



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:15 AM UTC

PDB ID : 2ZXA / pdb_00002zxa
Title : alpha-L-fucosidase complexed with inhibitor, FNJ-acetyl
Authors : Wu, H.-J.; Ko, T.-P.; Ho, C.-W.; Lin, C.-H.; Wang, A.H.-J.
Deposited on : 2008-12-22
Resolution : 2.57 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
Mogul : 2022.3.0, CSD as543be (2022)
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

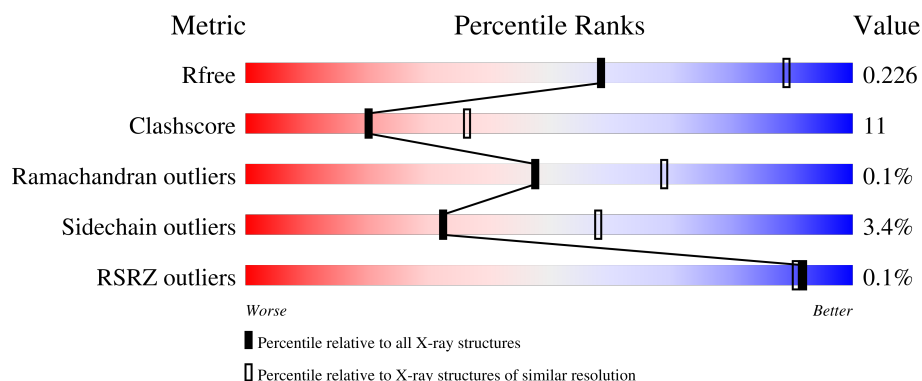
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	455	 65% 28% . .
1	B	455	 68% 26% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7716 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.

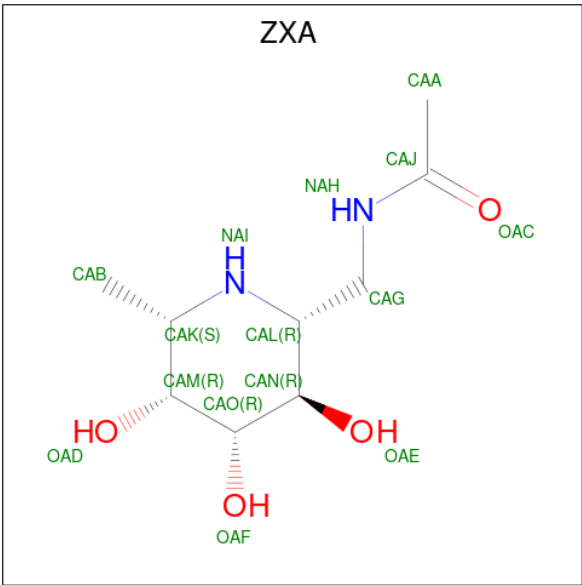
- Molecule 1 is a protein called Alpha-L-fucosidase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3648	2377	600	663	8			
1	B	442	Total	C	N	O	S	0	0	0
			3648	2377	600	663	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	450	HIS	-	expression tag	UNP Q9WYE2
A	451	HIS	-	expression tag	UNP Q9WYE2
A	452	HIS	-	expression tag	UNP Q9WYE2
A	453	HIS	-	expression tag	UNP Q9WYE2
A	454	HIS	-	expression tag	UNP Q9WYE2
A	455	HIS	-	expression tag	UNP Q9WYE2
B	450	HIS	-	expression tag	UNP Q9WYE2
B	451	HIS	-	expression tag	UNP Q9WYE2
B	452	HIS	-	expression tag	UNP Q9WYE2
B	453	HIS	-	expression tag	UNP Q9WYE2
B	454	HIS	-	expression tag	UNP Q9WYE2
B	455	HIS	-	expression tag	UNP Q9WYE2

- Molecule 2 is N- $\{[(2R,3R,4R,5R,6S)-3,4,5\text{-trihydroxy-6-methylpiperidin-2-yl}]methyl\}$ acetamide (CCD ID: ZXA) (formula: $C_9H_{18}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	9	2	4		
2	B	1	Total	C	N	O	0	0
			15	9	2	4		

