



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 30, 2022 – 02:25 PM JST

PDB ID : 7D66
Title : Crystal structure of retroviral protease-like domain of Ddi1 from *Toxoplasma gondii*
Authors : Biswas, I.B.; Killivalavan, A.K.; Suguna, K.S.
Deposited on : 2020-09-29
Resolution : 2.13 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

<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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
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)	:	2.31.3

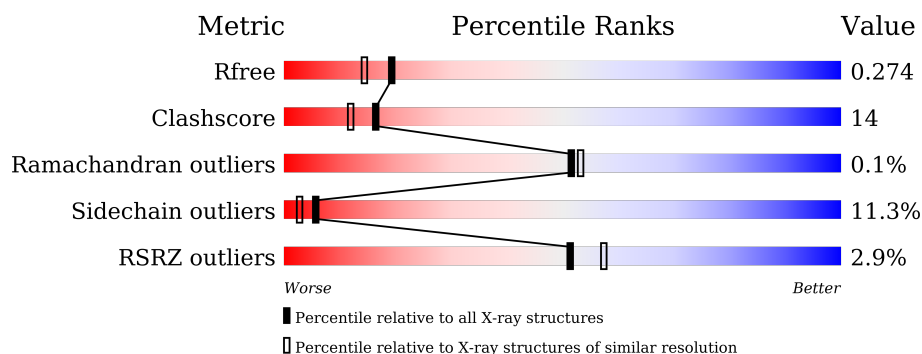
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	128	<div> <div>3%</div> <div>70% 23% 5% .</div> </div>
1	B	128	<div> <div>2%</div> <div>67% 23% . 6%</div> </div>
1	C	128	<div> <div>6%</div> <div>66% 27% 5% .</div> </div>
1	D	128	<div> <div>0%</div> <div>65% 28% . .</div> </div>
1	E	128	<div> <div>2%</div> <div>58% 25% . 14%</div> </div>
1	F	128	<div> <div>2%</div> <div>59% 28% 7% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	128	<div><div></div><div>3%</div><div>62%</div><div>27%</div><div>5%</div><div>6%</div></div>
1	H	128	<div><div></div><div>3%</div><div>64%</div><div>24%</div><div></div><div></div><div>7%</div></div>
1	I	128	<div><div></div><div>2%</div><div>66%</div><div>27%</div><div></div><div></div><div></div></div>
1	J	128	<div><div></div><div>4%</div><div>54%</div><div>36%</div><div></div><div></div><div>6%</div></div>
1	K	128	<div><div></div><div>5%</div><div>66%</div><div>26%</div><div></div><div></div><div></div></div>
1	L	128	<div><div></div><div>2%</div><div>62%</div><div>27%</div><div>6%</div><div></div></div>

2 Entry composition

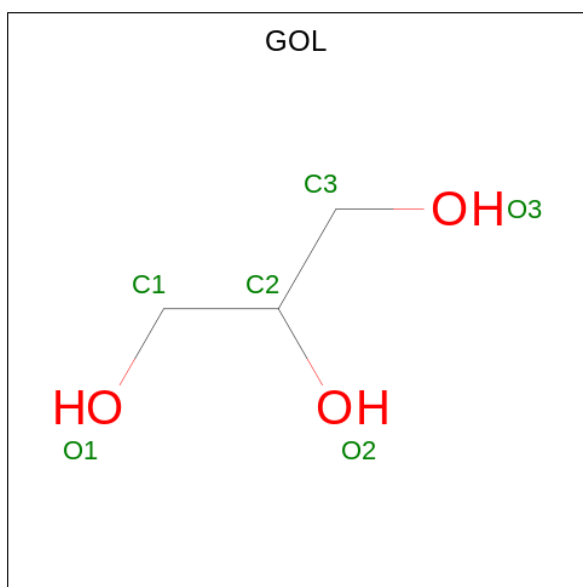
There are 3 unique types of molecules in this entry. The entry contains 23392 atoms, of which 11534 are hydrogens and 0 are deuteriums.

