WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:47 AM GMT

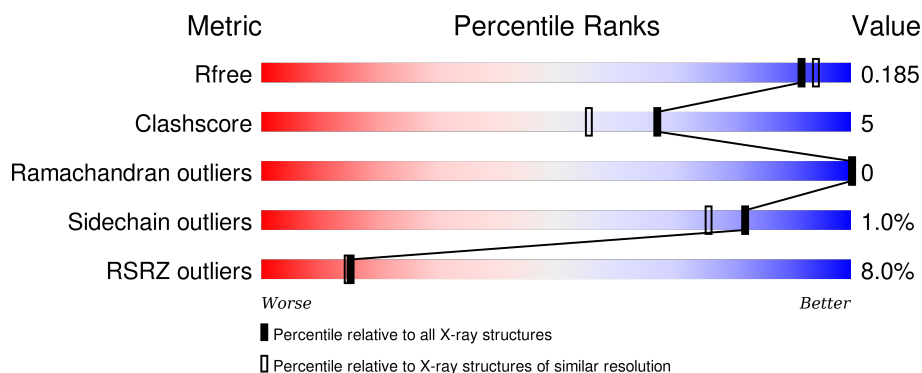|		
PDB ID	:	3PVJ
Title	:	Crystal structure of the Fe(II)/alpha-ketoglutarate dependent taurine dioxygenase from Pseudomonas putida KT2440
Authors	:	Knauer, S.H.; Spiegelhauer, O.; Schwarzinger, S.; Haenzelmann P.; Dobbek, H.
Deposited on	:	2010-12-07
Resolution	:	1.85 Å(reported)

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 1.85 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	Percentile Ranks	Value
Rfree		0.185
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		1.0%
RSRZ outliers		8.0%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	277	% 91% 8%
1	B	277	12% 89% 10%
1	C	277	9% 87% 12%
1	D	277	10% 89% 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 19060 atoms, of which 8831 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 Alpha-ketoglutarate-dependent taurine dioxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	275	Total 4467	C 1425	H 2225	N 404	O 410	S 3	0	10	0
1	B	276	Total 4446	C 1421	H 2207	N 406	O 410	S 2	0	8	0
1	C	276	Total 4432	C 1417	H 2202	N 403	O 408	S 2	0	6	0
1	D	276	Total 4424	C 1411	H 2197	N 407	O 407	S 2	0	5	0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Cl 2	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	388	Total 388	O 388	0	16
3	B	271	Total 271	O 271	0	3
3	C	333	Total 333	O 333	0	11
3	D	297	Total 297	O 297	0	2

3 Residue-property plots ⓘ

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.
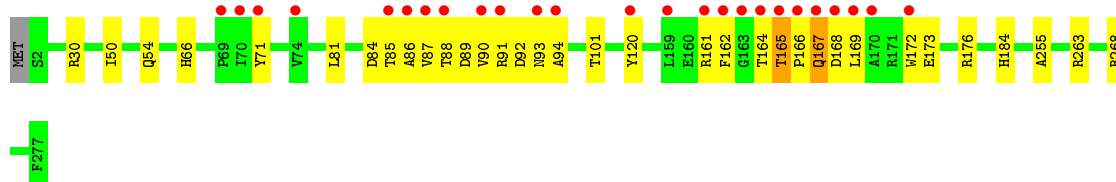
- Molecule 1: Alpha-ketoglutarate-dependent taurine dioxygenase

Chain A:

- Molecule 1: Alpha-ketoglutarate-dependent taurine dioxygenase

Chain B:
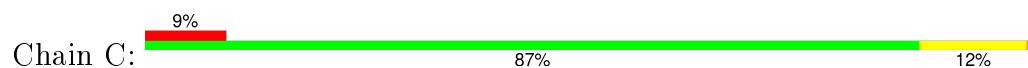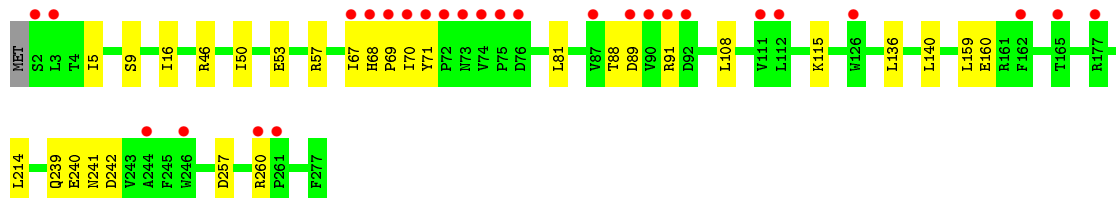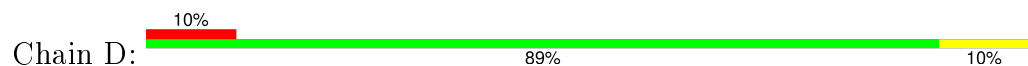
- Molecule 1: Alpha-ketoglutarate-dependent taurine dioxygenase

Chain C:

- Molecule 1: Alpha-ketoglutarate-dependent taurine dioxygenase

Chain D:
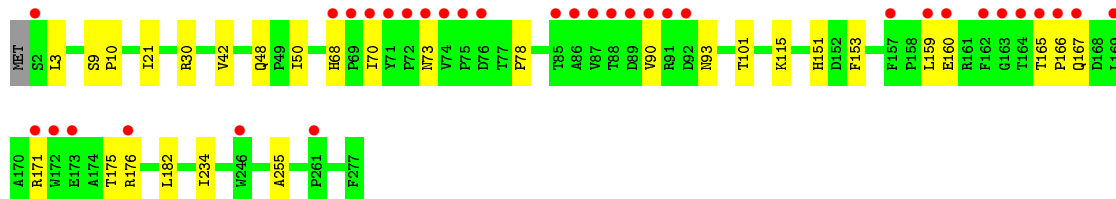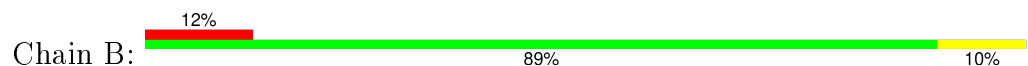
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.25Å 105.34Å 171.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.57 – 1.85 29.92 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.5 (28.57-1.85) 99.5 (29.92-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$<I/\sigma(I)>$ [1]	2.82 (at 1.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.157 , 0.191 0.149 , 0.185	Depositor DCC
R_{free} test set	5805 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Outliers	1 of 116115 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	19060	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 7.94% 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 (i)

5.1 Standard geometry (i)

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

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	0.46	0/2334	0.58	0/3189
1	B	0.40	0/2324	0.54	0/3176
1	C	0.45	0/2307	0.59	0/3153
1	D	0.40	0/2304	0.53	0/3148
All	All	0.43	0/9269	0.56	0/12666

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 (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	2242	2225	2207	15	0
1	B	2239	2207	2184	25	0
1	C	2230	2202	2188	31	0
1	D	2227	2197	2176	18	0
2	A	2	0	0	0	0
3	A	388	0	0	3	0
3	B	271	0	0	4	0
3	C	333	0	0	5	0
3	D	297	0	0	1	0
All	All	10229	8831	8755	85	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 5.

