



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:50 PM UTC

PDB ID : 1KHJ / pdb_00001khj
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

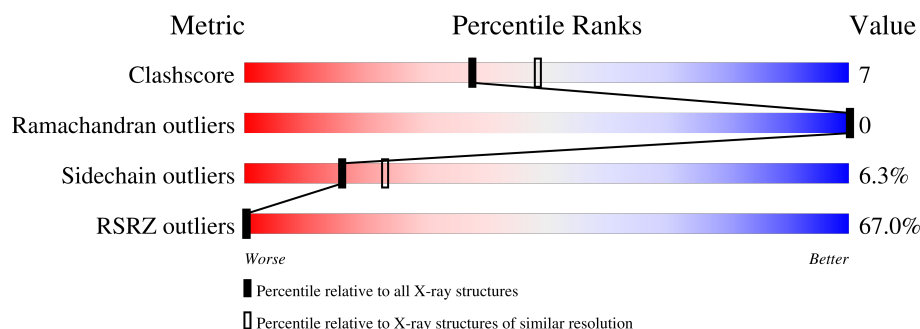
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	61% 78% 18% ..
1	B	449	71% 74% 23% ..

2 Entry composition

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	C	N	O	S	0	0	0
			3258	2013	579	655	11			
1	B	444	Total	C	N	O	S	0	0	0
			3258	2013	579	655	11			

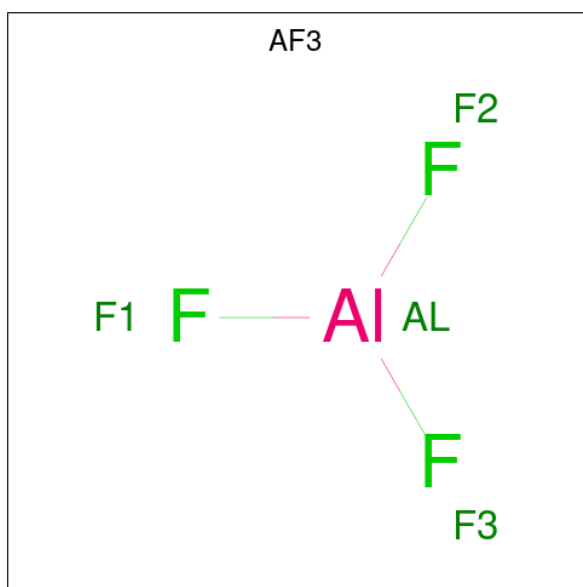
There are 14 discrepancies between the modelled and reference sequences:

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 (CCD ID: 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 (CCD ID: 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		

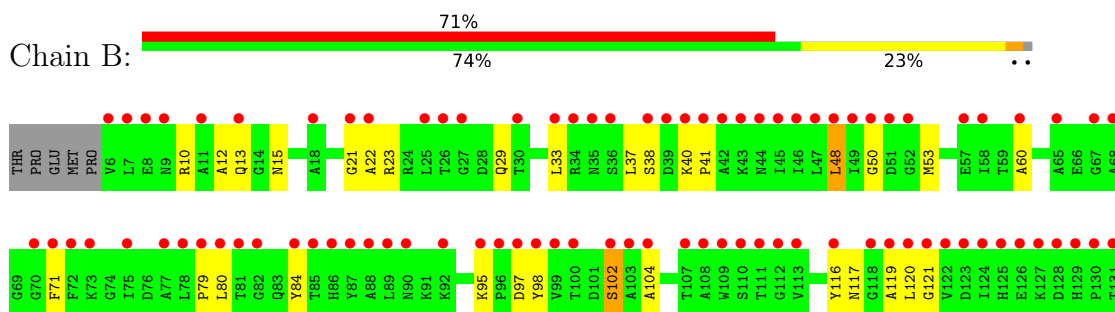
3 Residue-property plots [i](#)