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 Ubiquitin family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	120	Total	C	H	N	O	S	32	0	0
			1877	599	948	154	169	7			
1	A	124	Total	C	H	N	O	S	31	0	0
			1901	605	955	159	175	7			
1	D	124	Total	C	H	N	O	S	36	0	0
			1897	605	959	157	169	7			
1	C	126	Total	C	H	N	O	S	37	0	0
			1920	610	969	160	174	7			
1	F	121	Total	C	H	N	O	S	30	0	0
			1886	600	951	155	173	7			
1	E	110	Total	C	H	N	O	S	28	0	0
			1706	549	862	135	153	7			
1	H	119	Total	C	H	N	O	S	27	0	0
			1897	604	962	155	169	7			
1	G	120	Total	C	H	N	O	S	32	0	0
			1860	601	936	147	169	7			
1	J	120	Total	C	H	N	O	S	32	0	0
			1878	599	953	153	166	7			
1	I	124	Total	C	H	N	O	S	31	0	0
			1931	616	977	156	175	7			
1	L	123	Total	C	H	N	O	S	29	0	0
			1945	618	983	160	177	7			
1	K	123	Total	C	H	N	O	S	34	0	0
			1885	601	951	156	171	6			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	2	0
			14	3	8	3		
2	B	1	Total	C	H	O	2	0
			14	3	8	3		
2	B	1	Total	C	H	O	2	0
			14	3	8	3		
2	B	1	Total	C	H	O	2	0
			14	3	8	3		
2	A	1	Total	C	H	O	2	0
			14	3	8	3		
2	A	1	Total	C	H	O	2	0
			14	3	8	3		
2	A	1	Total	C	H	O	2	0
			14	3	8	3		
2	F	1	Total	C	H	O	2	0
			14	3	8	3		
2	F	1	Total	C	H	O	2	0
			14	3	8	3		
2	F	1	Total	C	H	O	2	0
			14	3	8	3		
2	F	1	Total	C	H	O	2	0
			14	3	8	3		
2	E	1	Total	C	H	O	2	0
			14	3	8	3		
2	H	1	Total	C	H	O	2	0
			14	3	8	3		
2	J	1	Total	C	H	O	2	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total	C	H	O	2	0
			14	3	8	3		
2	L	1	Total	C	H	O	2	0
			14	3	8	3		

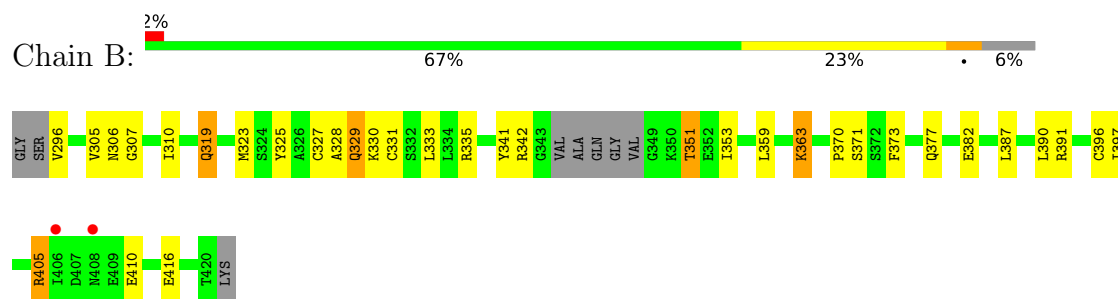
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	43	Total	O	0	0
			43	43		
3	A	53	Total	O	0	0
			53	53		
3	D	52	Total	O	0	0
			52	52		
3	C	47	Total	O	0	0
			47	47		
3	F	56	Total	O	0	0
			56	56		
3	E	41	Total	O	0	0
			41	41		
3	H	49	Total	O	0	0
			49	49		
3	G	53	Total	O	0	0
			53	53		
3	J	38	Total	O	0	0
			38	38		
3	I	48	Total	O	0	0
			48	48		
3	L	45	Total	O	0	0
			45	45		
3	K	60	Total	O	0	0
			60	60		

