Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 02:12 AM EST

PDB ID	:	1WNO
Title	:	Crystal structure of a native chitinase from Aspergillus fumigatus YJ-407
Authors	:	Hu, H.; Wang, G.; Yang, H.; Zhou, J.; Mo, L.; Yang, K.; Jin, C.; Jin, C.; Rao, Z.
Deposited on	:	2004-08-07
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

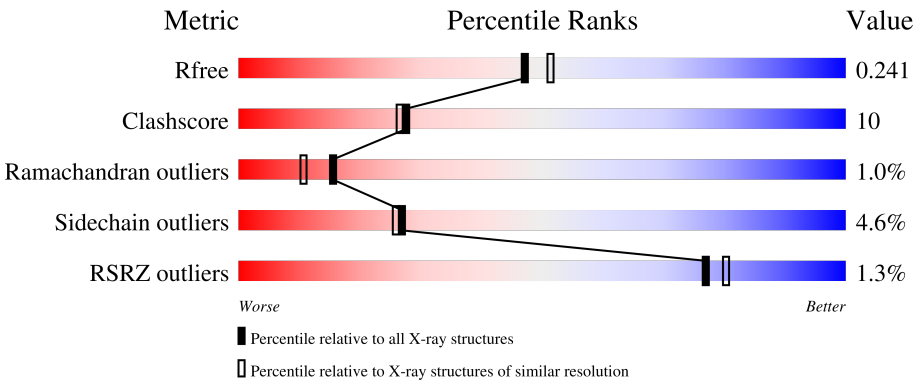
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

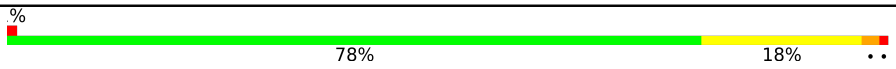
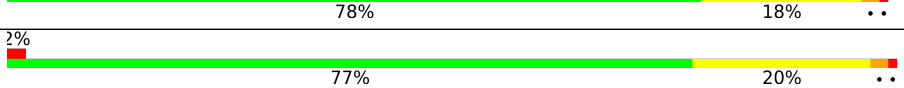
The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	395	
1	B	395	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6775 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.

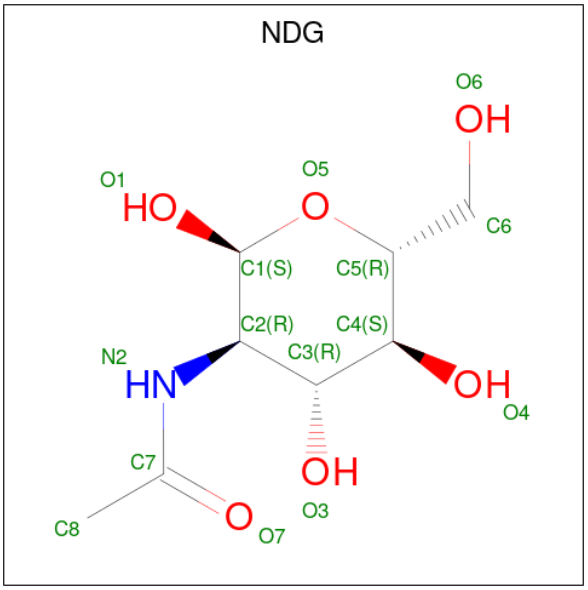
- Molecule 1 is a protein called Chitinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	394	3064	1943	516	597	8	0	0	0
1	B	394	3064	1943	516	597	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

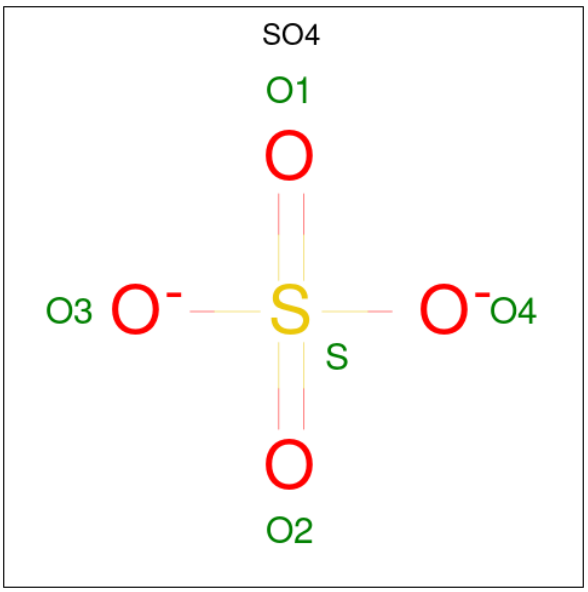
Chain	Residue	Modelled	Actual	Comment	Reference
A	49	TYR	HIS	conflict	UNP Q870C0
B	49	TYR	HIS	conflict	UNP Q870C0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	15	8	1	6	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

