Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 02:45 PM EDT

PDB ID	:	1EPP
Title	:	ENDOTHIA ASPARTIC PROTEINASE (ENDOTHIAPEPSIN) COMPLEXED WITH PD-130,693 (MAS PHE LYS+MTF STA MBA)
Authors	:	Wallace, B.A.; Cooper, J.B.; Blundell, T.L.
Deposited on	:	1994-07-27
Resolution	:	1.90 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 (i) 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 (1)) were used in the production of this report:

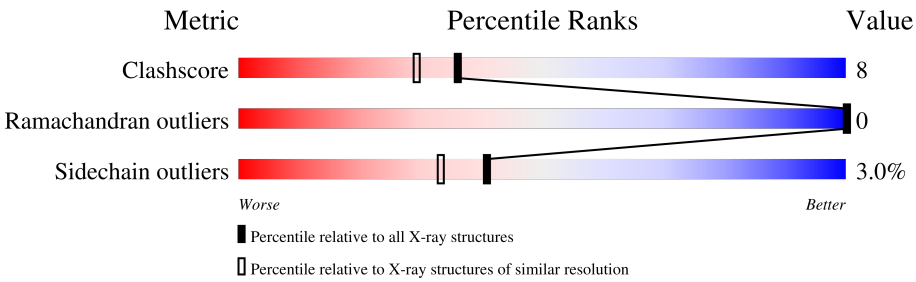
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	330	64% 32% .

2 Entry composition (i)

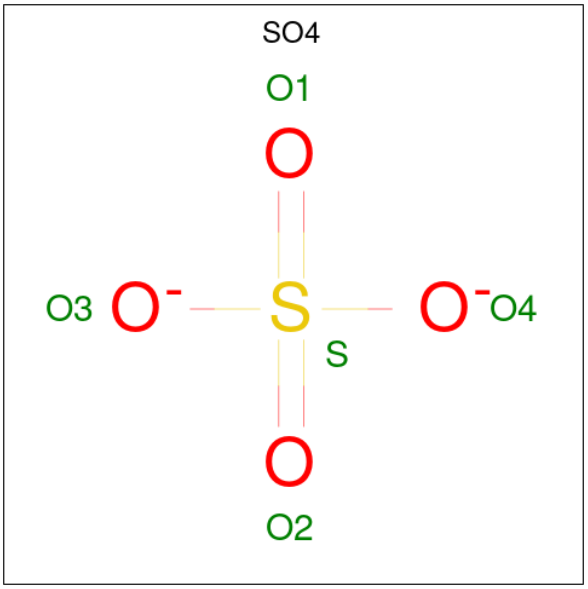
There are 4 unique types of molecules in this entry. The entry contains 2706 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENDOTHIAPEPSIN.

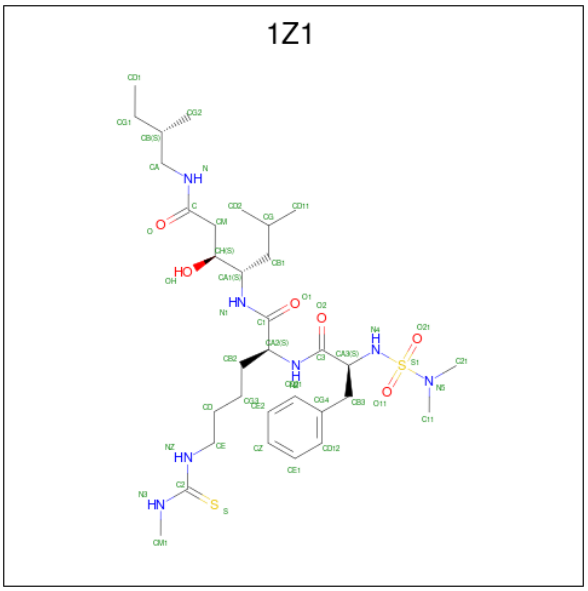
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	330	2389	1514	366	507	2	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is N-(dimethylsulfamoyl)-L-phenylalanyl-N-[(1S,2S)-2-hydroxy-4-{[(2S)-2-methylbutyl]amino}-1-(2-methylpropyl)-4-oxobutyl]-N 6 -(methylcarbamothioyl)-L-lysinamide (three-letter code: 1Z1) (formula: $C_{32}H_{57}N_7O_6S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	E	1	47	32	7	6	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	260	260	260	0	0

