



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:23 PM GMT

PDB ID : 4ER2
Title : The active site of aspartic proteinases
Authors : Bailey, D.; Veerapandian, B.; Cooper, J.B.; Blundell, T.L.
Deposited on : 1990-10-20
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

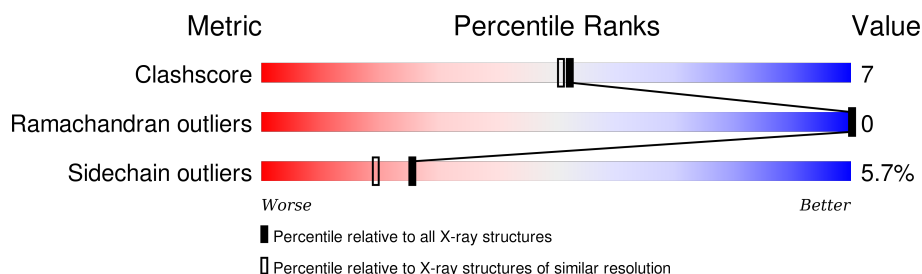
1 Overall quality at a glance

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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	330	
2	I	6	

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
3	SO4	E	920	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2795 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
1	E	330	Total	C	N	O	S	0	0	0
			2389	1514	366	507	2			

- Molecule 2 is a protein called PEPSTATIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	6	Total	C	N	O	0	0	0
			48	34	5	9			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

- Molecule 4 is water.

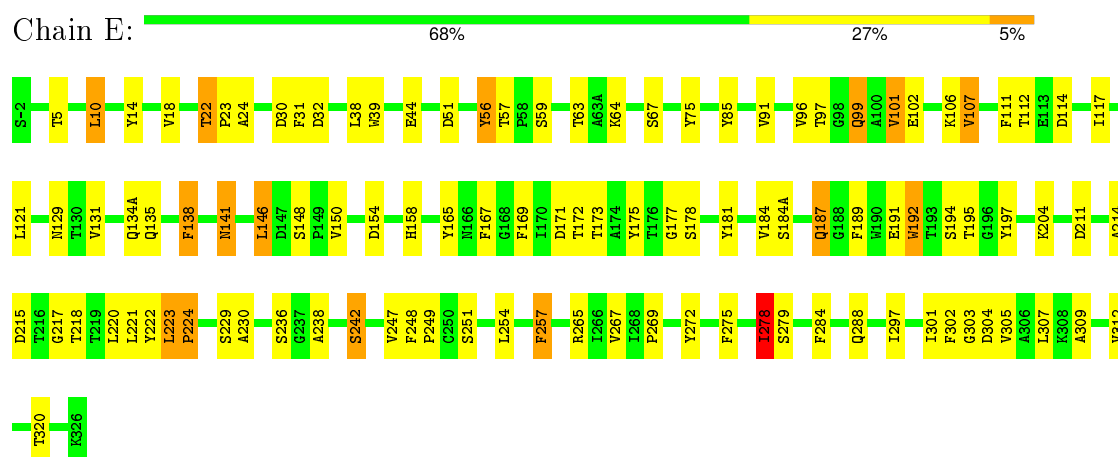
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	338	Total	O	0	0
			338	338		
4	I	5	Total	O	0	0
			5	5		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: ENDOTHIAPEPSIN



• Molecule 2: PEPSTATIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.10 Å 75.60 Å 42.90 Å 90.00° 97.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2795	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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, IVA, STA

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	1.36	5/2445 (0.2%)	2.13	90/3345 (2.7%)
2	I	0.88	0/17	2.28	1/21 (4.8%)
All	All	1.36	5/2462 (0.2%)	2.13	91/3366 (2.7%)

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	E	0	4
2	I	0	2
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	39	TRP	NE1-CE2	-7.99	1.27	1.37
1	E	75	TYR	CZ-OH	6.64	1.49	1.37
1	E	138	PHE	N-CA	5.72	1.57	1.46
1	E	99	GLN	CD-OE1	5.37	1.35	1.24
1	E	134(A)	GLN	CD-OE1	5.15	1.35	1.24

