



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:27 PM UTC

PDB ID : 2JFC / pdb_00002jfc
Title : M144L mutant of Nitrite Reductase from *Alcaligenes xylosoxidans* in space group P212121
Authors : Paraskevopoulos, K.; Hough, M.A.; Sawers, R.G.; Eady, R.R.; Hasnain, S.S.
Deposited on : 2007-01-31
Resolution : 2.40 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

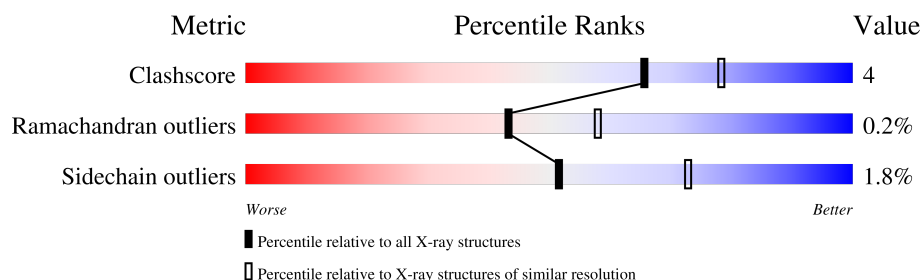
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	335	92% 7%
1	B	335	92% 8%
1	C	335	91% 8% .
1	D	335	91% 8% .
1	E	335	93% 7%
1	F	335	89% 10% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16613 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 DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2556	1632	440	474	10			
1	B	335	Total	C	N	O	S	0	0	0
			2556	1632	440	474	10			
1	C	335	Total	C	N	O	S	0	0	0
			2553	1630	439	474	10			
1	D	335	Total	C	N	O	S	0	0	0
			2549	1627	438	474	10			
1	E	335	Total	C	N	O	S	0	0	0
			2549	1627	438	474	10			
1	F	335	Total	C	N	O	S	0	0	0
			2552	1629	439	474	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	LEU	MET	engineered mutation	UNP O68601
B	144	LEU	MET	engineered mutation	UNP O68601
C	144	LEU	MET	engineered mutation	UNP O68601
D	144	LEU	MET	engineered mutation	UNP O68601
E	144	LEU	MET	engineered mutation	UNP O68601
F	144	LEU	MET	engineered mutation	UNP O68601

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		
2	C	2	Total	Cu	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total 2	Cu 2	0	0
2	E	2	Total 2	Cu 2	0	0
2	F	2	Total 2	Cu 2	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Cl 1	0	0
3	B	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0
3	F	1	Total 1	Cl 1	0	0

- Molecule 4 is water.

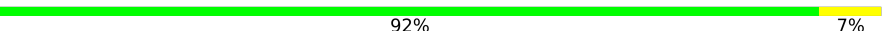
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	208	Total 208	O 208	0	0
4	B	211	Total 211	O 211	0	0
4	C	214	Total 214	O 214	0	0
4	D	211	Total 211	O 211	0	0
4	E	217	Total 217	O 217	0	0
4	F	221	Total 221	O 221	0	0

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: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain A:  92% 7%



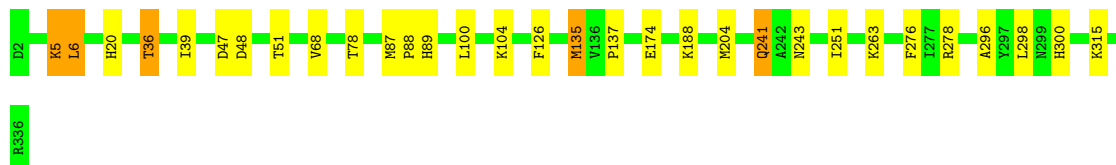
• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain B:  92% 8%



• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain C:  91% 8%

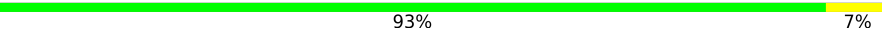


• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain D:  91% 8%



• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain E:  93% 7%



• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain F:

89%

10%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were 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	171.96Å 175.91Å 181.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.40	Depositor
% Data completeness (in resolution range)	97.6 (49.70-2.40)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.171 , 0.193	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16613	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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: CL, CU