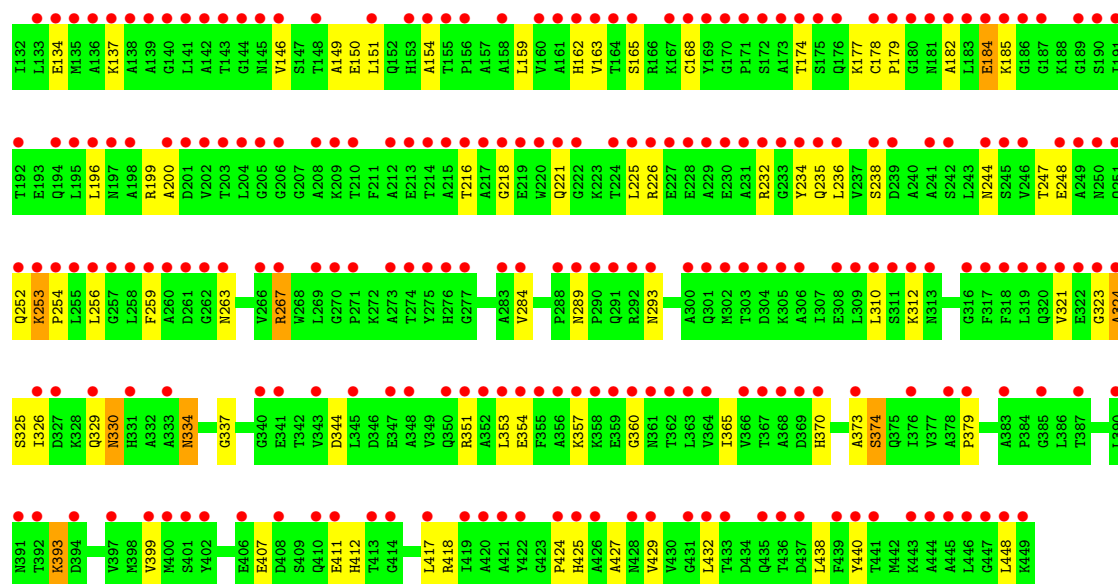
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

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 10.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (10.00-2.30) 98.5 (10.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.27Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.180 , 0.223 0.391 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	6967	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

5.1 Standard geometry

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

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	0.69	0/3312	1.12	26/4496 (0.6%)
1	B	0.70	0/3312	1.10	23/4496 (0.5%)
All	All	0.69	0/6624	1.11	49/8992 (0.5%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	ILE	N-CA-C	-9.50	100.93	110.62
1	A	324	ALA	N-CA-C	9.37	121.26	111.14
1	A	326	ILE	N-CA-C	-8.62	102.14	110.42
1	B	324	ALA	N-CA-C	7.78	119.83	111.36
1	A	373	ALA	N-CA-C	7.76	121.24	111.69
1	B	373	ALA	N-CA-C	7.38	120.77	111.69
1	A	325	SER	N-CA-C	7.17	121.72	113.19
1	A	98	TYR	N-CA-C	6.98	120.90	112.38
1	A	79	PRO	N-CA-C	6.97	122.74	113.40
1	A	411	GLU	N-CA-C	6.75	120.89	110.42
1	B	98	TYR	N-CA-C	6.71	119.42	111.71
1	B	411	GLU	N-CA-C	6.68	120.78	110.42
1	B	79	PRO	N-CA-C	6.51	122.58	113.53
1	A	374	SER	N-CA-C	6.41	119.66	110.24
1	A	429	VAL	N-CA-CB	-6.37	105.21	112.21
1	A	267	ARG	N-CA-C	6.26	118.19	111.36
1	B	267	ARG	N-CA-C	6.26	117.90	111.14
1	B	325	SER	N-CA-C	6.23	120.73	113.20
1	B	334	ASN	CA-C-N	6.13	125.62	119.24
1	B	334	ASN	C-N-CA	6.13	125.62	119.24
1	B	374	SER	N-CA-C	6.09	119.20	110.24
1	B	259	PHE	N-CA-C	5.86	120.42	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	GLN	N-CA-C	-5.82	100.51	109.76
1	B	13	GLN	N-CA-C	5.74	117.22	111.07
1	B	289	ASN	CA-C-N	5.68	125.30	119.56
1	B	289	ASN	C-N-CA	5.68	125.30	119.56
1	A	97	ASP	N-CA-C	-5.63	98.16	108.02
1	A	280	ASP	N-CA-C	5.51	120.00	113.28
1	A	172	SER	N-CA-C	5.47	117.24	111.28
1	A	200	ALA	N-CA-C	-5.47	102.79	110.50
1	A	360	GLY	N-CA-C	5.46	122.63	115.36
1	B	418	ARG	N-CA-C	5.46	118.14	110.23
1	A	334	ASN	CA-C-N	5.44	124.90	119.24
1	A	334	ASN	C-N-CA	5.44	124.90	119.24
1	B	200	ALA	N-CA-C	-5.40	102.88	110.50
1	A	77	ALA	N-CA-C	5.35	119.79	113.16
1	A	429	VAL	N-CA-C	-5.33	107.61	113.43
1	A	378	ALA	CA-C-N	5.27	125.33	119.32
1	A	378	ALA	C-N-CA	5.27	125.33	119.32
1	B	360	GLY	N-CA-C	5.25	122.33	115.40
1	A	142	ALA	N-CA-C	-5.25	103.47	110.55
1	A	160	VAL	N-CA-C	5.19	118.18	113.20
1	B	50	GLY	N-CA-C	-5.17	100.92	113.18
1	A	75	ILE	N-CA-C	5.15	116.49	110.62
1	B	97	ASP	N-CA-C	-5.12	98.94	107.99
1	B	323	GLY	N-CA-C	-5.06	101.18	113.18
1	B	53	MET	N-CA-C	5.05	117.20	109.62
1	A	310	LEU	N-CA-C	5.04	116.86	111.36
1	A	13	GLN	N-CA-C	5.00	116.73	111.28

