



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 05:10 AM BST

PDB ID : 3AIW
Title : Crystal structure of beta-glucosidase in rye complexed with 2-deoxy-2-fluorog
lucoside and dinitrophenol
Authors : Sue, M.; Nakamura, C.; Miyamoto, T.; Yajima, S.
Deposited on : 2010-05-18
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

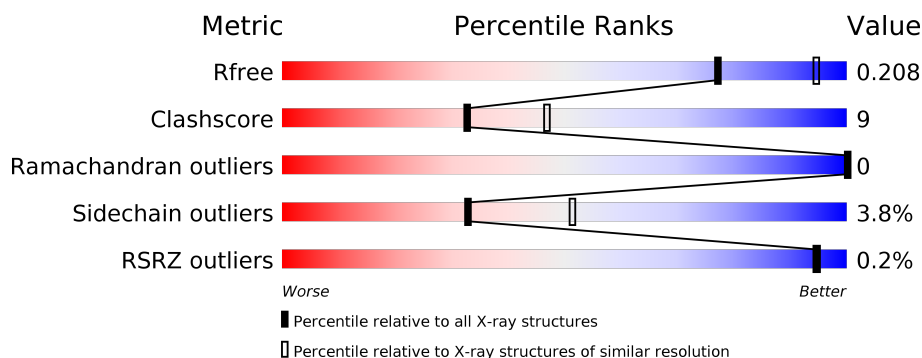
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	564	 66% 16% •• 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4340 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 Beta-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3932	2517	651	745	19			

There are 47 discrepancies between the modelled and reference sequences:

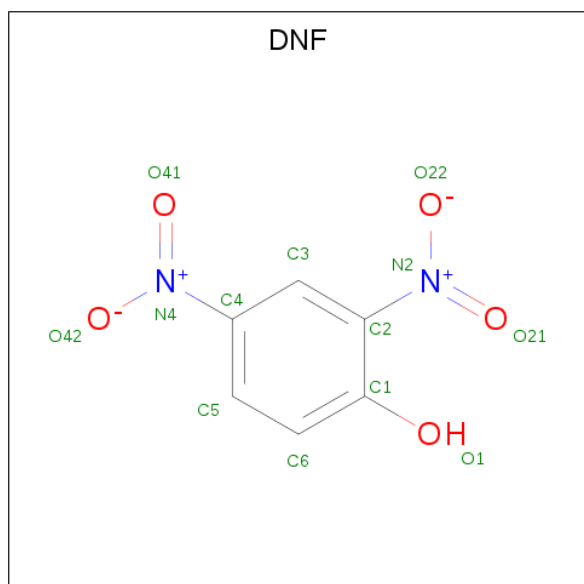
Chain	Residue	Modelled	Actual	Comment	Reference
A	-44	MET	-	expression tag	UNP Q9FYS3
A	-43	HIS	-	expression tag	UNP Q9FYS3
A	-42	HIS	-	expression tag	UNP Q9FYS3
A	-41	HIS	-	expression tag	UNP Q9FYS3
A	-40	HIS	-	expression tag	UNP Q9FYS3
A	-39	HIS	-	expression tag	UNP Q9FYS3
A	-38	HIS	-	expression tag	UNP Q9FYS3
A	-37	SER	-	expression tag	UNP Q9FYS3
A	-36	SER	-	expression tag	UNP Q9FYS3
A	-35	GLY	-	expression tag	UNP Q9FYS3
A	-34	LEU	-	expression tag	UNP Q9FYS3
A	-33	VAL	-	expression tag	UNP Q9FYS3
A	-32	PRO	-	expression tag	UNP Q9FYS3
A	-31	ARG	-	expression tag	UNP Q9FYS3
A	-30	GLY	-	expression tag	UNP Q9FYS3
A	-29	SER	-	expression tag	UNP Q9FYS3
A	-28	GLY	-	expression tag	UNP Q9FYS3
A	-27	MET	-	expression tag	UNP Q9FYS3
A	-26	LYS	-	expression tag	UNP Q9FYS3
A	-25	GLU	-	expression tag	UNP Q9FYS3
A	-24	THR	-	expression tag	UNP Q9FYS3
A	-23	ALA	-	expression tag	UNP Q9FYS3
A	-22	ALA	-	expression tag	UNP Q9FYS3
A	-21	ALA	-	expression tag	UNP Q9FYS3
A	-20	LYS	-	expression tag	UNP Q9FYS3
A	-19	PHE	-	expression tag	UNP Q9FYS3
A	-18	GLU	-	expression tag	UNP Q9FYS3