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	0.60	0/2627	0.78	0/3581
1	B	0.59	0/2627	0.77	1/3581 (0.0%)
1	C	0.60	0/2624	0.80	0/3578
1	D	0.58	0/2620	0.78	1/3574 (0.0%)
1	E	0.60	1/2620 (0.0%)	0.78	1/3574 (0.0%)
1	F	0.58	1/2623 (0.0%)	0.79	1/3577 (0.0%)
All	All	0.59	2/15741 (0.0%)	0.78	4/21465 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	136	VAL	CA-CB	5.36	1.57	1.54
1	F	28	SER	C-N	5.26	1.41	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	TYR	N-CA-C	5.96	117.46	110.97
1	D	197	TYR	N-CA-C	5.85	117.34	110.97
1	E	197	TYR	N-CA-C	5.13	116.57	110.97
1	F	197	TYR	N-CA-C	5.04	116.47	110.97

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	HIS	Peptide
1	B	300	HIS	Peptide
1	C	300	HIS	Peptide
1	D	300	HIS	Peptide
1	E	300	HIS	Peptide
1	F	300	HIS	Peptide

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	2556	0	2504	16	0
1	B	2556	0	2504	15	0
1	C	2553	0	2495	28	0
1	D	2549	0	2484	20	0
1	E	2549	0	2484	19	0
1	F	2552	0	2493	29	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
4	A	208	0	0	3	0
4	B	211	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	214	0	0	3	0
4	D	211	0	0	2	0
4	E	217	0	0	1	0
4	F	221	0	0	4	0
All	All	16613	0	14964	114	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 4.

