



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 30, 2021 – 02:52 PM EST

PDB ID : 3DUG
Title : Crystal structure of zn-dependent arginine carboxypeptidase complexed with zinc
Authors : Patskovsky, Y.; Ramagopal, U.A.; Toro, R.; Meyer, A.J.; Freeman, J.; Iizuka, M.; Bain, K.; Rodgers, L.; Raushel, F.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-07-17
Resolution : 2.62 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 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 : 2.16
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) : 2.16

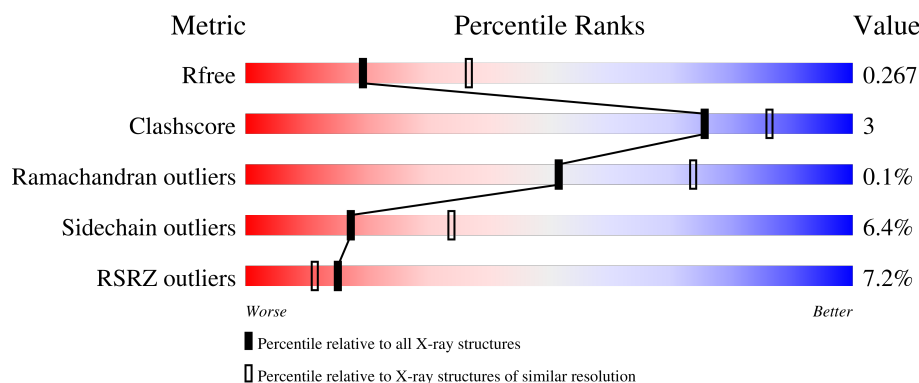
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 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	408	<div> <div>4%</div> <div>84%</div> <div>11%</div> <div>..</div> </div>
1	B	408	<div> <div>4%</div> <div>84%</div> <div>11%</div> <div>..</div> </div>
1	C	408	<div> <div>11%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>
1	D	408	<div> <div>7%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>
1	E	408	<div> <div>5%</div> <div>84%</div> <div>11%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	408	
1	G	408	
1	H	408	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	433	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24575 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 ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	2	0
			3012	1893	525	578	16			
1	B	394	Total	C	N	O	S	0	2	0
			3012	1893	525	578	16			
1	C	395	Total	C	N	O	S	0	2	0
			3026	1901	529	580	16			
1	D	394	Total	C	N	O	S	0	0	0
			3001	1886	522	577	16			
1	E	394	Total	C	N	O	S	0	0	0
			3001	1886	522	577	16			
1	F	395	Total	C	N	O	S	0	2	0
			3021	1898	524	583	16			
1	G	394	Total	C	N	O	S	0	0	0
			3001	1886	522	577	16			
1	H	394	Total	C	N	O	S	0	4	0
			3027	1902	529	580	16			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

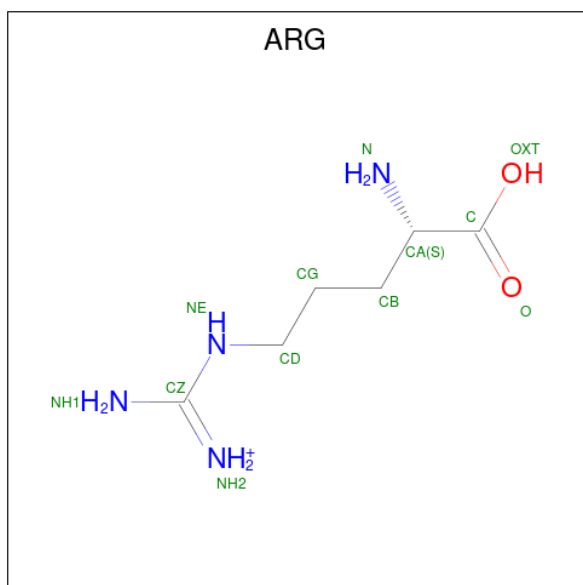
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	4	Total	Zn	0	0
			4	4		
2	D	4	Total	Zn	0	0
			4	4		
2	E	4	Total	Zn	0	0
			4	4		
2	H	4	Total	Zn	0	0
			4	4		
2	B	4	Total	Zn	0	0
			4	4		
2	C	4	Total	Zn	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Zn	0	0
			4	4		
2	F	4	Total	Zn	0	0
			4	4		

