



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:30 PM GMT

PDB ID : 1PCA
Title : THREE DIMENSIONAL STRUCTURE OF PORCINE PANCREATIC PRO-CARBOXYPEPTIDASE A. A COMPARISON OF THE A AND B ZYMOGENS AND THEIR DETERMINANTS FOR INHIBITION AND ACTIVATION
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Deposited on : 1991-10-28
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

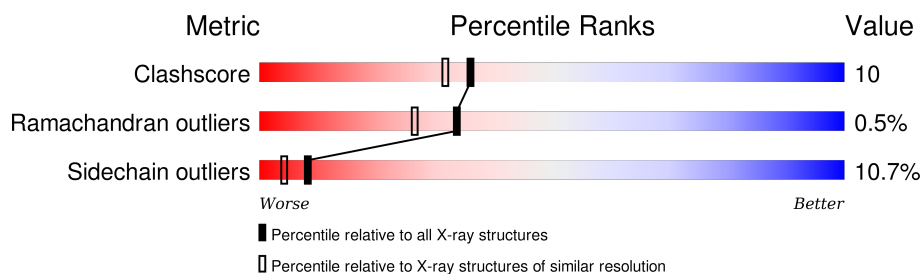
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	403	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3508 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 PROCARBOXYPEPTIDASE A PCPA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	402	3192	2036	540	609	7	129	0	0

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3A	LYS	ALA	CONFLICT	UNP P09954
A	31	ALA	GLN	CONFLICT	UNP P09954
A	40	ARG	SER	CONFLICT	UNP P09954
A	57	SER	ASN	CONFLICT	UNP P09954
A	66	SER	THR	CONFLICT	UNP P09954
A	74	ILE	VAL	CONFLICT	UNP P09954
A	89	ASN	ASP	CONFLICT	UNP P09954
A	93	ASN	ASP	CONFLICT	UNP P09954
A	94	SER	PRO	CONFLICT	UNP P09954
A	95	SER	ALA	CONFLICT	UNP P09954
A	102	SER	ASN	CONFLICT	UNP P09954
A	103	MET	LEU	CONFLICT	UNP P09954
A	114	ASN	ASP	CONFLICT	UNP P09954
A	122	ASP	GLU	CONFLICT	UNP P09954
A	125	LEU	MET	CONFLICT	UNP P09954
A	132	LYS	ARG	CONFLICT	UNP P09954
A	133	ALA	THR	CONFLICT	UNP P09954
A	137	LEU	PHE	CONFLICT	UNP P09954
A	141	SER	VAL	CONFLICT	UNP P09954
A	143	SER	PRO	CONFLICT	UNP P09954
A	159	SER	ASN	CONFLICT	UNP P09954
A	162	ALA	SER	CONFLICT	UNP P09954
A	169	TYR	PHE	CONFLICT	UNP P09954
A	180	THR	VAL	CONFLICT	UNP P09954
A	184	LYS	ASN	CONFLICT	UNP P09954
A	185	ASN	ASP	CONFLICT	UNP P09954
A	186	ASN	HIS	CONFLICT	UNP P09954

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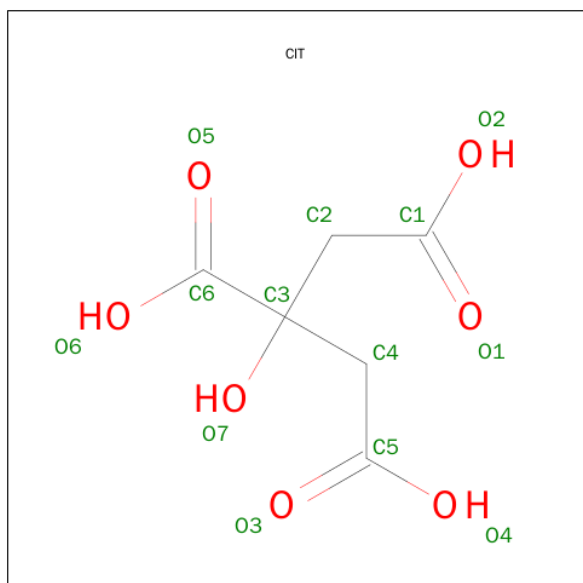
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Chain	Residue	Modelled	Actual	Comment	Reference
A	211	GLN	GLU	CONFLICT	UNP P09954
A	212	SER	ALA	CONFLICT	UNP P09954
A	217	SER	ASP	CONFLICT	UNP P09954
A	220	ASN	ASP	CONFLICT	UNP P09954
A	223	ALA	SER	CONFLICT	UNP P09954
A	231	LYS	THR	CONFLICT	UNP P09954
A	237	SER	LYS	CONFLICT	UNP P09954
A	238	TYR	PHE	CONFLICT	UNP P09954
A	239	LYS	GLN	CONFLICT	UNP P09954
A	246	VAL	THR	CONFLICT	UNP P09954
A	254	VAL	THR	CONFLICT	UNP P09954
A	277	ARG	TYR	CONFLICT	UNP P09954
A	307	ASN	HIS	CONFLICT	UNP P09954
A	308	SER	PRO	CONFLICT	UNP P09954