All (85) 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:C:169:LEU:O	1:C:173:GLU:HG2	1.93	0.68
1:C:164:THR:HG23	1:C:165:THR:HG22	1.75	0.68
1:B:153[A]:PHE:CE2	1:B:176:ARG:HA	2.29	0.67
1:A:93:ASN:HB3	1:A:255:ALA:HB3	1.78	0.66
1:C:94:ALA:O	3:C:631:HOH:O	2.14	0.65
1:A:159:LEU:HD23	1:B:176:ARG:NH1	2.12	0.64
1:C:93:ASN:HB3	1:C:255:ALA:HB3	1.78	0.64
1:D:69:PRO:HB2	1:D:70:ILE:HD12	1.83	0.60
1:C:71:TYR:HB2	1:C:81:LEU:HD11	1.84	0.59
1:A:42[B]:VAL:HG11	1:A:234:ILE:HD11	1.85	0.58
1:B:73:ASN:OD1	1:B:78:PRO:HA	2.03	0.58
1:B:151:HIS:HE1	3:B:520:HOH:O	1.88	0.57
1:B:90:VAL:O	1:B:90:VAL:HG23	2.03	0.57
1:D:5:ILE:HG12	1:D:16:ILE:CD1	2.35	0.56
1:C:165:THR:OG1	1:C:167:GLN:HG3	2.05	0.56
1:C:164:THR:HG23	1:C:165:THR:N	2.21	0.56
1:C:184:HIS:HD2	3:C:319:HOH:O	1.88	0.55
1:D:69:PRO:HB2	1:D:70:ILE:CD1	2.37	0.54
1:B:21:ILE:HG12	1:B:48:GLN:CG	2.38	0.53
1:A:99:ASP:OD1	1:A:253:HIS:HE1	1.91	0.53
1:A:176:ARG:NH2	1:B:159:LEU:HD22	2.23	0.53
1:D:71:TYR:HB2	1:D:81:LEU:HD11	1.91	0.53
1:B:101:THR:OG1	1:B:151:HIS:HD2	1.92	0.52
1:C:87:VAL:HG12	1:C:87:VAL:O	2.08	0.52
1:D:136:LEU:HD22	1:D:140:LEU:HD23	1.91	0.52
1:C:176:ARG:NH2	1:D:159:LEU:HD21	2.25	0.52
1:B:3:LEU:C	1:B:3:LEU:HD23	2.31	0.50
1:B:153[A]:PHE:HE2	1:B:176:ARG:HA	1.74	0.50
1:A:42[B]:VAL:HG23	1:A:246:TRP:HB3	1.93	0.50
1:C:86:ALA:HA	3:C:626:HOH:O	2.12	0.49
1:C:172:TRP:CH2	1:C:176:ARG:HD3	2.48	0.48
1:D:53:GLU:HG3	1:D:57:ARG:NH1	2.29	0.48
1:C:88:THR:CG2	1:C:89:ASP:N	2.76	0.48
1:D:67:ILE:N	1:D:67:ILE:HD12	2.29	0.48
1:C:84:ASP:HB3	1:C:87:VAL:H	1.77	0.48
1:B:165:THR:HB	1:B:166:PRO:HD2	1.96	0.48
1:D:46:ARG:HD3	1:D:242:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:THR:HB	1:C:263:ARG:HG3	1.96	0.47
1:C:92:ASP:HB3	1:C:161:ARG:HH12	1.78	0.47
1:C:162:PHE:CE1	1:C:172:TRP:HA	2.50	0.47
1:C:176:ARG:NH2	1:C:176:ARG:HB3	2.30	0.47
1:C:85:THR:CB	1:C:263:ARG:HA	2.45	0.47
1:A:46:ARG:NH2	1:A:239[B]:GLN:HG3	2.29	0.47
1:A:42[A]:VAL:HG22	1:A:246:TRP:HB2	1.96	0.47
1:C:66:HIS:HD2	3:C:536:HOH:O	1.98	0.47
1:B:160:GLU:HG3	3:B:536:HOH:O	2.15	0.46
1:B:182:LEU:C	1:B:182:LEU:HD12	2.36	0.46
1:B:68:HIS:CE1	1:B:70:ILE:HG22	2.51	0.46