All (114) 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:C:87:MET:SD	4:C:2141:HOH:O	2.10	1.09
1:F:160:GLN:OE1	4:F:2130:HOH:O	1.72	1.07
1:A:168:ARG:HD3	4:A:2111:HOH:O	1.54	1.05
1:E:87:MET:HE2	4:F:2080:HOH:O	1.64	0.95
1:F:44:MET:HE3	1:F:55:ALA:CB	1.97	0.93
1:F:87:MET:HE2	4:F:2118:HOH:O	1.71	0.90
1:F:44:MET:HE3	1:F:55:ALA:HB3	1.63	0.81
1:F:44:MET:CE	1:F:55:ALA:HB3	2.10	0.81
1:B:137:PRO:HB2	1:B:204:MET:HE1	1.62	0.81
1:C:87:MET:HE3	1:C:87:MET:HA	1.59	0.80
1:E:20:HIS:HE1	1:E:68:VAL:H	1.30	0.79
1:F:44:MET:CE	1:F:55:ALA:CB	2.59	0.79
1:A:87:MET:HE2	4:A:2100:HOH:O	1.85	0.75
1:B:20:HIS:HE1	1:B:68:VAL:H	1.37	0.73
1:A:20:HIS:HE1	1:A:68:VAL:H	1.36	0.71
1:D:87:MET:HE2	4:D:2104:HOH:O	1.88	0.71
1:E:188:LYS:HD2	4:E:2152:HOH:O	1.90	0.70
1:C:20:HIS:HE1	1:C:68:VAL:H	1.39	0.69
1:F:20:HIS:HE1	1:F:68:VAL:H	1.41	0.68
1:E:137:PRO:HB2	1:E:204:MET:HE1	1.77	0.66
1:D:20:HIS:HE1	1:D:68:VAL:H	1.42	0.66
1:F:135:MET:HG2	4:F:2118:HOH:O	1.95	0.66
1:E:20:HIS:CE1	1:E:68:VAL:H	2.15	0.65
1:C:188:LYS:HD2	4:C:2134:HOH:O	1.97	0.64
1:E:137:PRO:HB2	1:E:204:MET:CE	2.28	0.62
1:A:137:PRO:HB2	1:A:204:MET:CE	2.30	0.62
1:F:137:PRO:HB2	1:F:204:MET:HE1	1.81	0.61
1:A:137:PRO:HB2	1:A:204:MET:HE1	1.83	0.61
1:A:251:ILE:HD12	1:A:296:ALA:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:PRO:HB2	1:B:204:MET:CE	2.31	0.60
1:D:137:PRO:HB2	1:D:204:MET:HE1	1.84	0.58
1:B:251:ILE:HD11	1:B:298:LEU:HD21	1.85	0.58
1:D:137:PRO:HB2	1:D:204:MET:CE	2.35	0.57
1:C:47:ASP:OD1	1:C:51:THR:HB	2.05	0.56
1:C:47:ASP:CG	1:C:51:THR:HB	2.30	0.56
1:E:251:ILE:HD11	1:E:298:LEU:HD21	1.88	0.56
1:A:20:HIS:CE1	1:A:68:VAL:H	2.22	0.56
1:F:39:ILE:HD13	1:F:89:HIS:CB	2.36	0.56
1:C:251:ILE:HD12	1:C:296:ALA:HB3	1.88	0.55
1:E:126:PHE:CE2	1:E:263:LYS:HE3	2.41	0.55
1:C:276:PHE:HB2	1:F:278:ARG:HG2	1.89	0.54
1:F:294:VAL:HG22	1:F:315:LYS:HG2	1.89	0.54
1:C:251:ILE:HD11	1:C:298:LEU:HD21	1.89	0.54
1:D:251:ILE:HD12	1:D:296:ALA:HB3	1.90	0.54
1:E:210:SER:OG	1:E:211:HIS:HD2	1.89	0.53
1:A:251:ILE:HD11	1:A:298:LEU:HD21	1.89	0.53
1:C:137:PRO:HB2	1:C:204:MET:CE	2.38	0.53
1:D:276:PHE:HB2	1:E:278:ARG:HG2	1.92	0.52
1:F:126:PHE:CE2	1:F:263:LYS:HE3	2.45	0.51
1:F:251:ILE:HD12	1:F:296:ALA:HB3	1.91	0.51
1:D:210:SER:OG	1:D:211:HIS:HD2	1.92	0.51
1:D:20:HIS:CE1	1:D:68:VAL:H	2.25	0.51
1:F:44:MET:CE	1:F:55:ALA:HB1	2.42	0.50
1:B:39:ILE:HG21	1:B:89:HIS:CD2	2.46	0.50
1:B:20:HIS:CE1	1:B:68:VAL:H	2.22	0.50
1:F:137:PRO:HB2	1:F:204:MET:CE	2.42	0.50
1:D:39:ILE:HD13	1:D:89:HIS:CB	2.41	0.50
1:B:210:SER:OG	1:B:211:HIS:HD2	1.95	0.49
1:F:56:MET:HE2	1:F:193:LEU:HD11	1.95	0.48
1:C:174:GLU:HB3	1:C:241:GLN:HG2	1.95	0.48
1:A:276:PHE:HB2	1:D:278:ARG:HG2	1.96	0.48
1:C:20:HIS:CE1	1:C:68:VAL:H	2.24	0.48
1:C:36:THR:HB	1:C:78:THR:HB	1.95	0.48
1:F:44:MET:HE2	1:F:55:ALA:HB3	1.92	0.48
1:D:294:VAL:HG22	1:D:315:LYS:HG2	1.96	0.47
1:F:20:HIS:CE1	1:F:68:VAL:H	2.27	0.47
1:B:278:ARG:HG2	1:F:276:PHE:HB2	1.95	0.47
1:C:36:THR:HG22	4:C:2025:HOH:O	2.15	0.47
1:F:87:MET:HE3	1:F:88:PRO:HD2	1.97	0.47
1:F:251:ILE:HD11	1:F:298:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLU:HB3	1:A:241:GLN:HG2	1.98	0.46
1:C:39:ILE:HD13	1:C:89:HIS:HB2	1.98	0.46
1:E:39:ILE:HD13	1:E:89:HIS:HB2	1.98	0.46
1:E:87:MET:HA	1:E:87:MET:HE3	1.98	0.46
1:C:39:ILE:HG21	1:C:89:HIS:CD2	2.50	0.46
1:F:210:SER:OG	1:F:211:HIS:HD2	1.98	0.46
1:E:251:ILE:HD12	1:E:296:ALA:HB3	1.98	0.45
1:D:56:MET:HE2	1:D:193:LEU:HD11	1.97	0.45
1:D:18:GLN:HE22	1:D:168:ARG:HH11	1.65	0.45
1:D:62:MET:O	1:D:215:ASN:HA	2.16	0.45
1:C:5:LYS:O	1:C:6:LEU:O	2.34	0.45
1:B:276:PHE:HB2	1:C:278:ARG:HG2	1.99	0.44
1:C:39:ILE:HD13	1:C:89:HIS:CB	2.47	0.44
1:C:126:PHE:CE2	1:C:263:LYS:HE3	2.52	0.44
1:E:87:MET:HE1	1:F:84:THR:C	2.43	0.44
1:E:88:PRO:HG3	1:F:110:PRO:HG2	2.00	0.44
1:F:174:GLU:HB3	1:F:241:GLN:HG2	1.99	0.44
1:B:126:PHE:CE2	1:B:263:LYS:HE3	2.53	0.44
1:A:278:ARG:HG2	1:E:276:PHE:HB2	1.99	0.43
1:C:47:ASP:OD1	1:C:51:THR:N	2.51	0.43
1:C:47:ASP:OD2	1:C:51:THR:HB	2.18	0.43
1:B:236:LEU:HD11	1:B:284:ALA:HB1	2.00	0.43
1:D:39:ILE:HD13	1:D:89:HIS:HB2	2.01	0.43
1:F:257:TRP:CZ3	1:F:270:ARG:HB3	2.54	0.43
1:E:39:ILE:HG21	1:E:89:HIS:CD2	2.53	0.43
1:A:301:ASN:HA	1:D:243:ASN:O	2.19	0.43
1:B:87:MET:HE2	1:B:138:TRP:CZ3	2.54	0.43
1:D:251:ILE:HD11	1:D:298:LEU:HD21	2.00	0.42
1:A:168:ARG:NH1	4:A:2112:HOH:O	2.52	0.42
1:B:251:ILE:HG22	1:C:100:LEU:HA	2.02	0.42
1:C:47:ASP:OD1	1:C:47:ASP:N	2.53	0.42
1:D:174:GLU:HB3	1:D:241:GLN:HG2	2.02	0.42
1:A:236:LEU:HD11	1:A:284:ALA:HB1	2.02	0.42
1:D:36:THR:HG22	4:D:2029:HOH:O	2.19	0.42
1:C:47:ASP:OD2	1:C:51:THR:CB	2.68	0.42
1:C:137:PRO:HB2	1:C:204:MET:HE1	2.01	0.41
1:F:136:VAL:HB	1:F:137:PRO:HD3	2.02	0.41
1:B:301:ASN:HA	1:C:243:ASN:O	2.20	0.41
1:E:174:GLU:HB3	1:E:241:GLN:HG2	2.02	0.41
1:A:210:SER:OG	1:A:211:HIS:HD2	2.04	0.41
1:B:100:LEU:HA	1:F:251:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:PRO:HG2	1:C:135:MET:HE1	2.04	0.40
1:D:251:ILE:HG22	1:E:100:LEU:HA	2.03	0.40
1:A:6:LEU:O	1:A:8:HIS:HD2	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	333/335 (99%)	325 (98%)	8 (2%)	0	100	100
1	B	333/335 (99%)	325 (98%)	8 (2%)	0	100	100
1	C	333/335 (99%)	324 (97%)	7 (2%)	2 (1%)	21	32
1	D	333/335 (99%)	326 (98%)	7 (2%)	0	100	100
1	E	333/335 (99%)	325 (98%)	8 (2%)	0	100	100
1	F	333/335 (99%)	323 (97%)	9 (3%)	1 (0%)	36	50
All	All	1998/2010 (99%)	1948 (98%)	47 (2%)	3 (0%)	43	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	28	SER
1	C	5	LYS
1	C	6	LEU

