Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 03:21 am GMT

PDB ID	:	2JB3
Title	:	The structure of L-amino acid oxidase from Rhodococcus opacus in complex with o-aminobenzoate
Authors	:	Faust, A.; Niefind, K.; hummel, W.; Schomburg, D.
Deposited on	:	2006-12-01
Resolution	:	1.85 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:

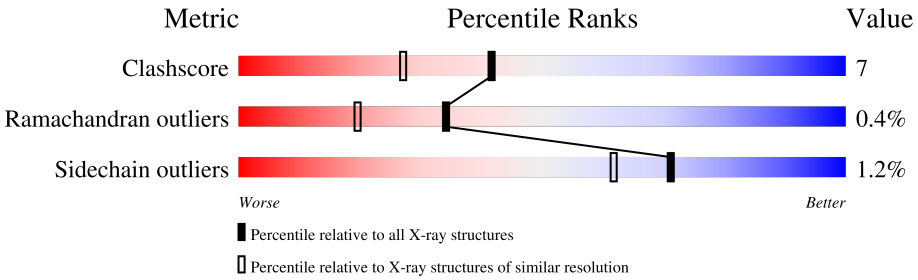
MolProbity	:	4.02b-467
Mogul	:	FAILED
Xtriage (Phenix)	:	FAILED
EDS	:	NOT EXECUTED
buster-report	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	489	86% 11%
1	B	489	82% 14%

2 Entry composition (i)

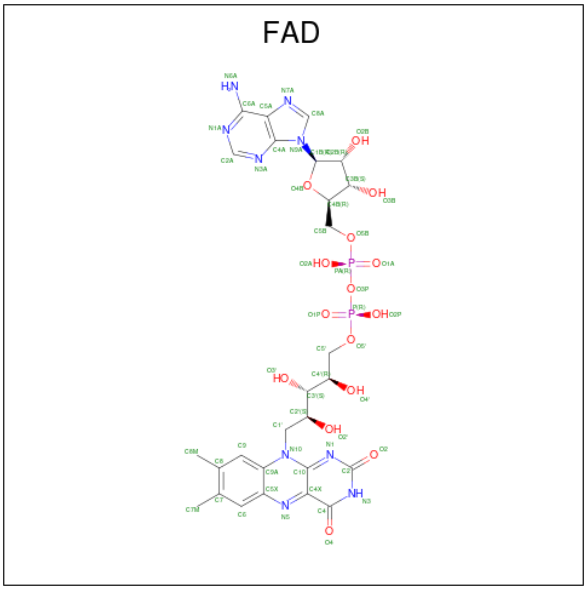
There are 4 unique types of molecules in this entry. The entry contains 8511 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-AMINO ACID OXIDASE.

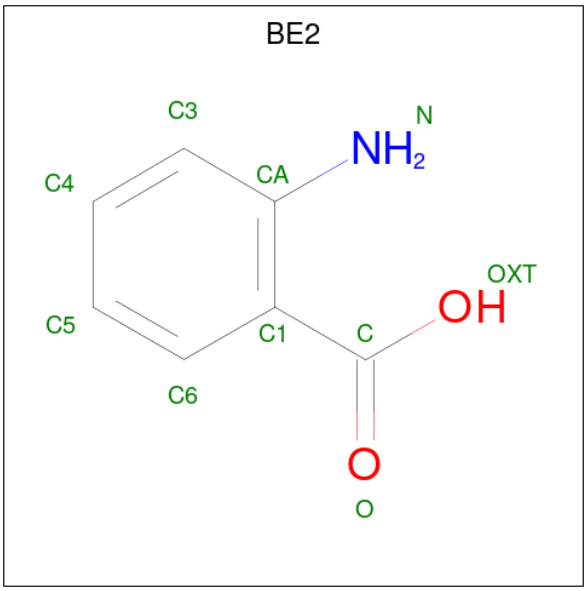
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	5	1
			3707	2311	649	735	12			
1	B	477	Total	C	N	O	S	0	0	0
			3693	2308	645	728	12			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 2-AMINOBENZOIC ACID (three-letter code: BE2) (formula: $C_7H_7NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 10 7 1 2	0	0
3	B	1	Total C N O 10 7 1 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	481	Total O 481 481	0	0
4	B	504	Total O 504 504	0	0