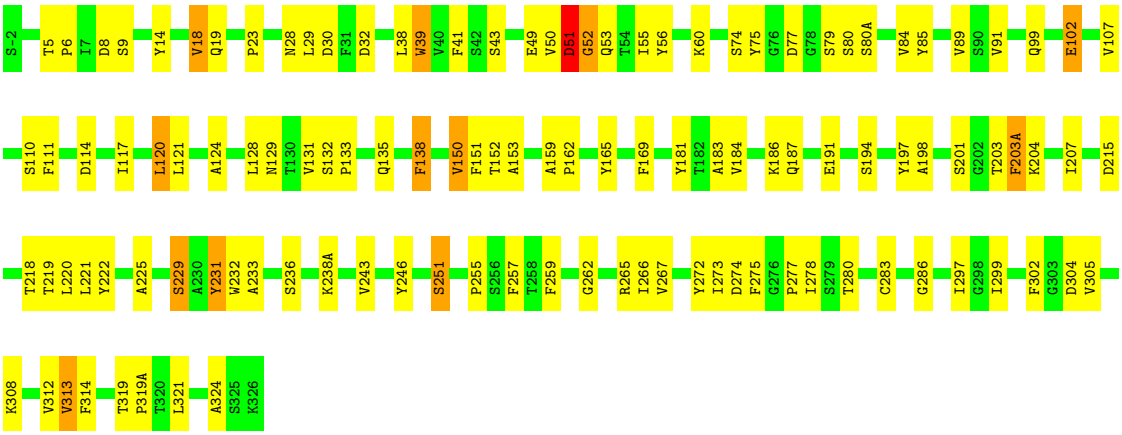
3 Residue-property plots (i)

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: ENDOTHIAPEPSIN

Chain E:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.10Å 75.60Å 42.90Å 90.00° 97.20° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
% Data completeness (in resolution range)	84.0 (20.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2706	wwPDB-VP
Average B, all atoms (Å^2)	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: 1Z1, 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	E	1.64	16/2445 (0.7%)	2.21	106/3345 (3.2%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	52	GLY	N-CA	8.47	1.58	1.46
1	E	39	TRP	N-CA	7.54	1.61	1.46
1	E	74	SER	CA-CB	-6.43	1.43	1.52
1	E	201	SER	CB-OG	6.07	1.50	1.42
1	E	53	GLN	CD-OE1	6.04	1.37	1.24
1	E	259	PHE	CG-CD2	5.82	1.47	1.38
1	E	251	SER	CB-OG	-5.74	1.34	1.42
1	E	187	GLN	CD-OE1	5.53	1.36	1.24
1	E	6	PRO	CA-CB	-5.38	1.42	1.53
1	E	262	GLY	N-CA	5.38	1.54	1.46
1	E	80	SER	CB-OG	5.21	1.49	1.42
1	E	229	SER	CB-OG	-5.17	1.35	1.42
1	E	19	GLN	CD-OE1	5.17	1.35	1.24
1	E	257	PHE	CG-CD1	5.17	1.46	1.38
1	E	165	TYR	CG-CD2	5.12	1.45	1.39
1	E	203(A)	PHE	CA-CB	-5.12	1.42	1.53