- Molecule 3 is ARGinine (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	6	4	2		
3	B	1	Total	C	N	O	0	0
			12	6	4	2		
3	C	1	Total	C	N	O	0	0
			12	6	4	2		
3	D	1	Total	C	N	O	0	0
			12	6	4	2		
3	E	1	Total	C	N	O	0	0
			12	6	4	2		
3	F	1	Total	C	N	O	0	0
			12	6	4	2		
3	G	1	Total	C	N	O	0	0
			12	6	4	2		
3	H	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total	O	0	0
			24	24		
5	B	37	Total	O	0	0
			37	37		

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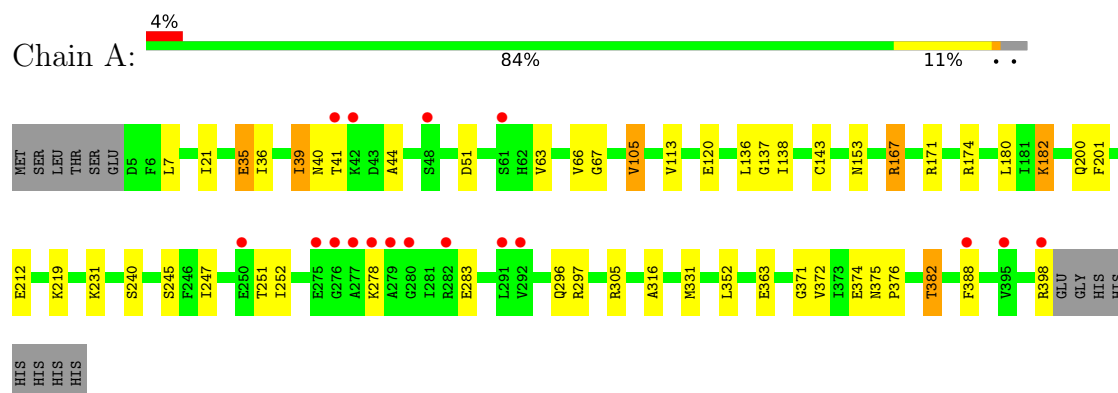
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	34	Total 34	O 34	0	0
5	D	27	Total 27	O 27	0	0
5	E	40	Total 40	O 40	0	0
5	F	40	Total 40	O 40	0	0
5	G	31	Total 31	O 31	0	0
5	H	53	Total 53	O 53	0	0

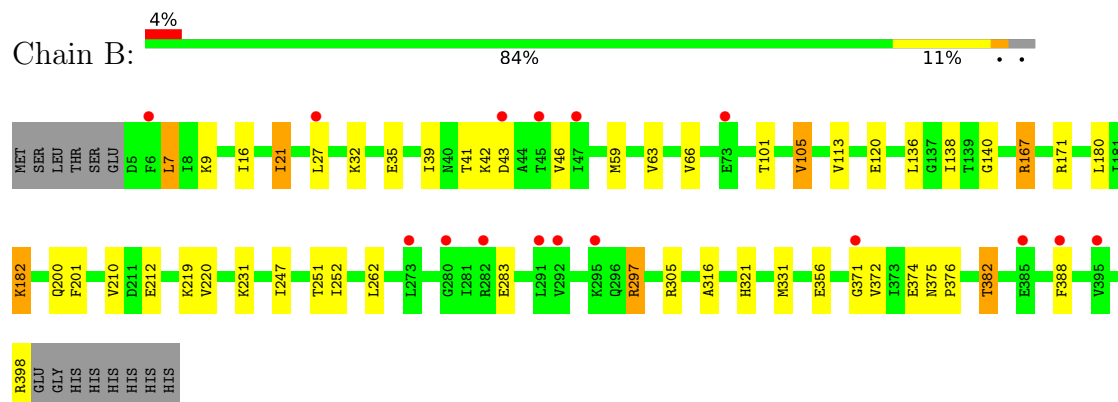
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

