



Full wwPDB EM Validation Report ⓘ

Jul 15, 2025 – 11:15 AM JST

PDB ID : 9IZW / pdb_00009izw
EMDB ID : EMD-61044
Title : Cryo-EM structure of ALDH6A1-S262Y
Authors : Su, G.; Xu, Y.; Luan, X.
Deposited on : 2024-08-01
Resolution : 3.12 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

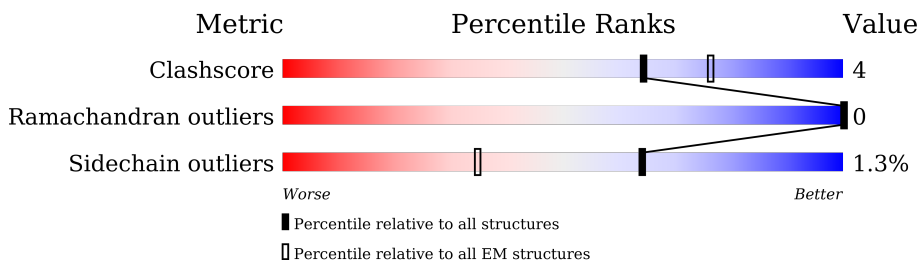
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.12 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	509	 91% 7% .
1	B	509	 88% 9% ..
1	C	509	 87% 10% .
1	D	509	 86% 11% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15196 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Methylmalonate-semialdehyde/malonate-semialdehyde dehydrogenase [acylating], mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	499	Total	C	N	O	S	0	0
			3799	2411	652	710	26		
1	B	499	Total	C	N	O	S	0	0
			3799	2411	652	710	26		
1	C	499	Total	C	N	O	S	0	0
			3799	2411	652	710	26		
1	D	499	Total	C	N	O	S	0	0
			3799	2411	652	710	26		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q02252
A	230	TYR	SER	engineered mutation	UNP Q02252
A	504	GLU	-	expression tag	UNP Q02252
A	505	ASN	-	expression tag	UNP Q02252
A	506	LEU	-	expression tag	UNP Q02252
A	507	TYR	-	expression tag	UNP Q02252
A	508	PHE	-	expression tag	UNP Q02252
A	509	GLN	-	expression tag	UNP Q02252
B	1	MET	-	initiating methionine	UNP Q02252
B	230	TYR	SER	engineered mutation	UNP Q02252
B	504	GLU	-	expression tag	UNP Q02252
B	505	ASN	-	expression tag	UNP Q02252
B	506	LEU	-	expression tag	UNP Q02252
B	507	TYR	-	expression tag	UNP Q02252
B	508	PHE	-	expression tag	UNP Q02252
B	509	GLN	-	expression tag	UNP Q02252
C	1	MET	-	initiating methionine	UNP Q02252
C	230	TYR	SER	engineered mutation	UNP Q02252
C	504	GLU	-	expression tag	UNP Q02252
C	505	ASN	-	expression tag	UNP Q02252
C	506	LEU	-	expression tag	UNP Q02252

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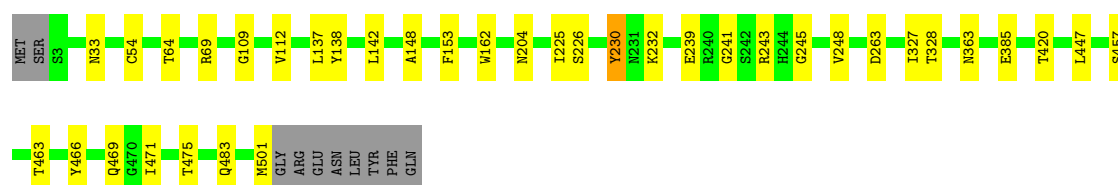
Chain	Residue	Modelled	Actual	Comment	Reference
C	507	TYR	-	expression tag	UNP Q02252
C	508	PHE	-	expression tag	UNP Q02252
C	509	GLN	-	expression tag	UNP Q02252
D	1	MET	-	initiating methionine	UNP Q02252
D	230	TYR	SER	engineered mutation	UNP Q02252
D	504	GLU	-	expression tag	UNP Q02252
D	505	ASN	-	expression tag	UNP Q02252
D	506	LEU	-	expression tag	UNP Q02252
D	507	TYR	-	expression tag	UNP Q02252
D	508	PHE	-	expression tag	UNP Q02252
D	509	GLN	-	expression tag	UNP Q02252

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.