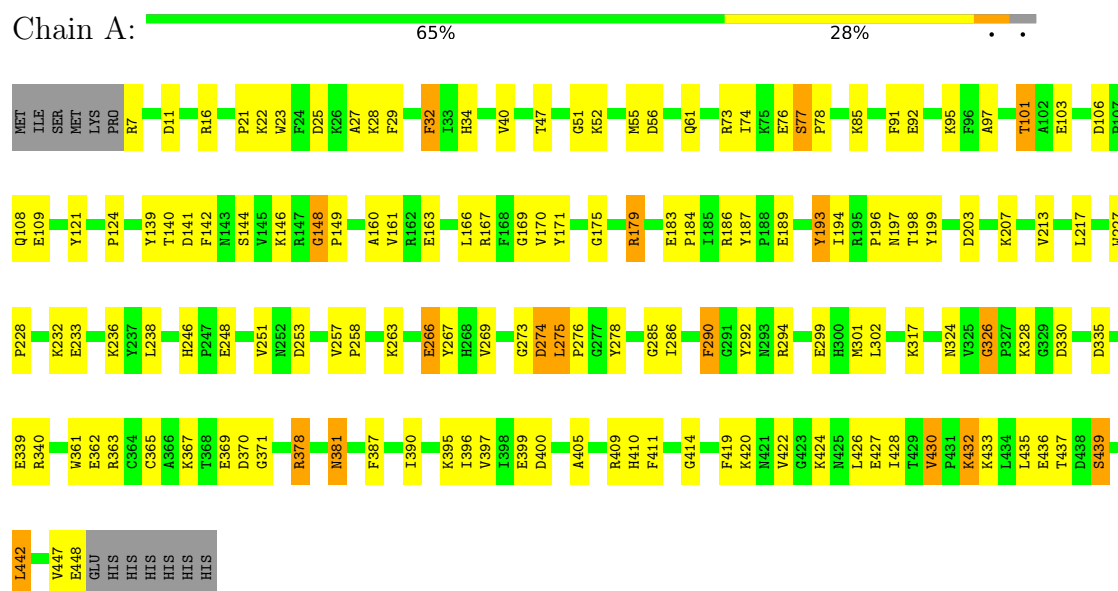
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	203	Total	O	0	0
			203	203		
3	B	187	Total	O	0	0
			187	187		

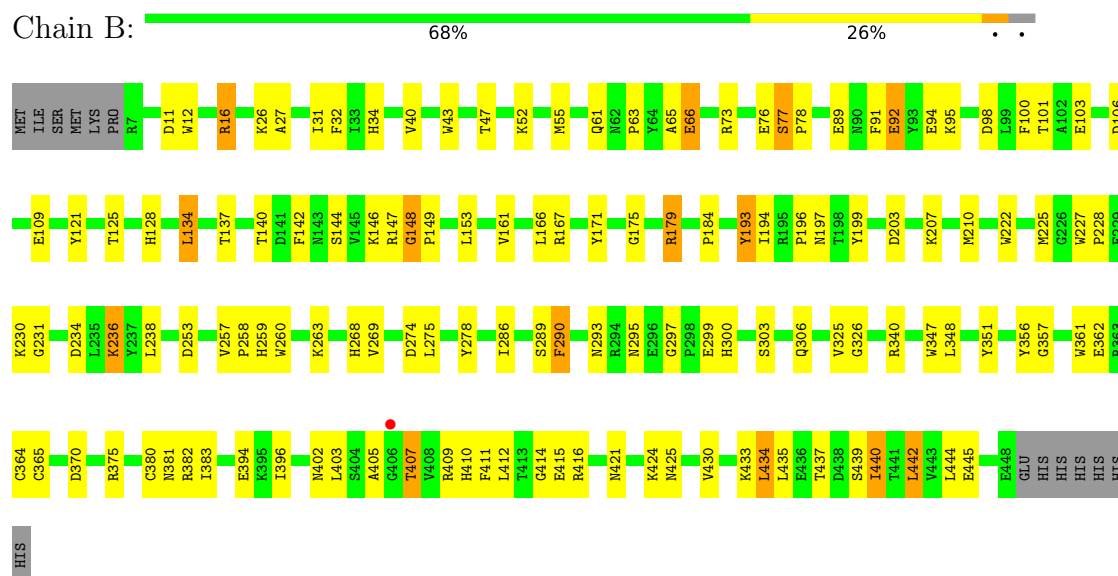
3 Residue-property plots

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: Alpha-L-fucosidase, putative



