



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 03:59 PM GMT

PDB ID : 1TLP
Title : CRYSTALLOGRAPHIC STRUCTURAL ANALYSIS OF PHOSPHORAMIDATES AS INHIBITORS AND TRANSITION-STATE ANALOGS OF THERMOLYSIN
Authors : Tronrud, D.E.; Monzingo, A.F.; Matthews, B.W.
Deposited on : 1987-06-29
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

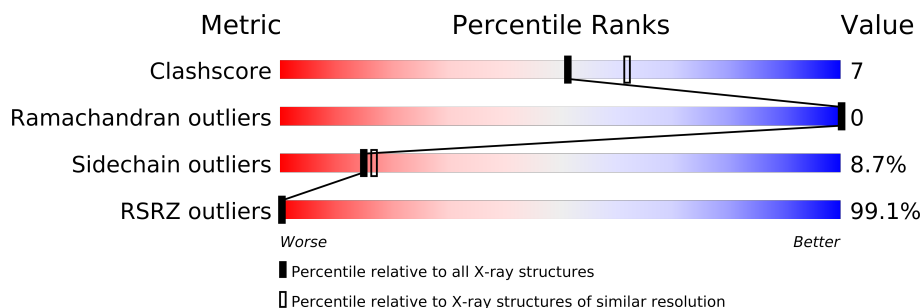
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	E	316	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	RDF	E	317	-	X
3	CA	E	319	-	X
3	CA	E	320	-	X
3	CA	E	321	-	X
4	ZN	E	322	-	X

2 Entry composition i

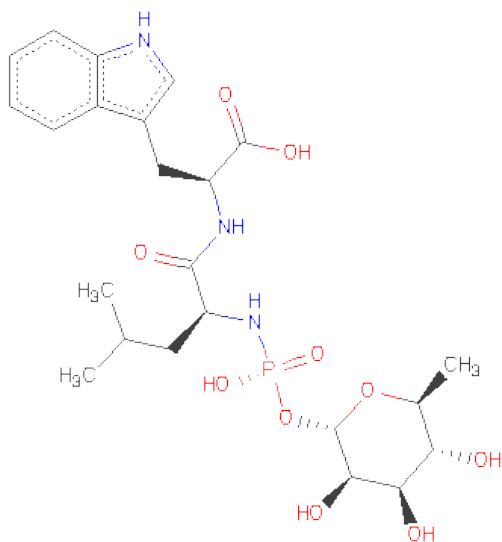
There are 5 unique types of molecules in this entry. The entry contains 2637 atoms, of which 0 are hydrogen and 0 are deuterium.

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 THERMOLYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	316	2432	1528	408	494	2	0	0	0

- Molecule 2 is N-ALPHA-L-RHAMNOPYRANOSYLOXY(HYDROXYPHOSPHINYL)-L-L EUCYL-L-TRYPTOPHAN (three-letter code: RDF) (formula: $C_{23}H_{34}N_3O_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	E	1	37	23	3	10	1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	4	Total	Ca	0	0
			4	4		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	Zn 1	0	0

- Molecule 5 is water.

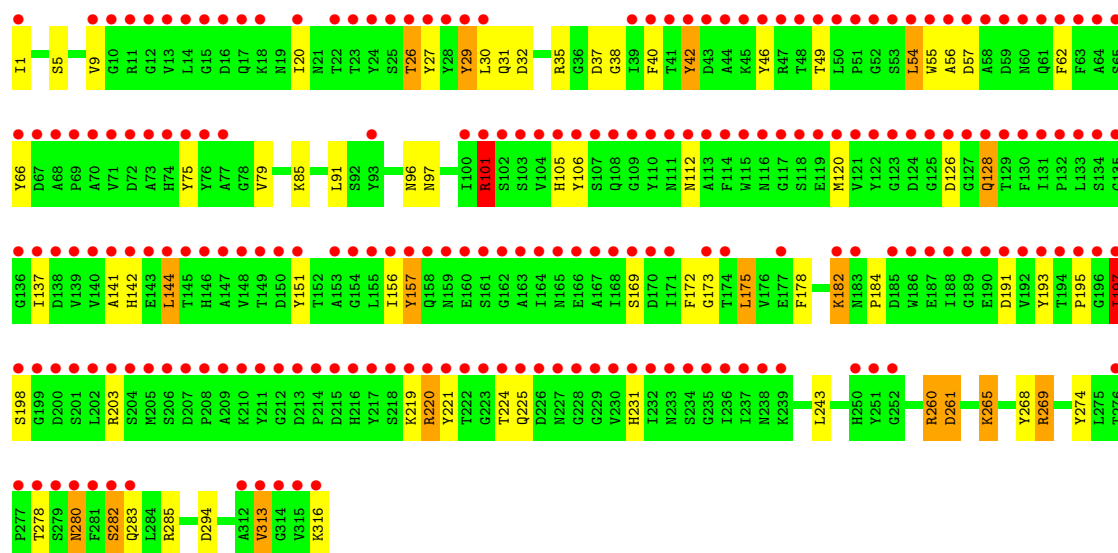
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	163	Total 163	O 163	0	0

