



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:03 PM GMT

PDB ID : 2DDF
Title : Crystal structure of TACE in complex with TAPI-2
Authors : Orth, P.
Deposited on : 2006-01-28
Resolution : 1.70 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>

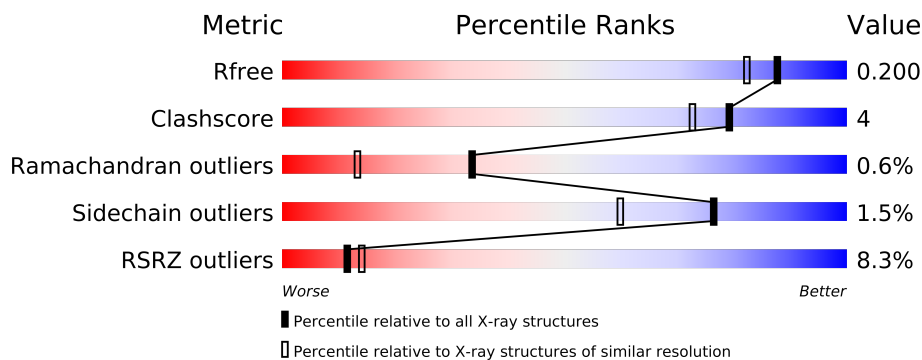
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.70 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))
R_{free}	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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	A	257	
1	B	257	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	IMD	B	475	-	X
7	IPA	B	501	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4323 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 ADAM 17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	1	0
			1969	1241	327	387	14			
1	B	254	Total	C	N	O	S	0	0	0
			1926	1215	323	375	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	ALA	SER	ENGINEERED	UNP P78536
A	353	GLY	VAL	ENGINEERED	UNP P78536
A	452	GLN	ASN	ENGINEERED	UNP P78536
B	266	ALA	SER	ENGINEERED	UNP P78536
B	353	GLY	VAL	ENGINEERED	UNP P78536
B	452	GLN	ASN	ENGINEERED	UNP P78536

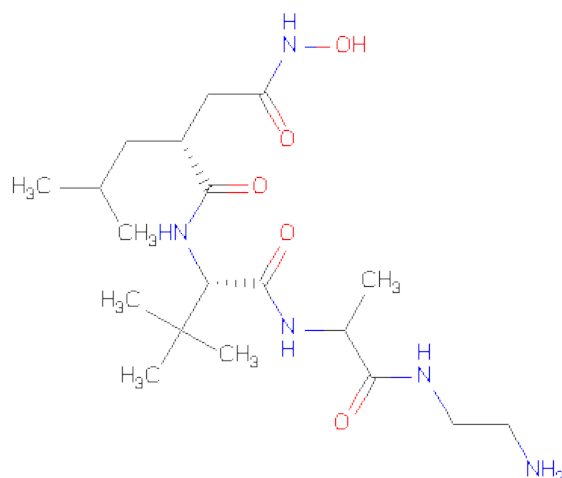
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

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

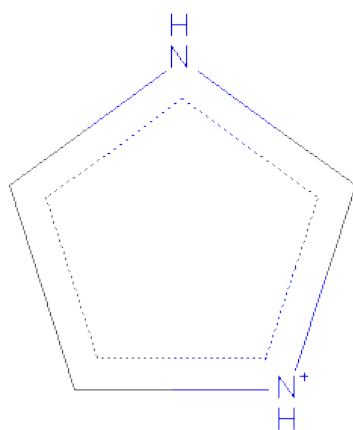
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is N-{(2R)-2-[2-(HYDROXYAMINO)-2-OXOETHYL]-4-METHYLPENTANOYL}-3-METHYL-L-VALYL-N-(2-AMINOETHYL)-L-ALANINAMIDE (three-letter code: INN) (formula: C₁₉H₃₇N₅O₅).