- Molecule 1: Alpha-L-fucosidase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	180.56Å 180.56Å 169.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.57 30.00 – 2.57	Depositor EDS
% Data completeness (in resolution range)	96.4 (30.00-2.57) 96.4 (30.00-2.57)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.70 (at 2.57Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.161 , 0.225 0.162 , 0.226	Depositor DCC
R_{free} test set	1613 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7716	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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

5.1 Standard geometry

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

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	1.21	7/3768 (0.2%)	1.31	44/5120 (0.9%)
1	B	1.17	4/3768 (0.1%)	1.30	40/5120 (0.8%)
All	All	1.19	11/7536 (0.1%)	1.31	84/10240 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	MET	SD-CE	7.00	1.97	1.79
1	B	55	MET	SD-CE	6.66	1.96	1.79
1	A	213	VAL	CA-CB	6.44	1.62	1.54
1	B	31	ILE	CA-CB	6.33	1.61	1.54
1	A	194	ILE	CA-C	6.23	1.58	1.53
1	A	101	THR	CA-CB	5.30	1.62	1.53
1	A	266	GLU	CA-C	5.28	1.58	1.52
1	B	210	MET	SD-CE	5.25	1.92	1.79
1	A	140	THR	CA-CB	5.09	1.61	1.53
1	B	63	PRO	CA-C	5.03	1.59	1.52
1	A	29	PHE	N-CA	-5.01	1.39	1.46