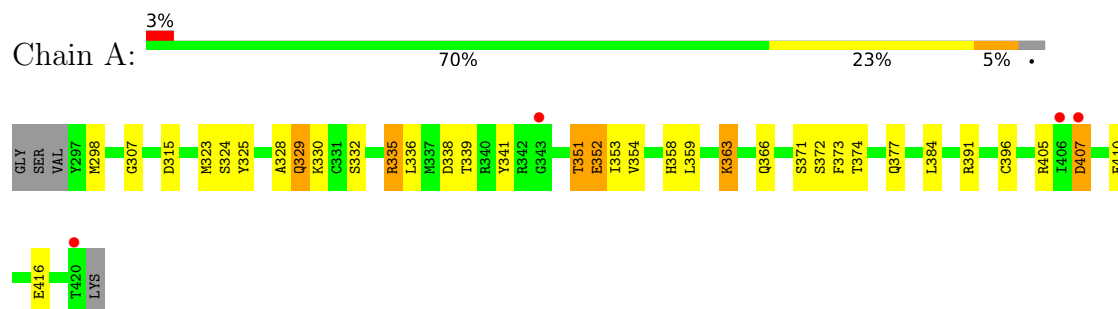
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

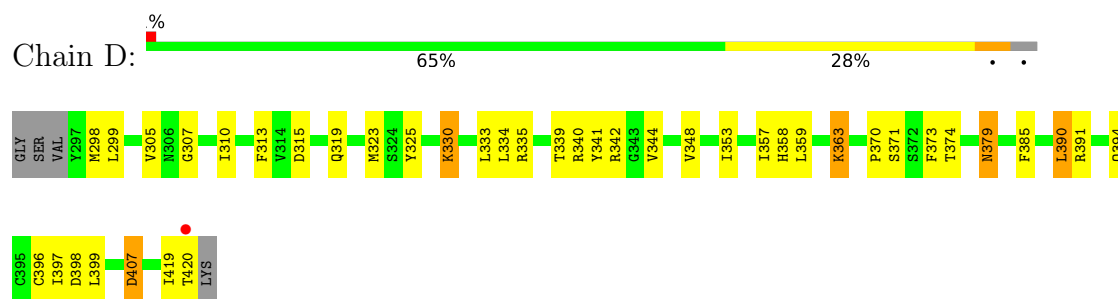
- Molecule 1: Ubiquitin family protein



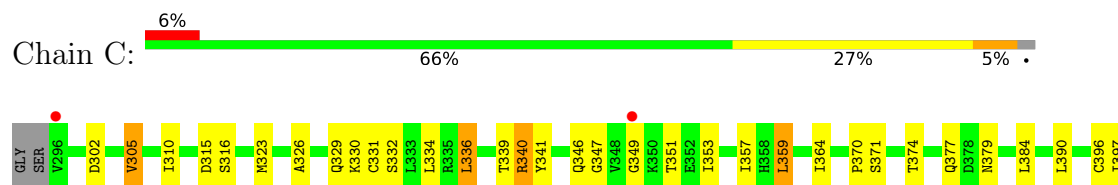
- Molecule 1: Ubiquitin family protein



- Molecule 1: Ubiquitin family protein

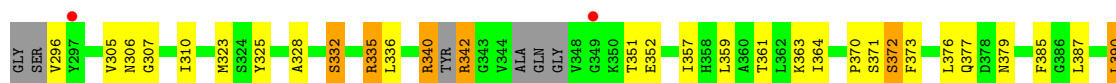


- Molecule 1: Ubiquitin family protein

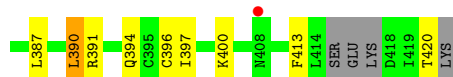




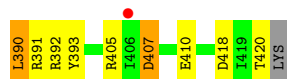
- Molecule 1: Ubiquitin family protein



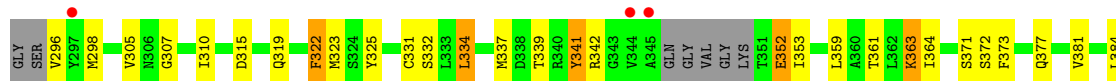
- Molecule 1: Ubiquitin family protein



- Molecule 1: Ubiquitin family protein

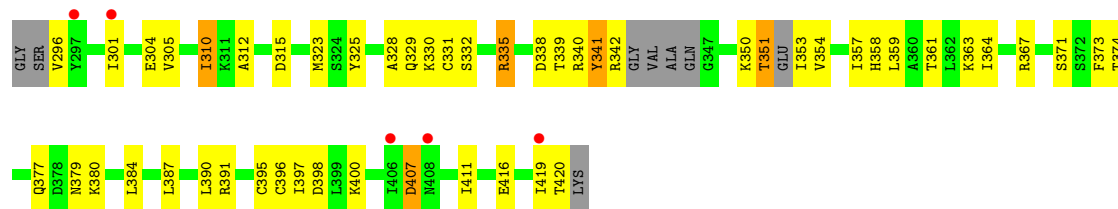


- Molecule 1: Ubiquitin family protein

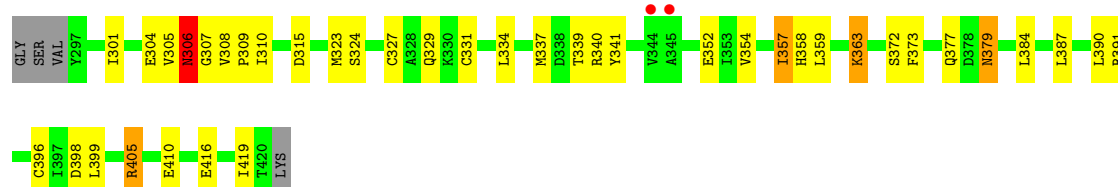


- Molecule 1: Ubiquitin family protein

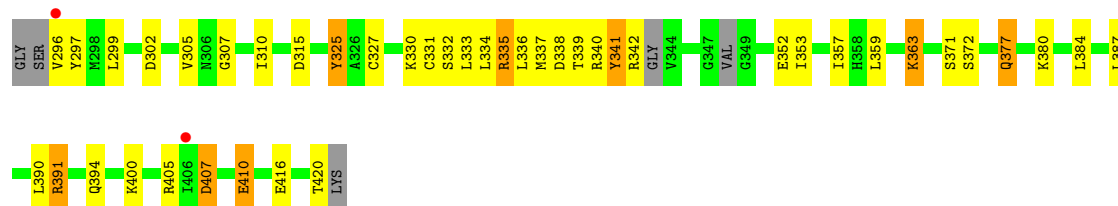