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	3258	0	3195	44	6
1	B	3258	0	3195	50	7

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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:A:135:MET:HE1	1:A:443:LYS:HE2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:177:LYS:C	1:A:179:PRO:HD3	2.37	0.49
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:B:177:LYS:C	1:B:179:PRO:HD3	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:250:ASN:OD1	1:A:252:GLN:HG2	2.19	0.42
1:B:330:ASN:HD21	1:B:374:SER:H	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:A:10:ARG:HH22	1:A:29:GLN:CD	2.28	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

5.3.1 Protein backbone

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

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%)	18	27
1	B	332/340 (98%)	309 (93%)	23 (7%)	14	20
All	All	664/680 (98%)	622 (94%)	42 (6%)	16	23

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	48	LEU
1	A	71	PHE
1	A	84	TYR
1	A	102	SER
1	A	146	VAL
1	A	151	LEU
1	A	184	GLU

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Mol	Chain	Res	Type
1	A	196	LEU
1	A	252	GLN
1	A	253	LYS
1	A	284	VAL
1	A	310	LEU
1	A	330	ASN
1	A	334	ASN
1	A	353	LEU
1	A	417	LEU
1	A	429	VAL
1	A	448	LEU
1	B	48	LEU
1	B	71	PHE
1	B	80	LEU
1	B	84	TYR
1	B	102	SER
1	B	146	VAL
1	B	151	LEU
1	B	184	GLU
1	B	196	LEU
1	B	225	LEU
1	B	232	ARG
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	393	LYS
1	B	407	GLU
1	B	417	LEU
1	B	429	VAL
1	B	448	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	15	ASN
1	A	35	ASN
1	A	83	GLN

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Mol	Chain	Res	Type
1	A	125	HIS
1	A	145	ASN
1	A	162	HIS
1	A	263	ASN
1	A	329	GLN
1	A	330	ASN
1	A	334	ASN
1	A	375	GLN
1	A	391	ASN
1	A	425	HIS
1	B	9	ASN
1	B	13	GLN
1	B	15	ASN
1	B	29	GLN
1	B	35	ASN
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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

6.1 Protein, DNA and RNA chains

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(Å ²)	Q<0.9
1	A	444/449 (98%)	2.42	275 (61%) 0 0	11, 21, 46, 72	0
1	B	444/449 (98%)	2.75	320 (72%) 0 0	10, 20, 46, 69	0
All	All	888/898 (98%)	2.58	595 (67%) 0 0	10, 20, 46, 72	0