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	30	ASP	CB-CG-OD1	13.00	130.00	118.30
1	E	246	TYR	CB-CG-CD1	-11.23	114.26	121.00
1	E	85	TYR	CB-CG-CD1	-10.54	114.67	121.00
1	E	138	PHE	CB-CG-CD1	9.96	127.77	120.80
1	E	181	TYR	CB-CG-CD1	-9.02	115.59	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	91	VAL	CA-CB-CG2	8.86	124.19	110.90
1	E	312	VAL	CA-CB-CG2	8.81	124.11	110.90
1	E	222	TYR	CB-CG-CD2	-8.78	115.73	121.00
1	E	181	TYR	CB-CG-CD2	8.76	126.25	121.00
1	E	89	VAL	CA-CB-CG2	8.70	123.95	110.90
1	E	150	VAL	CA-CB-CG1	8.56	123.74	110.90
1	E	324	ALA	N-CA-CB	8.56	122.08	110.10
1	E	165	TYR	CB-CG-CD2	-8.46	115.92	121.00
1	E	138	PHE	CB-CG-CD2	-8.45	114.88	120.80
1	E	246	TYR	CB-CG-CD2	8.24	125.94	121.00
1	E	151	PHE	O-C-N	-8.09	109.75	122.70
1	E	165	TYR	CG-CD2-CE2	-8.05	114.86	121.30
1	E	243	VAL	CA-CB-CG2	8.05	122.97	110.90
1	E	51	ASP	C-N-CA	-7.93	105.66	122.30
1	E	313	VAL	CA-CB-CG2	7.81	122.62	110.90
1	E	128	LEU	CB-CG-CD2	7.71	124.10	111.00
1	E	304	ASP	CB-CG-OD1	7.67	125.20	118.30
1	E	265	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	E	319(A)	PRO	O-C-N	-7.59	110.55	122.70
1	E	43	SER	O-C-N	-7.47	110.74	122.70
1	E	232	TRP	CE3-CZ3-CH2	7.34	129.28	121.20
1	E	107	VAL	CA-CB-CG2	7.28	121.81	110.90
1	E	266	ILE	O-C-N	7.24	134.28	122.70
1	E	56	TYR	O-C-N	7.22	134.26	122.70
1	E	232	TRP	CZ3-CH2-CZ2	-7.15	113.02	121.60
1	E	197	TYR	CD1-CE1-CZ	7.01	126.11	119.80
1	E	159	ALA	N-CA-CB	-6.98	100.33	110.10
1	E	232	TRP	CB-CG-CD1	-6.96	117.95	127.00
1	E	225	ALA	O-C-N	-6.96	111.56	122.70
1	E	23	PRO	O-C-N	-6.85	111.75	122.70
1	E	305	VAL	CA-CB-CG1	6.82	121.12	110.90
1	E	197	TYR	CG-CD1-CE1	-6.79	115.87	121.30
1	E	274	ASP	CB-CG-OD1	6.69	124.32	118.30
1	E	275	PHE	CB-CG-CD1	-6.68	116.12	120.80
1	E	151	PHE	CA-C-O	6.65	134.06	120.10
1	E	257	PHE	CB-CG-CD2	6.61	125.42	120.80
1	E	32	ASP	CB-CG-OD1	6.60	124.24	118.30
1	E	321	LEU	CB-CG-CD1	6.58	122.19	111.00
1	E	121	LEU	O-C-N	-6.57	112.04	123.20
1	E	169	PHE	CD1-CE1-CZ	-6.45	112.36	120.10
1	E	132	SER	C-N-CD	-6.42	106.47	120.60
1	E	184	VAL	CA-CB-CG2	6.38	120.47	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	236	SER	O-C-N	6.37	134.02	123.20
1	E	275	PHE	CG-CD2-CE2	-6.34	113.82	120.80
1	E	232	TRP	CB-CG-CD2	6.21	134.67	126.60
1	E	183	ALA	CB-CA-C	-6.16	100.86	110.10
1	E	80(A)	SER	N-CA-CB	6.14	119.70	110.50
1	E	75	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	E	50	VAL	CA-CB-CG2	6.00	119.90	110.90
