



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:58 AM UTC

PDB ID : 6BOL / pdb_00006bol
Title : Crystal structure of mutant 2-methylcitrate synthase mcsAG419A from *Aspergillus fumigatus*.
Authors : Schlachter, C.; Chruszcz, M.
Deposited on : 2017-11-20
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

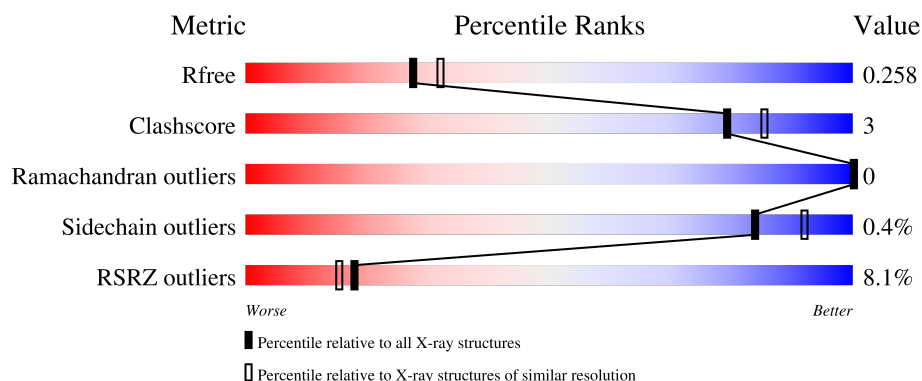
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	441	6% 88% 10%
1	B	441	10% 93% 6%

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	PO4	A	504	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6975 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.

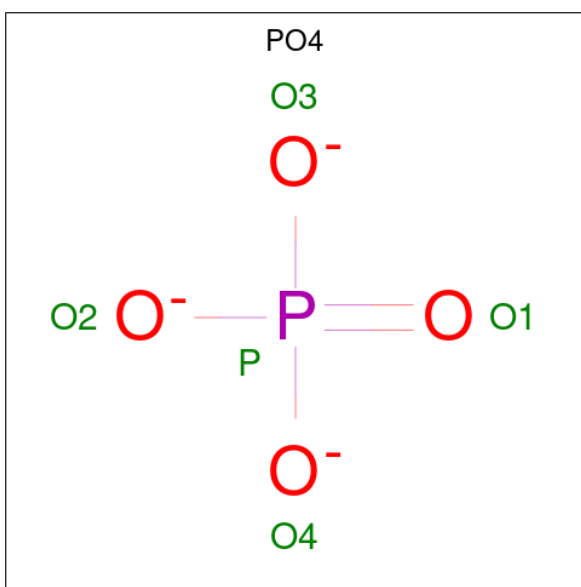
- Molecule 1 is a protein called 2-methylcitrate synthase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	434	Total	C	N	O	S	0	0	0
			3365	2157	579	620	9			
1	A	433	Total	C	N	O	S	0	0	0
			3352	2148	576	619	9			

There are 10 discrepancies between the modelled and reference sequences:

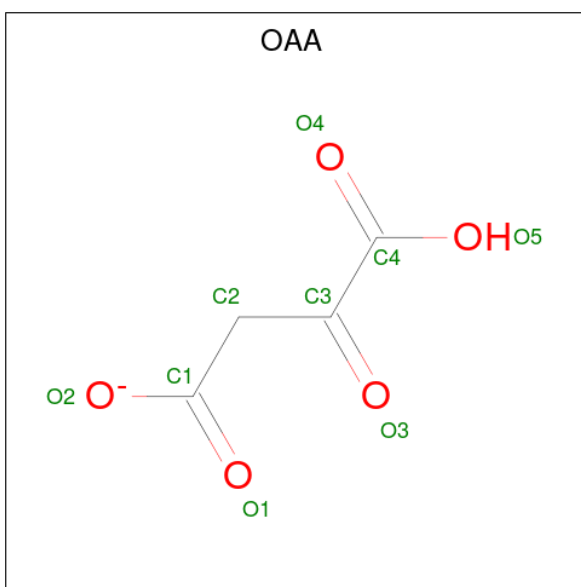
Chain	Residue	Modelled	Actual	Comment	Reference
B	25	SER	-	expression tag	UNP B0YD89
B	26	GLY	-	expression tag	UNP B0YD89
B	27	SER	-	expression tag	UNP B0YD89
B	28	GLY	-	expression tag	UNP B0YD89
B	419	ALA	GLY	engineered mutation	UNP B0YD89
A	25	SER	-	expression tag	UNP B0YD89
A	26	GLY	-	expression tag	UNP B0YD89
A	27	SER	-	expression tag	UNP B0YD89
A	28	GLY	-	expression tag	UNP B0YD89
A	419	ALA	GLY	engineered mutation	UNP B0YD89

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is OXALOACETATE ION (CCD ID: OAA) (formula: $C_4H_3O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	110	Total	O	0	0
			110	110		
5	A	114	Total	O	0	0
			114	114		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.64Å 103.59Å 135.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 40.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.4 (40.00-2.20) 95.4 (40.00-2.20)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.25	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.204 , 0.262 0.209 , 0.258	Depositor DCC
R_{free} test set	2119 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6975	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: CL, OAA, PO4