All (595) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	GLY	6.4
1	B	138	ALA	6.3
1	A	6	VAL	6.2
1	A	431	GLY	6.0
1	B	165	SER	5.9
1	A	293	ASN	5.9
1	B	250	ASN	5.8
1	B	218	GLY	5.8
1	A	221	GLN	5.7
1	B	168	CYS	5.6
1	B	6	VAL	5.5
1	B	173	ALA	5.5
1	B	129	HIS	5.4
1	B	174	THR	5.3
1	A	22	ALA	5.3
1	A	7	LEU	5.3
1	A	26	THR	5.1
1	B	119	ALA	5.1
1	B	182	ALA	5.1
1	B	89	LEU	5.0
1	B	448	LEU	5.0
1	B	183	LEU	5.0
1	B	212	ALA	5.0
1	A	18	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	43	LYS	4.9
1	B	111	THR	4.9
1	B	186	GLY	4.8
1	B	160	VAL	4.8
1	A	173	ALA	4.8
1	A	72	PHE	4.8
1	B	361	ASN	4.8
1	B	221	GLN	4.8
1	B	436	THR	4.7
1	B	102	SER	4.7
1	B	47	LEU	4.7
1	B	439	PHE	4.7
1	B	13	GLN	4.7
1	B	317	PHE	4.7
1	A	350	GLN	4.6
1	B	327	ASP	4.6
1	B	187	GLY	4.6
1	B	222	GLY	4.6
1	A	187	GLY	4.5
1	A	236	LEU	4.5
1	B	206	GLY	4.5
1	A	409	SER	4.5
1	B	161	ALA	4.5
1	A	254	PRO	4.5
1	B	230	GLU	4.5
1	B	82	GLY	4.5
1	B	151	LEU	4.4
1	B	45	ILE	4.4
1	A	360	GLY	4.4
1	A	313	ASN	4.4
1	B	319	LEU	4.4
1	B	131	THR	4.3
1	B	224	THR	4.3
1	A	230	GLU	4.3
1	A	30	THR	4.3
1	A	291	GLN	4.3
1	B	163	VAL	4.3
1	A	316	GLY	4.3
1	B	253	LYS	4.2
1	A	69	GLY	4.2
1	B	440	TYR	4.2
1	A	214	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	121	GLY	4.2
1	A	63	ASN	4.2
1	B	229	ALA	4.2
1	A	17	THR	4.2
1	B	219	GLU	4.1
1	B	128	ASP	4.1
1	A	445	ALA	4.1
1	A	392	THR	4.1
1	B	318	PHE	4.1
1	A	128	ASP	4.1
1	B	7	LEU	4.1
1	B	227	GLU	4.1
1	B	366	VAL	4.1
1	B	27	GLY	4.0
1	B	175	SER	4.0
1	A	37	LEU	4.0
1	A	103	ALA	4.0
1	B	255	LEU	4.0
1	B	109	TRP	4.0
1	A	217	ALA	4.0
1	B	217	ALA	4.0
1	B	251	GLN	4.0
1	B	123	ASP	4.0
1	B	135	MET	4.0
1	B	360	GLY	4.0
1	A	28	ASP	4.0
1	B	156	PRO	3.9
1	B	220	TRP	3.9
1	A	356	ALA	3.9
1	B	215	ALA	3.9
1	B	424	PRO	3.9
1	B	225	LEU	3.9
1	B	178	CYS	3.9
1	A	396	ALA	3.9
1	B	203	THR	3.9
1	A	74	GLY	3.9
1	B	340	GLY	3.9
1	B	107	THR	3.9
1	B	241	ALA	3.9
1	B	162	HIS	3.9
1	A	56	SER	3.8
1	A	314	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	429	VAL	3.8
1	B	170	GLY	3.8
1	A	65	ALA	3.8
1	B	254	PRO	3.8
1	B	98	TYR	3.8
1	A	299	LEU	3.8
1	A	32	ALA	3.8
1	B	42	ALA	3.8
1	A	290	PRO	3.8
1	A	232	ARG	3.8
1	A	257	GLY	3.8
1	A	363	LEU	3.8