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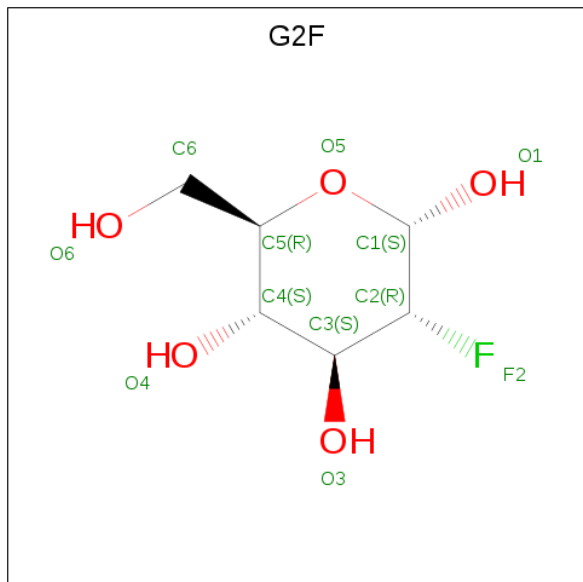
Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	ARG	-	expression tag	UNP Q9FYS3
A	-16	GLN	-	expression tag	UNP Q9FYS3
A	-15	HIS	-	expression tag	UNP Q9FYS3
A	-14	MET	-	expression tag	UNP Q9FYS3
A	-13	ASP	-	expression tag	UNP Q9FYS3
A	-12	SER	-	expression tag	UNP Q9FYS3
A	-11	PRO	-	expression tag	UNP Q9FYS3
A	-10	ASP	-	expression tag	UNP Q9FYS3
A	-9	LEU	-	expression tag	UNP Q9FYS3
A	-8	GLY	-	expression tag	UNP Q9FYS3
A	-7	THR	-	expression tag	UNP Q9FYS3
A	-6	ASP	-	expression tag	UNP Q9FYS3
A	-5	ASP	-	expression tag	UNP Q9FYS3
A	-4	ASP	-	expression tag	UNP Q9FYS3
A	-3	ASP	-	expression tag	UNP Q9FYS3
A	-2	LYS	-	expression tag	UNP Q9FYS3
A	-1	ALA	-	expression tag	UNP Q9FYS3
A	0	MET	-	expression tag	UNP Q9FYS3
A	323	ALA	GLY	SEE REMARK 999	UNP Q9FYS3
A	325	SER	LEU	SEE REMARK 999	UNP Q9FYS3

- Molecule 2 is 2,4-DINITROPHENOL (three-letter code: DNF) (formula: C₆H₄N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			26	12	4	10		

- Molecule 3 is 2-deoxy-2-fluoro- α -D-glucopyranose (three-letter code: G2F) (formula: $C_6H_{11}FO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	O	0	0
			11	6	1	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	371	Total	O	0	0
			371	371		

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.

