Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 10:45 am GMT

PDB ID	:	1DWG
Title	:	STUDY ON RADIATION DAMAGE ON A CRYOCOOLED CRYSTAL: PART 3 STRUCTURE AFTER IRRADIATION WITH 18.2*10E15 PHOTONS/MM2.
Authors	:	Burmeister, W.P.
Deposited on	:	1999-12-05
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
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:

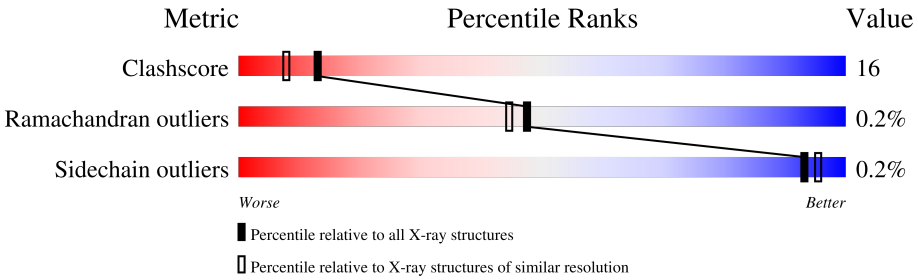
MolProbity	:	4.02b-467
Mogul	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (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 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	M	499	81% 16% .
2	A	2	50% 50%
2	D	2	50% 50%
3	B	5	100%
4	C	7	71% 29%

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
4	BMA	C	3	-	-	X	-
4	MAN	C	6	X	-	X	-
5	NAG	M	905	-	-	X	-
5	NAG	M	918	X	-	-	-
7	SO4	M	925	-	-	X	-
7	SO4	M	926	-	-	X	-
7	SO4	M	931	-	-	X	-
8	GOL	M	932	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5217 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 MYROSINASE MA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	M	499	4080	2616	660	788	16	0	20	0

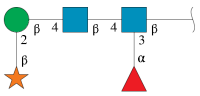
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	497	THR	SER	SEE REMARK 999	UNP P29736

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	A	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-xylopyranose-(1-2)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.

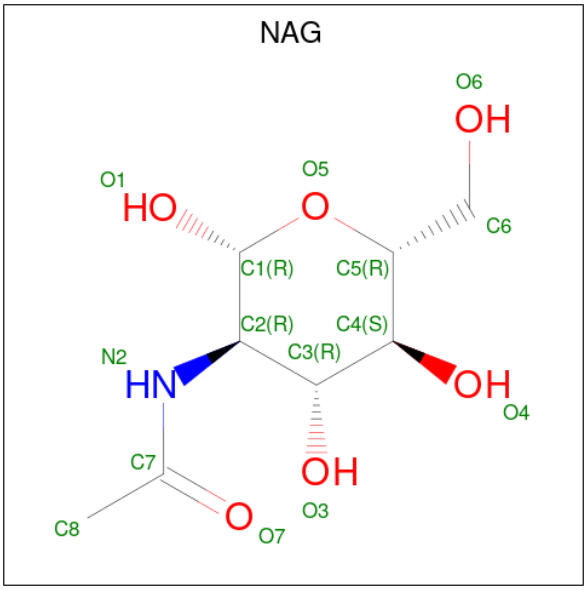


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	B	5	Total C N O 58 33 2 23	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)][alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	C	7	Total C N O 80 45 2 33	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

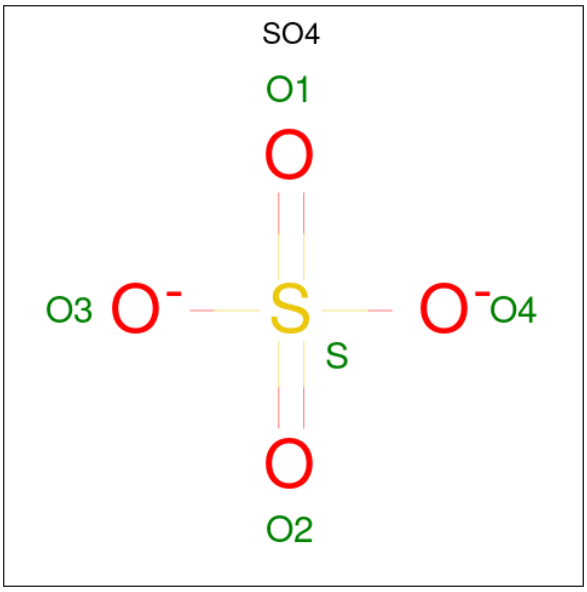


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total C N O 14 8 1 5	0	0
5	M	1	Total C N O 14 8 1 5	0	0
5	M	1	Total C N O 14 8 1 5	0	0
5	M	1	Total C N O 14 8 1 5	0	0
5	M	1	Total C N O 14 8 1 5	0	0
5	M	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

