Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 10:34 AM EST

PDB ID	:	6DXV
Title	:	Citrobacter freundii tyrosine phenol-lyase F448A mutant
Authors	:	Phillips, R.S.
Deposited on	:	2018-07-01
Resolution	:	2.20 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

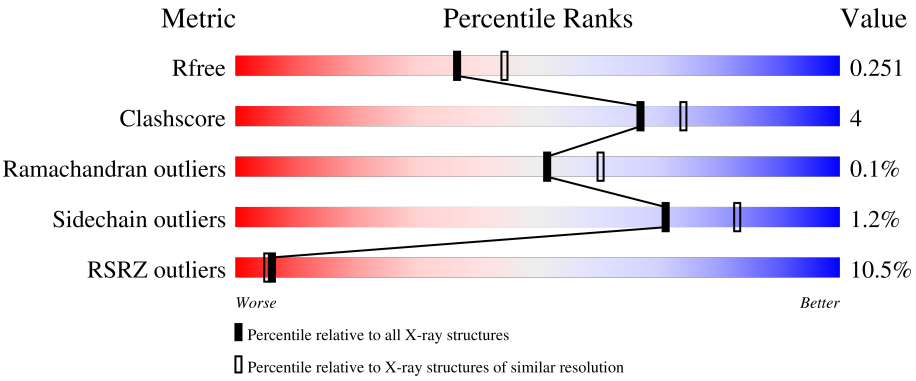
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	455	14% 86% 12% ·
1	B	455	7% 93% 7% ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7652 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 phenol-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	P	S	0	1	0
			3569	2259	616	668	1	25			
1	B	455	Total	C	N	O	P	S	0	0	0
			3613	2283	625	679	1	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	ALA	GLU	conflict	UNP P31013
A	448	ALA	PHE	engineered mutation	UNP P31013
B	205	ALA	GLU	conflict	UNP P31013
B	448	ALA	PHE	engineered mutation	UNP P31013

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		

- Molecule 3 is water.

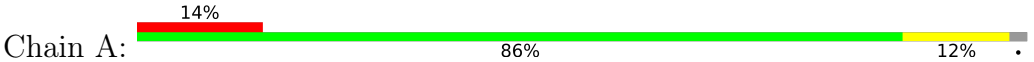
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	225	Total	O	0	0
			225	225		
3	B	243	Total	O	0	0
			243	243		

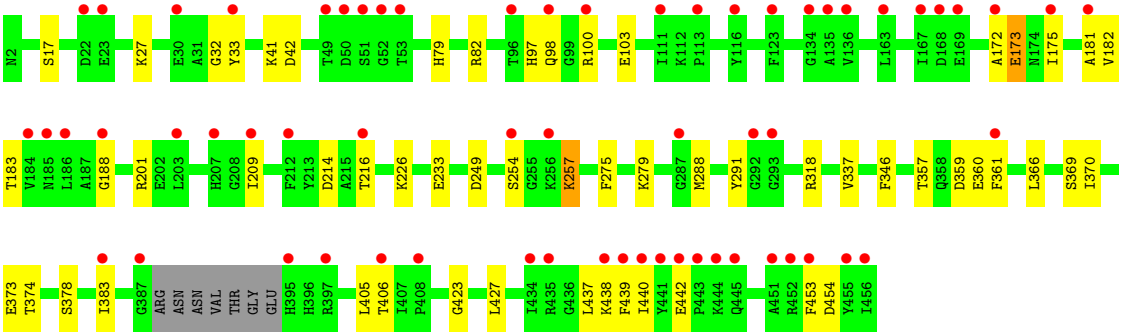
3 Residue-property plots (i)

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: Tyrosine phenol-lyase

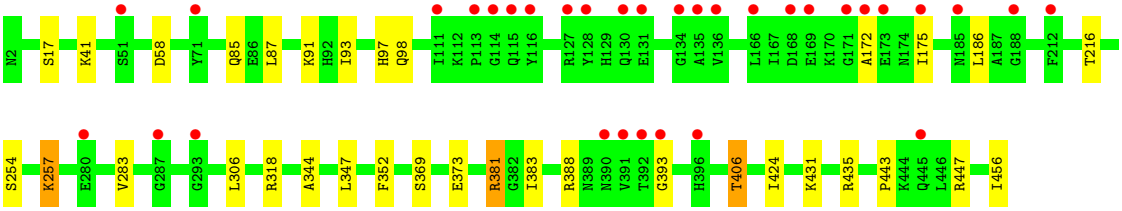
Chain A:





• Molecule 1: Tyrosine phenol-lyase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.35Å 132.18Å 145.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.48 – 2.20 37.48 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.3 (37.48-2.20) 96.3 (37.48-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.208 , 0.250 0.208 , 0.251	Depositor DCC
R_{free} test set	1950 reflections (3.45%)	wwPDB-VP
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 86.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7652	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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

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	0.31	0/3615	0.48	0/4867
1	B	0.30	0/3659	0.48	0/4928
All	All	0.31	0/7274	0.48	0/9795

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	3569	0	3505	37	0
1	B	3613	0	3549	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	225	0	0	2	0
3	B	243	0	0	0	0
All	All	7652	0	7054	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 4.

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:A:437:LEU:HB3	1:A:453:PHE:HB3	1.71	0.72
1:A:373:GLU:HG3	1:A:427:LEU:HD13	1.77	0.65
1:A:100:ARG:NH1	1:B:283:VAL:O	2.32	0.63
1:B:435:ARG:NH2	1:B:456:ILE:O	2.32	0.61
1:A:361:PHE:HD1	1:A:383:ILE:HD11	1.69	0.58
1:A:17:SER:OG	1:A:41:LYS:O	2.17	0.57
1:A:357:THR:HG22	1:A:360:GLU:HG3	1.88	0.56
1:B:17:SER:OG	1:B:41:LYS:O	2.22	0.55
1:A:172:ALA:HB1	1:A:209:ILE:HD11	1.88	0.55
1:B:443:PRO:HG2	1:B:447:ARG:HA	1.88	0.55
1:B:97:HIS:CD2	1:B:98:GLN:HG2	2.43	0.54
1:A:374:THR:HG21	1:A:423:GLY:HA3	1.91	0.52
1:B:216:THR:HG22	1:B:254:SER:H	1.77	0.51
1:B:383:ILE:O	1:B:447:ARG:NH2	2.44	0.50
1:A:97:HIS:CD2	1:A:98:GLN:HG2	2.46	0.50
1:B:85:GLN:NE2	1:B:91:LYS:O	2.41	0.49
1:A:172:ALA:HA	1:A:175:ILE:HD12	1.94	0.49
1:A:103:GLU:OE2	1:A:257:LLP:H6	2.13	0.48
1:B:98:GLN:HB2	1:B:257:LLP:OP1	2.14	0.48
1:B:369:SER:O	1:B:373:GLU:HG2	2.14	0.47
1:B:347:LEU:HD11	1:B:424:ILE:HD13	1.95	0.47
1:B:344:ALA:HB2	1:B:406:THR:HG23	1.96	0.47
1:B:381:ARG:HA	1:B:381:ARG:HD2	1.59	0.46
1:B:58:ASP:OD1	1:B:58:ASP:N	2.49	0.45
1:A:173:GLU:H	1:A:173:GLU:CD	2.20	0.45
1:A:33:TYR:HB2	1:A:453:PHE:HB2	1.99	0.44
1:A:378:SER:HB3	1:A:405:LEU:HD23	2.00	0.43
1:B:388:ARG:HD3	1:B:393:GLY:O	2.19	0.43
1:A:27:LYS:HD2	1:A:42:ASP:OD2	2.18	0.43
1:A:438:LYS:O	1:A:453:PHE:HA	2.18	0.43
1:A:374:THR:CG2	1:A:423:GLY:HA3	2.48	0.43
1:A:79[B]:HIS:HD2	1:A:82:ARG:HH11	1.66	0.43
1:A:82:ARG:HG3	3:A:622:HOH:O	2.19	0.43
1:A:98:GLN:HB2	1:A:257:LLP:OP1	2.18	0.43
1:A:216:THR:HG22	1:A:254:SER:H	1.84	0.43
1:A:216:THR:HB	1:A:257:LLP:HG2	2.01	0.43
1:A:438:LYS:HD2	1:A:454:ASP:HB3	2.00	0.42
1:B:352:PHE:O	1:B:431:LYS:HD2	2.19	0.42
1:A:357:THR:HG23	1:A:359:ASP:H	1.84	0.42
1:A:366:LEU:O	1:A:370:ILE:HG12	2.18	0.42
1:A:182:VAL:HA	1:A:183:THR:HA	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:SER:O	1:A:373:GLU:HG2	2.19	0.42
1:A:188:GLY:HA2	1:A:346:PHE:CE1	2.55	0.42
1:B:87:LEU:HD12	1:B:306:LEU:HG	2.01	0.42
1:A:32:GLY:O	1:A:453:PHE:N	2.52	0.42
1:B:172:ALA:HA	1:B:175:ILE:HD12	2.02	0.42
1:B:186:LEU:HD23	1:B:186:LEU:HA	1.86	0.41
1:A:181:ALA:HA	1:A:214:ASP:HB3	2.03	0.41
1:A:201:ARG:NH2	1:A:249:ASP:OD1	2.35	0.41
1:A:357:THR:HG23	1:A:359:ASP:N	2.36	0.41
1:A:439:PHE:CZ	1:A:442:GLU:HB2	2.56	0.41
1:A:275:PHE:CZ	1:A:279:LYS:HD3	2.56	0.40
1:A:33:TYR:CE2	1:A:454:ASP:HA	2.56	0.40
1:A:288:MET:HB2	1:A:291:TYR:CE2	2.56	0.40
1:A:226:LYS:NZ	3:A:613:HOH:O	2.54	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	444/455 (98%)	435 (98%)	8 (2%)	1 (0%)	47 55
1	B	452/455 (99%)	444 (98%)	8 (2%)	0	100 100
All	All	896/910 (98%)	879 (98%)	16 (2%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	440	ILE