1	E	75	TYR	C-N-CA	5.98	134.87	122.30
1	E	280	THR	O-C-N	-5.97	113.05	123.20
1	E	278	ILE	CB-CA-C	5.94	123.47	111.60
1	E	50	VAL	CA-CB-CG1	5.93	119.79	110.90
1	E	275	PHE	CD1-CG-CD2	5.89	125.96	118.30
1	E	111	PHE	CG-CD2-CE2	5.87	127.26	120.80
1	E	38	LEU	C-N-CA	-5.87	107.04	121.70
1	E	221	LEU	CB-CG-CD1	5.87	120.97	111.00
1	E	267	VAL	CG1-CB-CG2	-5.82	101.58	110.90
1	E	85	TYR	CG-CD1-CE1	-5.82	116.64	121.30
1	E	257	PHE	CB-CG-CD1	-5.80	116.74	120.80
1	E	219	THR	CA-CB-CG2	-5.80	104.28	112.40
1	E	8	ASP	CB-CG-OD1	5.78	123.51	118.30
1	E	9	SER	CA-C-N	5.77	129.90	117.20
1	E	84	VAL	CA-CB-CG2	5.77	119.56	110.90
1	E	308	LYS	CB-CG-CD	-5.66	96.89	111.60
1	E	120	LEU	CA-CB-CG	5.63	128.24	115.30
1	E	51	ASP	CB-CG-OD1	5.62	123.36	118.30
1	E	74	SER	N-CA-CB	5.61	118.92	110.50
1	E	273	ILE	CA-CB-CG2	5.61	122.12	110.90
1	E	236	SER	N-CA-CB	5.58	118.86	110.50
1	E	297	ILE	O-C-N	-5.54	113.79	123.20
1	E	231	TYR	CA-CB-CG	-5.51	102.94	113.40
1	E	302	PHE	CB-CG-CD1	5.50	124.65	120.80
1	E	102	GLU	OE1-CD-OE2	-5.49	116.71	123.30
1	E	278	ILE	CA-CB-CG1	5.49	121.44	111.00
1	E	203(A)	PHE	CB-CG-CD2	-5.49	116.96	120.80
1	E	85	TYR	CD1-CG-CD2	5.47	123.92	117.90
1	E	272	TYR	CG-CD1-CE1	-5.46	116.93	121.30
1	E	14	TYR	CB-CG-CD2	5.45	124.27	121.00
1	E	215	ASP	N-CA-CB	-5.41	100.86	110.60
1	E	80	SER	C-N-CA	5.41	135.22	121.70
1	E	169	PHE	N-CA-CB	5.39	120.30	110.60
1	E	191	GLU	OE1-CD-OE2	-5.35	116.88	123.30
1	E	225	ALA	CB-CA-C	-5.34	102.09	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	314	PHE	CG-CD1-CE1	-5.30	114.96	120.80
1	E	233	ALA	N-CA-CB	5.30	117.52	110.10
1	E	238(A)	LYS	CA-CB-CG	-5.28	101.78	113.40
1	E	124	ALA	CA-C-N	5.28	128.82	117.20
1	E	51	ASP	CA-CB-CG	5.28	125.01	113.40
1	E	14	TYR	O-C-N	-5.27	114.27	122.70
1	E	49	GLU	N-CA-CB	5.25	120.05	110.60
1	E	133	PRO	CA-N-CD	5.24	119.03	111.70
1	E	77	ASP	CB-CG-OD1	5.20	122.98	118.30
1	E	153	ALA	N-CA-CB	5.18	117.36	110.10
1	E	38	LEU	CB-CG-CD2	5.15	119.76	111.00
1	E	197	TYR	C-N-CA	5.14	134.54	121.70
1	E	43	SER	CA-C-N	5.13	128.50	117.20
1	E	18	VAL	CG1-CB-CG2	-5.12	102.71	110.90
1	E	30	ASP	OD1-CG-OD2	-5.10	113.61	123.30
1	E	218	THR	N-CA-CB	5.06	119.91	110.30
1	E	203	THR	C-N-CA	5.03	134.28	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	E	2389	0	2279	20	1
2	E	10	0	0	0	0
3	E	47	0	57	18	0
4	E	260	0	0	1	3
All	All	2706	0	2336	38	3