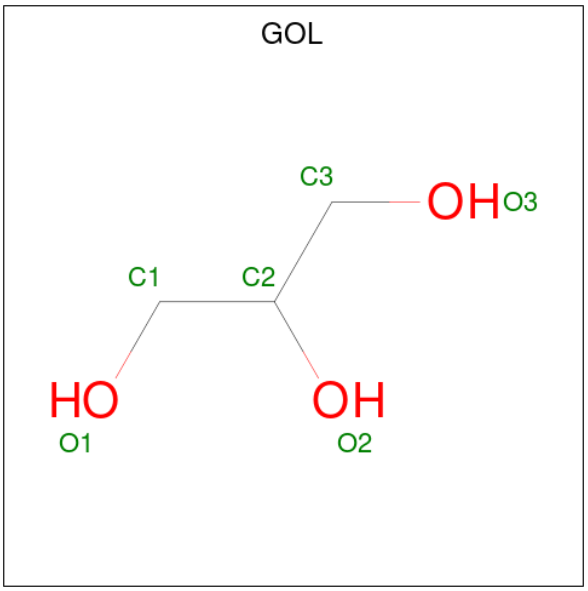
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	M	1	Total Zn 1 1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total C O 6 3 3	0	0
8	M	1	Total C O 6 3 3	0	0
8	M	1	Total C O 6 3 3	0	0
8	M	1	Total C O 6 3 3	0	0
8	M	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	788	Total O 788 788	0	0

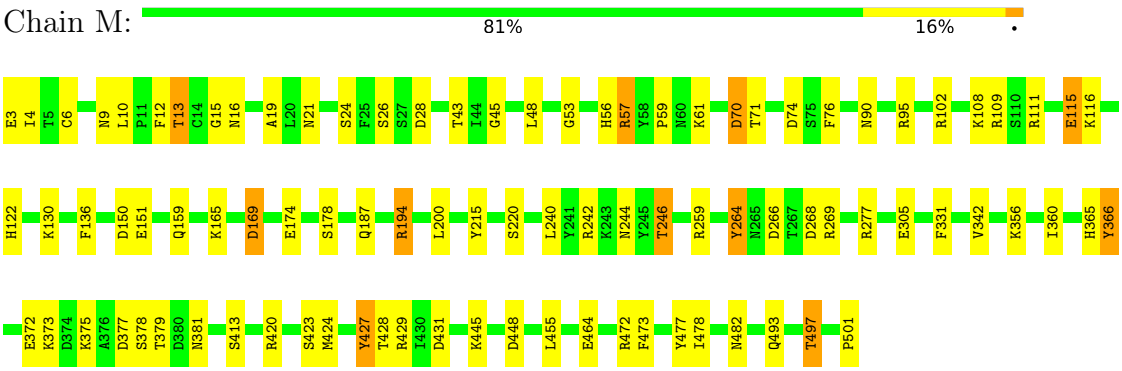
3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

• Molecule 1: MYROSINASE MA1

Chain M:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

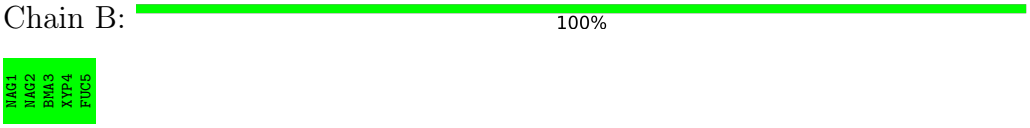
Chain A:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

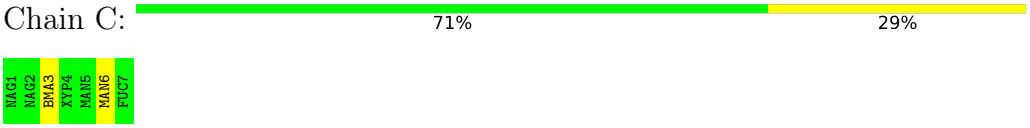
• Molecule 3: beta-D-xylopyranose-(1-2)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



