Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:28 PM GMT

PDB ID : 1KHJ

Title : E. COLI ALKALINE PHOSPHATASE MUTANT (D153HD330N) MIMIC OF THE TRANSITION STATES WITH ALUMINIUM FLUORIDE

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Deposited on : 2001-11-30

Resolution : 2.30 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865
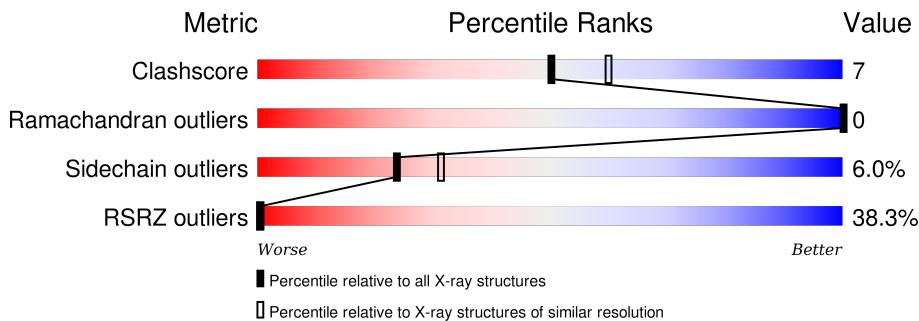
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
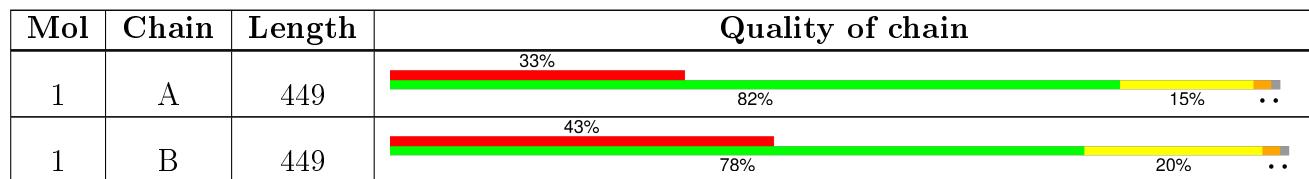
The reported resolution of this entry is 2.30 Å.

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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		6.0%
RSRZ outliers		38.3%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	449	33% / 82% / 15% / ..
1	B	449	43% / 78% / 20% / ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AF3	B	453	-	-	-	X

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
1	A	444	Total 3258	C 2013	N 579	O 655	S 11	0	0	0
1	B	444	Total 3258	C 2013	N 579	O 655	S 11	0	0	0
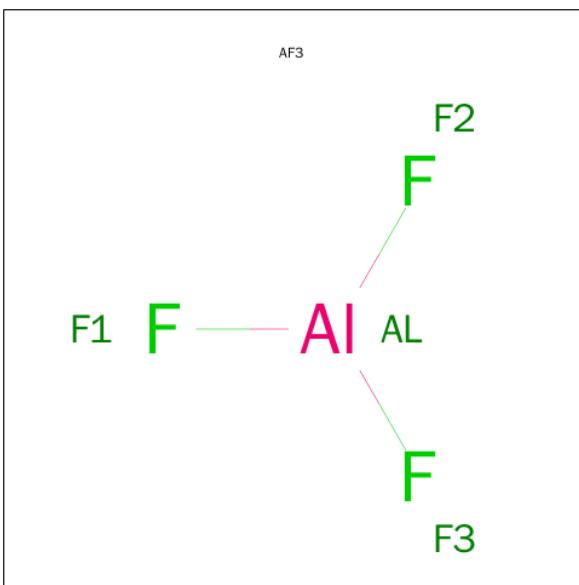
There are 14 discrepancies between the modelled and reference sequences:

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	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	UNP P00634
B	15	ASN	ASP	CONFLICT	UNP P00634
B	35	ASN	ASP	CONFLICT	UNP P00634
B	153	HIS	ASP	ENGINEERED	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	UNP P00634

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

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

- Molecule 3 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).

