



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:58 am BST

PDB ID : 1MPP  
Title : X-RAY ANALYSES OF ASPARTIC PROTEINASES. V. STRUCTURE AND REFINEMENT AT 2.0 ANGSTROMS RESOLUTION OF THE ASPARTIC PROTEINASE FROM MUCOR PUSILLUS  
Authors : Newman, M.; Watson, F.; Roychowdhury, P.; Jones, H.; Badasso, M.; Cleasby, A.; Wood, S.P.; Tickle, I.J.; Blundell, T.L.  
Deposited on : 1992-02-19  
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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

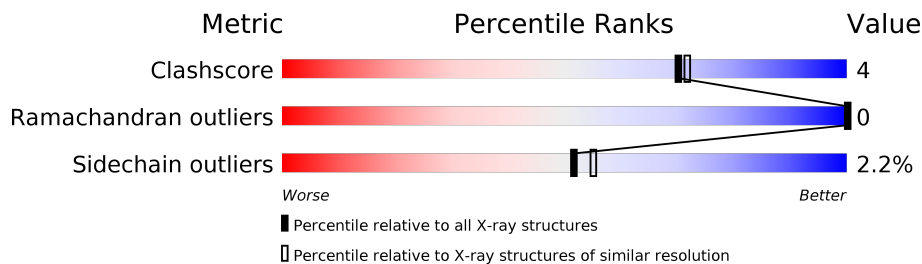
# 1 Overall quality at a glance

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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	361	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2864 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 PEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	357	2638	1686	414	530	8	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	ILE	MET	CONFLICT	UNP P09177
A	170	VAL	ALA	CONFLICT	UNP P09177
A	202	SER	ALA	CONFLICT	UNP P09177

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is water.

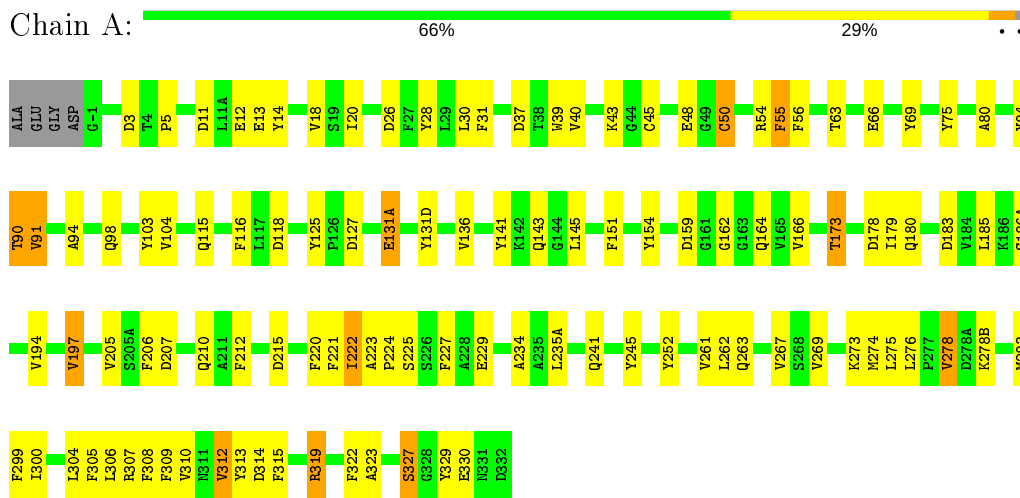
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	221	Total 221	O 221	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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: PEPSIN



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.00Å 104.00Å 46.30Å 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	X-PLOR	Depositor
R, $R_{free}$	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2864	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

## 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: SO4

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	1.42	8/2704 (0.3%)	2.35	140/3693 (3.8%)

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	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	SER	CA-CB	6.20	1.62	1.52
1	A	90	THR	CB-OG1	5.76	1.54	1.43
1	A	267	VAL	N-CA	5.34	1.57	1.46
1	A	305	PHE	CG-CD1	5.19	1.46	1.38
1	A	241	GLN	CD-OE1	5.17	1.35	1.24
1	A	98	GLN	CD-OE1	5.14	1.35	1.24
1	A	180	GLN	CD-OE1	5.07	1.35	1.24
1	A	210	GLN	CD-OE1	5.03	1.35	1.24