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	ALA	CA-C-N	-10.25	106.00	121.99
1	B	27	ALA	C-N-CA	-10.25	106.00	121.99
1	A	27	ALA	CA-C-N	-9.23	107.89	122.29
1	A	27	ALA	C-N-CA	-9.23	107.89	122.29
1	A	326	GLY	CA-C-N	8.81	129.35	119.92
1	A	326	GLY	C-N-CA	8.81	129.35	119.92
1	B	40	VAL	CA-C-N	-8.07	111.33	119.56
1	B	40	VAL	C-N-CA	-8.07	111.33	119.56
1	B	269	VAL	N-CA-C	8.05	119.80	108.93
1	A	365	CYS	N-CA-C	7.91	121.18	109.24
1	B	47	THR	N-CA-C	7.74	119.72	111.28
1	A	77	SER	N-CA-C	-7.64	95.91	108.82
1	B	148	GLY	N-CA-C	7.53	127.69	112.34
1	A	275	LEU	CA-C-N	7.34	129.01	119.84
1	A	275	LEU	C-N-CA	7.34	129.01	119.84
1	A	390	ILE	CA-C-N	7.32	127.30	119.76
1	A	390	ILE	C-N-CA	7.32	127.30	119.76
1	A	411	PHE	N-CA-C	7.10	118.67	111.07
1	B	365	CYS	N-CA-C	7.04	119.88	109.24
1	B	290	PHE	N-CA-C	-6.97	103.41	112.68
1	A	371	GLY	N-CA-C	6.96	125.80	115.08
1	B	410	HIS	N-CA-C	-6.93	98.65	109.25
1	B	77	SER	N-CA-C	-6.70	97.37	108.23
1	B	179	ARG	N-CA-C	-6.70	105.07	113.18
1	B	286	ILE	N-CA-C	-6.66	102.77	111.09
1	A	27	ALA	N-CA-C	-6.64	101.13	110.50
1	B	415	GLU	N-CA-C	6.54	119.70	109.96
1	A	183	GLU	CA-C-N	-6.54	114.05	120.52
1	A	183	GLU	C-N-CA	-6.54	114.05	120.52
1	A	430	VAL	CA-C-N	6.46	126.84	119.93
1	A	430	VAL	C-N-CA	6.46	126.84	119.93
1	A	290	PHE	N-CA-C	-6.46	105.05	113.12
1	A	232	LYS	N-CA-C	6.44	118.30	111.28
1	A	144	SER	N-CA-C	6.40	120.69	113.01
1	B	351	TYR	N-CA-C	6.37	121.05	113.28
1	B	101	THR	N-CA-C	6.34	121.16	113.17
1	B	439	SER	CA-C-N	-6.30	114.15	121.71
1	B	439	SER	C-N-CA	-6.30	114.15	121.71
1	A	148	GLY	CA-C-N	6.29	125.97	119.56
1	A	148	GLY	C-N-CA	6.29	125.97	119.56
1	B	55	MET	N-CA-C	6.23	120.34	112.87
1	B	442	LEU	N-CA-C	-6.21	100.39	110.20
1	A	40	VAL	CA-C-N	-6.21	112.61	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	VAL	C-N-CA	-6.21	112.61	119.19
1	A	139	TYR	N-CA-C	6.15	120.92	113.17
1	B	440	ILE	N-CA-C	-6.07	107.58	113.53
1	A	273	GLY	N-CA-C	-6.00	106.30	115.66
1	A	56	ASP	N-CA-C	-5.91	106.07	113.28
1	B	326	GLY	CA-C-N	5.91	126.24	119.92
1	B	326	GLY	C-N-CA	5.91	126.24	119.92
1	A	199	TYR	N-CA-C	-5.81	105.03	111.36
1	A	410	HIS	N-CA-C	-5.81	99.81	109.46
1	B	27	ALA	N-CA-C	-5.81	102.31	110.50
1	B	194	ILE	N-CA-C	5.80	112.42	106.21
1	A	193	TYR	CA-C-N	-5.75	115.60	122.22
1	A	193	TYR	C-N-CA	-5.75	115.60	122.22
1	A	47	THR	N-CA-C	5.68	118.24	111.71
1	B	61	GLN	N-CA-C	-5.64	102.00	110.06
1	B	144	SER	N-CA-C	5.62	119.40	112.54
1	B	259	HIS	N-CA-C	5.54	118.84	109.76
1	A	51	GLY	N-CA-C	-5.51	107.42	114.37
1	A	442	LEU	CA-C-N	-5.50	115.79	123.10
1	A	442	LEU	C-N-CA	-5.50	115.79	123.10
1	A	274	ASP	N-CA-C	5.50	115.49	108.24
1	B	412	LEU	N-CA-C	5.48	117.26	111.28
1	A	198	THR	N-CA-C	5.47	117.58	110.53
1	B	411	PHE	N-CA-C	5.42	120.27	111.37
1	A	439	SER	N-CA-C	5.37	119.78	111.56
1	A	269	VAL	N-CA-C	5.37	115.31	108.12
1	A	378	ARG	N-CA-C	5.34	117.80	109.52
1	A	179	ARG	N-CA-C	-5.32	106.74	113.18
1	B	193	TYR	CA-C-N	-5.23	116.74	121.65
1	B	193	TYR	C-N-CA	-5.23	116.74	121.65
1	B	380	CYS	CA-CB-SG	-5.21	102.41	114.40
1	B	148	GLY	CA-C-N	5.14	124.80	119.56
1	B	148	GLY	C-N-CA	5.14	124.80	119.56
1	A	363	ARG	N-CA-C	-5.13	101.49	109.24
1	B	146	LYS	N-CA-C	5.12	119.58	113.23
1	B	439	SER	N-CA-C	5.12	118.97	111.04
1	A	175	GLY	N-CA-C	5.11	119.31	112.77
1	A	442	LEU	N-CA-C	-5.09	101.00	109.46
1	B	405	ALA	CA-C-N	-5.08	117.40	123.44
1	B	405	ALA	C-N-CA	-5.08	117.40	123.44
1	B	394	GLU	N-CA-C	-5.05	107.07	113.18

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	193	TYR	Sidechain
1	B	193	TYR	Sidechain

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	3648	0	3512	89	0
1	B	3648	0	3512	77	1
2	A	15	0	18	0	0
2	B	15	0	18	1	0
3	A	203	0	0	1	0
3	B	187	0	0	4	2
All	All	7716	0	7060	163	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 11.

