



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 10:43 AM EDT

PDB ID : 1KHJ
Title : E. COLI ALKALINE PHOSPHATASE MUTANT (D153HD330N) MIMIC OF THE TRANSITION STATES WITH ALUMINIUM FLUORIDE
Authors : Le Du, M.H.; Lamoure, C.; Muller, B.H.; Bulgakov, O.V.; Lajeunesse, E.; Menez, A.; Boulain, J.C.
Deposited on : 2001-11-30
Resolution : 2.30 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 : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

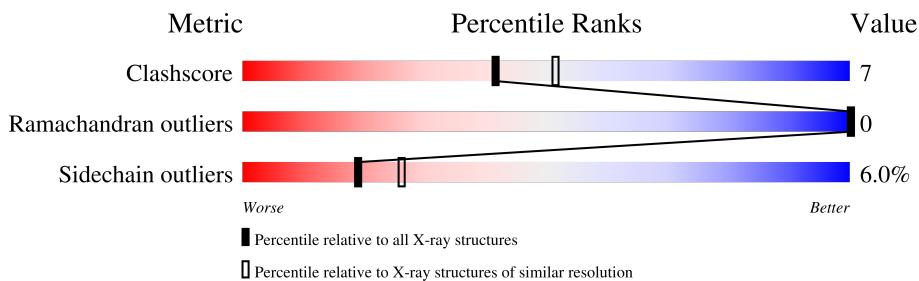
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	449	
1	B	449	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6967 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 Alkaline phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	444	3258	2013	579	655	11	0	0	0
1	B	444	3258	2013	579	655	11	0	0	0

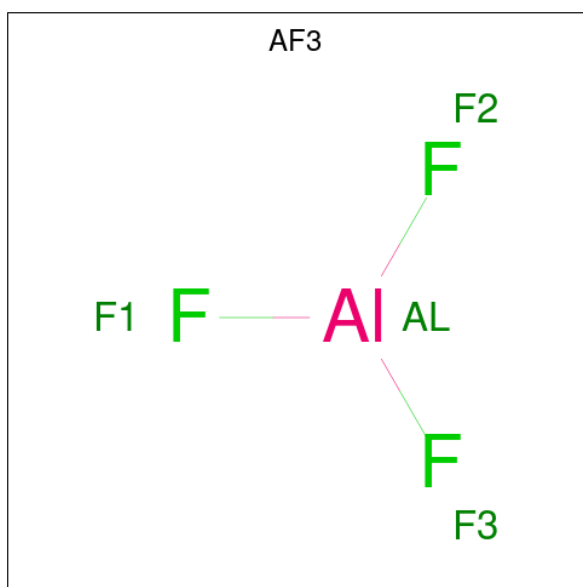
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ASN	ASP	conflict	UNP P00634
A	35	ASN	ASP	conflict	UNP P00634
A	153	HIS	ASP	engineered mutation	UNP P00634
A	176	GLN	GLU	conflict	UNP P00634
A	228	GLU	GLN	conflict	UNP P00634
A	230	GLU	GLN	conflict	UNP P00634
A	330	ASN	ASP	engineered mutation	UNP P00634
B	15	ASN	ASP	conflict	UNP P00634
B	35	ASN	ASP	conflict	UNP P00634
B	153	HIS	ASP	engineered mutation	UNP P00634
B	176	GLN	GLU	conflict	UNP P00634
B	228	GLU	GLN	conflict	UNP P00634
B	230	GLU	GLN	conflict	UNP P00634
B	330	ASN	ASP	engineered mutation	UNP P00634

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Al	F	0	0
			4	1	3		
3	B	1	Total	Al	F	0	0
			4	1	3		

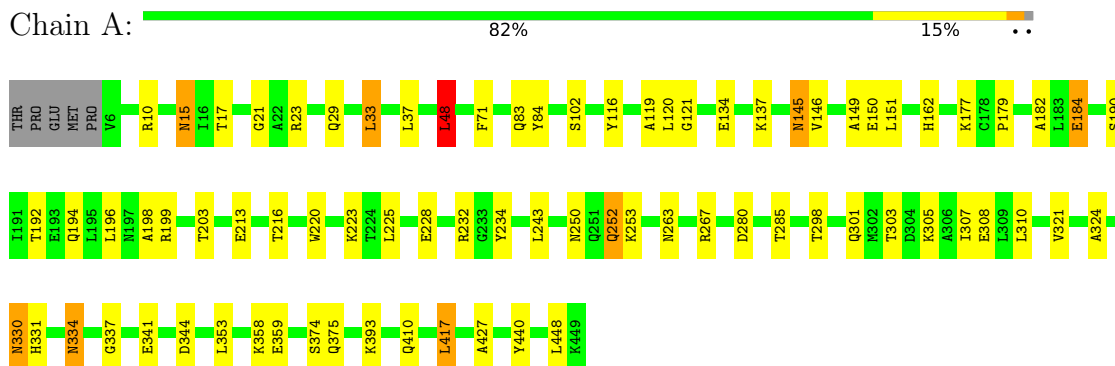
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	228	Total	O	0	0
			228	228		
4	B	211	Total	O	0	0
			211	211		

