



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:26 PM UTC

PDB ID : 1ESB / pdb_00001esb
Title : DIRECT STRUCTURE OBSERVATION OF AN ACYL-ENZYME INTER-MEDIATE IN THE HYDROLYSIS OF AN ESTER SUBSTRATE BY ELAS-TASE
Authors : Ding, X.; Rasmussen, B.; Petsko, G.A.; Ringe, D.
Deposited on : 1994-02-04
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

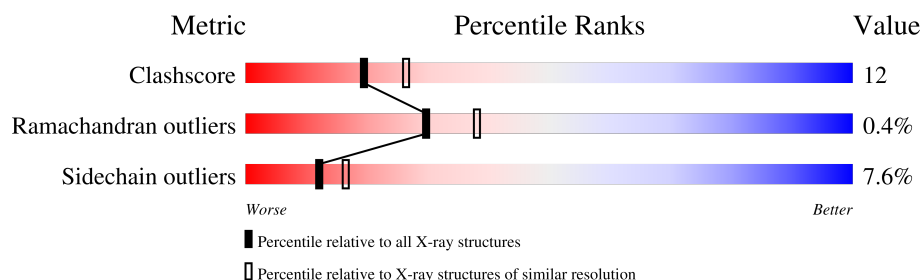
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	240	

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	BBL	A	256	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1968 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.

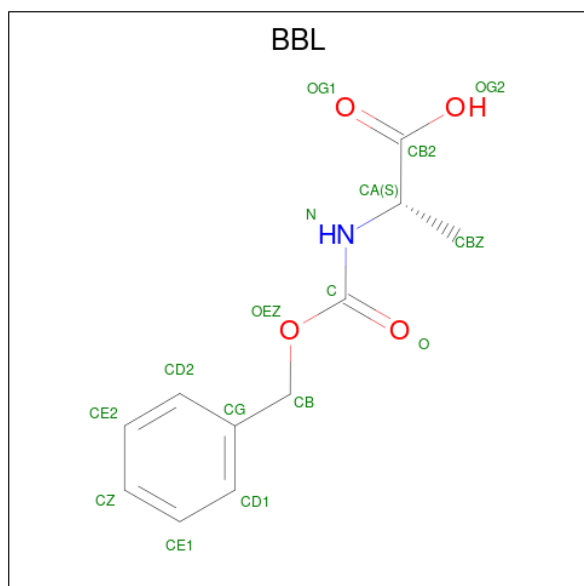
- Molecule 1 is a protein called PORCINE PANCREATIC ELASTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	240	1821	1135	330	346	10	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	ASN	ASP	conflict	UNP P00772

- Molecule 2 is N-[(BENZYLOXY)CARBONYL]-L-ALANINE (CCD ID: BBL) (formula: $C_{11}H_{13}NO_4$).

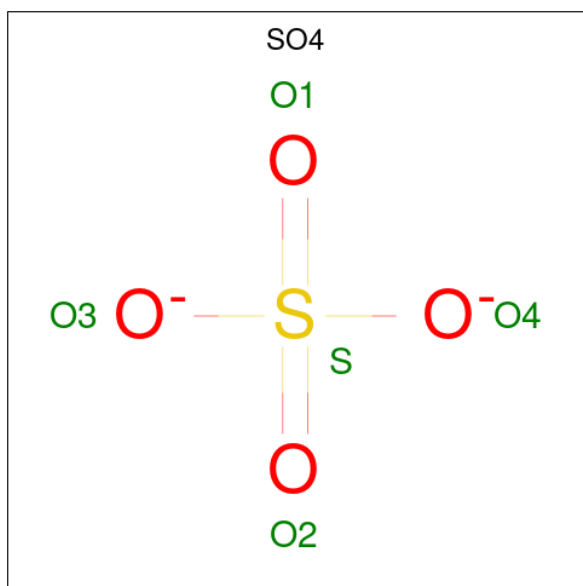


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	15	11	1	3	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is water.

