



Full wwPDB X-ray Structure Validation Report

Nov 5, 2014 – 03:51 AM EST

PDB ID : 4PI3
Title : Crystal structure analysis of cruzain bound to vinyl sulfone analog of WRR-483 (WRR-666)
Authors : Tochowicz, A.; McKerrow, J.H.
Deposited on : 2014-05-08
Resolution : 1.27 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>

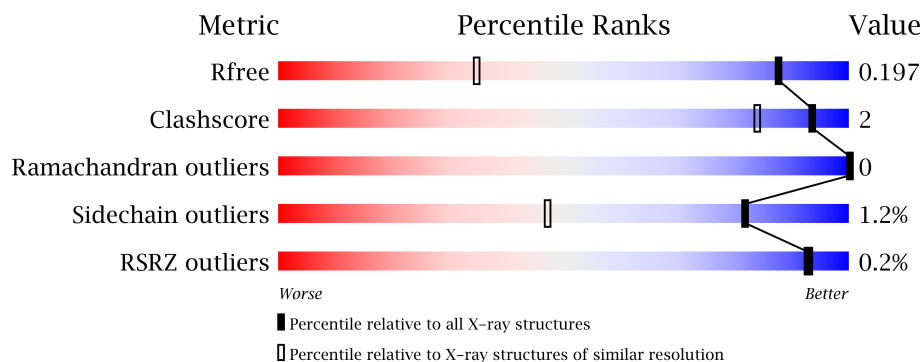
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance

The reported resolution of this entry is 1.27 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	1030 (1.32-1.24)
Clashscore	79885	1134 (1.32-1.24)
Ramachandran outliers	78287	1083 (1.32-1.24)
Sidechain outliers	78261	1082 (1.32-1.24)
RSRZ outliers	66119	1030 (1.32-1.24)

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	331	
1	B	331	

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	2V5	A	301	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3727 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.

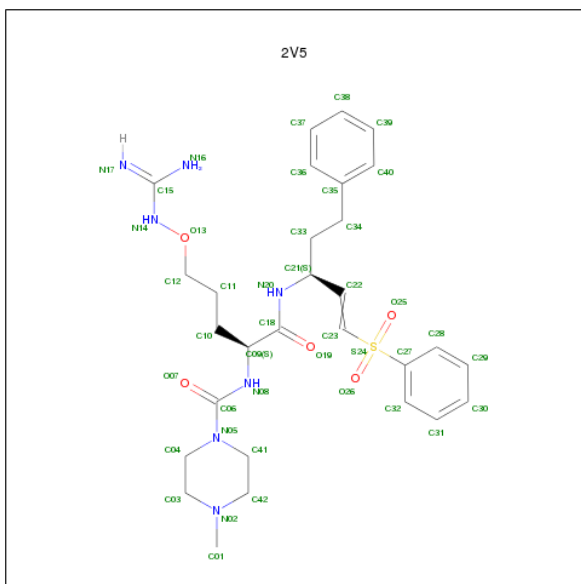
- Molecule 1 is a protein called Cruzipain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1592	995	266	319	12			
1	B	215	Total	C	N	O	S	0	0	0
			1592	995	266	319	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-115	ASP	-	expression tag	UNP P25779
A	-114	ILE	-	expression tag	UNP P25779
A	-113	HIS	-	expression tag	UNP P25779
A	-112	MET	-	expression tag	UNP P25779
A	-111	HIS	-	expression tag	UNP P25779
A	-110	HIS	-	expression tag	UNP P25779
A	-109	HIS	-	expression tag	UNP P25779
A	-108	HIS	-	expression tag	UNP P25779
A	-107	HIS	-	expression tag	UNP P25779
A	-106	HIS	-	expression tag	UNP P25779
A	-105	GLY	-	expression tag	UNP P25779
A	-104	SER	-	expression tag	UNP P25779
B	-115	ASP	-	expression tag	UNP P25779
B	-114	ILE	-	expression tag	UNP P25779
B	-113	HIS	-	expression tag	UNP P25779
B	-112	MET	-	expression tag	UNP P25779
B	-111	HIS	-	expression tag	UNP P25779
B	-110	HIS	-	expression tag	UNP P25779
B	-109	HIS	-	expression tag	UNP P25779
B	-108	HIS	-	expression tag	UNP P25779
B	-107	HIS	-	expression tag	UNP P25779
B	-106	HIS	-	expression tag	UNP P25779
B	-105	GLY	-	expression tag	UNP P25779
B	-104	SER	-	expression tag	UNP P25779