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 ($\text{RSRZ} > 2$). 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: THERMOLYSIN

Chain E: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	94.10Å 94.10Å 131.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.30 – 2.30 23.16 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (23.30-2.30) 86.8 (23.16-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.174 , (Not available) 0.159 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 123.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 13730 reflections	Xtriage
F_o, F_c correlation	0.26	EDS
Total number of atoms	2637	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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: ZN, RDF, CA

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	1.12	0/2491	1.59	37/3391 (1.1%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	220	ARG	NE-CZ-NH2	-12.45	114.08	120.30
1	E	29	TYR	CB-CG-CD1	-12.31	113.61	121.00
1	E	274	TYR	CB-CG-CD1	-10.04	114.98	121.00
1	E	151	TYR	CB-CG-CD2	-9.47	115.31	121.00
1	E	268	TYR	CB-CG-CD2	-8.29	116.03	121.00
1	E	220	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	E	46	TYR	CB-CG-CD1	-7.68	116.39	121.00
1	E	27	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	E	29	TYR	CB-CG-CD2	7.59	125.56	121.00
1	E	42	TYR	CB-CG-CD1	-7.54	116.48	121.00
1	E	35	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	E	313	VAL	CA-CB-CG1	7.06	121.49	110.90
1	E	260	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	E	75	TYR	CB-CG-CD1	-6.94	116.84	121.00
1	E	106	TYR	CB-CG-CD2	-6.91	116.86	121.00
1	E	260	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	E	26	THR	N-CA-CB	6.50	122.66	110.30
1	E	5	SER	N-CA-CB	6.08	119.62	110.50
1	E	9	VAL	CA-CB-CG2	6.05	119.98	110.90
1	E	274	TYR	CB-CG-CD2	5.85	124.51	121.00
1	E	203	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	E	101	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	E	57	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	E	282	SER	CB-CA-C	5.73	120.99	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	278	THR	N-CA-CB	-5.48	99.90	110.30
1	E	220	ARG	N-CA-CB	-5.37	100.93	110.60
1	E	156	ILE	CA-CB-CG2	5.34	121.58	110.90
1	E	157	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	E	197	ILE	CA-CB-CG1	5.33	121.12	111.00
1	E	9	VAL	CB-CA-C	-5.32	101.28	111.40
1	E	193	TYR	CG-CD1-CE1	-5.26	117.09	121.30
1	E	37	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	E	126	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	E	35	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	E	261	ASP	CB-CG-OD2	-5.09	113.71	118.30
1	E	172	PHE	CB-CG-CD2	-5.07	117.25	120.80
1	E	54	LEU	CB-CG-CD2	5.05	119.59	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2432	0	2267	29	0
2	E	37	0	32	9	0
3	E	4	0	0	0	0
4	E	1	0	0	0	0
5	E	163	0	0	3	2
All	All	2637	0	2299	35	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (35) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:317:RDF:HD1	2:E:317:RDF:CD11	0.97	1.08
1:E:285:ARG:HD3	1:E:316:LYS:HD3	1.45	0.98