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 (38) 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)
3:E:333:1Z1:HD12	3:E:333:1Z1:CD11	0.97	1.14
3:E:333:1Z1:CD11	3:E:333:1Z1:HD13	0.97	1.11
3:E:333:1Z1:CD11	3:E:333:1Z1:HD11	0.97	1.08
3:E:333:1Z1:HD25	3:E:333:1Z1:CD21	0.97	1.07
3:E:333:1Z1:CD12	3:E:333:1Z1:HD14	0.97	1.06
3:E:333:1Z1:CE2	3:E:333:1Z1:CG4	2.40	0.94
3:E:333:1Z1:HD14	3:E:333:1Z1:CG4	1.99	0.91
3:E:333:1Z1:HD12	3:E:333:1Z1:CG	2.04	0.88
3:E:333:1Z1:HD11	3:E:333:1Z1:CG	2.04	0.87
3:E:333:1Z1:HD13	3:E:333:1Z1:CG	2.04	0.86
3:E:333:1Z1:CG4	3:E:333:1Z1:CE1	2.47	0.86
3:E:333:1Z1:HD12	3:E:333:1Z1:HD13	1.58	0.85
3:E:333:1Z1:HD14	3:E:333:1Z1:CE1	2.05	0.85
3:E:333:1Z1:HD12	3:E:333:1Z1:HD11	1.58	0.84
3:E:333:1Z1:HD13	3:E:333:1Z1:HD11	1.58	0.83
3:E:333:1Z1:HD25	3:E:333:1Z1:CE2	2.07	0.83
3:E:333:1Z1:HD25	3:E:333:1Z1:CG4	2.08	0.82
1:E:129:ASN:ND2	1:E:135:GLN:H	1.93	0.66
1:E:18:VAL:HG21	1:E:29:LEU:HD12	1.81	0.63
1:E:114:ASP:OD2	1:E:117:ILE:HD12	2.00	0.62
1:E:5:THR:HG22	1:E:162:PRO:HB3	1.85	0.59
1:E:129:ASN:HD21	1:E:131:VAL:HB	1.71	0.55
1:E:198:ALA:HB2	1:E:203(A):PHE:HA	1.92	0.51
1:E:39:TRP:HA	1:E:102:GLU:O	2.11	0.50
1:E:129:ASN:ND2	1:E:131:VAL:H	2.11	0.48
1:E:277:PRO:HA	1:E:283:CYS:HA	1.95	0.48
3:E:333:1Z1:HE2	3:E:333:1Z1:HB3	1.48	0.46
1:E:79:SER:HB3	1:E:110:SER:OG	2.15	0.46
1:E:231:TYR:OH	1:E:255:PRO:HD2	2.15	0.46
1:E:60:LYS:HE2	1:E:60:LYS:HA	2.00	0.44
1:E:220:LEU:HD22	1:E:286:GLY:HA2	2.01	0.43
1:E:99:GLN:NE2	1:E:138:PHE:HA	2.35	0.42
1:E:114:ASP:HB2	4:E:548:HOH:O	2.19	0.42
1:E:152:THR:HG22	1:E:313:VAL:HG22	2.01	0.42
1:E:51:ASP:HB3	1:E:52:GLY:H	1.31	0.42
1:E:28:ASN:HD22	1:E:28:ASN:HA	1.68	0.41
1:E:41:PHE:HB3	1:E:55:ILE:HG22	2.03	0.41
1:E:194:SER:HB3	1:E:207:ILE:HB	2.02	0.40