- Molecule 2 is N-[(2S)-5-(carbamimidamidooxy)-1-oxo-1-{[(1E,3S)-5-phenyl-1-(phenylsulfonyl)pent-1-en-3-yl]amino}pentan-2-yl]-4-methylpiperazine-1-carboxamide (three-letter code: 2V5) (formula: C₂₉H₄₁N₇O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			42	29	7	5	1		
2	B	1	Total	C	N	O	S	0	0
			42	29	7	5	1		

- Molecule 3 is water.

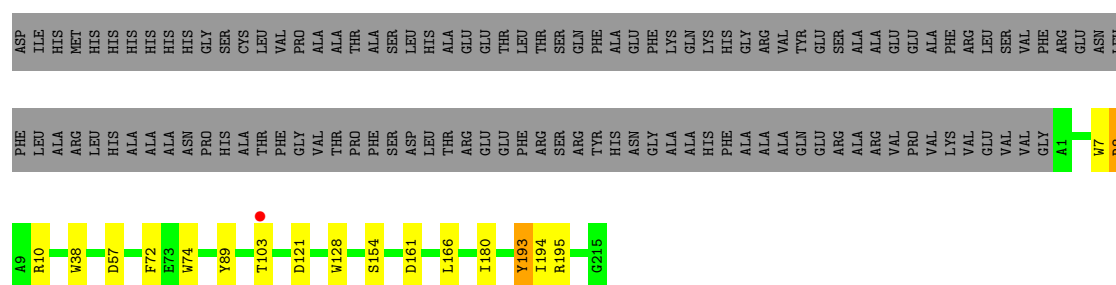
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	246	Total	O	0	0
			246	246		
3	B	213	Total	O	0	0
			213	213		

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.

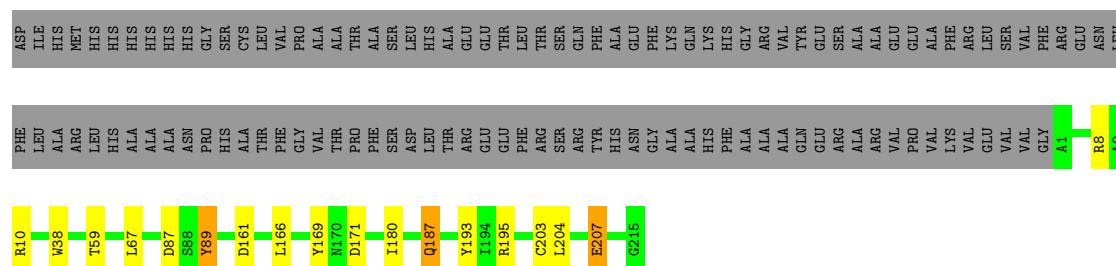
• Molecule 1: Cruzipain

Chain A: 



• Molecule 1: Cruzipain

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.92Å 38.67Å 94.65Å 90.00° 113.91° 90.00°	Depositor
Resolution (Å)	86.52 – 1.27 44.94 – 1.27	Depositor EDS
% Data completeness (in resolution range)	98.2 (86.52-1.27) 98.2 (44.94-1.27)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.27Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.174 , 0.197 0.174 , 0.197	Depositor DCC
R_{free} test set	5804 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 115216 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3727	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: 2V5

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	1.38	4/1631 (0.2%)	1.32	9/2232 (0.4%)
1	B	1.30	3/1631 (0.2%)	1.31	9/2232 (0.4%)
All	All	1.34	7/3262 (0.2%)	1.31	18/4464 (0.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	CYS	CB-SG	-6.70	1.70	1.82
1	A	154	SER	CB-OG	-5.77	1.34	1.42
1	B	38	TRP	CD2-CE2	5.63	1.48	1.41
1	A	128	TRP	CD2-CE2	5.24	1.47	1.41
1	A	7	TRP	CD2-CE2	5.24	1.47	1.41
1	A	74	TRP	CD2-CE2	5.16	1.47	1.41
1	B	207	GLU	CD-OE2	5.14	1.31	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ASP	CB-CG-OD1	10.29	127.56	118.30
1	B	195	ARG	NE-CZ-NH2	9.01	124.81	120.30
1	B	171	ASP	CB-CG-OD1	8.61	126.05	118.30
1	B	89	TYR	CB-CG-CD1	-8.23	116.06	121.00
1	B	161	ASP	CB-CG-OD1	8.18	125.66	118.30
1	B	87	ASP	CB-CG-OD2	7.85	125.36	118.30
1	B	10	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	121	ASP	CB-CG-OD1	7.26	124.83	118.30
1	A	161	ASP	CB-CG-OD2	6.88	124.49	118.30
1	A	8	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	B	169	TYR	CB-CG-CD1	-6.40	117.16	121.00
1	A	193	TYR	CB-CG-CD1	-6.26	117.24	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	72	PHE	CB-CG-CD1	5.83	124.88	120.80
1	A	195	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	38	TRP	CE2-CD2-CG	-5.43	102.96	107.30
1	B	67	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	B	207	GLU	OE1-CD-OE2	5.38	129.75	123.30