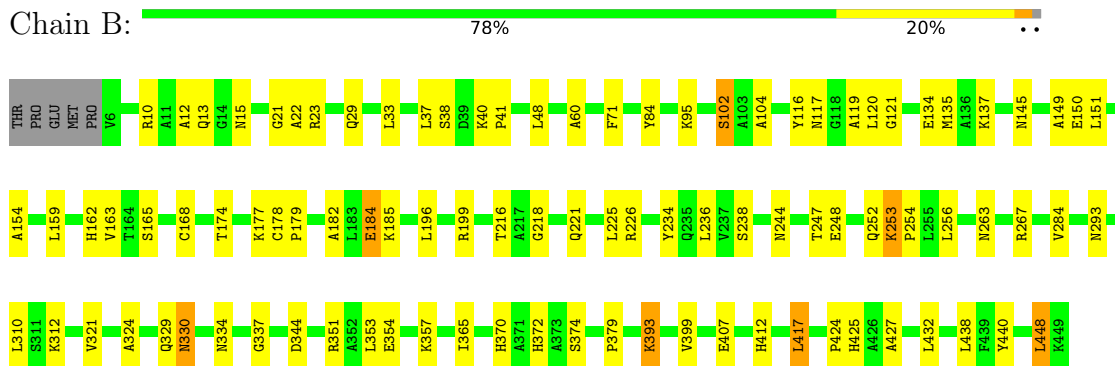
3 Residue-property plots [i](#)

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: Alkaline phosphatase



- Molecule 1: Alkaline phosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	163.51Å 163.51Å 138.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.30 49.90 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.7 (10.00-2.30) 98.1 (49.90-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.27Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.180 , 0.223 0.354 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtrriage
Anisotropy	0.425	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	6967	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, AF3

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	0.53	0/3312	0.77	2/4496 (0.0%)
1	B	0.54	0/3312	0.76	1/4496 (0.0%)
All	All	0.54	0/6624	0.77	3/8992 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	417	LEU	CA-CB-CG	7.85	133.36	115.30
1	A	417	LEU	CA-CB-CG	6.81	130.96	115.30
1	A	48	LEU	CA-CB-CG	6.38	129.97	115.30

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	3258	0	3195	43	6
1	B	3258	0	3195	51	7
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	228	0	0	2	8
4	B	211	0	0	5	5
All	All	6967	0	6390	90	14