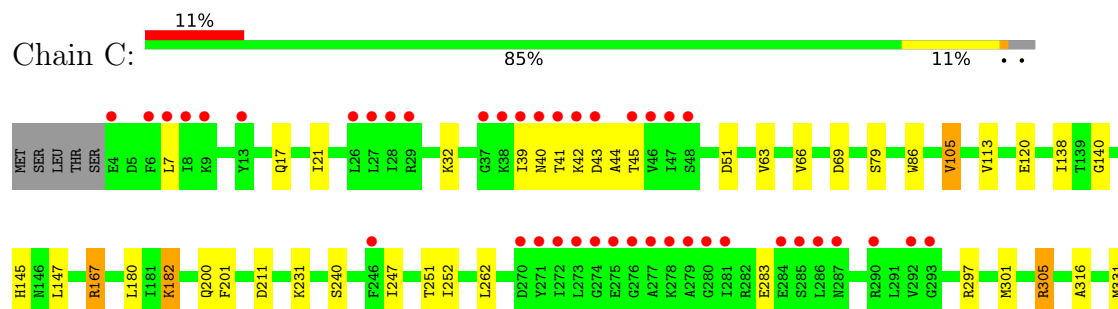
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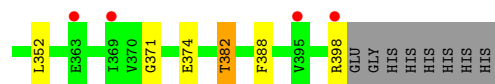


• Molecule 1: ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE

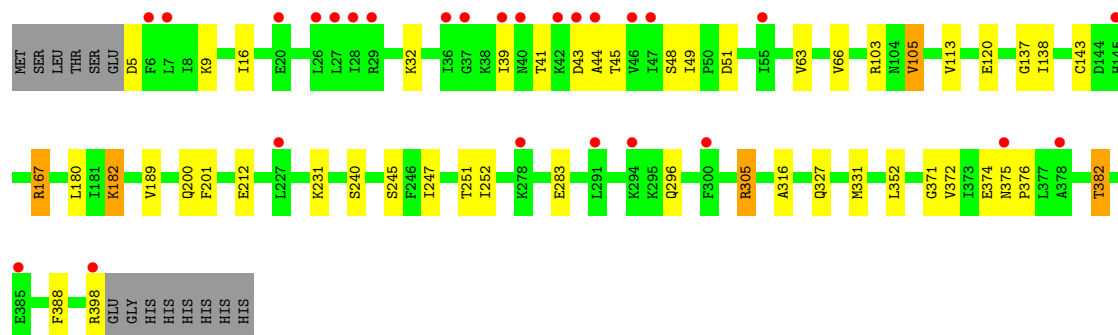
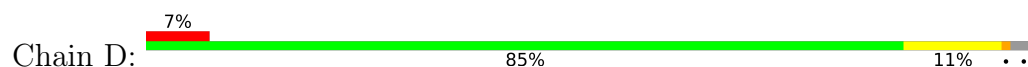


• Molecule 1: ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE

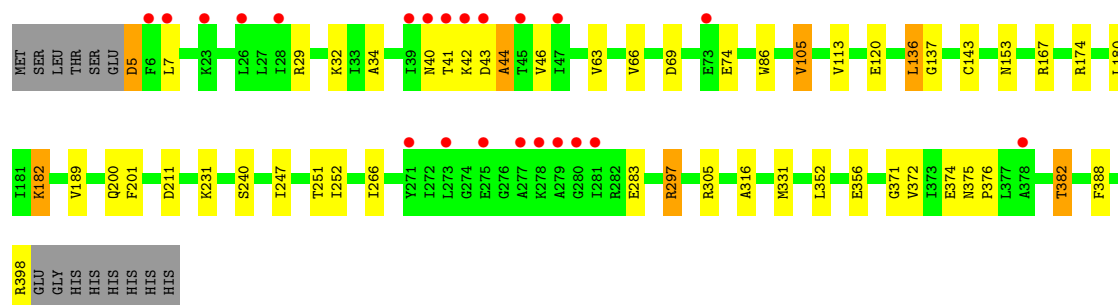
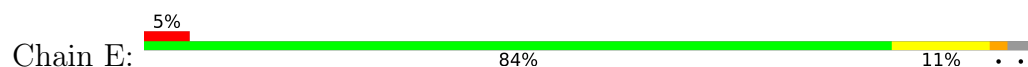