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	A	1592	0	1489	3	0
1	B	1592	0	1489	6	0
2	A	42	0	0	1	0
2	B	42	0	0	0	0
3	A	246	0	0	1	0
3	B	213	0	0	2	1
All	All	3727	0	2978	10	1

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 2.

All (10) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:204:LEU:HB3	1:B:207:GLU:HG3	1.66	0.78
1:B:59:THR:HG23	3:B:523:HOH:O	2.01	0.60
1:B:166:LEU:HD23	1:B:180:ILE:HG12	1.89	0.53
1:B:8:ARG:HD3	1:B:193:TYR:CE1	2.47	0.50
1:A:8:ARG:HD3	1:A:193:TYR:CE1	2.49	0.48
1:A:180:ILE:HB	1:A:194:ILE:HG23	1.99	0.45
1:B:187:GLN:OE1	1:B:187:GLN:HA	2.16	0.45
2:A:301:2V5:C03	3:A:638:HOH:O	2.65	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:166:LEU:HD23	1:A:180:ILE:HG12	2.02	0.41
1:B:59:THR:CG2	3:B:523:HOH:O	2.64	0.40

All (1) 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)
3:B:401:HOH:O	3:B:422:HOH:O[1_565]	1.93	0.27

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	213/331 (64%)	208 (98%)	5 (2%)	0	100	100
1	B	213/331 (64%)	208 (98%)	5 (2%)	0	100	100
All	All	426/662 (64%)	416 (98%)	10 (2%)	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	A	167/259 (64%)	165 (99%)	2 (1%)	82	47
1	B	167/259 (64%)	165 (99%)	2 (1%)	82	47
All	All	334/518 (64%)	330 (99%)	4 (1%)	82	47

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	TYR
1	A	103	THR
1	B	89	TYR
1	B	187	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

2 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	2V5	A	301	1	44,44,44	2.71	11 (25%)	58,58,58	2.34	21 (36%)
2	2V5	B	301	1	44,44,44	2.66	14 (31%)	58,58,58	2.48	21 (36%)

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	2V5	A	301	1	-	0/41/51/51	0/3/3/3
2	2V5	B	301	1	-	1/41/51/51	1/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	2V5	C23-C22	13.24	1.53	1.31
2	B	301	2V5	C23-C22	10.28	1.48	1.31
2	B	301	2V5	C06-N08	6.26	1.49	1.35
2	A	301	2V5	C37-C36	5.01	1.49	1.38
2	B	301	2V5	O13-N14	-4.68	1.28	1.41
2	A	301	2V5	C41-N05	-4.37	1.39	1.47
2	B	301	2V5	C31-C32	4.23	1.47	1.38
2	B	301	2V5	C39-C40	3.84	1.46	1.38
2	A	301	2V5	O13-N14	-3.79	1.31	1.41
2	B	301	2V5	O25-S24	3.78	1.48	1.44
2	B	301	2V5	C41-N05	-3.71	1.40	1.47
2	B	301	2V5	C15-N14	3.58	1.43	1.34
2	A	301	2V5	C06-N08	3.51	1.43	1.35
2	B	301	2V5	C37-C36	3.49	1.46	1.38
2	B	301	2V5	C06-N05	3.11	1.42	1.36
2	A	301	2V5	C39-C40	2.98	1.45	1.38
2	A	301	2V5	C15-N14	2.87	1.41	1.34
2	A	301	2V5	C32-C27	-2.83	1.34	1.38
2	B	301	2V5	C18-N20	2.74	1.40	1.34
2	B	301	2V5	C29-C28	2.73	1.44	1.38
2	A	301	2V5	C29-C28	2.40	1.43	1.38
2	A	301	2V5	O26-S24	2.29	1.46	1.44
2	B	301	2V5	C15-N17	2.17	1.41	1.32
2	B	301	2V5	C09-C18	2.11	1.58	1.52
2	A	301	2V5	C23-S24	2.07	1.78	1.75

