



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2POD / pdb_00002pod
Title : Crystal structure of a member of enolase superfamily from Burkholderia pseudomallei K96243
Authors : Patskovsky, Y.; Bonanno, J.; Sauder, J.M.; Gilmore, J.M.; Iizuka, M.; Ozyurt, S.; Wasserman, S.R.; Smith, D.; Gerlt, J.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2007-04-26
Resolution : 2.34 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

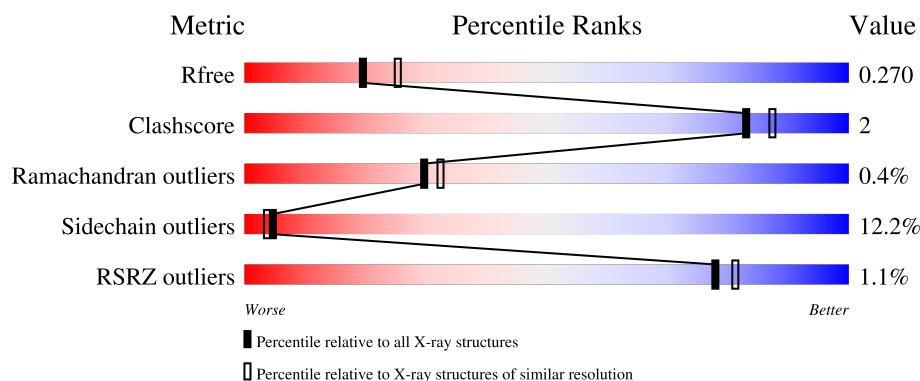
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	410	 79% 12% • 8%
1	B	410	 75% 16% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6132 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 Mandelate racemase / muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	Se	0	1	0
			2987	1900	516	557	6	8			
1	B	380	Total	C	N	O	S	Se	0	1	0
			2991	1901	514	562	6	8			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	cloning artifact	UNP Q63IJ7
A	0	SER	-	cloning artifact	UNP Q63IJ7
A	1	LEU	-	cloning artifact	UNP Q63IJ7
A	81	MSE	MET	modified residue	UNP Q63IJ7
A	173	MSE	MET	modified residue	UNP Q63IJ7
A	213	MSE	MET	modified residue	UNP Q63IJ7
A	216	MSE	MET	modified residue	UNP Q63IJ7
A	249	MSE	MET	modified residue	UNP Q63IJ7
A	291	MSE	MET	modified residue	UNP Q63IJ7
A	309	MSE	MET	modified residue	UNP Q63IJ7
A	383	MSE	MET	modified residue	UNP Q63IJ7
A	401	GLU	-	cloning artifact	UNP Q63IJ7
A	402	GLY	-	cloning artifact	UNP Q63IJ7
A	403	HIS	-	cloning artifact	UNP Q63IJ7
A	404	HIS	-	cloning artifact	UNP Q63IJ7
A	405	HIS	-	cloning artifact	UNP Q63IJ7
A	406	HIS	-	cloning artifact	UNP Q63IJ7
A	407	HIS	-	cloning artifact	UNP Q63IJ7
A	408	HIS	-	cloning artifact	UNP Q63IJ7
B	-1	MSE	-	cloning artifact	UNP Q63IJ7
B	0	SER	-	cloning artifact	UNP Q63IJ7
B	1	LEU	-	cloning artifact	UNP Q63IJ7
B	81	MSE	MET	modified residue	UNP Q63IJ7
B	173	MSE	MET	modified residue	UNP Q63IJ7
B	213	MSE	MET	modified residue	UNP Q63IJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	216	MSE	MET	modified residue	UNP Q63IJ7
B	249	MSE	MET	modified residue	UNP Q63IJ7
B	291	MSE	MET	modified residue	UNP Q63IJ7
B	309	MSE	MET	modified residue	UNP Q63IJ7
B	383	MSE	MET	modified residue	UNP Q63IJ7
B	401	GLU	-	cloning artifact	UNP Q63IJ7
B	402	GLY	-	cloning artifact	UNP Q63IJ7
B	403	HIS	-	cloning artifact	UNP Q63IJ7
B	404	HIS	-	cloning artifact	UNP Q63IJ7
B	405	HIS	-	cloning artifact	UNP Q63IJ7
B	406	HIS	-	cloning artifact	UNP Q63IJ7
B	407	HIS	-	cloning artifact	UNP Q63IJ7
B	408	HIS	-	cloning artifact	UNP Q63IJ7