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	275	PHE	CB-CG-CD1	-14.30	110.79	120.80
1	E	44	GLU	OE1-CD-OE2	-14.21	106.25	123.30
1	E	284	PHE	CB-CG-CD1	-13.06	111.66	120.80
1	E	284	PHE	CB-CG-CD2	11.82	129.07	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	154	ASP	CB-CG-OD2	11.43	128.58	118.30
1	E	175	TYR	CB-CG-CD1	-10.71	114.57	121.00
1	E	138	PHE	CB-CG-CD2	10.60	128.22	120.80
1	E	175	TYR	CB-CG-CD2	10.45	127.27	121.00
1	E	75	TYR	CB-CG-CD1	-10.36	114.79	121.00
1	E	265	ARG	NE-CZ-NH2	10.12	125.36	120.30
1	E	150	VAL	CA-CB-CG1	9.43	125.04	110.90
1	E	181	TYR	CB-CG-CD1	-9.15	115.51	121.00
1	E	102	GLU	OE1-CD-OE2	8.70	133.73	123.30
1	E	111	PHE	CB-CG-CD1	8.64	126.85	120.80
1	E	30	ASP	CB-CG-OD2	8.45	125.91	118.30
1	E	85	TYR	CB-CG-CD2	-8.36	115.98	121.00
1	E	181	TYR	CG-CD2-CE2	-8.26	114.69	121.30
1	E	146	LEU	CB-CG-CD1	8.19	124.92	111.00
1	E	304	ASP	CB-CG-OD2	-8.17	110.95	118.30
1	E	165	TYR	CB-CG-CD1	-8.10	116.14	121.00
1	E	39	TRP	CG-CD2-CE3	8.04	141.14	133.90
1	E	146	LEU	CB-CG-CD2	7.80	124.27	111.00
1	E	175	TYR	CG-CD1-CE1	-7.72	115.12	121.30
1	E	181	TYR	CD1-CE1-CZ	-7.65	112.92	119.80
1	E	111	PHE	CG-CD2-CE2	7.42	128.96	120.80
1	E	302	PHE	C-N-CA	7.40	137.84	122.30
1	E	107	VAL	CA-CB-CG1	7.36	121.94	110.90
1	E	175	TYR	CD1-CE1-CZ	7.28	126.35	119.80
1	E	154	ASP	CB-CG-OD1	-7.22	111.80	118.30
1	E	44	GLU	CG-CD-OE1	7.11	132.51	118.30
1	E	171	ASP	CB-CG-OD1	7.06	124.65	118.30
1	E	167	PHE	CB-CG-CD1	6.93	125.65	120.80
1	E	197	TYR	CB-CG-CD1	-6.88	116.87	121.00
1	E	312	VAL	CA-CB-CG2	6.67	120.91	110.90
1	E	14	TYR	CD1-CE1-CZ	6.65	125.78	119.80
1	E	85	TYR	CB-CG-CD1	6.58	124.95	121.00
1	E	165	TYR	CB-CG-CD2	6.50	124.90	121.00
1	E	320	THR	N-CA-CB	6.46	122.57	110.30
1	E	230	ALA	N-CA-CB	6.42	119.09	110.10
1	E	32	ASP	CB-CG-OD2	6.40	124.06	118.30
1	E	211	ASP	CB-CG-OD1	-6.35	112.59	118.30
1	E	31	PHE	CB-CG-CD1	-6.32	116.38	120.80
1	E	158	HIS	N-CA-CB	6.27	121.89	110.60
1	E	236	SER	O-C-N	-6.27	112.55	123.20
1	E	307	LEU	CB-CG-CD1	-6.16	100.53	111.00