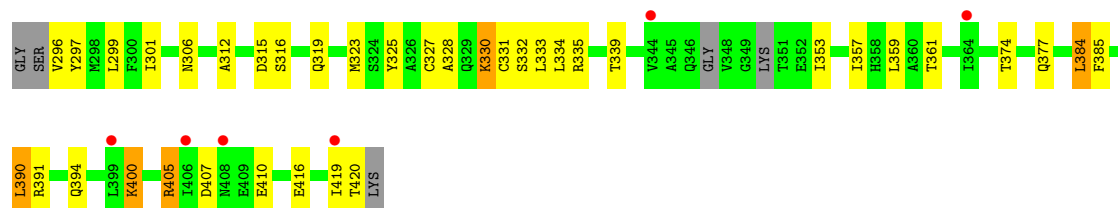
• Molecule 1: Ubiquitin family protein



• Molecule 1: Ubiquitin family protein



• Molecule 1: Ubiquitin family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	184.60Å 184.60Å 184.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.27 – 2.13 65.27 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.7 (65.27-2.13) 99.7 (65.27-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	22.18 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0266	Depositor
R, R_{free}	0.192 , 0.247 0.225 , 0.274	Depositor DCC
R_{free} test set	8844 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.049 for -h,-l,-k 0.044 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23392	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2204e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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