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:317:RDF:HD1	2:E:317:RDF:CG1	2.07	0.84
2:E:317:RDF:CG1	2:E:317:RDF:CE3	2.60	0.69
2:E:317:RDF:HD1	2:E:317:RDF:NE1	2.07	0.68
1:E:280:ASN:HD22	1:E:283:GLN:H	1.43	0.67
1:E:280:ASN:ND2	1:E:283:GLN:H	1.92	0.66
1:E:128:GLN:O	1:E:195:PRO:HD2	1.96	0.66
1:E:269:ARG:NH1	1:E:294:ASP:OD2	2.29	0.65
2:E:317:RDF:CE3	2:E:317:RDF:CE2	2.46	0.63
1:E:120:MET:SD	1:E:144:LEU:HD23	2.43	0.58
1:E:31:GLN:HG3	1:E:40:PHE:CE1	2.42	0.55
1:E:280:ASN:HD22	1:E:280:ASN:C	2.10	0.55
1:E:112:ASN:OD1	2:E:317:RDF:HB2	2.09	0.53
1:E:265:LYS:HE2	5:E:404:HOH:O	2.09	0.53
1:E:231:HIS:CE1	2:E:317:RDF:H1	2.44	0.51
1:E:32:ASP:O	1:E:38:GLY:HA2	2.12	0.49
2:E:317:RDF:O	2:E:317:RDF:HG	2.14	0.48
1:E:141:ALA:HB3	1:E:173:GLY:HA2	1.97	0.46
1:E:219:LYS:HE2	5:E:371:HOH:O	2.15	0.46
1:E:137:ILE:H	1:E:182:LYS:HZ2	1.63	0.45
1:E:29:TYR:CE1	1:E:56:ALA:HB2	2.52	0.45
1:E:221:TYR:OH	1:E:225:GLN:HG3	2.16	0.45
1:E:157:TYR:CE1	2:E:317:RDF:H61	2.53	0.44
1:E:20:ILE:HD11	1:E:62:PHE:CD2	2.52	0.44
1:E:175:LEU:HD11	1:E:260:ARG:HB2	2.01	0.43
1:E:85:LYS:HG3	1:E:91:LEU:HD23	1.99	0.43
1:E:30:LEU:HB2	1:E:55:TRP:HB3	2.00	0.43
1:E:197:ILE:HD13	1:E:197:ILE:N	2.34	0.43
1:E:178:PHE:CD1	1:E:184:PRO:HB2	2.54	0.43
1:E:191:ASP:HB2	5:E:339:HOH:O	2.19	0.42
1:E:66:TYR:O	1:E:105:HIS:NE2	2.40	0.42
1:E:42:TYR:HE2	1:E:101:ARG:HG3	1.85	0.42
1:E:97:ASN:HA	1:E:97:ASN:HD22	1.73	0.42
1:E:142:HIS:CG	1:E:169:SER:HB3	2.56	0.41

All (2) 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	Distance(Å)	Clash(Å)
5:E:434:HOH:O	5:E:434:HOH:O[7_555]	1.03	1.17
5:E:387:HOH:O	5:E:387:HOH:O[12_565]	1.86	0.34

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	314/316 (99%)	300 (96%)	14 (4%)	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	252/252 (100%)	230 (91%)	22 (9%)	15	17

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1	ILE
1	E	26	THR
1	E	49	THR
1	E	54	LEU
1	E	79	VAL
1	E	96	ASN
1	E	101	ARG
1	E	128	GLN
1	E	144	LEU
1	E	175	LEU
1	E	182	LYS
1	E	197	ILE
1	E	198	SER
1	E	220	ARG
1	E	224	THR
1	E	243	LEU

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Mol	Chain	Res	Type
1	E	261	ASP
1	E	265	LYS
1	E	269	ARG
1	E	280	ASN
1	E	282	SER
1	E	313	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	21	ASN
1	E	31	GLN
1	E	33	ASN
1	E	97	ASN
1	E	280	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	RDF	E	317	4	39,39,39	3.40	6 (15%)	57,57,57	2.09	18 (31%)

