



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 2, 2018 – 11:26 PM EST

PDB ID : 5JAW
Title : Structure of a beta galactosidase with inhibitor
Authors : Offen, W.; Davies, G.
Deposited on : 2016-04-12
Resolution : 1.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

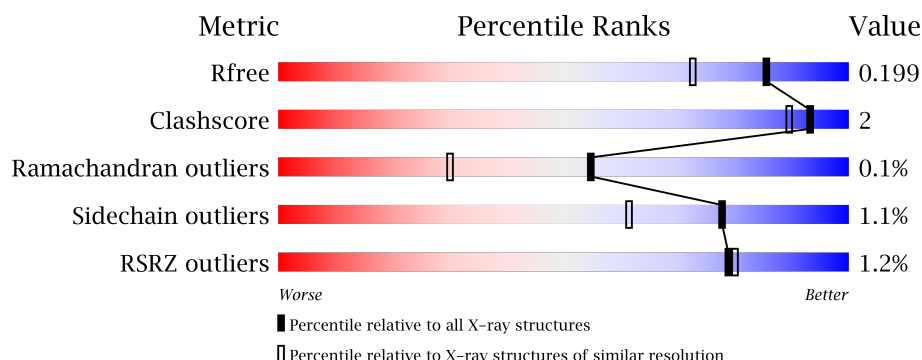
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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.




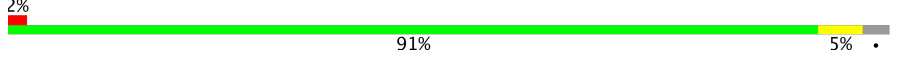

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2696 (1.60-1.60)
Clashscore	112137	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)
RSRZ outliers	101464	2714 (1.60-1.60)

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. 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	550	<div> <div></div> <div>89% 8% .</div> </div>
1	B	550	<div> <div></div> <div>90% 6% .</div> </div>
1	C	550	<div> <div></div> <div>90% 7% .</div> </div>
1	D	550	<div> <div></div> <div>91% 6% .</div> </div>
1	E	550	<div> <div></div> <div>90% 6% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	550	 .% 88% 7% 5%
1	G	550	 2% 91% 5% •
1	H	550	 3% 89% 7% •

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
3	NA	B	602	-	-	-	X
3	NA	F	603	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 35244 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-galactosidase, putative, bgl35A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	6	0
			4212	2697	716	782	17			
1	B	528	Total	C	N	O	S	0	6	0
			4189	2686	710	777	16			
1	C	536	Total	C	N	O	S	0	8	0
			4240	2714	726	784	16			
1	D	532	Total	C	N	O	S	0	2	0
			4163	2667	707	774	15			
1	E	533	Total	C	N	O	S	0	6	0
			4204	2690	716	781	17			
1	F	525	Total	C	N	O	S	0	4	0
			4142	2653	704	769	16			
1	G	531	Total	C	N	O	S	0	4	0
			4178	2681	708	772	17			
1	H	527	Total	C	N	O	S	0	4	0
			4154	2663	703	772	16			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	initiating methionine	UNP B3PBE0
A	27	GLY	-	expression tag	UNP B3PBE0
A	28	SER	-	expression tag	UNP B3PBE0
A	29	SER	-	expression tag	UNP B3PBE0
A	30	HIS	-	expression tag	UNP B3PBE0
A	31	HIS	-	expression tag	UNP B3PBE0
A	32	HIS	-	expression tag	UNP B3PBE0
A	33	HIS	-	expression tag	UNP B3PBE0
A	34	HIS	-	expression tag	UNP B3PBE0
A	35	HIS	-	expression tag	UNP B3PBE0
B	26	MET	-	initiating methionine	UNP B3PBE0
B	27	GLY	-	expression tag	UNP B3PBE0
B	28	SER	-	expression tag	UNP B3PBE0

