



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2018 – 09:43 PM EST

PDB ID : 6BMX
Title : Non-receptor Protein Tyrosine Phosphatase SHP2 in Complex with Allosteric Inhibitor SHP844
Authors : Stams, T.; Fodor, M.
Deposited on : 2017-11-15
Resolution : 2.42 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 : rb-20030736
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) : rb-20030736

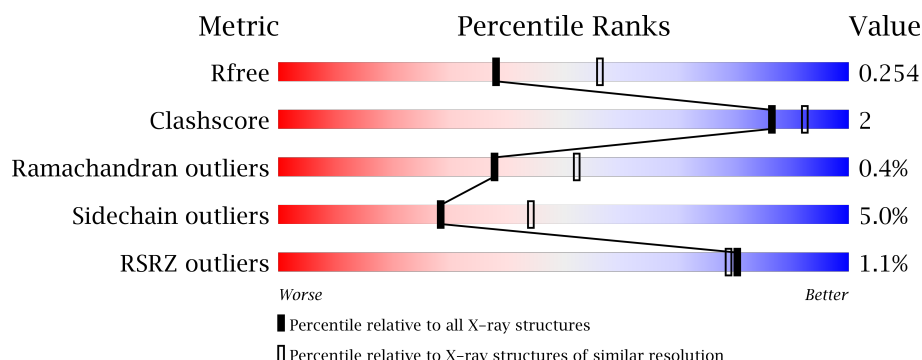
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	3709 (2.44-2.40)
Clashscore	112137	4241 (2.44-2.40)
Ramachandran outliers	110173	4178 (2.44-2.40)
Sidechain outliers	110143	4179 (2.44-2.40)
RSRZ outliers	101464	3740 (2.44-2.40)

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	526	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 83%, yellow 83%, yellow 90%, green 90%, green 99%, green 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%; text-align: center;">83% 9% • 7%</div> </div> </div>
1	B	526	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 81%, yellow 81%, yellow 90%, green 90%, green 99%, green 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%; text-align: center;">81% 9% • 9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	603	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8582 atoms, of which 0 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.

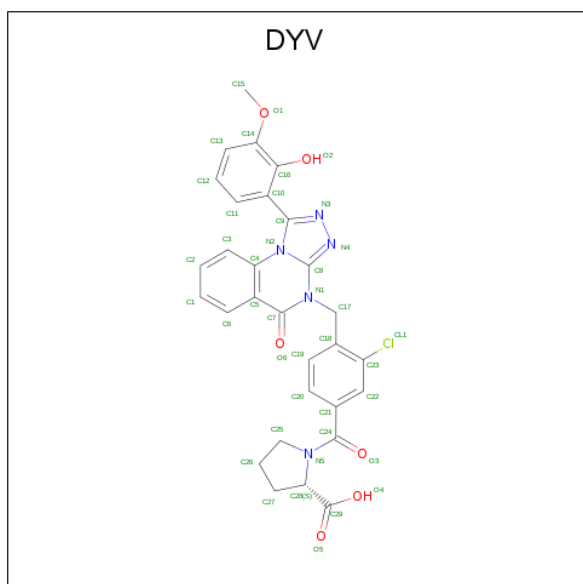
- Molecule 1 is a protein called Tyrosine-protein phosphatase non-receptor type 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	1	0
			3949	2489	700	741	19			
1	B	478	Total	C	N	O	S	0	3	0
			3886	2455	690	721	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q06124
B	0	SER	-	expression tag	UNP Q06124

- Molecule 2 is 1-(3-chloro-4-{[1-(2-hydroxy-3-methoxyphenyl)-5-oxo[1,2,4]triazolo[4,3-a]quinazolin-4(5H)-yl]methyl}benzene-1-carbonyl)-L-proline (three-letter code: DYV) (formula: C₂₉H₂₄ClN₅O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			41	29	1	5	6		
2	B	1	Total	C	Cl	N	O	0	0
			41	29	1	5	6		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

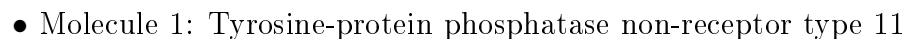


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	332	Total	O	0	0
			332	332		
5	B	307	Total	O	0	0
			307	307		

- Molecule 1: Tyrosine-protein phosphatase non-receptor type 11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.13 Å 215.00 Å 56.04 Å 90.00° 96.59° 90.00°	Depositor
Resolution (Å)	55.67 – 2.42 55.67 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.1 (55.67-2.42) 99.6 (55.67-2.42)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.42 Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.167 , 0.252 0.169 , 0.254	Depositor DCC
R_{free} test set	1936 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8582	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, DYV

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	0.52	0/4032	0.70	0/5434
1	B	0.51	0/3974	0.71	0/5354
All	All	0.51	0/8006	0.71	0/10788

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	3949	0	3889	20	0
1	B	3886	0	3850	19	0
2	A	41	0	0	0	0
2	B	41	0	0	0	0
3	A	15	0	0	0	0
3	B	5	0	0	0	0
4	B	6	0	8	0	0
5	A	332	0	0	1	0
5	B	307	0	0	0	0
All	All	8582	0	7747	39	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 2.

