



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:58 PM UTC

PDB ID : 1ELY / pdb_00001ely
Title : E. COLI ALKALINE PHOSPHATASE MUTANT (S102C)
Authors : Stec, B.; Hehir, M.; Brennan, C.; Nolte, M.; Kantrowitz, E.R.
Deposited on : 1998-02-10
Resolution : 2.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

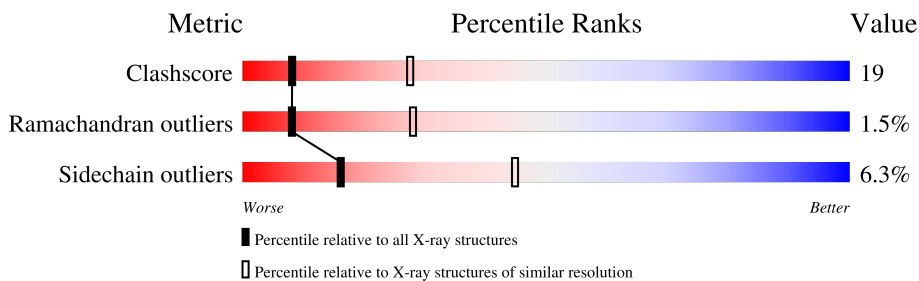
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	449	
1	B	449	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7088 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	449	Total	C	N	O	S	0	0	0
			3304	2042	581	668	13			
1	B	449	Total	C	N	O	S	0	0	0
			3304	2042	581	668	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	CYS	SER	engineered mutation	UNP P00634
B	102	CYS	SER	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

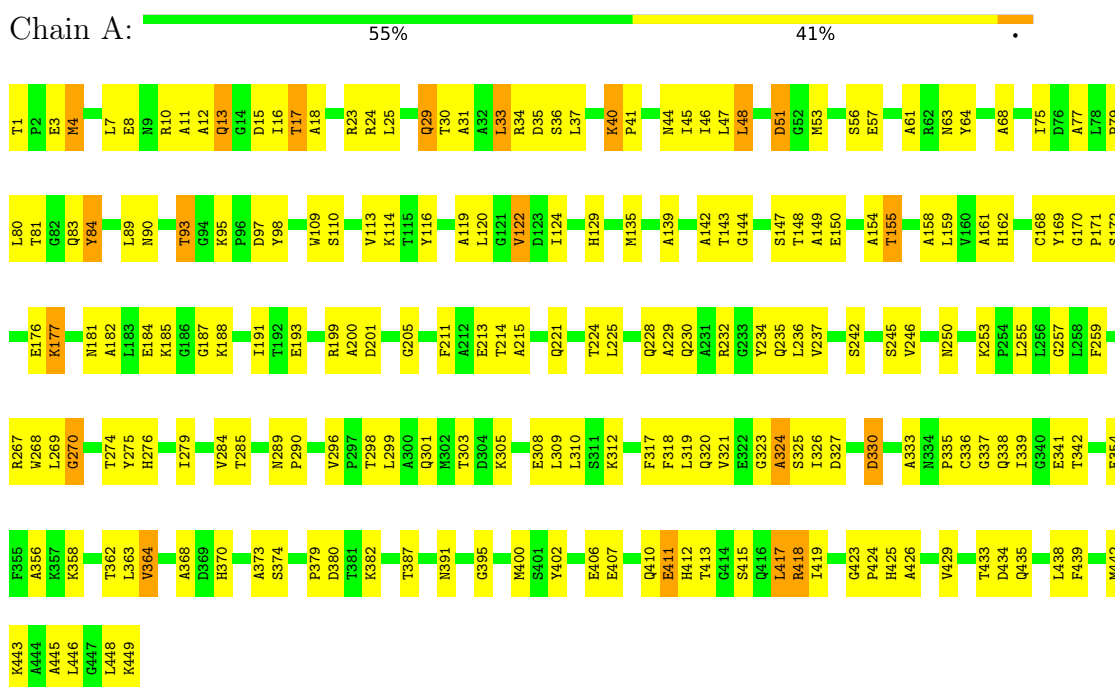
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	223	Total	O	0	0
			223	223		
5	B	241	Total	O	0	0
			241	241		

