



Full wwPDB X-ray Structure Validation Report

Jan 23, 2021 – 02:23 PM EST


PDB ID : 1KCX
Title : X-ray structure of NYSGRC target T-45
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Deposited on : 2001-11-11
Resolution : 2.12 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 following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : 2.16

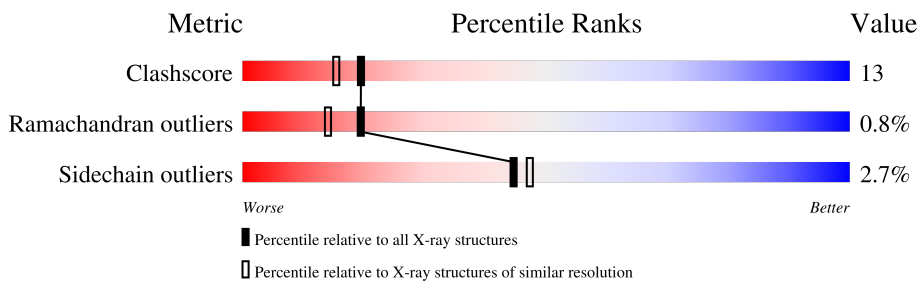
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)

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	518	
1	B	518	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8086 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 DIHYDROPYRIMIDINASE RELATED PROTEIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	476	3641	2312	616	695	18	0	0	0
1	B	476	3641	2312	616	695	18	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	421	421	421	0	0
2	B	383	383	383	0	0

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	123.40Å 152.11Å 157.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.12	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.12)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.233	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8086	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

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	0.55	5/3719 (0.1%)	0.75	8/5042 (0.2%)
1	B	0.40	0/3719	0.66	1/5042 (0.0%)
All	All	0.48	5/7438 (0.1%)	0.71	9/10084 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	417	MET	CG-SD	13.79	2.17	1.81
1	A	416	LYS	CG-CD	9.95	1.86	1.52
1	A	416	LYS	CB-CG	9.29	1.77	1.52
1	A	417	MET	SD-CE	8.63	2.26	1.77
1	A	416	LYS	CD-CE	7.74	1.70	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	MET	N-CA-C	11.21	141.25	111.00
1	A	417	MET	C-N-CA	-9.49	97.97	121.70
1	A	417	MET	CG-SD-CE	9.21	114.94	100.20
1	A	416	LYS	CD-CE-NZ	7.65	129.30	111.70
1	A	415	ASP	CB-CG-OD1	-6.89	112.10	118.30
1	A	415	ASP	N-CA-C	6.27	127.92	111.00
1	A	417	MET	O-C-N	-5.40	114.06	122.70
1	B	395	TYR	N-CA-C	5.36	125.47	111.00
1	A	416	LYS	CB-CG-CD	5.31	125.42	111.60

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	3641	0	3603	95	0
1	B	3641	0	3603	90	0
2	A	421	0	0	7	1
2	B	383	0	0	5	0
All	All	8086	0	7206	185	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 13.