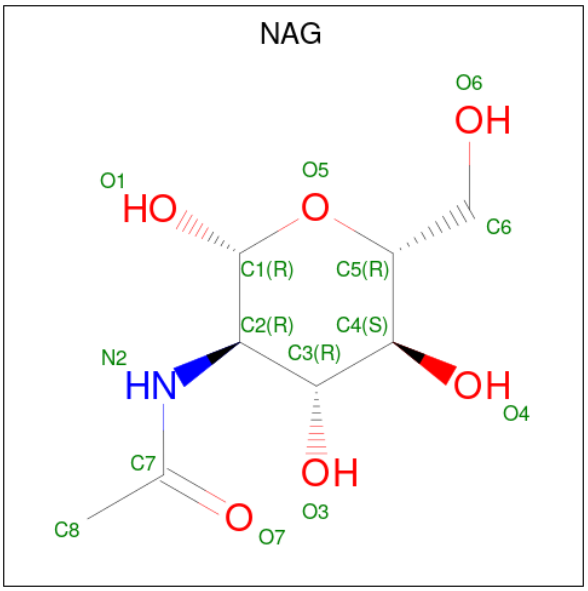


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0
			Total	Mg		
4	B	1	1	1	0	0

- Molecule 5 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		
5	B	1	15	8	1	6	0	0

- Molecule 6 is water.

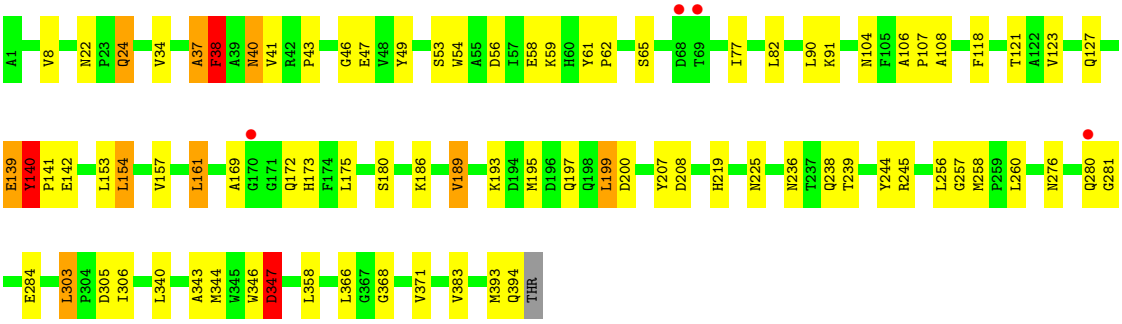
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	306	306	306	0	0
			Total	O		
6	B	279	279	279	0	0

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.

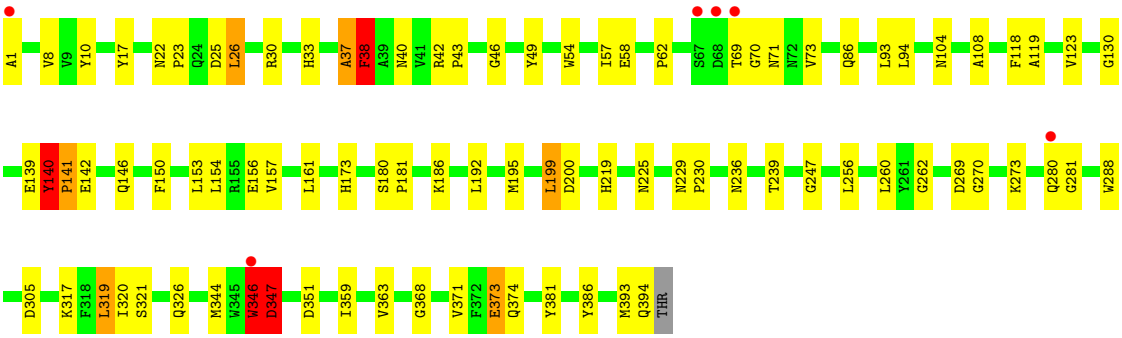
- Molecule 1: Chitinase

Chain A:



