



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 09:07 pm GMT

PDB ID : 1O37
Title : Elaborate Manifold of Short Hydrogen Bond Arrays Mediating Binding of Active Site-Directed Serine Protease Inhibitors
Authors : Katz, B.A.; Elrod, K.; Verner, E.; Mackman, R.L.; Luong, C.; Shrader, W.D.; Sendzik, M.; Spencer, J.R.; Sprengeler, P.A.; Kolesnikov, A.; Tai, V.W.; Hui, H.C.; Breitenbucher, J.G.; Allen, D.; Janc, J.W.
Deposited on : 2003-03-06
Resolution : 1.45 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

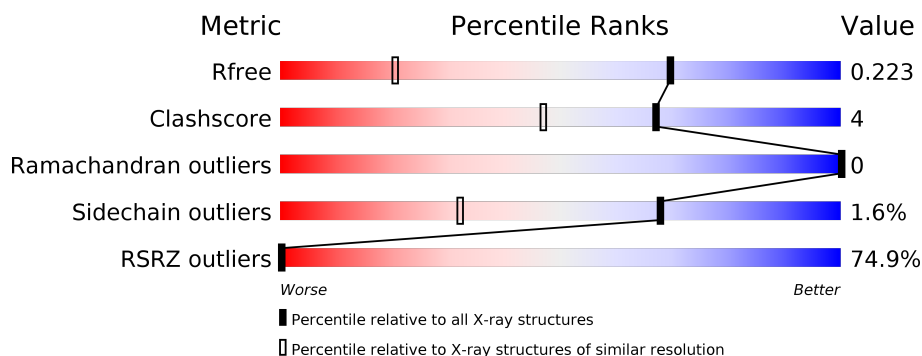
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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}	100719	1510 (1.48-1.44)
Clashscore	112137	1573 (1.48-1.44)
Ramachandran outliers	110173	1555 (1.48-1.44)
Sidechain outliers	110143	1555 (1.48-1.44)
RSRZ outliers	101464	1516 (1.48-1.44)

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.

Mol	Chain	Length	Quality of chain
1	A	223	<div> <div>75%</div> <div>88%</div> <div>10%</div> </div>

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.

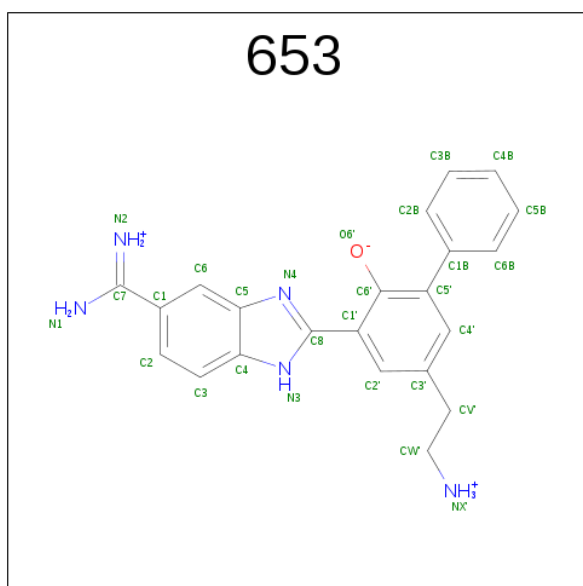
- Molecule 1 is a protein called BETA-TRYPSIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	223	Total	C	H	N	O	S	0	16	0
			3360	1047	1678	284	337	14			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is 5-(2-AMINOETHYL)-3-{5-[AMINO(IMINIO)METHYL]-1H-BENZIMIDAZO L-2-YL}-1,1'-BIPHENYL-2-OLATE (three-letter code: 653) (formula: C₂₂H₂₂N₅O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			50	22	22	5	1		