• Molecule 4: beta-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)][alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	134.30Å 136.40Å 80.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.8 (15.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	5.22 (at 1.99Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.184 , 0.193	Depositor
Wilson B-factor (Å^2)	19.4	Xtriage
Anisotropy	0.084	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
Total number of atoms	5217	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 5.20% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, XYP, GOL, FUC, ZN, NAG, MAN, BMA

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	M	1.15	18/4283 (0.4%)	1.32	41/5824 (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	M	0	1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	264	TYR	CE1-CZ	-21.78	1.10	1.38
1	M	264	TYR	CZ-OH	20.20	1.72	1.37
1	M	16	ASN	CG-ND2	12.66	1.64	1.32
1	M	356	LYS	CE-NZ	-11.08	1.21	1.49
1	M	423	SER	CB-OG	9.83	1.55	1.42
1	M	13	THR	C-O	-9.72	1.04	1.23
1	M	6	CYS	CB-SG	-9.15	1.66	1.82
1	M	178	SER	CB-OG	8.91	1.53	1.42
1	M	501	PRO	CA-C	7.25	1.67	1.52
1	M	24	SER	CB-OG	7.00	1.51	1.42
1	M	115	GLU	CD-OE2	6.86	1.33	1.25
1	M	26	SER	CB-OG	5.51	1.49	1.42
1	M	413	SER	CB-OG	-5.36	1.35	1.42
1	M	246	THR	CB-CG2	-5.35	1.34	1.52
1	M	61	LYS	CD-CE	-5.18	1.38	1.51
1	M	501	PRO	N-CD	5.17	1.55	1.47
1	M	242	ARG	NE-CZ	5.11	1.39	1.33
1	M	464	GLU	CG-CD	-5.06	1.44	1.51

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	448	ASP	CB-CG-OD2	-18.65	101.51	118.30
1	M	115	GLU	OE1-CD-OE2	-15.25	105.00	123.30
1	M	264	TYR	CZ-CE2-CD2	-12.25	108.77	119.80
1	M	264	TYR	CE1-CZ-CE2	11.60	138.36	119.80
1	M	109	ARG	NE-CZ-NH1	-11.36	114.62	120.30
1	M	269	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	M	372	GLU	OE1-CD-OE2	-10.19	111.07	123.30
1	M	169[A]	ASP	CB-CG-OD2	-9.73	109.55	118.30
1	M	169[B]	ASP	CB-CG-OD2	-9.73	109.55	118.30
1	M	194	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	M	242	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	M	268	ASP	CB-CG-OD1	8.74	126.17	118.30
1	M	269	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	M	266	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	M	74	ASP	CB-CG-OD1	7.91	125.42	118.30
1	M	427	TYR	CG-CD1-CE1	-7.74	115.11	121.30
1	M	448	ASP	OD1-CG-OD2	7.70	137.92	123.30
1	M	264	TYR	OH-CZ-CE2	-7.51	99.82	120.10
1	M	264	TYR	CD1-CE1-CZ	-6.94	113.55	119.80
1	M	372	GLU	CG-CD-OE2	6.55	131.39	118.30
1	M	109	ARG	NH1-CZ-NH2	6.45	126.50	119.40
1	M	246	THR	OG1-CB-CG2	-6.39	95.31	110.00
1	M	482	ASN	CB-CG-OD1	6.24	134.09	121.60
1	M	76	PHE	CB-CG-CD1	-6.10	116.53	120.80
1	M	482	ASN	CA-CB-CG	-6.03	100.13	113.40
1	M	194	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	M	70	ASP	CB-CG-OD1	5.82	123.54	118.30
1	M	377	ASP	O-C-N	-5.62	113.70	122.70
1	M	497	THR	OG1-CB-CG2	-5.55	97.24	110.00
1	M	102	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	M	420	ARG	CD-NE-CZ	5.51	131.31	123.60
1	M	429	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	M	420	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	M	277	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	M	427	TYR	CZ-CE2-CD2	-5.34	114.99	119.80
1	M	19	ALA	CB-CA-C	-5.24	102.24	110.10
1	M	366[A]	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	M	366[B]	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	M	57	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	M	473	PHE	CB-CG-CD2	5.14	124.40	120.80
1	M	478	ILE	CB-CG1-CD1	5.08	128.13	113.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	13	THR	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	M	4080	0	3828	108	4
2	A	28	0	24	3	0
2	D	28	0	25	1	0
3	B	58	0	42	0	0
4	C	80	0	58	9	0
5	M	84	0	77	21	0
6	M	1	0	0	0	1
7	M	40	0	0	10	0
8	M	30	0	39	4	0
9	M	788	0	0	78	13
All	All	5217	0	4093	139	17

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 16.