- Molecule 1: Chitinase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.68Å 100.46Å 134.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.10 33.54 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.00-2.10) 94.3 (33.54-2.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.245 0.219 , 0.241	Depositor DCC
R_{free} test set	6252 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å^2)	18.5	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 60.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6775	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: SO4, NAG, MG, NDG

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	0.57	8/3146 (0.3%)	0.89	20/4289 (0.5%)
1	B	0.54	7/3146 (0.2%)	0.86	21/4289 (0.5%)
All	All	0.56	15/6292 (0.2%)	0.88	41/8578 (0.5%)

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	3	2
1	B	2	1
All	All	5	3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	GLU	CB-CG	-10.68	1.31	1.52
1	A	37	ALA	CA-CB	9.92	1.73	1.52
1	B	140	TYR	C-N	9.87	1.52	1.34
1	B	37	ALA	C-O	8.78	1.40	1.23
1	A	38	PHE	N-CA	-8.24	1.29	1.46
1	B	140	TYR	C-O	7.99	1.38	1.23
1	A	347	ASP	CA-C	-7.65	1.33	1.52
1	A	140	TYR	C-N	7.16	1.47	1.34
1	B	38	PHE	C-O	7.08	1.36	1.23
1	B	141	PRO	N-CD	6.79	1.57	1.47
1	A	140	TYR	C-O	6.31	1.35	1.23
1	B	347	ASP	CA-CB	-5.21	1.42	1.53
1	B	140	TYR	N-CA	-5.13	1.36	1.46
1	A	141	PRO	N-CD	5.06	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	TYR	CA-C	-5.03	1.39	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	37	ALA	CA-C-N	-13.98	86.44	117.20
1	B	139	GLU	C-N-CA	12.19	152.16	121.70
1	B	37	ALA	C-N-CA	12.01	151.73	121.70
1	A	140	TYR	N-CA-C	11.63	142.40	111.00
1	A	37	ALA	C-N-CA	11.40	150.21	121.70
1	B	37	ALA	O-C-N	11.29	140.76	122.70
1	B	37	ALA	CA-C-N	-11.10	92.79	117.20
1	A	37	ALA	CA-C-O	10.54	142.24	120.10
1	A	347	ASP	CB-CG-OD2	-10.41	108.93	118.30
1	B	140	TYR	N-CA-C	9.26	136.00	111.00
1	A	346	TRP	CA-C-N	-9.14	97.10	117.20
1	A	346	TRP	C-N-CA	9.11	144.47	121.70
1	A	38	PHE	N-CA-C	9.05	135.43	111.00
1	A	139	GLU	C-N-CA	8.99	144.18	121.70
1	B	38	PHE	N-CA-C	8.33	133.49	111.00
1	B	38	PHE	CB-CG-CD2	8.04	126.43	120.80
1	A	347	ASP	N-CA-C	7.90	132.34	111.00
1	A	346	TRP	O-C-N	7.68	134.99	122.70
1	B	346	TRP	CA-C-N	-7.54	100.62	117.20
1	A	347	ASP	CB-CA-C	7.48	125.36	110.40
1	A	139	GLU	CA-C-N	-6.78	102.28	117.20
1	B	346	TRP	C-N-CA	6.78	138.65	121.70
1	B	347	ASP	N-CA-C	6.69	129.05	111.00
1	A	347	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	139	GLU	CB-CA-C	6.58	123.57	110.40
1	B	38	PHE	CB-CG-CD1	-6.50	116.25	120.80
1	A	346	TRP	CA-CB-CG	6.21	125.51	113.70
1	B	37	ALA	N-CA-C	6.08	127.41	111.00
1	A	140	TYR	C-N-CD	6.06	141.12	128.40
1	B	347	ASP	CB-CA-C	6.06	122.52	110.40
1	B	140	TYR	O-C-N	6.06	132.61	121.10
1	B	139	GLU	CA-C-N	-6.00	104.00	117.20
1	B	38	PHE	CA-C-N	-5.85	104.34	117.20
1	B	37	ALA	N-CA-CB	5.82	118.25	110.10
1	B	141	PRO	CA-N-CD	-5.52	103.77	111.50
1	B	346	TRP	O-C-N	5.46	131.44	122.70
1	A	140	TYR	O-C-N	5.31	131.18	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	139	GLU	O-C-N	5.25	131.11	122.70
1	B	38	PHE	O-C-N	5.17	130.97	122.70
1	B	347	ASP	CA-C-N	-5.17	105.84	117.20
1	A	37	ALA	O-C-N	5.03	130.75	122.70