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		
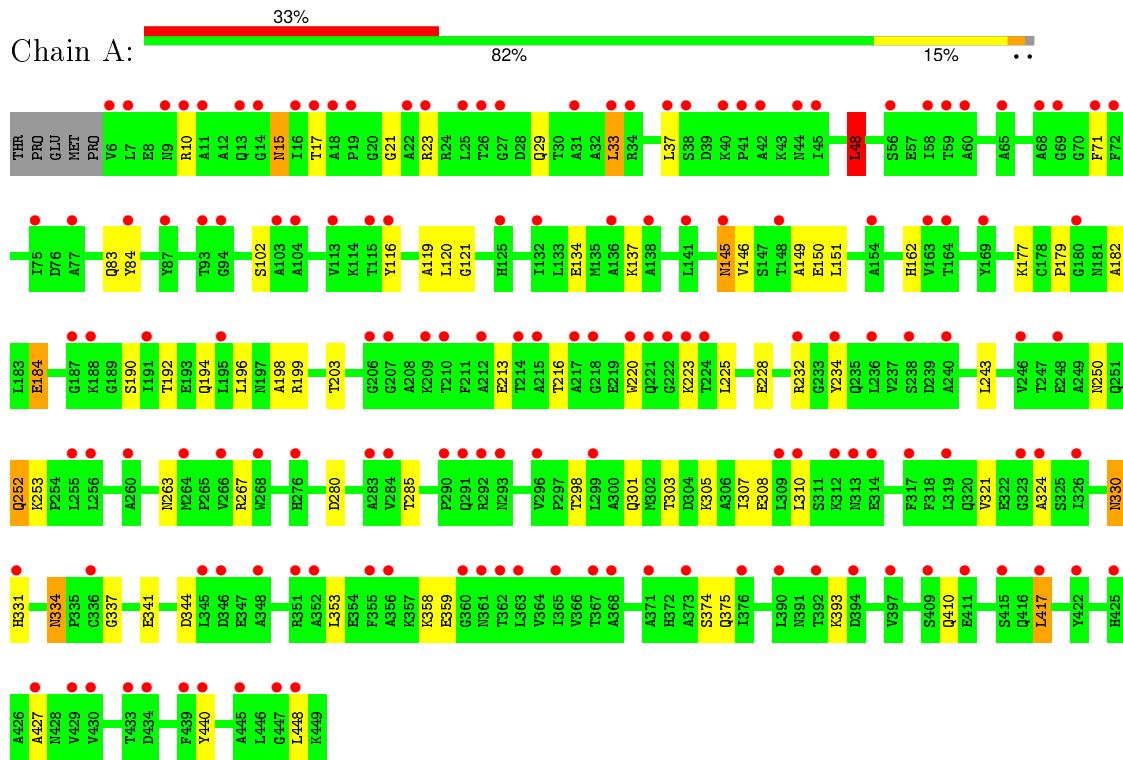
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	228	Total	O	0	0
			228	228		
4	B	211	Total	O	0	0
			211	211		
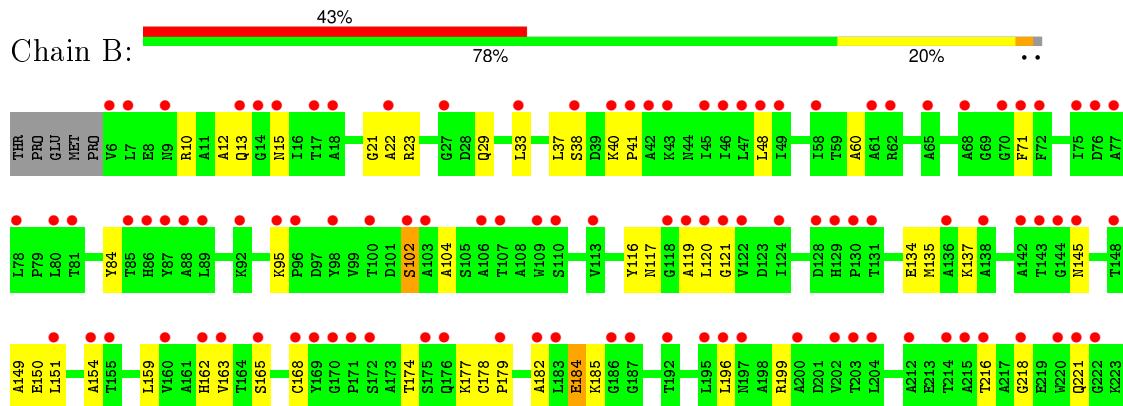
3 Residue-property plots (i)
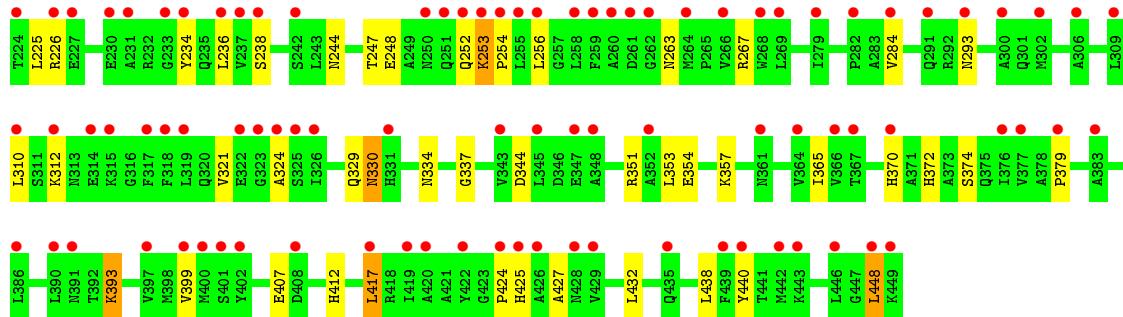
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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 (i)