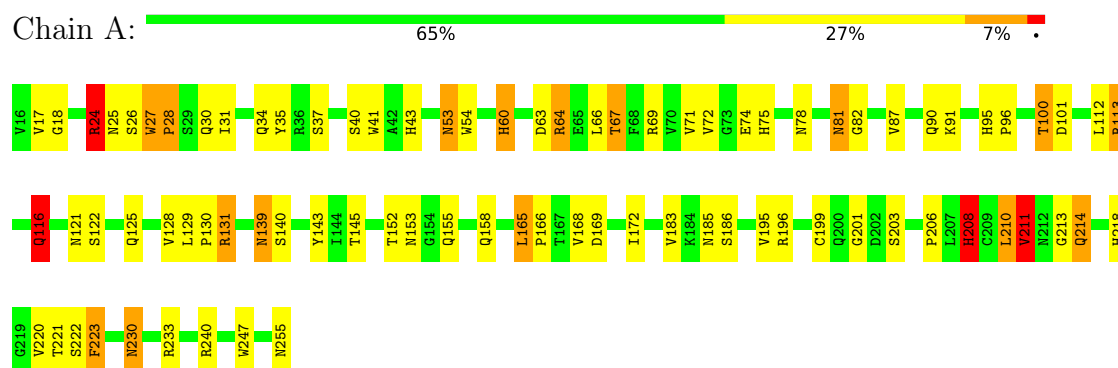
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	126	Total	O	0	0
			126	126		

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. 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: PORCINE PANCREATIC ELASTASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.02Å 57.22Å 74.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1968	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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: SO4, CA, BBL

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	1.27	10/1861 (0.5%)	1.99	57/2543 (2.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	HIS	CD2-NE2	-7.57	1.29	1.37
1	A	218	HIS	CD2-NE2	-7.10	1.30	1.37
1	A	75	HIS	CG-ND1	-6.49	1.31	1.38
1	A	43	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	220	VAL	CA-CB	6.15	1.61	1.53
1	A	75	HIS	CD2-NE2	-5.76	1.31	1.37
1	A	60	HIS	CD2-NE2	-5.63	1.31	1.37
1	A	211	VAL	CA-CB	5.27	1.61	1.54
1	A	208	HIS	CG-ND1	-5.21	1.32	1.38
1	A	130	PRO	CA-CB	-5.10	1.46	1.53

