wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:05 PM GMT

PDB ID	:	3SJB
Title	:	Crystal structure of S. cerevisiae Get3 in the open state in complex with Get1 cytosolic domain
Authors	:	Reitz, S.; Wild, K.; Sinning, I.
Deposited on	:	2011-06-21
Resolution	:	3.30 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.
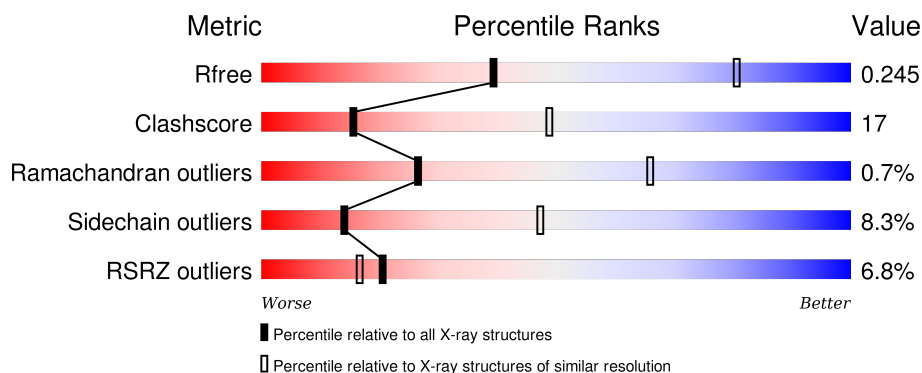
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 <=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	362	4% / 50% / 26% / • / 20%
1	B	362	5% / 52% / 28% / • / 17%
2	C	93	8% / 49% / 17% / • / 32%
2	D	93	10% / 48% / 27% / • / 23%

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
3	PO4	A	364	-	-	-	X
3	PO4	B	363	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5823 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 ATPase GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total 2280	C 1437	N 380	O 447	S 16	0	0	0
1	B	302	Total 2384	C 1503	N 396	O 468	S 17	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	LEU	-	EXPRESSION TAG	UNP Q12154
A	356	GLU	-	EXPRESSION TAG	UNP Q12154
A	357	HIS	-	EXPRESSION TAG	UNP Q12154
A	358	HIS	-	EXPRESSION TAG	UNP Q12154
A	359	HIS	-	EXPRESSION TAG	UNP Q12154
A	360	HIS	-	EXPRESSION TAG	UNP Q12154
A	361	HIS	-	EXPRESSION TAG	UNP Q12154
A	362	HIS	-	EXPRESSION TAG	UNP Q12154
B	355	LEU	-	EXPRESSION TAG	UNP Q12154
B	356	GLU	-	EXPRESSION TAG	UNP Q12154
B	357	HIS	-	EXPRESSION TAG	UNP Q12154
B	358	HIS	-	EXPRESSION TAG	UNP Q12154
B	359	HIS	-	EXPRESSION TAG	UNP Q12154
B	360	HIS	-	EXPRESSION TAG	UNP Q12154
B	361	HIS	-	EXPRESSION TAG	UNP Q12154
B	362	HIS	-	EXPRESSION TAG	UNP Q12154

- Molecule 2 is a protein called Golgi to ER traffic protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	63	Total 528	C 328	N 96	O 104	0	0	0
2	D	72	Total 610	C 379	N 115	O 116	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	18	MET	-	EXPRESSION TAG	UNP P53192
C	104	GLU	-	EXPRESSION TAG	UNP P53192
C	105	HIS	-	EXPRESSION TAG	UNP P53192
C	106	HIS	-	EXPRESSION TAG	UNP P53192
C	107	HIS	-	EXPRESSION TAG	UNP P53192
C	108	HIS	-	EXPRESSION TAG	UNP P53192
C	109	HIS	-	EXPRESSION TAG	UNP P53192
C	110	HIS	-	EXPRESSION TAG	UNP P53192
D	18	MET	-	EXPRESSION TAG	UNP P53192
D	104	GLU	-	EXPRESSION TAG	UNP P53192
D	105	HIS	-	EXPRESSION TAG	UNP P53192
D	106	HIS	-	EXPRESSION TAG	UNP P53192
D	107	HIS	-	EXPRESSION TAG	UNP P53192
D	108	HIS	-	EXPRESSION TAG	UNP P53192
D	109	HIS	-	EXPRESSION TAG	UNP P53192
D	110	HIS	-	EXPRESSION TAG	UNP P53192