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

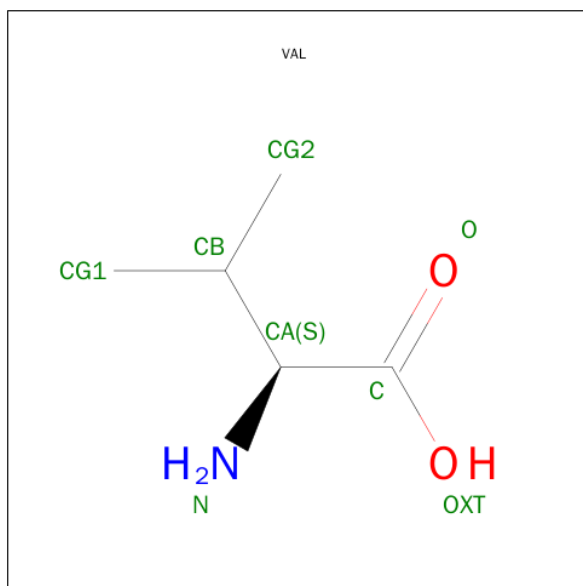
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0

- Molecule 4 is VALINE (three-letter code: VAL) (formula: $C_5H_{11}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	1	0
			8	5	1	2		

- Molecule 5 is water.

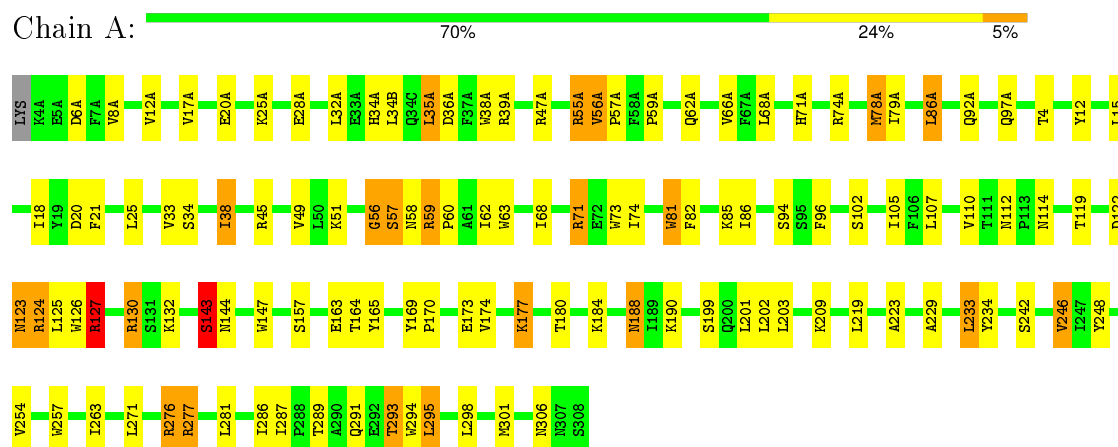
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	294	Total	O	0	0
			294	294		

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.

Note EDS was not executed.

• Molecule 1: PROCARBOXYPEPTIDASE A PCPA



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.06 Å 76.92 Å 47.52 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3508	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.05	11/3271 (0.3%)	1.30	17/4436 (0.4%)

