



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:54 am GMT

PDB ID : 1W62
Title : PROLINE RACEMASE IN COMPLEX WITH ONE MOLECULE OF
PYRROLE-2-CARBOXYLIC ACID (HEMI FORM)
Authors : Buschiazzo, A.; Alzari, P.
Deposited on : 2004-08-12
Resolution : 2.50 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 : trunk28620
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) : recalc28949

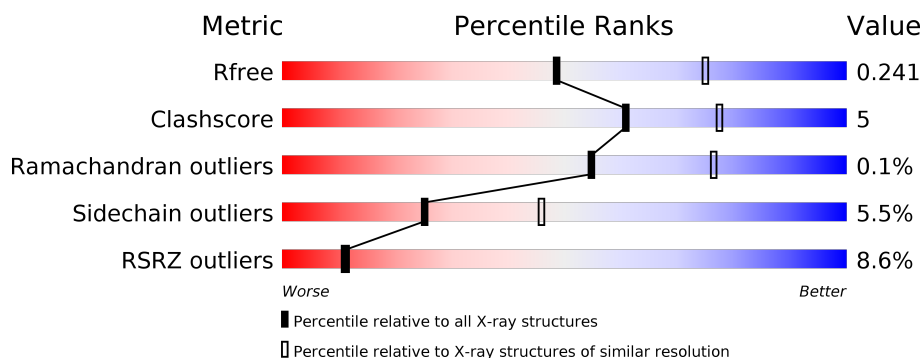
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	414	<div> <div>11%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	414	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>13%</div> <div>•</div> <div>15%</div> </div> </div>

2 Entry composition [i](#)

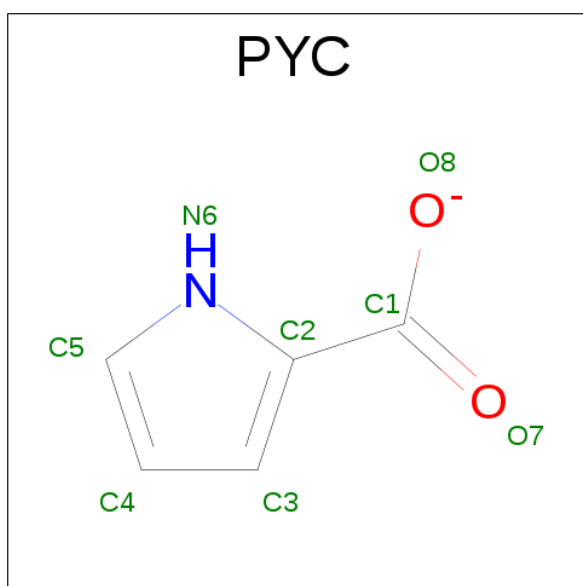
There are 3 unique types of molecules in this entry. The entry contains 5554 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 B-CELL MITOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2739	1736	465	522	16			
1	B	351	Total	C	N	O	S	0	0	0
			2656	1684	450	509	13			

- Molecule 2 is PYRROLE-2-CARBOXYLATE (three-letter code: PYC) (formula: $C_5H_4NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total	O	0	0
			73	73		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	78	Total	O	0	0
			78	78		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.02Å 89.38Å 84.46Å 90.00° 125.98° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 28.76 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.3 (30.00-2.50) 97.2 (28.76-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.170 , 0.236 0.179 , 0.241	Depositor DCC
R_{free} test set	2778 reflections (11.17%)	DCC
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5554	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: PYC

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	0.80	0/2794	0.95	12/3791 (0.3%)
1	B	0.88	0/2710	0.95	7/3682 (0.2%)
All	All	0.84	0/5504	0.95	19/7473 (0.3%)

