



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:14 AM GMT

PDB ID : 3LPG
Title : Structure of E. coli beta-Glucuronidase bound with a novel, potent inhibitor
3-(2-fluorophenyl)-1-(2-hydroxyethyl)-1-((6-methyl-2-oxo-1,2-dihydroquinolin
-3-yl)methyl)urea
Authors : Wallace, B.D.; Redinbo, M.R.
Deposited on : 2010-02-05
Resolution : 2.42 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

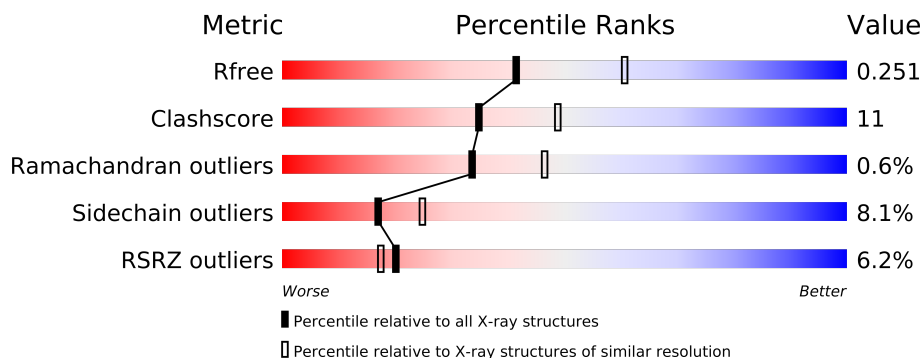
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.42 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}	66092	2496 (2.44-2.40)
Clashscore	79885	3124 (2.44-2.40)
Ramachandran outliers	78287	3067 (2.44-2.40)
Sidechain outliers	78261	3068 (2.44-2.40)
RSRZ outliers	66119	2499 (2.44-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	605	
1	B	605	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 10067 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

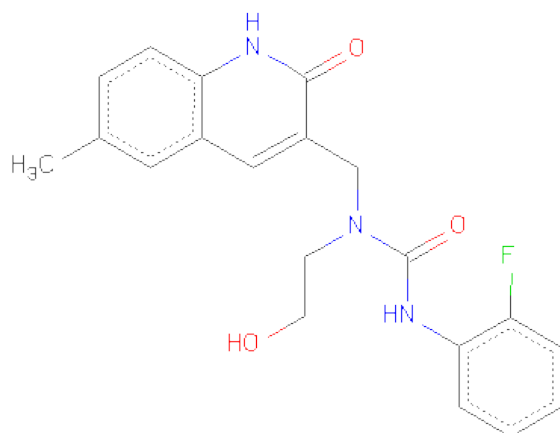
- Molecule 1 is a protein called Beta-glucuronidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	603	Total	C	N	O	S	Se	0	0	0
			4826	3063	834	907	9	13			
1	B	603	Total	C	N	O	S	Se	0	0	0
			4829	3066	834	907	9	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P05804
A	0	HIS	-	EXPRESSION TAG	UNP P05804
B	-1	SER	-	EXPRESSION TAG	UNP P05804
B	0	HIS	-	EXPRESSION TAG	UNP P05804

- Molecule 2 is 3-(2-FLUOROPHENYL)-1-(2-HYDROXYETHYL)-1-[(6-METHYL-2-OXO-1,2-DIHYDROQUINOLIN-3-YL)METHYL]UREA (three-letter code: Z78) (formula: $C_{20}H_{20}FN_3O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			27	20	1	3	3		
2	B	1	Total	C	F	N	O	0	0
			27	20	1	3	3		

- Molecule 3 is water.

