Full wwPDB X-ray Structure Validation Report (i)

Sep 28, 2024 – 01:47 PM EDT

PDB ID	:	3WMT
Title	:	Crystal structure of feruloyl esterase B from Aspergillus oryzae
Authors	:	Suzuki, K.; Ishida, T.; Igarashi, K.; Koseki, T.; Fushinobu, S.
Deposited on	:	2013-11-25
Resolution	:	1.50 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 (i) 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 (i)) were used in the production of this report:

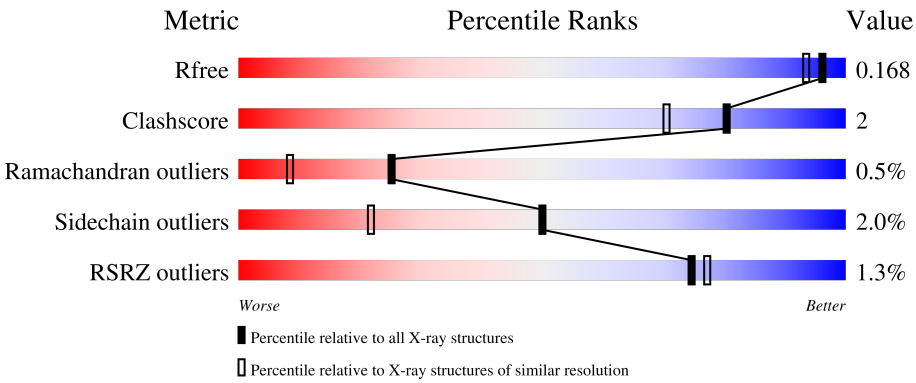
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.50 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}	164625	3717 (1.50-1.50)
Clashscore	180529	4048 (1.50-1.50)
Ramachandran outliers	177936	3970 (1.50-1.50)
Sidechain outliers	177891	3967 (1.50-1.50)
RSRZ outliers	164620	3718 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	522	% 85% 11% •
1	B	522	2% 84% 11% • 5%

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	NAG	A	603	-	-	X	-
2	NAG	A	605	-	-	X	-

2 Entry composition (i)

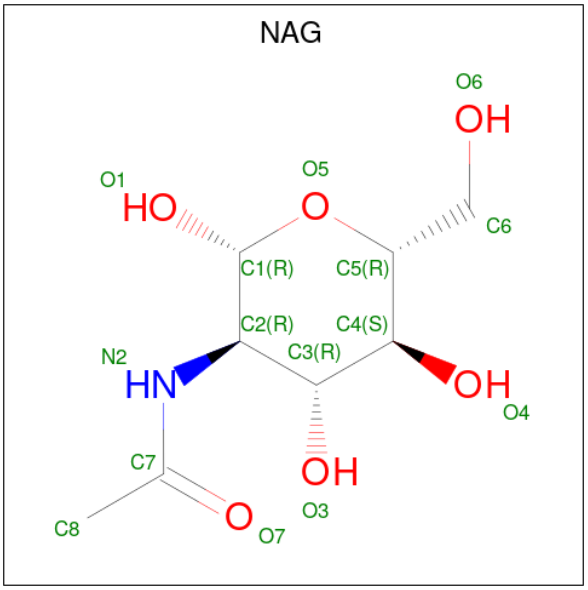
There are 4 unique types of molecules in this entry. The entry contains 8889 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Probable feruloyl esterase B-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	503	3859	2436	645	758	20	0	0	0
1	B	498	3829	2419	640	751	19	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	B	1	14	8	1	5	0	0
			Total	C	N	O		
2	B	1	14	8	1	5	0	0
			Total	C	N	O		
2	B	1	14	8	1	5	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	1	1	1	0	0
			Total	Ca		
3	B	1	1	1	0	0

- Molecule 4 is water.

