



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:46 AM GMT

PDB ID : 3C5N
Title : Structure of human TULP1 in complex with IP3
Authors : Busam, R.D.; Lehtio, L.; Arrowsmith, C.H.; Collins, R.; Dahlgren, L.G.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Hallberg, B.M.; Herman, M.D.; Johansson, A.; Johansson, I.; Kallas, A.; Karlberg, T.; Kotenyova, T.; Moche, M.; Nilsson, M.E.; Nordlund, P.; Nyman, T.; Persson, C.; Sagemark, J.; Svensson, L.; Thorsell, A.G.; Tresaugues, L.; Van den Berg, S.; Weigelt, J.; Welin, M.; Berglund, H.; Structural Genomics Consortium (SGC)
Deposited on : 2008-01-31
Resolution : 1.80 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

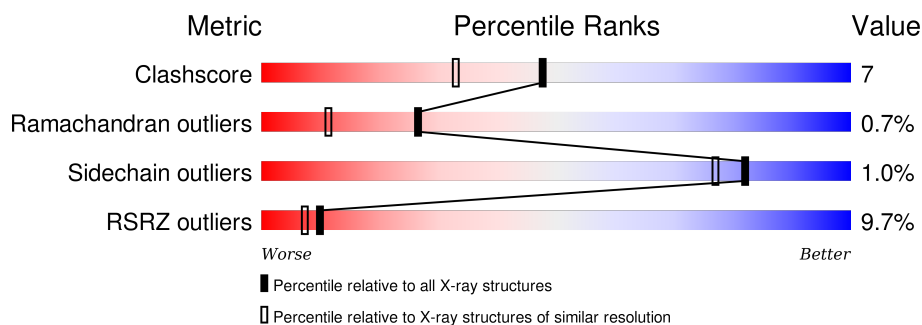
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	246	
1	B	246	

2 Entry composition [i](#)

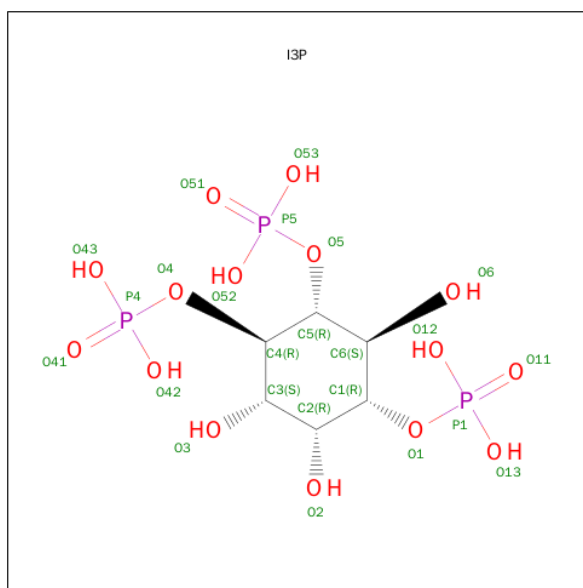
There are 3 unique types of molecules in this entry. The entry contains 7650 atoms, of which 3656 are hydrogens and 0 are deuteriums.

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 Tubby-related protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	231	Total	C	H	N	O	S	13	2	0
			3699	1176	1839	339	340	5			
1	B	223	Total	C	H	N	O	S	9	4	0
			3633	1154	1817	336	322	4			

- Molecule 2 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			24	6	15	3		
2	B	1	Total	C	O	P	0	0
			24	6	15	3		
2	B	1	Total	C	O	P	0	0
			24	6	15	3		

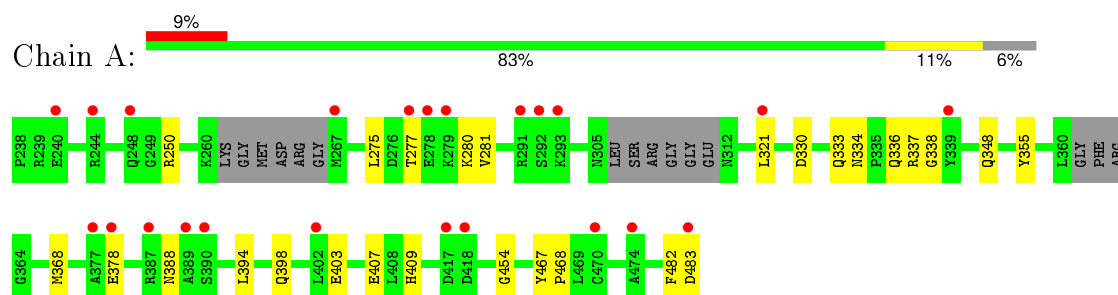
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	101	Total 101	O 101	0	0
3	B	145	Total 145	O 145	0	0