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
$< I/\sigma(I) >$ [1]	3.19 (at 2.27Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.180 , 0.223 0.357 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å²)	26.4	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.32 , 55.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	0 of 49146 reflections	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	6967	wwPDB-VP
Average B, all atoms (Å²)	24.0	wwPDB-VP

Xtriage'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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(^{o})	Ideal(^{o})
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:NZ	1:A:253:LYS:HB2	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:B:163:VAL:HB	4:B:1416:HOH:O	1.96	0.64
1:A:182:ALA:HB1	1:A:184:GLU:OE1	1.97	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:B:163:VAL:HG12	1:B:165:SER:H	1.67	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: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:329:GLN:HE21	1:B:334:ASN:HB3	1.76	0.49
1:B:137:LYS:HE3	1:B:199:ARG:O	2.12	0.49
1:B:120:LEU:HD12	4:B:1416:HOH:O	2.12	0.49
1:A:253:LYS:HZ2	1:A:253:LYS:HB2	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:B:174:THR:HG23	1:B:178:CYS:HB2	1.98	0.46
1:A:228:GLU:O	1:A:232:ARG:HG3	2.15	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:B:121:GLY:O	1:B:162:HIS:HD2	1.99	0.46
1:A:298:THR:OG1	1:A:301:GLN:HG3	2.15	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:B:150:GLU:H	1:B:263:ASN:ND2	2.15	0.44
1:A:37:LEU:HD22	1:A:427:ALA:HB2	1.99	0.44
1:B:379:PRO:HA	1:B:399:VAL:HG21	1.99	0.44
1:B:379:PRO:HA	1:B:399:VAL:CG2	2.49	0.43
1:B:60:ALA:HB2	4:B:1311:HOH:O	2.18	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:B:184:GLU:HG3	1:B:216:THR:OG1	2.20	0.41
1:B:102:SER:HB2	1:B:154:ALA:HB3	2.03	0.41
1:A:145:ASN:O	1:A:203:THR:HA	2.20	0.41
1:A:33:LEU:HA	1:A:33:LEU:HD22	1.92	0.40
1:A:337:GLY:O	1:A:341:GLU:HG2	2.21	0.40
1:B:370:HIS:CE1	1:B:412:HIS:CE1	3.09	0.40
1:B:234:TYR:CD2	1:B:254:PRO:HB2	2.56	0.40
1:A:116:TYR:CZ	1:A:119:ALA:HB2	2.56	0.40
1:B:104:ALA:HB2	1:B:117:ASN:HA	2.04	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%)	25	34
1	B	332/340 (98%)	311 (94%)	21 (6%)	22	29
All	All	664/680 (98%)	624 (94%)	40 (6%)	24	31

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

Some 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 carbohydrates 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

