN
1	B	64	GLN
1	B	181	GLN
1	B	184	HIS
1	B	300	HIS
1	B	302	ASN
1	B	354	ASN
1	B	364	ASN
1	B	378	HIS
1	B	456	HIS
1	B	461	GLN
1	B	473	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

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	AHR	A	550	1	9,9,10	1.19	1 (11%)	12,12,14	3.79	4 (33%)
2	AHR	B	550	1	9,9,10	0.54	0	12,12,14	3.70	3 (25%)

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	AHR	A	550	1	2/2/3/4	0/2/15/18	0/1/1/1
2	AHR	B	550	1	2/2/3/4	0/2/15/18	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	550	AHR	C1'-C2'	2.93	1.57	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	550	AHR	O4'-C1'-C2'	-2.59	100.87	106.16
2	B	550	AHR	O3'-C3'-C2'	3.46	119.91	111.68
2	B	550	AHR	O2'-C2'-C1'	3.75	122.83	111.20
2	A	550	AHR	O2'-C2'-C1'	3.95	123.42	111.20
2	A	550	AHR	O3'-C3'-C2'	4.67	122.78	111.68
2	A	550	AHR	O2'-C2'-C3'	10.98	132.30	111.23
2	B	550	AHR	O2'-C2'-C3'	11.34	132.99	111.23

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	550	AHR	C2'
2	B	550	AHR	C1'
2	A	550	AHR	C2'
2	A	550	AHR	C1'

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

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	497/502 (99%)	-0.08	20 (4%) 42 44	27, 38, 58, 73	0
1	B	497/502 (99%)	-0.08	16 (3%) 51 52	30, 41, 58, 69	0
All	All	994/1004 (99%)	-0.08	36 (3%) 46 48	27, 40, 58, 73	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	482	ASP	4.6
1	B	180	TRP	3.9
1	B	482	ASP	3.9
1	A	445	ASP	3.9
1	B	466	GLN	3.8
1	A	444	GLU	3.7
1	A	441	ARG	3.7
1	A	466	GLN	3.6
1	A	417	GLU	3.3
1	B	441	ARG	3.2
1	A	14	PHE	3.1
1	A	49	GLU	3.1
1	A	457	ASP	3.0
1	B	14	PHE	2.8
1	B	49	GLU	2.8
1	A	180	TRP	2.8
1	A	404	ASP	2.5
1	B	457	ASP	2.5
1	A	435	LEU	2.5
1	A	5	LYS	2.5
1	B	431	GLU	2.5
1	B	444	GLU	2.4
1	B	5	LYS	2.4
1	A	308	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	43	GLY	2.3
1	A	393	SER	2.3
1	A	307	LEU	2.2
1	B	445	ASP	2.2
1	A	405	VAL	2.2
1	B	483	ARG	2.2
1	B	481	SER	2.2
1	A	399	SER	2.1
1	B	435	LEU	2.1
1	B	467	SER	2.1
1	A	252	ASN	2.0
1	A	309	GLU	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^{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	LLDF	B-factors(Å^2)	Q<0.9
2	AHR	A	550	9/10	0.71	0.22	3.23	38,42,46,46	0
2	AHR	B	550	9/10	0.81	0.16	2.76	40,43,46,48	0

6.5 Other polymers (i)

There are no such residues in this entry.