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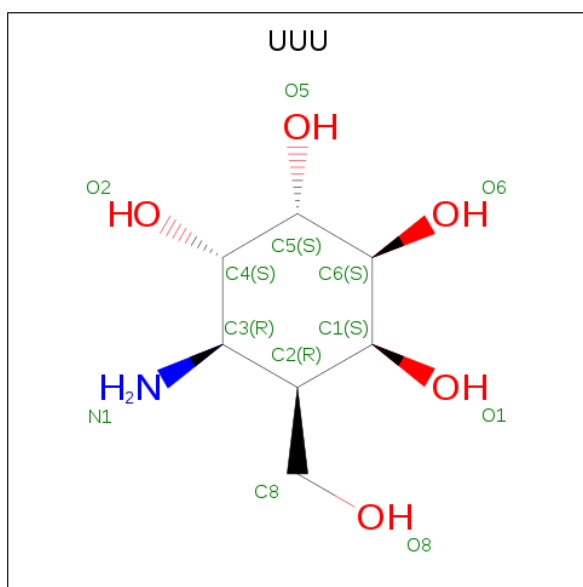
Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP B3PBE0
B	30	HIS	-	expression tag	UNP B3PBE0
B	31	HIS	-	expression tag	UNP B3PBE0
B	32	HIS	-	expression tag	UNP B3PBE0
B	33	HIS	-	expression tag	UNP B3PBE0
B	34	HIS	-	expression tag	UNP B3PBE0
B	35	HIS	-	expression tag	UNP B3PBE0
C	26	MET	-	initiating methionine	UNP B3PBE0
C	27	GLY	-	expression tag	UNP B3PBE0
C	28	SER	-	expression tag	UNP B3PBE0
C	29	SER	-	expression tag	UNP B3PBE0
C	30	HIS	-	expression tag	UNP B3PBE0
C	31	HIS	-	expression tag	UNP B3PBE0
C	32	HIS	-	expression tag	UNP B3PBE0
C	33	HIS	-	expression tag	UNP B3PBE0
C	34	HIS	-	expression tag	UNP B3PBE0
C	35	HIS	-	expression tag	UNP B3PBE0
D	26	MET	-	initiating methionine	UNP B3PBE0
D	27	GLY	-	expression tag	UNP B3PBE0
D	28	SER	-	expression tag	UNP B3PBE0
D	29	SER	-	expression tag	UNP B3PBE0
D	30	HIS	-	expression tag	UNP B3PBE0
D	31	HIS	-	expression tag	UNP B3PBE0
D	32	HIS	-	expression tag	UNP B3PBE0
D	33	HIS	-	expression tag	UNP B3PBE0
D	34	HIS	-	expression tag	UNP B3PBE0
D	35	HIS	-	expression tag	UNP B3PBE0
E	26	MET	-	initiating methionine	UNP B3PBE0
E	27	GLY	-	expression tag	UNP B3PBE0
E	28	SER	-	expression tag	UNP B3PBE0
E	29	SER	-	expression tag	UNP B3PBE0
E	30	HIS	-	expression tag	UNP B3PBE0
E	31	HIS	-	expression tag	UNP B3PBE0
E	32	HIS	-	expression tag	UNP B3PBE0
E	33	HIS	-	expression tag	UNP B3PBE0
E	34	HIS	-	expression tag	UNP B3PBE0
E	35	HIS	-	expression tag	UNP B3PBE0
F	26	MET	-	initiating methionine	UNP B3PBE0
F	27	GLY	-	expression tag	UNP B3PBE0
F	28	SER	-	expression tag	UNP B3PBE0
F	29	SER	-	expression tag	UNP B3PBE0
F	30	HIS	-	expression tag	UNP B3PBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	31	HIS	-	expression tag	UNP B3PBE0
F	32	HIS	-	expression tag	UNP B3PBE0
F	33	HIS	-	expression tag	UNP B3PBE0
F	34	HIS	-	expression tag	UNP B3PBE0
F	35	HIS	-	expression tag	UNP B3PBE0
G	26	MET	-	initiating methionine	UNP B3PBE0
G	27	GLY	-	expression tag	UNP B3PBE0
G	28	SER	-	expression tag	UNP B3PBE0
G	29	SER	-	expression tag	UNP B3PBE0
G	30	HIS	-	expression tag	UNP B3PBE0
G	31	HIS	-	expression tag	UNP B3PBE0
G	32	HIS	-	expression tag	UNP B3PBE0
G	33	HIS	-	expression tag	UNP B3PBE0
G	34	HIS	-	expression tag	UNP B3PBE0
G	35	HIS	-	expression tag	UNP B3PBE0
H	26	MET	-	initiating methionine	UNP B3PBE0
H	27	GLY	-	expression tag	UNP B3PBE0
H	28	SER	-	expression tag	UNP B3PBE0
H	29	SER	-	expression tag	UNP B3PBE0
H	30	HIS	-	expression tag	UNP B3PBE0
H	31	HIS	-	expression tag	UNP B3PBE0
H	32	HIS	-	expression tag	UNP B3PBE0
H	33	HIS	-	expression tag	UNP B3PBE0
H	34	HIS	-	expression tag	UNP B3PBE0
H	35	HIS	-	expression tag	UNP B3PBE0