Full wwPDB X-ray Structure Validation Report

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	1,2,4	0,3,3	0.00	-	0,3,3	0.00	-
3	AF3	B	453	1,2,4	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AF3	A	453	1,2,4	-	0/0/0/0	0/0/0/0
3	AF3	B	453	1,2,4	-	0/0/0/0	0/0/0/0

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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	444/449 (98%)	1.76	147 (33%)	0	0	11, 21, 46, 72	0
1	B	444/449 (98%)	1.97	193 (43%)	0	0	10, 20, 46, 69	0
All	All	888/898 (98%)	1.87	340 (38%)	0	0	10, 20, 46, 72	0

All (340) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	VAL	7.1
1	A	7	LEU	6.2
1	B	182	ALA	6.1
1	B	138	ALA	5.6
1	A	218	GLY	5.6
1	B	170	GLY	5.6
1	B	6	VAL	5.4
1	B	165	SER	5.2
1	B	258	LEU	5.2
1	A	22	ALA	5.0
1	A	240	ALA	5.0
1	A	293	ASN	4.8
1	B	236	LEU	4.8
1	B	448	LEU	4.7
1	B	215	ALA	4.5
1	B	408	ASP	4.4
1	A	324	ALA	4.4
1	B	22	ALA	4.4
1	B	310	LEU	4.4
1	A	187	GLY	4.4
1	B	163	VAL	4.3
1	A	13	GLN	4.3
1	B	142	ALA	4.3
1	B	89	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	160	VAL	4.2
1	B	216	THR	4.2
1	A	27	GLY	4.1
1	B	179	PRO	4.1
1	B	449	LYS	4.1
1	A	40	LYS	4.1
1	B	102	SER	4.0
1	B	33	LEU	4.0
1	B	196	LEU	4.0
1	B	221	GLN	4.0
1	B	293	ASN	3.9
1	A	72	PHE	3.9
1	B	318	PHE	3.9
1	B	129	HIS	3.9
1	B	151	LEU	3.9
1	A	236	LEU	3.8
1	B	183	LEU	3.8
1	A	397	VAL	3.8
1	B	325	SER	3.8
1	A	292	ARG	3.8
1	B	422	TYR	3.7
1	B	204	LEU	3.7
1	B	361	ASN	3.7
1	A	390	LEU	3.7
1	B	319	LEU	3.7
1	B	376	ILE	3.7
1	A	430	VAL	3.7
1	A	33	LEU	3.6
1	A	195	LEU	3.6
1	B	169	TYR	3.6
1	A	18	ALA	3.6
1	B	162	HIS	3.6
1	A	60	ALA	3.5
1	A	345	LEU	3.5
1	A	191	ILE	3.5
1	B	75	ILE	3.5
1	B	71	PHE	3.5
1	A	17	THR	3.5
1	B	343	VAL	3.5
1	A	310	LEU	3.5
1	B	13	GLN	3.5
1	B	203	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	377	VAL	3.4
1	A	68	ALA	3.4
1	B	175	SER	3.4
1	A	217	ALA	3.4
1	B	124	ILE	3.4
1	A	409	SER	3.4
1	B	118	GLY	3.4
1	B	41	PRO	3.4
1	A	220	TRP	3.3
1	B	260	ALA	3.3
1	B	43	LYS	3.3
1	B	324	ALA	3.3
1	A	26	THR	3.3
1	A	132	ILE	3.3
1	A	363	LEU	3.3
1	A	348	ALA	3.3
1	A	154	ALA	3.2
1	A	214	THR	3.2
1	A	84	TYR	3.2
1	B	45	ILE	3.2
1	B	326	ILE	3.2
1	B	18	ALA	3.2
1	A	447	GLY	3.2
1	B	212	ALA	3.2
1	A	260	ALA	3.2
1	B	47	LEU	3.2
1	A	296	VAL	3.1
1	B	439	PHE	3.1
1	A	141	LEU	3.1
1	B	331	HIS	3.1
1	B	266	VAL	3.1
