



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:25 PM GMT

PDB ID : 3ZGJ
Title : S221M V223F Y359A mutant of 4-Hydroxymandelate synthase from *Streptomyces coelicolor*
Authors : Pratter, S.; Straganz, G.; Grogan, G.
Deposited on : 2012-12-18
Resolution : 1.95 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 (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

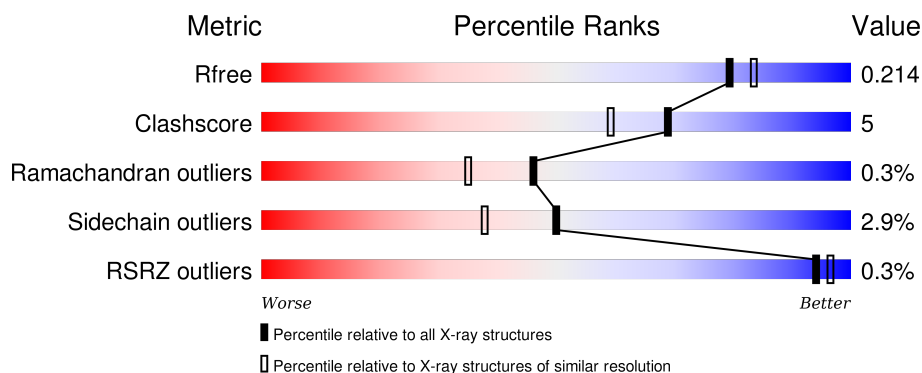
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	371	 78% 9% • 12%
1	B	371	 82% 9% • 8%

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
2	CO	A	1368	-	-	-	X
3	RMN	A	1369	-	-	-	X
3	RMN	B	1369	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5614 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 4-HYDROXYPHENYLPYRUVIC ACID DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	1	0
			2457	1559	419	473	6			
1	B	343	Total	C	N	O	S	0	0	0
			2602	1641	455	500	6			

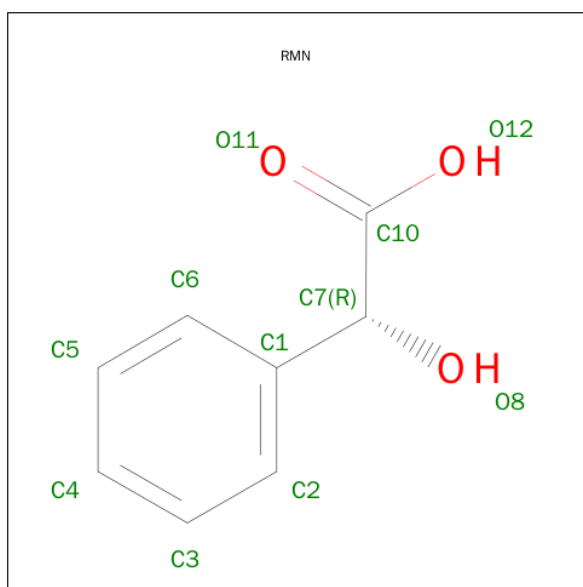
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	MET	SER	ENGINEERED MUTATION	UNP Q9Z4X7
A	223	PHE	VAL	ENGINEERED MUTATION	UNP Q9Z4X7
A	359	ALA	TYR	ENGINEERED MUTATION	UNP Q9Z4X7
B	221	MET	SER	ENGINEERED MUTATION	UNP Q9Z4X7
B	223	PHE	VAL	ENGINEERED MUTATION	UNP Q9Z4X7
B	359	ALA	TYR	ENGINEERED MUTATION	UNP Q9Z4X7

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

- Molecule 3 is (R)-MANDELIC ACID (three-letter code: RMN) (formula: C₈H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	8	3		
3	B	1	Total	C	O	0	0
			11	8	3		


- Molecule 4 is water.

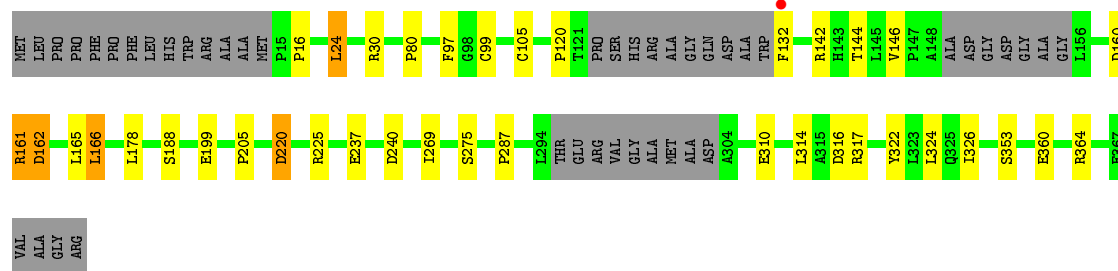
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	220	Total	O	0	0
			220	220		
4	B	311	Total	O	0	0
			311	311		

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.