- Molecule 2 is (1S,2S,3S,4S,5R,6R)-5-amino-6-(hydroxymethyl)cyclohexane-1,2,3,4-tetrol (three-letter code: UUU) (formula: C₇H₁₅NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	7	1	4		
2	B	1	Total	C	N	O	0	0
			12	7	1	4		
2	C	1	Total	C	N	O	0	0
			12	7	1	4		
2	D	1	Total	C	N	O	0	0
			12	7	1	4		
2	E	1	Total	C	N	O	0	0
			12	7	1	4		
2	F	1	Total	C	N	O	0	0
			12	7	1	4		
2	G	1	Total	C	N	O	0	0
			12	7	1	4		
2	H	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

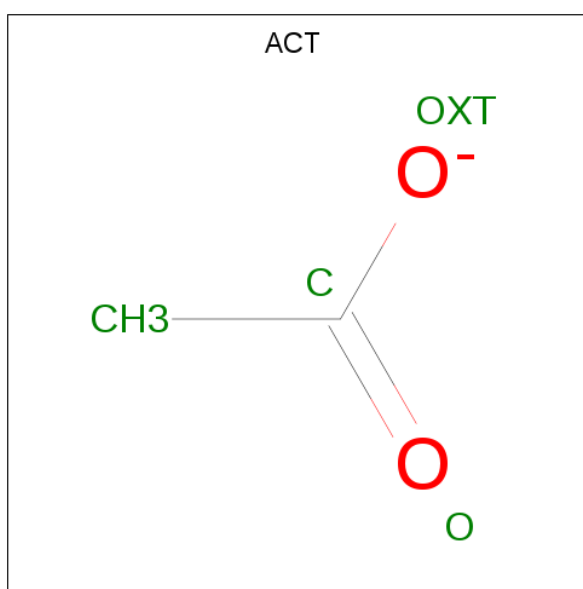
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	3	Total	Na	0	0
			3	3		
3	D	3	Total	Na	0	0
			3	3		
3	E	5	Total	Na	0	0
			5	5		
3	H	2	Total	Na	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total 3	Na 3	0	0
3	C	4	Total 4	Na 4	0	0
3	A	3	Total 3	Na 3	0	0
3	F	2	Total 2	Na 2	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total 4	C 2	O 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	241	Total 241	O 241	0	0
5	B	210	Total 210	O 210	0	0
5	C	264	Total 264	O 264	0	0
5	D	214	Total 214	O 214	0	0

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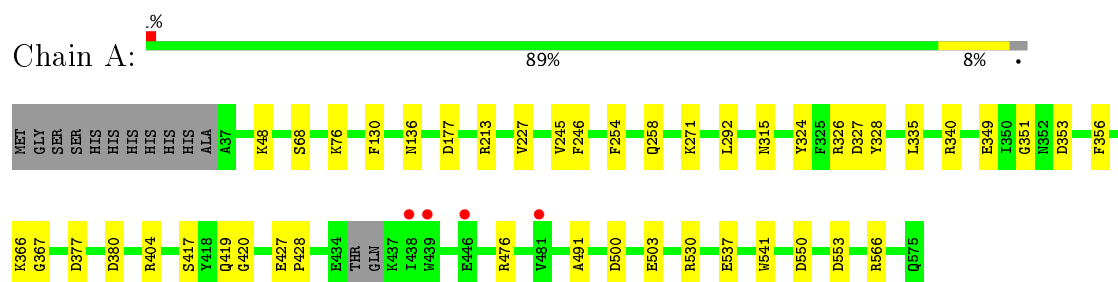
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	226	Total 226	O 226	0	0
5	F	165	Total 165	O 165	0	0
5	G	161	Total 161	O 161	0	0
5	H	155	Total 156	O 156	0	1