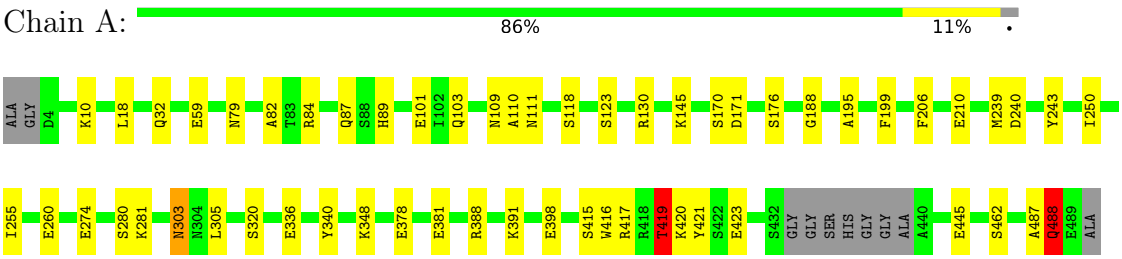
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

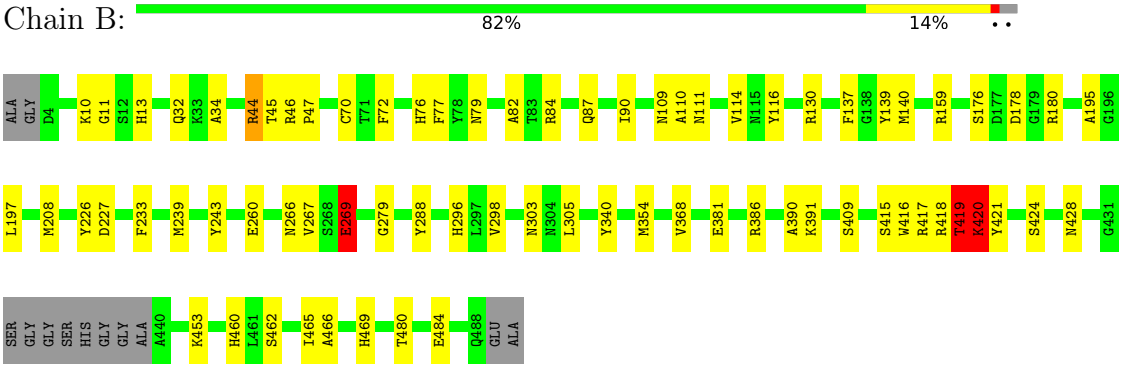
• Molecule 1: L-AMINO ACID OXIDASE

Chain A:



• Molecule 1: L-AMINO ACID OXIDASE

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) failed to run properly; EDS was not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.65Å 109.68Å 134.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.77 – 1.85	Depositor
% Data completeness (in resolution range)	99.2 (19.77-1.85)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.151 , 0.214	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8511	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, BE2

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	0.64	0/3811	0.69	1/5146 (0.0%)
1	B	0.65	0/3770	0.72	1/5086 (0.0%)
All	All	0.65	0/7581	0.70	2/10232 (0.0%)

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	17
1	B	0	20
All	All	0	37

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	388	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	419	THR	CB-CA-C	5.04	125.21	111.60