1	B	22	ALA	3.8
1	B	142	ALA	3.8
1	B	164	THR	3.8
1	B	201	ASP	3.8
1	B	444	ALA	3.8
1	A	296	VAL	3.8
1	B	192	THR	3.7
1	B	303	THR	3.7
1	B	200	ALA	3.7
1	B	408	ASP	3.7
1	A	268	TRP	3.7
1	B	292	ARG	3.7
1	A	64	TYR	3.7
1	B	228	GLU	3.7
1	B	378	ALA	3.7
1	B	130	PRO	3.7
1	B	258	LEU	3.7
1	B	447	GLY	3.7
1	B	145	ASN	3.7
1	B	197	ASN	3.7
1	A	60	ALA	3.7
1	A	36	SER	3.7
1	A	13	GLN	3.7
1	B	118	GLY	3.7
1	B	196	LEU	3.7
1	B	306	ALA	3.6
1	B	41	PRO	3.6
1	B	171	PRO	3.6
1	B	242	SER	3.6
1	A	337	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	408	ASP	3.6
1	B	343	VAL	3.6
1	B	21	GLY	3.6
1	A	346	ASP	3.6
1	A	127	LYS	3.6
1	A	324	ALA	3.6
1	B	71	PHE	3.6
1	B	35	ASN	3.6
1	B	331	HIS	3.6
1	B	290	PRO	3.6
1	B	248	GLU	3.6
1	A	292	ARG	3.5
1	A	345	LEU	3.5
1	B	309	LEU	3.5
1	B	81	THR	3.5
1	B	210	THR	3.5
1	A	212	ALA	3.5
1	A	300	ALA	3.5
1	B	333	ALA	3.5
1	B	36	SER	3.5
1	B	38	SER	3.5
1	B	110	SER	3.5
1	B	428	ASN	3.5
1	B	362	THR	3.5
1	A	195	LEU	3.5
1	A	425	HIS	3.5
1	B	204	LEU	3.5
1	A	237	VAL	3.5
1	A	284	VAL	3.5
1	B	154	ALA	3.5
1	B	100	THR	3.4
1	A	102	SER	3.4
1	B	134	GLU	3.4
1	B	180	GLY	3.4
1	A	244	ASN	3.4
1	A	430	VAL	3.4
1	A	33	LEU	3.4
1	B	80	LEU	3.4
1	B	155	THR	3.4
1	B	122	VAL	3.4
1	A	348	ALA	3.4
1	B	367	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	200	ALA	3.4
1	B	158	ALA	3.4
1	A	206	GLY	3.4
1	A	447	GLY	3.4
1	B	112	GLY	3.4
1	A	278	ASN	3.4
1	A	309	LEU	3.3
1	A	390	LEU	3.3
1	B	417	LEU	3.3
1	B	79	PRO	3.3
1	B	179	PRO	3.3
1	B	300	ALA	3.3
1	A	312	LYS	3.3
1	A	414	GLY	3.3
1	A	336	CYS	3.3
1	A	71	PHE	3.3
1	A	298	THR	3.3
1	A	362	THR	3.3
1	B	245	SER	3.3
1	A	104	ALA	3.3
1	A	427	ALA	3.3
1	B	144	GLY	3.3
1	A	448	LEU	3.3
1	B	113	VAL	3.3
1	B	310	LEU	3.3
1	B	234	TYR	3.3
1	A	12	ALA	3.2
1	A	429	VAL	3.3
1	B	18	ALA	3.2
1	B	68	ALA	3.2
1	B	104	ALA	3.2
1	B	261	ASP	3.2
1	B	347	GLU	3.2
1	A	58	ILE	3.2
1	A	365	ILE	3.2
1	B	92	LYS	3.2
1	A	440	TYR	3.2
1	A	138	ALA	3.2
1	B	231	ALA	3.2
1	A	180	GLY	3.2
1	B	97	ASP	3.2
1	B	235	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	435	GLN	3.2
1	A	376	ILE	3.2
1	A	15	ASN	3.2
1	B	422	TYR	3.2
1	B	95	LYS	3.1
1	B	443	LYS	3.1
1	B	311	SER	3.1
1	A	407	GLU	3.1
1	B	86	HIS	3.1