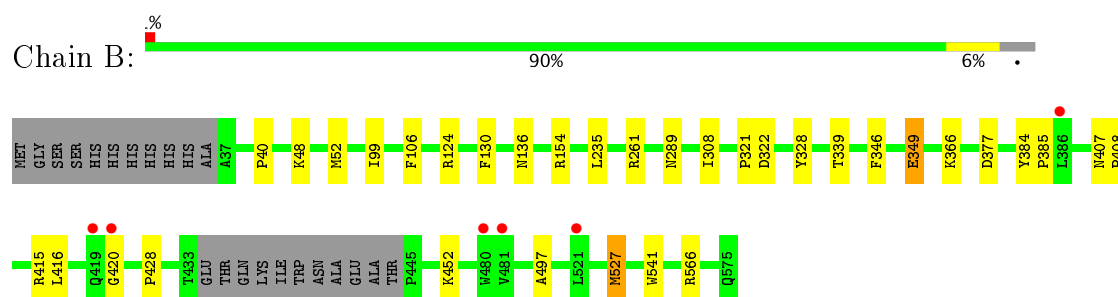
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

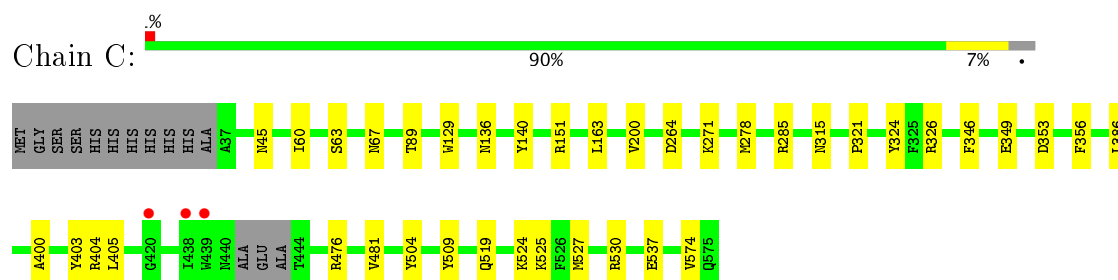
- Molecule 1: Beta-galactosidase, putative, bgl35A



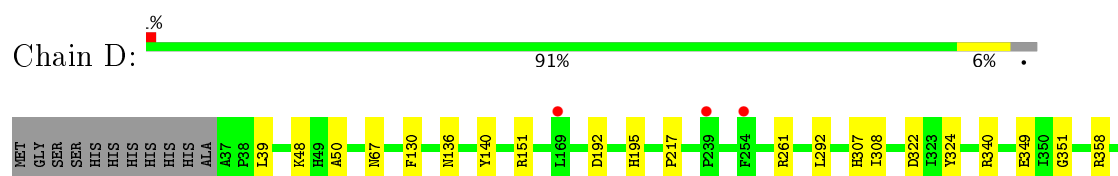
- Molecule 1: Beta-galactosidase, putative, bgl35A

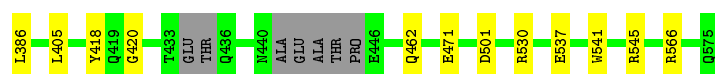


- Molecule 1: Beta-galactosidase, putative, bgl35A

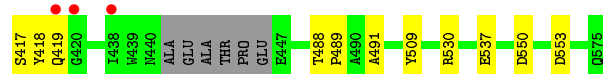
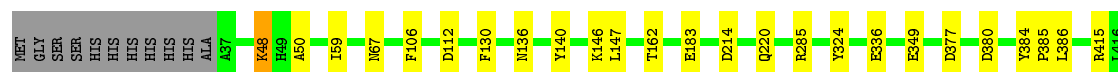
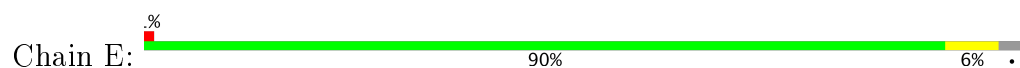


- Molecule 1: Beta-galactosidase, putative, bgl35A

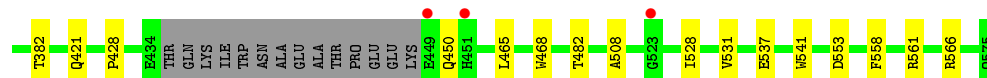
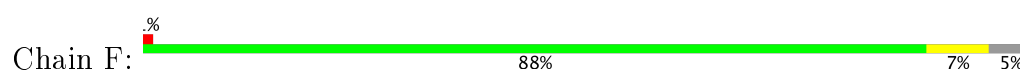




