wwPDB X-ray Structure Validation Summary Report (i)

Oct 8, 2024 – 02:50 AM EDT

PDB ID	:	4N5C
Title	:	Crystal structure of Ypp1
Authors	:	Wu, X.; Chi, R.J.; Baskin, J.M.; Lucast, L.; Burd, C.G.; De Camilli, P.; Reinisch, K.M.
Deposited on	:	2013-10-09
Resolution	:	3.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

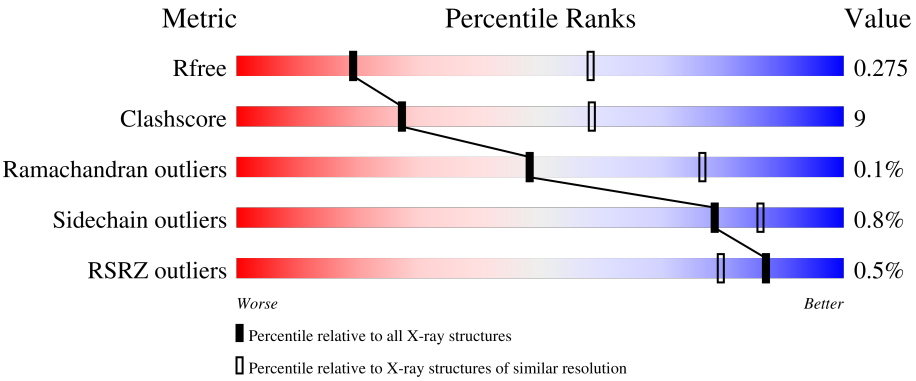
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.25 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}	164625	1482 (3.30-3.22)
Clashscore	180529	1546 (3.30-3.22)
Ramachandran outliers	177936	1536 (3.30-3.22)
Sidechain outliers	177891	1535 (3.30-3.22)
RSRZ outliers	164620	1483 (3.30-3.22)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	802	71% 21% 7%
1	B	802	72% 20% 8%
1	C	802	73% 18% 8%
1	D	802	72% 22% 6%
1	E	802	69% 21% 9%

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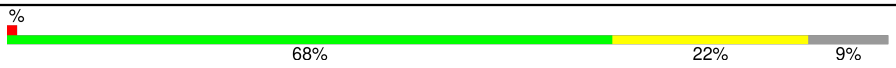
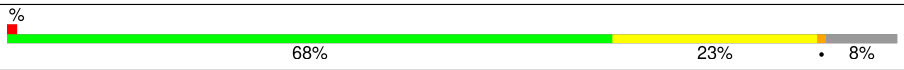
Mol	Chain	Length	Quality of chain
1	F	802	
1	G	802	
1	H	802	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 48674 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 Cargo-transport protein YPP1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	745	Total	C	N	O	S	Se	0	0	0
			6138	3963	987	1160	11	17			
1	B	741	Total	C	N	O	S	Se	0	0	0
			6109	3948	982	1151	11	17			
1	C	737	Total	C	N	O	S	Se	0	0	0
			6080	3930	977	1145	11	17			
1	D	757	Total	C	N	O	S	Se	0	0	0
			6241	4031	1003	1179	11	17			
1	E	727	Total	C	N	O	S	Se	0	0	0
			6000	3884	967	1123	11	15			
1	F	727	Total	C	N	O	S	Se	0	0	0
			5993	3872	967	1128	11	15			
1	G	735	Total	C	N	O	S	Se	0	0	0
			6056	3910	977	1143	11	15			
1	H	734	Total	C	N	O	S	Se	0	0	0
			6057	3916	976	1138	11	16			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLY	-	expression tag	UNP P46951
A	7	PRO	-	expression tag	UNP P46951
A	8	LEU	-	expression tag	UNP P46951
A	9	GLY	-	expression tag	UNP P46951
A	10	SER	-	expression tag	UNP P46951
A	?	-	LEU	deletion	UNP P46951
A	?	-	ASP	deletion	UNP P46951
A	?	-	LYS	deletion	UNP P46951
A	?	-	LYS	deletion	UNP P46951
A	?	-	PRO	deletion	UNP P46951
A	?	-	GLY	deletion	UNP P46951
A	?	-	LYS	deletion	UNP P46951
A	?	-	ARG	deletion	UNP P46951