3 Residue-property plots

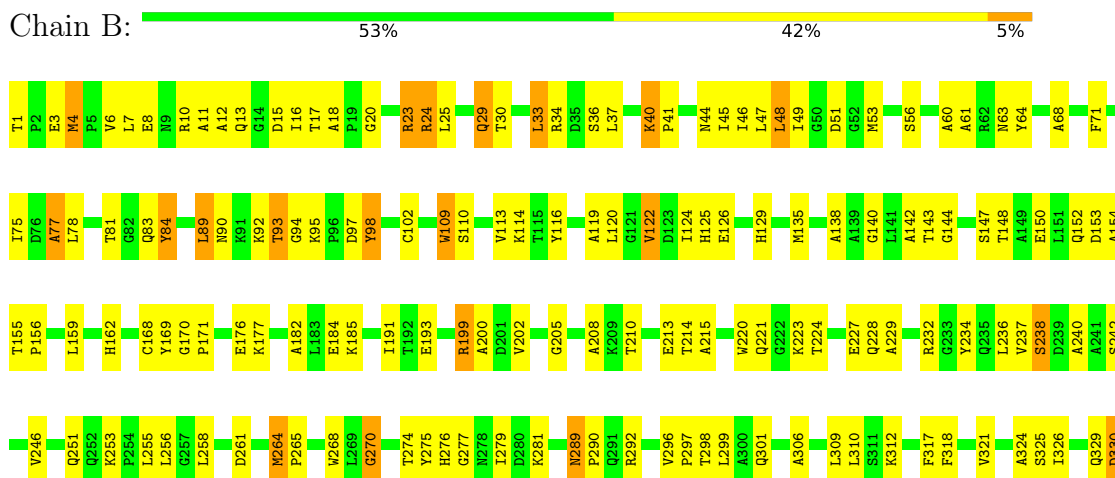
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: ALKALINE PHOSPHATASE



• Molecule 1: ALKALINE PHOSPHATASE



V429	T433	D434	Q435	T436	D437	L438	F439	Y440	T441	M442	K443	A444	A445	L446	K449	H351	A352	A353	R354	C356	G358	L363	V364	A368	H372	A373	S374	A378	P379	K382	A383	G385	V389	M400	S401	Y402	E406	E407	D408	S409	Q410	E411	H412	T413	L417	R418	I419	G423	P424	H425
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	163.44Å 163.44Å 139.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	9.00 – 2.80	Depositor
% Data completeness (in resolution range)	81.0 (9.00-2.80)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.143 , 0.193	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7088	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, PO4

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	0.83	1/3359 (0.0%)	1.30	41/4560 (0.9%)
1	B	0.81	1/3359 (0.0%)	1.29	46/4560 (1.0%)
All	All	0.82	2/6718 (0.0%)	1.30	87/9120 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	364	VAL	CA-CB	6.84	1.62	1.54
1	B	364	VAL	CA-CB	5.74	1.61	1.54

