



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 02:58 AM EDT

PDB ID : 3BEU  
Title : Na<sup>+</sup>-Dependent Allostery Mediates Coagulation Factor Protease Active Site Selectivity  
Authors : Page, M.J.; Carrell, C.J.; Di Cera, E.  
Deposited on : 2007-11-20  
Resolution : 1.05 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)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

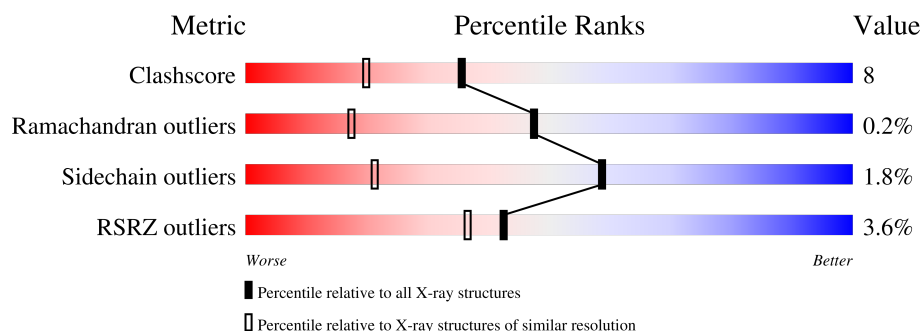
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.05 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	1252 (1.10-1.02)
Ramachandran outliers	138981	1204 (1.10-1.02)
Sidechain outliers	138945	1202 (1.10-1.02)
RSRZ outliers	127900	1178 (1.10-1.02)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	224	<div> <div>3%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	B	224	<div> <div>4%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>

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
2	SO4	A	6	-	X	-	-
2	SO4	B	10	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4054 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 Trypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	6	0
			1679	1051	291	327	10			
1	B	224	Total	C	N	O	S	0	4	0
			1666	1041	289	326	10			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	PHE	TYR	engineered mutation	UNP P00775
A	95	THR	ASN	engineered mutation	UNP P00775
A	96	LYS	GLY	engineered mutation	UNP P00775
A	97	GLU	THR	engineered mutation	UNP P00775
A	98	THR	-	SEE REMARK 999	UNP P00775
A	99	TYR	-	SEE REMARK 999	UNP P00775
A	171	SER	ALA	engineered mutation	UNP P00775
A	172	SER	TYR	engineered mutation	UNP P00775
A	173	SER	GLY	engineered mutation	UNP P00775
A	174	PHE	ASN	engineered mutation	UNP P00775
A	175	ILE	GLU	engineered mutation	UNP P00775
A	180	MET	GLU	engineered mutation	UNP P00775
A	?	-	PRO	SEE REMARK 999	UNP P00775
A	186	LYS	GLY	engineered mutation	UNP P00775
A	187	GLN	GLY	engineered mutation	UNP P00775
A	188	GLU	VAL	engineered mutation	UNP P00775
A	208	VAL	ILE	engineered mutation	UNP P00775
A	217	GLU	TYR	engineered mutation	UNP P00775
A	223	LYS	PRO	engineered mutation	UNP P00775
A	224	LYS	TYR	engineered mutation	UNP P00775
A	225	TYR	PRO	engineered mutation	UNP P00775
B	94	PHE	TYR	engineered mutation	UNP P00775
B	95	THR	ASN	engineered mutation	UNP P00775
B	96	LYS	GLY	engineered mutation	UNP P00775
B	97	GLU	THR	engineered mutation	UNP P00775

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Chain	Residue	Modelled	Actual	Comment	Reference
B	98	THR	-	SEE REMARK 999	UNP P00775
B	99	TYR	-	SEE REMARK 999	UNP P00775
B	171	SER	ALA	engineered mutation	UNP P00775
B	172	SER	TYR	engineered mutation	UNP P00775
B	173	SER	GLY	engineered mutation	UNP P00775
B	174	PHE	ASN	engineered mutation	UNP P00775
B	175	ILE	GLU	engineered mutation	UNP P00775
B	180	MET	GLU	engineered mutation	UNP P00775
B	?	-	PRO	SEE REMARK 999	UNP P00775
B	186	LYS	GLY	engineered mutation	UNP P00775
B	187	GLN	GLY	engineered mutation	UNP P00775
B	188	GLU	VAL	engineered mutation	UNP P00775
B	208	VAL	ILE	engineered mutation	UNP P00775
B	217	GLU	TYR	engineered mutation	UNP P00775
B	223	LYS	PRO	engineered mutation	UNP P00775
B	224	LYS	TYR	engineered mutation	UNP P00775
B	225	TYR	PRO	engineered mutation	UNP P00775