1	B	109	TRP	3.1
1	B	192	THR	3.1
1	B	222	GLY	3.1
1	A	365	ILE	3.1
1	B	58	ILE	3.1
1	B	309	LEU	3.1
1	B	400	MET	3.1
1	A	221	GLN	3.1
1	A	367	THR	3.1
1	B	443	LYS	3.1
1	B	171	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	168	CYS	3.0
1	A	222	GLY	3.0
1	A	314	GLU	3.0
1	B	40	LYS	3.0
1	A	164	THR	3.0
1	B	197	ASN	3.0
1	A	368	ALA	3.0
1	B	7	LEU	3.0
1	B	312	LYS	3.0
1	B	172	SER	3.0
1	A	440	TYR	3.0
1	B	420	ALA	2.9
1	B	92	LYS	2.9
1	B	259	PHE	2.9
1	A	58	ILE	2.9
1	A	37	LEU	2.9
1	A	212	ALA	2.9
1	B	122	VAL	2.9
1	A	16	ILE	2.9
1	A	71	PHE	2.9
1	A	207	GLY	2.9
1	A	362	THR	2.8
1	B	314	GLU	2.8
1	B	186	GLY	2.8
1	A	31	ALA	2.8
1	B	261	ASP	2.8
1	A	264	MET	2.8
1	B	446	LEU	2.8
1	B	428	ASN	2.8
1	A	115	THR	2.8
1	B	345	LEU	2.8
1	B	402	TYR	2.8
1	A	19	PRO	2.8
1	B	366	VAL	2.7
1	B	81	THR	2.7
1	A	439	PHE	2.7
1	B	49	ILE	2.7
1	A	169	TYR	2.7
1	B	268	TRP	2.7
1	B	120	LEU	2.7
1	B	264	MET	2.7
1	B	77	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	200	ALA	2.7
1	B	187	GLY	2.7
1	B	284	VAL	2.7
1	A	42	ALA	2.7
1	B	317	PHE	2.7
1	A	232	ARG	2.7
1	A	319	LEU	2.6
1	A	309	LEU	2.6
1	B	78	LEU	2.6
1	B	110	SER	2.6
1	B	269	LEU	2.6
1	A	125	HIS	2.6
1	A	427	ALA	2.6
1	B	279	ILE	2.6
1	B	230	GLU	2.6
1	A	266	VAL	2.6
1	B	85	THR	2.6
1	B	383	ALA	2.6
1	A	59	THR	2.6
1	B	419	ILE	2.6
1	A	23	ARG	2.6
1	A	238	SER	2.6
1	A	323	GLY	2.6
1	A	104	ALA	2.6
1	B	399	VAL	2.6
1	B	143	THR	2.6
1	B	391	ASN	2.6
1	B	424	PRO	2.6
1	A	422	TYR	2.6
1	A	425	HIS	2.6
1	B	87	TYR	2.6
1	A	10	ARG	2.6
1	A	25	LEU	2.6
1	A	429	VAL	2.6
1	B	80	LEU	2.6
1	B	440	TYR	2.5
1	B	231	ALA	2.5
1	A	246	VAL	2.5
1	A	355	PHE	2.5
1	A	352	ALA	2.5
1	B	154	ALA	2.5
1	B	214	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	291	GLN	2.5
1	A	94	GLY	2.5
1	A	180	GLY	2.5
1	B	86	HIS	2.5
1	B	65	ALA	2.5
1	B	315	LYS	2.5
1	A	299	LEU	2.5
1	A	284	VAL	2.5
1	B	218	GLY	2.5
1	B	429	VAL	2.5
1	A	41	PRO	2.5
1	B	348	ALA	2.5
1	A	87	TYR	2.5
1	A	56	SER	2.5
1	A	206	GLY	2.5
1	B	70	GLY	2.5
1	B	234	TYR	2.5
1	B	386	LEU	2.5
1	B	96	PRO	2.5
1	A	11	ALA	2.4
1	B	42	ALA	2.4
1	B	119	ALA	2.4
1	A	224	THR	2.4
1	A	434	ASP	2.4
1	B	62	ARG	2.4
1	B	291	GLN	2.4
1	B	253	LYS	2.4
1	B	14	GLY	2.4
1	B	401	SER	2.4
1	A	331	HIS	2.4
1	B	397	VAL	2.4
1	B	121	GLY	2.4
1	A	38	SER	2.4
1	A	223	LYS	2.4
1	B	425	HIS	2.4
1	A	65	ALA	2.4
1	A	283	ALA	2.4
1	B	322	GLU	2.4