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	139	GLU	CA
1	A	140	TYR	CA
1	A	347	ASP	CA
1	B	140	TYR	CA
1	B	347	ASP	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	GLU	Mainchain
1	A	347	ASP	Sidechain
1	B	346	TRP	Mainchain

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	3064	0	2909	63	0
1	B	3064	0	2908	64	0
2	A	15	0	12	4	0
3	A	15	0	0	1	0
3	B	15	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	15	0	15	2	0
6	A	306	0	0	2	0
6	B	279	0	0	7	0
All	All	6775	0	5844	120	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 10.

All (120) 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:40:ASN:HD22	1:A:41:VAL:H	1.23	0.84
1:A:40:ASN:ND2	1:A:41:VAL:H	1.77	0.82
1:A:37:ALA:HB1	1:A:38:PHE:CG	2.16	0.79
1:B:37:ALA:HB1	1:B:38:PHE:CG	2.19	0.78
1:B:173:HIS:HE1	1:B:200:ASP:OD2	1.67	0.76
1:A:106:ALA:HB3	1:A:107:PRO:HD3	1.67	0.75
1:A:53:SER:O	1:A:58:GLU:HG2	1.90	0.72
1:B:326:GLN:HG3	6:B:3469:HOH:O	1.90	0.70
1:A:225:ASN:HD21	2:A:1042:NDG:C1	2.06	0.68
1:A:40:ASN:HD22	1:A:41:VAL:N	1.91	0.68
1:B:43:PRO:HG3	1:B:104:ASN:OD1	1.93	0.68
1:B:23:PRO:O	1:B:26:LEU:HB2	1.95	0.67
1:A:281:GLY:HA3	1:A:284:GLU:O	1.96	0.66
1:A:225:ASN:ND2	2:A:1042:NDG:N2	2.47	0.63
1:B:140:TYR:CE2	1:B:181:PRO:HB3	2.34	0.62
1:A:37:ALA:HB1	1:A:38:PHE:CD1	2.35	0.62
1:B:8:VAL:O	1:B:344:MET:HA	1.98	0.62
1:A:225:ASN:ND2	2:A:1042:NDG:O1	2.26	0.61
1:B:319:LEU:HD13	1:B:320:ILE:N	2.15	0.61
1:A:82:LEU:HB3	1:B:62:PRO:HB2	1.82	0.61
1:A:236:ASN:ND2	1:A:239:THR:H	1.99	0.60
1:A:54:TRP:HA	1:A:58:GLU:HG3	1.84	0.60
1:A:173:HIS:HE1	1:A:200:ASP:OD1	1.83	0.60
1:A:24:GLN:NE2	6:A:1709:HOH:O	2.35	0.59
1:B:186:LYS:HE2	6:B:3611:HOH:O	2.01	0.59
1:A:37:ALA:HB1	1:A:38:PHE:CD2	2.37	0.59
1:B:54:TRP:HA	1:B:58:GLU:HB2	1.84	0.58
1:B:393:MET:O	1:B:394:GLN:HB2	2.03	0.57
1:B:373:GLU:HG2	1:B:374:GLN:N	2.19	0.57
1:A:140:TYR:O	1:A:142:GLU:HG3	2.05	0.56
1:B:57:ILE:HB	1:B:73:VAL:HG23	1.87	0.56
1:A:153:LEU:O	1:A:157:VAL:HG23	2.06	0.55
1:B:142:GLU:H	1:B:146:GLN:NE2	2.04	0.55
1:B:195:MET:O	1:B:199:LEU:HD22	2.06	0.54