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



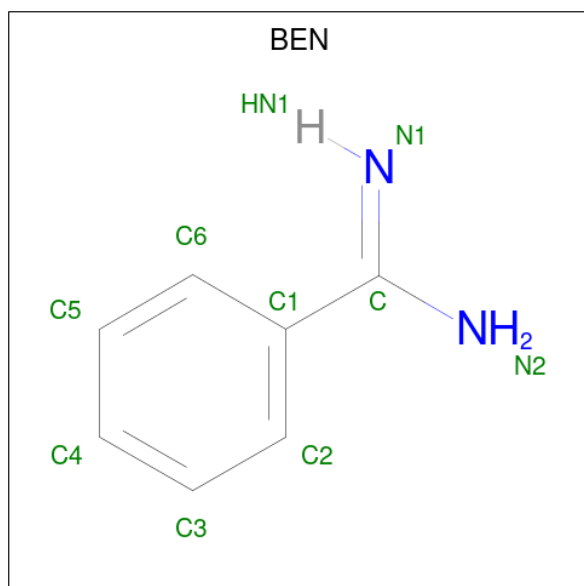
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is BENZAMIDINE (three-letter code: BEN) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	7	2		
3	A	1	Total	C	N	0	1
			18	14	4		
3	A	1	Total	C	N	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			9	7	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		

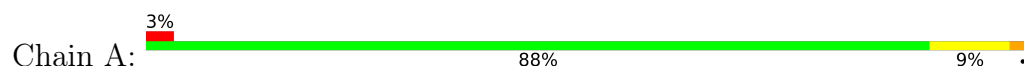
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	330	Total	O	0	0
			330	330		
6	B	275	Total	O	0	0
			275	275		

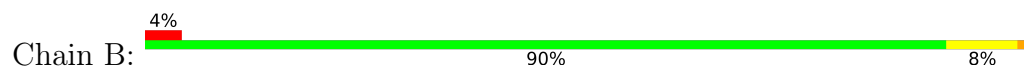
### 3 Residue-property plots [i](#)

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: Trypsin



- Molecule 1: Trypsin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.79Å 72.43Å 122.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.05 36.22 – 1.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.05) 95.7 (36.22-1.05)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 1.05Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.119 , 0.146 0.128 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.1	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	4054	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BEN, CA, NA, 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	0.79	1/1726 (0.1%)	1.24	15/2340 (0.6%)
1	B	0.71	0/1707	1.16	10/2313 (0.4%)
All	All	0.75	1/3433 (0.0%)	1.20	25/4653 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	ARG	CB-CG	-5.33	1.38	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ARG	NE-CZ-NH1	-18.96	110.82	120.30
1	A	243	ARG	NE-CZ-NH2	15.80	128.20	120.30
1	A	21	ARG	NE-CZ-NH2	-12.71	113.95	120.30
1	A	205	ASP	CB-CG-OD1	10.95	128.16	118.30
1	B	222	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	B	174	PHE	CB-CG-CD2	-8.62	114.77	120.80
1	A	205	ASP	CB-CG-OD2	-8.07	111.03	118.30
1	B	243	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	145	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	B	222	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	B	153	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	222	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	154	TYR	CG-CD1-CE1	-6.14	116.39	121.30
1	B	185(A)	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	145	ARG	CD-NE-CZ	5.84	131.78	123.60
1	B	21	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	174	PHE	N-CA-CB	-5.68	100.38	110.60
1	A	225	TYR	CG-CD2-CE2	5.60	125.78	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	TYR	CB-CG-CD1	-5.56	117.66	121.00
1	A	84	ARG	CG-CD-NE	-5.51	100.23	111.80
1	B	173	SER	O-C-N	-5.39	114.07	122.70
1	A	225	TYR	CZ-CE2-CD2	-5.38	114.96	119.80
1	A	21	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	172	SER	N-CA-CB	-5.24	102.64	110.50
1	B	145	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1679	0	1663	29	0
1	B	1666	0	1643	25	0
2	A	30	0	0	1	0
2	B	25	0	0	2	0
3	A	36	0	31	1	0
3	B	9	0	7	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	330	0	0	10	0
6	B	275	0	0	4	0
All	All	4054	0	3344	55	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 8.