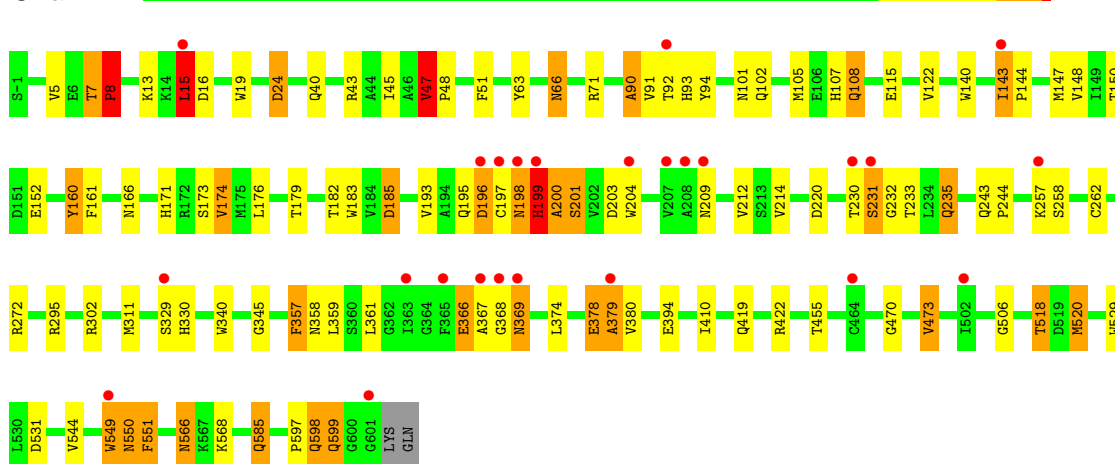
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	240	Total	O	0	0
			240	240		
3	B	118	Total	O	0	0
			118	118		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

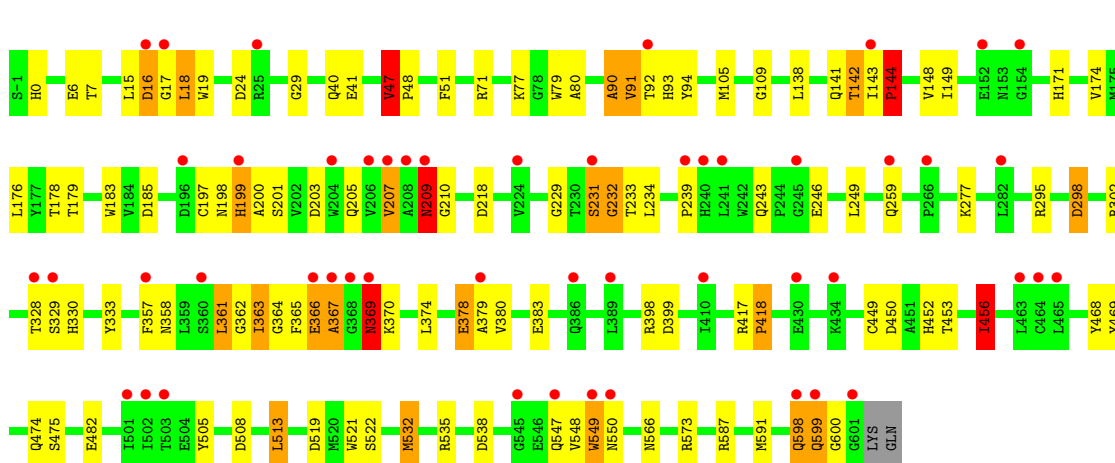
• Molecule 1: Beta-glucuronidase

Chain A:



• Molecule 1: Beta-glucuronidase

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.81Å 76.93Å 125.81Å 90.00° 124.75° 90.00°	Depositor
Resolution (Å)	30.86 – 2.42 30.86 – 2.42	Depositor EDS
% Data completeness (in resolution range)	89.5 (30.86-2.42) 98.0 (30.86-2.42)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.204 , 0.246 0.215 , 0.251	Depositor DCC
R_{free} test set	2488 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 49119 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10067	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: Z78

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	0.36	1/4943 (0.0%)	0.95	44/6704 (0.7%)
1	B	0.28	0/4946	1.12	59/6708 (0.9%)
All	All	0.32	1/9889 (0.0%)	1.04	103/13412 (0.8%)

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	1	2
1	B	1	2
All	All	2	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	PRO	N-CD	5.21	1.55	1.47