1:B:140:TYR:CD1	1:B:186:LYS:HE3	2.42	0.54
1:B:37:ALA:HB1	1:B:38:PHE:CD1	2.43	0.54
1:A:47:GLU:HG3	1:A:121:THR:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLN:HE22	1:A:245:ARG:HH22	1.55	0.54
1:A:8:VAL:O	1:A:344:MET:HA	2.09	0.53
1:B:46:GLY:O	1:B:118:PHE:HA	2.09	0.53
1:B:317:LYS:HE2	6:B:3621:HOH:O	2.08	0.53
1:A:40:ASN:HD21	1:A:104:ASN:HD22	1.55	0.52
1:A:62:PRO:N	1:B:86:GLN:HE22	2.07	0.52
1:B:37:ALA:HB1	1:B:38:PHE:CD2	2.44	0.52
1:B:1:ALA:HA	1:B:374:GLN:O	2.10	0.52
1:A:43:PRO:HG3	1:A:104:ASN:OD1	2.09	0.51
1:A:46:GLY:HA2	1:A:108:ALA:HB1	1.93	0.51
1:A:169:ALA:HB1	1:A:172:GLN:HB3	1.92	0.50
1:A:62:PRO:HA	1:B:86:GLN:HE21	1.77	0.50
1:B:73:VAL:HB	1:B:386:TYR:CG	2.47	0.50
1:A:40:ASN:ND2	1:A:41:VAL:N	2.52	0.50
1:A:303:LEU:HD23	1:A:306:ILE:HD11	1.93	0.50
1:A:186:LYS:O	1:A:189:VAL:HG13	2.11	0.50
1:B:368:GLY:O	1:B:371:VAL:HG22	2.12	0.50
1:B:393:MET:O	1:B:394:GLN:CB	2.60	0.50
1:A:46:GLY:O	1:A:118:PHE:HA	2.12	0.49
1:B:30:ARG:HB3	1:B:363:VAL:HG21	1.94	0.49
1:B:141:PRO:HA	1:B:146:GLN:HE21	1.77	0.49
1:B:305:ASP:HB2	6:B:3636:HOH:O	2.12	0.49
1:A:40:ASN:HB3	1:A:49:TYR:CZ	2.48	0.49
1:A:123:VAL:HG22	1:A:161:LEU:HD13	1.96	0.48
1:A:154:LEU:HG	1:A:199:LEU:HD11	1.96	0.48
1:B:269:ASP:HB3	1:B:273:LYS:HG2	1.96	0.48
1:B:22:ASN:O	1:B:25:ASP:HB2	2.14	0.48
1:B:69:THR:HG22	1:B:70:GLY:N	2.29	0.47
1:A:393:MET:O	1:A:394:GLN:HB2	2.15	0.47
1:A:305:ASP:OD1	3:A:1214:SO4:S	2.72	0.47
1:B:40:ASN:HB3	1:B:49:TYR:CZ	2.50	0.47
1:B:260:LEU:HD13	1:B:351:ASP:HB2	1.97	0.47
1:B:229:ASN:N	1:B:230:PRO:HD3	2.29	0.47
1:A:65:SER:HB2	1:B:394:GLN:HG2	1.97	0.46
1:B:236:ASN:ND2	1:B:239:THR:H	2.13	0.46
1:A:260:LEU:HD23	1:A:358:LEU:HD12	1.98	0.46
1:B:270:GLY:O	1:B:273:LYS:HB2	2.15	0.46
1:B:173:HIS:HD2	6:B:3552:HOH:O	1.98	0.45
1:B:262:GLY:HA2	1:B:321:SER:O	2.16	0.45
1:A:56:ASP:O	1:A:77:ILE:HG12	2.16	0.45
1:A:22:ASN:ND2	1:A:61:TYR:OH	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:GLY:HA2	1:B:108:ALA:HB1	1.98	0.45
1:A:195:MET:O	1:A:199:LEU:HD13	2.17	0.44
1:B:71:ASN:O	1:B:386:TYR:HA	2.17	0.44