All (185) 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:416:LYS:CG	1:A:416:LYS:CB	1.77	1.58
1:A:416:LYS:CG	1:A:416:LYS:CD	1.86	1.54
1:A:417:MET:SD	1:A:417:MET:CG	2.17	1.33
1:A:417:MET:SD	1:A:417:MET:CE	2.26	1.24
1:A:417:MET:SD	1:A:442:SER:OG	2.11	1.07
1:A:416:LYS:HE3	1:A:417:MET:CG	1.89	1.03
1:A:416:LYS:CE	1:A:417:MET:HG3	1.88	1.01
1:B:166:VAL:HB	1:B:176:MET:HE3	1.48	0.94
1:A:416:LYS:HE3	1:A:417:MET:HG3	0.95	0.93
1:A:218:THR:HB	1:A:346:ASP:O	1.69	0.92
1:B:389:ALA:HB1	1:B:395:TYR:HA	1.49	0.91
1:A:416:LYS:HG3	1:A:417:MET:SD	2.11	0.91
1:B:432:ASN:HD22	1:B:434:PHE:H	1.23	0.86
1:A:432:ASN:HD22	1:A:434:PHE:H	1.24	0.84
1:B:111:GLU:HB3	1:B:112:PRO:CD	2.08	0.84
1:B:416:LYS:O	1:B:416:LYS:HG3	1.79	0.82
1:B:166:VAL:HB	1:B:176:MET:CE	2.10	0.81
1:A:266:LEU:HD11	1:A:270:LYS:HE3	1.65	0.77
1:A:256:MET:HE1	1:A:279:ILE:HG12	1.68	0.76
1:A:416:LYS:O	1:A:417:MET:SD	2.44	0.76
1:B:111:GLU:HB3	1:B:112:PRO:HD2	1.68	0.75
1:A:416:LYS:HD2	1:A:417:MET:HB3	1.69	0.73
1:A:389:ALA:HB1	1:A:395:TYR:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:O	1:A:50:ILE:HG22	1.92	0.70
1:A:25:ILE:HB	1:A:66:ILE:HG22	1.75	0.69
1:B:138:HIS:HD2	1:B:163:SER:OG	1.76	0.69
1:A:256:MET:HG3	1:A:282:SER:HB3	1.77	0.67
1:A:417:MET:HE1	1:A:442:SER:H	1.60	0.67
1:B:210:LYS:O	1:B:214:GLU:HG2	1.95	0.66
1:A:149:ARG:O	1:A:153:GLU:HG3	1.96	0.66
1:B:432:ASN:ND2	1:B:434:PHE:H	1.93	0.66
1:B:141:ILE:HD13	1:B:144:TRP:HZ3	1.60	0.65
1:B:341:LYS:HA	1:B:352:PRO:HD2	1.77	0.65
1:A:432:ASN:ND2	1:A:434:PHE:H	1.94	0.64
1:A:395:TYR:O	1:A:398:LYS:O	2.15	0.64
1:A:16:ARG:HD3	1:A:36:TYR:OH	1.99	0.63
1:B:395:TYR:O	1:B:398:LYS:O	2.17	0.62
1:B:72:VAL:O	1:B:138:HIS:HE1	1.82	0.62
1:B:111:GLU:CB	1:B:112:PRO:CD	2.79	0.61
1:B:255:VAL:O	1:B:256:MET:HE3	2.01	0.61
1:B:25:ILE:HB	1:B:66:ILE:HG22	1.83	0.61
1:A:295:TRP:CZ2	1:A:345:LYS:HA	2.36	0.60
1:B:77:GLN:HE22	1:B:126:ALA:CB	2.15	0.60
1:A:415:ASP:O	1:A:416:LYS:HB3	2.00	0.60
1:A:256:MET:HA	1:A:256:MET:HE2	1.85	0.59
1:A:416:LYS:CD	1:A:417:MET:HB3	2.32	0.59
1:A:416:LYS:CG	1:A:416:LYS:CA	2.76	0.59
1:B:16:ARG:CZ	1:B:52:PRO:HG2	2.33	0.59
1:A:17:LEU:HD13	1:A:56:LYS:HD3	1.85	0.58
1:B:112:PRO:HA	2:B:556:HOH:O	2.04	0.58
1:B:245:ARG:HA	1:B:245:ARG:NE	2.19	0.57
1:B:258:LYS:HG2	1:B:316:TYR:CD2	2.39	0.57
1:A:138:HIS:HD2	1:A:163:SER:OG	1.88	0.57
1:A:417:MET:HE1	1:A:442:SER:O	2.05	0.56
1:B:64:MET:HE3	1:B:414:PRO:HD3	1.86	0.56
1:A:256:MET:HE2	1:A:256:MET:CA	2.36	0.56
1:B:64:MET:CE	1:B:414:PRO:HD3	2.36	0.56
1:A:255:VAL:O	1:A:256:MET:HE2	2.06	0.56
1:A:416:LYS:C	1:A:417:MET:SD	2.84	0.56
1:B:200:GLU:OE2	1:B:227:ARG:NH1	2.39	0.55
1:B:421:THR:HB	2:B:624:HOH:O	2.07	0.55
1:B:256:MET:HE2	1:B:279:ILE:HG12	1.89	0.55