- Chain A: 66% 16% .. 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	194.69 Å 194.69 Å 194.69 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 52.03 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.40) 100.0 (52.03-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.53 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.186 , 0.212 0.183 , 0.208	Depositor DCC
R_{free} test set	2516 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4340	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: G2F, DNF

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	1.72	70/4055 (1.7%)	1.14	19/5498 (0.3%)

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	LYS	CD-CE	11.29	1.79	1.51
1	A	488	LYS	CE-NZ	10.25	1.74	1.49
1	A	147	ASP	CB-CG	-9.81	1.31	1.51
1	A	317	GLU	CD-OE2	9.69	1.36	1.25
1	A	317	GLU	CG-CD	9.65	1.66	1.51
1	A	31	LYS	CD-CE	9.34	1.74	1.51
1	A	370	GLU	CD-OE1	8.75	1.35	1.25
1	A	86	GLU	CG-CD	8.71	1.65	1.51
1	A	418	GLU	CD-OE2	8.17	1.34	1.25
1	A	251	LYS	CE-NZ	8.04	1.69	1.49
1	A	93	LYS	CD-CE	7.89	1.71	1.51
1	A	320	GLU	CG-CD	7.78	1.63	1.51
1	A	396	GLU	CD-OE2	7.67	1.34	1.25
1	A	317	GLU	CD-OE1	7.51	1.33	1.25
1	A	25	LYS	CE-NZ	7.47	1.67	1.49
1	A	396	GLU	CG-CD	7.13	1.62	1.51
1	A	246	LYS	CD-CE	7.01	1.68	1.51
1	A	370	GLU	CG-CD	6.93	1.62	1.51
1	A	67	GLU	CG-CD	6.92	1.62	1.51
1	A	14	VAL	CB-CG1	6.87	1.67	1.52
1	A	120	LYS	CE-NZ	6.76	1.66	1.49
1	A	93	LYS	CE-NZ	6.74	1.65	1.49
1	A	251	LYS	N-CA	6.52	1.59	1.46
1	A	383	TYR	CG-CD2	6.35	1.47	1.39
1	A	170	TYR	CG-CD2	6.19	1.47	1.39
1	A	317	GLU	CB-CG	6.15	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	LYS	CG-CD	6.01	1.72	1.52
1	A	168	TYR	CD1-CE1	-5.99	1.30	1.39
1	A	81	SER	CA-CB	5.90	1.61	1.52
1	A	292	GLU	CB-CG	5.85	1.63	1.52
1	A	200	TYR	CD1-CE1	5.83	1.48	1.39
1	A	134	ARG	CG-CD	5.79	1.66	1.51
1	A	398	TYR	CZ-OH	5.79	1.47	1.37
1	A	384	PRO	CG-CD	5.78	1.69	1.50
1	A	170	TYR	CE1-CZ	5.74	1.46	1.38
1	A	61	PHE	CD1-CE1	5.74	1.50	1.39
1	A	462	GLU	CD-OE1	5.71	1.31	1.25
1	A	418	GLU	CD-OE1	5.71	1.31	1.25
1	A	396	GLU	CB-CG	5.66	1.62	1.52
1	A	170	TYR	CE2-CZ	5.65	1.46	1.38
1	A	58	TRP	CG-CD1	5.63	1.44	1.36
1	A	189	PHE	CE1-CZ	5.62	1.48	1.37
1	A	295	VAL	CB-CG2	5.47	1.64	1.52
1	A	147	ASP	CA-CB	5.45	1.66	1.53
1	A	156	TYR	CE2-CZ	5.44	1.45	1.38
1	A	461	PHE	CE1-CZ	5.43	1.47	1.37
1	A	31	LYS	CE-NZ	5.42	1.62	1.49
1	A	56	SER	CB-OG	5.41	1.49	1.42
1	A	42	TYR	CG-CD1	5.41	1.46	1.39
1	A	86	GLU	CD-OE2	5.40	1.31	1.25
1	A	414	GLU	CG-CD	5.35	1.59	1.51
1	A	269	TYR	CG-CD1	5.32	1.46	1.39
1	A	378	TYR	CG-CD1	5.31	1.46	1.39
1	A	329	MET	CG-SD	-5.29	1.67	1.81
1	A	342	VAL	CB-CG1	5.28	1.64	1.52
1	A	98	LYS	CE-NZ	5.27	1.62	1.49
1	A	48	TRP	CZ3-CH2	5.26	1.48	1.40
1	A	418	GLU	CG-CD	5.18	1.59	1.51
1	A	263	VAL	CB-CG1	5.15	1.63	1.52
1	A	383	TYR	CE1-CZ	5.14	1.45	1.38
1	A	156	TYR	CG-CD1	5.13	1.45	1.39
1	A	165	VAL	CA-CB	5.12	1.65	1.54
1	A	269	TYR	CE2-CZ	5.11	1.45	1.38
1	A	134	ARG	NE-CZ	5.11	1.39	1.33
1	A	36	GLY	CA-C	5.10	1.60	1.51
1	A	220	GLU	CB-CG	5.08	1.61	1.52
1	A	184	LYS	CD-CE	5.07	1.64	1.51
1	A	120	LYS	CD-CE	5.06	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	398	TYR	CE1-CZ	5.05	1.45	1.38
1	A	87	GLU	CB-CG	5.05	1.61	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ARG	NE-CZ-NH2	-21.39	109.61	120.30
1	A	279	ARG	NE-CZ-NH1	17.86	129.23	120.30
1	A	101	ARG	NE-CZ-NH2	-14.55	113.03	120.30
1	A	147	ASP	CB-CG-OD1	-13.86	105.83	118.30
1	A	147	ASP	N-CA-CB	-8.08	96.06	110.60
1	A	182	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	182	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	279	ARG	CG-CD-NE	-6.83	97.47	111.80
1	A	251	LYS	CB-CA-C	-6.64	97.12	110.40
1	A	147	ASP	CB-CG-OD2	6.44	124.10	118.30
1	A	279	ARG	CD-NE-CZ	6.24	132.34	123.60
1	A	298	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	70	SER	N-CA-CB	-5.72	101.92	110.50
1	A	254	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	27	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	A	337	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	101	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	480	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	14	VAL	CB-CA-C	-5.05	101.81	111.40