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP P46951
A	?	-	LYS	deletion	UNP P46951
B	6	GLY	-	expression tag	UNP P46951
B	7	PRO	-	expression tag	UNP P46951
B	8	LEU	-	expression tag	UNP P46951
B	9	GLY	-	expression tag	UNP P46951
B	10	SER	-	expression tag	UNP P46951
B	?	-	LEU	deletion	UNP P46951
B	?	-	ASP	deletion	UNP P46951
B	?	-	LYS	deletion	UNP P46951
B	?	-	LYS	deletion	UNP P46951
B	?	-	PRO	deletion	UNP P46951
B	?	-	GLY	deletion	UNP P46951
B	?	-	LYS	deletion	UNP P46951
B	?	-	ARG	deletion	UNP P46951
B	?	-	ALA	deletion	UNP P46951
B	?	-	LYS	deletion	UNP P46951
C	6	GLY	-	expression tag	UNP P46951
C	7	PRO	-	expression tag	UNP P46951
C	8	LEU	-	expression tag	UNP P46951
C	9	GLY	-	expression tag	UNP P46951
C	10	SER	-	expression tag	UNP P46951
C	?	-	LEU	deletion	UNP P46951
C	?	-	ASP	deletion	UNP P46951
C	?	-	LYS	deletion	UNP P46951
C	?	-	LYS	deletion	UNP P46951
C	?	-	PRO	deletion	UNP P46951
C	?	-	GLY	deletion	UNP P46951
C	?	-	LYS	deletion	UNP P46951
C	?	-	ARG	deletion	UNP P46951
C	?	-	ALA	deletion	UNP P46951
C	?	-	LYS	deletion	UNP P46951
D	6	GLY	-	expression tag	UNP P46951
D	7	PRO	-	expression tag	UNP P46951
D	8	LEU	-	expression tag	UNP P46951
D	9	GLY	-	expression tag	UNP P46951
D	10	SER	-	expression tag	UNP P46951
D	?	-	LEU	deletion	UNP P46951
D	?	-	ASP	deletion	UNP P46951
D	?	-	LYS	deletion	UNP P46951
D	?	-	LYS	deletion	UNP P46951
D	?	-	PRO	deletion	UNP P46951

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLY	deletion	UNP P46951
D	?	-	LYS	deletion	UNP P46951
D	?	-	ARG	deletion	UNP P46951
D	?	-	ALA	deletion	UNP P46951
D	?	-	LYS	deletion	UNP P46951
E	6	GLY	-	expression tag	UNP P46951
E	7	PRO	-	expression tag	UNP P46951
E	8	LEU	-	expression tag	UNP P46951
E	9	GLY	-	expression tag	UNP P46951
E	10	SER	-	expression tag	UNP P46951
E	?	-	LEU	deletion	UNP P46951
E	?	-	ASP	deletion	UNP P46951
E	?	-	LYS	deletion	UNP P46951
E	?	-	LYS	deletion	UNP P46951
E	?	-	PRO	deletion	UNP P46951
E	?	-	GLY	deletion	UNP P46951
E	?	-	LYS	deletion	UNP P46951
E	?	-	ARG	deletion	UNP P46951
E	?	-	ALA	deletion	UNP P46951
E	?	-	LYS	deletion	UNP P46951
F	6	GLY	-	expression tag	UNP P46951
F	7	PRO	-	expression tag	UNP P46951
F	8	LEU	-	expression tag	UNP P46951
F	9	GLY	-	expression tag	UNP P46951
F	10	SER	-	expression tag	UNP P46951
F	?	-	LEU	deletion	UNP P46951
F	?	-	ASP	deletion	UNP P46951
F	?	-	LYS	deletion	UNP P46951
F	?	-	LYS	deletion	UNP P46951
F	?	-	PRO	deletion	UNP P46951
F	?	-	GLY	deletion	UNP P46951
F	?	-	LYS	deletion	UNP P46951
F	?	-	ARG	deletion	UNP P46951
F	?	-	ALA	deletion	UNP P46951
F	?	-	LYS	deletion	UNP P46951
G	6	GLY	-	expression tag	UNP P46951
G	7	PRO	-	expression tag	UNP P46951
G	8	LEU	-	expression tag	UNP P46951
G	9	GLY	-	expression tag	UNP P46951
G	10	SER	-	expression tag	UNP P46951
G	?	-	LEU	deletion	UNP P46951
G	?	-	ASP	deletion	UNP P46951