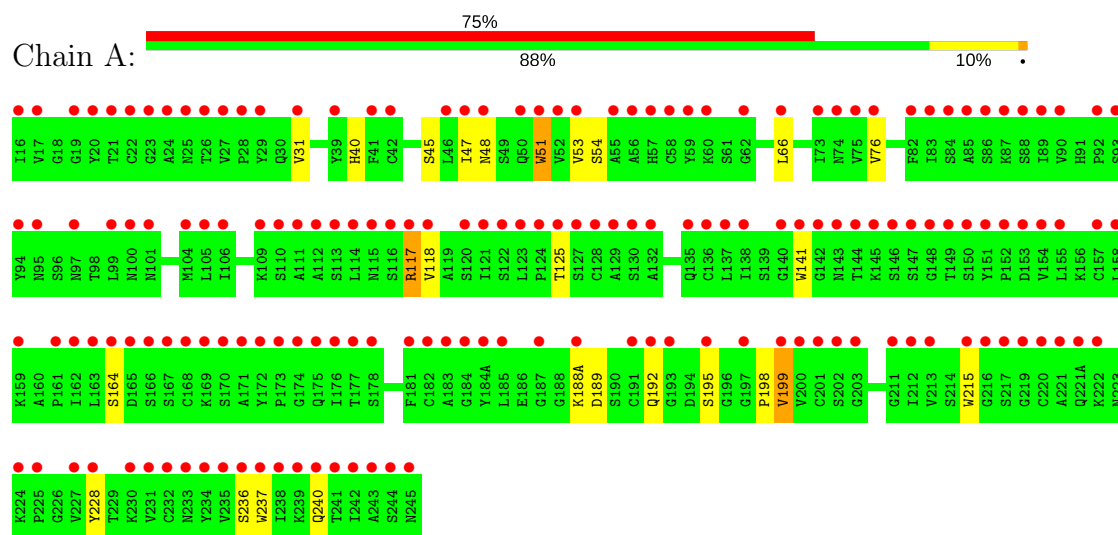
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	132	Total 399	H 266	O 133	0	2

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 the various outlier classes 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: BETA-TRYPSIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.09Å 62.18Å 70.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 1.45 7.00 – 1.45	Depositor EDS
% Data completeness (in resolution range)	84.2 (7.00-1.45) 84.2 (7.00-1.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.40 (at 1.45Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.225 , 0.241 0.231 , 0.223	Depositor DCC
R_{free} test set	4294 reflections (10.18%)	DCC
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3810	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: CA, 653

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	1.48	5/1773 (0.3%)	1.51	18/2399 (0.8%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	SER	CA-CB	7.36	1.64	1.52
1	A	40	HIS	CB-CG	5.71	1.60	1.50
1	A	199	VAL	CB-CG1	5.44	1.64	1.52
1	A	118	VAL	CA-CB	5.05	1.65	1.54
1	A	164	SER	CA-CB	5.03	1.60	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	TRP	CD1-NE1-CE2	9.92	117.93	109.00
1	A	237	TRP	CD1-NE1-CE2	9.74	117.77	109.00
1	A	215	TRP	CD1-NE1-CE2	9.06	117.16	109.00
1	A	51	TRP	CD1-NE1-CE2	8.96	117.06	109.00
1	A	237	TRP	NE1-CE2-CZ2	7.60	138.76	130.40
1	A	141	TRP	CG-CD1-NE1	-6.96	103.14	110.10
1	A	215	TRP	NE1-CE2-CZ2	6.83	137.92	130.40
1	A	237	TRP	NE1-CE2-CD2	-6.73	100.57	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	TRP	CG-CD1-NE1	-6.53	103.57	110.10
1	A	141	TRP	NE1-CE2-CZ2	6.50	137.55	130.40
1	A	141	TRP	NE1-CE2-CD2	-6.34	100.96	107.30
1	A	237	TRP	CG-CD1-NE1	-6.34	103.76	110.10
1	A	51	TRP	NE1-CE2-CZ2	6.21	137.24	130.40
1	A	199	VAL	N-CA-C	-6.20	94.27	111.00
1	A	215	TRP	NE1-CE2-CD2	-5.93	101.37	107.30
1	A	51	TRP	NE1-CE2-CD2	-5.88	101.42	107.30
1	A	51	TRP	CG-CD1-NE1	-5.55	104.55	110.10
1	A	76	VAL	N-CA-C	-5.21	96.93	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain

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	A	1682	1678	1643	15	0
2	A	1	0	0	0	0
3	A	28	22	22	4	0
4	A	133	266	0	2	0
All	All	1844	1966	1665	15	0

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 4.