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

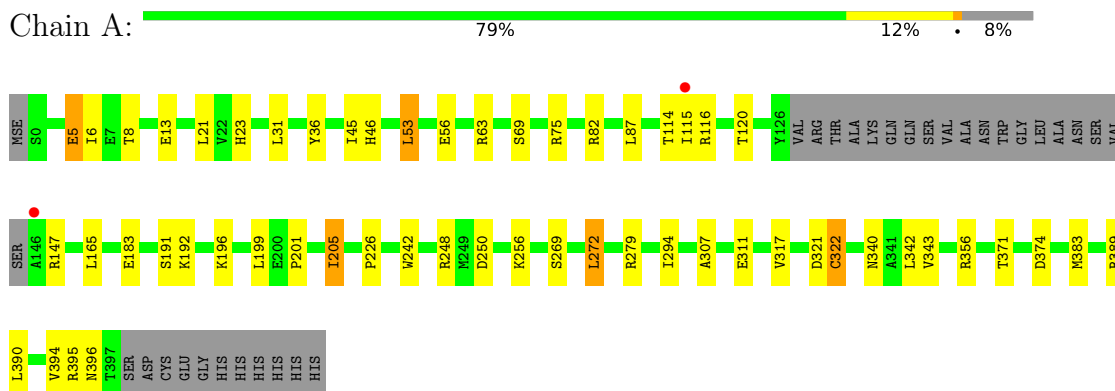
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	88	Total O 88 88	0	0
3	B	64	Total O 64 64	0	0

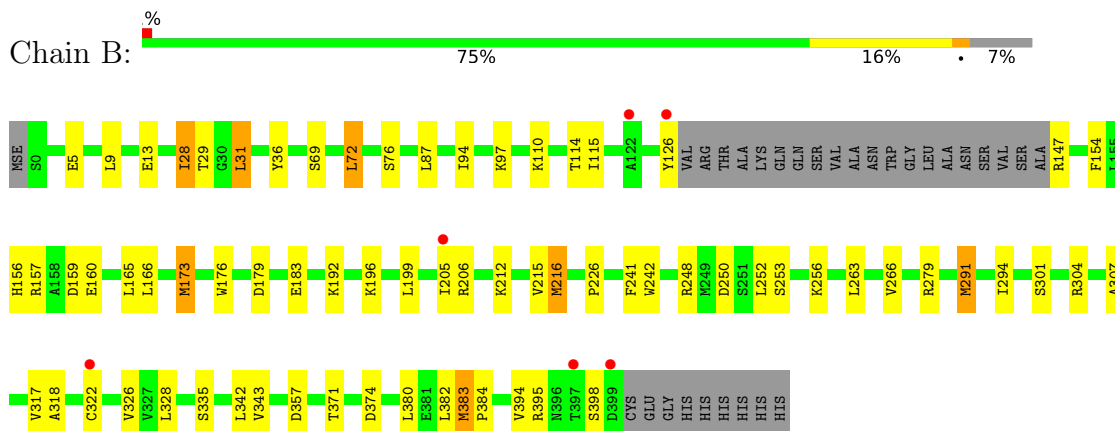
3 Residue-property plots

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: Mandelate racemase / muconate lactonizing enzyme



- Molecule 1: Mandelate racemase / muconate lactonizing enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	146.77Å 146.77Å 85.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.34 20.00 – 2.34	Depositor EDS
% Data completeness (in resolution range)	90.7 (20.00-2.34) 90.5 (20.00-2.34)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.209 , 0.275 0.205 , 0.270	Depositor DCC
R_{free} test set	1077 reflections (2.81%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.011 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6132	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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: NA

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	0.52	0/3056	0.94	2/4144 (0.0%)
1	B	0.55	2/3060 (0.1%)	0.95	5/4150 (0.1%)
All	All	0.54	2/6116 (0.0%)	0.94	7/8294 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	156	HIS	C-N	7.40	1.44	1.33
1	B	157	ARG	C-N	6.65	1.43	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	PRO	N-CA-C	6.18	118.24	110.70
1	A	226	PRO	N-CA-C	6.08	118.11	110.70
1	B	176	TRP	N-CA-C	5.28	117.16	109.30
1	B	179	ASP	N-CA-C	5.16	119.96	113.25
1	A	322	CYS	N-CA-C	5.15	118.86	112.47
1	B	226	PRO	CA-C-N	-5.11	113.78	119.19
1	B	226	PRO	C-N-CA	-5.11	113.78	119.19

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	2987	0	2931	13	0
1	B	2991	0	2927	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	88	0	0	0	0
3	B	64	0	0	0	0
All	All	6132	0	5858	28	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 2.