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ALA	CB-CA-C	-22.81	75.89	110.10
1	B	6	GLU	N-CA-C	17.13	157.26	111.00
1	B	15	LEU	CB-CA-C	-16.52	78.81	110.20
1	B	367	ALA	CB-CA-C	-16.27	85.69	110.10
1	A	551	PHE	N-CA-CB	-16.19	81.46	110.60
1	B	369	ASN	N-CA-C	15.23	152.12	111.00
1	B	599	GLN	CB-CA-C	14.81	140.02	110.40
1	B	366	GLU	CB-CA-C	-14.74	80.92	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	CYS	N-CA-C	-14.66	71.43	111.00
1	A	198	ASN	CB-CA-C	-14.33	81.74	110.40
1	B	369	ASN	CB-CA-C	-14.25	81.90	110.40
1	B	549	TRP	CB-CA-C	13.57	137.53	110.40
1	B	367	ALA	N-CA-C	13.54	147.56	111.00
1	A	198	ASN	N-CA-C	12.88	145.77	111.00
1	A	599	GLN	N-CA-CB	-12.81	87.54	110.60
1	A	230	THR	CB-CA-C	-12.64	77.48	111.60
1	A	598	GLN	N-CA-C	-12.49	77.28	111.00
1	B	16	ASP	N-CA-C	-12.35	77.66	111.00
1	B	379	ALA	N-CA-C	12.07	143.60	111.00
1	B	370	LYS	N-CA-C	-12.01	78.58	111.00
1	B	7	THR	N-CA-C	11.67	142.51	111.00
1	B	198	ASN	CB-CA-C	-11.59	87.22	110.40
1	A	366	GLU	N-CA-C	-11.50	79.95	111.00
1	B	18	LEU	N-CA-C	11.38	141.74	111.00
1	A	379	ALA	N-CA-C	11.12	141.01	111.00
1	B	363	ILE	N-CA-CB	-11.00	85.50	110.80
1	B	6	GLU	CB-CA-C	-10.97	88.46	110.40
1	A	90	ALA	CB-CA-C	10.40	125.71	110.10
1	B	366	GLU	N-CA-C	9.87	137.64	111.00
1	B	449	CYS	N-CA-C	-9.65	84.95	111.00
1	A	198	ASN	N-CA-CB	-9.63	93.26	110.60
1	A	367	ALA	N-CA-CB	-9.22	97.19	110.10
1	A	199	HIS	N-CA-CB	-9.10	94.22	110.60
1	B	7	THR	N-CA-CB	-9.02	93.16	110.30
1	A	108	GLN	N-CA-C	8.96	135.18	111.00
1	B	367	ALA	N-CA-CB	8.91	122.57	110.10
1	A	379	ALA	CB-CA-C	-8.84	96.84	110.10
1	B	378	GLU	CB-CA-C	8.76	127.92	110.40
1	B	90	ALA	CB-CA-C	8.63	123.04	110.10
1	B	232	GLY	N-CA-C	8.59	134.59	113.10
1	A	199	HIS	CB-CA-C	-8.42	93.55	110.40
1	B	600	GLY	N-CA-C	-8.27	92.43	113.10
1	A	200	ALA	N-CA-CB	-8.15	98.69	110.10
1	B	379	ALA	N-CA-CB	-7.88	99.07	110.10
1	B	379	ALA	CB-CA-C	-7.77	98.45	110.10
1	A	197	CYS	CB-CA-C	7.76	125.91	110.40
1	A	101	ASN	CB-CA-C	-7.67	95.07	110.40
1	A	231	SER	CB-CA-C	7.61	124.56	110.10
1	B	199	HIS	N-CA-CB	-7.40	97.29	110.60
1	A	366	GLU	CB-CA-C	7.36	125.12	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	549	TRP	N-CA-C	-7.30	91.29	111.00
1	A	209	ASN	N-CA-C	7.21	130.48	111.00
1	A	358	ASN	N-CA-CB	-7.20	97.64	110.60
1	B	380	VAL	N-CA-C	-7.20	91.57	111.00
1	A	15	LEU	N-CA-C	-7.05	91.96	111.00
1	B	450	ASP	N-CA-CB	7.02	123.24	110.60
1	B	358	ASN	N-CA-CB	-6.98	98.03	110.60
1	B	209	ASN	N-CA-C	6.93	129.71	111.00
1	B	231	SER	N-CA-C	-6.93	92.30	111.00
1	B	94	TYR	N-CA-CB	-6.90	98.17	110.60
1	A	232	GLY	N-CA-C	6.74	129.94	113.10
1	A	201	SER	N-CA-CB	-6.66	100.51	110.50
1	A	549	TRP	C-N-CA	-6.66	105.06	121.70
1	A	378	GLU	CB-CA-C	6.60	123.59	110.40
1	B	259	GLN	CB-CA-C	6.52	123.44	110.40
1	B	364	GLY	N-CA-C	-6.41	97.07	113.10
1	A	24	ASP	N-CA-C	-6.38	93.76	111.00
1	A	357	PHE	CB-CA-C	6.36	123.12	110.40
1	B	231	SER	CB-CA-C	-6.35	98.03	110.10
1	A	380	VAL	N-CA-C	-6.34	93.88	111.00
1	B	79	TRP	N-CA-C	-6.30	93.98	111.00
1	A	94	TYR	N-CA-CB	-6.27	99.31	110.60
1	B	200	ALA	N-CA-CB	-6.26	101.33	110.10