All (3) 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)
4:E:533:HOH:O	4:E:593:HOH:O[1_655]	0.42	1.78
4:E:554:HOH:O	4:E:569:HOH:O[2_656]	1.71	0.49
1:E:319:THR:OG1	4:E:583:HOH:O[2_555]	1.85	0.35

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	E	328/330 (99%)	321 (98%)	7 (2%)	0	100 100

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	E	263/263 (100%)	255 (97%)	8 (3%)	41 33

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	51	ASP
1	E	120	LEU
1	E	150	VAL
1	E	186	LYS
1	E	204	LYS
1	E	229	SER

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Mol	Chain	Res	Type
1	E	251	SER
1	E	299	ILE

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

Mol	Chain	Res	Type
1	E	28	ASN
1	E	99	GLN
1	E	129	ASN
1	E	134(A)	GLN
1	E	135	GLN
1	E	141	ASN
1	E	166	ASN
1	E	187	GLN
1	E	300	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)

3 ligands 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	$\#\|Z\| > 2$
2	SO4	E	327	-	4,4,4	0.16	0	6,6,6	0.13	0
3	1Z1	E	333	-	46,47,47	2.73	10 (21%)	58,62,62	2.96	24 (41%)
2	SO4	E	328	-	4,4,4	0.60	0	6,6,6	1.24	1 (16%)

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	1Z1	E	333	-	-	14/60/60/60	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	333	1Z1	C2-N3	9.97	1.42	1.32
3	E	333	1Z1	O11-S1	9.17	1.52	1.43
3	E	333	1Z1	C2-NZ	5.94	1.43	1.33
3	E	333	1Z1	S1-N4	5.38	1.69	1.61
3	E	333	1Z1	O21-S1	-5.09	1.37	1.43
3	E	333	1Z1	C21-N5	3.64	1.52	1.47
3	E	333	1Z1	CA1-N1	3.10	1.51	1.46
3	E	333	1Z1	CH-CA1	2.41	1.57	1.53
3	E	333	1Z1	C11-N5	2.05	1.50	1.47
3	E	333	1Z1	CD2-CG	2.03	1.62	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	333	1Z1	CM1-N3-C2	-12.80	113.64	124.07
3	E	333	1Z1	O21-S1-O11	-7.70	108.44	119.72
3	E	333	1Z1	CE-NZ-C2	-7.25	112.67	124.69
3	E	333	1Z1	C21-N5-C11	-4.57	105.54	114.79
3	E	333	1Z1	O21-S1-N5	4.18	113.74	107.00
3	E	333	1Z1	S-C2-N3	-3.88	118.54	123.76
3	E	333	1Z1	CE1-CD12-CG4	3.60	126.16	120.63
3	E	333	1Z1	O21-S1-N4	3.59	117.10	107.63
3	E	333	1Z1	CM-C-N	3.22	120.42	115.97
3	E	333	1Z1	CA-N-C	-3.16	115.80	122.69
3	E	333	1Z1	C11-N5-S1	-3.02	107.08	117.64
3	E	333	1Z1	CB2-CA2-N2	3.00	116.94	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	333	1Z1	CZ-CE1-CD12	-2.88	115.81	120.19
3	E	333	1Z1	CB2-CA2-C1	2.86	116.89	110.20
3	E	333	1Z1	C21-N5-S1	-2.81	107.83	117.64
3	E	333	1Z1	CA1-N1-C1	-2.74	118.23	123.07
3	E	333	1Z1	CG3-CD-CE	-2.64	101.08	113.56
3	E	333	1Z1	O11-S1-N5	-2.56	102.88	107.00
3	E	333	1Z1	CD-CG3-CB2	-2.48	104.85	113.62
3	E	333	1Z1	CA2-N2-C3	2.44	126.91	121.67
3	E	333	1Z1	CG-CB1-CA1	2.33	120.48	115.84
2	E	328	SO4	O3-S-O1	2.22	120.89	109.31
3	E	333	1Z1	NZ-C2-N3	2.19	120.22	116.14
3	E	333	1Z1	CB1-CA1-CH	-2.06	109.43	112.55
3	E	333	1Z1	O-C-CM	-2.03	118.52	121.50

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	333	1Z1	CA3-N4-S1-N5
3	E	333	1Z1	C21-N5-S1-N4
3	E	333	1Z1	C21-N5-S1-O11
3	E	333	1Z1	C11-N5-S1-O21
3	E	333	1Z1	N2-CA2-CB2-CG3
3	E	333	1Z1	CG3-CD-CE-NZ
3	E	333	1Z1	C1-CA2-CB2-CG3
3	E	333	1Z1	O1-C1-CA2-N2
3	E	333	1Z1	N1-C1-CA2-N2
3	E	333	1Z1	CG2-CB-CG1-CD1
3	E	333	1Z1	CA-CB-CG1-CD1
3	E	333	1Z1	S-C2-NZ-CE
3	E	333	1Z1	CD-CE-NZ-C2
3	E	333	1Z1	N3-C2-NZ-CE

There are no ring outliers.