All (28) 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:8:THR:OG1	1:A:46:HIS:HE1	1.86	0.58
1:B:216:MSE:HE2	1:B:241:PHE:HB3	1.89	0.55
1:B:28:ILE:HD11	1:B:94:ILE:HA	1.89	0.54
1:A:75:ARG:HB3	1:B:76[A]:SER:HB3	1.92	0.50
1:A:307:ALA:HA	1:A:317:VAL:HG21	1.92	0.50
1:B:165:LEU:HD13	1:B:173:MSE:HG2	1.95	0.49
1:B:291:MSE:HG2	1:B:318:ALA:O	2.13	0.49
1:A:56:GLU:OE1	1:A:63:ARG:NH2	2.46	0.48
1:B:115:ILE:HD13	1:B:335:SER:HB3	1.95	0.48
1:B:114:THR:HG22	1:B:371:THR:HB	1.95	0.47
1:B:5:GLU:HG3	1:B:398:SER:HB3	1.95	0.47
1:A:114:THR:HG22	1:A:371:THR:HB	1.97	0.46
1:B:31:LEU:HD11	1:B:382:LEU:HG	1.98	0.46
1:A:120:THR:HG21	1:A:322:CYS:SG	2.56	0.45
1:B:383:MSE:HA	1:B:384:PRO:HD3	1.89	0.45
1:A:321:ASP:CG	1:A:322:CYS:N	2.75	0.45
1:A:82:ARG:HD3	1:B:72:LEU:HD23	1.98	0.44
1:A:311:GLU:HG3	1:A:340:ASN:HB3	1.99	0.44
1:B:166:LEU:HD21	1:B:212:LYS:HD2	1.99	0.43
1:A:201:PRO:O	1:A:205:ILE:HG23	2.19	0.43
1:B:307:ALA:HA	1:B:317:VAL:HG21	2.00	0.43
1:B:28:ILE:HD13	1:B:97:LYS:HB2	2.01	0.43
1:A:5:GLU:HB3	1:A:23:HIS:HD2	1.84	0.42
1:B:301:SER:HA	1:B:304:ARG:HH11	1.85	0.42
1:A:269:SER:HB3	1:A:272:LEU:HD22	2.01	0.42
1:B:9:LEU:HD22	1:B:394:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:VAL:HG22	1:B:380:LEU:HD11	2.01	0.41
1:A:53:LEU:HA	1:A:56:GLU:HG3	2.01	0.41

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	376/410 (92%)	364 (97%)	11 (3%)	1 (0%)	36	41
1	B	377/410 (92%)	357 (95%)	18 (5%)	2 (0%)	24	26
All	All	753/820 (92%)	721 (96%)	29 (4%)	3 (0%)	30	32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	TYR
1	B	36	TYR
1	B	322	CYS

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	312/328 (95%)	276 (88%)	36 (12%)	5	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	314/328 (96%)	274 (87%)	40 (13%)	4	3
All	All	626/656 (95%)	550 (88%)	76 (12%)	5	4

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	6	ILE
1	A	13	GLU
1	A	21	LEU
1	A	31	LEU
1	A	45	ILE
1	A	53	LEU
1	A	69	SER
1	A	87	LEU
1	A	115	ILE
1	A	116	ARG
1	A	147	ARG
1	A	165	LEU
1	A	183	GLU
1	A	191	SER
1	A	192	LYS
1	A	196	LYS
1	A	199	LEU
1	A	205	ILE
1	A	242	TRP
1	A	248	ARG
1	A	250	ASP
1	A	256	LYS
1	A	272	LEU
1	A	279	ARG
1	A	294	ILE
1	A	342	LEU
1	A	343	VAL
1	A	356	ARG
1	A	374	ASP
1	A	383	MSE
1	A	389	ARG
1	A	390	LEU
1	A	394	VAL
1	A	395	ARG
1	A	396	ASN

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Mol	Chain	Res	Type
1	B	13	GLU
1	B	28	ILE
1	B	29	THR
1	B	31	LEU
1	B	69	SER
1	B	72	LEU
1	B	87	LEU
1	B	110	LYS
1	B	126	TYR
1	B	147	ARG
1	B	154	PHE
1	B	159	ASP
1	B	160	GLU
1	B	173	MSE
1	B	183	GLU
1	B	192	LYS
1	B	196	LYS
1	B	199	LEU
1	B	205	ILE
1	B	206	ARG
1	B	215	VAL
1	B	216	MSE
1	B	242	TRP
1	B	248	ARG
1	B	250	ASP
1	B	252	LEU
1	B	253	SER
1	B	256	LYS
1	B	263	LEU
1	B	266	VAL
1	B	279	ARG
1	B	291	MSE
1	B	294	ILE
1	B	328	LEU
1	B	342	LEU
1	B	343	VAL
1	B	357	ASP
1	B	374	ASP
1	B	383	MSE
1	B	395	ARG

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

Mol	Chain	Res	Type
1	A	46	HIS
1	A	156	HIS
1	A	369	HIS
1	B	16	ASN
1	B	125	HIS
1	B	344	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 oligosaccharides 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	371/410 (90%)	-0.05	2 (0%) 87 89	27, 47, 71, 104	1 (0%)
1	B	372/410 (90%)	0.08	6 (1%) 70 75	31, 50, 75, 109	1 (0%)
All	All	743/820 (90%)	0.02	8 (1%) 78 81	27, 48, 74, 109	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	ALA	4.0
1	B	397	THR	2.8
1	B	126	TYR	2.7
1	B	122	ALA	2.6
1	A	115	ILE	2.5
1	B	205	ILE	2.2
1	B	322	CYS	2.1
1	B	399	ASP	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 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($\text{\AA}^2$)	Q<0.9
2	NA	A	409	1/1	0.78	0.12	73,73,73,73	0
2	NA	B	409	1/1	0.94	0.10	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.