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ARG	NE-CZ-NH2	14.47	127.54	120.30
1	A	37	ASP	CB-CG-OD2	12.41	129.47	118.30
1	A	307	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	A	48	GLU	OE1-CD-OE2	-10.99	110.12	123.30
1	A	13	GLU	OE1-CD-OE2	-10.66	110.51	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	TYR	CB-CG-CD2	-10.57	114.66	121.00
1	A	75	TYR	CZ-CE2-CD2	9.82	128.64	119.80
1	A	314	ASP	CB-CG-OD2	-9.67	109.60	118.30
1	A	305	PHE	CB-CG-CD2	9.55	127.49	120.80
1	A	86	ARG	NE-CZ-NH2	-9.15	115.73	120.30
1	A	56	PHE	CB-CG-CD2	-9.13	114.41	120.80
1	A	305	PHE	CG-CD2-CE2	8.93	130.63	120.80
1	A	187	TYR	CB-CG-CD1	-8.86	115.68	121.00
1	A	207	ASP	C-N-CA	-8.84	103.74	122.30
1	A	309	PHE	CB-CG-CD1	-8.83	114.62	120.80
1	A	118	ASP	CB-CG-OD2	-8.83	110.36	118.30
1	A	261	VAL	CG1-CB-CG2	-8.80	96.82	110.90
1	A	86	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	A	84	TYR	CB-CG-CD2	-8.60	115.84	121.00
1	A	14	TYR	CG-CD1-CE1	-8.54	114.47	121.30
1	A	31	PHE	CG-CD1-CE1	-8.50	111.45	120.80
1	A	229	GLU	OE1-CD-OE2	-8.37	113.26	123.30
1	A	131(D)	TYR	CB-CG-CD1	8.36	126.02	121.00
1	A	31	PHE	CD1-CE1-CZ	8.29	130.04	120.10
1	A	310	VAL	CG1-CB-CG2	-8.21	97.76	110.90
1	A	86	ARG	CA-CB-CG	-8.11	95.56	113.40
1	A	11	ASP	CB-CG-OD2	8.10	125.59	118.30
1	A	269	VAL	CG1-CB-CG2	-8.07	97.99	110.90
1	A	299	PHE	CB-CG-CD2	-7.93	115.25	120.80
1	A	305	PHE	CD1-CE1-CZ	7.84	129.50	120.10
1	A	197	VAL	CA-CB-CG2	7.79	122.58	110.90
1	A	14	TYR	CB-CG-CD2	-7.76	116.34	121.00
1	A	91	VAL	CG1-CB-CG2	-7.71	98.56	110.90
1	A	314	ASP	CB-CG-OD1	7.71	125.23	118.30
1	A	151	PHE	CG-CD1-CE1	-7.62	112.42	120.80
1	A	28	TYR	CZ-CE2-CD2	7.47	126.52	119.80
1	A	69	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	A	178	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	A	262	LEU	CB-CG-CD1	-7.44	98.35	111.00
1	A	212	PHE	CG-CD2-CE2	-7.43	112.62	120.80
1	A	212	PHE	CB-CG-CD2	-7.41	115.61	120.80
1	A	28	TYR	CG-CD2-CE2	-7.34	115.43	121.30
1	A	55	PHE	CB-CG-CD2	-7.27	115.71	120.80
1	A	205	VAL	CA-CB-CG2	7.14	121.61	110.90
1	A	319	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	A	141	TYR	CB-CG-CD1	-6.96	116.83	121.00
1	A	98	GLN	CG-CD-NE2	6.88	133.22	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	PHE	O-C-N	-6.88	111.50	123.20
1	A	131(D)	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	A	188	PHE	CG-CD1-CE1	-6.87	113.25	120.80
1	A	20	ILE	O-C-N	6.68	134.56	123.20
1	A	183	ASP	CB-CG-OD1	6.67	124.31	118.30
1	A	55	PHE	CG-CD2-CE2	-6.65	113.48	120.80
1	A	241	GLN	O-C-N	6.60	133.26	122.70
1	A	313	TYR	CB-CG-CD1	-6.59	117.05	121.00
1	A	104	VAL	CA-CB-CG2	6.58	120.76	110.90
1	A	159	ASP	CB-CG-OD1	6.56	124.21	118.30
1	A	319	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	A	322	PHE	CD1-CE1-CZ	-6.55	112.24	120.10
1	A	12	GLU	OE1-CD-OE2	-6.50	115.50	123.30
1	A	86	ARG	CD-NE-CZ	6.49	132.68	123.60
1	A	178	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	308	PHE	CG-CD2-CE2	-6.45	113.70	120.80
1	A	13	GLU	CG-CD-OE1	6.45	131.19	118.30
1	A	308	PHE	CZ-CE2-CD2	6.44	127.83	120.10
1	A	55	PHE	CD1-CG-CD2	6.37	126.59	118.30
1	A	131(D)	TYR	CD1-CE1-CZ	-6.37	114.07	119.80
1	A	194	VAL	CG1-CB-CG2	-6.36	100.72	110.90
1	A	323	ALA	N-CA-CB	6.35	118.98	110.10