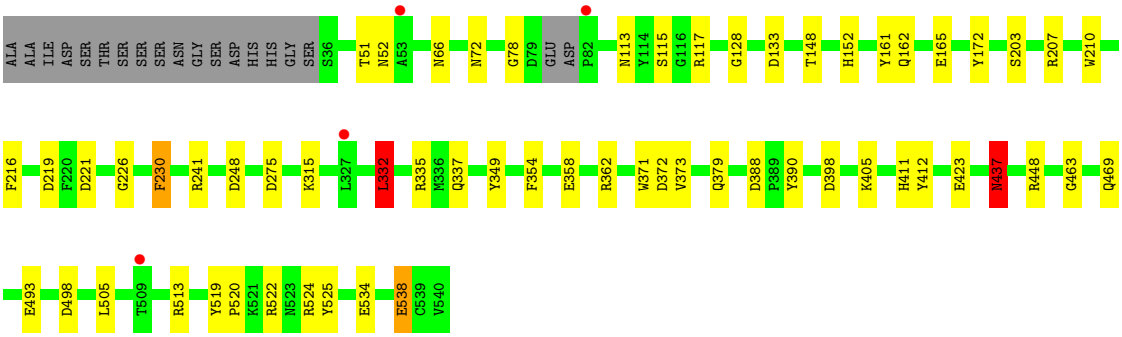
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	589	589	589	0	0
			Total	O		
4	B	498	498	498	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

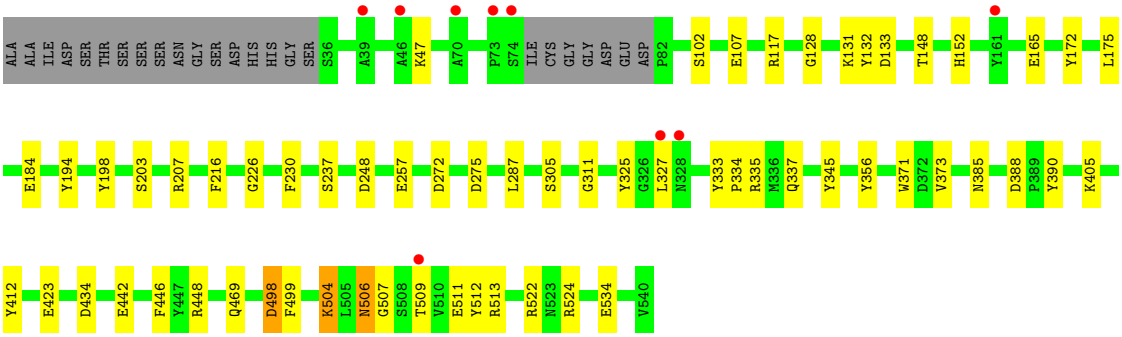
• Molecule 1: Probable feruloyl esterase B-1

Chain A:



• Molecule 1: Probable feruloyl esterase B-1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	93.95Å 142.94Å 73.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.73 – 1.50 35.73 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (35.73-1.50) 97.8 (35.73-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	6.86 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.141 , 0.168 0.141 , 0.168	Depositor DCC
R_{free} test set	7815 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	13.5	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8889	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.33	15/3962 (0.4%)	1.35	37/5392 (0.7%)
1	B	1.31	17/3932 (0.4%)	1.34	33/5352 (0.6%)
All	All	1.32	32/7894 (0.4%)	1.34	70/10744 (0.7%)