1	B	260	ALA	3.1
1	A	10	ARG	3.1
1	B	85	THR	3.1
1	B	358	LYS	3.1
1	B	291	GLN	3.1
1	A	310	LEU	3.1
1	B	25	LEU	3.1
1	B	88	ALA	3.1
1	B	46	ILE	3.1
1	A	81	THR	3.1
1	A	367	THR	3.1
1	B	190	SER	3.1
1	A	82	GLY	3.1
1	A	222	GLY	3.1
1	A	434	ASP	3.1
1	B	437	ASP	3.1
1	B	139	ALA	3.1
1	B	249	ALA	3.1
1	A	19	PRO	3.1
1	B	246	VAL	3.1
1	A	234	TYR	3.0
1	A	422	TYR	3.0
1	B	8	GLU	3.0
1	B	308	GLU	3.0
1	A	174	THR	3.0
1	A	301	GLN	3.0
1	A	361	ASN	3.0
1	B	90	ASN	3.0
1	B	259	PHE	3.0
1	B	127	LYS	3.0
1	A	424	PRO	3.0
1	B	256	LEU	3.0
1	B	399	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	175	SER	3.0
1	A	351	ARG	3.0
1	B	40	LYS	3.0
1	A	68	ALA	3.0
1	A	215	ALA	3.0
1	A	368	ALA	3.0
1	B	96	PRO	3.0
1	B	252	GLN	3.0
1	A	207	GLY	3.0
1	B	289	ASN	3.0
1	A	154	ALA	3.0
1	B	77	ALA	3.0
1	B	198	ALA	3.0
1	B	84	TYR	3.0
1	A	50	GLY	3.0
1	A	218	GLY	3.0
1	A	304	ASP	3.0
1	A	240	ALA	2.9
1	A	24	ARG	2.9
1	A	287	THR	2.9
1	B	214	THR	2.9
1	B	216	THR	2.9
1	A	420	ALA	2.9
1	B	136	ALA	2.9
1	B	345	LEU	2.9
1	A	209	LYS	2.9
1	B	226	ARG	2.9
1	B	284	VAL	2.9
1	B	44	ASN	2.9
1	A	61	ALA	2.9
1	B	60	ALA	2.9
1	B	176	GLN	2.9
1	A	238	SER	2.9
1	B	313	ASN	2.9
1	A	120	LEU	2.9
1	B	283	ALA	2.9
1	A	274	THR	2.9
1	B	75	ILE	2.9
1	A	394	ASP	2.9
1	B	316	GLY	2.8
1	B	414	GLY	2.8
1	A	116	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	267	ARG	2.8
1	A	269	LEU	2.8
1	B	120	LEU	2.8
1	B	108	ALA	2.8
1	B	184	GLU	2.8
1	B	26	THR	2.8
1	A	282	PRO	2.8
1	B	141	LEU	2.8
1	A	260	ALA	2.8
1	A	399	VAL	2.8
1	A	40	LYS	2.8
1	A	281	LYS	2.8
1	A	115	THR	2.8
1	A	191	ILE	2.8
1	B	387	THR	2.8
1	A	289	ASN	2.8
1	A	359	GLU	2.8
1	A	444	ALA	2.8
1	B	356	ALA	2.8
1	B	426	ALA	2.8
1	A	397	VAL	2.8
1	A	280	ASP	2.8
1	B	239	ASP	2.8
1	A	308	GLU	2.8
1	A	11	ALA	2.8
1	A	77	ALA	2.8
1	A	229	ALA	2.8
1	A	421	ALA	2.8
1	B	368	ALA	2.8
1	A	355	PHE	2.8
1	B	355	PHE	2.8
1	B	34	ARG	2.8
1	A	391	ASN	2.7
1	B	49	ILE	2.7
1	A	38	SER	2.7
1	B	140	GLY	2.7
1	B	271	PRO	2.7
1	B	446	LEU	2.7
1	A	139	ALA	2.7
1	A	241	ALA	2.7
1	A	39	ASP	2.7
1	A	224	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	205	GLY	2.7
1	A	225	LEU	2.7
1	A	255	LEU	2.7
1	B	116	TYR	2.7
1	B	420	ALA	2.7
1	B	72	PHE	2.7
1	A	29	GLN	2.7