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	1.12	1/3434 (0.0%)	1.12	4/4667 (0.1%)
1	B	1.11	3/3447 (0.1%)	1.10	5/4682 (0.1%)
All	All	1.12	4/6881 (0.1%)	1.11	9/9349 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	VAL	C-O	-6.07	1.16	1.24
1	B	43	ILE	CA-CB	5.24	1.57	1.54
1	B	170	SER	C-O	-5.17	1.18	1.24
1	A	210	ILE	CA-CB	5.09	1.57	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	LYS	N-CA-C	7.59	120.28	111.02
1	B	210	ILE	N-CA-CB	6.81	114.79	110.50
1	A	420	PHE	N-CA-C	-6.52	100.52	109.71
1	A	43	ILE	N-CA-CB	6.25	114.44	110.50
1	B	43	ILE	N-CA-CB	5.24	114.54	110.45
1	B	420	PHE	N-CA-C	-5.17	102.42	109.71
1	A	146	SER	N-CA-C	5.11	119.27	113.19
1	B	356	LYS	CA-C-N	-5.02	114.61	119.78
1	B	356	LYS	C-N-CA	-5.02	114.61	119.78

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	3352	0	3331	27	0
1	B	3365	0	3358	12	0
2	A	10	0	0	2	0
2	B	5	0	0	0	0
3	A	18	0	4	0	0
4	A	1	0	0	0	0
5	A	114	0	0	2	0
5	B	110	0	0	1	0
All	All	6975	0	6693	36	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 3.

All (36) 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:426:TYR:O	1:A:429:THR:HG22	1.87	0.74
1:A:218:PHE:CZ	1:A:425:TYR:HB3	2.29	0.68
1:B:323:ILE:HD11	1:B:335:TYR:HB2	1.82	0.60
1:A:313:LEU:HD22	1:A:426:TYR:HE2	1.67	0.59
1:A:86:LEU:HD11	1:A:354:LEU:CD1	2.34	0.56
1:B:171:ILE:HG23	1:A:171:ILE:HG23	1.87	0.55
1:A:86:LEU:HD11	1:A:354:LEU:HD11	1.89	0.55
1:A:319:MET:O	1:A:323:ILE:HG12	2.08	0.53
1:B:319:MET:HE1	1:B:332:VAL:HG13	1.90	0.52
1:A:166:MET:SD	1:A:427:THR:HG22	2.50	0.51
1:A:351:HIS:NE2	2:A:504:PO4:O2	2.45	0.50
1:B:77:LYS:HE2	1:A:456:LYS:HG2	1.93	0.49
1:B:434:ARG:O	1:B:438:PRO:HD2	2.14	0.48
1:B:454:ARG:NE	2:A:504:PO4:O4	2.46	0.48
1:A:218:PHE:CZ	1:A:420:PHE:CZ	3.03	0.47
1:A:218:PHE:CZ	1:A:425:TYR:CB	2.97	0.47
1:B:197:GLU:HB3	1:B:198:PRO:HD3	1.97	0.47
1:A:303:PRO:HA	1:A:307:LEU:HB2	1.96	0.47
1:B:184:LYS:NZ	5:B:601:HOH:O	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ALA:O	5:A:601:HOH:O	2.20	0.46
1:A:385:LYS:HD2	1:A:389:ILE:HD11	1.98	0.45
1:A:269:HIS:O	1:A:270:GLU:HB2	2.17	0.44
1:A:136:ARG:HD3	5:A:628:HOH:O	2.17	0.44
1:A:81:TRP:CE3	1:A:441:GLN:HG2	2.53	0.44
1:A:147:HIS:O	1:A:209:LYS:HE3	2.18	0.44
1:A:247:LYS:NZ	1:A:418:TYR:O	2.35	0.44
1:A:434:ARG:O	1:A:438:PRO:HD2	2.18	0.43
1:A:86:LEU:HD21	1:A:354:LEU:HD12	2.01	0.43
1:B:206:LEU:HD23	1:B:206:LEU:O	2.18	0.43
1:A:349:TYR:OH	1:A:387:SER:HA	2.20	0.42
1:B:262:TYR:CE1	1:B:429:THR:HG22	2.55	0.42
1:B:349:TYR:OH	1:B:387:SER:HA	2.20	0.42
1:A:362:GLN:NE2	1:A:366:ASP:OD1	2.52	0.41
1:A:81:TRP:CH2	1:A:276:ALA:HB1	2.56	0.41
1:A:313:LEU:HD22	1:A:426:TYR:CE2	2.50	0.40
1:B:56:ARG:NH2	1:A:464:LYS:HA	2.36	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	431/441 (98%)	420 (97%)	11 (3%)	0	100	100
1	B	432/441 (98%)	424 (98%)	8 (2%)	0	100	100
All	All	863/882 (98%)	844 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	354/365 (97%)	352 (99%)	2 (1%)	78	89
1	B	356/365 (98%)	355 (100%)	1 (0%)	86	93
All	All	710/730 (97%)	707 (100%)	3 (0%)	84	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	177	ASN
1	A	177	ASN
1	A	329	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	145	GLN
1	B	168	GLN
1	B	225	GLN
1	B	266	HIS
1	A	168	GLN
1	A	266	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
2	PO4	A	504	-	4,4,4	1.03	0	6,6,6	0.61	0
2	PO4	A	503	-	4,4,4	0.81	0	6,6,6	0.59	0
3	OAA	A	502	-	8,8,8	1.98	1 (12%)	8,10,10	1.46	1 (12%)
3	OAA	A	501	-	8,8,8	1.84	1 (12%)	8,10,10	1.10	0
2	PO4	B	501	-	4,4,4	0.93	0	6,6,6	0.52	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
3	OAA	A	502	-	-	6/8/8/8	-
3	OAA	A	501	-	-	7/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	OAA	C3-C4	-4.81	1.46	1.53
3	A	501	OAA	C3-C4	-4.18	1.47	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	OAA	O4-C4-C3	-2.71	118.44	121.81