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	2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	TRP	CG-CD1	10.93	1.52	1.36
1	A	423	GLU	CD-OE2	-9.86	1.14	1.25
1	B	423	GLU	CD-OE2	-9.81	1.14	1.25
1	A	534	GLU	CD-OE2	-9.81	1.14	1.25
1	B	442	GLU	CD-OE2	8.90	1.35	1.25
1	B	237	SER	CB-OG	7.09	1.51	1.42
1	A	522	ARG	CD-NE	-6.94	1.34	1.46
1	A	538	GLU	CD-OE1	6.43	1.32	1.25
1	A	493	GLU	CG-CD	-6.27	1.42	1.51
1	B	165	GLU	CD-OE2	6.27	1.32	1.25
1	A	522	ARG	CZ-NH2	-5.99	1.25	1.33
1	A	358	GLU	CD-OE2	5.80	1.32	1.25
1	A	115	SER	CB-OG	5.79	1.49	1.42
1	A	463	GLY	N-CA	-5.70	1.37	1.46
1	B	216	PHE	CB-CG	-5.69	1.41	1.51
1	B	442	GLU	CD-OE1	-5.69	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	534	GLU	CD-OE2	-5.69	1.19	1.25
1	B	356	TYR	CE1-CZ	-5.58	1.31	1.38
1	A	354	PHE	CB-CG	-5.54	1.42	1.51
1	B	390	TYR	CE1-CZ	-5.54	1.31	1.38
1	B	498	ASP	CG-OD2	5.50	1.38	1.25
1	B	327	LEU	C-O	5.41	1.33	1.23
1	B	305	SER	CB-OG	5.38	1.49	1.42
1	B	184	GLU	CD-OE1	5.37	1.31	1.25
1	B	499	PHE	CB-CG	-5.32	1.42	1.51
1	A	165	GLU	CD-OE2	5.23	1.31	1.25
1	B	194	TYR	CE1-CZ	-5.21	1.31	1.38
1	B	345	TYR	CE2-CZ	-5.15	1.31	1.38
1	B	522	ARG	CD-NE	-5.12	1.37	1.46
1	A	538	GLU	CG-CD	5.09	1.59	1.51
1	A	379	GLN	CD-OE1	5.07	1.35	1.24
1	A	161	TYR	CG-CD1	-5.02	1.32	1.39

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	522	ARG	NE-CZ-NH2	-18.71	110.94	120.30
1	B	498	ASP	CB-CG-OD1	-16.04	103.86	118.30
1	A	522	ARG	NE-CZ-NH1	15.49	128.05	120.30
1	B	513	ARG	NE-CZ-NH1	12.77	126.68	120.30
1	A	513	ARG	NE-CZ-NH1	11.22	125.91	120.30
1	A	117	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	B	335	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	A	133	ASP	CB-CG-OD1	9.88	127.19	118.30
1	B	513	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	B	275	ASP	CB-CG-OD2	9.33	126.69	118.30
1	B	133	ASP	CB-CG-OD1	9.31	126.68	118.30
1	B	522	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	B	498	ASP	CB-CG-OD2	9.04	126.43	118.30
1	B	512	TYR	CB-CG-CD2	8.68	126.21	121.00
1	A	248	ASP	CB-CG-OD2	8.40	125.86	118.30
1	A	513	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	B	107	GLU	OE1-CD-OE2	8.08	133.00	123.30
1	A	133	ASP	CB-CG-OD2	-7.86	111.22	118.30
1	A	315	LYS	CD-CE-NZ	-7.86	93.61	111.70
1	A	388	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	B	325	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	A	117	ARG	NE-CZ-NH1	7.60	124.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	210	TRP	CG-CD1-NE1	-7.58	102.52	110.10
1	B	207	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	A	448	ARG	NE-CZ-NH1	-7.37	116.62	120.30
1	B	175	LEU	CB-CG-CD2	7.17	123.19	111.00
1	A	248	ASP	CB-CG-OD1	-7.13	111.89	118.30
1	A	207	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	B	442	GLU	OE1-CD-OE2	-7.01	114.89	123.30
1	B	272	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	B	504	LYS	CD-CE-NZ	-6.82	96.02	111.70
1	A	332	LEU	CB-CG-CD2	6.82	122.59	111.00
1	B	448	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	B	165	GLU	OE1-CD-OE2	-6.68	115.28	123.30
1	A	498	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	332	LEU	CB-CG-CD1	-6.57	99.84	111.00
1	B	117	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	335	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	499	PHE	CB-CG-CD2	-6.37	116.34	120.80
1	B	257	GLU	OE1-CD-OE2	6.35	130.92	123.30
1	B	325	TYR	OH-CZ-CE2	-6.27	103.16	120.10
1	A	275	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	524	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	230	PHE	CB-CG-CD2	-6.10	116.53	120.80
1	A	216	PHE	CB-CG-CD1	-5.90	116.67	120.80
1	A	398	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	390	TYR	CB-CG-CD2	5.88	124.53	121.00
1	A	423	GLU	CG-CD-OE2	-5.81	106.68	118.30
1	A	411	HIS	N-CA-CB	-5.73	100.28	110.60
1	B	194	TYR	CB-CG-CD1	-5.71	117.58	121.00
1	A	538	GLU	CG-CD-OE2	-5.54	107.23	118.30
1	B	446	PHE	CB-CG-CD1	-5.50	116.95	120.80
1	B	272	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	248	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	349	TYR	CB-CG-CD2	-5.44	117.74	121.00
1	A	362	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	B	133	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	388	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	A	372	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	198	TYR	CZ-CE2-CD2	5.34	124.61	119.80
1	A	388	ASP	OD1-CG-OD2	5.33	133.44	123.30
1	A	525	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	A	221	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	A	241	ARG	NE-CZ-NH2	-5.21	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	434	ASP	CB-CG-OD1	5.21	122.98	118.30
1	A	219	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	325	TYR	CD1-CE1-CZ	-5.16	115.15	119.80
1	A	241	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	B	287	LEU	CB-CG-CD1	5.07	119.62	111.00
1	B	132	TYR	CD1-CE1-CZ	5.02	124.32	119.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	437	ASN	Sidechain
1	A	538	GLU	Sidechain