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
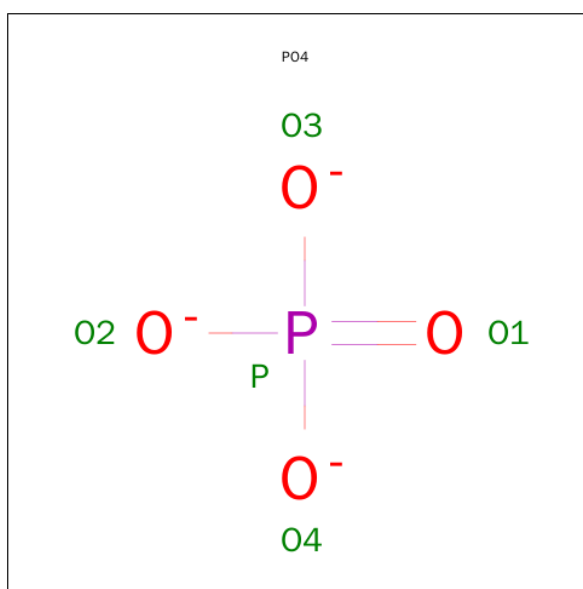
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	P 1	0	0
3	B	1	Total 5	O 4	P 1	0	0
3	A	1	Total 5	O 4	P 1	0	0

Continued from previous page...

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

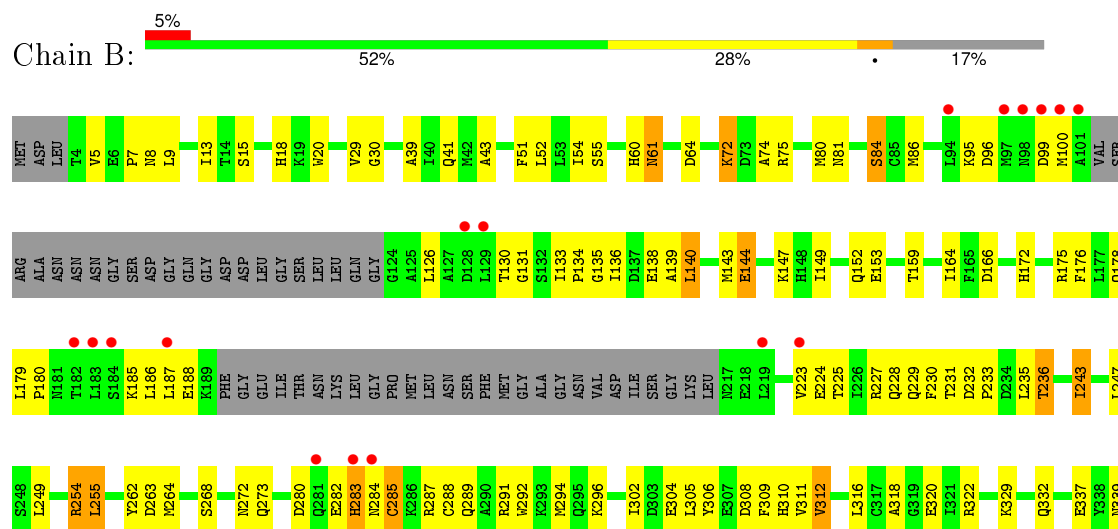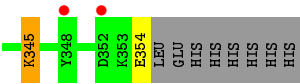| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Zn 1	0	0