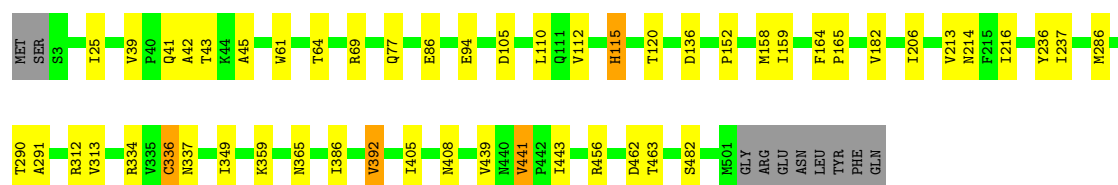
- Molecule 1: Methylmalonate-semialdehyde/malonate-semialdehyde dehydrogenase [acylating], mitochondrial

Chain A:  91% 7% .



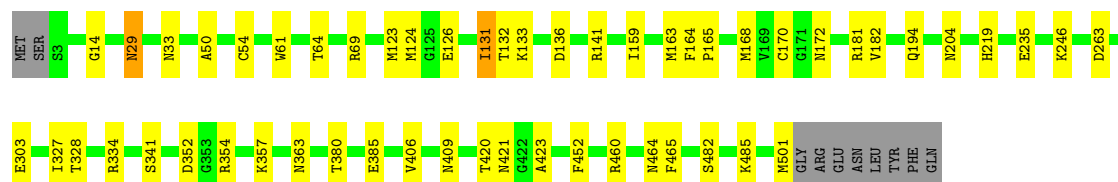
- Molecule 1: Methylmalonate-semialdehyde/malonate-semialdehyde dehydrogenase [acylating], mitochondrial

Chain B:  88% 9% ..




- Molecule 1: Methylmalonate-semialdehyde/malonate-semialdehyde dehydrogenase [acylating], mitochondrial

Chain C:  87% 10% .



- Molecule 1: Methylmalonate-semialdehyde/malonate-semialdehyde dehydrogenase [acylating], mitochondrial

Chain D:  86% 11% ..

MET	SER	S3	S19	K20	N29	N33	Q41	A42	C54	W61	T64	Y76	E94	T132	K133	D136	L137	Y138	N154	F164	P165	M166	A167	M168	V169	R181	V182	L189	N204	H219	F227	V228	G229	Y230	N231	K232	K246	A250	N251
M252	G253	E267	N271	V274	L293	K298	E303	N314	A315	I327	T328	D340	R354	I386	L399	P410	Y411	T420	V439	S457	R460	I471	T475	E487	L491	M501	GLY	ARG	GLU	ASN	LEU	TYR	PHE	GLN					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175674	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.13	0/3877	0.27	0/5257
1	B	0.12	0/3877	0.29	0/5257
1	C	0.12	0/3877	0.29	1/5257 (0.0%)
1	D	0.25	2/3877 (0.1%)	0.38	2/5257 (0.0%)
All	All	0.17	2/15508 (0.0%)	0.31	3/21028 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	228	VAL	CA-C	-6.74	1.44	1.52
1	D	228	VAL	N-CA	-5.36	1.39	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	228	VAL	N-CA-C	-12.48	90.15	108.12
1	D	229	GLY	N-CA-C	-5.98	101.39	111.08
1	C	131	ILE	N-CA-C	-5.25	107.30	111.81

There are no chirality outliers.

There are no planarity outliers.