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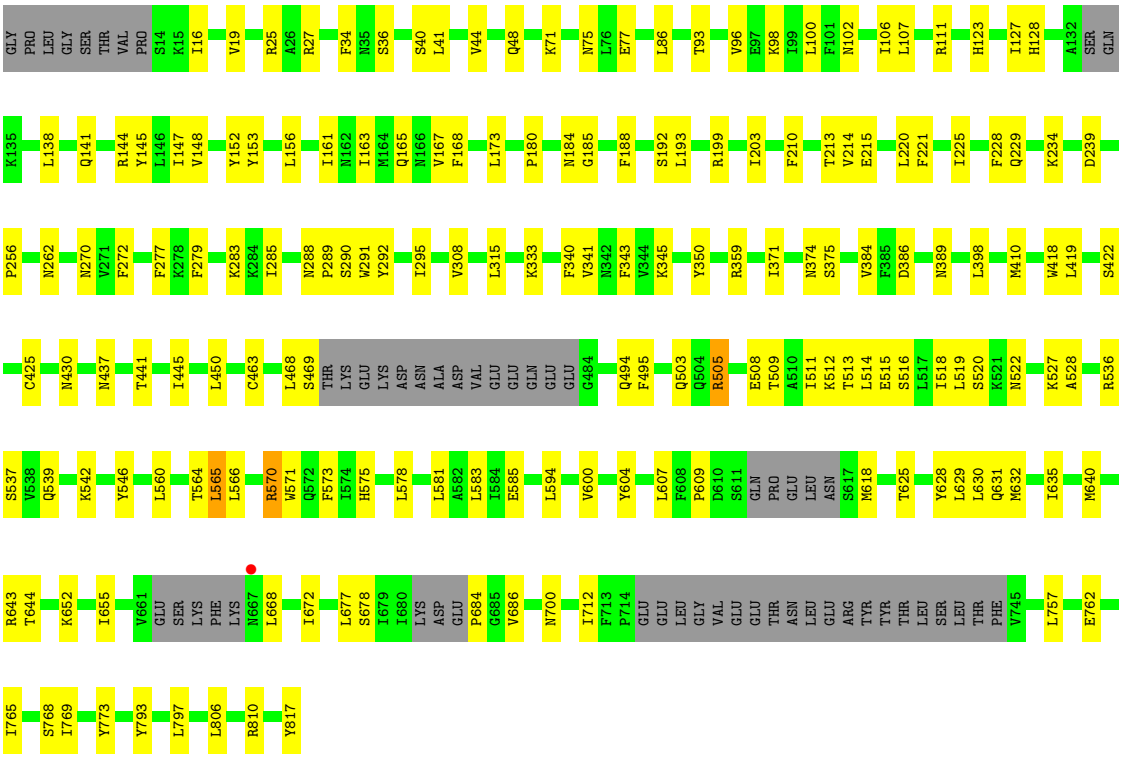
Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	LYS	deletion	UNP P46951
G	?	-	LYS	deletion	UNP P46951
G	?	-	PRO	deletion	UNP P46951
G	?	-	GLY	deletion	UNP P46951
G	?	-	LYS	deletion	UNP P46951
G	?	-	ARG	deletion	UNP P46951
G	?	-	ALA	deletion	UNP P46951
G	?	-	LYS	deletion	UNP P46951
H	6	GLY	-	expression tag	UNP P46951
H	7	PRO	-	expression tag	UNP P46951
H	8	LEU	-	expression tag	UNP P46951
H	9	GLY	-	expression tag	UNP P46951
H	10	SER	-	expression tag	UNP P46951
H	?	-	LEU	deletion	UNP P46951
H	?	-	ASP	deletion	UNP P46951
H	?	-	LYS	deletion	UNP P46951
H	?	-	LYS	deletion	UNP P46951
H	?	-	PRO	deletion	UNP P46951
H	?	-	GLY	deletion	UNP P46951
H	?	-	LYS	deletion	UNP P46951
H	?	-	ARG	deletion	UNP P46951
H	?	-	ALA	deletion	UNP P46951
H	?	-	LYS	deletion	UNP P46951

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 (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.

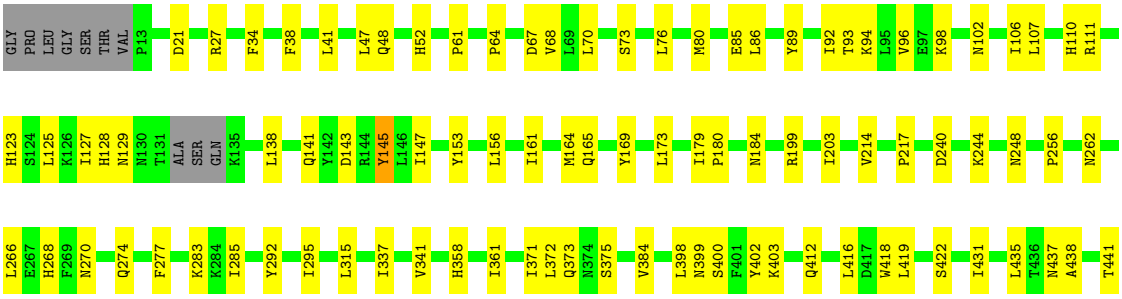
• Molecule 1: Cargo-transport protein YPP1

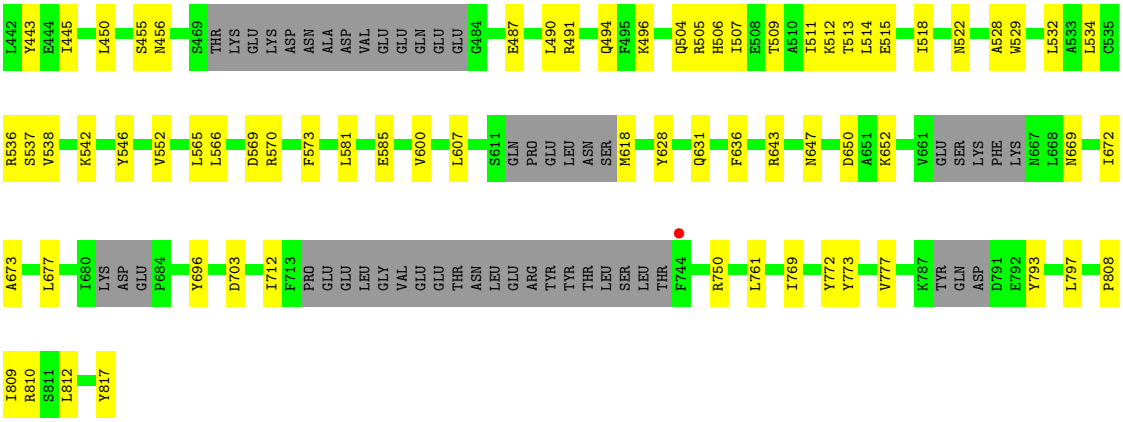
Chain A:



• Molecule 1: Cargo-transport protein YPP1

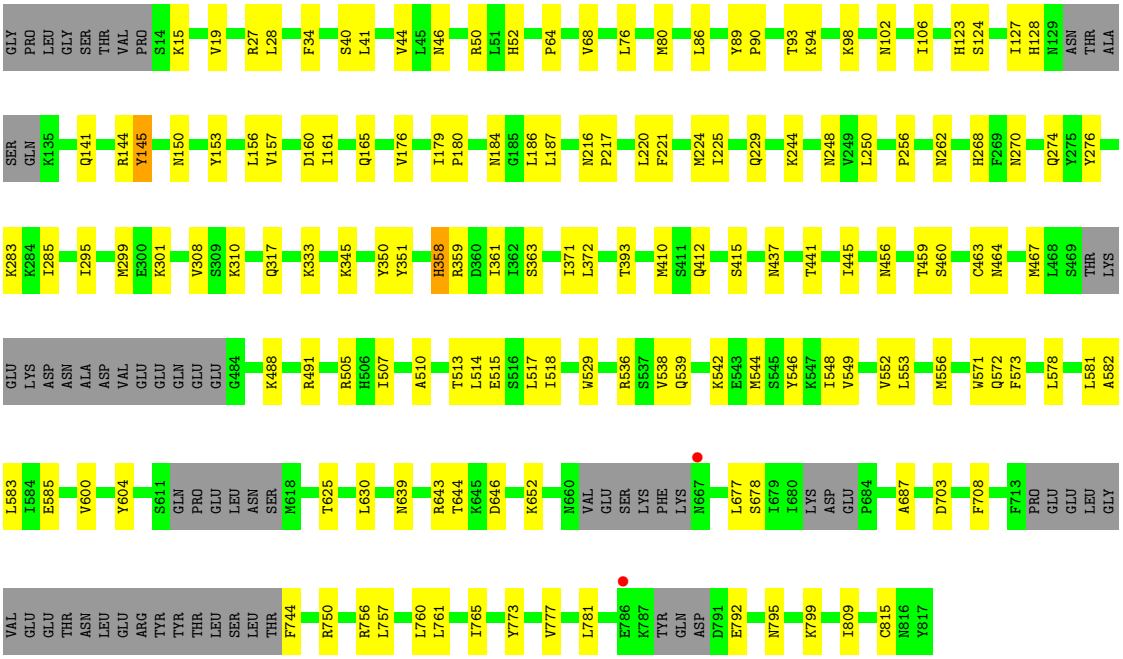
Chain B:





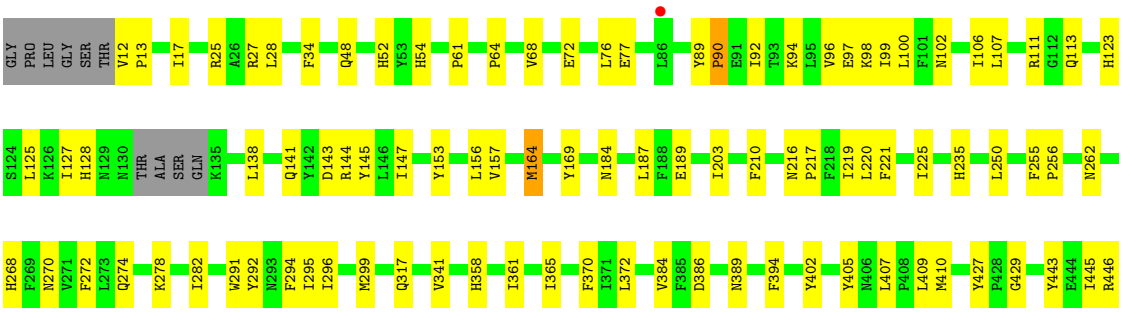
• Molecule 1: Cargo-transport protein YPP1

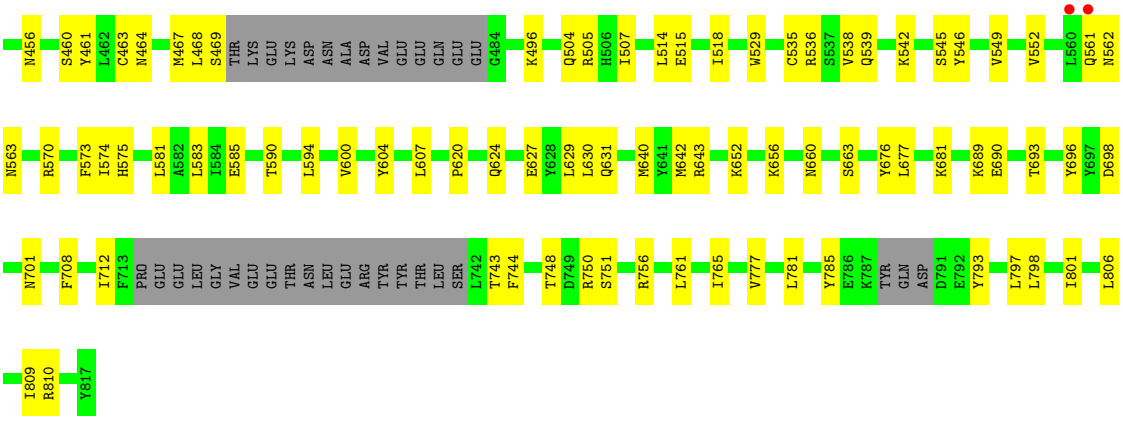
Chain C:



• Molecule 1: Cargo-transport protein YPP1

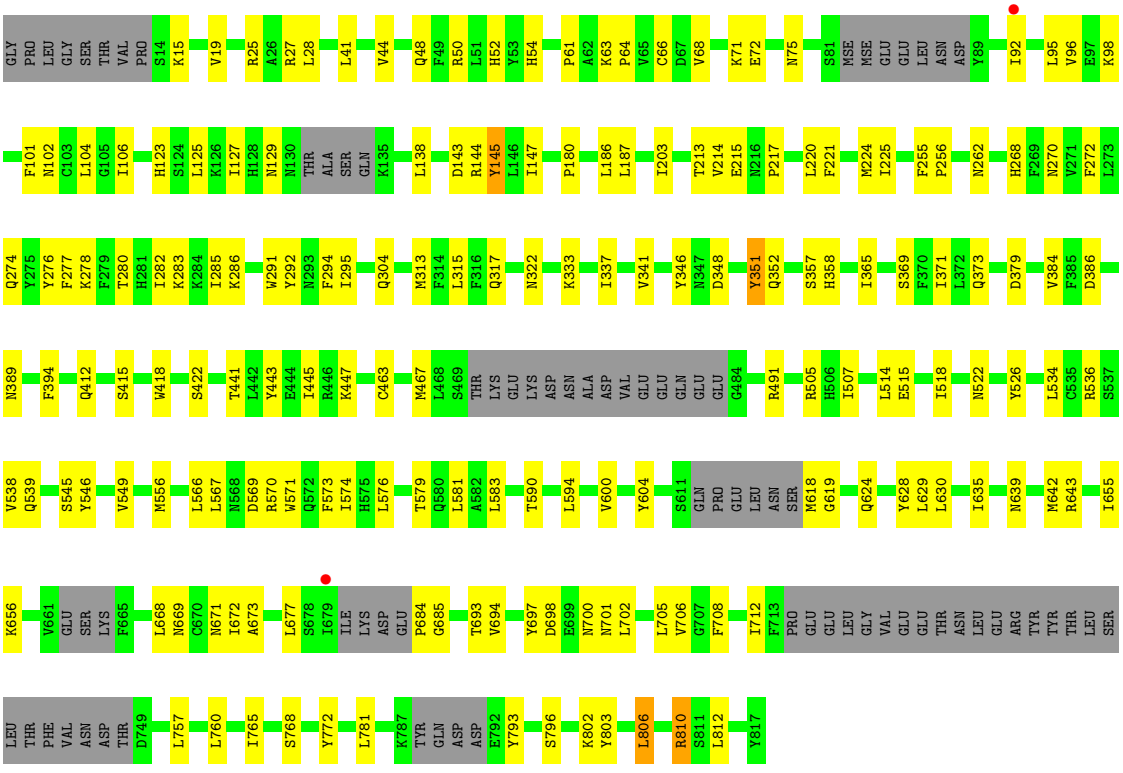
Chain D:





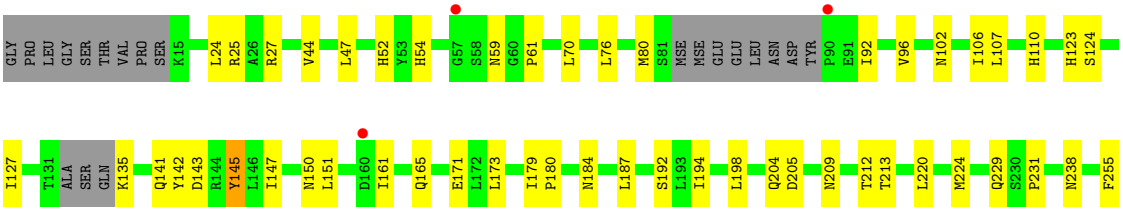
• Molecule 1: Cargo-transport protein YPP1