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ASP	CA-CB-CG	11.58	124.18	112.60
1	A	27	TRP	CA-C-N	9.60	129.26	119.56
1	A	27	TRP	C-N-CA	9.60	129.26	119.56
1	A	95	HIS	CA-CB-CG	-9.15	104.65	113.80
1	A	139	ASN	CA-CB-CG	-8.71	103.89	112.60
1	A	116	GLN	OE1-CD-NE2	-8.06	114.54	122.60
1	A	172	ILE	N-CA-C	-7.63	103.01	110.72
1	A	131	ARG	CA-CB-CG	6.93	127.95	114.10
1	A	129	LEU	CA-C-N	6.75	126.72	120.03
1	A	129	LEU	C-N-CA	6.75	126.72	120.03
1	A	220	VAL	CA-C-O	-6.68	113.13	120.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	GLN	CG-CD-NE2	6.58	126.27	116.40
1	A	28	PRO	N-CA-C	6.52	122.00	113.86
1	A	113	ARG	CA-C-O	6.41	127.78	120.54
1	A	81	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	A	113	ARG	CA-CB-CG	6.19	126.48	114.10
1	A	81	ASN	CB-CG-ND2	6.14	125.62	116.40
1	A	223	PHE	O-C-N	6.14	129.43	123.29
1	A	223	PHE	CA-CB-CG	5.96	119.76	113.80
1	A	240	ARG	CB-CG-CD	-5.86	97.83	111.30
1	A	17	VAL	CB-CA-C	-5.85	104.24	111.08
1	A	208	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	A	112	LEU	CA-C-N	-5.77	114.06	122.19
1	A	112	LEU	C-N-CA	-5.77	114.06	122.19
1	A	158	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	A	95	HIS	CA-C-N	5.55	126.78	119.84
1	A	95	HIS	C-N-CA	5.55	126.78	119.84
1	A	128	VAL	O-C-N	-5.53	116.20	122.94
1	A	199	CYS	O-C-N	-5.51	117.47	123.26
1	A	100	THR	N-CA-C	5.50	117.98	111.33
1	A	67	THR	CA-CB-OG1	-5.48	101.38	109.60
1	A	218	HIS	CB-CG-CD2	-5.48	124.08	131.20
1	A	152	THR	N-CA-C	-5.47	101.54	109.59
1	A	165	LEU	O-C-N	-5.45	116.36	121.32
1	A	168	VAL	N-CA-C	-5.40	99.86	107.75
1	A	25	ASN	CA-CB-CG	5.40	118.00	112.60
1	A	63	ASP	CA-C-O	-5.38	115.17	120.82
1	A	41	TRP	CG-CD2-CE3	5.38	139.28	133.90
1	A	101	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	195	VAL	N-CA-C	-5.35	107.39	111.62
1	A	41	TRP	CG-CD1-NE1	-5.33	103.28	110.20
1	A	27	TRP	CG-CD2-CE3	5.30	139.20	133.90
1	A	186	SER	N-CA-C	-5.26	106.71	113.02
1	A	53	ASN	CA-CB-CG	5.20	117.80	112.60
1	A	218	HIS	CB-CG-ND1	5.16	130.44	122.70
1	A	26	SER	CA-C-O	-5.13	115.06	120.55
1	A	24	ARG	NE-CZ-NH2	-5.13	114.58	119.20
1	A	54	TRP	CG-CD2-CE3	5.09	138.99	133.90
1	A	247	TRP	CG-CD2-CE3	5.08	138.98	133.90
1	A	214	GLN	OE1-CD-NE2	5.08	127.68	122.60
1	A	121	ASN	O-C-N	-5.07	117.05	122.88
1	A	78	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	A	168	VAL	O-C-N	-5.07	117.83	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	PRO	N-CA-C	5.06	120.13	111.68
1	A	27	TRP	CB-CG-CD1	-5.06	119.32	126.90
1	A	221	THR	CA-C-O	5.05	126.47	120.96
1	A	30	GLN	CA-C-O	5.02	126.59	120.81

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	1821	0	1758	40	5
2	A	15	0	12	12	0
3	A	1	0	0	0	0
4	A	5	0	0	0	1
5	A	126	0	0	7	3
All	All	1968	0	1770	41	7

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 12.

All (41) 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:SER:CB	2:A:256:BBL:CB2	2.38	1.01
1:A:213:GLY:N	5:A:349:HOH:O	1.96	0.97
1:A:81:ASN:HB3	5:A:310:HOH:O	1.66	0.94
2:A:256:BBL:HD1	5:A:505:HOH:O	1.72	0.90
1:A:222:SER:O	2:A:256:BBL:HE1	1.85	0.77
1:A:34:GLN:HE22	1:A:69:ARG:HH21	1.31	0.77
1:A:230:ASN:H	1:A:230:ASN:HD22	1.36	0.71
1:A:122:SER:O	5:A:393:HOH:O	2.07	0.71
1:A:203:SER:HB2	2:A:256:BBL:CB2	2.20	0.71
1:A:34:GLN:NE2	1:A:69:ARG:HH21	1.91	0.68
1:A:91:LYS:HB3	1:A:113:ARG:HG2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:PRO:HB2	1:A:125:GLN:HB2	1.82	0.62
1:A:60:HIS:CD2	2:A:256:BBL:CE2	2.82	0.62
1:A:223:PHE:HB3	2:A:256:BBL:HE1	1.83	0.60
1:A:222:SER:O	2:A:256:BBL:CE1	2.51	0.58
1:A:31:ILE:HG22	1:A:72:VAL:HG12	1.85	0.58
1:A:24:ARG:HH22	1:A:81:ASN:HD22	1.50	0.57
1:A:60:HIS:CG	2:A:256:BBL:HE2	2.40	0.56
1:A:87:VAL:HG23	1:A:116:GLN:HE21	1.70	0.56
1:A:60:HIS:CE1	2:A:256:BBL:CZ	2.89	0.55
1:A:28:PRO:HD2	5:A:334:HOH:O	2.08	0.54
1:A:60:HIS:CG	2:A:256:BBL:CE2	2.92	0.52
1:A:230:ASN:H	1:A:230:ASN:ND2	2.06	0.51
1:A:34:GLN:HE21	1:A:69:ARG:HE	1.60	0.49
1:A:24:ARG:NH2	1:A:81:ASN:HD22	2.11	0.48
1:A:64:ARG:HB3	1:A:66:LEU:HG	1.96	0.48
1:A:201:GLY:N	2:A:256:BBL:OG1	2.46	0.47
1:A:210:LEU:HD12	5:A:536:HOH:O	2.15	0.47
1:A:211:VAL:O	1:A:214:GLN:HG2	2.16	0.46
1:A:18:GLY:O	1:A:196:ARG:HG2	2.15	0.46
1:A:31:ILE:CG2	1:A:72:VAL:HG12	2.46	0.46
1:A:35:TYR:HA	1:A:67:THR:O	2.16	0.45
1:A:27:TRP:CD1	1:A:145:THR:HG21	2.53	0.44
1:A:140:SER:O	1:A:166:PRO:HA	2.19	0.43
1:A:64:ARG:HE	1:A:66:LEU:HD21	1.84	0.43
1:A:74:GLU:HB3	5:A:322:HOH:O	2.19	0.42
1:A:143:TYR:O	1:A:208:HIS:HD2	2.02	0.42
1:A:71:VAL:HG12	1:A:74:GLU:HB2	2.02	0.42
1:A:233:ARG:HH11	1:A:233:ARG:HD3	1.73	0.41
1:A:201:GLY:H	2:A:256:BBL:HBZ3	1.86	0.40
1:A:53:ASN:HD22	1:A:113:ARG:NH2	2.19	0.40