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	3859	0	3595	24	0
1	B	3829	0	3573	11	0
2	A	70	0	64	15	0
2	B	42	0	38	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	589	0	0	4	0
4	B	498	0	0	4	0
All	All	8889	0	7270	37	0

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 2.

All (37) 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:332:LEU:HD11	2:A:603:NAG:H61	1.26	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HD11	2:A:603:NAG:C6	1.94	0.98
1:A:162:GLN:HA	2:A:605:NAG:H81	1.53	0.91
1:B:385:ASN:HB2	4:B:1182:HOH:O	1.86	0.75
1:A:332:LEU:HD12	2:A:603:NAG:O5	1.88	0.73
2:A:605:NAG:H3	2:A:605:NAG:H83	1.67	0.73
1:A:113:ASN:HB2	4:A:1049:HOH:O	1.91	0.70
1:A:332:LEU:CD1	2:A:603:NAG:O5	2.40	0.69
1:B:524:ARG:HD2	4:B:1060:HOH:O	1.97	0.64
1:A:162:GLN:HG2	2:A:605:NAG:H82	1.80	0.63
1:B:506:ASN:O	1:B:509:THR:HG22	1.98	0.63
1:B:131:LYS:HE2	4:B:1187:HOH:O	1.99	0.62
1:A:162:GLN:CA	2:A:605:NAG:H81	2.28	0.60
1:A:437:ASN:ND2	4:A:848:HOH:O	2.35	0.60
1:A:332:LEU:CD1	2:A:603:NAG:C6	2.77	0.60
1:A:162:GLN:HA	2:A:605:NAG:C8	2.32	0.54
1:A:226:GLY:HA3	1:A:412:TYR:CZ	2.46	0.50
2:A:605:NAG:H83	2:A:605:NAG:C3	2.39	0.48
1:A:162:GLN:HG2	2:A:605:NAG:C8	2.43	0.48
1:B:226:GLY:HA3	1:B:412:TYR:CZ	2.50	0.47
1:B:333:TYR:CG	1:B:334:PRO:HD2	2.50	0.47
1:A:51:THR:O	1:A:52:ASN:HB2	2.15	0.46
1:B:506:ASN:HB2	1:B:511:GLU:OE1	2.14	0.46
1:A:332:LEU:HD11	2:A:603:NAG:C5	2.45	0.46
1:A:72:ASN:O	1:A:78:GLY:HA2	2.17	0.45
1:B:102:SER:HB2	4:B:822:HOH:O	2.18	0.44
1:A:332:LEU:CD1	2:A:603:NAG:C5	2.96	0.43
1:B:371:TRP:CZ3	1:B:373:VAL:HA	2.54	0.42
1:B:128:GLY:HA2	1:B:152:HIS:O	2.20	0.42
1:A:128:GLY:HA2	1:A:152:HIS:O	2.20	0.42
1:A:332:LEU:HD12	1:A:332:LEU:HA	1.73	0.42
1:A:437:ASN:HD21	1:B:311:GLY:H	1.66	0.41
1:A:66:ASN:ND2	4:A:1028:HOH:O	2.53	0.41
1:A:371:TRP:CZ3	1:A:373:VAL:HA	2.55	0.41
2:A:605:NAG:H3	2:A:605:NAG:C8	2.44	0.40
1:A:505:LEU:CD1	4:A:1206:HOH:O	2.70	0.40
1:A:519:TYR:CG	1:A:520:PRO:HA	2.56	0.40

There are no symmetry-related clashes.