There are no chirality outliers.

There are no planarity outliers.

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	3932	0	3693	66	0
2	A	26	0	7	1	0
3	A	11	0	9	0	0
4	A	371	0	0	12	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4340	0	3709	67	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 9.

All (67) 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:25:LYS:CD	1:A:25:LYS:CE	1.79	1.60
1:A:25:LYS:NZ	1:A:25:LYS:CE	1.67	1.56
1:A:251:LYS:NZ	1:A:251:LYS:CE	1.69	1.56
1:A:31:LYS:CE	1:A:31:LYS:CD	1.74	1.55
1:A:488:LYS:CE	1:A:488:LYS:NZ	1.74	1.47
1:A:364:THR:HB	4:A:880:HOH:O	1.38	1.20
1:A:162:LYS:HB2	4:A:828:HOH:O	1.57	1.04
1:A:126:ASN:ND2	1:A:182:ARG:HH22	1.61	0.97
1:A:126:ASN:HD22	1:A:182:ARG:HH22	1.04	0.93
1:A:60:HIS:O	1:A:64:THR:HG23	1.73	0.87
1:A:188:THR:HG23	1:A:257:ILE:HD11	1.63	0.80
1:A:74:ASN:HD22	1:A:76:ASP:H	1.32	0.78
1:A:74:ASN:ND2	1:A:76:ASP:H	1.83	0.77
1:A:170:TYR:HD1	4:A:822:HOH:O	1.68	0.76
1:A:313:MET:HE3	4:A:667:HOH:O	1.85	0.75
1:A:364:THR:CB	4:A:880:HOH:O	2.08	0.75
1:A:245:PHE:HZ	1:A:255:SER:HB3	1.58	0.68
1:A:364:THR:HG22	1:A:370:GLU:HG2	1.75	0.67
1:A:232:HIS:HD2	1:A:299:TYR:OH	1.78	0.66
1:A:181:ASP:OD2	1:A:182:ARG:HD3	1.95	0.66
1:A:159:PHE:O	1:A:233:HIS:HD2	1.79	0.66
1:A:126:ASN:HD22	1:A:182:ARG:NH2	1.87	0.64
1:A:162:LYS:HG2	1:A:233:HIS:CE1	2.34	0.63
1:A:397:LYS:HE2	1:A:398:TYR:CZ	2.34	0.62
1:A:266:TYR:O	1:A:279:ARG:HD2	1.99	0.62
1:A:19:LYS:NZ	4:A:563:HOH:O	2.26	0.60
1:A:251:LYS:NZ	1:A:251:LYS:CD	2.62	0.59
1:A:60:HIS:O	1:A:64:THR:CG2	2.51	0.58
1:A:315:THR:OG1	1:A:317:GLU:HG3	2.05	0.56
1:A:162:LYS:HE3	1:A:233:HIS:HE1	1.71	0.55
1:A:349:THR:HG22	4:A:862:HOH:O	2.06	0.55
1:A:341:HIS:HE1	1:A:343:ASP:OD1	1.88	0.55
