



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:13 AM GMT

PDB ID : 1IEC  
Title : CRYSTAL STRUCTURE OF THE CATALYTIC SITE MUTANT (H157A)  
OF THE HUMAN CYTOMEGALOVIRUS PROTEASE  
Authors : Khayat, R.; Batra, R.; Massariol, M.J.; Lagace, L.; Tong, L.  
Deposited on : 2001-04-09  
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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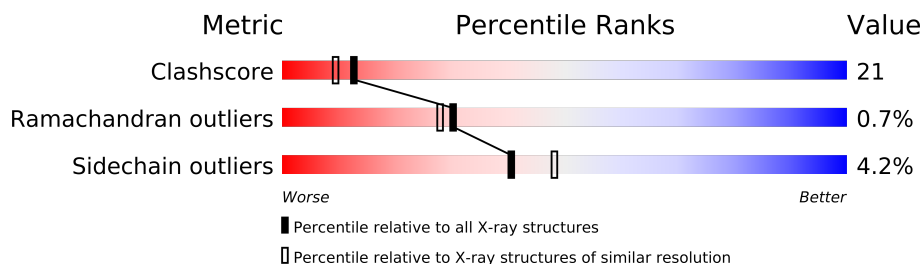
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
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 2.20 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	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	256	
1	B	256	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3492 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 CAPSID PROTEIN P40: ASSEMBLIN PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1629	1029	292	303	5			
1	B	219	Total	C	N	O	S	0	0	0
			1719	1080	307	327	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	SEB	SER	MODIFIED RESIDUE	UNP P16753
A	143	GLN	ALA	ENGINEERED	UNP P16753
A	157	ALA	HIS	ENGINEERED	UNP P16753
B	432	SEB	SER	MODIFIED RESIDUE	UNP P16753
B	443	GLN	ALA	ENGINEERED	UNP P16753
B	457	ALA	HIS	ENGINEERED	UNP P16753

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	62	Total	O	0	0
			62	62		
2	B	82	Total	O	0	0
			82	82		



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.10Å 76.10Å 169.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.15 – 2.20	Depositor
% Data completeness (in resolution range)	96.7 (29.15-2.20)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.226 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3492	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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: SEB

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	0.34	0/1644	0.60	0/2225
1	B	0.33	0/1733	0.58	0/2345
All	All	0.33	0/3377	0.59	0/4570

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1629	0	1613	85	0
1	B	1719	0	1690	61	1
2	A	62	0	0	2	0
2	B	82	0	0	1	0
All	All	3492	0	3303	139	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 21.