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	GLU	Sidechain
1	A	199	PHE	Sidechain
1	A	206	PHE	Sidechain
1	A	210	GLU	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	240	ASP	Sidechain
1	A	243	TYR	Sidechain
1	A	255	ILE	Mainchain
1	A	260	GLU	Sidechain
1	A	274	GLU	Sidechain
1	A	280	SER	Mainchain
1	A	336	GLU	Sidechain
1	A	378	GLU	Sidechain
1	A	391	LYS	Mainchain
1	A	419	THR	Mainchain
1	A	423	GLU	Sidechain
1	A	488	GLN	Mainchain
1	A	59	GLU	Sidechain
1	B	11	GLY	Mainchain
1	B	159	ARG	Sidechain
1	B	180	ARG	Sidechain
1	B	227	ASP	Sidechain
1	B	233	PHE	Sidechain
1	B	243	TYR	Sidechain
1	B	260	GLU	Sidechain
1	B	269	GLU	Mainchain
1	B	279	GLY	Mainchain
1	B	288	TYR	Sidechain
1	B	298	VAL	Mainchain
1	B	34	ALA	Mainchain
1	B	386	ARG	Sidechain
1	B	409	SER	Mainchain
1	B	417	ARG	Sidechain
1	B	418	ARG	Sidechain
1	B	419	THR	Mainchain
1	B	44	ARG	Sidechain
1	B	460	HIS	Mainchain
1	B	77	PHE	Sidechain

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	3707	0	3547	37	0
1	B	3693	0	3533	75	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	10	0	3	1	0
3	B	10	0	3	1	0
4	A	481	0	0	8	1
4	B	504	0	0	15	1
All	All	8511	0	7148	102	1

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 7.