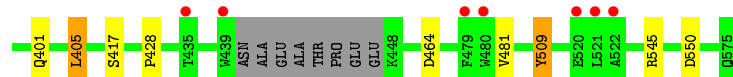
- Molecule 1: Beta-galactosidase, putative, bgl35A



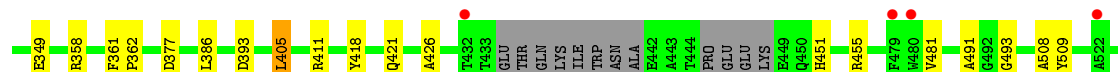
- Molecule 1: Beta-galactosidase, putative, bgl35A



- Molecule 1: Beta-galactosidase, putative, bgl35A



- Molecule 1: Beta-galactosidase, putative, bgl35A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.17Å 115.66Å 115.94Å 90.15° 90.11° 90.11°	Depositor
Resolution (Å)	81.99 – 1.60 81.99 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.5 (81.99-1.60) 94.5 (81.99-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.197 , 0.214 0.186 , 0.199	Depositor DCC
R_{free} test set	32563 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 25.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.207 for h,l,-k 0.207 for h,-l,k 0.155 for h,-k,-l 0.090 for -h,k,-l 0.088 for -h,-k,l 0.086 for -h,l,k 0.087 for -h,-l,-k	Xtriage
Reported twinning fraction	0.649 for H, K, L 0.052 for h,-k,-l 0.142 for H, L, -K 0.158 for H, -L, K	Depositor
Outliers	0 of 650569 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	35244	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: UUU, NA, ACT

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	1.04	2/4328 (0.0%)	1.12	20/5898 (0.3%)
1	B	0.91	1/4310 (0.0%)	1.00	10/5873 (0.2%)
1	C	1.01	4/4359 (0.1%)	1.07	8/5938 (0.1%)
1	D	0.97	1/4275 (0.0%)	1.05	9/5826 (0.2%)
1	E	0.98	3/4320 (0.1%)	1.05	10/5888 (0.2%)
1	F	0.86	1/4258 (0.0%)	0.95	9/5802 (0.2%)
1	G	0.85	2/4296 (0.0%)	0.97	7/5854 (0.1%)
1	H	0.84	1/4270 (0.0%)	0.97	11/5818 (0.2%)
All	All	0.94	15/34416 (0.0%)	1.02	84/46897 (0.2%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	GLU	CD-OE1	15.22	1.42	1.25
1	C	349	GLU	CD-OE1	12.07	1.39	1.25
1	H	349	GLU	CD-OE1	11.41	1.38	1.25
1	B	349	GLU	CD-OE1	9.93	1.36	1.25
1	G	349	GLU	CD-OE1	9.85	1.36	1.25

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	ARG	NE-CZ-NH1	9.43	125.01	120.30
1	A	353	ASP	CB-CG-OD2	-9.38	109.86	118.30
1	A	500	ASP	CB-CG-OD1	8.71	126.14	118.30
1	G	550	ASP	CB-CG-OD2	-8.24	110.89	118.30
1	C	151	ARG	NE-CZ-NH1	7.80	124.20	120.30

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	4212	0	4031	15	0
1	B	4189	0	4035	17	0
1	C	4240	0	4070	22	0
1	D	4163	0	3988	12	0
1	E	4204	0	4030	18	0
1	F	4142	0	3988	13	0
1	G	4178	0	4015	11	0
1	H	4154	0	3990	12	0
2	A	12	0	0	0	0
2	B	12	0	0	0	0
2	C	12	0	0	0	0
2	D	12	0	0	0	0
2	E	12	0	0	0	0
2	F	12	0	0	0	0
2	G	12	0	0	0	0
2	H	12	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
3	E	5	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	H	2	0	0	0	0
4	E	4	0	3	1	0
5	A	241	0	0	1	0
5	B	210	0	0	0	0
5	C	264	0	0	0	0
5	D	214	0	0	1	0
5	E	226	0	0	1	0
5	F	165	0	0	1	0
5	G	161	0	0	0	0
5	H	156	0	0	0	0
All	All	35244	0	32150	112	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.