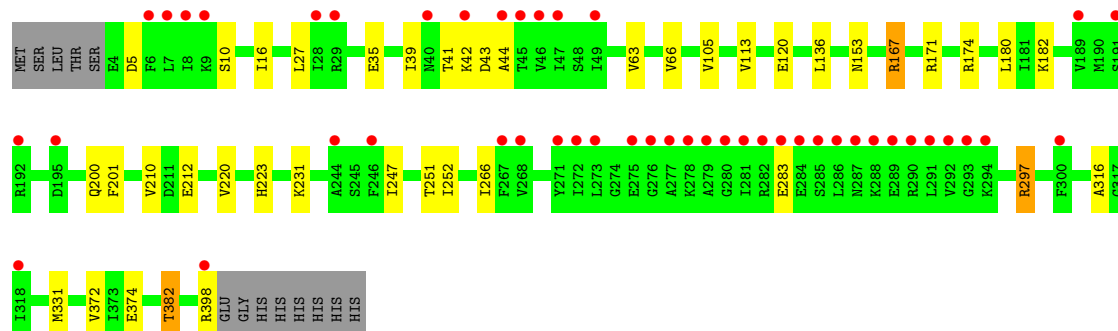
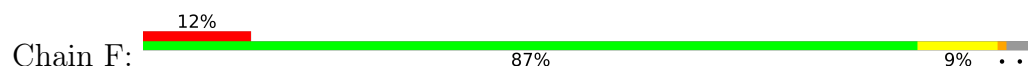
• Molecule 1: ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE



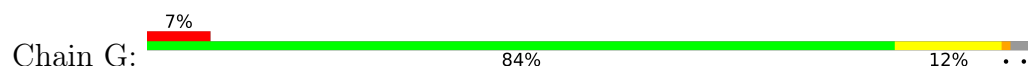
• Molecule 1: ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE

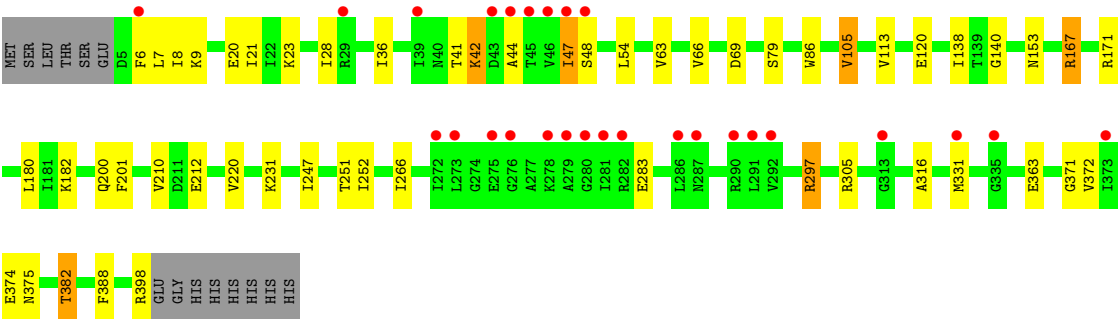


• Molecule 1: ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE

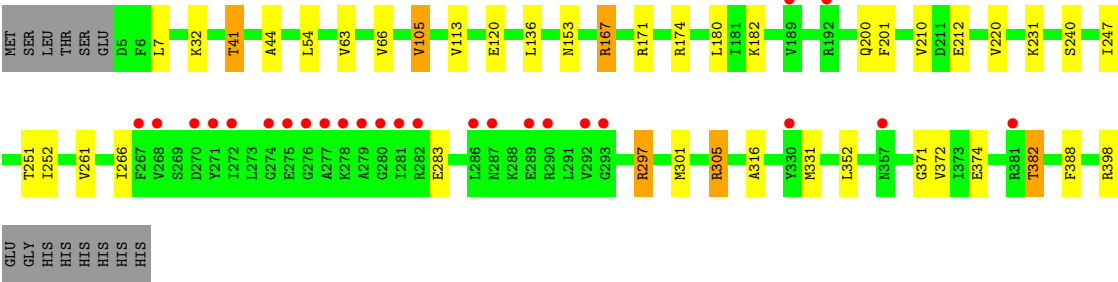
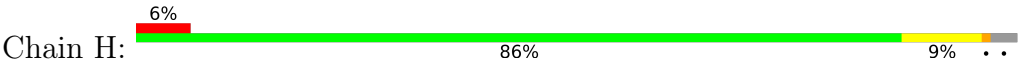