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	7

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	TRP	NE1-CE2	-8.76	1.26	1.37
1	A	294	TRP	NE1-CE2	-7.57	1.27	1.37
1	A	126	TRP	NE1-CE2	-7.51	1.27	1.37
1	A	257	TRP	NE1-CE2	-7.09	1.28	1.37
1	A	81	TRP	NE1-CE2	-6.67	1.28	1.37
1	A	63	TRP	NE1-CE2	-6.31	1.29	1.37
1	A	38(A)	TRP	NE1-CE2	-6.22	1.29	1.37
1	A	73	TRP	NE1-CE2	-5.65	1.30	1.37
1	A	57	SER	CB-OG	5.44	1.49	1.42
1	A	143	SER	CB-OG	5.07	1.48	1.42
1	A	223	ALA	CA-CB	5.05	1.63	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	ARG	NE-CZ-NH1	10.59	125.60	120.30
1	A	276	ARG	NE-CZ-NH2	-9.09	115.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	A	277	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	A	127	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	A	277	ARG	CD-NE-CZ	7.86	134.61	123.60
1	A	246	VAL	CA-CB-CG2	6.65	120.87	110.90
1	A	277	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	A	47(A)	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	74(A)	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	A	276	ARG	CD-NE-CZ	6.11	132.16	123.60
1	A	78(A)	MET	CG-SD-CE	-5.63	91.19	100.20
1	A	209	LYS	N-CA-CB	-5.52	100.67	110.60
1	A	12	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	A	71	ARG	CD-NE-CZ	-5.32	116.16	123.60
1	A	59	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	55(A)	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	LYS	Mainchain
1	A	201	LEU	Mainchain
1	A	202	LEU	Mainchain
1	A	263	ILE	Mainchain
1	A	306	ASN	Mainchain
1	A	56	GLY	Mainchain
1	A	59(A)	PRO	Mainchain

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	3192	0	3105	58	1
2	A	1	0	0	0	0
3	A	13	0	5	1	0
4	A	8	0	8	0	0
5	A	294	0	0	7	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3508	0	3118	58	1

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 10.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HD21	1:A:246:VAL:HG22	1.57	0.86
1:A:180:THR:HG22	1:A:184:LYS:HE3	1.56	0.85
1:A:62:ILE:HD13	1:A:301:MET:HG2	1.63	0.81
1:A:56:GLY:HA3	1:A:59:ARG:HD3	1.64	0.79
1:A:144:ASN:OD1	1:A:254:VAL:HG23	1.97	0.64
1:A:233:LEU:HD13	1:A:234:TYR:CE2	2.36	0.60
1:A:242:SER:O	1:A:246:VAL:HG13	2.02	0.59
1:A:62(A):GLN:O	1:A:66(A):VAL:HG23	2.03	0.58
1:A:107:LEU:HD22	5:A:925:HOH:O	2.03	0.58
1:A:12(A):VAL:HG13	1:A:79(A):ILE:HB	1.86	0.58
1:A:74:ILE:HD11	1:A:286:ILE:HA	1.88	0.56
1:A:71(A):HIS:HB3	3:A:600:CIT:O4	2.07	0.54
1:A:56:GLY:HA3	1:A:59:ARG:CD	2.36	0.53
1:A:271:LEU:HD22	1:A:293:THR:HG21	1.89	0.53
1:A:82:PHE:O	1:A:86:ILE:HG13	2.09	0.52
1:A:119:THR:HA	1:A:123:ASN:O	2.10	0.51
1:A:289:THR:O	1:A:293:THR:HG23	2.11	0.50
1:A:86:ILE:HD11	5:A:925:HOH:O	2.10	0.50
1:A:188:ASN:HB3	5:A:838:HOH:O	2.10	0.50
1:A:173:GLU:HG3	5:A:961:HOH:O	2.11	0.49
1:A:86:ILE:HG23	1:A:96:PHE:CZ	2.48	0.48
1:A:4:THR:HG21	1:A:25:LEU:CD1	2.43	0.48
1:A:180:THR:CG2	1:A:184:LYS:HE3	2.35	0.48
1:A:74:ILE:HD13	1:A:281:LEU:HD23	1.96	0.48
1:A:157:SER:O	1:A:165:TYR:HA	2.13	0.48
1:A:45:ARG:HH11	1:A:114:ASN:HD22	1.61	0.48
1:A:287:ILE:O	1:A:291:GLN:HG3	2.13	0.48
1:A:177:LYS:HD3	5:A:733:HOH:O	2.13	0.47
1:A:86(A):LEU:HD11	1:A:124:ARG:CG	2.45	0.47
1:A:86(A):LEU:HD13	1:A:86(A):LEU:HA	1.70	0.47
1:A:123:ASN:HD22	1:A:123:ASN:C	2.17	0.47
1:A:203:LEU:CD2	1:A:246:VAL:HG22	2.35	0.46
1:A:45:ARG:HH11	1:A:114:ASN:ND2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ILE:O	1:A:21:PHE:HB3	2.16	0.46
1:A:34(B):LEU:HB3	1:A:35(A):LEU:HD13	1.97	0.46
1:A:298:LEU:HD23	1:A:301:MET:HE3	1.98	0.45
1:A:169:TYR:HB2	1:A:170:PRO:HD2	1.98	0.45
1:A:15:LEU:HD23	1:A:110:VAL:HG11	1.99	0.45
1:A:81:TRP:CH2	1:A:85:LYS:HG3	2.52	0.45
1:A:33:VAL:HA	1:A:51:LYS:O	2.17	0.44
1:A:86(A):LEU:HD11	1:A:124:ARG:HG2	1.99	0.44
1:A:124:ARG:HD2	1:A:124:ARG:HH11	1.65	0.43
1:A:229:ALA:O	1:A:295:LEU:HD23	2.19	0.42
1:A:68:ILE:HG21	1:A:68:ILE:HD13	1.81	0.42
1:A:127:ARG:HD3	1:A:163:GLU:O	2.20	0.42
1:A:4:THR:HG21	1:A:25:LEU:HD13	2.01	0.42
1:A:56(A):VAL:HA	1:A:57(A):PRO:HD3	1.85	0.42
1:A:86:ILE:HG23	1:A:96:PHE:HZ	1.83	0.42
1:A:71:ARG:HD3	5:A:703:HOH:O	2.20	0.41
1:A:36(A):ASP:HB3	1:A:55(A):ARG:HB3	2.03	0.41
1:A:25(A):LYS:HA	1:A:25(A):LYS:HD3	1.85	0.41
1:A:143:SER:HA	5:A:961:HOH:O	2.20	0.41
1:A:38:ILE:HD12	1:A:49:VAL:CG2	2.51	0.41
1:A:105:ILE:HG21	1:A:105:ILE:HD13	1.88	0.41
1:A:6(A):ASP:HB2	1:A:8(A):VAL:HG23	2.02	0.40
1:A:28(A):GLU:O	1:A:32(A):LEU:HD13	2.21	0.40
1:A:124:ARG:O	1:A:124:ARG:HD2	2.21	0.40
1:A:34(B):LEU:HD23	1:A:34(B):LEU:HA	1.88	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:SER:O	5:A:980:HOH:O[3_646]	2.00	0.20