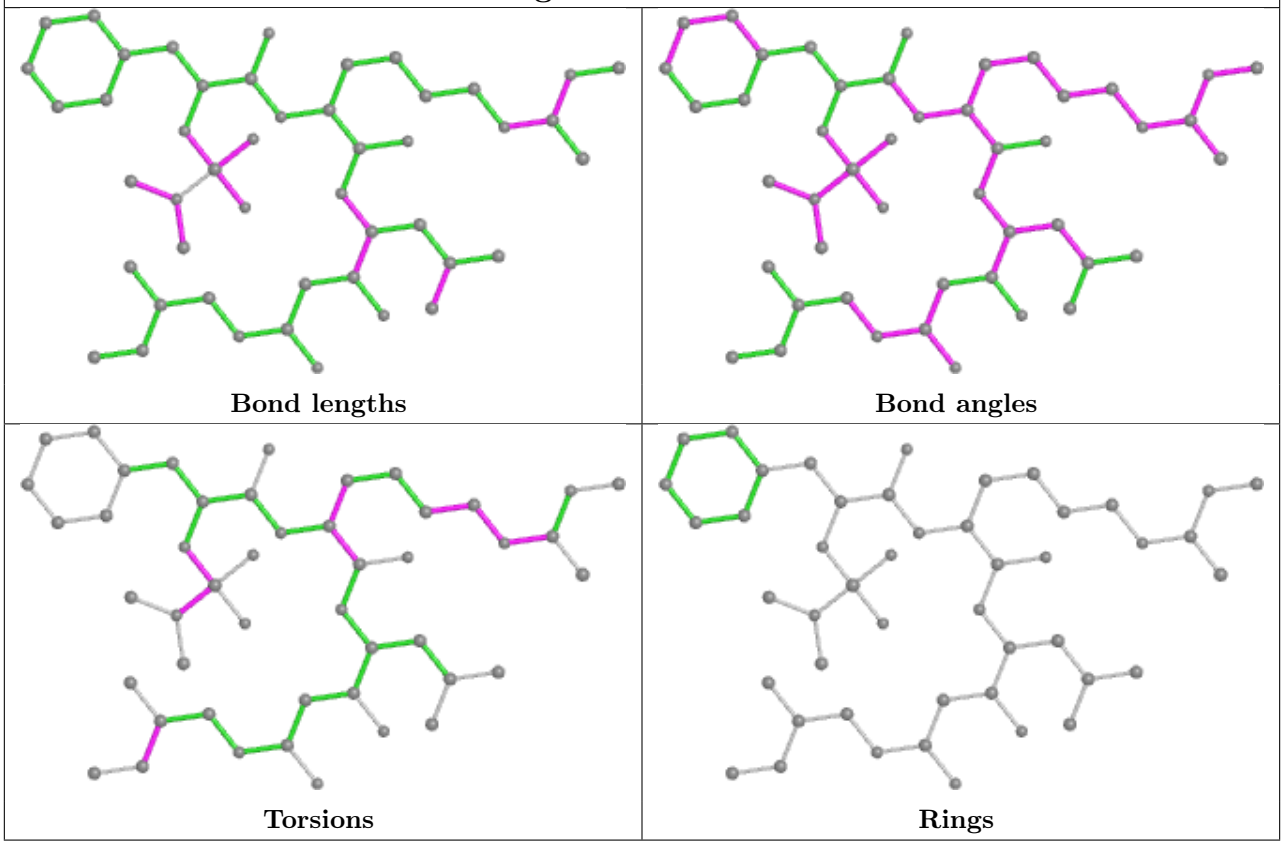
1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	333	1Z1	18	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 1Z1 E 333



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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.