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	499/522 (96%)	485 (97%)	12 (2%)	2 (0%)	30 12
1	B	494/522 (95%)	479 (97%)	12 (2%)	3 (1%)	22 6
All	All	993/1044 (95%)	964 (97%)	24 (2%)	5 (0%)	25 8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	507	GLY
1	B	172	TYR
1	B	203	SER
1	A	172	TYR
1	A	203	SER

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	408/423 (96%)	401 (98%)	7 (2%)	56 29
1	B	405/423 (96%)	396 (98%)	9 (2%)	47 18
All	All	813/846 (96%)	797 (98%)	16 (2%)	50 22

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	THR

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Mol	Chain	Res	Type
1	A	230	PHE
1	A	332	LEU
1	A	337	GLN
1	A	405	LYS
1	A	437	ASN
1	A	469	GLN
1	B	47	LYS
1	B	148	THR
1	B	230	PHE
1	B	337	GLN
1	B	405	LYS
1	B	469	GLN
1	B	498	ASP
1	B	504	LYS
1	B	506	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	NAG	A	603	1	14,14,15	1.61	2 (14%)	17,19,21	1.53	3 (17%)
2	NAG	B	603	1	14,14,15	1.31	2 (14%)	17,19,21	1.81	5 (29%)
2	NAG	A	601	1	14,14,15	1.10	1 (7%)	17,19,21	1.27	2 (11%)
2	NAG	B	601	1	14,14,15	1.33	2 (14%)	17,19,21	2.77	5 (29%)
2	NAG	A	602	1	14,14,15	1.11	1 (7%)	17,19,21	3.25	3 (17%)
2	NAG	A	604	1	14,14,15	1.32	3 (21%)	17,19,21	2.03	4 (23%)
2	NAG	A	605	1	14,14,15	3.54	3 (21%)	17,19,21	1.30	3 (17%)
2	NAG	B	602	1	14,14,15	1.15	2 (14%)	17,19,21	1.49	1 (5%)