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	370/375 (99%)	365 (99%)	5 (1%)	67 80
1	B	375/375 (100%)	371 (99%)	4 (1%)	73 85
All	All	745/750 (99%)	736 (99%)	9 (1%)	71 83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	GLU
1	A	233	GLU
1	A	318	ARG
1	A	337	VAL
1	A	406	THR
1	B	93	ILE
1	B	318	ARG
1	B	381	ARG
1	B	406	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	LLP	A	257	1	23,24,25	1.88	6 (26%)	25,32,34	1.09	3 (12%)
1	LLP	B	257	1	23,24,25	2.01	6 (26%)	25,32,34	1.28	4 (16%)

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
1	LLP	A	257	1	-	5/16/17/19	0/1/1/1
1	LLP	B	257	1	-	6/16/17/19	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	257	LLP	C4-C4'	4.49	1.55	1.46
1	A	257	LLP	C4-C4'	4.29	1.54	1.46
1	B	257	LLP	C4-C5	-3.72	1.37	1.42
1	B	257	LLP	P-OP2	3.46	1.68	1.54
1	A	257	LLP	C4-C5	-3.17	1.38	1.42
1	A	257	LLP	C4-C3	-2.87	1.36	1.40
1	B	257	LLP	C4-C3	-2.81	1.36	1.40
1	A	257	LLP	P-OP3	2.74	1.65	1.54
1	A	257	LLP	P-OP2	2.72	1.65	1.54
1	B	257	LLP	C2'-C2	2.72	1.55	1.50
1	B	257	LLP	P-OP3	2.69	1.65	1.54
1	A	257	LLP	C2'-C2	2.42	1.54	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	257	LLP	CD-CE-NZ	-2.54	104.71	110.93
1	A	257	LLP	C4-C4'-NZ	-2.37	113.43	124.31
1	B	257	LLP	C3-C4-C5	2.30	120.02	118.26
1	B	257	LLP	C5-C6-N1	-2.29	120.00	123.82
1	A	257	LLP	C5-C6-N1	-2.11	120.30	123.82
1	A	257	LLP	C3-C4-C5	2.08	119.86	118.26
1	B	257	LLP	C4-C4'-NZ	-2.05	114.89	124.31