All (15) 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:A:195[A]:SER:HB2	4:A:383[A]:HOH:O	1.90	0.72
1:A:31:VAL:HG12	1:A:66[A]:LEU:CD2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195[A]:SER:CB	4:A:383[A]:HOH:O	2.54	0.53
1:A:199:VAL:HG21	1:A:228:TYR:CD1	2.44	0.52
1:A:47:ILE:HD13	1:A:53[B]:VAL:CG2	2.39	0.52
1:A:192:GLN:NE2	3:A:246:653:C3'	2.75	0.49
1:A:188(A):LYS:O	1:A:189:ASP:HB2	2.17	0.44
1:A:192:GLN:HE21	3:A:246:653:C4'	2.31	0.44
1:A:48:ASN:ND2	1:A:51:TRP:HB2	2.33	0.43
1:A:45:SER:OG	1:A:198:PRO:HB3	2.19	0.42
1:A:31:VAL:CG1	1:A:66[A]:LEU:CD2	2.97	0.42
1:A:31:VAL:HG12	1:A:66[A]:LEU:HD23	2.01	0.42
1:A:192:GLN:NE2	3:A:246:653:CV'	2.83	0.41
1:A:195[A]:SER:HG	3:A:246:653:HN3	1.66	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	237/223 (106%)	229 (97%)	8 (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	A	200/184 (109%)	196 (98%)	4 (2%)	60 23

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

Mol	Chain	Res	Type
1	A	117	ARG
1	A	125	THR
1	A	236[A]	SER
1	A	236[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	192	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 2 ligands modelled in this entry, 1 is 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
3	653	A	246	-	30,31,31	1.88	8 (26%)	38,44,44	2.28	7 (18%)

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	653	A	246	-	-	0/12/15/15	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	246	653	C5'-C1B	-5.92	1.39	1.49
3	A	246	653	CV'-C3'	-3.02	1.42	1.51
3	A	246	653	C8-N3	-2.76	1.28	1.34
3	A	246	653	C1'-C8	-2.16	1.43	1.48
3	A	246	653	C5-N4	-2.13	1.31	1.39
3	A	246	653	C1-C7	-2.02	1.44	1.48
3	A	246	653	C3-C4	-2.01	1.37	1.40
3	A	246	653	C6-C1	3.89	1.44	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	246	653	CV'-C3'-C4'	-8.84	106.04	120.56
3	A	246	653	C2-C1-C6	-2.23	116.43	119.28
3	A	246	653	C2'-C1'-C6'	-2.21	115.68	118.46
3	A	246	653	C2-C3-C4	-2.16	116.59	119.41
3	A	246	653	C5-C4-N3	2.06	107.62	105.89
3	A	246	653	C3-C2-C1	2.53	123.89	120.80
3	A	246	653	CV'-C3'-C2'	7.95	133.60	120.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	246	653	4	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