All (39) 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:294:ASP:HB2	1:A:343:ARG:HE	1.39	0.88
1:B:232:GLU:HA	1:B:235:LYS:HE2	1.72	0.70
1:B:88:LEU:HG	1:B:96:ILE:HG23	1.75	0.67
1:A:294:ASP:CB	1:A:343:ARG:HE	2.11	0.64
1:A:272:GLU:HB3	1:A:301:VAL:HG11	1.80	0.63
1:B:222:ASN:O	1:B:225:GLU:HG2	2.01	0.60
1:A:272:GLU:CB	1:A:301:VAL:HG11	2.35	0.57
1:B:356:THR:OG1	1:B:459:CYS:HB3	2.04	0.57
1:B:65:LEU:HD23	1:B:68:GLY:HA3	1.92	0.52
1:A:47:ARG:HH21	1:A:94:ASP:HB3	1.75	0.51
1:A:294:ASP:HB2	1:A:343:ARG:NE	2.16	0.51
1:B:126:LEU:HD22	1:B:152:ARG:HB2	1.94	0.50
1:A:390:GLU:HG2	1:A:399:ARG:HG2	1.93	0.50
1:A:125:LEU:HB3	1:A:216:LEU:HD21	1.93	0.49
1:A:290:VAL:HG11	1:A:344:MET:HG3	1.94	0.49
1:B:390:GLU:HG2	1:B:399:ARG:HG2	1.96	0.47
1:B:330:THR:HG23	1:B:458:HIS:HB3	1.96	0.47
1:A:295:GLY:H	1:A:343:ARG:NH2	2.13	0.46
1:B:432:PRO:HG3	1:B:516[A]:MET:HG2	1.97	0.46
1:A:399:ARG:HD2	1:A:417:GLN:OE1	2.15	0.46
1:A:309:ILE:HD13	1:A:328:ILE:HG12	1.97	0.46
1:A:294:ASP:HB2	1:A:343:ARG:HH21	1.82	0.45
1:A:326:SER:HB3	1:A:454:PRO:HB3	1.98	0.45
1:A:147:PHE:HB2	1:A:172:ILE:HB	2.00	0.44
1:B:125:LEU:HB3	1:B:216:LEU:HD21	1.99	0.44
1:A:475:LEU:HA	1:A:478:ILE:HD12	1.99	0.43
1:B:328:ILE:HD11	1:B:348:GLU:HG3	2.01	0.43
1:A:4:ARG:HH21	1:A:74:LEU:HB2	1.83	0.43
1:B:525:LEU:HD12	1:B:525:LEU:HA	1.95	0.42
1:A:107:PRO:HG3	1:A:190:LEU:HD12	2.02	0.42
1:A:463:ILE:HG12	5:A:805:HOH:O	2.20	0.42
1:A:88:LEU:HG	1:A:96:ILE:HD12	2.02	0.42
1:B:223:ALA:HB3	1:B:484:VAL:O	2.19	0.41
1:B:65:LEU:HD21	1:B:88:LEU:HD13	2.00	0.41
1:B:45:VAL:HB	1:B:96:ILE:HD11	2.03	0.41
1:B:107:PRO:HG3	1:B:190:LEU:HD12	2.03	0.41
1:B:211:GLN:HB3	1:B:213:LYS:HG3	2.03	0.41
1:B:290:VAL:HG11	1:B:344:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:GLY:HA2	1:B:507:THR:HG23	2.03	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	475/526 (90%)	456 (96%)	16 (3%)	3 (1%)	28	40
1	B	467/526 (89%)	453 (97%)	13 (3%)	1 (0%)	51	66
All	All	942/1052 (90%)	909 (96%)	29 (3%)	4 (0%)	38	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	VAL
1	A	295	GLY
1	A	505	VAL
1	B	505	VAL

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	434/468 (93%)	408 (94%)	26 (6%)	22	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	428/468 (92%)	410 (96%)	18 (4%)	34 52
All	All	862/936 (92%)	818 (95%)	44 (5%)	28 43

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	111	ARG
1	A	131	LYS
1	A	149	LEU
1	A	151	VAL
1	A	152	ARG
1	A	177	LEU
1	A	211	GLN
1	A	245	GLN
1	A	249	GLU
1	A	294	ASP
1	A	311	MET
1	A	325	LYS
1	A	326	SER
1	A	413	ARG
1	A	430	SER
1	A	439	LEU
1	A	447	GLU
1	A	477	ASP
1	A	480	ARG
1	A	484	VAL
1	A	502	SER
1	A	508	GLU
1	A	512	ARG
1	A	516[A]	MET
1	A	516[B]	MET
1	B	47	ARG
1	B	70	LYS
1	B	87	GLN
1	B	94	ASP
1	B	96	ILE
1	B	151	VAL
1	B	152	ARG
1	B	166	LYS
1	B	218	THR
1	B	275	ASN