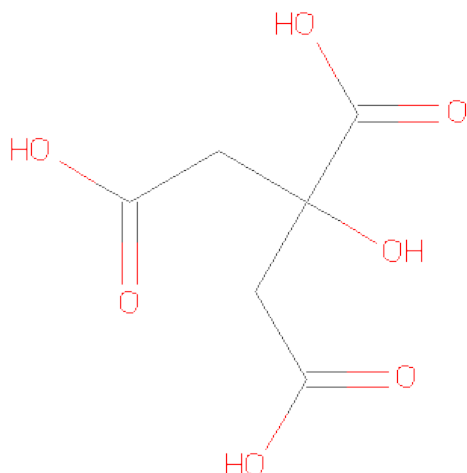
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			29	19	5	5		
4	A	1	Total	C	N	O	0	0
			29	19	5	5		

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



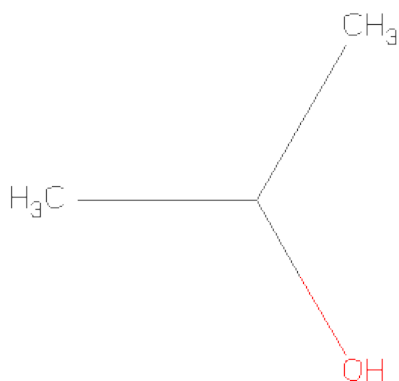
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 7 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	3	1		
7	A	1	Total	C	O	0	0
			4	3	1		
7	B	1	Total	C	O	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	3	1		

- Molecule 8 is water.

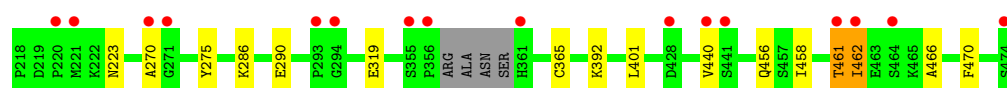
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	189	Total	O	0	0
			189	189		
8	B	144	Total	O	0	0
			144	144		

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.

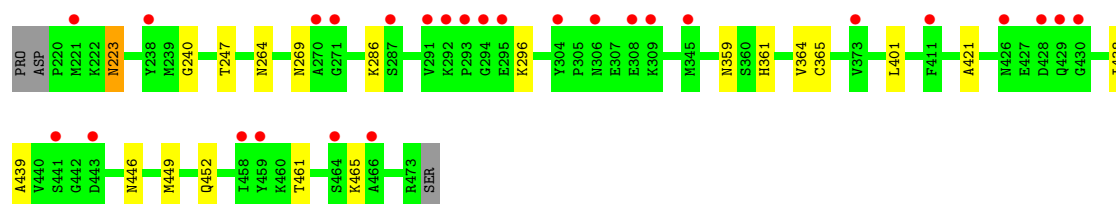
• Molecule 1: ADAM 17

Chain A: 



• Molecule 1: ADAM 17

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.39Å 75.64Å 103.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 19.65 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (20.00-1.70) 97.8 (19.65-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.204 , 0.230 0.218 , 0.200	Depositor DCC
R_{free} test set	1258 reflections (2.02%)	DCC
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 55.5	EDS
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 63554 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4323	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, IPA, IMD, CA, INN, CIT

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	0.65	0/2019	0.68	0/2729
1	B	0.58	0/1971	0.62	0/2674
All	All	0.62	0/3990	0.65	0/5403

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	461	THR	Peptide

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	A	1969	0	1845	8	0
1	B	1926	0	1770	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
4	A	29	0	36	0	0
4	B	29	0	36	4	0
5	B	5	0	5	1	0
6	B	13	0	5	0	0
7	A	4	0	8	0	0
7	B	12	0	24	2	0
8	A	189	0	0	3	0
8	B	144	0	0	3	0
All	All	4323	0	3729	27	0

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 4.