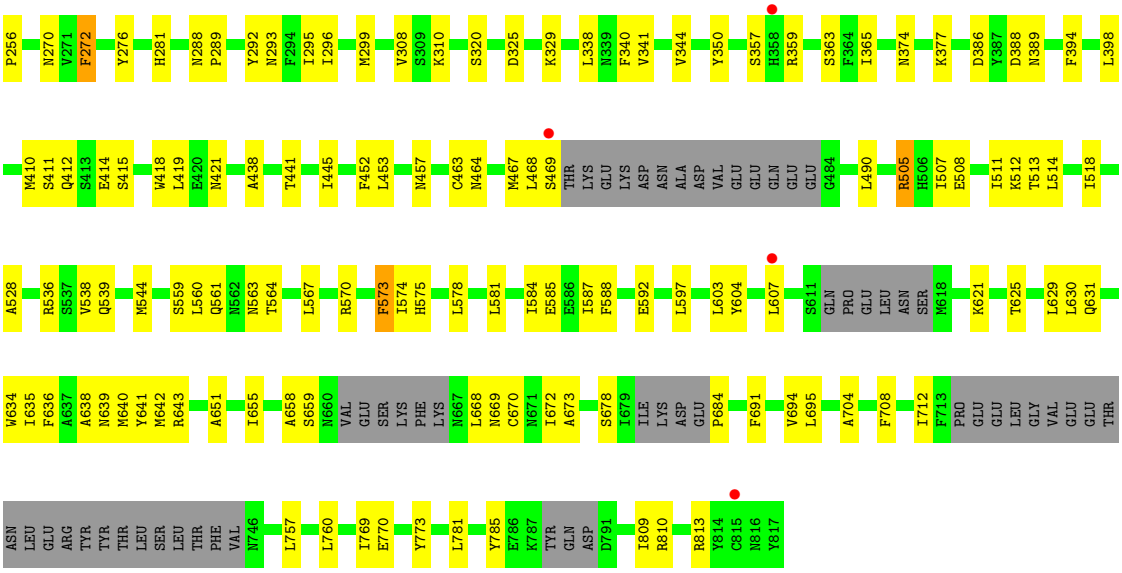
Chain E:



• Molecule 1: Cargo-transport protein YPP1

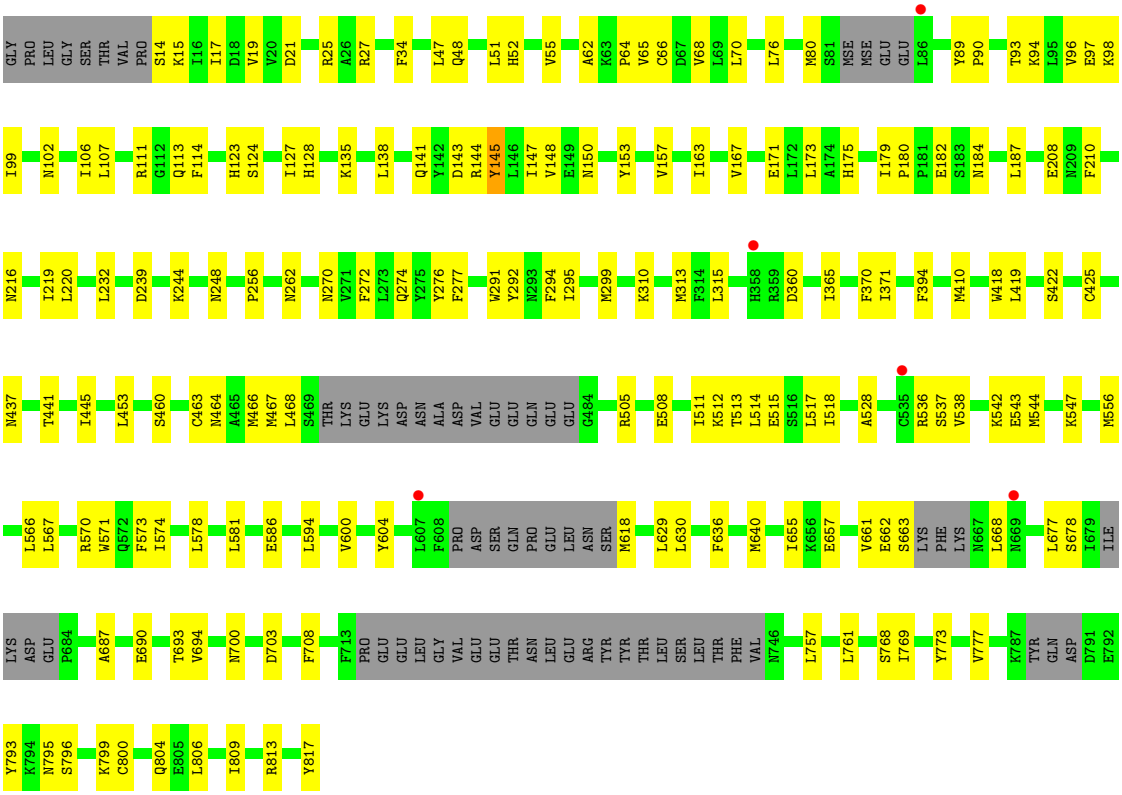
Chain F:





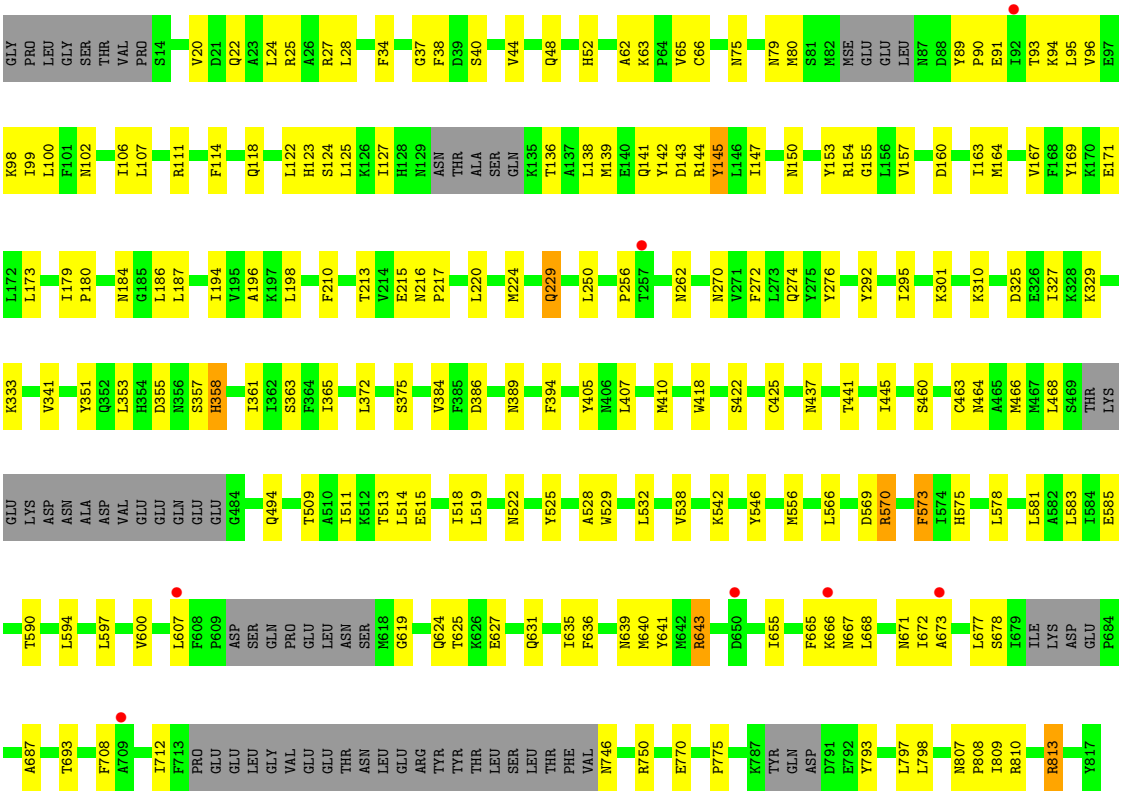
• Molecule 1: Cargo-transport protein YPP1

Chain G:



• Molecule 1: Cargo-transport protein YPP1

Chain H:


GLY PRO LEU GLY SER THR VAL PRO S14 V20 D21 Q22 A23 L24 R25 A26 R27 L28 F34 G37 F38 D39 S40 V44 Q48 H52 A62 K63 P64 V65 C66 N75 N79 M80 S81 M82 MSE GLU GLU LEU N87 D88 Y89 P90 E91 I92 T93 K94 L95 V96 E97
K98 I99 L100 F101 N102 I106 L107 R111 F114 Q118 L122 H123 S124 L125 K126 I127 H128 N129 ASN THR ALA SER GLN K135 T136 A137 L138 M139 E140 Q141 Y142 D143 R144 Y145 L146 I147 N150 Y153 R154 G155 L156 V157 D160 I163 M164 V167 F168 Y169 K170 E171
L172 L173 I179 P180 N184 G185 L186 L187 I194 V195 A196 K197 L198 F210 T213 V214 E215 N216 P217 L220 M224 Q229 L250 P256 T257 N262 N270 V271 F272 L273 Q274 Y275 Y276 Y292 I295 K301 K310 D325 E326 I327 K328 K329
K333 V341 Y351 Q352 L353 H354 D355 N356 S357 H358 I361 I362 S363 F364 I365 L372 S375 V384 F385 D386 N389 F394 Y405 N406 L407 M410 W418 S422 C425 N437 T441 I445 S460 C463 N464 A465 M466 M467 L468 S469 THR LYS
GLU LYS ASP ASN ALA ASP VAL GLU GLU GLN GLU GLU G484 Q494 T509 A510 I511 K512 T513 L514 E515 I518 L519 N522 Y525 A528 W529 L532 V538 K542 Y546 M556 L566 D569 R570 F573 I574 H575 L578 L581 A582 L583 I584 E585
T590 L594 L597 V600 L607 F608 P609 ASP SER GLN PRO GLU LEU ASN SER M618 G619 Q624 T625 K626 E627 Q631 I635 F636 N639 M640 Y641 M642 R643 D650 I655 F665 K666 N667 L668 N671 I672 A673 L677 S678 I679 ILE LYS ASP GLU P684
A687 T693 F708 A709 I712 F713 PRO GLU GLU LEU GLY VAL GLU GLU THR ASN LEU GLU ARG TYR TYR THR LEU SER LEU THR PHE VAL N746 R750 E770 P775 K787 TYR GLN ASP D791 E792 Y793 L797 L798 N807 P808 I809 R810 R813 Y817