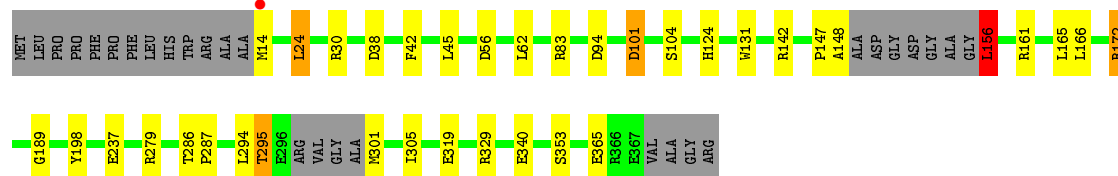
• Molecule 1: 4-HYDROXYPHENYLPYRUVIC ACID DIOXYGENASE

Chain A: 



• Molecule 1: 4-HYDROXYPHENYLPYRUVIC ACID DIOXYGENASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	122.87Å 122.87Å 54.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.95 – 1.95 54.95 – 1.88	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.95-1.95) 100.0 (54.95-1.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.175 , 0.215 0.174 , 0.214	Depositor DCC
R_{free} test set	3048 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.3	EDS
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 66951 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5614	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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, 0.375 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: CO, RMN

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	0.98	0/2515	1.00	5/3432 (0.1%)
1	B	1.10	2/2661 (0.1%)	1.08	10/3629 (0.3%)
All	All	1.04	2/5176 (0.0%)	1.04	15/7061 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	340	GLU	CD-OE1	5.87	1.32	1.25
1	B	161	ARG	CD-NE	-5.38	1.37	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	ARG	NE-CZ-NH2	-12.90	113.85	120.30
1	A	162	ASP	N-CA-CB	-11.53	89.86	110.60
1	B	161	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	A	166	LEU	CA-CB-CG	7.29	132.06	115.30
1	A	240	ASP	CB-CG-OD1	7.12	124.71	118.30
1	B	101	ASP	CB-CG-OD1	6.94	124.54	118.30
1	B	94	ASP	CB-CG-OD1	6.75	124.37	118.30
1	A	240	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	B	24	LEU	CA-CB-CG	6.23	129.64	115.30
1	B	56	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	156	LEU	CA-CB-CG	5.68	128.37	115.30
1	B	45	LEU	CB-CG-CD1	-5.63	101.42	111.00
1	B	24	LEU	CB-CG-CD2	5.58	120.48	111.00
1	A	24	LEU	CA-CB-CG	5.56	128.09	115.30
1	B	198	TYR	CA-CB-CG	-5.14	103.63	113.40