1:A:101:ARG:NH2	1:A:190:ASN:OD1	2.29	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLY:HA2	1:A:149:PRO:HG2	1.91	0.53
1:A:281:ARG:HH22	1:A:341:HIS:HD2	1.56	0.53
1:A:78:ALA:HA	1:A:467:TYR:OH	2.10	0.52
1:A:257:ILE:HD13	1:A:258:GLY:N	2.25	0.52
1:A:232:HIS:CD2	1:A:299:TYR:OH	2.62	0.51
1:A:313:MET:CE	4:A:667:HOH:O	2.51	0.49
1:A:479:GLU:HG3	4:A:818:HOH:O	2.13	0.49
1:A:349:THR:HG22	1:A:350:PRO:HD2	1.94	0.49
1:A:364:THR:HG22	1:A:370:GLU:CG	2.43	0.48
1:A:317:GLU:HG2	4:A:813:HOH:O	2.14	0.47
1:A:101:ARG:HA	1:A:140:TYR:O	2.14	0.47
1:A:374:ILE:HG22	1:A:376:GLY:H	1.78	0.47
1:A:159:PHE:O	1:A:233:HIS:CD2	2.66	0.46
1:A:93:LYS:HE2	1:A:93:LYS:HB3	1.73	0.46
1:A:392:LEU:HA	1:A:392:LEU:HD13	1.83	0.46
1:A:162:LYS:HG2	1:A:233:HIS:HE1	1.80	0.46
1:A:106:TRP:HB2	4:A:666:HOH:O	2.17	0.45
1:A:74:ASN:HD22	1:A:74:ASN:C	2.20	0.45
2:A:800[A]:DNF:O21	2:A:800[A]:DNF:O1	2.34	0.45
1:A:462:GLU:HG3	1:A:462:GLU:O	2.16	0.44
1:A:109:ILE:HD13	1:A:122:ILE:CG1	2.47	0.44
1:A:190:ASN:ND2	1:A:191:GLU:HG3	2.33	0.44
1:A:258:GLY:HA3	1:A:328:ILE:O	2.18	0.43
1:A:495:LYS:HB3	1:A:495:LYS:HE2	1.53	0.43
1:A:188:THR:CG2	1:A:257:ILE:HD11	2.42	0.43
1:A:482:ASN:HD22	1:A:482:ASN:HA	1.68	0.42
1:A:162:LYS:HE3	1:A:233:HIS:CE1	2.54	0.42
1:A:483:LYS:HD2	1:A:485:LYS:HE2	2.00	0.42
1:A:455:TRP:HA	1:A:456:GLY:HA2	1.84	0.42
1:A:126:ASN:ND2	1:A:182:ARG:NH2	2.46	0.41
1:A:31:LYS:CG	1:A:31:LYS:CE	2.88	0.41
1:A:215:ASP:OD1	1:A:215:ASP:C	2.59	0.41
1:A:317:GLU:CG	4:A:813:HOH:O	2.69	0.41
1:A:186:TRP:HB2	1:A:257:ILE:HG12	2.04	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)
4:A:854:HOH:O	4:A:899:HOH:O 24_444	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:893:HOH:O	4:A:899:HOH:O[24_444]	2.09	0.11
4:A:566:HOH:O	4:A:639:HOH:O[12_455]	2.10	0.10