All (139) 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:M:244:ASN:HD21	5:M:905:NAG:C1	0.96	1.56
1:M:90:ASN:ND2	5:M:902:NAG:C1	1.72	1.53
1:M:21:ASN:HD21	5:M:901:NAG:C1	0.90	1.52
1:M:244:ASN:ND2	5:M:905:NAG:C1	1.77	1.46
1:M:264:TYR:OH	1:M:264:TYR:CZ	1.72	1.42
1:M:21:ASN:ND2	5:M:901:NAG:C1	1.75	1.42
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:CZ	1.57	1.37
8:M:932:GOL:C1	9:M:1011:HOH:O	1.71	1.34
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CZ	2.14	1.30
1:M:15:GLY:HA3	9:M:1077:HOH:O	1.25	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:427:TYR:HE2	9:M:1022:HOH:O	1.19	1.25
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:OH	1.33	1.24
1:M:428:THR:HG23	9:M:1109:HOH:O	1.27	1.24
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CE2	2.22	1.23
2:A:1:NAG:C3	2:A:1:NAG:O3	1.89	1.19
1:M:477:TYR:HE1	9:M:1021:HOH:O	1.21	1.18
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:CE2	1.78	1.17
1:M:431:ASP:OD1	9:M:1004:HOH:O	1.66	1.10
1:M:477:TYR:CE1	9:M:1021:HOH:O	1.94	1.08
8:M:932:GOL:H11	9:M:1011:HOH:O	1.27	1.08
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CE2	2.33	1.07
1:M:215:TYR:O	9:M:1005:HOH:O	1.69	1.07
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CD2	1.92	1.05
8:M:932:GOL:C2	9:M:1011:HOH:O	1.91	1.04
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:OH	2.03	1.03
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CE2	1.91	1.02
1:M:427:TYR:CE2	9:M:1022:HOH:O	1.95	1.01
7:M:926:SO4:O2	7:M:931:SO4:S	2.19	1.00
1:M:165:LYS:NZ	5:M:905:NAG:H82	1.76	0.99
5:M:918:NAG:H61	9:M:1622:HOH:O	1.62	0.98
1:M:259:ARG:HG2	9:M:1061:HOH:O	1.64	0.96
1:M:472:ARG:CZ	9:M:1021:HOH:O	2.12	0.95
1:M:246:THR:HG22	9:M:1309:HOH:O	1.66	0.94
1:M:150:ASP:OD2	9:M:1007:HOH:O	1.88	0.91
1:M:379:THR:HG23	9:M:1573:HOH:O	1.71	0.90
1:M:53:GLY:O	9:M:1008:HOH:O	1.90	0.89
4:C:3:BMA:H61	4:C:6:MAN:C6	2.03	0.89
7:M:926:SO4:O2	7:M:931:SO4:O2	1.91	0.88
1:M:130:LYS:HB3	9:M:1579:HOH:O	1.72	0.88
4:C:3:BMA:H61	4:C:6:MAN:H61	1.55	0.88
1:M:215:TYR:HB2	9:M:1478:HOH:O	1.72	0.86
1:M:165:LYS:HZ1	5:M:905:NAG:H82	1.34	0.86
1:M:130:LYS:HG3	9:M:1387:HOH:O	1.76	0.84
1:M:15:GLY:CA	9:M:1077:HOH:O	1.93	0.84
1:M:21:ASN:HD21	5:M:901:NAG:C2	1.88	0.83
1:M:151:GLU:OE1	9:M:1009:HOH:O	1.97	0.82
4:C:3:BMA:C6	4:C:6:MAN:H61	2.11	0.81
1:M:381:ASN:ND2	9:M:1018:HOH:O	2.14	0.79
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CD2	2.61	0.78
7:M:931:SO4:O1	9:M:1010:HOH:O	2.00	0.78
1:M:70:ASP:HB3	9:M:1540:HOH:O	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:1578:HOH:O	2:D:2:NAG:H83	1.86	0.76
4:C:3:BMA:C6	4:C:6:MAN:C6	2.65	0.74
1:M:373:LYS:NZ	9:M:1018:HOH:O	2.21	0.74
1:M:130:LYS:HB3	9:M:1675:HOH:O	1.87	0.74
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:CZ	2.22	0.74
1:M:90:ASN:ND2	5:M:902:NAG:C2	2.53	0.72
1:M:264:TYR:OH	1:M:264:TYR:CE2	2.42	0.71
1:M:360[B]:ILE:HG13	1:M:366[B]:TYR:CE2	2.24	0.71
1:M:9:ASN:HB2	9:M:1497:HOH:O	1.91	0.70
1:M:116:LYS:HG2	9:M:1452:HOH:O	1.92	0.70
9:M:1013:HOH:O	2:A:1:NAG:O3	2.10	0.70
1:M:472:ARG:NE	9:M:1021:HOH:O	2.20	0.70