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	2V5	C01-N02-C03	7.25	122.25	110.63
2	A	301	2V5	C01-N02-C03	6.99	121.83	110.63
2	B	301	2V5	C41-C42-N02	6.75	118.06	110.81
2	B	301	2V5	N14-C15-N17	-4.96	111.21	120.27
2	A	301	2V5	C01-N02-C42	4.75	118.24	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	2V5	C42-N02-C03	4.67	115.84	109.52
2	B	301	2V5	O07-C06-N05	4.58	128.47	121.83
2	B	301	2V5	O26-S24-O25	-4.50	114.80	118.78
2	A	301	2V5	C22-C23-S24	-4.45	110.85	122.92
2	B	301	2V5	C01-N02-C42	4.36	117.62	110.63
2	A	301	2V5	C38-C39-C40	-4.29	113.89	120.20
2	A	301	2V5	C41-C42-N02	4.28	115.41	110.81
2	B	301	2V5	C41-N05-C04	4.24	120.61	112.57
2	B	301	2V5	C38-C39-C40	-3.77	114.66	120.20
2	A	301	2V5	C37-C36-C35	-3.74	114.65	120.66
2	A	301	2V5	N14-C15-N17	-3.73	113.47	120.27
2	A	301	2V5	C09-N08-C06	-3.59	113.00	120.84
2	A	301	2V5	C39-C38-C37	3.57	126.35	119.91
2	B	301	2V5	C42-C41-N05	-3.53	102.11	110.56
2	B	301	2V5	C39-C38-C37	3.53	126.28	119.91
2	B	301	2V5	C09-N08-C06	-3.52	113.16	120.84
2	A	301	2V5	O26-S24-O25	-3.44	115.75	118.78
2	A	301	2V5	C41-N05-C04	3.24	118.72	112.57
2	A	301	2V5	C40-C35-C36	3.06	123.12	118.13
2	A	301	2V5	O25-S24-C27	3.03	111.23	107.93
2	B	301	2V5	C34-C33-C21	-2.92	107.06	112.99
2	B	301	2V5	C22-C21-N20	-2.77	106.75	110.96
2	A	301	2V5	C03-C04-N05	2.72	117.08	110.56
2	B	301	2V5	C22-C23-S24	-2.68	115.65	122.92
2	B	301	2V5	C40-C35-C36	2.60	122.38	118.13
2	B	301	2V5	N16-C15-N17	2.58	128.64	120.31
2	A	301	2V5	C28-C27-S24	-2.57	115.70	119.51
2	A	301	2V5	C34-C33-C21	-2.49	107.94	112.99
2	A	301	2V5	O13-N14-C15	2.38	118.95	113.67
2	A	301	2V5	C21-C22-C23	-2.37	115.06	126.34
2	B	301	2V5	C28-C27-S24	-2.36	116.00	119.51
2	A	301	2V5	C30-C31-C32	-2.33	116.78	120.20
2	B	301	2V5	C04-N05-C06	-2.30	113.56	122.10
2	B	301	2V5	C29-C28-C27	-2.28	116.46	118.96
2	A	301	2V5	C31-C32-C27	2.26	121.44	118.96
2	B	301	2V5	C28-C27-C32	2.16	123.78	120.40
2	B	301	2V5	N08-C06-N05	-2.11	112.78	117.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	2V5	C21-C22-C23-S24

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	2V5	C03-C04-C41-C42-N02-N05

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	215/331 (64%)	-0.29	1 (0%) 88 90	9, 12, 21, 36	0
1	B	215/331 (64%)	-0.26	0 100 100	10, 14, 24, 31	0
All	All	430/662 (64%)	-0.27	1 (0%) 93 93	9, 13, 22, 36	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	THR	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
2	2V5	A	301	42/42	0.08	2.20	9,14,24,34	0
2	2V5	B	301	42/42	0.07	1.19	9,14,25,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.