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	0.82	1/960 (0.1%)	0.96	0/1295
1	B	0.87	2/943 (0.2%)	0.96	0/1270
1	C	0.84	0/965	1.00	2/1302 (0.2%)
1	D	0.79	0/953	0.95	1/1285 (0.1%)
1	E	0.82	0/856	0.96	0/1153
1	F	0.88	2/947 (0.2%)	1.09	7/1274 (0.5%)
1	G	0.81	1/939 (0.1%)	0.97	1/1267 (0.1%)
1	H	0.86	0/948	1.06	3/1271 (0.2%)
1	I	0.86	3/969 (0.3%)	1.03	1/1306 (0.1%)
1	J	0.81	0/938	1.02	3/1262 (0.2%)
1	K	0.79	0/946	0.95	1/1276 (0.1%)
1	L	0.94	2/975 (0.2%)	1.01	0/1309
All	All	0.84	11/11339 (0.1%)	1.00	19/15270 (0.1%)

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	D	0	1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	409	GLU	CD-OE1	9.46	1.36	1.25
1	B	416	GLU	CD-OE1	-6.23	1.18	1.25
1	L	410	GLU	CD-OE2	-5.85	1.19	1.25
1	I	309	PRO	C-O	-5.72	1.11	1.23
1	I	306	ASN	CG-OD1	5.65	1.36	1.24

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	342	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	F	392	ARG	NE-CZ-NH2	8.06	124.33	120.30
1	K	297	TYR	CB-CA-C	6.73	123.86	110.40
1	H	335	ARG	CG-CD-NE	-6.61	97.92	111.80
1	F	335	ARG	NE-CZ-NH2	6.58	123.59	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	344	VAL	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	946	955	936	36	2
1	B	929	948	929	27	5
1	C	951	969	942	34	29
1	D	938	959	934	38	0
1	E	844	862	843	35	0
1	F	935	951	934	32	29
1	G	924	936	916	23	5
1	H	935	962	950	30	2
1	I	954	977	961	31	8
1	J	925	953	933	36	8
1	K	934	951	926	37	1
1	L	962	983	969	49	0
2	A	18	24	24	3	0
2	B	24	32	32	0	0
2	E	6	8	8	0	0
2	F	24	32	32	1	0
2	H	6	8	8	0	0
2	I	6	8	8	0	0
2	J	6	8	8	0	0
2	L	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	53	0	0	0	0
3	B	43	0	0	0	0
3	C	47	0	0	0	0
3	D	52	0	0	0	0
3	E	41	0	0	1	0
3	F	56	0	0	3	0
3	G	53	0	0	1	0
3	H	49	0	0	1	0
3	I	48	0	0	0	0
3	J	38	0	0	1	0
3	K	60	0	0	0	0
3	L	45	0	0	2	1
All	All	11858	11534	11301	322	46

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 14.

The worst 5 of 322 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:D:339:THR:O	1:E:420:THR:HG22	1.41	1.19
1:H:325:TYR:OH	1:K:325:TYR:CE2	2.07	1.08
1:L:331:CYS:HB2	1:L:333:LEU:HD12	1.41	1.01
1:B:329:GLN:HE21	1:I:334:LEU:HD12	1.29	0.96
1:C:379:ASN:HD22	1:J:341:TYR:HE2	1.14	0.95

The worst 5 of 46 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)
1:C:336:LEU:CD1	1:F:306:ASN:O[4_454]	0.87	1.33
1:C:359:LEU:CD2	1:F:361:THR:CG2[4_454]	1.17	1.03
1:J:361:THR:HG1	1:I:359:LEU:HD23[4_454]	0.60	1.00
1:C:332:SER:O	1:F:332:SER:OG[4_454]	1.22	0.98
1:C:336:LEU:CG	1:F:306:ASN:O[4_454]	1.29	0.91