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	3799	0	3832	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3799	0	3832	28	0
1	C	3799	0	3832	31	0
1	D	3799	0	3832	36	0
All	All	15196	0	15328	120	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 (120) 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:D:136:ASP:OD2	1:D:138:TYR:OH	1.89	0.89
1:B:136:ASP:OD1	1:B:482:SER:OG	2.00	0.79
1:C:219:HIS:O	1:C:246:LYS:NZ	2.19	0.76
1:C:33:ASN:ND2	1:C:363:ASN:O	2.20	0.74
1:A:263:ASP:O	1:A:420:THR:OG1	2.04	0.74
1:D:54:CYS:SG	1:D:204:ASN:ND2	2.62	0.73
1:C:181:ARG:O	1:C:181:ARG:NH1	2.21	0.73
1:C:54:CYS:SG	1:C:204:ASN:ND2	2.62	0.73
1:C:64:THR:O	1:C:69:ARG:NH1	2.21	0.73
1:D:471:ILE:O	1:D:475:THR:OG1	2.04	0.73
1:B:334:ARG:NH2	1:B:386:ILE:O	2.24	0.71
1:B:64:THR:O	1:B:69:ARG:NH1	2.24	0.70
1:B:206:ILE:HD11	1:B:216:ILE:HD11	1.73	0.70
1:C:406:VAL:O	1:C:409:ASN:ND2	2.24	0.70
1:D:227:PHE:CZ	1:D:229:GLY:HA3	2.27	0.68
1:C:263:ASP:O	1:C:420:THR:OG1	2.10	0.68
1:C:124:MET:O	1:C:141:ARG:N	2.28	0.66
1:D:410:PRO:O	1:D:457:SER:OG	2.13	0.66
1:A:420:THR:O	1:C:421:ASN:ND2	2.30	0.65
1:A:463:THR:HG21	1:A:469:GLN:HB3	1.79	0.65
1:A:501:MET:HA	1:A:501:MET:HE3	1.81	0.63
1:C:50:ALA:O	1:C:204:ASN:ND2	2.33	0.62
1:C:132:THR:HG23	1:C:501:MET:HG3	1.81	0.62
1:A:142:LEU:O	1:A:475:THR:OG1	2.13	0.60
1:A:230:TYR:OH	1:A:385:GLU:HB2	2.02	0.60
1:B:41:GLN:NE2	1:B:42:ALA:O	2.35	0.59
1:C:132:THR:HG22	1:C:133:LYS:H	1.67	0.59
1:A:112:VAL:HG11	1:A:162:TRP:CD1	2.42	0.55
1:A:225:ILE:HB	1:A:248:VAL:HG12	1.88	0.55
1:C:131:ILE:O	1:C:501:MET:HE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:ASP:OD1	1:D:354:ARG:NH1	2.40	0.54
1:C:452:PHE:O	1:C:464:ASN:ND2	2.42	0.53
1:C:136:ASP:OD2	1:C:482:SER:OG	2.16	0.52
1:D:61:TRP:O	1:D:64:THR:OG1	2.27	0.52
1:C:14:GLY:O	1:C:194:GLN:NE2	2.40	0.51
1:C:61:TRP:NE1	1:C:168:MET:O	2.41	0.51
1:B:86:GLU:N	1:B:86:GLU:OE1	2.43	0.50
1:D:132:THR:HG22	1:D:133:LYS:H	1.77	0.50
1:B:290:THR:HG22	1:B:291:ALA:H	1.77	0.50
1:B:349:ILE:O	1:B:349:ILE:HG23	2.12	0.50
1:C:235:GLU:OE1	1:C:460:ARG:NH1	2.45	0.50
1:B:77:GLN:HG3	1:B:110:LEU:HD11	1.94	0.49
1:D:181:ARG:HE	1:D:328:THR:HG22	1.76	0.49
1:A:239:GLU:OE2	1:A:243:ARG:NH2	2.46	0.49
1:B:439:VAL:HG13	1:B:439:VAL:O	2.12	0.49
1:B:405:ILE:O	1:B:408:ASN:ND2	2.46	0.48
1:D:229:GLY:O	1:D:252:MET:HA	2.13	0.48
1:B:312:ARG:NH2	1:B:313:VAL:O	2.46	0.48
1:B:456:ARG:NE	1:B:456:ARG:O	2.46	0.48
1:D:164:PHE:N	1:D:165:PRO:CD	2.77	0.48
1:D:327:ILE:HG23	1:D:328:THR:HG23	1.95	0.48
1:B:462:ASP:OD2	1:B:463:THR:N	2.47	0.47
1:A:112:VAL:HG11	1:A:162:TRP:HD1	1.78	0.47
1:D:439:VAL:O	1:D:439:VAL:HG23	2.14	0.47
1:C:126:GLU:N	1:C:126:GLU:OE2	2.46	0.47
1:A:153:PHE:CD1	1:A:327:ILE:HG21	2.50	0.47
1:A:327:ILE:HG23	1:A:328:THR:HG23	1.96	0.47
1:A:501:MET:HE3	1:A:501:MET:CA	2.44	0.47