• Molecule 1: ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE





● Molecule 1: ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.33Å 146.04Å 255.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.62 37.37 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.62) 99.1 (37.37-2.62)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.264 0.233 , 0.267	Depositor DCC
R_{free} test set	3818 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24575	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: GOL, ZN, KCX

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	0.37	0/3052	0.58	1/4115 (0.0%)
1	B	0.38	0/3052	0.59	2/4115 (0.0%)
1	C	0.39	0/3066	0.57	0/4133
1	D	0.38	0/3035	0.57	0/4093
1	E	0.38	0/3035	0.58	1/4093 (0.0%)
1	F	0.40	0/3061	0.59	0/4128
1	G	0.38	0/3035	0.58	0/4093
1	H	0.39	0/3071	0.59	1/4141 (0.0%)
All	All	0.38	0/24407	0.58	5/32911 (0.0%)

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	0	1
1	B	0	1
1	C	0	2
1	D	0	1
1	E	0	2
1	F	0	1
1	G	0	2
1	H	0	2
All	All	0	12

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	ARG	CG-CD-NE	5.72	123.82	111.80
1	A	136	LEU	CA-CB-CG	5.58	128.12	115.30
1	B	297	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	E	136	LEU	CA-CB-CG	5.23	127.34	115.30
1	H	136	LEU	CA-CB-CG	5.16	127.18	115.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	ALA	Peptide
1	B	42	LYS	Peptide
1	C	42	LYS	Peptide
1	C	44	ALA	Peptide
1	D	43	ASP	Peptide

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	3012	0	3020	20	0
1	B	3012	0	3019	20	0
1	C	3026	0	3034	18	0
1	D	3001	0	3002	23	0
1	E	3001	0	3002	22	0
1	F	3021	0	3019	16	0
1	G	3001	0	3002	20	0
1	H	3027	0	3032	18	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
3	A	12	0	12	0	0
3	B	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	12	0	12	0	0
3	D	12	0	12	1	0
3	E	12	0	12	1	0
3	F	12	0	12	1	0
3	G	12	0	12	0	0
3	H	12	0	12	0	0
4	A	6	0	8	1	0
4	B	24	0	32	2	0
4	D	6	0	8	0	0
4	E	12	0	16	0	0
4	G	6	0	8	0	0
4	H	6	0	8	0	0
5	A	24	0	0	0	0
5	B	37	0	0	0	0
5	C	34	0	0	0	0
5	D	27	0	0	1	0
5	E	40	0	0	0	0
5	F	40	0	0	0	0
5	G	31	0	0	0	0
5	H	53	0	0	0	0
All	All	24575	0	24306	149	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 3.

The worst 5 of 149 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:E:305:ARG:HG2	1:E:305:ARG:HH21	1.16	1.07
1:D:305:ARG:HH21	1:D:305:ARG:HG2	1.19	1.06
1:D:305:ARG:NH2	1:D:305:ARG:HG2	1.78	0.93
1:E:305:ARG:CG	1:E:305:ARG:HH21	1.83	0.91
1:D:305:ARG:CG	1:D:305:ARG:HH21	1.85	0.88

There are no symmetry-related clashes.