All (163) 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:433:LYS:HG3	1:B:434:LEU:HD23	1.56	0.87
1:B:434:LEU:O	1:B:437:THR:HG22	1.78	0.83
1:A:381:ASN:HD22	1:A:381:ASN:H	1.30	0.79
1:B:297:GLY:H	1:B:300:HIS:HD2	1.30	0.76
1:A:361:TRP:CG	1:A:362:GLU:H	2.03	0.74
1:A:108:GLN:HE22	1:A:163:GLU:HB2	1.51	0.74
1:A:290:PHE:HA	1:A:324:ASN:ND2	2.04	0.73
1:A:381:ASN:HD22	1:A:381:ASN:N	1.86	0.73
1:A:381:ASN:H	1:A:381:ASN:ND2	1.89	0.70
1:B:106:ASP:CG	1:B:109:GLU:HG3	2.18	0.69
1:B:263:LYS:HD3	1:B:278:TYR:CE1	2.27	0.69
1:A:74:ILE:O	1:A:77:SER:HB3	1.93	0.68
1:B:409:ARG:NH1	1:B:414:GLY:O	2.27	0.67
1:A:395:LYS:HD2	1:A:427:GLU:HG2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ASP:O	1:A:28:LYS:HE2	1.95	0.65
1:A:16:ARG:HD2	1:B:16:ARG:HH21	1.63	0.63
1:B:94:GLU:H	1:B:94:GLU:CD	2.07	0.63
1:B:434:LEU:HD23	1:B:434:LEU:N	2.14	0.61
1:B:171:TYR:CD2	1:B:171:TYR:C	2.79	0.61
1:A:91:PHE:CE2	1:A:95:LYS:HB3	2.36	0.61
1:B:238:LEU:C	1:B:238:LEU:HD23	2.25	0.61
1:A:108:GLN:NE2	1:A:163:GLU:HB2	2.15	0.60
1:B:134:LEU:HD13	1:B:153:LEU:HD12	1.84	0.59
1:A:141:ASP:OD1	1:A:146:LYS:HD2	2.02	0.59
1:B:402:ASN:HA	1:B:421:ASN:OD1	2.02	0.59
1:B:407:THR:HB	1:B:416:ARG:NH1	2.17	0.59
1:A:367:LYS:HE3	1:A:399:GLU:OE1	2.03	0.59
1:A:171:TYR:CD2	1:A:171:TYR:C	2.81	0.59
1:A:301:MET:HE2	1:A:340:ARG:HD2	1.85	0.58
1:B:26:LYS:HD3	1:B:357:GLY:HA2	1.85	0.58
1:B:433:LYS:HG3	1:B:434:LEU:CD2	2.33	0.57
1:A:395:LYS:HD3	1:A:396:ILE:N	2.20	0.57
1:A:196:PRO:O	1:A:197:ASN:HB2	2.05	0.56
1:A:400:ASP:HA	1:A:424:LYS:O	2.06	0.56
1:A:286:ILE:CG2	1:A:301:MET:HE3	2.36	0.55
1:B:34:HIS:CG	1:B:290:PHE:HB3	2.41	0.55
1:A:16:ARG:HG3	1:B:260:TRP:CZ2	2.42	0.55
1:A:217:LEU:HD11	1:A:246:HIS:HB2	1.88	0.54
1:A:427:GLU:C	1:A:428:ILE:HG13	2.30	0.54
1:B:434:LEU:O	1:B:435:LEU:C	2.49	0.54
1:A:203:ASP:O	1:A:207:LYS:HG3	2.08	0.54
1:A:285:GLY:HA2	1:A:324:ASN:HB3	1.89	0.54
1:B:52:LYS:HG3	1:B:268:HIS:CD2	2.43	0.54
1:B:396:ILE:HD12	1:B:430:VAL:CG2	2.37	0.54
1:B:203:ASP:O	1:B:207:LYS:HG3	2.08	0.54
1:A:420:LYS:HE3	1:A:422:VAL:HG22	1.90	0.53
1:B:340:ARG:HH11	1:B:340:ARG:HG3	1.71	0.53
1:B:137:THR:HG21	1:B:140:THR:HG22	1.90	0.53
1:B:92:GLU:CB	1:B:94:GLU:OE2	2.57	0.53
1:A:61:GLN:HE22	1:A:78:PRO:HG2	1.73	0.53
1:A:274:ASP:CG	1:A:275:LEU:H	2.17	0.53
1:A:34:HIS:CG	1:A:290:PHE:HB3	2.44	0.53
1:A:369:GLU:HB2	1:A:397:VAL:HB	1.92	0.52
1:B:407:THR:HB	1:B:416:ARG:HH11	1.73	0.52