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	2457	0	2341	22	0
1	B	2602	0	2488	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	11	0	6	0	0
3	B	11	0	6	0	0
4	A	220	0	0	7	0
4	B	311	0	0	11	0
All	All	5614	0	4841	45	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 (45) 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:319:GLU:HG3	4:B:2281:HOH:O	1.82	0.80
1:B:294:LEU:O	1:B:295:THR:OG1	2.01	0.79
1:B:30:ARG:NH2	4:B:2023:HOH:O	2.09	0.78
1:B:83:ARG:NH2	4:B:2089:HOH:O	2.20	0.73
1:A:30[B]:ARG:HD2	4:A:2022:HOH:O	1.89	0.72
1:B:301:MET:O	1:B:305:ILE:HG12	1.92	0.69
1:B:38:ASP:OD1	4:B:2043:HOH:O	2.13	0.67
1:A:80:PRO:HD2	4:A:2053:HOH:O	1.99	0.62
1:A:220:ASP:OD2	1:B:172:ARG:NH1	2.34	0.60
1:A:199:GLU:HG2	1:A:205:PRO:HA	1.83	0.60
1:A:99:CYS:HG	1:A:105:CYS:CB	2.14	0.60
1:A:310:GLU:OE2	4:A:2194:HOH:O	2.16	0.60
1:A:16:PRO:HB3	1:A:97:PHE:HB3	1.85	0.59
1:B:279:ARG:NH1	4:B:2258:HOH:O	2.35	0.57
1:A:269:ILE:HD11	1:A:326:ILE:HG22	1.90	0.53
1:B:131:TRP:O	1:B:147:PRO:HG3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ASP:CG	1:B:104:SER:HB3	2.30	0.51
1:B:294:LEU:O	1:B:295:THR:CB	2.59	0.51
1:A:178:LEU:C	1:A:178:LEU:HD12	2.31	0.51
1:B:30:ARG:NE	4:B:2023:HOH:O	2.44	0.50
1:B:142:ARG:HD2	4:B:2052:HOH:O	2.10	0.49
1:A:99:CYS:SG	1:A:105:CYS:SG	3.11	0.49
1:B:156:LEU:CB	4:B:2167:HOH:O	2.60	0.48
1:B:329:ARG:HD3	1:B:365:GLU:OE2	2.13	0.48
1:B:30:ARG:CZ	4:B:2023:HOH:O	2.56	0.47
1:A:316:ASP:OD2	1:A:353:SER:HB3	2.14	0.47
1:B:42:PHE:HB3	1:B:62:LEU:HB3	1.98	0.46
1:A:188:SER:HA	1:A:237:GLU:HG3	1.98	0.46
1:A:142:ARG:NE	4:A:2096:HOH:O	2.44	0.45
1:B:156:LEU:HB3	4:B:2167:HOH:O	2.15	0.44
1:A:30[B]:ARG:NH1	4:A:2022:HOH:O	2.24	0.44
1:A:205:PRO:HD2	1:A:225:ARG:O	2.18	0.44
1:B:295:THR:HG22	1:B:295:THR:O	2.17	0.43
1:B:14:MET:N	1:B:104:SER:HG	2.17	0.43
1:A:160:ASP:OD1	1:A:161:ARG:HD3	2.18	0.43
1:A:317:ARG:HA	1:A:322:TYR:HA	2.01	0.42
1:B:148:ALA:C	4:B:2163:HOH:O	2.57	0.42
1:A:144:THR:HG22	1:A:146:VAL:HG13	2.02	0.42
1:B:156:LEU:HD12	1:B:156:LEU:C	2.41	0.41
1:B:286:THR:HA	1:B:287:PRO:HD3	1.86	0.41
1:A:314:LEU:O	1:A:324:LEU:HA	2.20	0.41
1:B:189:GLY:N	1:B:237:GLU:OE2	2.49	0.41
1:A:287:PRO:HD3	1:A:364:ARG:CZ	2.51	0.41
1:A:142:ARG:NH2	4:A:2096:HOH:O	2.46	0.40
1:A:360:GLU:OE1	4:A:2217:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	320/371 (86%)	314 (98%)	5 (2%)	1 (0%)	46	35
1	B	337/371 (91%)	331 (98%)	5 (2%)	1 (0%)	46	35
All	All	657/742 (88%)	645 (98%)	10 (2%)	2 (0%)	46	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	295	THR
1	A	120	PRO

5.3.2 Protein sidechains ⓘ

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	248/289 (86%)	240 (97%)	8 (3%)	46	33
1	B	264/289 (91%)	257 (97%)	7 (3%)	52	41
All	All	512/578 (89%)	497 (97%)	15 (3%)	50	38

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	132	PHE
1	A	161	ARG
1	A	162	ASP
1	A	165	LEU
1	A	166	LEU
1	A	220	ASP
1	A	275	SER
1	B	24	LEU
1	B	124	HIS
1	B	156	LEU
1	B	165	LEU
1	B	166	LEU
1	B	172	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	353	SER

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

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	RMN	A	1369	2	8,11,11	2.00	1 (12%)	11,14,14	0.90	0
3	RMN	B	1369	2	8,11,11	2.17	1 (12%)	11,14,14	1.45	2 (18%)

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	RMN	A	1369	2	-	0/4/8/8	0/1/1/1
3	RMN	B	1369	2	-	0/4/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1369	RMN	C1-C7	-5.62	1.42	1.52
3	A	1369	RMN	C1-C7	-5.07	1.43	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1369	RMN	O8-C7-C10	-3.00	105.53	111.00
3	B	1369	RMN	C10-C7-C1	-2.96	106.66	112.05

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	327/371 (88%)	-0.05	1 (0%) 94 96	21, 35, 61, 75	0
1	B	343/371 (92%)	-0.13	1 (0%) 94 96	16, 28, 55, 74	0
All	All	670/742 (90%)	-0.09	2 (0%) 94 96	16, 32, 58, 75	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	14	MET	2.6
1	A	132	PHE	2.1

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	RMN	A	1369	11/11	0.94	0.13	4.50	34,41,45,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CO	A	1368	1/1	0.99	0.11	3.35	27,27,27,27	0
3	RMN	B	1369	11/11	0.92	0.13	2.70	33,46,50,51	0
2	CO	B	1368	1/1	1.00	0.12	1.63	21,21,21,21	0

6.5 Other polymers

There are no such residues in this entry.