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	NAG	A	603	1	-	2/6/23/26	0/1/1/1
2	NAG	B	603	1	-	0/6/23/26	0/1/1/1
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1
2	NAG	B	601	1	-	4/6/23/26	0/1/1/1
2	NAG	A	602	1	-	2/6/23/26	0/1/1/1
2	NAG	A	604	1	-	0/6/23/26	0/1/1/1
2	NAG	A	605	1	-	3/6/23/26	0/1/1/1
2	NAG	B	602	1	-	1/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	NAG	C8-C7	-9.23	1.31	1.50
2	A	605	NAG	O7-C7	8.61	1.42	1.23
2	A	603	NAG	O5-C1	3.65	1.49	1.43
2	A	605	NAG	O5-C1	-3.46	1.37	1.43
2	B	603	NAG	O5-C5	-3.39	1.36	1.43
2	A	604	NAG	O5-C1	2.86	1.48	1.43
2	B	601	NAG	C8-C7	-2.76	1.44	1.50
2	A	603	NAG	C2-N2	2.49	1.50	1.46
2	B	602	NAG	C2-N2	2.45	1.50	1.46
2	A	604	NAG	O7-C7	2.24	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAG	O5-C1	2.17	1.47	1.43
2	B	601	NAG	O7-C7	2.09	1.27	1.23
2	B	603	NAG	O6-C6	-2.07	1.33	1.42
2	B	602	NAG	O4-C4	2.04	1.48	1.43
2	A	602	NAG	O7-C7	2.01	1.27	1.23
2	A	604	NAG	C2-N2	2.01	1.49	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	602	NAG	O7-C7-C8	-9.24	105.60	122.05
2	A	602	NAG	O7-C7-N2	8.75	137.44	121.98
2	B	601	NAG	C2-N2-C7	6.87	132.11	122.90
2	B	601	NAG	O7-C7-C8	-6.07	111.25	122.05
2	B	602	NAG	O5-C1-C2	-5.02	103.52	111.29
2	A	604	NAG	C1-C2-N2	-4.54	103.27	110.43
2	A	603	NAG	O5-C1-C2	-4.19	104.81	111.29
2	B	601	NAG	C8-C7-N2	4.08	122.88	116.12
2	A	604	NAG	O6-C6-C5	-4.03	97.61	111.33
2	B	601	NAG	O4-C4-C3	-3.57	101.97	110.38
2	A	604	NAG	O5-C1-C2	-3.44	105.97	111.29
2	A	603	NAG	O5-C5-C6	3.20	113.89	107.66
2	B	603	NAG	C4-C3-C2	-3.17	106.37	111.02
2	B	603	NAG	O5-C5-C4	-3.14	103.18	110.83
2	A	601	NAG	C3-C4-C5	3.00	115.68	110.23
2	B	603	NAG	O6-C6-C5	-2.83	101.69	111.33
2	B	603	NAG	C6-C5-C4	2.82	119.95	113.02
2	B	603	NAG	O5-C1-C2	-2.79	106.97	111.29
2	A	601	NAG	O5-C1-C2	-2.79	106.98	111.29
2	A	605	NAG	C4-C3-C2	-2.36	107.56	111.02
2	B	601	NAG	O7-C7-N2	2.20	125.86	121.98
2	A	604	NAG	C3-C4-C5	-2.16	106.31	110.23
2	A	603	NAG	C6-C5-C4	2.12	118.22	113.02
2	A	602	NAG	O3-C3-C4	-2.04	105.56	110.38
2	A	605	NAG	O7-C7-N2	-2.03	118.40	121.98
2	A	605	NAG	O6-C6-C5	-2.02	104.45	111.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	603	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	603	NAG	C4-C5-C6-O6
2	A	605	NAG	C8-C7-N2-C2
2	A	605	NAG	O7-C7-N2-C2
2	B	601	NAG	C8-C7-N2-C2
2	B	601	NAG	O7-C7-N2-C2
2	B	602	NAG	C4-C5-C6-O6
2	A	602	NAG	C3-C2-N2-C7
2	A	605	NAG	C3-C2-N2-C7
2	B	601	NAG	C3-C2-N2-C7
2	A	602	NAG	C1-C2-N2-C7
2	B	601	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	NAG	7	0
2	A	605	NAG	8	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	503/522 (96%)	-0.34	4 (0%)	82	86	8, 12, 26, 43	0
1	B	498/522 (95%)	-0.11	9 (1%)	67	70	9, 14, 30, 47	0
All	All	1001/1044 (95%)	-0.23	13 (1%)	74	77	8, 13, 29, 47	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	SER	3.0
1	B	46	ALA	2.9
1	B	327	LEU	2.9
1	A	82	PRO	2.6
1	B	39	ALA	2.6
1	A	327	LEU	2.6
1	A	509	THR	2.5
1	B	73	PRO	2.4
1	B	70	ALA	2.1
1	B	509	THR	2.1
1	A	53	ALA	2.0
1	B	161	TYR	2.0
1	B	328	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	NAG	A	601	14/15	0.83	0.12	25,32,38,38	0
2	NAG	A	603	14/15	0.85	0.10	20,23,27,28	0
2	NAG	B	602	14/15	0.86	0.10	19,23,28,29	0
2	NAG	B	601	14/15	0.92	0.08	18,22,31,37	0
2	NAG	A	604	14/15	0.95	0.07	14,17,23,26	0
2	NAG	A	605	14/15	0.95	0.06	8,12,20,23	0
2	NAG	A	602	14/15	0.96	0.08	12,18,30,30	0
2	NAG	B	603	14/15	0.96	0.06	12,16,22,26	0
3	CA	A	606	1/1	1.00	0.02	10,10,10,10	0
3	CA	B	604	1/1	1.00	0.02	10,10,10,10	0

6.5 Other polymers (i)

There are no such residues in this entry.