All (7) 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:82:GLY:O	5:A:502:HOH:O[4_566]	1.44	0.76
4:A:290:SO4:O1	5:A:513:HOH:O[2_665]	1.56	0.64
1:A:81:ASN:O	1:A:196:ARG:NH1[4_566]	1.70	0.50
5:A:520:HOH:O	5:A:558:HOH:O[4_566]	1.99	0.21
1:A:131:ARG:NH2	1:A:153:ASN:ND2[2_665]	2.15	0.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLN:OE1	1:A:185:ASN:OD1[2_664]	2.16	0.04
1:A:131:ARG:NE	1:A:153:ASN:ND2[2_665]	2.17	0.03

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	238/240 (99%)	228 (96%)	9 (4%)	1 (0%)	30	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PRO

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	198/198 (100%)	183 (92%)	15 (8%)	12	16

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

Mol	Chain	Res	Type
1	A	24	ARG
1	A	37	SER
1	A	40	SER

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Mol	Chain	Res	Type
1	A	64	ARG
1	A	90	GLN
1	A	100	THR
1	A	116	GLN
1	A	139	ASN
1	A	165	LEU
1	A	183	VAL
1	A	208	HIS
1	A	210	LEU
1	A	211	VAL
1	A	230	ASN
1	A	255	ASN

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

Mol	Chain	Res	Type
1	A	34	GLN
1	A	53	ASN
1	A	78	ASN
1	A	95	HIS
1	A	99	ASN
1	A	116	GLN
1	A	158	GLN
1	A	230	ASN
1	A	249	ASN
1	A	250	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
2	BBL	A	256	1	14,15,16	2.35	2 (14%)	16,18,20	2.54	3 (18%)
4	SO4	A	290	-	4,4,4	0.55	0	6,6,6	0.36	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
2	BBL	A	256	1	-	4/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	256	BBL	OEZ-C	7.67	1.50	1.35
2	A	256	BBL	CA-N	-3.20	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	256	BBL	CBZ-CA-N	-6.14	102.74	109.68
2	A	256	BBL	CA-N-C	5.45	127.13	121.62
2	A	256	BBL	OG1-CB2-CA	-5.44	106.99	123.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	256	BBL	CB2-CA-N-C
2	A	256	BBL	CG-CB-OEZ-C

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Mol	Chain	Res	Type	Atoms
2	A	256	BBL	N-C-OEZ-CB
2	A	256	BBL	O-C-OEZ-CB

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	256	BBL	12	0
4	A	290	SO4	0	1

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.