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	223/223 (100%)	3.05	167 (74%) 0 0	12, 21, 31, 54	24 (10%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	SER	13.3
1	A	115	ASN	10.1
1	A	149	THR	8.0
1	A	162	ILE	7.1
1	A	187	GLY	7.0
1	A	151	TYR	6.9
1	A	185	LEU	6.7
1	A	148	GLY	6.5
1	A	242	ILE	6.3
1	A	31	VAL	6.3
1	A	158	LEU	6.2
1	A	51	TRP	6.2
1	A	125	THR	6.1
1	A	111	ALA	6.0
1	A	193	GLY	6.0
1	A	145	LYS	5.5
1	A	175[A]	GLN	5.5
1	A	21	THR	5.1
1	A	87[A]	LYS	5.1
1	A	154	VAL	4.9
1	A	144	THR	4.8
1	A	237	TRP	4.7
1	A	75	VAL	4.7
1	A	217[A]	SER	4.6
1	A	243	ALA	4.6
1	A	117	ARG	4.5
1	A	114	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	20	TYR	4.5
1	A	202	SER	4.5
1	A	116	SER	4.5
1	A	195[A]	SER	4.4
1	A	147	SER	4.4
1	A	177	THR	4.4
1	A	97	ASN	4.3
1	A	124	PRO	4.3
1	A	231	VAL	4.2
1	A	132	ALA	4.2
1	A	232	CYS	4.2
1	A	127	SER	4.2
1	A	176	ILE	4.2
1	A	220	CYS	4.1
1	A	159[A]	LYS	4.1
1	A	215	TRP	4.1
1	A	170[A]	SER	4.0
1	A	123	LEU	4.0
1	A	99	LEU	4.0
1	A	105	LEU	3.9
1	A	128	CYS	3.9
1	A	62	GLY	3.9
1	A	142	GLY	3.9
1	A	184(A)	TYR	3.9
1	A	150	SER	3.8
1	A	92	PRO	3.8
1	A	28	PRO	3.8
1	A	171	ALA	3.8
1	A	135	GLN	3.8
1	A	16	ILE	3.8
1	A	181	PHE	3.7
1	A	166	SER	3.7
1	A	130[A]	SER	3.7
1	A	59	TYR	3.7
1	A	76	VAL	3.7
1	A	27	VAL	3.6
1	A	48	ASN	3.6
1	A	219	GLY	3.5
1	A	228	TYR	3.5
1	A	17	VAL	3.5
1	A	188(A)	LYS	3.5
1	A	178	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	168	CYS	3.5
1	A	23	GLY	3.5
1	A	86[A]	SER	3.5
1	A	83	ILE	3.4
1	A	24	ALA	3.4
1	A	53[A]	VAL	3.4
1	A	22	CYS	3.4
1	A	152	PRO	3.4
1	A	227	VAL	3.4
1	A	164	SER	3.4
1	A	184	GLY	3.4
1	A	213	VAL	3.4
1	A	173	PRO	3.4
1	A	52	VAL	3.3
1	A	113[A]	SER	3.2
1	A	85	ALA	3.2
1	A	238	ILE	3.2
1	A	230[A]	LYS	3.2
1	A	73	ILE	3.2
1	A	235	VAL	3.2
1	A	165[A]	ASP	3.1
1	A	109	LYS	3.1
1	A	47	ILE	3.1
1	A	66[A]	LEU	3.1
1	A	172	TYR	3.1
1	A	41	PHE	3.0
1	A	225	PRO	3.0
1	A	167	SER	3.0
1	A	199	VAL	2.9
1	A	241	THR	2.9
1	A	104	MET	2.9
1	A	192	GLN	2.9
1	A	58	CYS	2.9
1	A	222	LYS	2.9
1	A	122	SER	2.9
1	A	89	ILE	2.9
1	A	203	GLY	2.9
1	A	129	ALA	2.9
1	A	197	GLY	2.8
1	A	118	VAL	2.8
1	A	39	TYR	2.8
1	A	120	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	157	CYS	2.8
1	A	212	ILE	2.8
1	A	82	PHE	2.8
1	A	224	LYS	2.7
1	A	221(A)	GLN	2.7
1	A	239	LYS	2.7
1	A	94	TYR	2.7
1	A	183	ALA	2.7
1	A	163	LEU	2.7
1	A	244[A]	SER	2.7
1	A	100	ASN	2.7
1	A	84	SER	2.7
1	A	60	LYS	2.6
1	A	112	ALA	2.6
1	A	90	VAL	2.6
1	A	236[A]	SER	2.6
1	A	55	ALA	2.6
1	A	221	ALA	2.6
1	A	191	CYS	2.6
1	A	121	ILE	2.6
1	A	245	ASN	2.5
1	A	101	ASN	2.5
1	A	137	LEU	2.5
1	A	95	ASN	2.5
1	A	136	CYS	2.5
1	A	50	GLN	2.5
1	A	25	ASN	2.5
1	A	155	LEU	2.4
1	A	42	CYS	2.4
1	A	211	GLY	2.4
1	A	234	TYR	2.4
1	A	216	GLY	2.4
1	A	143	ASN	2.4
1	A	174	GLY	2.4
1	A	29	TYR	2.4
1	A	233	ASN	2.3
1	A	200	VAL	2.3
1	A	57	HIS	2.3
1	A	182	CYS	2.3
1	A	19	GLY	2.3
1	A	240	GLN	2.3
1	A	106	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	153	ASP	2.2
1	A	141	TRP	2.2
1	A	110[A]	SER	2.2
1	A	26	THR	2.2
1	A	161	PRO	2.2
1	A	56	ALA	2.1
1	A	88	SER	2.1
1	A	93	SER	2.1
1	A	74	ASN	2.1
1	A	201	CYS	2.1
1	A	138	ILE	2.1
1	A	169	LYS	2.1
1	A	140	GLY	2.1
1	A	46	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	653	A	246	28/28	0.66	0.25	0.42	22,26,36,37	7
2	CA	A	247	1/1	0.80	0.18	-0.44	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.