1:B:304:SER:HA	1:B:305:PRO:C	2.28	0.55
1:B:256:MET:HG3	1:B:282:SER:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:CD1	1:A:270:LYS:HE3	2.36	0.54
1:A:304:SER:HA	1:A:305:PRO:C	2.27	0.54
1:B:139:VAL:HG23	1:B:161:VAL:HG11	1.90	0.54
1:A:413:ASP:HB3	1:A:417:MET:HE3	1.91	0.53
1:A:208:GLU:O	1:A:212:ILE:HG12	2.09	0.53
1:A:413:ASP:O	1:A:417:MET:HE1	2.07	0.53
1:B:295:TRP:CZ2	1:B:345:LYS:HA	2.44	0.53
1:B:459:ILE:HD12	1:B:461:VAL:HG13	1.91	0.52
1:B:47:GLU:O	1:B:48:ASN:CB	2.56	0.52
1:B:342:ALA:C	1:B:344:GLY:H	2.13	0.52
1:B:369:ALA:HB1	1:B:375:MET:HG2	1.90	0.52
1:A:72:VAL:O	1:A:138:HIS:HE1	1.93	0.52
1:B:397:ARG:HG3	1:B:398:LYS:HG2	1.93	0.51
1:B:256:MET:HA	1:B:256:MET:HE3	1.93	0.51
1:A:395:TYR:O	1:A:396:PRO:C	2.49	0.50
1:B:49:LEU:C	1:B:50:ILE:HG13	2.32	0.50
1:A:49:LEU:O	1:A:50:ILE:HB	2.11	0.50
1:B:256:MET:CA	1:B:256:MET:HE3	2.41	0.50
1:A:327:GLN:N	1:A:327:GLN:CD	2.65	0.50
1:A:334:CYS:O	1:A:354:GLY:HA3	2.11	0.50
1:B:395:TYR:CG	1:B:396:PRO:N	2.79	0.50
1:B:64:MET:CE	1:B:414:PRO:HB3	2.42	0.50
1:A:50:ILE:O	1:A:50:ILE:CG2	2.60	0.50
1:A:270:LYS:HD2	2:A:880:HOH:O	2.12	0.49
1:B:77:GLN:HE21	1:B:89:PHE:HD2	1.58	0.49
1:B:208:GLU:O	1:B:212:ILE:HG12	2.13	0.49
1:B:75:TYR:HB3	1:B:78:LYS:HB2	1.94	0.49
1:A:56:LYS:HE2	1:A:452:ILE:HD12	1.95	0.49
1:B:108:VAL:HG22	1:B:123:TRP:CG	2.48	0.49
1:A:417:MET:CE	1:A:442:SER:O	2.61	0.48
1:B:228:PRO:HG2	1:B:231:LEU:HG	1.96	0.48
1:B:200:GLU:CD	1:B:227:ARG:NH1	2.67	0.48
1:B:90:PHE:CD1	1:B:463:LYS:HG3	2.49	0.48
1:B:198:HIS:HE1	1:B:200:GLU:OE2	1.97	0.48
1:B:16:ARG:HD3	1:B:55:VAL:HG22	1.96	0.48
1:B:432:ASN:C	1:B:432:ASN:HD22	2.17	0.48
1:A:83:MET:HE3	1:A:352:PRO:HG3	1.96	0.47
1:A:442:SER:HB2	1:A:443:PRO:CD	2.44	0.47
1:B:255:VAL:C	1:B:256:MET:HE3	2.34	0.47
1:B:303:THR:HB	1:B:355:VAL:HG13	1.96	0.47
1:B:295:TRP:CH2	1:B:342:ALA:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:HIS:HD2	2:A:569:HOH:O	1.99	0.46
1:A:432:ASN:HD22	1:A:432:ASN:C	2.18	0.46
1:B:77:GLN:HE22	1:B:126:ALA:HB1	1.81	0.46
1:B:175:GLN:OE1	1:B:202:GLY:HA3	2.15	0.46
1:B:64:MET:HE1	1:B:414:PRO:HB3	1.97	0.46
1:A:421:THR:HG21	1:A:423:LYS:HZ3	1.80	0.46
1:A:49:LEU:O	1:A:50:ILE:CB	2.63	0.46
1:B:77:GLN:NE2	1:B:89:PHE:CD2	2.84	0.46
1:A:15:ASP:HB2	2:A:828:HOH:O	2.15	0.46
1:B:111:GLU:HB2	1:B:114:SER:OG	2.15	0.46
1:A:417:MET:CG	1:A:442:SER:OG	2.63	0.46
1:A:59:GLU:HB3	1:A:61:ASN:OD1	2.16	0.46
1:B:169:ALA:HB2	1:B:200:GLU:HB2	1.97	0.46
1:A:75:TYR:HB3	1:A:78:LYS:HB2	1.97	0.45
1:B:68:GLY:HA3	1:B:102:THR:OG1	2.16	0.45
1:B:16:ARG:NH1	1:B:52:PRO:HG2	2.31	0.45
1:B:141:ILE:HD13	1:B:144:TRP:CZ3	2.47	0.45
1:B:246:ILE:O	1:B:247:ASN:HB3	2.17	0.45
1:B:200:GLU:OE1	1:B:227:ARG:NH1	2.48	0.45