1:B:153[A]:PHE:CZ	1:B:176:ARG:HA	2.50	0.46
3:B:400:HOH:O	1:D:214:LEU:HD11	2.15	0.46
1:D:68:HIS:HA	1:D:69:PRO:HD3	1.81	0.45
1:C:89:ASP:OD2	1:C:91:ARG:HG3	2.16	0.45
1:B:167:GLN:O	1:B:171:ARG:HG3	2.16	0.45
1:D:50:ILE:O	1:D:115:LYS:NZ	2.49	0.45
1:C:50[B]:ILE:HG13	1:C:54:GLN:HB2	1.98	0.45
1:C:90:VAL:O	1:C:90:VAL:HG23	2.17	0.45
1:D:108:LEU:HD23	1:D:108:LEU:C	2.36	0.45
1:B:165:THR:HB	1:B:166:PRO:CD	2.47	0.45
1:A:3:LEU:N	3:A:671:HOH:O	2.50	0.45
1:D:257:ASP:OD2	1:D:260:ARG:NH1	2.50	0.45
1:B:21:ILE:HG12	1:B:48:GLN:HG2	1.98	0.44
1:A:157:PHE:HA	1:A:161:ARG:HD3	2.00	0.44
1:A:229:ARG:NH1	3:A:472:HOH:O	2.49	0.44
1:B:93:ASN:HB3	1:B:255:ALA:HB3	2.00	0.44
1:C:30:ARG:HD3	1:C:30:ARG:C	2.38	0.43
1:A:68:HIS:CE1	1:A:71:TYR:CD2	3.06	0.43
1:C:164:THR:CG2	1:C:165:THR:N	2.82	0.43
1:B:42:VAL:HG11	1:B:234:ILE:HD11	2.01	0.42
1:D:89:ASP:OD2	1:D:91:ARG:HB2	2.18	0.42
1:B:10:PRO:HG3	1:C:120[A]:TYR:CE1	2.54	0.42
1:C:165:THR:CB	1:C:166:PRO:CD	2.97	0.42
1:C:176:ARG:HB3	1:C:176:ARG:CZ	2.49	0.42
1:C:120[A]:TYR:C	1:C:120[A]:TYR:CD1	2.94	0.42
1:B:50:ILE:O	1:B:115:LYS:NZ	2.53	0.41
1:A:260:ARG:HG2	3:A:381:HOH:O	2.20	0.41
1:A:169:LEU:O	1:A:173:GLU:HG3	2.21	0.41
1:C:176:ARG:HD2	3:C:609:HOH:O	2.21	0.41
1:D:46:ARG:NH1	1:D:239[A]:GLN:HG3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:GLU:O	1:D:241:ASN:HB2	2.21	0.41
1:A:108:LEU:HD23	1:A:108:LEU:C	2.41	0.40
1:B:160:GLU:CG	3:B:536:HOH:O	2.69	0.40
1:D:160:GLU:CG	3:D:352:HOH:O	2.69	0.40
1:C:101:THR:O	1:C:184:HIS:HE1	2.05	0.40
1:B:153[B]:PHE:CZ	1:B:175:THR:HG21	2.57	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	283/277 (102%)	277 (98%)	6 (2%)	0	100	100
1	B	282/277 (102%)	273 (97%)	9 (3%)	0	100	100
1	C	280/277 (101%)	273 (98%)	7 (2%)	0	100	100
1	D	279/277 (101%)	273 (98%)	6 (2%)	0	100	100
All	All	1124/1108 (101%)	1096 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	243/235 (103%)	241 (99%)	2 (1%)	86	82
1	B	241/235 (103%)	239 (99%)	2 (1%)	86	82
1	C	239/235 (102%)	235 (98%)	4 (2%)	68	54
1	D	239/235 (102%)	237 (99%)	2 (1%)	86	82
All	All	962/940 (102%)	952 (99%)	10 (1%)	82	76