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	RDF	E	317	4	-	0/29/50/50	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	317	RDF	P-N	-17.65	1.42	1.61
2	E	317	RDF	P-O1P	7.33	1.55	1.46
2	E	317	RDF	P-O1	-5.72	1.52	1.57
2	E	317	RDF	P-O2P	-3.13	1.46	1.55
2	E	317	RDF	CB1-CG1	-2.76	1.47	1.51
2	E	317	RDF	O2-C2	2.41	1.48	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	317	RDF	O1-C1-C2	-6.20	97.02	108.38
2	E	317	RDF	O1P-P-N	-5.08	103.54	113.25
2	E	317	RDF	O3-C3-C2	-4.38	100.53	110.35
2	E	317	RDF	O2-C2-C3	-3.60	102.28	110.35
2	E	317	RDF	O5-C5-C6	3.28	113.93	106.70
2	E	317	RDF	CZ3-CE3-CD21	-3.10	116.36	120.88
2	E	317	RDF	CB1-CA1-C7	3.06	116.72	110.72
2	E	317	RDF	C4-C3-C2	-2.95	105.37	110.82
2	E	317	RDF	P-O1-C1	2.86	130.18	122.30
2	E	317	RDF	O6-C7-CA1	-2.80	111.64	121.86
2	E	317	RDF	O-C-CA	-2.58	114.65	120.31
2	E	317	RDF	CA1-N1-C	2.55	127.26	121.63
2	E	317	RDF	O5-C5-C4	-2.35	105.55	109.53
2	E	317	RDF	O-C-N1	2.33	127.41	122.93
2	E	317	RDF	O2P-P-O1	2.28	113.66	107.09
2	E	317	RDF	C6-C5-C4	2.27	116.76	113.06
2	E	317	RDF	C1-C2-C3	-2.23	105.66	110.00
2	E	317	RDF	C-CA-N	2.19	117.31	110.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 ²)	Q<0.9
1	E	209/316 (66%)	12.05	208 (99%) 0 0	5, 11, 27, 35	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	123	GLY	31.3
1	E	137	ILE	27.4
1	E	140	VAL	24.9
1	E	104	VAL	22.2
1	E	173	GLY	21.5
1	E	105	HIS	21.5
1	E	136	GLY	21.4
1	E	186	TRP	21.2
1	E	156	ILE	20.5
1	E	68	ALA	20.0
1	E	171	ILE	19.8
1	E	121	VAL	19.7
1	E	149	THR	19.6
1	E	177	GLU	19.6
1	E	66	TYR	19.1
1	E	157	TYR	18.9
1	E	122	TYR	18.8
1	E	100	ILE	18.7
1	E	48	THR	18.5
1	E	282	SER	18.5
1	E	168	ILE	18.4
1	E	276	THR	18.2
1	E	251	TYR	18.2
1	E	114	PHE	18.1
1	E	110	TYR	17.8
1	E	153	ALA	17.8
1	E	312	ALA	17.8

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Mol	Chain	Res	Type	RSRZ
1	E	145	THR	17.7
1	E	46	TYR	17.7
1	E	106	TYR	17.7
1	E	120	MET	17.6
1	E	217	TYR	17.6
1	E	154	GLY	17.5
1	E	39	ILE	17.3
1	E	207	ASP	17.3
1	E	218	SER	17.3
1	E	141	ALA	17.0
1	E	103	SER	16.9
1	E	117	GLY	16.9
1	E	314	GLY	16.8
1	E	51	PRO	16.7
1	E	93	TYR	16.6
1	E	142	HIS	16.6
1	E	115	TRP	16.5
1	E	205	MET	16.4
1	E	250	HIS	16.0
1	E	146	HIS	16.0
1	E	167	ALA	15.7
1	E	236	ILE	15.7
1	E	281	PHE	15.6
1	E	107	SER	15.5
1	E	164	ILE	15.4
1	E	315	VAL	15.4
1	E	187	GLU	15.3
1	E	163	ALA	15.3
1	E	52	GLY	15.2
1	E	49	THR	15.2
1	E	23	THR	15.2
1	E	151	TYR	15.1
1	E	206	SER	15.0
1	E	155	LEU	14.9
1	E	50	LEU	14.9
1	E	44	ALA	14.8
1	E	277	PRO	14.8
1	E	313	VAL	14.7
1	E	170	ASP	14.7
1	E	169	SER	14.6
1	E	280	ASN	14.5
1	E	237	ILE	14.4

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Mol	Chain	Res	Type	RSRZ
1	E	64	ALA	14.3
1	E	138	ASP	14.2
1	E	278	THR	14.1
1	E	279	SER	14.0
1	E	147	ALA	14.0
1	E	165	ASN	14.0
1	E	238	ASN	13.9
1	E	215	ASP	13.9
1	E	108	GLN	13.9
1	E	234	SER	13.8
1	E	183	ASN	13.8
1	E	118	SER	13.8
1	E	161	SER	13.7
1	E	15	GLY	13.7
1	E	144	LEU	13.5
1	E	119	GLU	13.5
1	E	239	LYS	13.4
1	E	65	SER	13.3
1	E	195	PRO	13.1
1	E	116	ASN	13.0
1	E	229	GLY	13.0
1	E	174	THR	13.0
1	E	109	GLY	12.7
1	E	17	GLN	12.6
1	E	45	LYS	12.5
1	E	139	VAL	12.5
1	E	223	GLY	12.4
1	E	252	GLY	12.3
1	E	55	TRP	12.2
1	E	124	ASP	12.2
1	E	162	GLY	12.1
1	E	143	GLU	12.1
1	E	47	ARG	12.1
1	E	222	THR	11.8
1	E	230	VAL	11.8
1	E	28	TYR	11.8
1	E	25	SER	11.7
1	E	150	ASP	11.5
1	E	185	ASP	11.2
1	E	208	PRO	11.2
1	E	56	ALA	11.2
1	E	231	HIS	11.0