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	393/408 (96%)	379 (96%)	14 (4%)	0	100	100
1	B	393/408 (96%)	377 (96%)	16 (4%)	0	100	100
1	C	394/408 (97%)	375 (95%)	18 (5%)	1 (0%)	41	62
1	D	391/408 (96%)	374 (96%)	17 (4%)	0	100	100
1	E	391/408 (96%)	370 (95%)	20 (5%)	1 (0%)	41	62
1	F	394/408 (97%)	376 (95%)	18 (5%)	0	100	100
1	G	391/408 (96%)	375 (96%)	16 (4%)	0	100	100
1	H	395/408 (97%)	378 (96%)	17 (4%)	0	100	100
All	All	3142/3264 (96%)	3004 (96%)	136 (4%)	2 (0%)	51	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	40	ASN
1	E	40	ASN

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	318/329 (97%)	297 (93%)	21 (7%)	16	32
1	B	318/329 (97%)	295 (93%)	23 (7%)	14	27
1	C	319/329 (97%)	296 (93%)	23 (7%)	14	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	316/329 (96%)	298 (94%)	18 (6%)	20	39
1	E	316/329 (96%)	296 (94%)	20 (6%)	18	35
1	F	319/329 (97%)	302 (95%)	17 (5%)	22	43
1	G	316/329 (96%)	294 (93%)	22 (7%)	15	29
1	H	320/329 (97%)	302 (94%)	18 (6%)	21	40
All	All	2542/2632 (97%)	2380 (94%)	162 (6%)	17	34

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	51	ASP
1	E	74	GLU
1	H	105	VAL
1	D	105	VAL
1	D	372	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	40	ASN
1	C	360	GLN
1	F	17	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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
1	KCX	G	182	1,2	7,11,12	0.67	0	4,12,14	1.07	0
1	KCX	A	182	1,2	7,11,12	0.84	0	4,12,14	1.23	1 (25%)
1	KCX	C	182	1	7,11,12	0.76	0	4,12,14	1.27	1 (25%)
1	KCX	F	182	1	7,11,12	0.66	0	4,12,14	1.15	0
1	KCX	H	182	1	7,11,12	0.72	0	4,12,14	0.93	0
1	KCX	B	182	1,2	7,11,12	0.57	0	4,12,14	1.24	1 (25%)
1	KCX	D	182	1,2	7,11,12	0.71	0	4,12,14	1.37	1 (25%)
1	KCX	E	182	1,2	7,11,12	0.68	0	4,12,14	1.39	1 (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
1	KCX	G	182	1,2	-	2/7/10/12	-
1	KCX	A	182	1,2	-	2/7/10/12	-
1	KCX	C	182	1	-	2/7/10/12	-
1	KCX	F	182	1	-	2/7/10/12	-
1	KCX	H	182	1	-	2/7/10/12	-
1	KCX	B	182	1,2	-	2/7/10/12	-
1	KCX	D	182	1,2	-	2/7/10/12	-
1	KCX	E	182	1,2	-	2/7/10/12	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	182	KCX	CE-NZ-CX	-2.44	118.81	122.95
1	D	182	KCX	CE-NZ-CX	-2.42	118.85	122.95
1	C	182	KCX	CE-NZ-CX	-2.28	119.09	122.95
1	A	182	KCX	CE-NZ-CX	-2.15	119.31	122.95
1	B	182	KCX	CE-NZ-CX	-2.12	119.35	122.95

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	182	KCX	CG-CD-CE-NZ
1	D	182	KCX	CG-CD-CE-NZ
1	F	182	KCX	CG-CD-CE-NZ
1	G	182	KCX	CG-CD-CE-NZ
1	H	182	KCX	CG-CD-CE-NZ