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	400/403 (99%)	382 (96%)	16 (4%)	2 (0%)	34	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	SER
1	A	60	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	344/345 (100%)	307 (89%)	37 (11%)	8	4

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17(A)	VAL
1	A	20(A)	GLU
1	A	34(A)	HIS
1	A	35(A)	LEU
1	A	39(A)	ARG
1	A	56(A)	VAL
1	A	68(A)	LEU
1	A	78(A)	MET
1	A	86(A)	LEU
1	A	92(A)	GLN
1	A	97(A)	GLN
1	A	20	ASP
1	A	34	SER
1	A	38	ILE
1	A	58	ASN
1	A	94	SER
1	A	102	SER

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Mol	Chain	Res	Type
1	A	112	ASN
1	A	122	ASP
1	A	123	ASN
1	A	124	ARG
1	A	125	LEU
1	A	127	ARG
1	A	130	ARG
1	A	143	SER
1	A	164	THR
1	A	174	VAL
1	A	177	LYS
1	A	188	ASN
1	A	190	LYS
1	A	219	LEU
1	A	233	LEU
1	A	248	TYR
1	A	276	ARG
1	A	277	ARG
1	A	293	THR
1	A	295	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11(A)	GLN
1	A	90(A)	GLN
1	A	92(A)	GLN
1	A	37	GLN
1	A	112	ASN
1	A	114	ASN
1	A	123	ASN
1	A	171	ASN
1	A	220	ASN
1	A	249	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
3	CIT	A	600	-	3,12,12	2.77	2 (66%)	3,17,17	3.19	3 (100%)
4	VAL	A	700	-	3,7,7	0.36	0	3,9,9	2.27	1 (33%)

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
3	CIT	A	600	-	-	0/6/16/16	0/0/0/0
4	VAL	A	700	-	-	0/4/8/8	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	CIT	C2-C3	2.79	1.59	1.54
3	A	600	CIT	C4-C3	3.86	1.60	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	VAL	CG2-CB-CG1	-3.91	99.15	110.67
3	A	600	CIT	C3-C2-C1	-3.69	109.05	114.96
3	A	600	CIT	C3-C4-C5	-3.28	109.71	114.96
3	A	600	CIT	C4-C3-C2	2.46	115.69	109.81

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
3	A	600	CIT	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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.