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	411	GLU	N-CA-C	11.27	126.26	109.24
1	A	289	ASN	CA-C-N	11.20	131.59	119.28
1	A	289	ASN	C-N-CA	11.20	131.59	119.28
1	A	411	GLU	N-CA-C	11.10	126.73	109.52
1	B	326	ILE	N-CA-C	-9.03	101.75	110.42
1	A	170	GLY	CA-C-N	8.75	130.78	119.84
1	A	170	GLY	C-N-CA	8.75	130.78	119.84
1	B	97	ASP	N-CA-C	-8.71	92.51	108.02
1	B	289	ASN	CA-C-N	8.70	128.85	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	289	ASN	C-N-CA	8.70	128.85	119.28
1	B	373	ALA	N-CA-C	8.66	120.72	111.28
1	A	406	GLU	N-CA-C	-8.56	103.35	113.88
1	B	324	ALA	N-CA-C	8.49	120.22	110.97
1	A	325	SER	N-CA-C	8.44	123.23	113.19
1	B	330	ASP	N-CA-C	-8.15	102.47	111.36
1	A	373	ALA	N-CA-C	8.13	120.14	111.28
1	A	324	ALA	N-CA-C	8.12	120.86	111.11
1	B	374	SER	N-CA-C	8.09	122.14	110.24
1	B	170	GLY	CA-C-N	8.03	129.88	119.84
1	B	170	GLY	C-N-CA	8.03	129.88	119.84
1	A	40	LYS	N-CA-C	-7.85	99.67	109.64
1	A	93	THR	N-CA-C	7.68	122.75	113.23
1	B	150	GLU	N-CA-C	-7.18	99.85	110.48
1	A	97	ASP	N-CA-C	-7.13	95.55	108.02
1	B	40	LYS	N-CA-C	-6.93	101.63	109.60
1	A	395	GLY	N-CA-C	-6.83	105.77	114.37
1	A	270	GLY	CA-C-N	-6.76	113.72	120.21
1	A	270	GLY	C-N-CA	-6.76	113.72	120.21
1	A	374	SER	N-CA-C	6.69	119.68	110.24
1	A	150	GLU	N-CA-C	-6.62	101.17	110.50
1	A	326	ILE	N-CA-C	-6.60	104.08	110.42
1	B	395	GLY	N-CA-C	-6.52	106.45	114.92
1	A	330	ASP	N-CA-C	-6.43	104.19	111.14
1	B	334	ASN	CA-C-N	6.42	126.64	119.32
1	B	334	ASN	C-N-CA	6.42	126.64	119.32
1	B	81	THR	N-CA-C	6.40	119.61	109.50
1	B	325	SER	N-CA-C	6.38	120.78	113.19
1	B	406	GLU	N-CA-C	-6.36	105.83	113.97
1	B	378	ALA	CA-C-N	6.29	125.78	119.24
1	B	378	ALA	C-N-CA	6.29	125.78	119.24
1	A	407	GLU	N-CA-C	-6.25	102.25	110.43
1	B	429	VAL	N-CA-C	-6.19	106.18	113.42
1	A	423	GLY	CA-C-N	6.12	126.44	119.83
1	A	423	GLY	C-N-CA	6.12	126.44	119.83
1	A	161	ALA	N-CA-C	6.08	119.11	109.50
1	A	13	GLN	N-CA-C	6.07	118.69	111.71
1	B	407	GLU	N-CA-C	-6.05	102.12	110.35
1	A	81	THR	N-CA-C	5.91	118.68	109.52
1	A	75	ILE	N-CA-C	5.82	116.55	110.62
1	A	172	SER	N-CA-C	5.79	117.39	111.14
1	B	423	GLY	CA-C-N	5.75	126.04	119.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	423	GLY	C-N-CA	5.75	126.04	119.83
1	A	201	ASP	N-CA-C	5.71	118.23	111.33
1	B	93	THR	N-CA-C	5.69	120.35	112.90
1	B	29	GLN	N-CA-C	5.67	119.92	112.89
1	A	418	ARG	N-CA-C	5.60	117.77	110.43
1	B	75	ILE	N-CA-C	5.58	116.31	110.62
1	B	6	VAL	N-CA-C	-5.57	100.41	108.87
1	B	238	SER	N-CA-C	5.57	120.23	113.38
1	A	79	PRO	N-CA-C	5.55	121.14	113.65
1	A	342	THR	N-CA-C	-5.53	105.27	112.23
1	A	155	THR	CA-C-N	-5.50	112.96	119.84
1	A	155	THR	C-N-CA	-5.50	112.96	119.84
1	B	270	GLY	CA-C-N	-5.47	114.95	120.21
1	B	270	GLY	C-N-CA	-5.47	114.95	120.21
1	A	259	PHE	N-CA-C	5.47	118.96	112.72
1	B	383	ALA	N-CA-C	5.47	117.83	110.29
1	B	264	MET	CA-C-N	5.44	125.45	119.90
1	B	264	MET	C-N-CA	5.44	125.45	119.90
1	A	296	VAL	N-CA-C	5.43	112.50	107.56
1	B	98	TYR	N-CA-C	5.37	118.93	112.38
1	B	18	ALA	CA-C-N	5.26	126.08	119.98
1	B	18	ALA	C-N-CA	5.26	126.08	119.98
1	B	296	VAL	CA-C-N	5.22	125.22	119.90
1	B	296	VAL	C-N-CA	5.22	125.22	119.90
1	A	29	GLN	N-CA-C	5.16	119.29	112.89
1	B	24	ARG	N-CA-C	-5.14	106.09	112.93
1	A	18	ALA	CA-C-N	5.14	125.38	119.83
1	A	18	ALA	C-N-CA	5.14	125.38	119.83
1	B	102	CYS	N-CA-C	5.14	117.62	111.71
1	B	78	LEU	CA-C-N	5.13	124.93	119.28
1	B	78	LEU	C-N-CA	5.13	124.93	119.28
1	A	177	LYS	N-CA-C	5.09	119.12	113.01
1	B	199	ARG	N-CA-C	5.09	118.26	111.24
1	B	94	GLY	N-CA-C	-5.05	107.31	115.08
1	A	326	ILE	CB-CA-C	-5.03	105.53	111.97
1	A	323	GLY	N-CA-C	-5.03	101.27	113.18

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	64	TYR	Sidechain

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	3304	0	3248	138	0
1	B	3304	0	3249	138	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	223	0	0	9	0
5	B	241	0	0	6	1
All	All	7088	0	6497	254	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 19.