The worst 5 of 112 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:C:530[B]:ARG:CG	1:C:530[B]:ARG:HH11	1.65	1.07
1:C:530[B]:ARG:HG2	1:C:530[B]:ARG:NH1	1.51	0.96
1:D:530:ARG:NH1	5:D:701:HOH:O	1.93	0.92
1:A:326[A]:ARG:NH1	5:A:702:HOH:O	2.03	0.92
1:B:48[A]:LYS:NZ	1:B:420:GLY:O	2.02	0.91

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	539/550 (98%)	518 (96%)	20 (4%)	1 (0%)	51	27
1	B	530/550 (96%)	510 (96%)	20 (4%)	0	100	100
1	C	540/550 (98%)	520 (96%)	20 (4%)	0	100	100
1	D	528/550 (96%)	510 (97%)	18 (3%)	0	100	100
1	E	535/550 (97%)	513 (96%)	21 (4%)	1 (0%)	51	27
1	F	525/550 (96%)	503 (96%)	22 (4%)	0	100	100
1	G	531/550 (96%)	509 (96%)	22 (4%)	0	100	100
1	H	525/550 (96%)	502 (96%)	21 (4%)	2 (0%)	38	16
All	All	4253/4400 (97%)	4085 (96%)	164 (4%)	4 (0%)	55	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	491	ALA
1	A	491	ALA
1	H	491	ALA

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Mol	Chain	Res	Type
1	H	138	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/461 (93%)	425 (99%)	4 (1%)	82	69
1	B	433/461 (94%)	431 (100%)	2 (0%)	91	84
1	C	433/461 (94%)	429 (99%)	4 (1%)	82	69
1	D	426/461 (92%)	421 (99%)	5 (1%)	75	58
1	E	431/461 (94%)	426 (99%)	5 (1%)	75	58
1	F	427/461 (93%)	419 (98%)	8 (2%)	62	37
1	G	428/461 (93%)	423 (99%)	5 (1%)	75	58
1	H	427/461 (93%)	423 (99%)	4 (1%)	82	69
All	All	3434/3688 (93%)	3397 (99%)	37 (1%)	78	61

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	136	ASN
1	F	136	ASN
1	H	220	GLN
1	E	220	GLN
1	E	336	GLU

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

Mol	Chain	Res	Type
1	G	498	GLN
1	H	451	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 25 are monoatomic - leaving 9 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	UUU	A	601	1	12,12,13	1.07	1 (8%)	12,17,19	0.64	0
2	UUU	B	601	1	12,12,13	1.08	1 (8%)	12,17,19	1.15	0
2	UUU	C	601	1	12,12,13	1.30	2 (16%)	12,17,19	1.24	1 (8%)
2	UUU	D	601	1	12,12,13	0.81	0	12,17,19	1.06	0
2	UUU	E	601	1	12,12,13	0.97	1 (8%)	12,17,19	0.81	0
4	ACT	E	607	3	1,3,3	0.50	0	0,3,3	0.00	-
2	UUU	F	601	1	12,12,13	1.13	1 (8%)	12,17,19	0.90	0
2	UUU	G	601	1	12,12,13	0.88	1 (8%)	12,17,19	0.63	0
2	UUU	H	601	1	12,12,13	0.73	0	12,17,19	1.55	3 (25%)

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	UUU	A	601	1	-	0/2/22/26	0/1/1/1
2	UUU	B	601	1	-	0/2/22/26	0/1/1/1
2	UUU	C	601	1	-	0/2/22/26	0/1/1/1
2	UUU	D	601	1	-	0/2/22/26	0/1/1/1
2	UUU	E	601	1	-	0/2/22/26	0/1/1/1
4	ACT	E	607	3	-	0/0/0/0	0/0/0/0
2	UUU	F	601	1	-	0/2/22/26	0/1/1/1
2	UUU	G	601	1	-	0/2/22/26	0/1/1/1
2	UUU	H	601	1	-	0/2/22/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	UUU	C8-C2	-2.23	1.48	1.52
2	G	601	UUU	C5-C6	2.11	1.55	1.52
2	E	601	UUU	O1-C1	2.39	1.48	1.43
2	A	601	UUU	C5-C6	2.99	1.56	1.52
2	B	601	UUU	C2-C1	3.02	1.56	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	UUU	C4-C5-C6	-2.85	106.87	110.59
2	C	601	UUU	C4-C5-C6	-2.54	107.27	110.59
2	H	601	UUU	C4-C3-C2	-2.02	108.43	111.53
2	H	601	UUU	O5-C5-C4	3.03	117.35	110.02