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	266/270 (98%)	260 (98%)	6 (2%)	44	66
1	B	266/270 (98%)	261 (98%)	5 (2%)	50	71
1	C	265/270 (98%)	259 (98%)	6 (2%)	44	66
1	D	264/270 (98%)	260 (98%)	4 (2%)	57	77
1	E	264/270 (98%)	262 (99%)	2 (1%)	73	86
1	F	265/270 (98%)	260 (98%)	5 (2%)	50	71
All	All	1590/1620 (98%)	1562 (98%)	28 (2%)	51	73

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	36	THR
1	A	46	ILE
1	A	48	ASP
1	A	133	GLU
1	A	241	GLN
1	B	36	THR
1	B	46	ILE
1	B	104	LYS
1	B	168	ARG
1	B	241	GLN
1	C	36	THR
1	C	48	ASP
1	C	104	LYS
1	C	135	MET
1	C	241	GLN
1	C	315	LYS
1	D	36	THR
1	D	104	LYS
1	D	241	GLN
1	D	315	LYS
1	E	36	THR
1	E	241	GLN
1	F	9	THR
1	F	36	THR
1	F	133	GLU
1	F	135	MET

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Mol	Chain	Res	Type
1	F	241	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	20	HIS
1	A	76	GLN
1	A	113	GLN
1	A	202	GLN
1	A	211	HIS
1	B	8	HIS
1	B	18	GLN
1	B	20	HIS
1	B	76	GLN
1	B	113	GLN
1	B	211	HIS
1	C	18	GLN
1	C	20	HIS
1	C	76	GLN
1	C	113	GLN
1	C	211	HIS
1	D	18	GLN
1	D	20	HIS
1	D	76	GLN
1	D	113	GLN
1	D	202	GLN
1	D	211	HIS
1	E	8	HIS
1	E	18	GLN
1	E	20	HIS
1	E	113	GLN
1	E	202	GLN
1	E	211	HIS
1	F	8	HIS
1	F	20	HIS
1	F	76	GLN
1	F	113	GLN
1	F	160	GLN
1	F	165	HIS
1	F	211	HIS

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 16 ligands modelled in this entry, 16 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

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.