2	I	2	VAL	CA-CB-CG2	6.14	120.11	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	23	PRO	CA-N-CD	6.09	120.22	111.70
1	E	288	GLN	CG-CD-NE2	6.05	131.23	116.70
1	E	192	TRP	NE1-CE2-CZ2	-6.02	123.78	130.40
1	E	267	VAL	CA-CB-CG2	5.97	119.85	110.90
1	E	278	ILE	C-N-CA	5.96	136.60	121.70
1	E	309	ALA	N-CA-CB	-5.92	101.81	110.10
1	E	5	THR	N-CA-CB	-5.87	99.15	110.30
1	E	18	VAL	CA-CB-CG1	5.85	119.67	110.90
1	E	24	ALA	N-CA-CB	-5.84	101.93	110.10
1	E	91	VAL	CA-CB-CG1	-5.82	102.17	110.90
1	E	169	PHE	CG-CD2-CE2	5.77	127.14	120.80
1	E	75	TYR	C-N-CA	5.76	134.40	122.30
1	E	39	TRP	CH2-CZ2-CE2	5.75	123.16	117.40
1	E	138	PHE	N-CA-CB	-5.69	100.36	110.60
1	E	222	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	E	22	THR	C-N-CD	-5.57	108.36	120.60
1	E	275	PHE	CA-CB-CG	-5.57	100.54	113.90
1	E	215	ASP	CB-CG-OD1	5.53	123.28	118.30
1	E	221	LEU	CB-CG-CD1	5.53	120.40	111.00
1	E	269	PRO	O-C-N	-5.53	113.81	123.20
1	E	217	GLY	O-C-N	5.50	131.50	122.70
1	E	192	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	E	175	TYR	CG-CD2-CE2	5.40	125.62	121.30
1	E	172	THR	O-C-N	-5.37	114.11	122.70
1	E	278	ILE	CA-CB-CG2	5.36	121.63	110.90
1	E	214	ALA	O-C-N	5.36	131.28	122.70
1	E	148	SER	N-CA-CB	-5.34	102.48	110.50
1	E	181	TYR	CG-CD1-CE1	5.34	125.57	121.30
1	E	111	PHE	CZ-CE2-CD2	-5.28	113.76	120.10
1	E	257	PHE	CG-CD2-CE2	5.28	126.61	120.80
1	E	305	VAL	O-C-N	-5.27	114.27	122.70
1	E	275	PHE	CD1-CG-CD2	5.26	125.13	118.30
1	E	57	THR	CA-CB-CG2	-5.24	105.06	112.40
1	E	111	PHE	CD1-CE1-CZ	5.22	126.36	120.10
1	E	59	SER	CB-CA-C	5.21	120.00	110.10
1	E	121	LEU	CB-CG-CD2	5.20	119.83	111.00
1	E	242	SER	N-CA-CB	5.18	118.28	110.50
1	E	56	TYR	O-C-N	-5.16	114.45	122.70
1	E	236	SER	CA-C-N	5.12	126.44	116.20
1	E	223	LEU	N-CA-CB	5.11	120.61	110.40
1	E	272	TYR	CG-CD1-CE1	-5.07	117.25	121.30
1	E	195	THR	O-C-N	-5.07	114.59	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	97	THR	CA-C-N	5.04	126.27	116.20
1	E	224	PRO	N-CA-CB	-5.02	97.07	102.60
1	E	101	VAL	CG1-CB-CG2	-5.00	102.89	110.90