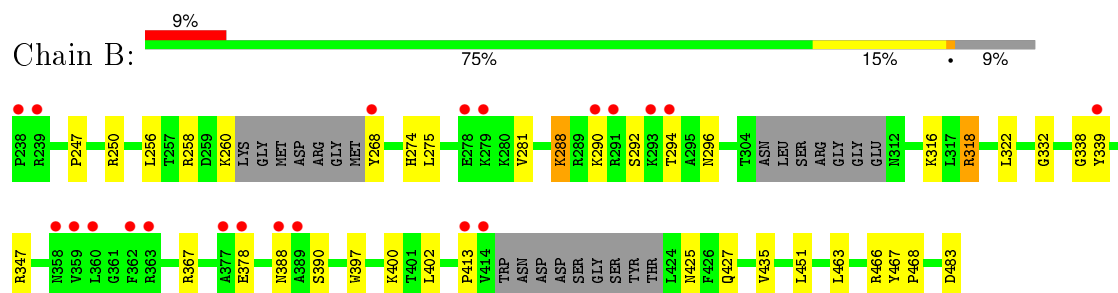
3 Residue-property plots [i](#)

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: Tubby-related protein 1



• Molecule 1: Tubby-related protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.31Å 83.63Å 57.68Å 90.00° 94.01° 90.00°	Depositor
Resolution (Å)	23.70 – 1.80 23.70 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (23.70-1.80) 97.6 (23.70-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.189 , 0.221 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.3	EDS
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 48245 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7650	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: I3P

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	0.56	0/1898	0.67	0/2567
1	B	0.58	0/1852	0.70	0/2500
All	All	0.57	0/3750	0.68	0/5067

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	1860	1839	1846	18	0
1	B	1816	1817	1819	37	0
2	A	24	0	9	0	0
2	B	48	0	18	0	0
3	A	101	0	0	4	0
3	B	145	0	0	13	0
All	All	3994	3656	3692	55	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 7.