All (139) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:163:VAL:HG12	1:A:238:LEU:HD13	1.43	0.96
1:A:132:SEB:HE3	1:A:165:ARG:H	1.32	0.91
1:A:92:ARG:HG2	1:A:92:ARG:HH11	1.34	0.91
1:A:136:ARG:HA	1:A:136:ARG:HE	1.41	0.84
1:B:376:GLN:HE22	1:B:494:GLY:HA3	1.42	0.82
1:A:232:ARG:NE	1:B:539:ARG:HH22	1.78	0.81
1:A:248:THR:HB	1:A:251:GLU:OE1	1.81	0.81
1:B:361:ILE:HD11	1:B:393:PHE:CE1	2.16	0.80
1:B:432:SEB:HE3	1:B:465:ARG:HE	1.49	0.76
1:B:431:LEU:HD13	1:B:471:ALA:HB2	1.68	0.76
1:B:398:ARG:HB3	1:B:398:ARG:HH11	1.52	0.75
1:B:463:VAL:HG12	1:B:538:LEU:HD13	1.68	0.75
1:A:177:PRO:HA	1:A:180:VAL:HG12	1.68	0.74
1:A:132:SEB:HE3	1:A:165:ARG:N	2.03	0.73
1:A:248:THR:HG21	1:A:250:ARG:HE	1.55	0.72
1:A:92:ARG:HG2	1:A:92:ARG:NH1	2.03	0.71
1:A:132:SEB:HH1	1:A:163:VAL:O	1.91	0.71
1:A:62:ASN:HD21	1:A:132:SEB:CJ	2.03	0.71
1:A:248:THR:HG21	1:A:250:ARG:NE	2.05	0.70
1:A:248:THR:HG22	1:A:250:ARG:H	1.58	0.69
1:B:311:VAL:HG12	1:B:311:VAL:O	1.93	0.68
1:B:542:LYS:HG2	1:B:548:THR:HG23	1.76	0.67
1:B:336:ARG:O	1:B:340:GLU:HG3	1.94	0.67
1:A:232:ARG:HE	1:B:539:ARG:HH22	1.43	0.66
1:A:75:MET:HE1	1:A:82:LEU:HD21	1.77	0.66
1:A:35:PRO:O	1:A:38:VAL:HG22	1.96	0.65
1:A:88:VAL:HG12	1:A:94:LEU:HD21	1.76	0.65
1:B:311:VAL:HG13	1:B:394:LEU:HB3	1.80	0.64
1:A:177:PRO:HA	1:A:180:VAL:CG1	2.27	0.64
1:A:178:GLU:OE1	1:A:196:ARG:NE	2.32	0.62
1:A:163:VAL:HG12	1:A:238:LEU:CD1	2.24	0.62
1:A:232:ARG:HH11	1:A:233:GLU:H	1.48	0.62
1:A:232:ARG:NH1	1:A:233:GLU:H	1.98	0.62
1:B:361:ILE:HD11	1:B:393:PHE:CZ	2.36	0.61
1:A:90:SER:O	1:A:94:LEU:HD23	2.00	0.61
1:A:132:SEB:HH2	1:A:132:SEB:OD1	2.02	0.60
1:A:39:VAL:O	1:A:43:LEU:HD13	2.02	0.60
1:A:181:THR:HG22	1:A:192:ARG:HD3	1.83	0.60
1:B:339:VAL:O	1:B:343:LEU:HB2	2.01	0.60
1:A:193:ASP:HA	1:A:196:ARG:NH1	2.16	0.59
1:A:229:LEU:HD23	1:B:529:LEU:HD23	1.84	0.59
1:A:131:LEU:HD21	1:A:171:ALA:HA	1.85	0.59
1:B:532:ARG:NH1	1:B:533:GLU:HG2	2.18	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:136:ARG:HB3	1:A:156:LYS:HG3	1.83	0.58
1:A:232:ARG:HH21	1:B:539:ARG:HH12	1.49	0.58
1:A:132:SEB:CE	1:A:165:ARG:H	2.11	0.58
1:B:463:VAL:CG1	1:B:534:ARG:HG3	2.35	0.56
1:B:463:VAL:HG11	1:B:534:ARG:HG3	1.87	0.56
1:B:398:ARG:NH1	1:B:398:ARG:HB3	2.18	0.56
1:B:496:ARG:HA	1:B:499:TRP:NE1	2.21	0.56
1:A:12:ALA:HA	2:A:278:HOH:O	2.06	0.56
1:B:479:TRP:O	1:B:483:ARG:HD2	2.07	0.55
1:A:75:MET:CE	1:A:82:LEU:HD21	2.36	0.55
1:B:463:VAL:HG12	1:B:538:LEU:CD1	2.37	0.55
1:A:179:TRP:O	1:A:183:ARG:HD2	2.07	0.55
1:A:232:ARG:HE	1:B:539:ARG:NH2	2.03	0.54
1:B:542:LYS:HE3	1:B:548:THR:HG22	1.90	0.54
1:B:545:VAL:HG23	1:B:547:VAL:HG23	1.89	0.53
1:A:11:VAL:O	1:A:11:VAL:HG12	2.08	0.53
1:B:493:ASP:HA	1:B:496:ARG:NH1	2.24	0.53
1:A:63:HIS:CE1	1:A:132:SEB:OG	2.62	0.52
1:A:63:HIS:CE1	1:A:132:SEB:HH2	2.45	0.52
1:A:196:ARG:HA	1:A:199:TRP:NE1	2.25	0.52
1:B:479:TRP:O	1:B:483:ARG:CD	2.57	0.52
1:A:242:LYS:HG2	1:A:247:VAL:O	2.10	0.52
1:A:85:LEU:HD21	1:A:180:VAL:HG11	1.91	0.51
1:A:232:ARG:NE	1:B:539:ARG:NH2	2.55	0.51
1:B:385:LEU:HD13	1:B:386:GLY:N	2.25	0.51
1:B:483:ARG:HD2	1:B:483:ARG:N	2.25	0.51
1:A:162:SER:O	1:A:163:VAL:HG13	2.10	0.51