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	OAA	C2-C3-C4-O5
3	A	502	OAA	O3-C3-C4-O4
3	A	502	OAA	C2-C3-C4-O4
3	A	502	OAA	C2-C3-C4-O5
3	A	501	OAA	O2-C1-C2-C3
3	A	501	OAA	C1-C2-C3-O3
3	A	501	OAA	O3-C3-C4-O4
3	A	502	OAA	C1-C2-C3-O3
3	A	501	OAA	C2-C3-C4-O4
3	A	501	OAA	O1-C1-C2-C3
3	A	501	OAA	O3-C3-C4-O5
3	A	502	OAA	O1-C1-C2-C3
3	A	502	OAA	O2-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	PO4	2	0

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	433/441 (98%)	0.61	27 (6%) 26 23	16, 27, 49, 74	0
1	B	434/441 (98%)	0.70	43 (9%) 13 10	16, 28, 57, 90	0
All	All	867/882 (98%)	0.66	70 (8%) 18 15	16, 27, 55, 90	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	325	THR	6.8
1	A	354	LEU	5.8
1	A	420	PHE	4.8
1	B	31	ALA	4.7
1	A	424	LEU	4.1
1	A	353	VAL	4.1
1	A	423	PRO	4.1
1	B	420	PHE	4.0
1	A	401	LYS	3.8
1	B	382	LEU	3.7
1	B	397	HIS	3.5
1	B	321	ASP	3.4
1	B	327	PHE	3.4
1	B	423	PRO	3.1
1	B	323	ILE	3.0
1	B	422	GLN	3.0
1	B	322	LYS	3.0
1	B	352	GLY	3.0
1	B	338	ASP	3.0
1	A	419	ALA	2.9
1	B	454	ARG	2.9
1	A	400	THR	2.9
1	A	193	ALA	2.9
1	B	144	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	424	LEU	2.8
1	B	306	GLY	2.8
1	B	403	PRO	2.8
1	B	315	TRP	2.8
1	A	310	GLN	2.8
1	B	188	LYS	2.7
1	A	194	ASP	2.7
1	A	429	THR	2.7
1	B	326	LYS	2.7
1	B	324	GLY	2.6
1	B	332	VAL	2.6
1	A	432	VAL	2.6
1	B	61	ILE	2.5
1	B	421	GLN	2.5
1	A	218	PHE	2.4
1	B	342	SER	2.4
1	A	321	ASP	2.4
1	A	352	GLY	2.4
1	A	356	LYS	2.4
1	A	355	ARG	2.3
1	A	422	GLN	2.3
1	A	223	VAL	2.3
1	B	353	VAL	2.3
1	B	383	VAL	2.3
1	B	75	GLY	2.3
1	B	377	ASN	2.2
1	A	402	ASN	2.2
1	B	354	LEU	2.2
1	B	393	VAL	2.2
1	B	337	TRP	2.2
1	B	329	ASP	2.2
1	B	372	PRO	2.1
1	B	392	ALA	2.1
1	B	362	GLN	2.1
1	A	90	GLU	2.1
1	B	402	ASN	2.1
1	A	96	GLY	2.1
1	B	411	SER	2.1
1	B	389	ILE	2.1
1	B	328	THR	2.0
1	B	319	MET	2.0
1	A	76	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	266	HIS	2.0
1	B	336	LEU	2.0
1	A	224	ASP	2.0
1	A	88	PRO	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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
2	PO4	A	503	5/5	0.56	0.19	97,98,106,107	0
3	OAA	A	501	9/9	0.69	0.21	70,75,81,83	0
3	OAA	A	502	9/9	0.69	0.18	79,86,90,93	0
2	PO4	B	501	5/5	0.70	0.13	93,93,96,96	0
4	CL	A	505	1/1	0.90	0.11	36,36,36,36	0
2	PO4	A	504	5/5	0.92	0.22	49,50,55,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.