1:B:98:ASP:CG	1:B:147:ARG:HH21	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:ARG:NE	1:B:445:GLU:OE1	2.36	0.52
1:A:378:ARG:HH11	1:A:378:ARG:HG2	1.74	0.52
1:A:189:GLU:H	1:A:189:GLU:CD	2.14	0.52
1:A:238:LEU:C	1:A:238:LEU:HD23	2.35	0.51
1:A:378:ARG:HG2	1:A:378:ARG:NH1	2.25	0.51
1:B:196:PRO:O	1:B:197:ASN:HB2	2.10	0.51
1:B:92:GLU:HB2	1:B:94:GLU:OE2	2.11	0.51
1:A:124:PRO:HD2	1:A:169:GLY:O	2.10	0.50
1:A:426:LEU:HD23	1:A:428:ILE:HD11	1.93	0.50
1:B:347:TRP:CD1	1:B:440:ILE:HD12	2.46	0.50
1:A:106:ASP:CG	1:A:109:GLU:HG3	2.36	0.50
1:B:433:LYS:HE2	1:B:434:LEU:CD2	2.42	0.50
1:B:66:GLU:H	1:B:66:GLU:CD	2.20	0.49
1:A:335:ASP:O	1:A:339:GLU:HG3	2.12	0.49
1:A:395:LYS:HD2	1:A:427:GLU:CG	2.42	0.49
1:A:108:GLN:NE2	1:A:160:ALA:HA	2.28	0.48
1:A:189:GLU:OE1	1:A:189:GLU:N	2.30	0.48
1:B:433:LYS:HG3	1:B:434:LEU:N	2.28	0.48
1:A:121:TYR:HB3	1:A:167:ARG:HB2	1.96	0.48
1:A:292:TYR:HB2	1:A:326:GLY:O	2.13	0.48
1:A:263:LYS:HD3	1:A:278:TYR:CE1	2.49	0.48
1:B:293:ASN:OD1	1:B:295:ASN:HB2	2.14	0.47
1:A:370:ASP:OD2	1:A:370:ASP:C	2.56	0.47
1:A:405:ALA:HA	1:A:448:GLU:HA	1.96	0.47
1:B:361:TRP:CG	1:B:362:GLU:H	2.32	0.47
1:B:396:ILE:HD12	1:B:430:VAL:HG21	1.95	0.47
1:A:161:VAL:HG13	1:A:166:LEU:HB2	1.97	0.47
1:B:297:GLY:H	1:B:300:HIS:CD2	2.21	0.47
1:A:395:LYS:NZ	3:A:616:HOH:O	2.46	0.47
1:A:433:LYS:O	1:A:437:THR:HG23	2.15	0.46
1:B:26:LYS:CD	1:B:357:GLY:HA2	2.45	0.46
1:A:328:LYS:HB2	1:A:330:ASP:OD2	2.16	0.46
1:A:106:ASP:OD2	1:A:109:GLU:HG3	2.15	0.46
1:B:257:VAL:HB	1:B:258:PRO:CD	2.45	0.46
1:A:97:ALA:O	1:A:148:GLY:CA	2.64	0.46
1:A:233:GLU:OE1	1:A:236:LYS:CE	2.64	0.46
1:B:12:TRP:CZ2	1:B:236:LYS:HG2	2.50	0.46
1:B:257:VAL:HB	1:B:258:PRO:HD2	1.97	0.45
1:A:395:LYS:HD3	1:A:396:ILE:H	1.81	0.45
1:B:73:ARG:HB2	1:B:184:PRO:HB3	1.98	0.45
1:A:274:ASP:OD2	1:A:275:LEU:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ALA:HB1	1:A:447:VAL:O	2.15	0.45
1:B:199:TYR:CZ	1:B:230:LYS:HE2	2.51	0.45
1:B:91:PHE:CZ	1:B:95:LYS:HG2	2.52	0.45
1:B:26:LYS:HD3	3:B:482:HOH:O	2.17	0.45
1:A:142:PHE:CE2	1:A:179:ARG:HD2	2.52	0.45
1:A:275:LEU:HA	1:A:276:PRO:HD3	1.71	0.44
1:B:77:SER:O	1:B:78:PRO:C	2.58	0.44
1:A:395:LYS:CD	1:A:427:GLU:HG2	2.46	0.44
1:A:32:PHE:HB3	1:A:324:ASN:HA	1.99	0.44
1:A:432:LYS:O	1:A:436:GLU:HB2	2.17	0.44
1:A:419:PHE:CB	1:A:428:ILE:HG12	2.48	0.44
1:B:125:THR:HA	1:B:171:TYR:HB3	1.98	0.44
1:B:370:ASP:OD1	3:B:639:HOH:O	2.21	0.43
1:B:424:LYS:HG3	1:B:425:ASN:OD1	2.18	0.43
1:A:409:ARG:HD3	1:A:414:GLY:O	2.19	0.43