All (27) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:269:ASN:HD21	1:B:452:GLN:HE22	1.32	0.74
1:B:269:ASN:HD21	1:B:452:GLN:NE2	1.91	0.66
1:A:319:GLU:HG3	8:A:636:HOH:O	1.95	0.65
1:B:438:ILE:CG2	4:B:2:INN:H151	2.35	0.56
1:B:446:ASN:HA	1:B:449:MET:HE3	1.87	0.56
1:B:438:ILE:HG21	4:B:2:INN:H151	1.85	0.56
1:B:264:ASN:ND2	8:B:603:HOH:O	2.40	0.54
1:B:421:ALA:HA	7:B:501:IPA:H31	1.89	0.53
1:A:290:GLU:OE2	8:A:614:HOH:O	2.18	0.53
1:A:466:ALA:HA	1:A:470:PHE:CG	2.44	0.53
1:B:439:ALA:HA	4:B:2:INN:H31	1.91	0.52
1:A:286:LYS:HE3	8:A:654:HOH:O	2.09	0.52
1:B:359:ASN:O	5:B:475:IMD:H2	2.13	0.48
4:B:2:INN:O3	4:B:2:INN:N4	2.46	0.47
1:A:401:LEU:HD13	1:A:440:VAL:HG23	1.96	0.47
1:B:446:ASN:HA	1:B:449:MET:CE	2.45	0.45
1:A:458:ILE:O	1:A:461:THR:N	2.50	0.45
1:B:223:ASN:C	1:B:223:ASN:HD22	2.20	0.45
1:B:452:GLN:NE2	8:B:570:HOH:O	2.50	0.44
1:B:361:HIS:HD2	8:B:575:HOH:O	2.02	0.42
1:B:364:VAL:HG23	1:B:465:LYS:HD3	2.02	0.42
1:A:275:TYR:CE1	1:A:462:ILE:HG21	2.54	0.42
1:B:401:LEU:HD23	1:B:401:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:286:LYS:H	7:B:502:IPA:H11	1.85	0.41
1:A:401:LEU:HD13	1:A:440:VAL:O	2.20	0.41
1:B:461:THR:HG23	1:B:465:LYS:HD2	2.01	0.41
1:B:240:GLY:HA3	1:B:247:THR:OG1	2.20	0.41

There are no symmetry-related clashes.

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	A	250/257 (97%)	242 (97%)	6 (2%)	2 (1%)	27	8
1	B	252/257 (98%)	247 (98%)	4 (2%)	1 (0%)	43	22
All	All	502/514 (98%)	489 (97%)	10 (2%)	3 (1%)	33	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	CYS
1	B	365	CYS
1	A	270	ALA

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	A	207/219 (94%)	203 (98%)	4 (2%)	69	50
1	B	195/219 (89%)	193 (99%)	2 (1%)	85	76
All	All	402/438 (92%)	396 (98%)	6 (2%)	76	60

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

Mol	Chain	Res	Type
1	A	223	ASN
1	A	392	LYS
1	A	456	GLN
1	A	462	ILE
1	B	223	ASN
1	B	296	LYS

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

Mol	Chain	Res	Type
1	A	223	ASN
1	A	281	GLN
1	A	456	GLN
1	A	471	GLN
1	B	223	ASN
1	B	278	GLN
1	B	361	HIS
1	B	452	GLN
1	B	471	GLN

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 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	$\# Z > 2$
4	INN	A	3	2	28,28,28	0.48	0	38,38,38	1.30	5 (13%)
7	IPA	A	476	-	3,3,3	0.73	0	3,3,3	0.46	0
4	INN	B	2	2	28,28,28	0.52	0	38,38,38	1.90	8 (21%)
5	IMD	B	475	-	5,5,5	1.31	1 (20%)	5,5,5	0.35	0
6	CIT	B	500	-	12,12,12	0.63	0	17,17,17	1.70	1 (5%)
7	IPA	B	501	-	3,3,3	0.59	0	3,3,3	0.37	0
7	IPA	B	502	-	3,3,3	0.68	0	3,3,3	0.17	0
7	IPA	B	503	-	3,3,3	0.63	0	3,3,3	0.26	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
4	INN	A	3	2	-	0/40/40/40	0/0/0/0
7	IPA	A	476	-	-	0/0/0/0	0/0/0/0
4	INN	B	2	2	-	0/40/40/40	0/0/0/0
5	IMD	B	475	-	-	0/0/0/0	0/1/1/1
6	CIT	B	500	-	-	0/16/16/16	0/0/0/0
7	IPA	B	501	-	-	0/0/0/0	0/0/0/0
7	IPA	B	502	-	-	0/0/0/0	0/0/0/0
7	IPA	B	503	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	475	IMD	C2-N1	2.09	1.35	1.31