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	257	LLP	C5-C4-C4'-NZ
1	A	257	LLP	O-C-CA-CB
1	B	257	LLP	C5-C4-C4'-NZ
1	B	257	LLP	O-C-CA-CB
1	B	257	LLP	CG-CD-CE-NZ
1	A	257	LLP	C3-C4-C4'-NZ
1	B	257	LLP	C3-C4-C4'-NZ
1	A	257	LLP	CD-CE-NZ-C4'
1	B	257	LLP	CD-CE-NZ-C4'
1	B	257	LLP	C-CA-CB-CG
1	A	257	LLP	C4-C5-C5'-OP4

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	257	LLP	3	0
1	B	257	LLP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

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	447/455 (98%)	0.57	62 (13%) 2 2	47, 87, 146, 198	0
1	B	454/455 (99%)	0.21	33 (7%) 15 14	49, 85, 135, 189	0
All	All	901/910 (99%)	0.39	95 (10%) 6 5	47, 85, 141, 198	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	455	TYR	12.2
1	B	391	VAL	8.1
1	B	390	ASN	6.3
1	A	456	ILE	5.1
1	A	387	GLY	4.8
1	A	33	TYR	4.4
1	B	166	LEU	4.4
1	A	163	LEU	4.2
1	A	395	HIS	4.2
1	A	51	SER	4.1
1	B	116	TYR	4.1
1	A	439	PHE	4.1
1	A	167	ILE	3.9
1	A	444	LYS	3.7
1	B	71	TYR	3.7
1	B	172	ALA	3.7
1	A	435	ARG	3.6
1	B	130	GLN	3.6
1	A	361	PHE	3.6
1	A	116	TYR	3.6
1	B	114	GLY	3.6
1	A	53	THR	3.6
1	A	254	SER	3.6
1	A	168	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	123	PHE	3.6
1	A	256	LYS	3.5
1	A	445	GLN	3.5
1	B	135	ALA	3.4
1	A	293	GLY	3.4
1	B	113	PRO	3.3
1	A	453	PHE	3.3
1	A	185	ASN	3.3
1	A	135	ALA	3.2
1	B	445	GLN	3.2
1	A	207	HIS	3.2
1	B	128	TYR	3.2
1	A	452	ARG	3.1
1	B	173	GLU	3.1
1	A	52	GLY	3.0
1	A	113	PRO	3.0
1	A	169	GLU	3.0
1	A	434	ILE	2.9
1	A	440	ILE	2.9
1	A	397	ARG	2.9
1	A	186	LEU	2.9
1	B	131	GLU	2.8
1	A	100	ARG	2.8
1	A	442	GLU	2.8
1	A	216	THR	2.8
1	A	96	THR	2.7
1	A	181	ALA	2.7
1	B	134	GLY	2.7
1	A	441	TYR	2.7
1	A	134	GLY	2.7
1	A	287	GLY	2.7
1	B	111	ILE	2.6
1	B	136	VAL	2.6
1	B	168	ASP	2.6
1	A	451	ALA	2.6
1	B	115	GLN	2.6
1	B	127	ARG	2.6
1	A	438	LYS	2.6
1	B	293	GLY	2.6
1	A	136	VAL	2.6
1	A	49	THR	2.5
1	A	212	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	393	GLY	2.5
1	A	184	VAL	2.5
1	B	287	GLY	2.5
1	A	22	ASP	2.5
1	A	23	GLU	2.4
1	A	172	ALA	2.4
1	B	169	GLU	2.4
1	A	443	PRO	2.4
1	A	383	ILE	2.4
1	A	203	LEU	2.4
1	B	171	GLY	2.3
1	B	175	ILE	2.3
1	A	408	PRO	2.3
1	A	98	GLN	2.3
1	A	209	ILE	2.3
1	A	30	GLU	2.2
1	A	175	ILE	2.2
1	B	188	GLY	2.2
1	B	212	PHE	2.2
1	B	392	THR	2.1
1	B	51	SER	2.1
1	B	185	ASN	2.1
1	A	292	GLY	2.1
1	A	188	GLY	2.1
1	B	396	HIS	2.0
1	A	111	ILE	2.0
1	B	280	GLU	2.0
1	A	50	ASP	2.0
1	A	406	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
1	LLP	B	257	24/25	0.93	0.19	56,97,115,117	0
1	LLP	A	257	24/25	0.95	0.34	52,83,96,108	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	K	B	501	1/1	0.91	0.06	69,69,69,69	0
2	K	A	501	1/1	0.93	0.07	70,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.