1:A:193:ASP:HA	1:A:196:ARG:HH12	1.75	0.51
1:A:63:HIS:HE1	1:A:132:SEB:HH2	1.76	0.51
1:A:63:HIS:HE1	1:A:132:SEB:OG	1.94	0.51
1:B:315:TYR:CD2	1:B:477:PRO:HG3	2.46	0.50
1:B:323:TYR:CD2	1:B:381:GLY:HA2	2.46	0.49
1:B:431:LEU:HD13	1:B:471:ALA:CB	2.40	0.49
1:A:95:GLU:OE1	1:A:98:ARG:NH1	2.46	0.49
1:B:478:GLU:O	1:B:482:GLN:HG2	2.14	0.48
1:A:177:PRO:CA	1:A:180:VAL:HG12	2.41	0.48
1:A:113:SER:HB3	1:A:114:PRO:CD	2.43	0.48
1:A:181:THR:CG2	1:A:192:ARG:HD3	2.44	0.48
1:B:483:ARG:NH2	1:B:550:ARG:HG3	2.29	0.47
1:A:10:ALA:HA	1:A:175:ARG:HH22	1.80	0.47
1:B:478:GLU:OE1	1:B:496:ARG:NE	2.31	0.47
1:A:85:LEU:HD13	1:A:86:GLY:N	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:177:PRO:O	1:A:180:VAL:CG1	2.62	0.47
1:A:38:VAL:HG23	1:A:39:VAL:N	2.29	0.47
1:A:23:TYR:CE2	1:A:81:GLY:HA2	2.51	0.46
1:A:136:ARG:NE	1:A:136:ARG:HA	2.20	0.46
1:B:361:ILE:CD1	1:B:393:PHE:CE1	2.92	0.46
1:B:392:ARG:O	1:B:396:ILE:HG12	2.15	0.46
1:B:371:HIS:CD2	1:B:505:THR:HG21	2.51	0.46
1:B:535:LEU:HB2	1:B:536:PRO:HD3	1.97	0.46
1:B:307:GLN:HG3	1:B:398:ARG:HE	1.81	0.45
1:B:315:TYR:CE2	1:B:477:PRO:HG3	2.51	0.45
1:B:432:SEB:HH2	1:B:432:SEB:OD1	2.17	0.45
1:A:136:ARG:H	1:A:156:LYS:HG2	1.82	0.45
1:A:248:THR:HG22	1:A:249:GLU:N	2.32	0.45
1:B:542:LYS:HG2	1:B:548:THR:CG2	2.45	0.45
1:A:38:VAL:CG2	1:A:39:VAL:N	2.80	0.45
1:A:10:ALA:HA	1:A:175:ARG:NH2	2.32	0.45
1:B:413:SER:CB	1:B:414:PRO:CD	2.95	0.44
1:A:15:TYR:HD2	1:A:85:LEU:HD11	1.82	0.44
1:A:28:ASP:N	1:A:28:ASP:OD2	2.50	0.44
1:B:311:VAL:CG1	1:B:311:VAL:O	2.64	0.44
1:A:11:VAL:O	1:A:11:VAL:CG1	2.66	0.44
1:A:248:THR:CG2	1:A:250:ARG:HE	2.26	0.44
1:A:133:LEU:HD21	1:A:155:PHE:CD1	2.52	0.43
1:B:496:ARG:HA	1:B:499:TRP:CE2	2.53	0.43
1:B:477:PRO:O	1:B:480:VAL:HG13	2.18	0.43
1:A:111:PRO:HD3	1:A:122:GLU:OE2	2.19	0.43
1:B:462:SER:O	1:B:463:VAL:HG13	2.19	0.43
1:B:477:PRO:O	1:B:480:VAL:CG1	2.67	0.43
1:A:132:SEB:HE2	1:A:132:SEB:HB3	1.59	0.43
1:A:136:ARG:CB	1:A:156:LYS:HG3	2.47	0.43
1:A:27:PRO:HG3	2:A:298:HOH:O	2.18	0.43
1:A:62:ASN:HD21	1:A:132:SEB:HJ	1.79	0.42
1:B:376:GLN:NE2	1:B:494:GLY:HA3	2.23	0.42
1:A:103:LYS:HG3	1:B:520:GLY:HA2	2.01	0.42
1:B:462:SER:OG	1:B:531:ILE:HD12	2.18	0.42
1:A:27:PRO:HD2	1:A:33:LEU:HD23	2.01	0.42
1:A:184:PHE:HA	1:A:185:PRO:HD3	1.88	0.42
1:A:235:LEU:HB2	1:A:236:PRO:HD3	2.02	0.42
1:A:233:GLU:C	1:A:236:PRO:HD2	2.40	0.42
1:B:523:GLY:O	1:B:526:VAL:HG12	2.20	0.42
1:A:63:HIS:CD2	1:A:134:SER:HB3	2.56	0.41
1:A:196:ARG:O	1:A:200:GLN:HB3	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:10:ALA:HB1	1:A:120:VAL:HG21	2.02	0.41
1:B:391:PRO:HD2	1:B:512:ASP:OD2	2.21	0.41
1:A:129:ALA:HB3	1:A:238:LEU:HD21	2.03	0.41
1:B:481:THR:HG23	1:B:487:LEU:CD1	2.51	0.41
1:A:177:PRO:O	1:A:180:VAL:HG13	2.21	0.41
1:B:419:LYS:HG3	2:B:16:HOH:O	2.19	0.41
1:A:167:ARG:NE	1:A:167:ARG:HA	2.36	0.41
1:A:177:PRO:C	1:A:180:VAL:HG12	2.42	0.40
1:B:550:ARG:HG3	1:B:551:GLU:H	1.86	0.40
1:A:163:VAL:CG1	1:A:234:ARG:HG3	2.52	0.40
1:B:481:THR:CG2	1:B:492:ARG:HG2	2.52	0.40
1:B:481:THR:HG23	1:B:487:LEU:HD13	2.04	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:550:ARG:NH1	1:B:550:ARG:NH1[7_646]	2.12	0.08