1	A	115	GLN	CB-CA-C	-6.32	97.75	110.40
1	A	164	GLN	O-C-N	-6.30	112.62	122.70
1	A	115	GLN	CA-CB-CG	-6.29	99.55	113.40
1	A	235(A)	LEU	CB-CG-CD1	-6.26	100.35	111.00
1	A	212	PHE	CD1-CE1-CZ	-6.24	112.62	120.10
1	A	206	PHE	CB-CG-CD2	-6.23	116.44	120.80
1	A	261	VAL	CA-CB-CG1	-6.16	101.66	110.90
1	A	330	GLU	OE1-CD-OE2	-6.15	115.92	123.30
1	A	305	PHE	CZ-CE2-CD2	-6.14	112.72	120.10
1	A	252	TYR	CG-CD1-CE1	-6.13	116.40	121.30
1	A	327	SER	C-N-CA	-6.12	109.44	122.30
1	A	131(D)	TYR	CG-CD1-CE1	6.10	126.18	121.30
1	A	220	PHE	CB-CG-CD2	6.10	125.07	120.80
1	A	312	VAL	CA-CB-CG1	-6.06	101.81	110.90
1	A	330	GLU	CA-CB-CG	-6.03	100.14	113.40
1	A	278	VAL	CG1-CB-CG2	-5.98	101.34	110.90
1	A	39	TRP	CG-CD1-NE1	-5.96	104.14	110.10
1	A	154	TYR	CB-CG-CD2	-5.91	117.46	121.00
1	A	278(B)	LYS	CA-C-O	5.89	132.46	120.10
1	A	143	GLN	O-C-N	-5.86	113.24	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	PHE	CB-CG-CD1	5.81	124.87	120.80
1	A	37	ASP	CB-CG-OD1	-5.79	113.08	118.30
1	A	245	TYR	CG-CD1-CE1	-5.77	116.68	121.30
1	A	164	GLN	N-CA-CB	-5.77	100.22	110.60
1	A	80	ALA	N-CA-CB	-5.77	102.03	110.10
1	A	215	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	A	286	VAL	CG1-CB-CG2	-5.75	101.69	110.90
1	A	322	PHE	O-C-N	5.71	131.83	122.70
1	A	54	ARG	NH1-CZ-NH2	-5.70	113.13	119.40
1	A	274	MET	O-C-N	-5.69	113.60	122.70
1	A	252	TYR	CZ-CE2-CD2	-5.69	114.68	119.80
1	A	162	GLY	CA-C-O	5.64	130.76	120.60
1	A	306	LEU	CA-CB-CG	-5.59	102.43	115.30
1	A	50	CYS	CA-CB-SG	-5.59	103.94	114.00
1	A	252	TYR	CB-CG-CD1	-5.56	117.66	121.00
1	A	26	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	131(D)	TYR	CZ-CE2-CD2	5.55	124.80	119.80
1	A	45	CYS	C-N-CA	5.54	135.56	121.70
1	A	136	VAL	CA-CB-CG2	5.50	119.15	110.90
1	A	185	LEU	CB-CG-CD2	5.50	120.35	111.00
1	A	164	GLN	CA-C-O	5.45	131.54	120.10
1	A	315	PHE	CA-C-O	5.39	131.42	120.10
1	A	145	LEU	O-C-N	-5.32	114.19	122.70
1	A	127	ASP	CB-CG-OD1	5.32	123.08	118.30
1	A	305	PHE	CG-CD1-CE1	-5.30	114.97	120.80
1	A	11	ASP	OD1-CG-OD2	-5.28	113.27	123.30
1	A	66	GLU	O-C-N	-5.28	114.26	122.70
1	A	5	PRO	CA-N-CD	5.24	119.04	111.70
1	A	125	TYR	CB-CG-CD1	5.24	124.14	121.00
1	A	88	SER	CA-CB-OG	-5.22	97.10	111.20
1	A	28	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	A	234	ALA	CA-C-N	5.21	128.65	117.20
1	A	186(A)	SER	CA-C-O	-5.20	109.19	120.10
1	A	3	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	A	225	SER	O-C-N	-5.19	114.40	122.70
1	A	26	ASP	O-C-N	5.19	131.00	122.70
1	A	166	VAL	CA-CB-CG1	-5.16	103.16	110.90
1	A	173	THR	CA-CB-CG2	-5.14	105.20	112.40
1	A	12	GLU	CA-CB-CG	-5.14	102.09	113.40
1	A	252	TYR	CD1-CG-CD2	5.11	123.53	117.90
1	A	14	TYR	CD1-CG-CD2	5.09	123.50	117.90
1	A	273	LYS	CA-CB-CG	-5.09	102.20	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	VAL	CA-CB-CG2	5.09	118.54	110.90
1	A	307	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
1	A	252	TYR	CA-C-O	-5.08	109.42	120.10
1	A	191	ASP	CA-CB-CG	-5.07	102.24	113.40
1	A	14	TYR	CA-CB-CG	5.05	123.00	113.40
1	A	245	TYR	CD1-CE1-CZ	5.04	124.34	119.80
1	A	30	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	A	116	PHE	C-N-CA	5.02	134.25	121.70
1	A	86	ARG	CB-CG-CD	-5.01	98.58	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	319	ARG	Sidechain