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
4	E	607	ACT	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	537/550 (97%)	0.00	4 (0%)	87 88	14, 21, 37, 69	2 (0%)
1	B	528/550 (96%)	0.01	6 (1%)	80 82	17, 23, 35, 65	3 (0%)
1	C	536/550 (97%)	0.00	3 (0%)	89 89	15, 21, 36, 53	7 (1%)
1	D	532/550 (96%)	0.03	3 (0%)	89 89	14, 23, 40, 58	1 (0%)
1	E	533/550 (96%)	0.01	3 (0%)	89 89	15, 22, 36, 65	0
1	F	525/550 (95%)	0.15	7 (1%)	77 78	17, 25, 38, 52	4 (0%)
1	G	531/550 (96%)	0.15	13 (2%)	59 59	18, 26, 40, 58	3 (0%)
1	H	527/550 (95%)	0.17	14 (2%)	55 54	18, 26, 40, 60	1 (0%)
All	All	4249/4400 (96%)	0.06	53 (1%)	79 80	14, 23, 38, 69	21 (0%)

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	521	LEU	5.9
1	C	438	ILE	4.6
1	C	439	TRP	4.0
1	H	522	ALA	4.0
1	A	438	ILE	3.8

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	NA	F	603	1/1	0.99	0.14	5.10	24,24,24,24	0
3	NA	B	602	1/1	0.91	0.16	2.17	45,45,45,45	0
2	UUU	C	601	12/13	0.96	0.10	0.59	13,15,16,19	0
3	NA	G	603	1/1	0.98	0.09	0.39	27,27,27,27	0
3	NA	G	604	1/1	0.97	0.11	0.31	29,29,29,29	0
2	UUU	D	601	12/13	0.95	0.10	0.05	16,17,19,20	0
2	UUU	F	601	12/13	0.93	0.09	-0.21	17,19,21,21	0
3	NA	D	604	1/1	0.97	0.09	-0.27	24,24,24,24	0
2	UUU	B	601	12/13	0.95	0.08	-0.43	15,18,20,22	0
3	NA	E	604	1/1	0.96	0.07	-0.48	25,25,25,25	0
2	UUU	G	601	12/13	0.95	0.08	-0.51	16,18,21,21	12
2	UUU	E	601	12/13	0.95	0.08	-0.63	14,16,18,19	0
3	NA	E	605	1/1	0.89	0.10	-0.67	27,27,27,27	0
3	NA	E	606	1/1	0.99	0.07	-1.11	21,21,21,21	0
2	UUU	H	601	12/13	0.94	0.07	-1.11	18,20,24,25	0
3	NA	C	602	1/1	0.98	0.07	-1.13	22,22,22,22	0
3	NA	D	602	1/1	0.99	0.07	-1.34	23,23,23,23	0
3	NA	A	603	1/1	0.96	0.07	-1.39	25,25,25,25	0
3	NA	F	602	1/1	0.91	0.07	-1.54	32,32,32,32	0
2	UUU	A	601	12/13	0.98	0.06	-1.54	14,15,16,17	0
3	NA	B	604	1/1	0.93	0.05	-1.75	32,32,32,32	0
3	NA	H	602	1/1	0.95	0.06	-1.75	25,25,25,25	0
3	NA	H	603	1/1	0.95	0.07	-1.91	29,29,29,29	0
3	NA	A	602	1/1	0.98	0.04	-2.94	21,21,21,21	0
3	NA	C	604	1/1	0.96	0.07	-3.07	23,23,23,23	0
3	NA	B	603	1/1	0.96	0.15	-	34,34,34,34	0
3	NA	G	602	1/1	0.88	0.08	-	33,33,33,33	0
3	NA	D	603	1/1	0.98	0.05	-	26,26,26,26	0
4	ACT	E	607	4/4	0.84	0.16	-	28,32,34,36	0
3	NA	A	604	1/1	0.98	0.12	-	26,26,26,26	0
3	NA	C	603	1/1	0.94	0.07	-	24,24,24,24	0
3	NA	E	603	1/1	0.93	0.10	-	23,23,23,23	0
3	NA	E	602	1/1	0.95	0.11	-	27,27,27,27	0
3	NA	C	605	1/1	0.96	0.10	-	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.