1:A:368:GLY:O	1:A:371:VAL:HG22	2.18	0.44
1:B:225:ASN:CG	5:B:2042:NAG:O1	2.57	0.43
1:A:54:TRP:HA	1:A:58:GLU:CG	2.46	0.43
1:B:141:PRO:HA	1:B:146:GLN:NE2	2.32	0.43
1:A:225:ASN:ND2	2:A:1042:NDG:C7	2.82	0.43
1:B:141:PRO:HD2	6:B:3521:HOH:O	2.18	0.43
1:A:258:MET:CE	1:A:343:ALA:HB1	2.48	0.43
1:B:8:VAL:HG22	1:B:33:HIS:HB2	2.01	0.43
1:A:394:GLN:HE21	1:A:394:GLN:HA	1.83	0.43
1:A:34:VAL:HG23	1:A:90:LEU:HD11	2.01	0.43
1:A:65:SER:CB	1:B:394:GLN:HG2	2.48	0.43
1:B:140:TYR:CE1	1:B:186:LYS:HE3	2.54	0.43
1:A:180:SER:HB2	1:A:244:TYR:OH	2.19	0.43
1:A:127:GLN:HG3	1:A:383:VAL:HG23	2.00	0.42
1:A:257:GLY:HA2	1:A:344:MET:HB3	2.01	0.42
1:A:193:LYS:O	1:A:197:GLN:HG2	2.19	0.42
1:A:62:PRO:CA	1:B:86:GLN:NE2	2.83	0.42
1:A:207:TYR:O	1:A:208:ASP:HB2	2.20	0.42
1:B:130:GLY:HA2	1:B:381:TYR:CZ	2.54	0.42
1:B:225:ASN:OD1	5:B:2042:NAG:O1	2.37	0.42
1:B:281:GLY:HA2	1:B:288:TRP:CE2	2.55	0.42
1:A:59:LYS:HD3	1:A:61:TYR:CE1	2.55	0.41
1:B:153:LEU:O	1:B:157:VAL:HG23	2.20	0.41
1:B:119:ALA:O	1:B:123:VAL:HG23	2.21	0.41
1:A:140:TYR:CE1	1:A:186:LYS:HD3	2.55	0.41
1:B:130:GLY:HA2	1:B:381:TYR:CE2	2.55	0.41
1:B:219:HIS:HE1	6:B:3480:HOH:O	2.03	0.41
1:B:359:ILE:O	1:B:363:VAL:HG23	2.20	0.41
1:B:93:LEU:HD12	1:B:93:LEU:N	2.36	0.41
1:A:62:PRO:HG3	1:B:86:GLN:NE2	2.35	0.41
1:A:236:ASN:HD21	1:A:239:THR:H	1.68	0.41
1:A:118:PHE:CD1	1:A:153:LEU:HD11	2.56	0.41
1:B:10:TYR:CB	1:B:346:TRP:HE3	2.33	0.40
1:A:303:LEU:HB3	1:A:306:ILE:HG12	2.03	0.40
1:B:192:LEU:HD12	1:B:247:GLY:HA3	2.03	0.40
1:A:154:LEU:HD12	1:A:154:LEU:HA	1.97	0.40
1:A:219:HIS:HD2	6:A:1615:HOH:O	2.03	0.40
1:B:10:TYR:HB2	1:B:346:TRP:HE3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ARG:HA	1:B:43:PRO:HD3	1.92	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	392/395 (99%)	380 (97%)	9 (2%)	3 (1%)	19 15
1	B	392/395 (99%)	376 (96%)	11 (3%)	5 (1%)	12 7
All	All	784/790 (99%)	756 (96%)	20 (3%)	8 (1%)	15 11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	PHE
1	B	38	PHE
1	A	140	TYR
1	A	347	ASP
1	B	140	TYR
1	B	347	ASP
1	B	17	TYR
1	B	280	GLN