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2	INN	C0-C-N	6.25	119.03	114.69
6	B	500	CIT	O6-C6-C3	5.27	120.56	112.89
4	B	2	INN	C15-C14-N3	4.87	121.47	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2	INN	C6-C5-N1	-3.88	108.57	112.29
4	B	2	INN	CA-CB-C1	-3.42	111.77	115.95
4	A	3	INN	CA-CB-C1	-3.13	112.11	115.95
4	A	3	INN	C12-C11-N2	2.57	115.25	110.31
4	B	2	INN	O1-C4-CA	-2.48	119.29	121.89
4	A	3	INN	C0-C-N	2.42	116.37	114.69
4	B	2	INN	CA-C0-C	-2.24	107.14	112.23
4	B	2	INN	O-C-C0	-2.24	118.03	121.24
4	A	3	INN	O2-C10-C5	-2.13	117.78	121.05
4	B	2	INN	O2-C10-N2	-2.12	118.85	122.93
4	A	3	INN	C0-CA-C4	-2.09	106.83	110.06

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	A	253/257 (98%)	0.33	16 (6%) 19 24	24, 32, 49, 55	0
1	B	254/257 (98%)	0.54	27 (10%) 7 9	26, 38, 54, 62	0
All	All	507/514 (98%)	0.44	43 (8%) 11 13	24, 35, 52, 62	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	428	ASP	4.5
1	A	361	HIS	4.0
1	A	428	ASP	4.0
1	B	308	GLU	3.8
1	A	474	SER	3.8
1	B	293	PRO	3.7
1	A	461	THR	3.7
1	B	294	GLY	3.7
1	B	429	GLN	3.6
1	A	271	GLY	3.4
1	B	466	ALA	3.4
1	B	221	MET	3.3
1	A	356	PRO	3.3
1	A	355	SER	3.2
1	B	270	ALA	3.2
1	B	304	TYR	3.2
1	A	440	VAL	3.0
1	A	220	PRO	2.9
1	A	221	MET	2.9
1	B	238	TYR	2.8
1	B	458	ILE	2.8
1	B	426	ASN	2.8
1	A	293	PRO	2.8
1	A	270	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	291	VAL	2.7
1	B	287	SER	2.7
1	B	306	ASN	2.6
1	B	271	GLY	2.6
1	A	294	GLY	2.5
1	A	441	SER	2.5
1	B	309	LYS	2.5
1	B	292	LYS	2.5
1	B	459	TYR	2.4
1	B	441	SER	2.4
1	B	430	GLY	2.4
1	B	295	GLU	2.4
1	B	443	ASP	2.3
1	A	462	ILE	2.3
1	A	464	SER	2.3
1	B	373	VAL	2.3
1	B	464	SER	2.1
1	B	345	MET	2.1
1	B	411	PHE	2.1

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
5	IMD	B	475	5/5	0.21	11.14	47,48,48,48	0
7	IPA	B	501	4/4	0.19	2.30	55,56,56,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	IPA	B	502	4/4	0.25	1.70	58,60,61,61	0
4	INN	B	2	29/29	0.12	0.93	27,32,55,58	0
6	CIT	B	500	13/13	0.17	0.93	38,42,45,46	0
3	CA	A	475	1/1	0.11	0.48	35,35,35,35	0
7	IPA	A	476	4/4	0.10	0.18	27,36,37,37	0
7	IPA	B	503	4/4	0.13	0.10	57,58,58,58	0
4	INN	A	3	29/29	0.09	-0.32	23,27,44,49	0
2	ZN	A	1	1/1	0.04	-1.85	29,29,29,29	0
2	ZN	B	4	1/1	0.02	-4.79	31,31,31,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.