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 (90) 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:334:ASN:HD22	1:A:337:GLY:H	1.35	0.73
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.72	0.69
1:A:253:LYS:HB2	1:A:253:LYS:NZ	2.08	0.68
1:B:182:ALA:HB1	1:B:184:GLU:OE1	1.93	0.67
1:B:38:SER:OG	1:B:40:LYS:HG2	1.96	0.66
1:A:182:ALA:HB1	1:A:184:GLU:OE1	1.97	0.64
1:B:163:VAL:HB	4:B:1416:HOH:O	1.96	0.64
1:A:440:TYR:CD2	1:B:23:ARG:HD3	2.32	0.64
1:A:334:ASN:ND2	1:A:337:GLY:H	1.97	0.63
1:B:334:ASN:HD22	1:B:337:GLY:H	1.45	0.62
1:B:10:ARG:HH22	1:B:29:GLN:NE2	1.99	0.61
1:A:267:ARG:HD3	1:A:344:ASP:HB2	1.82	0.61
1:A:48:LEU:HD13	1:A:321:VAL:HB	1.83	0.60
1:A:303:THR:O	1:A:307:ILE:HG13	2.01	0.60
1:B:15:ASN:O	1:B:21:GLY:HA3	2.01	0.60
1:B:163:VAL:HG12	1:B:165:SER:H	1.67	0.60
1:B:267:ARG:HD2	1:B:344:ASP:HB2	1.84	0.59
1:A:330:ASN:HD21	1:A:374:SER:H	1.50	0.59
1:B:247:THR:O	1:B:312:LYS:NZ	2.37	0.58
1:B:134:GLU:OE2	1:B:162:HIS:HE1	1.86	0.57
1:A:10:ARG:HH22	1:A:29:GLN:NE2	2.01	0.57
1:B:163:VAL:CG1	1:B:178:CYS:SG	2.94	0.56
1:A:358:LYS:HD3	1:A:359:GLU:N	2.21	0.55
1:B:159:LEU:HG	4:B:1342:HOH:O	2.08	0.53
1:A:15:ASN:ND2	4:A:1073:HOH:O	2.41	0.53
1:A:184:GLU:HG3	1:A:216:THR:OG1	2.08	0.52
1:B:149:ALA:HB2	1:B:324:ALA:CB	2.39	0.52
1:B:182:ALA:HB3	1:B:185:LYS:HD2	1.92	0.52
1:B:365:ILE:HD13	1:B:438:LEU:HD11	1.91	0.52
1:B:353:LEU:O	1:B:357:LYS:HG3	2.10	0.52
1:B:393:LYS:O	1:B:393:LYS:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLU:O	1:A:225:LEU:HD13	2.11	0.51
1:B:236:LEU:HD11	1:B:256:LEU:HD23	1.93	0.50
1:A:121:GLY:O	1:A:162:HIS:HD2	1.94	0.50
1:B:163:VAL:HG11	1:B:168:CYS:HB2	1.93	0.50
1:B:137:LYS:HE3	1:B:199:ARG:O	2.12	0.49
1:B:329:GLN:HE21	1:B:334:ASN:HB3	1.76	0.49
1:B:120:LEU:HD12	4:B:1416:HOH:O	2.12	0.49
1:A:253:LYS:HB2	1:A:253:LYS:HZ2	1.76	0.48
1:A:149:ALA:HB2	1:A:324:ALA:CB	2.43	0.48
1:A:10:ARG:HD2	1:B:432:LEU:O	2.13	0.48
1:B:149:ALA:HA	1:B:263:ASN:HD22	1.78	0.48
1:B:218:GLY:O	1:B:221:GLN:HG2	2.13	0.48
1:A:190:SER:O	1:A:194:GLN:HG3	2.14	0.48
1:A:192:THR:CG2	1:A:225:LEU:HD23	2.44	0.47
1:B:244:ASN:HB2	4:B:1291:HOH:O	2.14	0.47
1:A:134:GLU:OE2	1:A:162:HIS:HE1	1.98	0.47
1:B:37:LEU:HD22	1:B:427:ALA:HB2	1.96	0.47
1:A:15:ASN:O	1:A:21:GLY:HA3	2.14	0.47
1:A:228:GLU:O	1:A:232:ARG:HG3	2.15	0.46
1:B:174:THR:HG23	1:B:178:CYS:HB2	1.98	0.46
1:A:427:ALA:HB1	1:B:33:LEU:HD12	1.98	0.46
1:B:116:TYR:CZ	1:B:119:ALA:HB2	2.51	0.46
1:A:298:THR:OG1	1:A:301:GLN:HG3	2.15	0.46
1:B:121:GLY:O	1:B:162:HIS:HD2	1.99	0.46
1:A:120:LEU:O	1:A:162:HIS:HA	2.16	0.46
1:B:40:LYS:HB2	1:B:41:PRO:HD2	1.99	0.45
1:A:177:LYS:C	1:A:179:PRO:HD3	2.37	0.45
1:A:23:ARG:HD2	1:B:440:TYR:CE2	2.53	0.44
1:A:37:LEU:HD22	1:A:427:ALA:HB2	1.99	0.44
1:B:150:GLU:H	1:B:263:ASN:ND2	2.15	0.44
1:B:379:PRO:HA	1:B:399:VAL:HG21	1.99	0.44
1:B:60:ALA:HB2	4:B:1311:HOH:O	2.18	0.43
1:B:379:PRO:HA	1:B:399:VAL:CG2	2.49	0.43
1:B:424:PRO:O	1:B:425:HIS:HB2	2.18	0.43
1:A:150:GLU:H	1:A:263:ASN:ND2	2.16	0.43
1:B:253:LYS:HB2	1:B:253:LYS:NZ	2.33	0.43
1:B:12:ALA:HB1	1:B:22:ALA:HA	2.01	0.43
1:A:137:LYS:HE3	1:A:198:ALA:O	2.18	0.42
1:A:15:ASN:ND2	1:A:17:THR:H	2.17	0.42
1:A:243:LEU:O	1:A:305:LYS:HE2	2.19	0.42
1:A:199:ARG:HA	1:A:234:TYR:OH	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASN:OD1	1:A:252:GLN:HG2	2.19	0.42
1:B:177:LYS:C	1:B:179:PRO:HD3	2.39	0.42
1:B:330:ASN:HD21	1:B:374:SER:H	1.66	0.42
1:A:220:TRP:HD1	1:A:223:LYS:HZ1	1.66	0.42
1:A:331:HIS:ND1	1:A:410:GLN:O	2.50	0.42
1:A:375:GLN:NE2	4:A:1035:HOH:O	2.43	0.42
1:A:149:ALA:HA	1:A:263:ASN:HD22	1.84	0.41
1:B:178:CYS:N	1:B:179:PRO:HD3	2.35	0.41
1:B:135:MET:HE2	1:B:448:LEU:HB3	2.03	0.41
1:A:145:ASN:O	1:A:203:THR:HA	2.20	0.41
1:B:102:SER:HB2	1:B:154:ALA:HB3	2.03	0.41
1:B:184:GLU:HG3	1:B:216:THR:OG1	2.20	0.41
1:A:33:LEU:HD22	1:A:33:LEU:HA	1.92	0.40
1:A:116:TYR:CZ	1:A:119:ALA:HB2	2.56	0.40
1:A:337:GLY:O	1:A:341:GLU:HG2	2.21	0.40
1:B:104:ALA:HB2	1:B:117:ASN:HA	2.04	0.40
1:B:234:TYR:CD2	1:B:254:PRO:HB2	2.56	0.40
1:B:370:HIS:CE1	1:B:412:HIS:CE1	3.09	0.40