All (102) 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:420:LYS:HG3	4:B:2056:HOH:O	1.40	1.18
1:B:419:THR:HG23	1:B:420:LYS:CE	1.77	1.14
1:B:420:LYS:HG2	1:B:420:LYS:O	1.51	1.08
1:B:420:LYS:CG	4:B:2056:HOH:O	1.98	1.00
1:B:420:LYS:HB3	4:B:2437:HOH:O	1.62	0.99
1:B:419:THR:CG2	1:B:420:LYS:HE2	1.94	0.98
1:B:419:THR:HG23	1:B:420:LYS:HE2	0.97	0.97
1:B:419:THR:C	1:B:420:LYS:HD3	1.86	0.95
1:B:390:ALA:C	1:B:391:LYS:CA	2.39	0.90
1:B:420:LYS:CB	4:B:2056:HOH:O	2.18	0.89
1:B:419:THR:OG1	1:B:420:LYS:HD2	1.74	0.88
1:A:303:ASN:HD22	1:A:305:LEU:H	1.22	0.87
1:B:420:LYS:O	1:B:420:LYS:CG	2.19	0.87
1:B:419:THR:CB	1:B:420:LYS:HD3	2.04	0.87
1:B:420:LYS:HB2	4:B:2056:HOH:O	1.75	0.84
1:A:145:LYS:NZ	4:A:2168:HOH:O	2.10	0.83
1:B:419:THR:CA	1:B:420:LYS:HD3	2.08	0.83
1:B:419:THR:OG1	1:B:420:LYS:CD	2.27	0.82
1:B:90:ILE:H	1:B:469:HIS:HD2	1.24	0.81
1:A:87:GLN:HE22	1:B:109:ASN:HD21	1.28	0.81
1:A:79:ASN:HD21	1:A:239:MET:H	1.27	0.80
1:B:45:THR:C	1:B:46:ARG:CA	2.50	0.80
1:A:109:ASN:HD21	1:B:87:GLN:HE22	1.30	0.80
1:B:32:GLN:NE2	4:B:2021:HOH:O	2.15	0.78
1:B:79:ASN:HD21	1:B:239:MET:H	1.32	0.77
1:B:269:GLU:OE2	4:B:2297:HOH:O	2.02	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:NH2	1:B:420:LYS:HE3	2.02	0.75
1:A:87:GLN:HE21	1:B:340:TYR:H	1.31	0.74
1:A:171:ASP:OD2	4:A:2191:HOH:O	2.05	0.74
1:B:303:ASN:HD22	1:B:305:LEU:H	1.36	0.74
1:A:487:ALA:O	1:A:488:GLN:HB2	1.89	0.73
1:B:419:THR:CB	1:B:420:LYS:CD	2.67	0.73
1:B:296:HIS:CD2	4:B:2334:HOH:O	2.44	0.71
4:A:2178:HOH:O	1:B:208:MET:HB3	1.91	0.69
1:A:87:GLN:NE2	1:B:340:TYR:H	1.91	0.68
1:A:170[B]:SER:OG	4:A:2190:HOH:O	2.10	0.68
1:B:419:THR:CG2	1:B:420:LYS:CE	2.63	0.68
1:B:296:HIS:HD2	4:B:2334:HOH:O	1.77	0.67
1:A:111:ASN:HD21	1:A:130:ARG:HH21	1.44	0.65
1:B:139:TYR:CE1	1:B:208:MET:HG2	2.31	0.64
1:A:416:TRP:HA	1:A:419:THR:HG23	1.80	0.64
1:B:82:ALA:HA	2:B:1489:FAD:C4X	2.29	0.62
1:A:82:ALA:HA	2:A:1489:FAD:C4X	2.29	0.62
1:B:415:SER:O	1:B:419:THR:HG22	2.00	0.62
1:A:103:GLN:NE2	4:A:2111:HOH:O	2.32	0.61
1:B:137:PHE:HD1	1:B:140:MET:HE1	1.65	0.61
1:A:110:ALA:HB1	1:A:130:ARG:HB3	1.84	0.59
1:B:90:ILE:H	1:B:469:HIS:CD2	2.15	0.59
1:B:13:HIS:HD2	4:B:2316:HOH:O	1.85	0.59
1:B:46:ARG:NH1	4:B:2042:HOH:O	2.40	0.55
1:B:44:ARG:HH21	1:B:420:LYS:HE3	1.72	0.55
1:B:419:THR:OG1	1:B:420:LYS:HD3	1.99	0.55
1:A:111:ASN:ND2	1:A:130:ARG:HH21	2.06	0.54
1:A:281:LYS:NZ	4:A:2311:HOH:O	2.35	0.54
1:A:84:ARG:HH21	3:A:1490:BE2:C	2.23	0.52
1:B:76:HIS:HD2	4:B:2395:HOH:O	1.92	0.52
1:A:195:ALA:HA	1:B:462:SER:HA	1.92	0.51
1:A:415:SER:O	1:A:419:THR:HG22	2.09	0.51
1:B:419:THR:HG23	1:B:420:LYS:CD	2.39	0.51
1:A:32:GLN:HB2	4:A:2010:HOH:O	2.12	0.50
1:B:44:ARG:NH2	1:B:420:LYS:HG2	2.27	0.50
1:B:44:ARG:HH21	1:B:420:LYS:CE	2.24	0.50
1:B:208:MET:HG3	4:B:2237:HOH:O	2.11	0.49
1:B:419:THR:CG2	1:B:420:LYS:CD	2.90	0.49
1:B:266:ASN:HD21	1:B:453:LYS:H	1.61	0.48
1:B:111:ASN:ND2	1:B:130:ARG:HE	2.11	0.47
1:B:84:ARG:HH21	3:B:1490:BE2:C	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:TYR:H	1:B:87:GLN:NE2	2.12	0.47
1:B:44:ARG:HH21	1:B:420:LYS:CG	2.28	0.47
1:B:419:THR:C	1:B:420:LYS:CD	2.72	0.47
1:A:320[A]:SER:OG	1:A:381:GLU:OE1	2.17	0.47
1:B:10:LYS:O	1:B:13:HIS:CE1	2.68	0.47
1:B:79:ASN:ND2	1:B:239:MET:H	2.08	0.47
1:B:47:PRO:C	4:B:2042:HOH:O	2.53	0.46
1:A:79:ASN:ND2	1:A:239:MET:H	2.05	0.46
1:A:415:SER:O	1:A:419:THR:CG2	2.63	0.46
1:B:420:LYS:O	1:B:421:TYR:HB2	2.16	0.46
1:B:354:MET:HB2	1:B:368:VAL:HB	1.98	0.46
1:B:465:ILE:O	1:B:466:ALA:HB3	2.16	0.45
1:B:176:SER:OG	1:B:178:ASP:OD2	2.31	0.45
1:B:110:ALA:HB1	1:B:130:ARG:HB3	1.97	0.45
1:B:267:VAL:O	1:B:453:LYS:NZ	2.50	0.45
1:B:296:HIS:CD2	1:B:296:HIS:H	2.33	0.45
1:B:381:GLU:HG3	1:B:415:SER:OG	2.17	0.44
1:A:445:GLU:HG2	1:B:197:LEU:HD21	1.99	0.44
1:A:419:THR:HG21	4:A:2431:HOH:O	2.17	0.44
1:A:348:LYS:HE2	1:A:398:GLU:OE1	2.17	0.44
1:B:419:THR:HG21	4:B:2436:HOH:O	2.16	0.44
1:A:340:TYR:H	1:B:87:GLN:HE21	1.66	0.44
1:A:303:ASN:ND2	1:A:305:LEU:H	2.03	0.43
1:B:10:LYS:O	1:B:13:HIS:HE1	2.02	0.42
1:B:70:CYS:SG	1:B:72:PHE:CD2	3.11	0.42
1:A:18:LEU:HD12	1:A:18:LEU:N	2.34	0.42
1:A:32:GLN:HE22	1:A:250:ILE:HA	1.84	0.42
1:A:188:GLY:HA2	1:B:226:TYR:CE1	2.54	0.42
1:A:118:SER:O	1:A:123:SER:HB2	2.21	0.41
1:A:420:LYS:HG2	1:A:421:TYR:CD2	2.56	0.41
1:B:480:THR:O	1:B:484:GLU:HG3	2.20	0.41
1:A:462:SER:HA	1:B:195:ALA:HA	2.03	0.41
1:B:416:TRP:CZ3	1:B:420:LYS:NZ	2.85	0.41
1:B:114:VAL:HB	1:B:116:TYR:CE2	2.56	0.40
1:A:111:ASN:ND2	1:A:130:ARG:HE	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2297:HOH:O	4:B:2235:HOH:O[3_645]	2.16	0.04