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9[A]	SER
1	A	9[B]	SER
1	B	9	SER
1	B	30	ARG
1	C	165	THR
1	C	167	GLN
1	C	168	ASP
1	C	268	ARG
1	D	9	SER
1	D	88	THR

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	253	HIS
1	B	151	HIS
1	B	201	ASN
1	C	184	HIS
1	C	201	ASN
1	C	209	ASN
1	D	201	ASN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

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 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 (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	275/277 (99%)	-0.31	2 (0%)	89	88	11, 18, 45, 72	0
1	B	276/277 (99%)	0.22	34 (12%)	5	5	13, 26, 77, 132	0
1	C	276/277 (99%)	0.14	25 (9%)	11	11	13, 20, 88, 207	0
1	D	276/277 (99%)	0.19	27 (9%)	10	9	14, 24, 66, 160	0
All	All	1103/1108 (99%)	0.06	88 (7%)	15	14	11, 22, 70, 207	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	70	ILE	9.3
1	C	87	VAL	8.3
1	C	85	THR	7.7
1	D	71	TYR	7.1
1	B	164	THR	6.1
1	C	88	THR	6.1
1	B	70	ILE	5.9
1	D	69	PRO	5.8
1	C	170	ALA	5.8
1	B	71	TYR	5.7
1	C	86	ALA	5.7
1	C	91	ARG	5.4
1	C	165	THR	5.4
1	B	169	LEU	5.4
1	C	166	PRO	5.3
1	B	162	PHE	5.2
1	C	93	ASN	5.2
1	D	75	PRO	5.1
1	B	87	VAL	4.9
1	B	165	THR	4.7
1	C	164	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	162	PHE	4.5
1	C	168	ASP	4.3
1	B	74	VAL	4.1
1	B	90	VAL	4.0
1	C	90	VAL	3.9
1	C	169	LEU	3.9
1	D	67	ILE	3.9
1	D	91	ARG	3.6
1	C	94	ALA	3.6
1	D	76	ASP	3.6
1	B	163	GLY	3.5
1	A	161	ARG	3.5
1	D	162	PHE	3.5
1	C	71	TYR	3.4
1	D	246	TRP	3.4
1	D	87	VAL	3.4
1	D	2	SER	3.4
1	A	162	PHE	3.3
1	B	166	PRO	3.3
1	D	72	PRO	3.3
1	B	72	PRO	3.2
1	D	68	HIS	3.2
1	B	160	GLU	3.2
1	D	90	VAL	3.2
1	B	76	ASP	3.2
1	B	89	ASP	3.2
1	C	172	TRP	3.2
1	D	126	TRP	3.1
1	B	69	PRO	3.1
1	D	74	VAL	3.1
1	B	159	LEU	2.9
1	B	75	PRO	2.9
1	C	163	GLY	2.7
1	C	69	PRO	2.7
1	D	112	LEU	2.7
1	C	159	LEU	2.7
1	C	161	ARG	2.7
1	D	3	LEU	2.7
1	B	167	GLN	2.6
1	D	92	ASP	2.6
1	B	2	SER	2.6
1	C	70	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	261	PRO	2.6
1	D	73	ASN	2.6
1	C	74	VAL	2.5
1	D	111	VAL	2.5
1	B	68	HIS	2.5
1	B	261	PRO	2.4
1	B	157	PHE	2.4
1	C	120[A]	TYR	2.4
1	B	88	THR	2.4
1	B	73	ASN	2.3
1	B	172	TRP	2.3
1	B	171	ARG	2.3
1	D	177	ARG	2.3
1	D	165	THR	2.3
1	B	91	ARG	2.3
1	B	92	ASP	2.3
1	D	89	ASP	2.3
1	B	173	GLU	2.2
1	B	86	ALA	2.1
1	B	176	ARG	2.1
1	B	246	TRP	2.1
1	D	244	ALA	2.1
1	C	167	GLN	2.0
1	D	260	ARG	2.0
1	B	85	THR	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	CL	A	278	1/1	1.00	0.09	-0.15	21,21,21,21	0
2	CL	A	279	1/1	0.99	0.09	-0.77	24,24,24,24	0

6.5　Other polymers (i)

There are no such residues in this entry.