1	A	131	THR	2.7
1	A	380	ASP	2.7
1	B	51	ASP	2.7
1	B	58	ILE	2.7
1	B	302	MET	2.7
1	B	33	LEU	2.7
1	B	11	ALA	2.7
1	A	35	ASN	2.7
1	A	186	GLY	2.7
1	A	323	GLY	2.7
1	B	270	GLY	2.7
1	B	323	GLY	2.7
1	A	379	PRO	2.7
1	B	353	LEU	2.7
1	A	136	ALA	2.6
1	B	383	ALA	2.6
1	B	421	ALA	2.6
1	B	169	TYR	2.6
1	B	209	LYS	2.6
1	A	334	ASN	2.6
1	B	293	ASN	2.6
1	B	441	THR	2.6
1	A	23	ARG	2.6
1	A	62	ARG	2.6
1	A	384	PRO	2.6
1	A	151	LEU	2.6
1	B	236	LEU	2.6
1	B	185	LYS	2.6
1	B	449	LYS	2.6
1	B	445	ALA	2.6
1	B	413	THR	2.6
1	B	153	HIS	2.6
1	B	370	HIS	2.6
1	A	306	ALA	2.6
1	A	426	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	181	ASN	2.6
1	B	202	VAL	2.6
1	B	385	GLY	2.6
1	B	392	THR	2.6
1	B	402	TYR	2.6
1	B	433	THR	2.6
1	B	124	ILE	2.6
1	B	376	ILE	2.6
1	B	425	HIS	2.6
1	A	358	LYS	2.6
1	B	354	GLU	2.6
1	B	99	VAL	2.6
1	A	84	TYR	2.6
1	A	223	LYS	2.6
1	B	350	GLN	2.5
1	B	304	ASP	2.5
1	A	140	GLY	2.5
1	B	146	VAL	2.5
1	B	266	VAL	2.5
1	A	327	ASP	2.5
1	B	373	ALA	2.5
1	A	96	PRO	2.5
1	A	247	THR	2.5
1	A	413	THR	2.5
1	B	30	THR	2.5
1	A	235	GLN	2.5
1	A	349	VAL	2.5
1	B	301	GLN	2.5
1	A	98	TYR	2.5
1	A	44	ASN	2.5
1	A	182	ALA	2.5
1	A	197	ASN	2.5
1	B	348	ALA	2.5
1	B	391	ASN	2.5
1	B	125	HIS	2.5
1	B	194	GLN	2.5
1	B	419	ILE	2.5
1	A	31	ALA	2.5
1	A	252	GLN	2.5
1	A	148	THR	2.4
1	A	164	THR	2.4
1	B	57	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	213	GLU	2.4
1	A	147	SER	2.4
1	A	183	LEU	2.4
1	A	275	TYR	2.4
1	B	133	LEU	2.4
1	B	432	LEU	2.4
1	B	357	LYS	2.4
1	B	9	ASN	2.4
1	B	369	ASP	2.4
1	A	142	ALA	2.4
1	A	288	PRO	2.4
1	B	322	GLU	2.4
1	B	406	GLU	2.4
1	B	172	SER	2.4
1	A	132	ILE	2.4
1	A	272	LYS	2.4
1	B	167	LYS	2.4
1	B	195	LEU	2.4
1	A	248	GLU	2.4
1	A	341	GLU	2.4
1	B	126	GLU	2.4
1	B	277	GLY	2.4
1	A	210	THR	2.4
1	B	305	LYS	2.4
1	A	25	LEU	2.4
1	A	276	HIS	2.4
1	A	149	ALA	2.4
1	A	192	THR	2.4
1	A	342	THR	2.4
1	A	357	LYS	2.4
1	B	238	SER	2.4
1	A	45	ILE	2.4
1	B	191	ILE	2.4
1	B	321	VAL	2.4
1	B	397	VAL	2.4
1	B	320	GLN	2.4
1	B	410	GLN	2.4
1	A	145	ASN	2.3
1	A	369	ASP	2.3
1	A	170	GLY	2.3
1	A	253	LYS	2.3
1	B	65	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	137	LYS	2.3
1	A	319	LEU	2.3
1	B	48	LEU	2.3
1	B	263	ASN	2.3