1	B	199	HIS	CB-CA-C	-6.11	98.17	110.40
1	A	520	MSE	N-CA-C	6.07	127.40	111.00
1	A	199	HIS	N-CA-C	6.02	127.24	111.00
1	A	231	SER	N-CA-CB	5.97	119.46	110.50
1	B	17	GLY	N-CA-C	-5.96	98.20	113.10
1	B	246	GLU	CB-CA-C	-5.94	98.52	110.40
1	B	449	CYS	CB-CA-C	5.91	122.22	110.40
1	A	196	ASP	N-CA-C	5.84	126.77	111.00
1	A	8	PRO	N-CA-C	-5.80	97.02	112.10
1	B	200	ALA	CB-CA-C	-5.71	101.53	110.10
1	B	361	LEU	N-CA-C	5.62	126.18	111.00
1	A	8	PRO	N-CA-CB	5.57	109.99	103.30
1	A	91	VAL	N-CA-C	-5.57	95.97	111.00
1	B	469	TYR	N-CA-CB	5.54	120.58	110.60
1	B	456	ILE	CB-CA-C	-5.54	100.52	111.60
1	A	102	GLN	N-CA-CB	5.53	120.55	110.60
1	A	200	ALA	N-CA-C	5.53	125.92	111.00
1	A	369	ASN	CB-CA-C	5.53	121.45	110.40
1	B	468	TYR	N-CA-C	-5.52	96.10	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	THR	N-CA-C	-5.37	96.49	111.00
1	A	200	ALA	CB-CA-C	-5.35	102.08	110.10
1	B	450	ASP	N-CA-C	-5.28	96.75	111.00
1	B	234	LEU	N-CA-C	-5.28	96.75	111.00
1	B	144	PRO	N-CA-C	-5.18	98.63	112.10
1	B	197	CYS	CB-CA-C	5.18	120.76	110.40
1	A	380	VAL	N-CA-CB	5.14	122.80	111.50
1	B	365	PHE	N-CA-C	-5.11	97.21	111.00
1	B	91	VAL	N-CA-C	-5.07	97.30	111.00
1	B	522	SER	N-CA-CB	5.04	118.06	110.50
1	B	80	ALA	N-CA-CB	-5.01	103.09	110.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	231	SER	CA
1	B	18	LEU	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	ILE	Peptide
1	A	47	VAL	Peptide
1	B	369	ASN	Peptide
1	B	47	VAL	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4826	0	0	60	0
1	B	4829	0	0	45	1
2	A	27	0	0	1	0
2	B	27	0	0	3	0
3	A	240	0	0	9	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	118	0	0	3	0
All	All	10067	0	0	104	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (104) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:209:ASN:ND2	1:B:209:ASN:O	1.91	1.03
1:B:361:LEU:O	2:B:604:Z78:OAC	1.77	1.03
1:A:108:GLN:CG	1:A:108:GLN:O	2.09	1.01
1:A:90:ALA:O	3:A:650:HOH:O	1.78	0.99
1:A:15:LEU:CD1	1:A:173:SER:CB	2.46	0.93
1:A:378:GLU:O	3:A:625:HOH:O	1.86	0.93
1:A:15:LEU:CD1	1:A:173:SER:OG	2.17	0.93
1:A:24:ASP:O	1:A:63:TYR:OH	1.87	0.92
1:A:597:PRO:C	1:A:598:GLN:O	1.93	0.92
1:B:378:GLU:O	3:B:647:HOH:O	1.92	0.86
1:A:549:TRP:CE3	1:A:549:TRP:O	2.30	0.84
1:B:513:LEU:CD1	1:B:521:TRP:O	2.26	0.83
1:A:140:TRP:CE3	1:A:379:ALA:O	2.33	0.81
1:B:367:ALA:O	3:B:676:HOH:O	1.98	0.81
1:A:198:ASN:ND2	1:A:198:ASN:O	2.15	0.80
1:B:142:THR:CG2	1:B:144:PRO:O	2.29	0.79
1:A:7:THR:O	3:A:792:HOH:O	2.00	0.79
1:B:363:ILE:O	1:B:363:ILE:CG2	2.31	0.78
1:B:144:PRO:CG	1:B:144:PRO:O	2.35	0.72
1:B:598:GLN:O	1:B:598:GLN:CG	2.40	0.70
1:A:361:LEU:O	2:A:604:Z78:OAC	2.09	0.69
1:A:108:GLN:O	3:A:666:HOH:O	2.10	0.69
1:B:538:ASP:O	1:B:599:GLN:O	2.12	0.68
1:A:520:MSE:O	3:A:826:HOH:O	2.11	0.67
1:B:90:ALA:O	3:B:715:HOH:O	2.12	0.66
1:A:549:TRP:CD2	1:A:549:TRP:O	2.49	0.66
1:A:105:MSE:CE	1:A:115:GLU:CA	2.75	0.64
1:A:199:HIS:ND1	1:A:200:ALA:N	2.46	0.63
1:A:15:LEU:CD1	1:A:173:SER:CA	2.76	0.63
1:A:357:PHE:O	1:A:374:LEU:CD2	2.49	0.61
1:A:13:LYS:O	1:A:174:VAL:O	2.20	0.60
1:A:143:ILE:O	1:A:143:ILE:CG2	2.50	0.60
1:A:198:ASN:C	1:A:198:ASN:ND2	2.54	0.60