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	480/489 (98%)	466 (97%)	12 (2%)	2 (0%)	34	19
1	B	469/489 (96%)	454 (97%)	13 (3%)	2 (0%)	34	19
All	All	949/978 (97%)	920 (97%)	25 (3%)	4 (0%)	34	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	488	GLN
1	B	420	LYS
1	A	176	SER
1	B	424	SER

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	392/390 (100%)	386 (98%)	6 (2%)	65	53
1	B	384/390 (98%)	381 (99%)	3 (1%)	81	76
All	All	776/780 (100%)	767 (99%)	9 (1%)	71	62

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	89	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	303	ASN
1	A	417	ARG
1	A	419	THR
1	A	488	GLN
1	B	269	GLU
1	B	420	LYS
1	B	428	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	76	HIS
1	A	79	ASN
1	A	87	GLN
1	A	89	HIS
1	A	111	ASN
1	A	150	GLN
1	A	247	GLN
1	A	266	ASN
1	A	302	GLN
1	A	303	ASN
1	A	377	GLN
1	A	481	HIS
1	B	13	HIS
1	B	76	HIS
1	B	79	ASN
1	B	87	GLN
1	B	111	ASN
1	B	266	ASN
1	B	296	HIS
1	B	303	ASN
1	B	345	ASN
1	B	377	GLN
1	B	428	ASN
1	B	463	ASN
1	B	468	GLN
1	B	469	HIS
1	B	481	HIS
1	B	488	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

Mogul failed to run properly - this section is therefore empty.

5.5 Carbohydrates

Mogul failed to run properly - this section is therefore empty.

5.6 Ligand geometry

Mogul failed to run properly - this section is therefore empty.

5.7 Other polymers

Mogul failed to run properly - this section is therefore empty.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.