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 (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	ASP	CB-CG-OD2	9.87	127.18	118.30
1	B	108	ASP	CB-CG-OD2	8.36	125.83	118.30
1	A	115	ASP	CB-CG-OD2	8.04	125.54	118.30
1	A	161	ASP	CB-CG-OD2	7.38	124.94	118.30
1	A	122	ASP	CB-CG-OD2	6.81	124.43	118.30
1	A	100	ASP	CB-CG-OD2	6.72	124.35	118.30
1	B	318	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	99	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	296	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	115	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	85	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	269	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	386	LYS	CD-CE-NZ	-5.51	99.03	111.70
1	B	383	ASP	CB-CG-OD2	5.37	123.13	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	212	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	89	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	168	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	89	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	GLN	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	2739	0	2706	29	0
1	B	2656	0	2627	36	0
2	A	8	0	4	0	0
3	A	73	0	0	0	0
3	B	78	0	0	0	0
All	All	5554	0	5337	56	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 (56) 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:329:LEU:CD1	1:B:391:LEU:HD21	2.15	0.77
1:A:394:TYR:N	1:B:235:GLN:HE22	1.92	0.65
1:B:48:CYS:HB3	1:B:61:VAL:HA	1.78	0.65
1:A:155:ASN:ND2	1:A:172:HIS:ND1	2.48	0.62
1:B:84:MET:HE1	1:B:87:LEU:HD11	1.82	0.61
1:A:235:GLN:HA	1:B:393:GLN:NE2	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ARG:NH2	1:B:393:GLN:O	2.36	0.59
1:B:47:THR:HG22	1:B:62:THR:OG1	2.03	0.59
1:B:84:MET:CE	1:B:87:LEU:HD11	2.33	0.58
1:B:155:ASN:ND2	1:B:172:HIS:ND1	2.52	0.57
1:B:242:GLU:O	1:B:246:LEU:HD23	2.05	0.56
1:A:225:ALA:HB2	1:A:232:ILE:HD11	1.90	0.54
1:B:200:VAL:HG21	1:B:247:LEU:HD12	1.88	0.54
1:A:51:MET:SD	1:A:140:ALA:HB2	2.49	0.53
1:B:377:MET:C	1:B:378:LEU:HD23	2.29	0.53
1:B:292:ASN:H	1:B:294:GLN:HE21	1.57	0.53
1:A:96:ARG:HB3	1:A:377:MET:CE	2.40	0.51
1:B:200:VAL:HG23	1:B:202:LEU:HD13	1.93	0.51
1:A:394:TYR:N	1:B:235:GLN:NE2	2.59	0.51
1:A:308:MET:CE	1:A:363:ALA:HB1	2.41	0.50
1:A:213:ILE:HA	1:A:220:PHE:O	2.11	0.50
1:A:348:VAL:HB	1:A:349:PRO:CD	2.41	0.50
1:B:73:MET:CE	1:B:119:VAL:HG23	2.42	0.49
1:B:206:TYR:HE2	1:B:230:ILE:HD11	1.78	0.49
1:B:317:LEU:HD12	1:B:321:GLU:CD	2.33	0.49
1:A:211:VAL:HG21	1:A:251:ILE:HD11	1.94	0.48
1:A:259:HIS:CE1	1:A:261:GLN:HE21	2.30	0.48
1:A:102:PHE:HD2	1:A:133:ASN:HD22	1.61	0.48
1:B:259:HIS:HE1	1:B:261:GLN:NE2	2.11	0.47
1:A:266:ASN:C	1:A:266:ASN:HD22	2.17	0.47
1:A:394:TYR:H	1:B:235:GLN:HE22	1.60	0.46
1:B:259:HIS:CE1	1:B:261:GLN:NE2	2.84	0.46
1:A:299:PRO:O	1:A:300:CYS:HB3	2.17	0.45
1:B:212:ASP:OD1	1:B:314:LYS:NZ	2.42	0.45
1:B:299:PRO:O	1:B:300:CYS:HB3	2.16	0.45
1:A:329:LEU:HD12	1:B:391:LEU:HD21	1.97	0.45
1:A:247:LEU:CD2	1:A:251:ILE:HD12	2.47	0.44
1:A:96:ARG:HB3	1:A:377:MET:HE1	1.99	0.44
1:B:223:VAL:O	1:B:223:VAL:HG13	2.18	0.44
1:B:368:LYS:HE3	1:B:370:PHE:CE1	2.52	0.44
1:B:259:HIS:CE1	1:B:261:GLN:HE21	2.35	0.44
1:A:134:SER:O	1:A:138:VAL:HG23	2.19	0.43
1:B:78:ALA:HA	1:B:81:GLN:HE21	1.84	0.42
1:B:150:PRO:HB2	1:B:153:ALA:HB2	2.01	0.42
1:B:245:GLU:OE2	1:B:248:ARG:NH2	2.49	0.42
1:A:329:LEU:HD11	1:B:391:LEU:HD21	2.00	0.42
1:A:393:GLN:HA	1:B:235:GLN:HE22	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:VAL:HG22	1:B:391:LEU:HD22	2.01	0.42
1:A:131:GLY:HA3	1:A:301:GLY:HA3	2.02	0.41
1:B:68:ILE:HD13	1:B:80:LEU:HD21	2.02	0.41
1:B:245:GLU:O	1:B:249:THR:HG23	2.20	0.41
1:A:348:VAL:HB	1:A:349:PRO:HD2	2.03	0.41
1:A:259:HIS:HE1	1:A:261:GLN:HE21	1.67	0.41
1:B:348:VAL:HB	1:B:349:PRO:CD	2.50	0.41
1:A:344:PRO:HA	1:A:356:GLU:O	2.21	0.41
1:A:337:VAL:HG13	1:A:361:VAL:HB	2.04	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	360/414 (87%)	344 (96%)	16 (4%)	0	100	100
1	B	349/414 (84%)	337 (97%)	11 (3%)	1 (0%)	44	66
All	All	709/828 (86%)	681 (96%)	27 (4%)	1 (0%)	55	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	MET