1:D:19:SER:OG	1:D:20:LYS:N	2.48	0.47
1:A:112:VAL:HG23	1:A:466:TYR:CE1	2.51	0.46
1:B:152:PRO:HD2	1:B:159:ILE:HD13	1.97	0.46
1:D:136:ASP:N	1:D:136:ASP:OD1	2.47	0.46
1:A:64:THR:O	1:A:69:ARG:NH1	2.48	0.46
1:D:219:HIS:O	1:D:246:LYS:NZ	2.47	0.46
1:D:76:TYR:OH	1:D:189:LEU:O	2.30	0.46
1:D:94:GLU:HB2	1:D:182:VAL:HG23	1.97	0.46
1:B:290:THR:HG23	1:B:392:VAL:HG23	1.98	0.46
1:D:61:TRP:NE1	1:D:168:MET:O	2.48	0.45
1:B:164:PHE:N	1:B:165:PRO:CD	2.79	0.45
1:C:163:MET:HE2	1:C:465:PHE:HE1	1.80	0.45
1:D:491:LEU:HD23	1:D:491:LEU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:GLU:OE1	1:D:303:GLU:N	2.45	0.45
1:D:181:ARG:NH2	1:D:327:ILE:O	2.44	0.44
1:D:267:GLU:OE2	1:D:271:ASN:ND2	2.47	0.44
1:C:164:PHE:N	1:C:165:PRO:CD	2.81	0.44
1:B:214:ASN:OD1	1:B:236:TYR:OH	2.35	0.44
1:D:94:GLU:CB	1:D:182:VAL:HG23	2.48	0.44
1:D:293:LEU:HD13	1:D:298:LYS:HA	2.00	0.44
1:D:314:ASN:OD1	1:D:315:ALA:N	2.49	0.44
1:B:43:THR:HG23	1:B:45:ALA:H	1.82	0.43
1:C:334:ARG:NH2	1:C:385:GLU:O	2.51	0.43
1:A:54:CYS:SG	1:A:204:ASN:ND2	2.91	0.43
1:D:132:THR:HG22	1:D:133:LYS:N	2.33	0.43
1:C:123:MET:O	1:C:124:MET:C	2.62	0.43
1:B:25:ILE:O	1:B:39:VAL:N	2.41	0.43
1:A:33:ASN:ND2	1:A:363:ASN:O	2.51	0.43
1:C:182:VAL:HG22	1:C:182:VAL:O	2.19	0.43
1:B:94:GLU:CB	1:B:182:VAL:HG13	2.49	0.42
1:C:170:CYS:O	1:C:172:ASN:ND2	2.52	0.42
1:C:421:ASN:OD1	1:C:423:ALA:N	2.49	0.42
1:D:420:THR:O	1:D:420:THR:HG22	2.19	0.42
1:A:137:LEU:HD23	1:A:138:TYR:N	2.33	0.42
1:B:336:CYS:SG	1:B:337:ASN:N	2.92	0.42
1:D:182:VAL:O	1:D:182:VAL:HG22	2.19	0.42
1:A:471:ILE:O	1:A:475:THR:HG22	2.20	0.42
1:A:483:GLN:NE2	1:B:441:VAL:HG12	2.34	0.42
1:A:457:SER:O	1:A:457:SER:OG	2.34	0.42
1:C:352:ASP:OD1	1:C:354:ARG:NH1	2.52	0.42
1:D:230:TYR:HA	1:D:253:GLY:H	1.85	0.42
1:A:225:ILE:HG22	1:A:226:SER:H	1.83	0.42
1:B:112:VAL:O	1:B:115:HIS:ND1	2.42	0.42
1:C:341:SER:OG	1:C:380:THR:OG1	2.29	0.42
1:C:327:ILE:HG23	1:C:328:THR:N	2.34	0.42
1:D:166:MET:HA	1:D:169:VAL:HG12	2.02	0.42
1:D:399:LEU:O	1:D:399:LEU:HD23	2.19	0.42
1:B:105:ASP:HA	1:B:158:MET:HE2	2.01	0.42
1:A:109:GLY:O	1:A:112:VAL:HG12	2.20	0.41
1:A:148:ALA:HB3	1:A:225:ILE:HG23	2.03	0.41
1:A:248:VAL:O	1:A:248:VAL:HG23	2.21	0.41
1:D:154:ASN:CG	1:D:230:TYR:HH	2.28	0.41
1:B:286:MET:SD	1:B:286:MET:N	2.94	0.41
1:C:29:ASN:O	1:C:33:ASN:N	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:GLN:O	1:D:42:ALA:C	2.64	0.41
1:A:225:ILE:HG22	1:A:226:SER:N	2.36	0.41
1:B:61:TRP:O	1:B:69:ARG:NH1	2.53	0.41
1:A:241:GLY:O	1:A:245:GLY:N	2.53	0.41
1:B:213:VAL:HG21	1:B:237:ILE:HD11	2.02	0.40
1:D:29:ASN:O	1:D:33:ASN:N	2.42	0.40
1:D:250:ALA:HB3	1:D:460:ARG:HB3	2.04	0.40
1:C:159:ILE:HG23	1:C:163:MET:HE3	2.03	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 PDB entries followed by that with respect to all EM entries.