1:B:327:GLN:CD	1:B:327:GLN:N	2.70	0.45
1:B:342:ALA:C	1:B:344:GLY:N	2.70	0.45
1:A:416:LYS:HD3	2:A:922:HOH:O	2.15	0.45
1:A:242:ILE:HG22	1:A:246:ILE:HD12	1.99	0.45
1:A:269:LYS:HE3	2:B:738:HOH:O	2.17	0.45
1:A:481:ARG:O	1:A:485:ARG:HG3	2.17	0.45
1:B:51:VAL:HA	1:B:52:PRO:HD3	1.89	0.45
1:A:413:ASP:HB3	1:A:417:MET:CE	2.47	0.44
1:B:94:LYS:HG2	1:B:459:ILE:HD13	1.98	0.44
1:B:95:ALA:O	1:B:359:GLU:HG3	2.17	0.44
1:B:196:LEU:HG	1:B:251:TYR:CD1	2.53	0.44
1:B:75:TYR:HB2	1:B:334:CYS:HB3	2.00	0.44
1:A:58:ILE:HD11	1:A:452:ILE:HD11	2.00	0.44
1:B:169:ALA:O	1:B:170:TYR:HB2	2.18	0.44
1:B:334:CYS:O	1:B:354:GLY:HA3	2.18	0.43
1:A:20:ARG:HE	1:A:20:ARG:HB3	1.56	0.43
1:A:446:VAL:HB	1:A:454:PHE:HB3	2.00	0.43
1:B:124:HIS:CE1	1:B:128:ASP:OD2	2.71	0.43
1:B:444:LEU:HA	1:B:444:LEU:HD23	1.88	0.43
1:A:38:GLU:HB3	1:A:43:LYS:NZ	2.34	0.43
1:A:77:GLN:HE22	1:A:126:ALA:HB1	1.84	0.43
1:B:141:ILE:HG21	1:B:144:TRP:CZ3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLN:OE1	1:A:202:GLY:HA3	2.19	0.43
1:A:83:MET:CE	1:A:352:PRO:HG3	2.48	0.43
1:B:17:LEU:HD12	1:B:56:LYS:O	2.19	0.43
1:B:321:LEU:HD12	1:B:326:LEU:O	2.19	0.43
1:A:319:SER:OG	1:A:374:LYS:HE3	2.18	0.42
1:A:23:ARG:NH1	1:A:25:ILE:HD11	2.34	0.42
1:A:355:VAL:HA	2:A:933:HOH:O	2.19	0.42
1:A:38:GLU:HB3	1:A:43:LYS:HG3	2.00	0.42
1:A:77:GLN:HE21	1:A:89:PHE:HD2	1.66	0.42
1:A:347:ASN:HB3	1:A:350:LEU:HD12	2.02	0.42
1:A:108:VAL:HG22	1:A:123:TRP:CG	2.55	0.42
1:B:77:GLN:HG2	2:B:814:HOH:O	2.19	0.42
1:B:77:GLN:NE2	1:B:89:PHE:HD2	2.16	0.42
1:B:395:TYR:O	1:B:396:PRO:C	2.58	0.42
1:A:227:ARG:NH2	2:A:600:HOH:O	2.52	0.42
1:B:18:LEU:HD12	1:B:35:VAL:O	2.20	0.42
1:A:341:LYS:HA	1:A:352:PRO:HD2	2.02	0.42
1:A:417:MET:SD	1:A:442:SER:CB	3.05	0.42
1:B:395:TYR:C	1:B:395:TYR:CD1	2.91	0.42
1:A:145:TYR:OH	1:A:151:GLU:OE2	2.33	0.41
1:A:266:LEU:O	1:A:269:LYS:HG2	2.20	0.41
1:A:294:ASN:C	1:A:294:ASN:OD1	2.57	0.41
1:A:479:TYR:O	1:A:483:ARG:HG3	2.20	0.41
1:A:138:HIS:CD2	1:A:163:SER:OG	2.71	0.41
1:A:427:SER:OG	1:A:429:VAL:HG22	2.19	0.41
1:A:308:SER:HA	1:A:309:PRO:HD3	1.90	0.41
1:A:417:MET:CE	1:A:442:SER:OG	2.69	0.41
1:A:395:TYR:CG	1:A:396:PRO:N	2.84	0.41
1:A:423:LYS:HE2	2:A:766:HOH:O	2.20	0.41
1:A:259:SER:O	1:A:263:ILE:HG12	2.21	0.41
1:A:150:GLU:O	1:A:154:VAL:HG23	2.21	0.41
1:B:108:VAL:HG13	1:B:123:TRP:CE3	2.56	0.41
1:B:430:GLU:HG3	2:B:702:HOH:O	2.21	0.41
1:A:221:GLU:N	1:A:221:GLU:OE1	2.53	0.40
1:B:94:LYS:HG2	1:B:459:ILE:CD1	2.51	0.40
1:B:245:ARG:NE	1:B:245:ARG:CA	2.84	0.40
1:B:446:VAL:HB	1:B:454:PHE:HB3	2.03	0.40
1:B:249:PRO:HD3	1:B:482:VAL:HG21	2.03	0.40
1:A:255:VAL:C	1:A:256:MET:HE2	2.41	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)
2:A:758:HOH:O	2:A:758:HOH:O[4_555]	2.09	0.11