1:A:430:VAL:HG12	1:A:435:LEU:HG	2.00	0.43
1:A:286:ILE:CG2	1:A:301:MET:CE	2.95	0.43
1:A:91:PHE:C	1:A:91:PHE:CD2	2.96	0.43
1:B:161:VAL:HG13	1:B:166:LEU:HB2	1.99	0.43
1:A:275:LEU:HD23	1:A:317:LYS:HA	1.99	0.43
1:B:227:TRP:CG	1:B:228:PRO:HD2	2.54	0.43
1:A:101:THR:OG1	1:A:103:GLU:HG2	2.18	0.43
1:B:142:PHE:CE2	1:B:179:ARG:HD2	2.54	0.43
1:A:381:ASN:N	1:A:381:ASN:ND2	2.53	0.42
1:B:92:GLU:HB3	1:B:94:GLU:OE2	2.18	0.42
1:B:231:GLY:O	1:B:234:ASP:HB2	2.18	0.42
1:A:257:VAL:HB	1:A:258:PRO:CD	2.49	0.42
1:B:16:ARG:HD2	3:B:458:HOH:O	2.19	0.42
1:A:16:ARG:CG	1:B:260:TRP:CE2	3.02	0.42
1:A:274:ASP:CG	1:A:275:LEU:N	2.76	0.42
1:B:12:TRP:CE2	1:B:236:LYS:HD3	2.54	0.42
1:B:253:ASP:CG	1:B:263:LYS:HA	2.45	0.42
1:B:65:ALA:H	1:B:289:SER:HG	1.65	0.42
1:B:175:GLY:HA3	1:B:225:MET:O	2.20	0.42
1:A:148:GLY:HA3	1:A:149:PRO:HD3	1.78	0.42
1:B:364:CYS:O	1:B:375:ARG:HA	2.20	0.42
1:A:227:TRP:CG	1:A:228:PRO:HD2	2.55	0.41
1:B:147:ARG:HD3	3:B:536:HOH:O	2.20	0.41
1:B:396:ILE:HD12	1:B:430:VAL:HG23	2.01	0.41
1:A:184:PRO:HG2	1:A:186:ARG:NH2	2.35	0.41
1:A:302:LEU:O	1:A:340:ARG:NE	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LEU:HD22	1:B:356:TYR:CZ	2.55	0.41
1:B:361:TRP:CZ2	1:B:383:ILE:HD13	2.55	0.41
1:A:286:ILE:HG22	1:A:301:MET:HE3	2.02	0.41
1:B:43:TRP:NE1	1:B:295:ASN:HD21	2.18	0.41
1:B:128:HIS:CE1	2:B:902:ZXA:OAF	2.73	0.41
1:B:274:ASP:CG	1:B:275:LEU:H	2.28	0.41
1:B:361:TRP:CE2	1:B:383:ILE:HD13	2.55	0.41
1:A:22:LYS:HB2	1:A:22:LYS:HE3	1.84	0.41
1:A:21:PRO:HG3	1:A:248:GLU:O	2.20	0.41
1:A:266:GLU:O	1:A:267:TYR:C	2.64	0.41
1:B:100:PHE:O	1:B:149:PRO:HD3	2.21	0.41
1:A:23:TRP:CE3	1:A:23:TRP:C	2.99	0.41
1:A:426:LEU:CD2	1:A:428:ILE:HD11	2.50	0.41
1:B:11:ASP:HA	1:B:236:LYS:HD2	2.03	0.41
1:A:187:TYR:HB3	1:A:189:GLU:OE1	2.21	0.41
1:A:253:ASP:CG	1:A:263:LYS:HA	2.46	0.41
1:A:387:PHE:HB2	1:A:442:LEU:HB3	2.02	0.41
1:B:442:LEU:HD11	1:B:444:LEU:HD21	2.02	0.41
1:B:121:TYR:HB3	1:B:167:ARG:HB2	2.02	0.40
1:A:73:ARG:HB2	1:A:184:PRO:HB3	2.03	0.40
1:B:100:PHE:O	1:B:149:PRO:CD	2.69	0.40
1:B:403:LEU:H	1:B:421:ASN:HD21	1.68	0.40
1:A:121:TYR:HA	1:A:167:ARG:O	2.21	0.40
1:B:303:SER:OG	1:B:306:GLN:HG3	2.21	0.40
1:A:170:VAL:O	1:A:170:VAL:HG23	2.21	0.40
1:A:233:GLU:OE1	1:A:236:LYS:HE3	2.19	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:B:568:HOH:O	3:B:568:HOH:O[4_556]	0.75	1.45
3:B:502:HOH:O	3:B:502:HOH:O[5_556]	1.92	0.28
1:B:89:GLU:N	1:B:103:GLU:OE1[5_556]	2.03	0.17