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	497/509 (98%)	474 (95%)	23 (5%)	0	100	100
1	B	497/509 (98%)	472 (95%)	25 (5%)	0	100	100
1	C	497/509 (98%)	475 (96%)	22 (4%)	0	100	100
1	D	497/509 (98%)	476 (96%)	21 (4%)	0	100	100
All	All	1988/2036 (98%)	1897 (95%)	91 (5%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	411/420 (98%)	408 (99%)	3 (1%)	81	90
1	B	411/420 (98%)	403 (98%)	8 (2%)	52	73
1	C	411/420 (98%)	407 (99%)	4 (1%)	73	85
1	D	411/420 (98%)	404 (98%)	7 (2%)	56	76
All	All	1644/1680 (98%)	1622 (99%)	22 (1%)	64	80

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	TYR
1	A	232	LYS
1	A	447	LEU
1	B	115	HIS
1	B	120	THR
1	B	336	CYS
1	B	359	LYS
1	B	365	ASN
1	B	392	VAL
1	B	441	VAL
1	B	443	ILE
1	C	29	ASN
1	C	303	GLU
1	C	357	LYS
1	C	485	LYS
1	D	136	ASP
1	D	154	ASN
1	D	232	LYS
1	D	274	VAL
1	D	386	ILE
1	D	411	TYR
1	D	487	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	ASN
1	A	257	HIS
1	A	314	ASN
1	A	374	ASN
1	A	440	ASN

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Mol	Chain	Res	Type
1	A	483	GLN
1	B	251	ASN
1	B	421	ASN
1	B	469	GLN
1	B	483	GLN
1	C	154	ASN
1	C	204	ASN
1	C	249	GLN
1	C	268	ASN
1	D	204	ASN
1	D	231	ASN
1	D	268	ASN
1	D	374	ASN
1	D	472	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](#)

There are no ligands in this entry.

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.