## 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	2638	0	2415	18	0
2	A	5	0	0	0	0
3	A	221	0	0	0	0
All	All	2864	0	2415	18	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 4.

All (18) 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:278:VAL:HG11	1:A:283:MET:HB2	1.57	0.86
1:A:275:LEU:C	1:A:276:LEU:HD23	2.01	0.81
1:A:276:LEU:HD23	1:A:276:LEU:N	2.07	0.68
1:A:131(A):GLU:O	1:A:131(A):GLU:HG3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:VAL:CG1	1:A:283:MET:HB2	2.34	0.54
1:A:222:ILE:HB	1:A:300:ILE:HB	1.91	0.51
1:A:40:VAL:O	1:A:103:TYR:HA	2.12	0.50
1:A:197:VAL:HG21	1:A:227:PHE:CZ	2.48	0.49
1:A:50:CYS:HB3	1:A:55:PHE:HE1	1.80	0.47
1:A:43:LYS:HA	1:A:55:PHE:HB3	1.97	0.46
1:A:90:THR:HA	1:A:94:ALA:O	2.15	0.46
1:A:173:THR:HG22	1:A:173:THR:O	2.16	0.45
1:A:275:LEU:O	1:A:276:LEU:HD23	2.17	0.43
1:A:223:ALA:HB1	1:A:224:PRO:HD2	2.01	0.42
1:A:18:VAL:HG12	1:A:91:VAL:HG12	2.01	0.42
1:A:179:ILE:HD13	1:A:312:VAL:HG21	2.03	0.41
1:A:304:LEU:HD23	1:A:304:LEU:HA	1.82	0.40
1:A:287:LEU:HA	1:A:288:PRO:HD3	1.91	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	355/361 (98%)	349 (98%)	6 (2%)	0	<a href="#">100</a> <a href="#">100</a>

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	272/298 (91%)	266 (98%)	6 (2%)	52   55

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	THR
1	A	131(A)	GLU
1	A	221	PHE
1	A	222	ILE
1	A	263	GLN
1	A	327	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	72	ASN
1	A	311	ASN

### 5.3.3 RNA [i](#)

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](#)

1 ligand is 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	SO4	A	501	-	4,4,4	0.28	0	6,6,6	0.50	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.