5.3 Torsion angles

5.3.1 Protein backbone

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	440/455 (97%)	417 (95%)	23 (5%)	0	100	100
1	B	440/455 (97%)	416 (94%)	23 (5%)	1 (0%)	43	63
All	All	880/910 (97%)	833 (95%)	46 (5%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	GLY

5.3.2 Protein sidechains

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	382/395 (97%)	369 (97%)	13 (3%)	32	58
1	B	382/395 (97%)	369 (97%)	13 (3%)	32	58
All	All	764/790 (97%)	738 (97%)	26 (3%)	32	58

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	11	ASP
1	A	32	PHE
1	A	52	LYS
1	A	76	GLU

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Mol	Chain	Res	Type
1	A	85	LYS
1	A	92	GLU
1	A	251	VAL
1	A	294	ARG
1	A	299	GLU
1	A	381	ASN
1	A	432	LYS
1	A	439	SER
1	B	16	ARG
1	B	32	PHE
1	B	66	GLU
1	B	76	GLU
1	B	92	GLU
1	B	134	LEU
1	B	222	TRP
1	B	236	LYS
1	B	299	GLU
1	B	325	VAL
1	B	381	ASN
1	B	407	THR
1	B	434	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	108	GLN
1	A	268	HIS
1	A	324	ASN
1	A	381	ASN
1	A	402	ASN
1	B	208	GLN
1	B	300	HIS
1	B	381	ASN
1	B	402	ASN

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](#)

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	ZXA	A	901	-	15,15,15	0.68	0	19,21,21	1.44	3 (15%)
2	ZXA	B	902	-	15,15,15	0.65	0	19,21,21	1.61	3 (15%)

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	ZXA	A	901	-	-	1/5/25/25	0/1/1/1
2	ZXA	B	902	-	-	1/5/25/25	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	ZXA	CAL-CAG-NAH	-4.35	102.94	112.78
2	A	901	ZXA	CAK-NAI-CAL	-3.56	109.44	112.96
2	A	901	ZXA	CAO-CAN-CAL	-3.35	106.10	111.02
2	B	902	ZXA	CAK-NAI-CAL	-3.06	109.94	112.96
2	B	902	ZXA	CAO-CAN-CAL	-2.56	107.27	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	901	ZXA	CAL-CAG-NAH	-2.03	108.19	112.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	ZXA	CAL-CAG-NAH-CAJ
2	B	902	ZXA	CAL-CAG-NAH-CAJ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	902	ZXA	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	442/455 (97%)	-0.66	0 100 100	12, 30, 58, 76	0
1	B	442/455 (97%)	-0.57	1 (0%) 91 90	15, 31, 58, 75	0
All	All	884/910 (97%)	-0.62	1 (0%) 92 90	12, 30, 59, 76	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	406	GLY	2.4

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(Å ²)	Q<0.9
2	ZXA	B	902	15/15	0.94	0.08	22,29,36,40	0
2	ZXA	A	901	15/15	0.97	0.05	22,27,36,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.