All (14) 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)
1:A:308:GLU:OE1	4:B:1308:HOH:O[9_766]	1.47	0.73
1:B:95:LYS:CE	4:A:1376:HOH:O[9_766]	1.54	0.66
4:A:1118:HOH:O	4:A:1201:HOH:O[9_766]	1.66	0.54
4:A:1189:HOH:O	4:A:1189:HOH:O[9_766]	1.76	0.44
1:A:393:LYS:NZ	4:A:1290:HOH:O[9_766]	1.85	0.35
4:A:1110:HOH:O	4:B:1358:HOH:O[11_655]	1.90	0.30
1:B:354:GLU:OE2	4:B:1244:HOH:O[11_655]	2.04	0.16
1:A:280:ASP:OD2	1:B:226:ARG:NH2[3_665]	2.05	0.15
1:B:238:SER:OG	4:A:1274:HOH:O[2_655]	2.09	0.11
1:A:285:THR:CG2	4:A:1190:HOH:O[9_766]	2.10	0.10
1:B:95:LYS:NZ	4:A:1376:HOH:O[9_766]	2.13	0.07
1:B:351:ARG:NH1	4:B:1430:HOH:O[11_655]	2.13	0.07
1:A:280:ASP:OD1	1:B:226:ARG:NE[3_665]	2.15	0.05
1:A:301:GLN:CG	4:B:1347:HOH:O[9_766]	2.17	0.03

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	442/449 (98%)	434 (98%)	8 (2%)	0	100	100
1	B	442/449 (98%)	435 (98%)	7 (2%)	0	100	100
All	All	884/898 (98%)	869 (98%)	15 (2%)	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 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	332/340 (98%)	313 (94%)	19 (6%)	20	28
1	B	332/340 (98%)	311 (94%)	21 (6%)	18	24
All	All	664/680 (98%)	624 (94%)	40 (6%)	19	26

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	33	LEU
1	A	48	LEU
1	A	71	PHE
1	A	83	GLN
1	A	84	TYR
1	A	102	SER
1	A	145	ASN

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Mol	Chain	Res	Type
1	A	146	VAL
1	A	151	LEU
1	A	184	GLU
1	A	196	LEU
1	A	252	GLN
1	A	310	LEU
1	A	330	ASN
1	A	334	ASN
1	A	353	LEU
1	A	417	LEU
1	A	448	LEU
1	B	13	GLN
1	B	71	PHE
1	B	84	TYR
1	B	102	SER
1	B	145	ASN
1	B	151	LEU
1	B	184	GLU
1	B	196	LEU
1	B	225	LEU
1	B	248	GLU
1	B	252	GLN
1	B	253	LYS
1	B	284	VAL
1	B	293	ASN
1	B	310	LEU
1	B	330	ASN
1	B	372	HIS
1	B	393	LYS
1	B	407	GLU
1	B	417	LEU
1	B	448	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	29	GLN
1	A	35	ASN
1	A	83	GLN
1	A	145	ASN
1	A	162	HIS

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Mol	Chain	Res	Type
1	A	235	GLN
1	A	263	ASN
1	A	329	GLN
1	A	330	ASN
1	A	334	ASN
1	A	375	GLN
1	B	15	ASN
1	B	29	GLN
1	B	35	ASN
1	B	83	GLN
1	B	145	ASN
1	B	162	HIS
1	B	176	GLN
1	B	235	GLN
1	B	263	ASN
1	B	329	GLN
1	B	330	ASN
1	B	334	ASN

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](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	AF3	A	453	4,1,2	0,3,3	-	-	-		
3	AF3	B	453	4,1,2	0,3,3	-	-	-		

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.