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Mol	Chain	Res	Type	RSRZ
1	E	199	GLY	10.9
1	E	58	ALA	10.8
1	E	76	TYR	10.7
1	E	41	THR	10.7
1	E	70	ALA	10.6
1	E	316	LYS	10.6
1	E	133	LEU	10.5
1	E	216	HIS	10.5
1	E	226	ASP	10.3
1	E	192	VAL	10.3
1	E	13	VAL	10.2
1	E	188	ILE	10.1
1	E	211	TYR	10.1
1	E	283	GLN	9.9
1	E	200	ASP	9.8
1	E	112	ASN	9.8
1	E	16	ASP	9.7
1	E	135	GLY	9.7
1	E	191	ASP	9.7
1	E	235	GLY	9.6
1	E	1	ILE	9.6
1	E	14	LEU	9.6
1	E	131	ILE	9.6
1	E	132	PRO	9.5
1	E	71	VAL	9.4
1	E	24	TYR	9.3
1	E	40	PHE	9.3
1	E	203	ARG	9.2
1	E	213	ASP	9.2
1	E	166	GLU	9.2
1	E	102	SER	9.2
1	E	193	TYR	9.2
1	E	233	ASN	9.1
1	E	221	TYR	9.1
1	E	27	TYR	8.9
1	E	134	SER	8.9
1	E	204	SER	8.8
1	E	9	VAL	8.8
1	E	63	PHE	8.7
1	E	42	TYR	8.6
1	E	220	ARG	8.5
1	E	158	GLN	8.4

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Mol	Chain	Res	Type	RSRZ
1	E	197	ILE	8.4
1	E	130	PHE	8.4
1	E	12	GLY	8.3
1	E	125	GLY	8.1
1	E	126	ASP	8.0
1	E	113	ALA	8.0
1	E	67	ASP	7.9
1	E	20	ILE	7.9
1	E	190	GLU	7.7
1	E	212	GLY	7.7
1	E	159	ASN	7.6
1	E	219	LYS	7.5
1	E	62	PHE	7.5
1	E	53	SER	7.5
1	E	202	LEU	7.4
1	E	10	GLY	7.3
1	E	129	THR	7.3
1	E	148	VAL	7.3
1	E	60	ASN	7.2
1	E	160	GLU	7.0
1	E	111	ASN	7.0
1	E	127	GLY	7.0
1	E	224	THR	6.9
1	E	214	PRO	6.9
1	E	43	ASP	6.8
1	E	54	LEU	6.8
1	E	69	PRO	6.7
1	E	26	THR	6.7
1	E	182	LYS	6.7
1	E	227	ASN	6.6
1	E	232	ILE	6.6
1	E	22	THR	6.5
1	E	198	SER	6.5
1	E	30	LEU	6.1
1	E	61	GLN	6.1
1	E	57	ASP	6.0
1	E	189	GLY	5.8
1	E	194	THR	5.8
1	E	196	GLY	5.7
1	E	201	SER	5.6
1	E	77	ALA	5.5
1	E	225	GLN	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	29	TYR	5.4
1	E	72	ASP	5.0
1	E	59	ASP	5.0
1	E	11	ARG	4.9
1	E	228	GLY	4.9
1	E	209	ALA	4.9
1	E	74	HIS	4.7
1	E	128	GLN	4.6
1	E	101	ARG	4.3
1	E	210	LYS	3.9
1	E	73	ALA	3.6
1	E	75	TYR	2.8
1	E	18	LYS	2.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CA	E	320	1/1	1.08	6.48	14,14,14,14	0
3	CA	E	319	1/1	2.33	4.30	13,13,13,13	0
4	ZN	E	322	1/1	1.17	1.27	8,8,8,8	0
2	RDF	E	317	37/37	0.93	0.54	5,20,35,49	0
3	CA	E	321	1/1	0.58	-0.49	20,20,20,20	0
3	CA	E	318	1/1	0.20	-2.10	12,12,12,12	0

6.5 Other polymers ⓘ

There are no such residues in this entry.