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	474/518 (92%)	449 (95%)	22 (5%)	3 (1%)	25	20
1	B	474/518 (92%)	446 (94%)	23 (5%)	5 (1%)	14	9
All	All	948/1036 (92%)	895 (94%)	45 (5%)	8 (1%)	19	14

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	395	TYR
1	B	111	GLU
1	B	395	TYR
1	A	417	MET
1	B	50	ILE
1	B	48	ASN
1	B	334	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	388/428 (91%)	378 (97%)	10 (3%)	46	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	388/428 (91%)	377 (97%)	11 (3%)	43	46
All	All	776/856 (91%)	755 (97%)	21 (3%)	44	47

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	63	ARG
1	A	123	TRP
1	A	146	ASP
1	A	256	MET
1	A	417	MET
1	A	425	HIS
1	A	432	ASN
1	A	440	HIS
1	A	462	SER
1	B	15	ASP
1	B	29	GLN
1	B	63	ARG
1	B	123	TRP
1	B	256	MET
1	B	345	LYS
1	B	416	LYS
1	B	425	HIS
1	B	432	ASN
1	B	440	HIS
1	B	459	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	77	GLN
1	A	138	HIS
1	A	198	HIS
1	A	209	GLN
1	A	247	ASN
1	A	432	ASN
1	A	477	HIS
1	B	29	GLN
1	B	61	ASN

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Mol	Chain	Res	Type
1	B	77	GLN
1	B	124	HIS
1	B	138	HIS
1	B	198	HIS
1	B	209	GLN
1	B	432	ASN
1	B	477	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 monosaccharides 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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.