All (55) 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:95:THR:HG22	1:A:96:LYS:HG3	1.25	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:THR:HG21	1:A:174:PHE:HB3	1.42	1.01
1:B:96:LYS:HB3	1:B:99:TYR:HB2	1.42	1.01
1:B:98:THR:HG21	1:B:174:PHE:HB3	1.51	0.93
1:B:99:TYR:CE1	1:B:175:ILE:HD12	2.04	0.93
1:B:99:TYR:HE1	1:B:175:ILE:HD12	1.33	0.91
1:A:98:THR:CG2	1:A:174:PHE:HB3	2.09	0.82
1:B:185(B):THR:HG22	1:B:223:LYS:HG3	1.64	0.79
1:A:95:THR:HG22	1:A:96:LYS:CG	2.08	0.77
1:A:97:GLU:O	6:A:387:HOH:O	2.04	0.75
3:A:7[B]:BEN:H4	6:A:513:HOH:O	1.88	0.73
1:B:192:GLN:HB2	6:B:490:HOH:O	1.91	0.69
1:B:96:LYS:HE3	1:B:98:THR:HB	1.74	0.67
1:A:101:LYS:HD2	6:A:510:HOH:O	1.95	0.66
1:A:96:LYS:HE2	1:A:99:TYR:HB2	1.77	0.66
1:A:175:ILE:HA	6:A:559:HOH:O	1.96	0.65
1:B:84:ARG:NH2	2:B:10:SO4:O3	2.29	0.64
1:B:204:ASN:HB2	6:B:388:HOH:O	1.96	0.64
1:B:96:LYS:HE2	1:B:99:TYR:CD1	2.33	0.64
1:B:185(A):ASP:OD2	1:B:185(B):THR:HG23	1.99	0.63
1:B:96:LYS:O	1:B:99:TYR:N	2.30	0.62
1:A:97:GLU:C	1:A:99:TYR:H	2.02	0.61
1:A:96:LYS:HD3	1:A:99:TYR:CD2	2.35	0.61
1:B:96:LYS:CE	1:B:98:THR:HB	2.31	0.60
1:A:96:LYS:HE2	1:A:99:TYR:CG	2.37	0.59
1:A:192:GLN:HB2	6:A:467:HOH:O	2.02	0.59
1:A:98:THR:O	1:A:98:THR:HG22	2.03	0.58
1:B:98:THR:CG2	1:B:174:PHE:HB3	2.31	0.56
1:B:98:THR:HG22	1:B:98:THR:O	2.06	0.56
1:A:97:GLU:O	1:A:99:TYR:N	2.40	0.55
1:A:96:LYS:O	1:A:99:TYR:HB2	2.07	0.55
1:B:96:LYS:HB3	1:B:99:TYR:CB	2.25	0.55
1:A:96:LYS:HE2	1:A:99:TYR:CB	2.36	0.54
1:B:185(B):THR:CG2	1:B:223:LYS:HE3	2.40	0.52
1:B:96:LYS:CB	1:B:99:TYR:HB2	2.27	0.51
1:B:97:GLU:C	1:B:99:TYR:H	2.14	0.51
1:A:169:ARG:NH1	1:A:176:LEU:HB3	2.26	0.50
1:A:81[A]:VAL:HG11	6:A:484:HOH:O	2.13	0.49
1:A:97:GLU:C	1:A:99:TYR:N	2.65	0.49
1:A:96:LYS:HB2	1:A:96:LYS:HE3	1.43	0.47
1:B:84:ARG:NH2	2:B:10:SO4:O2	2.42	0.47
1:A:211:GLY:HA2	1:A:229:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:THR:O	2:A:11:SO4:O3	2.34	0.46
1:B:211:GLY:HA2	1:B:229:THR:O	2.17	0.45
1:B:185(B):THR:HG22	1:B:223:LYS:HE3	1.99	0.44
1:B:96:LYS:NZ	6:B:483:HOH:O	2.51	0.44
1:A:122:LYS:NZ	6:A:567:HOH:O	2.51	0.44
1:A:95:THR:C	1:A:96:LYS:HG3	2.32	0.43
1:B:119:PRO:HB2	6:B:463:HOH:O	2.18	0.43
1:A:187:GLN:NE2	6:A:556:HOH:O	2.49	0.43
1:A:175:ILE:HD13	1:A:175:ILE:HG21	1.83	0.43
1:A:223:LYS:NZ	6:A:472:HOH:O	2.50	0.42
1:A:145:ARG:NH2	6:A:498:HOH:O	2.52	0.42
1:A:98:THR:O	1:A:175:ILE:HG12	2.20	0.41
1:B:186:LYS:HE2	1:B:188:GLU:OE2	2.20	0.41