1:A:195:GLN:O	3:A:669:HOH:O	2.17	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:311:MSE:CE	1:A:340:TRP:CB	2.81	0.59
1:A:140:TRP:CD2	1:A:379:ALA:O	2.55	0.58
1:A:92:THR:OG1	1:A:171:HIS:ND1	2.37	0.58
1:A:15:LEU:O	1:A:16:ASP:C	2.40	0.57
1:A:506:GLY:N	1:A:529:TRP:CZ3	2.73	0.57
1:B:505:TYR:CD2	1:B:547:GLN:O	2.59	0.56
1:B:548:VAL:C	1:B:549:TRP:O	2.38	0.56
1:B:357:PHE:O	1:B:374:LEU:CD2	2.55	0.54
1:B:47:VAL:CG2	1:B:47:VAL:O	2.55	0.53
1:A:8:PRO:O	1:B:77:LYS:NZ	2.42	0.53
1:A:585:GLN:CG	3:A:840:HOH:O	2.56	0.53
1:A:147:MSE:CE	1:A:161:PHE:CZ	2.93	0.52
1:B:144:PRO:CD	1:B:144:PRO:O	2.57	0.52
1:A:19:TRP:CD1	1:A:47:VAL:CG1	2.92	0.52
1:B:143:ILE:N	1:B:144:PRO:CD	2.74	0.51
1:A:368:GLY:O	1:A:369:ASN:C	2.49	0.51
1:A:357:PHE:O	1:A:374:LEU:CD1	2.59	0.51
1:A:7:THR:CB	1:A:8:PRO:CD	2.88	0.50
1:B:138:LEU:CD2	1:B:144:PRO:CG	2.89	0.50
1:A:518:THR:OG1	1:A:518:THR:O	2.30	0.49
1:B:92:THR:OG1	1:B:171:HIS:ND1	2.46	0.49
1:A:47:VAL:CG2	1:A:47:VAL:O	2.60	0.49
1:B:207:VAL:CG1	1:B:210:GLY:N	2.75	0.49
1:B:456:ILE:CG2	1:B:456:ILE:O	2.56	0.48
1:B:19:TRP:CD1	1:B:47:VAL:CG1	2.96	0.48
1:A:199:HIS:N	3:A:786:HOH:O	2.46	0.48
1:B:295:ARG:O	1:B:329:SER:CB	2.63	0.47
1:A:244:PRO:O	1:A:345:GLY:O	2.33	0.47
1:B:362:GLY:CA	2:B:604:Z78:OAC	2.64	0.46
1:A:204:TRP:CA	1:A:231:SER:O	2.63	0.46
1:A:182:THR:OG1	1:A:258:SER:OG	2.33	0.46
1:A:183:TRP:N	1:A:183:TRP:CD1	2.84	0.46
1:B:330:HIS:CD2	1:B:330:HIS:N	2.81	0.46
1:A:200:ALA:CA	1:A:235:GLN:O	2.64	0.46
1:A:257:LYS:CD	1:A:262:CYS:SG	3.04	0.46
1:B:519:ASP:OD2	1:B:519:ASP:N	2.49	0.46
1:B:474:GLN:O	1:B:475:SER:C	2.53	0.46
1:B:93:HIS:O	1:B:109:GLY:O	2.35	0.45
1:B:295:ARG:O	1:B:333:TYR:OH	2.34	0.45
1:B:0:HIS:N	1:B:0:HIS:CD2	2.84	0.44
1:A:549:TRP:CD2	1:A:549:TRP:C	2.89	0.44
1:A:422:ARG:NH1	1:A:455:THR:O	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:505:TYR:CE2	1:B:547:GLN:O	2.71	0.44
1:B:203:ASP:OD1	1:B:233:THR:OG1	2.35	0.44
1:B:203:ASP:O	1:B:232:GLY:CA	2.65	0.44
1:B:398:ARG:NE	1:B:399:ASP:OD1	2.50	0.44
1:B:298:ASP:OD1	1:B:573:ARG:NH2	2.51	0.43
1:A:330:HIS:N	1:A:330:HIS:CD2	2.85	0.43
1:A:160:TYR:N	1:A:160:TYR:CD2	2.87	0.43
1:B:482:GLU:CB	1:B:532:MSE:CE	2.96	0.43
1:B:417:ARG:N	1:B:418:PRO:CD	2.82	0.42
1:A:107:HIS:CE1	1:A:394:GLU:OE1	2.73	0.42
1:A:183:TRP:CZ3	1:A:185:ASP:CB	3.03	0.42
1:B:361:LEU:C	2:B:604:Z78:OAC	2.55	0.42
1:A:66:ASN:N	1:A:66:ASN:ND2	2.68	0.41
1:B:366:GLU:O	1:B:366:GLU:CG	2.54	0.41
1:B:179:THR:CG2	1:B:183:TRP:CB	2.97	0.41
1:A:51:PHE:C	1:A:51:PHE:CD1	2.93	0.41
1:B:91:VAL:O	1:B:92:THR:C	2.59	0.41
1:A:295:ARG:O	1:A:329:SER:CB	2.68	0.41
1:A:470:GLY:N	1:A:473:VAL:O	2.53	0.41
1:B:229:GLY:O	1:B:231:SER:O	2.38	0.41
1:A:550:ASN:O	1:A:551:PHE:C	2.55	0.41
1:A:566:ASN:ND2	1:A:568:LYS:N	2.69	0.41
1:B:51:PHE:CD1	1:B:51:PHE:C	2.93	0.41
1:A:93:HIS:CE1	1:A:166:ASN:OD1	2.74	0.41
1:B:24:ASP:OD2	1:B:29:GLY:N	2.54	0.40
1:A:597:PRO:O	1:A:598:GLN:C	2.51	0.40
1:A:107:HIS:CD2	3:A:828:HOH:O	2.73	0.40
1:A:203:ASP:OD2	1:A:203:ASP:C	2.59	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:B:366:GLU:OE1	3:A:839:HOH:O[2_555]	1.87	0.33