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	324/326 (99%)	307 (95%)	17 (5%)	23	21
1	B	324/326 (99%)	311 (96%)	13 (4%)	31	32
All	All	648/652 (99%)	618 (95%)	30 (5%)	27	26

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	38	PHE
1	A	40	ASN
1	A	91	LYS
1	A	140	TYR
1	A	154	LEU
1	A	161	LEU
1	A	175	LEU
1	A	189	VAL
1	A	199	LEU
1	A	256	LEU
1	A	276	ASN
1	A	280	GLN
1	A	303	LEU
1	A	340	LEU
1	A	347	ASP
1	A	366	LEU
1	B	26	LEU
1	B	94	LEU
1	B	140	TYR
1	B	150	PHE
1	B	154	LEU
1	B	156	GLU
1	B	161	LEU
1	B	180	SER
1	B	199	LEU
1	B	256	LEU
1	B	319	LEU
1	B	347	ASP
1	B	373	GLU

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

Mol	Chain	Res	Type
1	A	22	ASN
1	A	24	GLN
1	A	33	HIS
1	A	40	ASN
1	A	172	GLN
1	A	173	HIS
1	A	191	HIS
1	A	203	ASN
1	A	219	HIS
1	A	225	ASN
1	A	236	ASN
1	A	276	ASN
1	A	285	ASN
1	A	364	ASN
1	A	394	GLN
1	B	33	HIS
1	B	86	GLN
1	B	146	GLN
1	B	148	ASN
1	B	173	HIS
1	B	219	HIS
1	B	229	ASN
1	B	236	ASN
1	B	316	ASN
1	B	391	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 monosaccharides 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	NDG	A	1042	-	15,15,15	0.50	0	21,21,21	0.71	1 (4%)
3	SO4	A	1212	-	4,4,4	0.65	0	6,6,6	0.20	0
3	SO4	A	1213	-	4,4,4	0.64	0	6,6,6	0.25	0
3	SO4	B	2213	-	4,4,4	0.62	0	6,6,6	0.21	0
3	SO4	B	2214	-	4,4,4	0.66	0	6,6,6	0.22	0
3	SO4	B	2212	-	4,4,4	0.68	0	6,6,6	0.22	0
5	NAG	B	2042	-	15,15,15	0.45	0	21,21,21	0.63	0
3	SO4	A	1214	-	4,4,4	0.68	0	6,6,6	0.23	0

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	NDG	A	1042	-	-	4/6/26/26	0/1/1/1
5	NAG	B	2042	-	-	2/6/26/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1042	NDG	O5-C1-C2	2.08	111.61	109.52

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1042	NDG	O7-C7-N2-C2
2	A	1042	NDG	C8-C7-N2-C2
5	B	2042	NAG	O5-C5-C6-O6
2	A	1042	NDG	O5-C5-C6-O6
5	B	2042	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	1042	NDG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1042	NDG	4	0
5	B	2042	NAG	2	0
3	A	1214	SO4	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	394/395 (99%)	-0.32	4 (1%)	82	85	12, 19, 31, 53	0
1	B	394/395 (99%)	-0.26	6 (1%)	73	77	13, 21, 33, 52	0
All	All	788/790 (99%)	-0.29	10 (1%)	77	80	12, 20, 32, 53	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	GLY	5.1
1	B	69	THR	4.6
1	A	68	ASP	4.3
1	A	280	GLN	3.9
1	B	1	ALA	3.2
1	A	69	THR	3.0
1	B	280	GLN	2.8
1	B	67	SER	2.8
1	B	68	ASP	2.4
1	B	346	TRP	2.3

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
4	MG	B	3439	1/1	0.58	0.13	41,41,41,41	0
3	SO4	B	2212	5/5	0.63	0.23	79,79,80,81	0
2	NDG	A	1042	15/15	0.65	0.24	52,55,57,58	0
5	NAG	B	2042	15/15	0.70	0.26	57,59,60,61	0
3	SO4	B	2214	5/5	0.74	0.20	79,79,80,81	0
3	SO4	B	2213	5/5	0.77	0.31	78,78,78,79	0
3	SO4	A	1214	5/5	0.81	0.19	68,69,70,70	0
3	SO4	A	1213	5/5	0.81	0.23	78,79,79,79	0
4	MG	A	1439	1/1	0.84	0.24	39,39,39,39	0
3	SO4	A	1212	5/5	0.87	0.17	72,72,72,73	0

6.5 Other polymers (i)

There are no such residues in this entry.