All (55) 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:B:294:THR:HG21	1:B:318:ARG:HD3	1.55	0.87
1:B:296:ASN:ND2	1:B:316:LYS:HE2	2.03	0.74
1:B:275:LEU:HD12	1:B:281:VAL:CG1	2.17	0.73
1:B:400:LYS:HE3	3:B:568:HOH:O	1.93	0.67
1:A:482:PHE:O	1:A:483:ASP:HB3	1.95	0.67
1:B:275:LEU:HD12	1:B:281:VAL:HG12	1.78	0.66
1:B:260:LYS:HD2	3:B:528:HOH:O	1.96	0.64
1:A:275:LEU:HD12	1:A:281:VAL:CG1	2.28	0.64
1:B:316:LYS:CD	3:B:573:HOH:O	2.48	0.62
1:A:454:GLY:N	3:A:564:HOH:O	2.33	0.61
1:B:322:LEU:HD23	3:B:602:HOH:O	2.05	0.57
1:B:397:TRP:O	1:B:400:LYS:HD2	2.05	0.56
1:B:268:TYR:HE1	1:B:290:LYS:HA	1.70	0.55
1:B:274:HIS:HD2	3:B:485:HOH:O	1.89	0.54
1:B:288:LYS:HB2	3:B:501:HOH:O	2.09	0.53
1:A:275:LEU:HD12	1:A:281:VAL:HG12	1.89	0.53
1:A:378:GLU:O	1:A:378:GLU:HG3	2.08	0.53
1:B:397:TRP:HA	1:B:402:LEU:HD21	1.92	0.52
1:A:407:GLU:OE2	1:A:409:HIS:HE1	1.94	0.51
1:B:451:LEU:HD11	1:B:463:LEU:HD11	1.91	0.51
1:A:355:TYR:CE1	1:A:368:MET:HG2	2.45	0.51
1:B:268:TYR:CE1	1:B:290:LYS:HG2	2.46	0.50
1:B:435[A]:VAL:HG12	1:B:435[A]:VAL:O	2.12	0.50
1:B:466:ARG:HA	3:B:536:HOH:O	2.12	0.50
1:B:292:SER:HB2	3:B:616:HOH:O	2.12	0.49
1:B:268:TYR:CD1	1:B:288:LYS:HB3	2.47	0.49
1:A:275:LEU:HD12	1:A:281:VAL:HG11	1.94	0.48
1:A:334:ASN:HB3	1:A:337:ARG:HG3	1.96	0.48
1:B:247:PRO:HB2	1:B:250:ARG:HG3	1.96	0.48
1:B:316:LYS:HD3	3:B:573:HOH:O	2.11	0.47
1:B:467:TYR:CD1	1:B:468:PRO:HA	2.50	0.47
1:B:258:ARG:CZ	1:B:260:LYS:HE2	2.45	0.46
1:B:339:TYR:HE2	3:B:533:HOH:O	1.98	0.46
1:B:467:TYR:CG	1:B:468:PRO:HA	2.51	0.45
1:A:403:GLU:HB2	3:A:582:HOH:O	2.17	0.45
1:A:250:ARG:HB3	3:A:557:HOH:O	2.16	0.45
1:B:294:THR:HG21	1:B:318:ARG:HH11	1.81	0.45
1:A:277[B]:THR:HG22	3:A:515:HOH:O	2.17	0.45
1:A:394:LEU:O	1:A:398:GLN:HG2	2.18	0.44
1:B:316:LYS:NZ	1:B:318:ARG:NH1	2.65	0.44
1:A:333:GLN:HG2	1:A:334:ASN:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ARG:HG3	3:B:558:HOH:O	2.17	0.44
1:A:336:GLN:HE22	1:A:388:ASN:HA	1.83	0.43
1:A:330:ASP:OD2	1:A:348:GLN:HG2	2.19	0.42
1:B:378:GLU:CD	1:B:378:GLU:N	2.73	0.42
1:B:316:LYS:HE3	3:B:573:HOH:O	2.20	0.42
1:A:275:LEU:HB2	1:A:281:VAL:HG12	2.00	0.42
1:B:316:LYS:HZ2	1:B:318:ARG:NH1	2.17	0.41
1:B:483:ASP:HB3	3:B:580:HOH:O	2.20	0.41
1:A:467:TYR:CG	1:A:468:PRO:HA	2.56	0.41
1:B:388:ASN:C	1:B:390:SER:H	2.24	0.41
1:B:258:ARG:NE	1:B:260:LYS:HE2	2.36	0.41
1:B:332:GLY:O	1:B:347:ARG:HB3	2.21	0.41
1:B:425:ASN:ND2	1:B:427:GLN:H	2.19	0.40
1:B:256:LEU:C	1:B:256:LEU:HD23	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	224/246 (91%)	216 (96%)	6 (3%)	2 (1%)	21	7
1	B	217/246 (88%)	207 (95%)	9 (4%)	1 (0%)	34	17
All	All	441/492 (90%)	423 (96%)	15 (3%)	3 (1%)	26	11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	LYS
1	A	338	GLY
1	B	338	GLY

5.3.2 Protein sidechains [i](#)

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	202/213 (95%)	201 (100%)	1 (0%)	92	91
1	B	197/213 (92%)	194 (98%)	3 (2%)	72	62
All	All	399/426 (94%)	395 (99%)	4 (1%)	82	77

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

Mol	Chain	Res	Type
1	A	321	LEU
1	B	288	LYS
1	B	318	ARG
1	B	413	PRO

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	333	GLN
1	A	336	GLN
1	A	379	ASN
1	A	409	HIS
1	A	416	ASN
1	B	274	HIS
1	B	296	ASN
1	B	336	GLN
1	B	425	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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$
2	I3P	A	2	-	24,24,24	1.16	4 (16%)	33,39,39	1.33	5 (15%)
2	I3P	B	1	-	24,24,24	1.34	4 (16%)	33,39,39	1.28	5 (15%)
2	I3P	B	3	-	24,24,24	1.19	4 (16%)	33,39,39	1.38	4 (12%)