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	601/605 (99%)	575 (96%)	23 (4%)	3 (0%)	38	52
1	B	601/605 (99%)	566 (94%)	31 (5%)	4 (1%)	30	42
All	All	1202/1210 (99%)	1141 (95%)	54 (4%)	7 (1%)	33	46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	PRO
1	A	144	PRO
1	B	48	PRO
1	A	8	PRO
1	B	144	PRO
1	B	239	PRO
1	B	418	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	510/500 (102%)	468 (92%)	42 (8%)	17	24
1	B	511/500 (102%)	470 (92%)	41 (8%)	17	26
All	All	1021/1000 (102%)	938 (92%)	83 (8%)	17	25

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	7	THR
1	A	15	LEU
1	A	40	GLN
1	A	43	ARG
1	A	45	ILE
1	A	47	VAL
1	A	66	ASN
1	A	71	ARG

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Mol	Chain	Res	Type
1	A	122	VAL
1	A	148	VAL
1	A	150	THR
1	A	152	GLU
1	A	160	TYR
1	A	174	VAL
1	A	176	LEU
1	A	179	THR
1	A	185	ASP
1	A	193	VAL
1	A	196	ASP
1	A	199	HIS
1	A	201	SER
1	A	212	VAL
1	A	214	VAL
1	A	220	ASP
1	A	233	THR
1	A	235	GLN
1	A	243	GLN
1	A	272	ARG
1	A	302	ARG
1	A	359	LEU
1	A	366	GLU
1	A	410	ILE
1	A	419	GLN
1	A	473	VAL
1	A	518	THR
1	A	531	ASP
1	A	544	VAL
1	A	550	ASN
1	A	566	ASN
1	A	585	GLN
1	A	599	GLN
1	B	16	ASP
1	B	18	LEU
1	B	40	GLN
1	B	41	GLU
1	B	47	VAL
1	B	71	ARG
1	B	105	MSE
1	B	141	GLN
1	B	142	THR