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Mol	Chain	Res	Type
1	B	325	LYS
1	B	413	ARG
1	B	426	HIS
1	B	447	GLU
1	B	451	ASP
1	B	477	ASP
1	B	492	LYS
1	B	525	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	256	GLN
1	A	269	GLN
1	A	408	GLN
1	B	87	GLN
1	B	256	GLN
1	B	281	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

7 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	DYV	A	601	-	38,46,46	1.72	6 (15%)	46,68,68	1.82	9 (19%)
3	PO4	A	602	-	4,4,4	2.61	1 (25%)	6,6,6	0.51	0
3	PO4	A	603	-	4,4,4	2.63	1 (25%)	6,6,6	0.44	0
3	PO4	A	604	-	4,4,4	2.06	1 (25%)	6,6,6	0.45	0
2	DYV	B	601	-	38,46,46	1.83	5 (13%)	46,68,68	1.42	6 (13%)
3	PO4	B	602	-	4,4,4	2.58	1 (25%)	6,6,6	0.77	0
4	GOL	B	603	-	5,5,5	0.18	0	5,5,5	0.27	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
2	DYV	A	601	-	-	0/18/32/32	0/6/6/6
3	PO4	A	602	-	-	0/0/0/0	0/0/0/0
3	PO4	A	603	-	-	0/0/0/0	0/0/0/0
3	PO4	A	604	-	-	0/0/0/0	0/0/0/0
2	DYV	B	601	-	-	0/18/32/32	0/6/6/6
3	PO4	B	602	-	-	0/0/0/0	0/0/0/0
4	GOL	B	603	-	-	0/4/4/4	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	DYV	C1-C6	2.06	1.41	1.36
2	B	601	DYV	C14-C16	2.21	1.43	1.40
2	B	601	DYV	C1-C6	2.23	1.41	1.36
2	A	601	DYV	C2-C3	2.23	1.41	1.36
2	A	601	DYV	C20-C21	2.24	1.43	1.39
2	B	601	DYV	C20-C21	2.24	1.43	1.39
2	A	601	DYV	C22-C21	2.29	1.42	1.39
3	A	604	PO4	P-O1	2.82	1.56	1.50
2	B	601	DYV	C5-C4	3.72	1.44	1.41
2	A	601	DYV	C5-C4	4.12	1.44	1.41
3	B	602	PO4	P-O1	4.53	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	PO4	P-O1	4.61	1.60	1.50
3	A	602	PO4	P-O1	4.62	1.60	1.50
2	A	601	DYV	C7-C5	6.16	1.51	1.41
2	B	601	DYV	C7-C5	6.96	1.52	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	DYV	C25-N5-C28	-6.98	105.55	111.81
2	B	601	DYV	C5-C4-N2	-3.97	117.19	119.50
2	A	601	DYV	C5-C4-N2	-3.67	117.36	119.50
2	A	601	DYV	C22-C23-C18	-2.33	120.21	122.46
2	A	601	DYV	C13-C14-C16	-2.05	117.97	120.00
2	B	601	DYV	C17-N1-C7	2.03	120.25	117.79
2	A	601	DYV	C17-N1-C7	2.04	120.25	117.79
2	A	601	DYV	C18-C17-N1	2.12	116.83	113.31
2	A	601	DYV	C10-C16-C14	2.32	121.44	120.30
2	B	601	DYV	C10-C16-C14	2.39	121.48	120.30
2	B	601	DYV	C26-C25-N5	2.47	107.06	103.22
2	A	601	DYV	C15-O1-C14	3.08	121.97	117.54
2	B	601	DYV	C18-C17-N1	3.30	118.79	113.31
2	B	601	DYV	C15-O1-C14	3.80	123.01	117.54
2	A	601	DYV	C6-C5-C4	4.73	120.22	118.04

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	488/526 (92%)	-0.14	5 (1%) 82 80	21, 42, 68, 93	0
1	B	478/526 (90%)	-0.10	6 (1%) 77 75	22, 43, 68, 93	0
All	All	966/1052 (91%)	-0.12	11 (1%) 80 79	21, 42, 68, 93	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	GLY	4.3
1	A	95	VAL	3.8
1	B	426	HIS	3.5
1	B	86	GLY	3.1
1	B	177	LEU	2.7
1	B	120	LYS	2.5
1	B	248	TRP	2.1
1	A	94	ASP	2.1
1	B	85	HIS	2.1
1	A	85	HIS	2.1
1	A	120	LYS	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
4	GOL	B	603	6/6	0.82	0.19	2.93	57,69,70,72	0
2	DYV	A	601	41/41	0.95	0.18	1.06	34,40,69,71	0
2	DYV	B	601	41/41	0.94	0.18	0.62	27,37,81,84	0
3	PO4	A	603	5/5	0.91	0.16	-0.13	90,90,91,93	0
3	PO4	A	602	5/5	0.97	0.14	-0.25	79,80,81,81	0
3	PO4	A	604	5/5	0.81	0.16	-0.95	108,109,109,110	0
3	PO4	B	602	5/5	0.97	0.13	-1.08	52,53,55,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.