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CZ	2.67	0.69
1:M:493:GLN:NE2	9:M:1024:HOH:O	2.24	0.69
7:M:926:SO4:S	7:M:931:SO4:O3	2.51	0.68
1:M:45:GLY:HA2	9:M:1180:HOH:O	1.93	0.68
1:M:70:ASP:OD2	9:M:1014:HOH:O	2.11	0.68
7:M:925:SO4:O2	9:M:1016:HOH:O	2.14	0.66
1:M:115:GLU:HG3	9:M:1020:HOH:O	1.95	0.66
4:C:3:BMA:H61	4:C:6:MAN:H62	1.76	0.66
1:M:111:ARG:O	9:M:1017:HOH:O	2.14	0.66
1:M:71:THR:HG23	9:M:1651:HOH:O	1.94	0.65
1:M:169[B]:ASP:HB2	1:M:240:LEU:HD21	1.78	0.65
1:M:472:ARG:NH2	9:M:1021:HOH:O	2.26	0.65
1:M:220[A]:SER:OG	9:M:1019:HOH:O	2.15	0.64
1:M:4:ILE:HD11	1:M:445:LYS:HD2	1.80	0.64
7:M:925:SO4:O4	9:M:1016:HOH:O	2.16	0.63
1:M:200:LEU:HB3	9:M:1222:HOH:O	1.98	0.63
7:M:926:SO4:O2	7:M:931:SO4:O3	2.15	0.63
8:M:932:GOL:O2	9:M:1011:HOH:O	2.01	0.61
7:M:926:SO4:O1	7:M:931:SO4:O3	2.20	0.60
1:M:365:HIS:HE1	9:M:1216:HOH:O	1.83	0.60
1:M:342[A]:VAL:HG13	9:M:1019:HOH:O	2.02	0.60
7:M:926:SO4:S	7:M:931:SO4:S	3.00	0.59
1:M:45:GLY:HA2	9:M:1079:HOH:O	2.03	0.58
1:M:159:GLN:NE2	9:M:1034:HOH:O	2.36	0.58
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CZ	2.33	0.58
1:M:115:GLU:CD	9:M:1020:HOH:O	2.42	0.58
1:M:90:ASN:ND2	5:M:902:NAG:O5	2.36	0.58
1:M:115:GLU:OE2	9:M:1020:HOH:O	2.17	0.57
1:M:21:ASN:CG	5:M:901:NAG:C1	2.67	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CG	2.40	0.56
1:M:424:MET:HE3	9:M:1024:HOH:O	2.05	0.56
1:M:194:ARG:NH1	7:M:931:SO4:O4	2.40	0.55
1:M:331:PHE:CD1	9:M:1061:HOH:O	2.53	0.55
1:M:165:LYS:HZ2	5:M:905:NAG:H82	1.67	0.55
9:M:1006:HOH:O	4:C:3:BMA:C6	2.47	0.55
1:M:21:ASN:ND2	5:M:901:NAG:C2	2.58	0.54
1:M:90:ASN:CG	5:M:902:NAG:C1	2.68	0.52
1:M:4:ILE:HD11	1:M:445:LYS:CD	2.39	0.52
1:M:244:ASN:HD21	5:M:905:NAG:C2	1.98	0.52
9:M:1023:HOH:O	4:C:6:MAN:C4	2.58	0.52
1:M:472:ARG:HG2	9:M:1445:HOH:O	2.11	0.51
2:A:1:NAG:O3	2:A:1:NAG:C2	2.56	0.51
1:M:21:ASN:ND2	5:M:901:NAG:O5	2.40	0.51
1:M:130:LYS:CB	9:M:1579:HOH:O	2.43	0.51
1:M:28:ASP:HA	9:M:1604:HOH:O	2.10	0.51
1:M:115:GLU:CG	9:M:1020:HOH:O	2.56	0.50
1:M:360[A]:ILE:HG23	9:M:1628:HOH:O	2.10	0.50
1:M:10:LEU:HD23	9:M:1025:HOH:O	2.12	0.49
1:M:108:LYS:HD2	9:M:1124:HOH:O	2.12	0.49
1:M:15:GLY:C	9:M:1077:HOH:O	2.34	0.48
1:M:70:ASP:CB	9:M:1540:HOH:O	2.51	0.48
1:M:360[A]:ILE:CG2	9:M:1628:HOH:O	2.61	0.48
1:M:95:ARG:HA	1:M:136:PHE:O	2.14	0.47
1:M:59:PRO:HB3	9:M:1228:HOH:O	2.14	0.47
9:M:1023:HOH:O	4:C:6:MAN:C5	2.62	0.47
4:C:3:BMA:O6	4:C:6:MAN:C6	2.49	0.46
1:M:12:PHE:HD2	9:M:1025:HOH:O	2.00	0.45
1:M:165:LYS:CE	5:M:905:NAG:H82	2.46	0.45
1:M:373:LYS:NZ	1:M:378:SER:OG	2.46	0.44
1:M:45:GLY:CA	9:M:1180:HOH:O	2.57	0.44
1:M:122:HIS:HE1	1:M:174:GLU:O	1.99	0.44
1:M:95:ARG:HB2	1:M:455:LEU:HD13	2.00	0.43
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:OH	2.05	0.43
1:M:497:THR:HG23	9:M:1584:HOH:O	2.19	0.42
1:M:59:PRO:HG3	9:M:1640:HOH:O	2.19	0.42
1:M:244:ASN:ND2	5:M:905:NAG:O5	2.42	0.42
1:M:4:ILE:CD1	1:M:445:LYS:HD2	2.49	0.42
1:M:12:PHE:N	9:M:1025:HOH:O	2.26	0.42
5:M:918:NAG:C6	9:M:1622:HOH:O	2.41	0.41
1:M:244:ASN:ND2	5:M:905:NAG:C2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:48:LEU:N	9:M:1032:HOH:O	2.35	0.40
1:M:111:ARG:C	9:M:1017:HOH:O	2.58	0.40