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	182	KCX	1	0
1	A	182	KCX	1	0
1	C	182	KCX	1	0
1	F	182	KCX	1	0
1	H	182	KCX	1	0
1	B	182	KCX	1	0
1	D	182	KCX	1	0
1	E	182	KCX	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 32 are monoatomic - leaving 18 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	$\# Z > 2$
4	GOL	E	430	-	5,5,5	0.36	0	5,5,5	0.33	0
3	ARG	H	429	-	7,11,11	0.57	0	6,13,13	0.28	0
4	GOL	A	430	-	5,5,5	0.46	0	5,5,5	0.10	0
3	ARG	F	429	-	7,11,11	0.46	0	6,13,13	0.55	0
4	GOL	B	432	-	5,5,5	0.30	0	5,5,5	0.38	0
3	ARG	A	429	-	7,11,11	0.52	0	6,13,13	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	431	-	5,5,5	0.45	0	5,5,5	0.25	0
4	GOL	E	431	-	5,5,5	0.37	0	5,5,5	0.19	0
4	GOL	H	430	-	5,5,5	0.40	0	5,5,5	0.52	0
4	GOL	D	430	-	5,5,5	0.34	0	5,5,5	0.32	0
4	GOL	B	430	-	5,5,5	0.37	0	5,5,5	0.28	0
3	ARG	G	429	-	7,11,11	0.49	0	6,13,13	0.60	0
3	ARG	D	429	-	7,11,11	0.51	0	6,13,13	0.53	0
3	ARG	E	429	-	7,11,11	0.48	0	6,13,13	0.33	0
3	ARG	B	429	-	7,11,11	0.59	0	6,13,13	0.45	0
3	ARG	C	429	-	7,11,11	0.53	0	6,13,13	0.38	0
4	GOL	B	433	-	5,5,5	0.36	0	5,5,5	0.37	0
4	GOL	G	430	-	5,5,5	0.48	0	5,5,5	0.53	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
4	GOL	E	430	-	-	2/4/4/4	-
3	ARG	H	429	-	-	3/7/11/11	-
4	GOL	A	430	-	-	4/4/4/4	-
3	ARG	F	429	-	-	0/7/11/11	-
4	GOL	B	432	-	-	2/4/4/4	-
3	ARG	A	429	-	-	1/7/11/11	-
4	GOL	B	431	-	-	4/4/4/4	-
4	GOL	E	431	-	-	2/4/4/4	-
4	GOL	H	430	-	-	2/4/4/4	-
4	GOL	D	430	-	-	4/4/4/4	-
4	GOL	B	430	-	-	2/4/4/4	-
3	ARG	G	429	-	-	0/7/11/11	-
3	ARG	D	429	-	-	1/7/11/11	-
3	ARG	E	429	-	-	1/7/11/11	-
3	ARG	B	429	-	-	0/7/11/11	-
3	ARG	C	429	-	-	1/7/11/11	-
4	GOL	B	433	-	-	2/4/4/4	-
4	GOL	G	430	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	430	GOL	C1-C2-C3-O3
4	B	430	GOL	O1-C1-C2-C3
3	C	429	ARG	C-CA-CB-CG
4	B	432	GOL	C1-C2-C3-O3
4	A	430	GOL	O1-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	430	GOL	1	0
3	F	429	ARG	1	0
4	B	432	GOL	1	0
3	D	429	ARG	1	0
3	E	429	ARG	1	0
4	B	433	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 ⓘ

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	393/408 (96%)	0.15	17 (4%)	35	29	45, 73, 104, 136	0
1	B	393/408 (96%)	0.26	16 (4%)	37	31	45, 74, 111, 136	0
1	C	394/408 (96%)	0.39	45 (11%)	5	3	47, 76, 114, 136	0
1	D	393/408 (96%)	0.35	27 (6%)	16	12	43, 75, 113, 142	0
1	E	393/408 (96%)	0.26	22 (5%)	24	19	45, 74, 110, 143	0
1	F	394/408 (96%)	0.56	47 (11%)	4	3	46, 72, 106, 136	0
1	G	393/408 (96%)	0.30	27 (6%)	16	12	39, 74, 110, 136	0
1	H	393/408 (96%)	0.26	25 (6%)	19	15	45, 69, 104, 136	0
All	All	3146/3264 (96%)	0.32	226 (7%)	15	11	39, 73, 110, 143	0

The worst 5 of 226 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	280	GLY	8.7
1	F	279	ALA	8.7
1	F	268	VAL	8.2
1	F	285	SER	7.7
1	F	286	LEU	7.2

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

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
1	KCX	D	182	12/13	0.92	0.25	54,63,103,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	A	182	12/13	0.93	0.26	56,66,102,108	0
1	KCX	F	182	12/13	0.93	0.18	54,63,103,111	0
1	KCX	H	182	12/13	0.93	0.21	56,65,102,109	0
1	KCX	G	182	12/13	0.93	0.21	57,66,103,109	0
1	KCX	E	182	12/13	0.94	0.32	54,67,103,108	0
1	KCX	C	182	12/13	0.95	0.23	55,66,102,108	0
1	KCX	B	182	12/13	0.95	0.20	55,64,104,109	0