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	122/128 (95%)	114 (93%)	8 (7%)	0	100	100
1	B	116/128 (91%)	112 (97%)	4 (3%)	0	100	100
1	C	124/128 (97%)	117 (94%)	6 (5%)	1 (1%)	19	14
1	D	122/128 (95%)	114 (93%)	8 (7%)	0	100	100
1	E	104/128 (81%)	100 (96%)	4 (4%)	0	100	100
1	F	115/128 (90%)	112 (97%)	3 (3%)	0	100	100
1	G	116/128 (91%)	114 (98%)	2 (2%)	0	100	100
1	H	113/128 (88%)	107 (95%)	6 (5%)	0	100	100
1	I	122/128 (95%)	114 (93%)	8 (7%)	0	100	100
1	J	114/128 (89%)	113 (99%)	1 (1%)	0	100	100
1	K	117/128 (91%)	113 (97%)	4 (3%)	0	100	100
1	L	117/128 (91%)	115 (98%)	2 (2%)	0	100	100
All	All	1402/1536 (91%)	1345 (96%)	56 (4%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	349	GLY

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	101/113 (89%)	92 (91%)	9 (9%)	9	6
1	B	100/113 (88%)	93 (93%)	7 (7%)	15	11
1	C	99/113 (88%)	89 (90%)	10 (10%)	7	4
1	D	98/113 (87%)	86 (88%)	12 (12%)	5	2
1	E	92/113 (81%)	82 (89%)	10 (11%)	6	3
1	F	102/113 (90%)	90 (88%)	12 (12%)	5	2
1	G	99/113 (88%)	83 (84%)	16 (16%)	2	1
1	H	103/113 (91%)	89 (86%)	14 (14%)	3	2
1	I	103/113 (91%)	91 (88%)	12 (12%)	5	2
1	J	100/113 (88%)	87 (87%)	13 (13%)	4	2
1	K	99/113 (88%)	89 (90%)	10 (10%)	7	4
1	L	105/113 (93%)	94 (90%)	11 (10%)	7	3
All	All	1201/1356 (89%)	1065 (89%)	136 (11%)	6	3