All (17) 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)
6:M:923:ZN:ZN	6:M:923:ZN:ZN[3_656]	1.10	1.10
9:M:1009:HOH:O	9:M:1009:HOH:O[3_656]	1.10	1.10
9:M:1720:HOH:O	9:M:1720:HOH:O[4_576]	1.42	0.78
9:M:1576:HOH:O	9:M:1576:HOH:O[4_576]	1.44	0.76
9:M:1174:HOH:O	9:M:1174:HOH:O[4_576]	1.63	0.57
9:M:1663:HOH:O	9:M:1663:HOH:O[4_576]	1.63	0.57
9:M:1046:HOH:O	9:M:1075:HOH:O[6_564]	1.71	0.49
9:M:1436:HOH:O	9:M:1629:HOH:O[3_656]	1.76	0.44
1:M:45:GLY:N	1:M:57:ARG:O[3_656]	1.95	0.25
9:M:1330:HOH:O	9:M:1461:HOH:O[4_576]	2.01	0.19
1:M:375:LYS:O	1:M:375:LYS:CD[4_576]	2.04	0.16
9:M:1496:HOH:O	9:M:1620:HOH:O[6_564]	2.06	0.14
1:M:379:THR:CG2	9:M:1108:HOH:O[4_576]	2.07	0.13
9:M:1174:HOH:O	9:M:1519:HOH:O[4_576]	2.08	0.12
1:M:43:THR:OG1	1:M:56:HIS:O[3_656]	2.10	0.10
9:M:1180:HOH:O	9:M:1555:HOH:O[3_656]	2.12	0.08
9:M:1497:HOH:O	9:M:1497:HOH:O[4_576]	2.12	0.08

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	M	517/499 (104%)	503 (97%)	13 (2%)	1 (0%)	47 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	187	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	M	455/435 (105%)	454 (100%)	1 (0%)	93 95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	3	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	244	ASN
1	M	365	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

Mogul failed to run properly - this section is therefore empty.

5.5 Carbohydrates (i)

Mogul failed to run properly - this section is therefore empty.

5.6 Ligand geometry (i)

Mogul failed to run properly - this section is therefore empty.

5.7 Other polymers (i)

Mogul failed to run properly - this section is therefore empty.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.