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 (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.
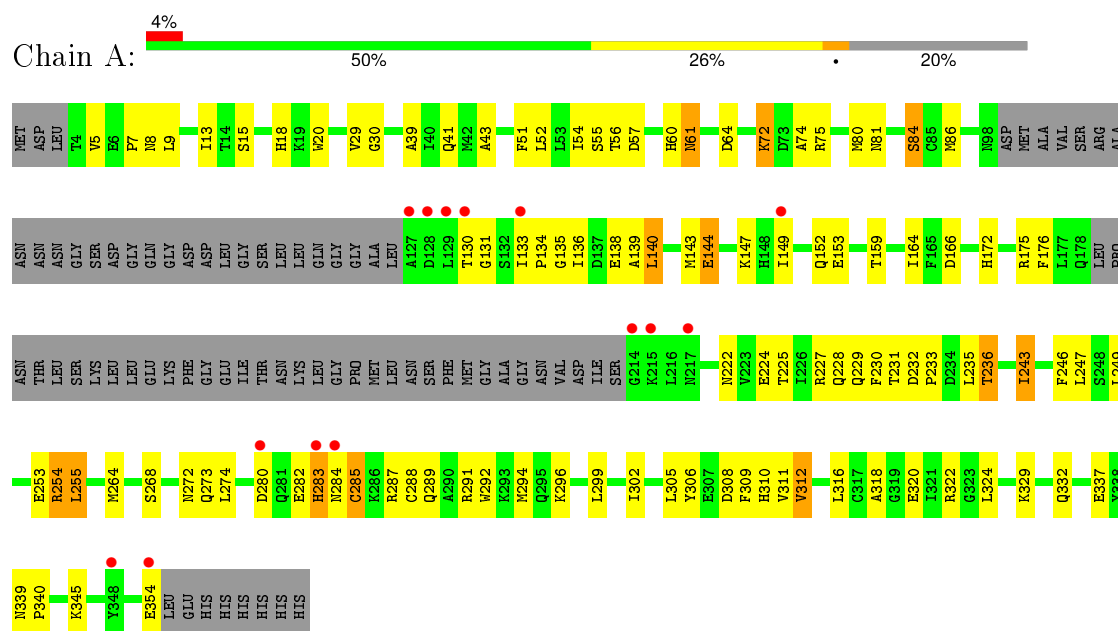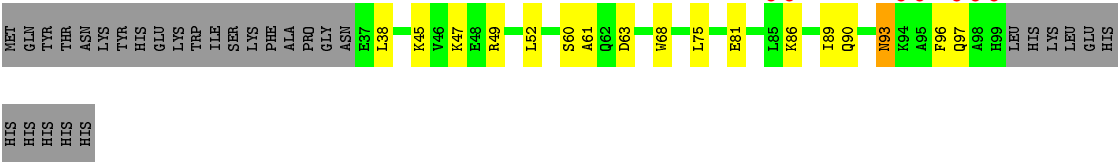
- Molecule 1: ATPase GET3

- Molecule 1: ATPase GET3

K345 Y348 D352 K353 E354 LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 2: Golgi to ER traffic protein 1

Chain C:

8%

49%   17% • 32%

MET GLN TYR THR ASN LYS TYR HIS GLU LYS TRP ILE SER LYS PHE ALA PRO GLY ASN E37 L38 K45 V46 K47 E48 R49 L52 S60 A61 Q62 D63 W68 L75 E81 L85 K86 I89 Q90 N93 K94 A95 F96 Q97 A98 H99 LEU HIS LYS LEU GLU HIS

HIS HIS HIS HIS

• Molecule 2: Golgi to ER traffic protein 1

Chain D:

10%

48%   27% • 23%

MET GLN TYR THR ASN LYS TYR HIS GLU LYS TRP ILE SER LYS PHE ALA PRO GLY N36 E37 L38 S39 K40 K41 K45 V46 K47 E48 R49 L52 S60 A61 Q62 D63 A66 K67 W68 L75 E81 K86 I89 Q90 N93 K94 A95 F96 Q97 A98 H99 L100 H101

K102 L103 E104 H105 H106 H107 HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	112.90Å 112.90Å 310.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.89 – 3.30 48.89 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.89-3.30) 99.6 (48.89-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.195 , 0.243 0.192 , 0.245	Depositor DCC
R_{free} test set	940 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	110.7	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 103.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.31$	Xtriage
Outliers	0 of 18399 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5823	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, PO4