1	A	448	LEU	2.4
1	B	256	LEU	2.4
1	A	75	ILE	2.4
1	A	113	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	394	ASP	2.4
1	A	373	ALA	2.4
1	B	100	THR	2.4
1	B	148	THR	2.4
1	A	255	LEU	2.4
1	B	390	LEU	2.4
1	A	268	TRP	2.4
1	B	103	ALA	2.4
1	B	352	ALA	2.4
1	B	176	GLN	2.4
1	A	9	ASN	2.3
1	B	250	ASN	2.3
1	A	69	GLY	2.3
1	B	238	SER	2.3
1	A	312	LYS	2.3
1	A	138	ALA	2.3
1	A	234	TYR	2.3
1	B	106	ALA	2.3
1	B	107	THR	2.3
1	A	417	LEU	2.3
1	A	411	GLU	2.3
1	B	254	PRO	2.3
1	A	148	THR	2.3
1	B	136	ALA	2.3
1	B	155	THR	2.3
1	B	233	GLY	2.3
1	B	227	GLU	2.3
1	B	130	PRO	2.3
1	A	116	TYR	2.3
1	A	392	THR	2.3
1	B	98	TYR	2.3
1	B	426	ALA	2.3
1	B	251	GLN	2.3
1	B	242	SER	2.3
1	B	255	LEU	2.3
1	B	282	PRO	2.3
1	B	46	ILE	2.3
1	A	103	ALA	2.3
1	B	262	GLY	2.3
1	B	95	LYS	2.3
1	B	144	GLY	2.2
1	A	376	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	364	VAL	2.2
1	A	326	ILE	2.2
1	B	61	ALA	2.2
1	B	68	ALA	2.2
1	A	145	ASN	2.2
1	B	17	THR	2.2
1	B	306	ALA	2.2
1	B	237	VAL	2.2
1	B	72	PHE	2.2
1	B	347	GLU	2.2
1	B	48	LEU	2.2
1	B	224	THR	2.2
1	B	370	HIS	2.2
1	B	435	GLN	2.2
1	B	220	TRP	2.2
1	A	163	VAL	2.2
1	B	202	VAL	2.2
1	A	14	GLY	2.2
1	A	34	ARG	2.2
1	A	351	ARG	2.2
1	B	226	ARG	2.2
1	A	210	THR	2.2
1	B	38	SER	2.2
1	A	215	ALA	2.2
1	B	300	ALA	2.2
1	A	360	GLY	2.2
1	A	77	ALA	2.2
1	A	346	ASP	2.1
1	A	248	GLU	2.1
1	A	317	PHE	2.1
1	A	445	ALA	2.1
1	B	15	ASN	2.1
1	A	415	SER	2.1
1	B	442	MET	2.1
1	B	367	THR	2.1
1	B	88	ALA	2.1
1	B	76	ASP	2.1
1	A	93	THR	2.1
1	A	336	CYS	2.1
1	B	113	VAL	2.1
1	A	209	LYS	2.1
1	B	27	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	128	ASP	2.1
1	B	379	PRO	2.1
1	A	433	THR	2.1
1	B	131	THR	2.1
1	A	44	ASN	2.1
1	B	145	ASN	2.1
1	B	417	LEU	2.1
1	B	252	GLN	2.1
1	B	9	ASN	2.0
1	B	323	GLY	2.0
1	A	256	LEU	2.0
1	B	195	LEU	2.0
1	A	290	PRO	2.0
1	A	188	LYS	2.0
1	A	136	ALA	2.0
1	B	302	MET	2.0
1	A	276	HIS	2.0
1	A	45	ILE	2.0
1	A	313	ASN	2.0
1	A	361	ASN	2.0
1	A	356	ALA	2.0
1	A	371	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	AF3	B	453	4/4	0.54	0.38	2.35	35,39,40,41	0
3	AF3	A	453	4/4	0.88	0.22	-0.14	31,34,37,38	0
2	ZN	B	451	1/1	0.67	0.12	-2.07	26,26,26,26	0
2	ZN	B	450	1/1	0.84	0.12	-2.27	20,20,20,20	0
2	ZN	A	451	1/1	0.90	0.12	-3.90	27,27,27,27	0
2	ZN	A	450	1/1	0.69	0.10	-4.06	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.