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	I3P	A	2	-	-	0/15/39/39	0/1/1/1
2	I3P	B	1	-	-	0/15/39/39	0/1/1/1
2	I3P	B	3	-	-	0/15/39/39	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	I3P	P4-O43	2.02	1.62	1.54
2	A	2	I3P	P4-O43	2.10	1.62	1.54
2	B	3	I3P	P4-O42	2.16	1.62	1.54
2	A	2	I3P	P1-O13	2.20	1.62	1.54
2	A	2	I3P	P1-O12	2.21	1.62	1.54
2	B	1	I3P	O3-C3	2.31	1.48	1.43
2	A	2	I3P	P4-O42	2.32	1.63	1.54
2	B	3	I3P	P5-O53	2.35	1.63	1.54
2	B	1	I3P	P4-O43	2.37	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	I3P	P1-O13	2.64	1.64	1.54
2	B	1	I3P	P1-O12	2.75	1.64	1.54
2	B	1	I3P	P1-O13	2.80	1.64	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	I3P	O3-C3-C4	-2.78	103.29	109.87
2	A	2	I3P	O3-C3-C2	-2.77	104.10	110.34
2	B	1	I3P	O3-C3-C2	-2.47	104.78	110.34
2	B	1	I3P	C6-C1-C2	-2.46	107.64	110.89
2	B	3	I3P	O3-C3-C2	-2.31	105.15	110.34
2	A	2	I3P	P1-O1-C1	-2.25	116.18	121.56
2	B	1	I3P	O5-P5-O51	2.02	112.14	107.11
2	A	2	I3P	O1-C1-C6	2.18	113.15	108.38
2	A	2	I3P	O1-P1-O11	2.27	112.77	107.11
2	B	1	I3P	O1-P1-O11	2.53	113.42	107.11
2	B	3	I3P	O1-P1-O11	2.55	113.48	107.11
2	B	1	I3P	O42-P4-O41	2.94	120.04	110.58
2	B	3	I3P	O5-P5-O51	3.80	116.60	107.11
2	A	2	I3P	P4-O4-C4	3.99	131.13	121.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	231/246 (93%)	0.48	23 (9%) 9 7	13, 29, 67, 92	1 (0%)
1	B	223/246 (90%)	0.66	21 (9%) 11 8	13, 27, 74, 117	0
All	All	454/492 (92%)	0.57	44 (9%) 10 7	13, 28, 71, 117	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	414	VAL	10.8
1	B	360	LEU	9.6
1	B	359	VAL	6.5
1	B	291	ARG	4.9
1	A	483	ASP	4.7
1	B	278	GLU	4.5
1	B	268	TYR	4.1
1	A	279	LYS	3.9
1	A	377	ALA	3.8
1	B	389	ALA	3.8
1	A	389	ALA	3.6
1	A	292	SER	3.6
1	A	277[A]	THR	3.5
1	A	321	LEU	3.2
1	A	378	GLU	3.1
1	B	378	GLU	3.0
1	A	339	TYR	3.0
1	B	413	PRO	3.0
1	A	293	LYS	2.9
1	B	239	ARG	2.9
1	A	244	ARG	2.8
1	A	291	ARG	2.8
1	B	339	TYR	2.7
1	A	240	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	387	ARG	2.6
1	A	418	ASP	2.6
1	A	390	SER	2.4
1	B	293	LYS	2.4
1	A	267	MET	2.4
1	A	278[A]	GLU	2.3
1	A	248	GLN	2.3
1	B	290	LYS	2.3
1	B	377	ALA	2.3
1	A	402	LEU	2.2
1	B	363	ARG	2.2
1	B	388	ASN	2.2
1	B	279[A]	LYS	2.2
1	B	238	PRO	2.2
1	A	417	ASP	2.2
1	B	362	PHE	2.1
1	B	294	THR	2.1
1	B	358	ASN	2.1
1	A	474	ALA	2.0
1	A	470	CYS	2.0

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
2	I3P	A	2	24/24	0.95	0.27	0.69	25,46,74,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	I3P	B	3	24/24	0.92	0.24	0.57	35,45,64,70	0
2	I3P	B	1	24/24	0.96	0.17	0.42	21,27,63,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.