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	97.55Å 136.65Å 154.12Å 76.69° 85.67° 72.74°	Depositor
Resolution (Å)	25.00 – 3.25 25.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	98.7 (25.00-3.25) 91.9 (25.00-3.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 3.23Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.240 , 0.277 0.239 , 0.275	Depositor DCC
R_{free} test set	1973 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å^2)	71.2	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 29.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	48674	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.5695e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.28	0/6252	0.49	1/8423 (0.0%)
1	B	0.28	0/6223	0.49	0/8382
1	C	0.28	0/6193	0.49	1/8340 (0.0%)
1	D	0.29	0/6359	0.51	1/8569 (0.0%)
1	E	0.27	0/6114	0.48	0/8234
1	F	0.27	0/6105	0.49	0/8223
1	G	0.29	0/6169	0.49	0/8312
1	H	0.29	0/6171	0.52	1/8310 (0.0%)
All	All	0.28	0/49586	0.49	4/66793 (0.0%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	663	SER	N-CA-C	-5.50	96.14	111.00
1	C	756	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	565	LEU	CA-CB-CG	5.31	127.51	115.30
1	H	353	LEU	CA-CB-CG	5.23	127.33	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	LYS	Peptide

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	6138	0	6060	112	0
1	B	6109	0	6038	101	1
1	C	6080	0	6008	99	0
1	D	6241	0	6171	115	0
1	E	6000	0	5943	104	1
1	F	5993	0	5927	114	0
1	G	6056	0	5984	115	0
1	H	6057	0	5993	124	0
All	All	48674	0	48124	873	1

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 9.

The worst 5 of 873 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:581:LEU:HD11	1:A:600:VAL:HG21	1.63	0.79
1:C:514:LEU:HD12	1:C:518:ILE:HD11	1.64	0.79
1:D:189:GLU:OE2	1:D:429:GLY:N	2.15	0.78
1:D:402:TYR:HB3	1:D:409:LEU:HD11	1.66	0.77
1:C:581:LEU:HD11	1:C:600:VAL:HG21	1.66	0.75

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	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:TYR:OH	1:E:671:ASN:OD1[1_655]	2.17	0.03

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	731/802 (91%)	714 (98%)	17 (2%)	0	100 100
1	B	725/802 (90%)	704 (97%)	21 (3%)	0	100 100
1	C	721/802 (90%)	701 (97%)	20 (3%)	0	100 100
1	D	747/802 (93%)	727 (97%)	19 (2%)	1 (0%)	48 77
1	E	709/802 (88%)	691 (98%)	18 (2%)	0	100 100
1	F	709/802 (88%)	688 (97%)	20 (3%)	1 (0%)	48 77
1	G	719/802 (90%)	699 (97%)	19 (3%)	1 (0%)	48 77
1	H	718/802 (90%)	700 (98%)	18 (2%)	0	100 100
All	All	5779/6416 (90%)	5624 (97%)	152 (3%)	3 (0%)	48 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	662	GLU
1	D	90	PRO
1	F	231	PRO

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	688/724 (95%)	683 (99%)	5 (1%)	81 87
1	B	685/724 (95%)	682 (100%)	3 (0%)	89 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	681/724 (94%)	677 (99%)	4 (1%)	84 89
1	D	701/724 (97%)	695 (99%)	6 (1%)	75 84
1	E	671/724 (93%)	664 (99%)	7 (1%)	73 82
1	F	671/724 (93%)	667 (99%)	4 (1%)	84 89
1	G	678/724 (94%)	672 (99%)	6 (1%)	75 84
1	H	678/724 (94%)	670 (99%)	8 (1%)	67 79
All	All	5453/5792 (94%)	5410 (99%)	43 (1%)	79 86

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	573	PHE
1	H	145	TYR
1	G	89	TYR
1	G	556	MSE
1	H	351	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	238	ASN
1	G	412	GLN
1	H	358	HIS
1	H	150	ASN
1	H	229	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} 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	728/802 (90%)	-0.30	1 (0%)	92	91	26, 69, 112, 156	0
1	B	724/802 (90%)	-0.25	1 (0%)	92	91	35, 67, 107, 142	0
1	C	720/802 (89%)	-0.28	2 (0%)	90	85	30, 68, 106, 140	0
1	D	740/802 (92%)	-0.32	3 (0%)	89	82	27, 61, 102, 144	0
1	E	712/802 (88%)	-0.27	2 (0%)	90	85	30, 62, 101, 131	0
1	F	712/802 (88%)	-0.23	7 (0%)	79	68	25, 69, 117, 155	0
1	G	720/802 (89%)	-0.22	5 (0%)	84	75	27, 75, 116, 144	0
1	H	718/802 (89%)	-0.12	7 (0%)	79	68	34, 77, 126, 152	0
All	All	5774/6416 (89%)	-0.25	28 (0%)	87	80	25, 68, 112, 156	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	669	ASN	4.7
1	H	666	LYS	3.1
1	E	92	ILE	3.0
1	C	667	ASN	2.9
1	H	650	ASP	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.