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	0.47	0/2318	0.63	0/3125
1	B	0.45	0/2423	0.61	0/3268
2	C	0.39	0/535	0.47	0/713
2	D	0.35	0/621	0.48	0/829
All	All	0.45	0/5897	0.60	0/7935

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	2280	0	2246	82	0
1	B	2384	0	2357	91	0
2	C	528	0	523	10	0
2	D	610	0	598	19	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	1	0	0	0	0
All	All	5823	0	5724	198	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 17.

The worst 5 of 198 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:20:TRP:HB2	1:B:236:THR:HB	1.45	0.98
1:A:20:TRP:HB2	1:A:236:THR:HB	1.47	0.96
1:A:29:VAL:HG12	1:A:243:ILE:HD13	1.44	0.96
1:B:29:VAL:HG12	1:B:243:ILE:HD13	1.44	0.95
1:A:72:LYS:HD3	1:A:72:LYS:N	1.87	0.87

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	282/362 (78%)	254 (90%)	26 (9%)	2 (1%)	26	66
1	B	296/362 (82%)	272 (92%)	22 (7%)	2 (1%)	26	66
2	C	61/93 (66%)	57 (93%)	4 (7%)	0	100	100
2	D	70/93 (75%)	66 (94%)	3 (4%)	1 (1%)	14	50
All	All	709/910 (78%)	649 (92%)	55 (8%)	5 (1%)	26	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	283	HIS
1	B	60	HIS
1	B	283	HIS
2	D	103	LEU

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	257/317 (81%)	233 (91%)	24 (9%)	11	40
1	B	269/317 (85%)	243 (90%)	26 (10%)	10	38
2	C	58/86 (67%)	56 (97%)	2 (3%)	44	77
2	D	67/86 (78%)	65 (97%)	2 (3%)	48	79
All	All	651/806 (81%)	597 (92%)	54 (8%)	14	47

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	61	ASN
1	B	84	SER
1	B	354	GLU
1	B	64	ASP
1	B	75	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	HIS
1	B	61	ASN
1	B	289	GLN
1	A	326	ASN
1	B	326	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)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	PO4	A	363	-	4,4,4	0.41	0	6,6,6	0.30	0
3	PO4	A	364	-	4,4,4	0.44	0	6,6,6	0.28	0
3	PO4	B	363	-	4,4,4	0.39	0	6,6,6	0.27	0
3	PO4	B	364	-	4,4,4	0.38	0	6,6,6	0.28	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
3	PO4	A	363	-	-	0/0/0/0	0/0/0/0
3	PO4	A	364	-	-	0/0/0/0	0/0/0/0
3	PO4	B	363	-	-	0/0/0/0	0/0/0/0
3	PO4	B	364	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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 (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	288/362 (79%)	0.16	14 (4%)	33	27	65, 109, 218, 258	0
1	B	302/362 (83%)	0.26	19 (6%)	23	19	64, 111, 223, 268	0
2	C	63/93 (67%)	0.38	7 (11%)	7	6	86, 129, 202, 219	0
2	D	72/93 (77%)	0.43	9 (12%)	5	4	87, 139, 229, 256	0
All	All	725/910 (79%)	0.25	49 (6%)	20	17	64, 114, 221, 268	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	ASP	6.2
1	B	128	ASP	6.2
1	B	223	VAL	5.8
1	B	219	LEU	5.2
1	B	184	SER	4.8

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	PO4	A	364	5/5	0.85	0.41	5.60	140,151,158,175	0
3	PO4	B	363	5/5	0.93	0.37	3.38	166,169,178,184	0
3	PO4	A	363	5/5	0.93	0.35	1.58	150,152,160,172	0
3	PO4	B	364	5/5	0.84	0.28	1.02	122,143,153,179	0
4	ZN	A	365	1/1	1.00	0.10	-	106,106,106,106	0

6.5　Other polymers ⓘ

There are no such residues in this entry.