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	294/347 (85%)	277 (94%)	17 (6%)	23	43
1	B	286/347 (82%)	271 (95%)	15 (5%)	27	49
All	All	580/694 (84%)	548 (94%)	32 (6%)	25	46

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	MET
1	A	48	CYS
1	A	174	GLN
1	A	177	THR
1	A	231	ASP
1	A	237	LEU
1	A	248	ARG
1	A	251	ILE
1	A	256	LYS
1	A	261	GLN
1	A	266	ASN
1	A	319	ILE
1	A	325	TYR
1	A	329	LEU
1	A	355	GLU
1	A	393	GLN
1	A	394	TYR
1	B	47	THR
1	B	202	LEU
1	B	208	GLU
1	B	226	GLU
1	B	245	GLU
1	B	249	THR
1	B	256	LYS
1	B	261	GLN
1	B	266	ASN
1	B	286	ASN
1	B	293	ARG
1	B	314	LYS
1	B	325	TYR
1	B	336	ARG
1	B	393	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	196	GLN
1	A	236	ASN
1	A	261	GLN
1	A	266	ASN
1	A	387	ASN
1	B	81	GLN
1	B	155	ASN
1	B	195	GLN
1	B	235	GLN
1	B	236	ASN
1	B	258	GLN
1	B	259	HIS
1	B	261	GLN
1	B	266	ASN
1	B	294	GLN
1	B	316	GLN
1	B	387	ASN
1	B	393	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	PYC	A	700	-	5,8,8	0.57	0	4,10,10	1.48	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	PYC	A	700	-	-	0/0/4/4	0/1/1/1

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, 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	362/414 (87%)	0.54	46 (12%) 4 3	26, 42, 55, 71	0
1	B	351/414 (84%)	0.16	15 (4%) 36 38	27, 38, 50, 64	0
All	All	713/828 (86%)	0.35	61 (8%) 11 11	26, 40, 53, 71	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	ALA	6.2
1	A	394	TYR	6.2
1	A	178	GLU	5.7
1	A	175	SER	5.6
1	A	204	LYS	4.7
1	A	179	SER	4.6
1	A	177	THR	4.4
1	A	35	GLN	4.4
1	A	176	GLY	4.3
1	A	203	PRO	3.9
1	A	153	ALA	3.8
1	A	393	GLN	3.6
1	B	394	TYR	3.6
1	A	34	GLN	3.6
1	A	150	PRO	3.5
1	A	280	PRO	3.5
1	A	120	PHE	3.4
1	B	178	GLU	3.4
1	A	174	GLN	3.4
1	A	130	CYS	3.3
1	A	180	GLU	3.3
1	B	393	GLN	3.3
1	A	149	VAL	3.2
1	B	177	THR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	33	HIS	3.1
1	B	346	VAL	3.1
1	A	173	LEU	2.9
1	A	39	ILE	2.7
1	A	57	ALA	2.7
1	A	132	HIS	2.7
1	A	133	ASN	2.7
1	B	130	CYS	2.6
1	A	112	GLU	2.6
1	A	302	THR	2.5
1	A	347	LYS	2.5
1	A	300	CYS	2.5
1	A	38	GLU	2.5
1	A	154	THR	2.5
1	B	150	PRO	2.5
1	B	280	PRO	2.5
1	B	153	ALA	2.5
1	A	36	LYS	2.5
1	A	37	ARG	2.4
1	B	175	SER	2.3
1	B	151	ALA	2.3
1	A	253	ARG	2.3
1	B	263	PRO	2.3
1	A	131	GLY	2.3
1	A	345	GLY	2.3
1	B	345	GLY	2.3
1	A	53	THR	2.2
1	A	148	SER	2.2
1	B	201	VAL	2.2
1	A	270	CYS	2.2
1	A	129	MET	2.1
1	A	40	MET	2.1
1	A	104	ALA	2.1
1	A	152	LYS	2.1
1	A	127	LEU	2.1
1	B	343	ILE	2.1
1	A	58	ALA	2.0

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 [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(\AA^2)	Q<0.9
2	PYC	A	700	8/8	0.97	0.22	-1.76	42,43,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.