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	228/224 (102%)	222 (97%)	5 (2%)	1 (0%)	34	11
1	B	226/224 (101%)	221 (98%)	5 (2%)	0	100	100
All	All	454/448 (101%)	443 (98%)	10 (2%)	1 (0%)	47	17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	THR

### 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	177/171 (104%)	173 (98%)	4 (2%)	50	13
1	B	175/171 (102%)	173 (99%)	2 (1%)	73	40
All	All	352/342 (103%)	346 (98%)	6 (2%)	59	23

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

Mol	Chain	Res	Type
1	A	96	LYS
1	A	99	TYR
1	A	175	ILE
1	A	192	GLN
1	B	99	TYR
1	B	192	GLN

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	159	ASN
1	A	187	GLN
1	B	110	GLN
1	B	159	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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$
2	SO4	B	246	-	4,4,4	0.90	0	6,6,6	0.75	0
2	SO4	A	6	-	4,4,4	1.69	2 (50%)	6,6,6	2.85	3 (50%)
2	SO4	B	2	-	4,4,4	0.97	0	6,6,6	1.34	1 (16%)
2	SO4	A	3	-	4,4,4	1.32	1 (25%)	6,6,6	0.98	0
2	SO4	B	4	-	4,4,4	1.55	1 (25%)	6,6,6	0.82	0
2	SO4	A	9	-	4,4,4	1.76	1 (25%)	6,6,6	1.36	1 (16%)
2	SO4	B	5	-	4,4,4	1.33	0	6,6,6	0.46	0
2	SO4	B	10	-	4,4,4	1.46	1 (25%)	6,6,6	1.21	1 (16%)
3	BEN	A	8	-	9,9,9	1.35	1 (11%)	7,11,11	1.43	2 (28%)
3	BEN	B	247	-	9,9,9	1.19	1 (11%)	7,11,11	1.65	1 (14%)
2	SO4	A	11	-	4,4,4	1.52	1 (25%)	6,6,6	0.47	0
3	BEN	A	247	-	9,9,9	1.56	3 (33%)	7,11,11	1.63	2 (28%)
2	SO4	A	246	-	4,4,4	0.58	0	6,6,6	0.80	0
3	BEN	A	7[B]	-	9,9,9	1.60	3 (33%)	7,11,11	5.41	4 (57%)
2	SO4	A	1	-	4,4,4	1.01	0	6,6,6	0.38	0
3	BEN	A	7[A]	-	9,9,9	1.24	1 (11%)	7,11,11	2.87	5 (71%)