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Mol	Chain	Res	Type
1	B	144	PRO
1	B	148	VAL
1	B	149	ILE
1	B	174	VAL
1	B	176	LEU
1	B	178	THR
1	B	185	ASP
1	B	199	HIS
1	B	201	SER
1	B	205	GLN
1	B	207	VAL
1	B	209	ASN
1	B	218	ASP
1	B	243	GLN
1	B	249	LEU
1	B	277	LYS
1	B	298	ASP
1	B	302	ARG
1	B	369	ASN
1	B	383	GLU
1	B	452	HIS
1	B	453	THR
1	B	456	ILE
1	B	508	ASP
1	B	513	LEU
1	B	532	MSE
1	B	535	ARG
1	B	550	ASN
1	B	566	ASN
1	B	587	ARG
1	B	591	MSE
1	B	598	GLN

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

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 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	Z78	A	604	-	29,29,29	3.74	13 (44%)	38,40,40	2.98	13 (34%)
2	Z78	B	604	-	29,29,29	3.71	13 (44%)	38,40,40	2.97	13 (34%)

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	Z78	A	604	-	-	0/15/15/15	0/1/3/3
2	Z78	B	604	-	-	0/15/15/15	0/1/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	604	Z78	CAW-CAU	11.26	1.53	1.38
2	A	604	Z78	CAW-CAU	11.16	1.52	1.38
2	A	604	Z78	OAC-CAX	8.56	1.41	1.24
2	B	604	Z78	OAC-CAX	8.12	1.40	1.24
2	A	604	Z78	CAS-N3	6.38	1.46	1.36
2	B	604	Z78	CAS-N3	6.28	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	604	Z78	CAK-CAJ	5.82	1.49	1.36
2	A	604	Z78	CAK-CAJ	5.74	1.48	1.36
2	A	604	Z78	CAS-N2	5.27	1.47	1.36
2	B	604	Z78	CAS-N2	5.16	1.47	1.36
2	B	604	Z78	OAD-CAN	-4.24	1.19	1.42
2	A	604	Z78	OAD-CAN	-4.24	1.19	1.42
2	A	604	Z78	CAM-CAV	3.95	1.41	1.35
2	B	604	Z78	CAX-N1	3.94	1.43	1.37
2	A	604	Z78	CAL-CAY	3.93	1.50	1.42
2	B	604	Z78	CAL-CAY	3.86	1.50	1.42
2	B	604	Z78	CAM-CAV	3.81	1.41	1.35
2	A	604	Z78	CAX-N1	3.61	1.43	1.37
2	B	604	Z78	CAG-CAF	3.47	1.47	1.37
2	A	604	Z78	CAG-CAF	3.42	1.47	1.37
2	A	604	Z78	CAL-CAT	2.73	1.41	1.37
2	B	604	Z78	CAL-CAT	2.59	1.41	1.37
2	A	604	Z78	CAW-N3	2.35	1.46	1.41
2	B	604	Z78	CAW-N3	2.23	1.46	1.41
2	B	604	Z78	CAJ-CAT	2.07	1.45	1.38
2	A	604	Z78	CAJ-CAT	2.06	1.45	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	604	Z78	CAW-N3-CAS	13.96	159.54	126.10
2	A	604	Z78	CAW-N3-CAS	13.39	158.17	126.10
2	A	604	Z78	CAM-CAV-CAX	6.25	120.40	115.58
2	B	604	Z78	CAM-CAV-CAX	5.37	119.73	115.58
2	B	604	Z78	N3-CAS-N2	3.69	120.06	115.88
2	A	604	Z78	N3-CAS-N2	3.62	119.98	115.88
2	A	604	Z78	CAV-CAM-CAY	-3.49	119.45	122.52
2	B	604	Z78	CAV-CAM-CAY	-3.39	119.54	122.52
2	A	604	Z78	OAB-CAS-N3	-3.31	117.63	124.16
2	B	604	Z78	OAB-CAS-N3	-3.15	117.95	124.16
2	A	604	Z78	CAP-N2-CAS	-3.08	110.67	122.50
2	A	604	Z78	CAH-CAU-CAW	-2.93	120.18	123.44