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	296	VAL
1	L	337	MET
1	K	377	GLN
1	F	419	ILE
1	F	418	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	329	GLN
1	J	379	ASN
1	J	377	GLN
1	I	319	GLN
1	D	394	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	GOL	B	454	-	5,5,5	0.23	0	5,5,5	0.41	0
2	GOL	L	451	-	5,5,5	0.24	0	5,5,5	0.45	0
2	GOL	A	451	-	5,5,5	0.18	0	5,5,5	0.21	0
2	GOL	A	453	-	5,5,5	0.26	0	5,5,5	0.44	0
2	GOL	E	451	-	5,5,5	0.27	0	5,5,5	1.10	0
2	GOL	B	451	-	5,5,5	0.32	0	5,5,5	0.47	0
2	GOL	F	454	-	5,5,5	0.51	0	5,5,5	0.77	0
2	GOL	I	451	-	5,5,5	0.42	0	5,5,5	0.71	0
2	GOL	B	453	-	5,5,5	0.12	0	5,5,5	0.35	0
2	GOL	A	452	-	5,5,5	0.46	0	5,5,5	0.36	0
2	GOL	F	451	-	5,5,5	0.28	0	5,5,5	0.50	0
2	GOL	F	452	-	5,5,5	0.41	0	5,5,5	0.77	0
2	GOL	B	452	-	5,5,5	0.45	0	5,5,5	0.89	0
2	GOL	J	451	-	5,5,5	0.26	0	5,5,5	0.46	0
2	GOL	F	453	-	5,5,5	0.27	0	5,5,5	0.64	0
2	GOL	H	451	-	5,5,5	0.16	0	5,5,5	0.42	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	GOL	B	454	-	-	0/4/4/4	-
2	GOL	L	451	-	-	2/4/4/4	-
2	GOL	A	451	-	-	1/4/4/4	-
2	GOL	A	453	-	-	3/4/4/4	-
2	GOL	E	451	-	-	0/4/4/4	-
2	GOL	B	451	-	-	2/4/4/4	-
2	GOL	F	454	-	-	2/4/4/4	-
2	GOL	I	451	-	-	1/4/4/4	-
2	GOL	B	453	-	-	4/4/4/4	-
2	GOL	A	452	-	-	4/4/4/4	-
2	GOL	F	451	-	-	2/4/4/4	-
2	GOL	F	452	-	-	4/4/4/4	-
2	GOL	B	452	-	-	0/4/4/4	-
2	GOL	J	451	-	-	2/4/4/4	-
2	GOL	F	453	-	-	2/4/4/4	-
2	GOL	H	451	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	451	GOL	C1-C2-C3-O3
2	B	451	GOL	O2-C2-C3-O3
2	B	453	GOL	O1-C1-C2-O2
2	F	451	GOL	C1-C2-C3-O3
2	F	453	GOL	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	451	GOL	1	0
2	A	453	GOL	1	0
2	A	452	GOL	1	0
2	F	453	GOL	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	124/128 (96%)	0.35	4 (3%) 47 54	25, 33, 46, 53	0
1	B	120/128 (93%)	0.15	2 (1%) 70 74	22, 33, 44, 54	0
1	C	126/128 (98%)	0.24	8 (6%) 20 24	19, 34, 45, 58	0
1	D	124/128 (96%)	0.05	1 (0%) 86 88	23, 33, 44, 52	0
1	E	110/128 (85%)	0.18	2 (1%) 68 72	23, 33, 47, 55	0
1	F	121/128 (94%)	0.30	2 (1%) 70 74	24, 32, 43, 50	0
1	G	120/128 (93%)	0.18	4 (3%) 46 53	23, 34, 45, 57	0
1	H	119/128 (92%)	0.45	4 (3%) 45 51	23, 31, 44, 52	0
1	I	124/128 (96%)	0.37	2 (1%) 72 76	24, 33, 45, 53	0
1	J	120/128 (93%)	0.33	5 (4%) 36 42	21, 33, 48, 55	0
1	K	123/128 (96%)	0.19	6 (4%) 29 35	23, 35, 46, 55	0
1	L	123/128 (96%)	0.20	2 (1%) 72 76	23, 34, 44, 60	0
All	All	1454/1536 (94%)	0.25	42 (2%) 51 57	19, 33, 46, 60	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	406	ILE	5.8
1	L	296	VAL	4.4
1	C	349	GLY	4.3
1	J	406	ILE	4.1
1	B	408	ASN	4.1

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(\AA^2)	Q<0.9
2	GOL	B	452	6/6	0.57	0.27	36,46,53,54	2
2	GOL	A	453	6/6	0.79	0.17	43,47,51,52	2
2	GOL	F	451	6/6	0.80	0.24	43,49,55,60	2
2	GOL	A	452	6/6	0.83	0.14	36,46,50,52	2
2	GOL	I	451	6/6	0.83	0.17	40,55,67,69	2
2	GOL	F	454	6/6	0.85	0.17	29,41,48,49	2
2	GOL	A	451	6/6	0.86	0.11	41,43,47,48	2
2	GOL	E	451	6/6	0.86	0.15	43,50,57,62	2
2	GOL	F	453	6/6	0.86	0.19	37,43,51,67	2
2	GOL	L	451	6/6	0.86	0.17	41,44,48,49	2
2	GOL	F	452	6/6	0.88	0.18	43,47,50,50	2
2	GOL	B	451	6/6	0.89	0.14	32,49,59,59	2
2	GOL	B	453	6/6	0.89	0.23	42,45,53,54	2
2	GOL	H	451	6/6	0.90	0.18	43,44,50,50	2
2	GOL	J	451	6/6	0.92	0.13	38,43,46,49	2
2	GOL	B	454	6/6	0.97	0.16	37,43,49,53	2

6.5 Other polymers [i](#)

There are no such residues in this entry.