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	484/564 (86%)	466 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	418/483 (86%)	402 (96%)	16 (4%)	33	51

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

Mol	Chain	Res	Type
1	A	31	LYS
1	A	64	THR
1	A	70	SER
1	A	74	ASN
1	A	77	VAL
1	A	109	ILE

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Mol	Chain	Res	Type
1	A	114	THR
1	A	182	ARG
1	A	212	PRO
1	A	218	VAL
1	A	257	ILE
1	A	317	GLU
1	A	331	LEU
1	A	349	THR
1	A	419	MET
1	A	495	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	119	GLN
1	A	126	ASN
1	A	127	ASN
1	A	145	HIS
1	A	166	ASN
1	A	232	HIS
1	A	233	HIS
1	A	341	HIS
1	A	369	ASN
1	A	482	ASN
1	A	497	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

3 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	DNF	A	800[B]	-	11,13,13	4.54	4 (36%)	12,18,18	1.31	2 (16%)
2	DNF	A	800[A]	-	11,13,13	4.62	4 (36%)	12,18,18	2.46	6 (50%)
3	G2F	A	700	1	11,11,12	2.11	1 (9%)	10,15,17	1.38	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	DNF	A	800[B]	-	-	0/4/8/8	0/1/1/1
2	DNF	A	800[A]	-	-	0/4/8/8	0/1/1/1
3	G2F	A	700	1	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800[B]	DNF	O41-N4	10.64	1.40	1.22
2	A	800[A]	DNF	O41-N4	9.49	1.38	1.22
2	A	800[A]	DNF	O21-N2	9.16	1.38	1.22
2	A	800[B]	DNF	O21-N2	7.22	1.35	1.22
3	A	700	G2F	C2-C3	6.42	1.60	1.51
2	A	800[B]	DNF	C2-N2	-5.71	1.35	1.45
2	A	800[A]	DNF	C2-N2	-5.36	1.35	1.45
2	A	800[A]	DNF	C4-N4	-5.02	1.33	1.45
2	A	800[B]	DNF	C4-N4	-4.66	1.34	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	800[A]	DNF	C3-C4-N4	-4.79	114.52	118.75
2	A	800[A]	DNF	C5-C6-C1	-3.71	116.69	120.50
2	A	800[A]	DNF	C5-C4-N4	3.20	121.78	119.38
2	A	800[A]	DNF	C6-C1-C2	2.85	122.78	118.95
2	A	800[A]	DNF	C5-C4-C3	2.82	123.67	120.09
2	A	800[B]	DNF	C5-C4-C3	2.56	123.33	120.09
2	A	800[B]	DNF	C6-C5-C4	-2.46	116.66	120.08
2	A	800[A]	DNF	C4-C3-C2	-2.00	116.63	119.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800[A]	DNF	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	486/564 (86%)	-0.83	1 (0%) 95 94	13, 22, 37, 55	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	ASP	2.5

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	DNF	A	800[B]	13/13	0.89	0.30	25,29,34,34	13
2	DNF	A	800[A]	13/13	0.89	0.30	19,22,29,31	13
3	G2F	A	700	11/12	0.97	0.09	17,21,26,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.