1	B	87	TYR	2.3
1	B	52	GLY	2.3
1	B	208	ALA	2.3
1	B	324	ALA	2.3
1	A	377	VAL	2.3
1	A	9	ASN	2.3
1	A	294	ASP	2.3
1	A	344	ASP	2.3
1	B	73	LYS	2.3
1	B	244	ASN	2.3
1	B	233	GLY	2.3
1	B	262	GLY	2.3
1	B	431	GLY	2.3
1	A	49	ILE	2.3
1	A	43	LYS	2.3
1	A	239	ASP	2.3
1	B	70	GLY	2.3
1	A	264	MET	2.3
1	A	220	TRP	2.3
1	A	387	THR	2.3
1	A	110	SER	2.3
1	B	411	GLU	2.3
1	B	326	ILE	2.3
1	B	364	VAL	2.3
1	B	267	ARG	2.2
1	B	351	ARG	2.2
1	A	93	THR	2.2
1	A	150	GLU	2.2
1	A	283	ALA	2.2
1	A	402	TYR	2.2
1	B	103	ALA	2.2
1	B	143	THR	2.2
1	B	312	LYS	2.2
1	B	39	ASP	2.2
1	A	21	GLY	2.2
1	A	375	GLN	2.2
1	A	203	THR	2.2
1	A	249	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	401	SER	2.2
1	A	326	ILE	2.2
1	A	34	ARG	2.2
1	A	121	GLY	2.2
1	B	189	GLY	2.2
1	B	329	GLN	2.2
1	A	59	THR	2.2
1	A	436	THR	2.2
1	B	275	TYR	2.2
1	A	78	LEU	2.2
1	B	78	LEU	2.2
1	A	41	PRO	2.2
1	B	341	GLU	2.2
1	B	50	GLY	2.2
1	A	190	SER	2.2
1	A	242	SER	2.2
1	A	245	SER	2.2
1	B	274	THR	2.2
1	A	47	LEU	2.1
1	B	269	LEU	2.1
1	A	428	ASN	2.1
1	A	347	GLU	2.1
1	A	331	HIS	2.1
1	A	372	HIS	2.1
1	B	257	GLY	2.1
1	A	107	THR	2.1
1	A	333	ALA	2.1
1	A	381	THR	2.1
1	A	133	LEU	2.1
1	A	188	LYS	2.1
1	A	305	LYS	2.1
1	B	394	ASP	2.1
1	A	194	GLN	2.1
1	B	276	HIS	2.1
1	A	259	PHE	2.1
1	A	439	PHE	2.1
1	B	67	GLY	2.1
1	A	352	ALA	2.1
1	A	405	SER	2.1
1	B	400	MET	2.1
1	A	141	LEU	2.1
1	B	359	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	307	ILE	2.1
1	B	390	LEU	2.1
1	A	317	PHE	2.1
1	A	119	ALA	2.1
1	A	161	ALA	2.1
1	A	231	ALA	2.1
1	B	273	ALA	2.1
1	A	219	GLU	2.1
1	B	379	PRO	2.1
1	A	143	THR	2.0
1	A	286	CYS	2.0
1	A	388	GLN	2.0
1	A	243	LEU	2.0
1	B	363	LEU	2.0
1	A	419	ILE	2.0
1	B	288	PRO	2.0
1	A	385	GLY	2.0
1	A	109	TRP	2.0
1	A	135	MET	2.0
1	A	354	GLU	2.0
1	B	148	THR	2.0
1	A	373	ALA	2.0
1	B	352	ALA	2.0
1	A	338	GLN	2.0
1	B	232	ARG	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	AF3	B	453	4/4	0.32	0.37	35,39,40,41	0
2	ZN	B	450	1/1	0.58	0.11	20,20,20,20	0
2	ZN	A	450	1/1	0.61	0.09	23,23,23,23	0
2	ZN	A	451	1/1	0.61	0.12	27,27,27,27	0
2	ZN	B	451	1/1	0.66	0.10	26,26,26,26	0
3	AF3	A	453	4/4	0.84	0.16	31,34,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.