2	B	604	Z78	CAO-N2-CAS	-2.84	110.37	120.46
2	B	604	Z78	CAH-CAU-CAW	-2.83	120.30	123.44
2	A	604	Z78	CAO-N2-CAS	-2.79	110.56	120.46
2	A	604	Z78	CAP-N2-CAO	-2.76	108.80	116.69
2	A	604	Z78	CAY-CAZ-N1	2.71	120.42	118.23
2	A	604	Z78	OAB-CAS-N2	-2.67	117.85	121.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	604	Z78	FAE-CAU-CAW	2.58	120.04	117.48
2	B	604	Z78	CAP-N2-CAO	-2.53	109.48	116.69
2	B	604	Z78	CAP-N2-CAS	-2.51	112.88	122.50
2	B	604	Z78	CAI-CAW-CAU	2.49	119.64	117.09
2	B	604	Z78	OAB-CAS-N2	-2.45	118.18	121.73
2	A	604	Z78	CAI-CAW-CAU	2.23	119.37	117.09
2	A	604	Z78	CAV-CAP-N2	2.22	117.06	113.35
2	B	604	Z78	CAY-CAZ-N1	2.21	120.02	118.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	603/605 (99%)	0.24	25 (4%)	35 32	21, 49, 99, 132	0
1	B	603/605 (99%)	0.48	50 (8%)	11 10	34, 82, 156, 189	0
All	All	1206/1210 (99%)	0.36	75 (6%)	20 17	21, 66, 138, 189	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	ASN	8.5
1	A	368	GLY	6.3
1	B	601	GLY	5.2
1	B	367	ALA	5.1
1	A	199	HIS	5.0
1	A	367	ALA	4.9
1	A	207	VAL	4.9
1	A	208	ALA	4.8
1	A	231	SER	4.6
1	B	196	ASP	4.5
1	B	259	GLN	4.4
1	B	503	THR	4.4
1	B	204	TRP	4.3
1	B	207	VAL	4.2
1	A	365	PHE	4.2
1	B	241	LEU	4.0
1	B	369	ASN	4.0
1	B	357	PHE	4.0
1	A	369	ASN	3.7
1	B	199	HIS	3.6
1	A	230	THR	3.6
1	A	198	ASN	3.5
1	B	366	GLU	3.4
1	A	601	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	368	GLY	3.2
1	A	204	TRP	3.2
1	A	549	TRP	3.1
1	B	386	GLN	3.1
1	B	501	ILE	2.9
1	B	545	GLY	2.9
1	B	245	GLY	2.9
1	B	329	SER	2.8
1	A	363	ILE	2.8
1	B	547	GLN	2.8
1	B	434	LYS	2.8
1	B	239	PRO	2.8
1	B	231	SER	2.8
1	B	464	CYS	2.7
1	B	549	TRP	2.7
1	A	209	ASN	2.7
1	B	152	GLU	2.5
1	B	16	ASP	2.5
1	B	282	LEU	2.5
1	A	464	CYS	2.5
1	B	240	HIS	2.5
1	A	329	SER	2.4
1	B	598	GLN	2.4
1	B	463	LEU	2.4
1	B	154	GLY	2.4
1	A	379	ALA	2.3
1	B	143	ILE	2.3
1	B	208	ALA	2.3
1	B	328	THR	2.3
1	B	92	THR	2.3
1	B	502	ILE	2.3
1	A	197	CYS	2.3
1	A	257	LYS	2.3
1	B	17	GLY	2.2
1	A	502	ILE	2.2
1	B	410	ILE	2.2
1	B	550	ASN	2.2
1	B	360	SER	2.2
1	B	25	ARG	2.2
1	A	196	ASP	2.1
1	A	143	ILE	2.1
1	B	379	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	224	VAL	2.1
1	A	92	THR	2.1
1	A	15	LEU	2.1
1	B	266	PRO	2.0
1	B	465	LEU	2.0
1	B	430	GLU	2.0
1	B	206	VAL	2.0
1	B	389	LEU	2.0
1	B	599	GLN	2.0

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	Z78	A	604	27/27	0.26	1.35	52,64,100,101	0
2	Z78	B	604	27/27	0.26	0.65	86,94,111,112	0

6.5 Other polymers ⓘ

There are no such residues in this entry.