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	ZN	F	428	1/1	0.66	0.15	127,127,127,127	1
2	ZN	G	427	1/1	0.72	0.20	74,74,74,74	1
4	GOL	B	433	6/6	0.72	0.44	93,96,98,99	0
4	GOL	A	430	6/6	0.75	0.32	77,89,90,93	0
3	ARG	F	429	12/12	0.77	0.26	98,108,130,132	0
4	GOL	B	432	6/6	0.78	0.32	75,92,94,95	0
3	ARG	A	429	12/12	0.79	0.26	81,84,86,87	0
4	GOL	G	430	6/6	0.81	0.29	58,70,74,77	0
2	ZN	H	428	1/1	0.81	0.19	127,127,127,127	1
4	GOL	D	430	6/6	0.81	0.28	85,95,99,100	0
3	ARG	C	429	12/12	0.83	0.24	85,92,100,105	0
2	ZN	A	427	1/1	0.84	0.10	122,122,122,122	0
4	GOL	E	431	6/6	0.84	0.43	87,94,97,105	0
4	GOL	B	431	6/6	0.85	0.25	60,75,79,84	0
3	ARG	D	429	12/12	0.86	0.17	78,84,85,85	0
3	ARG	H	429	12/12	0.86	0.21	68,82,106,108	0
4	GOL	E	430	6/6	0.87	0.23	84,89,93,101	0
2	ZN	F	427	1/1	0.87	0.24	113,113,113,113	0
2	ZN	A	428	1/1	0.89	0.28	106,106,106,106	1
3	ARG	B	429	12/12	0.89	0.17	61,74,94,95	0
3	ARG	G	429	12/12	0.89	0.25	87,95,102,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	C	426	1/1	0.89	0.19	117,117,117,117	0
3	ARG	E	429	12/12	0.90	0.17	66,71,76,77	0
4	GOL	H	430	6/6	0.91	0.29	67,81,86,100	0
4	GOL	B	430	6/6	0.91	0.28	95,100,103,106	0
2	ZN	C	427	1/1	0.91	0.21	67,67,67,67	1
2	ZN	D	427	1/1	0.92	0.32	78,78,78,78	1
2	ZN	D	426	1/1	0.92	0.18	128,128,128,128	0
2	ZN	C	428	1/1	0.92	0.15	106,106,106,106	1
2	ZN	H	427	1/1	0.93	0.08	118,118,118,118	0
2	ZN	E	428	1/1	0.93	0.20	91,91,91,91	1
2	ZN	B	428	1/1	0.94	0.15	87,87,87,87	1
2	ZN	G	426	1/1	0.94	0.37	78,78,78,78	1
2	ZN	D	428	1/1	0.95	0.20	89,89,89,89	1
2	ZN	B	426	1/1	0.95	0.35	77,77,77,77	1
2	ZN	A	426	1/1	0.95	0.15	104,104,104,104	0
2	ZN	F	425	1/1	0.95	0.16	93,93,93,93	0
2	ZN	G	428	1/1	0.95	0.21	101,101,101,101	1
2	ZN	E	427	1/1	0.95	0.33	76,76,76,76	1
2	ZN	B	427	1/1	0.96	0.38	80,80,80,80	1
2	ZN	B	425	1/1	0.96	0.22	85,85,85,85	0
2	ZN	F	426	1/1	0.97	0.22	98,98,98,98	0
2	ZN	H	425	1/1	0.97	0.15	93,93,93,93	0
2	ZN	E	426	1/1	0.97	0.17	102,102,102,102	0
2	ZN	C	425	1/1	0.97	0.18	93,93,93,93	0
2	ZN	G	425	1/1	0.97	0.22	93,93,93,93	0
2	ZN	E	425	1/1	0.97	0.22	88,88,88,88	0
2	ZN	A	425	1/1	0.97	0.23	92,92,92,92	0
2	ZN	D	425	1/1	0.98	0.19	88,88,88,88	0
2	ZN	H	426	1/1	0.98	0.12	95,95,95,95	0

6.5 Other polymers ⓘ

There are no such residues in this entry.