## 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	198/256 (77%)	187 (94%)	9 (4%)	2 (1%)	22	18
1	B	208/256 (81%)	200 (96%)	7 (3%)	1 (0%)	38	38
All	All	406/512 (79%)	387 (95%)	16 (4%)	3 (1%)	30	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	SER
1	B	413	SER
1	A	114	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	172/213 (81%)	166 (96%)	6 (4%)	48	57
1	B	183/213 (86%)	174 (95%)	9 (5%)	35	40
All	All	355/426 (83%)	340 (96%)	15 (4%)	40	48

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	84	CYS
1	A	92	ARG
1	A	136	ARG
1	A	183	ARG
1	A	238	LEU
1	B	322	ARG
1	B	362	ASN
1	B	365	ASP
1	B	376	GLN
1	B	384	CYS
1	B	394	LEU
1	B	431	LEU
1	B	476	ASP
1	B	538	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	63	HIS
1	A	76	GLN
1	A	182	GLN
1	B	306	GLN
1	B	362	ASN
1	B	371	HIS
1	B	376	GLN
1	B	482	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 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	SEB	A	132	1	16,16,17	5.02	5 (31%)	19,21,23	1.55	5 (26%)
1	SEB	B	432	1	16,16,17	4.79	6 (37%)	19,21,23	1.58	5 (26%)

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	SEB	A	132	1	-	2/11/13/15	0/1/1/1
1	SEB	B	432	1	-	0/11/13/15	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	SEB	O-C	18.35	1.24	1.11
1	B	432	SEB	O-C	17.83	1.23	1.11
1	A	132	SEB	CE-SD	5.42	1.83	1.78
1	B	432	SEB	CE-SD	4.26	1.82	1.78
1	A	132	SEB	OD2-SD	4.17	1.54	1.43
1	B	432	SEB	OD2-SD	3.07	1.51	1.43
1	A	132	SEB	CA-C	2.74	1.53	1.48
1	B	432	SEB	CA-C	2.73	1.53	1.48
1	A	132	SEB	OD1-SD	2.69	1.50	1.43
1	B	432	SEB	OG-SD	2.45	1.64	1.56
1	B	432	SEB	OD1-SD	2.41	1.49	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	432	SEB	CB-OG-SD	-3.41	111.98	119.37
1	A	132	SEB	CB-OG-SD	-3.33	112.15	119.37
1	A	132	SEB	OD1-SD-CE	3.23	111.42	107.36
1	B	432	SEB	C-CA-N	-3.10	110.73	113.83
1	B	432	SEB	CZ-CE-SD	-2.63	109.65	112.52
1	A	132	SEB	C-CA-N	-2.61	111.22	113.83
1	B	432	SEB	OG-CB-CA	2.61	111.72	107.37
1	A	132	SEB	OD1-SD-OD2	-2.39	108.05	116.56
1	A	132	SEB	OG-SD-CE	2.34	110.34	103.64
1	B	432	SEB	OD1-SD-OD2	-2.09	109.14	116.56

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	132	SEB	CH2-CZ-CE-SD
1	A	132	SEB	CH1-CZ-CE-SD

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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 ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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