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	101	VAL	Mainchain
1	E	22	THR	Peptide
1	E	257	PHE	Mainchain
1	E	56	TYR	Mainchain
2	I	4	STA	Mainchain,Peptide

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	E	2389	0	2278	32	1
2	I	48	0	60	1	0
3	E	15	0	0	1	5
4	E	338	0	0	2	7
4	I	5	0	0	0	0
All	All	2795	0	2338	32	8

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 7.

All (32) 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:E:187:GLN:O	1:E:187:GLN:HG3	1.54	1.03
1:E:51:ASP:OD1	1:E:112:THR:HG22	1.76	0.86
1:E:187:GLN:HG2	1:E:189:PHE:CD1	2.15	0.81
1:E:129:ASN:ND2	1:E:135:GLN:H	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:LYS:HE2	4:E:1264:HOH:O	1.91	0.69
1:E:220:LEU:O	1:E:303:GLY:HA3	1.93	0.69
1:E:10:LEU:N	1:E:10:LEU:HD23	2.11	0.66
1:E:187:GLN:HG2	1:E:189:PHE:HD1	1.57	0.64
1:E:248:PHE:CZ	1:E:254:LEU:HD11	2.38	0.59
1:E:192:TRP:CH2	1:E:194:SER:HB2	2.39	0.57
1:E:51:ASP:OD1	1:E:112:THR:CG2	2.53	0.55
1:E:129:ASN:HD22	1:E:135:GLN:H	1.55	0.55
1:E:10:LEU:N	1:E:10:LEU:CD2	2.70	0.54
1:E:187:GLN:HG2	1:E:189:PHE:CE1	2.42	0.54
1:E:96:VAL:HG11	1:E:141:ASN:HB3	1.92	0.51
1:E:10:LEU:HD22	4:E:967:HOH:O	2.11	0.50
1:E:297:ILE:HG21	1:E:301:ILE:HD11	1.95	0.48
1:E:187:GLN:CG	1:E:189:PHE:CD1	2.94	0.47
1:E:297:ILE:HD13	1:E:301:ILE:HD12	1.97	0.46
1:E:238:ALA:HA	1:E:247:VAL:O	2.16	0.46
1:E:99:GLN:NE2	1:E:138:PHE:HA	2.31	0.46
1:E:187:GLN:CG	1:E:189:PHE:CE1	3.00	0.45
1:E:38:LEU:C	1:E:38:LEU:HD23	2.38	0.44
1:E:247:VAL:CG1	1:E:278:ILE:HD11	2.48	0.44
1:E:247:VAL:HG12	1:E:278:ILE:HD11	2.00	0.43
1:E:178:SER:HA	3:E:930:SO4:O2	2.19	0.42
1:E:223:LEU:HB3	1:E:224:PRO:CD	2.50	0.41
1:E:184:VAL:HA	1:E:191:GLU:O	2.20	0.41
1:E:114:ASP:OD2	1:E:117:ILE:HD12	2.19	0.41
1:E:129:ASN:HD21	1:E:131:VAL:HB	1.86	0.41
1:E:218:THR:HA	2:I:2:VAL:O	2.22	0.40
1:E:249:PRO:C	1:E:251:SER:H	2.24	0.40

All (8) 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)
3:E:920:SO4:S	4:E:1087:HOH:O[2_556]	0.61	1.59
3:E:920:SO4:O2	4:E:1087:HOH:O[2_556]	0.97	1.23
3:E:920:SO4:O3	4:E:1087:HOH:O[2_556]	1.60	0.60
3:E:920:SO4:O4	4:E:1087:HOH:O[2_556]	1.61	0.59
4:E:1033:HOH:O	4:E:1119:HOH:O[2_545]	1.85	0.35
4:E:1084:HOH:O	4:E:1190:HOH:O[2_555]	1.85	0.35
3:E:920:SO4:O1	4:E:1087:HOH:O[2_556]	1.96	0.24
1:E:64:LYS:NZ	1:E:177:GLY:O[2_655]	2.16	0.04

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	E	328/330 (99%)	318 (97%)	10 (3%)	0	100	100
2	I	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
All	All	331/336 (98%)	320 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	E	263/263 (100%)	249 (95%)	14 (5%)	28	22
2	I	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	265/265 (100%)	250 (94%)	15 (6%)	25	19

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

Mol	Chain	Res	Type
1	E	10	LEU
1	E	63	THR
1	E	67	SER
1	E	107	VAL
1	E	141	ASN
1	E	146	LEU
1	E	173	THR
1	E	184(A)	SER

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Mol	Chain	Res	Type
1	E	187	GLN
1	E	204	LYS
1	E	229	SER
1	E	242	SER
1	E	278	ILE
1	E	279	SER
2	I	2	VAL

Some 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	234	GLN
1	E	300	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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	$\# Z > 2$
2	STA	I	4	2	10,10,11	1.12	1 (10%)	10,12,14	1.55	2 (20%)
2	STA	I	6	2	8,11,11	1.09	0	8,14,14	0.63	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	STA	I	4	2	-	0/11/11/12	0/0/0/0
2	STA	I	6	2	-	0/10/12/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	4	STA	CD2-CG	2.54	1.66	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4	STA	O-C-CM	-3.45	112.66	125.24
2	I	4	STA	CH-CM-C	-2.36	109.70	113.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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
3	SO4	E	910	-	4,4,4	0.28	0	6,6,6	0.20	0
3	SO4	E	920	-	4,4,4	0.29	0	6,6,6	0.22	0
3	SO4	E	930	-	4,4,4	0.79	0	6,6,6	0.34	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
3	SO4	E	910	-	-	0/0/0/0	0/0/0/0
3	SO4	E	920	-	-	0/0/0/0	0/0/0/0
3	SO4	E	930	-	-	0/0/0/0	0/0/0/0

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.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	920	SO4	0	5
3	E	930	SO4	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](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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