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	BEN	B	247	-	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BEN	A	8	-	-	0/4/4/4	0/1/1/1
3	BEN	A	247	-	-	1/4/4/4	0/1/1/1
3	BEN	A	7[B]	-	-	2/4/4/4	0/1/1/1
3	BEN	A	7[A]	-	-	1/4/4/4	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	8	BEN	C1-C	-3.13	1.41	1.47
3	A	247	BEN	C6-C1	-2.92	1.34	1.39
2	A	9	SO4	O2-S	2.75	1.60	1.46
3	A	7[B]	BEN	C-N1	2.60	1.39	1.28
2	A	6	SO4	O1-S	2.59	1.60	1.46
2	A	3	SO4	O3-S	2.48	1.68	1.47
2	B	4	SO4	O2-S	2.47	1.59	1.46
3	A	7[B]	BEN	C6-C1	-2.32	1.35	1.39
3	B	247	BEN	C6-C1	-2.31	1.35	1.39
3	A	7[A]	BEN	C-N1	2.29	1.37	1.28
3	A	247	BEN	C5-C6	2.11	1.43	1.38
2	B	10	SO4	O1-S	2.10	1.57	1.46
2	A	6	SO4	O4-S	2.08	1.65	1.47
3	A	7[B]	BEN	C-N2	-2.02	1.28	1.33
3	A	247	BEN	C-N1	2.01	1.36	1.28
2	A	11	SO4	O1-S	2.00	1.56	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	7[B]	BEN	C1-C-N2	11.54	135.45	118.05
3	A	7[B]	BEN	C6-C1-C2	-5.61	110.59	118.59
3	A	7[B]	BEN	C5-C6-C1	4.83	126.06	120.34
3	A	7[A]	BEN	C1-C-N2	4.45	124.76	118.05
2	A	6	SO4	O3-S-O2	4.38	132.15	109.31
2	A	6	SO4	O4-S-O1	-4.03	88.26	109.31
3	A	7[A]	BEN	C3-C2-C1	3.72	124.75	120.34
3	A	7[B]	BEN	C3-C2-C1	3.25	124.19	120.34
3	A	7[A]	BEN	C5-C4-C3	-2.98	114.39	119.93
3	A	7[A]	BEN	C4-C5-C6	2.95	124.69	120.19
2	A	6	SO4	O4-S-O2	-2.64	95.55	109.31
3	A	247	BEN	C5-C6-C1	2.52	123.32	120.34
3	A	7[A]	BEN	C6-C1-C2	-2.45	115.09	118.59
3	A	8	BEN	C6-C1-C2	-2.45	115.10	118.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	10	SO4	O3-S-O1	-2.29	97.34	109.31
2	B	2	SO4	O4-S-O3	-2.24	99.50	109.06
3	A	8	BEN	C3-C2-C1	2.23	122.98	120.34
3	B	247	BEN	C5-C4-C3	-2.23	115.79	119.93
2	A	9	SO4	O4-S-O1	2.10	120.27	109.31
3	A	247	BEN	C6-C1-C2	-2.04	115.68	118.59

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	247	BEN	N2-C-C1-C2
3	A	7[B]	BEN	N2-C-C1-C2
3	A	7[A]	BEN	N1-C-C1-C2
3	A	7[B]	BEN	N1-C-C1-C2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	10	SO4	2	0
2	A	11	SO4	1	0
3	A	7[B]	BEN	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	224/224 (100%)	-0.23	6 (2%) 54 49	7, 10, 28, 43	0
1	B	224/224 (100%)	-0.12	10 (4%) 33 28	8, 11, 32, 49	0
All	All	448/448 (100%)	-0.18	16 (3%) 42 36	7, 11, 30, 49	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	TYR	14.4
1	B	98	THR	9.8
1	A	99	TYR	7.4
1	A	98	THR	7.2
1	A	175	ILE	6.7
1	B	96	LYS	5.8
1	B	175	ILE	5.3
1	A	94	PHE	4.2
1	A	174	PHE	4.1
1	B	174	PHE	3.6
1	B	170	SER	2.9
1	B	223	LYS	2.8
1	B	95	THR	2.7
1	A	96	LYS	2.4
1	B	173	SER	2.3
1	B	172	SER	2.0

### 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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	BEN	A	8	9/9	0.77	0.18	17,18,25,29	0
2	SO4	A	9	5/5	0.79	0.21	39,39,62,71	0
3	BEN	A	7[B]	9/9	0.81	0.22	12,17,25,48	9
3	BEN	A	7[A]	9/9	0.81	0.22	14,17,19,22	9
2	SO4	A	11	5/5	0.84	0.22	60,62,79,79	0
2	SO4	B	10	5/5	0.86	0.19	31,36,54,54	0
2	SO4	B	5	5/5	0.89	0.28	20,23,27,29	0
2	SO4	B	4	5/5	0.91	0.19	26,30,42,42	0
2	SO4	A	6	5/5	0.91	0.18	17,30,50,52	0
2	SO4	A	3	5/5	0.96	0.10	18,19,24,24	0
3	BEN	B	247	9/9	0.96	0.07	12,14,15,17	0
2	SO4	B	2	5/5	0.97	0.12	13,23,45,51	0
2	SO4	B	246	5/5	0.98	0.11	16,19,27,28	0
3	BEN	A	247	9/9	0.98	0.05	11,13,15,17	0
2	SO4	A	246	5/5	0.98	0.09	15,17,44,49	0
4	NA	B	248	1/1	0.98	0.12	20,20,20,20	0
4	NA	A	248	1/1	0.99	0.12	17,17,17,17	0
2	SO4	A	1	5/5	1.00	0.04	13,13,17,21	0
5	CA	A	249	1/1	1.00	0.04	9,9,9,9	0
5	CA	B	249	1/1	1.00	0.02	11,11,11,11	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.