All (254) 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:B:45:ILE:HD12	1:B:446:LEU:HG	1.52	0.90
1:A:402:TYR:HB3	1:A:410:GLN:HG3	1.64	0.79
1:A:7:LEU:HD13	1:A:10:ARG:HD2	1.62	0.78
1:B:228:GLN:O	1:B:232:ARG:HG3	1.85	0.77
1:B:199:ARG:HD3	1:B:251:GLN:OE1	1.84	0.76
1:A:250:ASN:HB2	5:A:665:HOH:O	1.85	0.75
1:B:246:VAL:HG21	1:B:255:LEU:HD13	1.69	0.75
1:B:92:LYS:HD3	5:B:503:HOH:O	1.85	0.75
1:A:142:ALA:HB3	1:A:317:PHE:HB3	1.69	0.75
1:B:402:TYR:HB3	1:B:410:GLN:HG3	1.69	0.74
1:A:34:ARG:HG2	1:B:37:LEU:HD13	1.67	0.74
1:A:182:ALA:HB3	1:A:185:LYS:HD2	1.69	0.74
1:A:41:PRO:HA	1:A:425:HIS:HE1	1.54	0.72
1:A:17:THR:HB	1:B:124:ILE:HD11	1.71	0.72
1:A:48:LEU:HD13	1:A:321:VAL:HB	1.71	0.71
1:A:228:GLN:O	1:A:232:ARG:HG3	1.90	0.71
1:A:44:ASN:HB2	1:A:362:THR:HG23	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LEU:O	1:A:162:HIS:HA	1.91	0.70
1:B:44:ASN:HB2	1:B:362:THR:HG23	1.73	0.69
1:A:246:VAL:HG21	1:A:255:LEU:HD13	1.74	0.69
1:B:182:ALA:HB3	1:B:185:LYS:HD2	1.75	0.68
1:B:4:MET:HG2	1:B:36:SER:HA	1.76	0.68
1:B:41:PRO:HA	1:B:425:HIS:HE1	1.59	0.68
1:B:120:LEU:O	1:B:162:HIS:HA	1.93	0.68
1:A:142:ALA:HB3	1:A:317:PHE:CB	2.24	0.68
1:A:124:ILE:HD11	1:B:17:THR:HB	1.76	0.67
1:B:7:LEU:HB2	1:B:77:ALA:HA	1.75	0.67
1:B:330:ASP:HA	1:B:338:GLN:NE2	2.10	0.67
1:A:168:CYS:O	1:A:191:ILE:HG13	1.94	0.67
1:A:411:GLU:HB2	5:A:643:HOH:O	1.95	0.66
1:B:93:THR:OG1	1:B:95:LYS:HB2	1.96	0.66
1:B:309:LEU:HA	1:B:312:LYS:HE2	1.78	0.65
1:B:330:ASP:HA	1:B:338:GLN:HE21	1.63	0.64
1:A:135:MET:HE1	1:A:439:PHE:HZ	1.62	0.64
1:A:51:ASP:O	1:A:327:ASP:HB2	1.98	0.64
1:B:60:ALA:HB1	1:B:400:MET:HE3	1.79	0.64
1:B:333:ALA:O	1:B:335:PRO:HD3	1.98	0.64
1:B:214:THR:HG22	1:B:224:THR:HA	1.79	0.63
1:B:51:ASP:HA	5:B:685:HOH:O	1.99	0.62
1:A:93:THR:OG1	1:A:95:LYS:HB2	2.00	0.60
1:B:443:LYS:HE2	1:B:449:LYS:HA	1.83	0.60
1:A:229:ALA:O	1:A:234:TYR:HB2	2.00	0.60
1:A:434:ASP:HB2	1:B:24:ARG:HG3	1.84	0.60
1:B:418:ARG:HG2	1:B:419:ILE:N	2.17	0.59
1:A:45:ILE:HD12	1:A:446:LEU:HG	1.84	0.59
1:B:368:ALA:HB3	1:B:417:LEU:HD13	1.84	0.59
1:A:7:LEU:HB2	1:A:77:ALA:HA	1.85	0.59
1:A:135:MET:HE1	1:A:439:PHE:CZ	2.37	0.58
1:B:135:MET:HE1	1:B:439:PHE:CZ	2.38	0.58
1:B:379:PRO:HA	1:B:399:VAL:HG21	1.85	0.58
1:A:368:ALA:HB3	1:A:417:LEU:HD13	1.85	0.58
1:B:46:ILE:HG22	1:B:48:LEU:HD22	1.86	0.58
1:A:47:LEU:HD23	1:A:320:GLN:HG3	1.86	0.58
1:B:135:MET:HE1	1:B:439:PHE:HZ	1.66	0.58
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.84	0.57
1:B:60:ALA:CB	1:B:400:MET:HE3	2.35	0.57
1:A:215:ALA:HB3	1:A:221:GLN:HA	1.85	0.57
1:A:363:LEU:HD13	1:A:424:PRO:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:THR:OG1	1:B:301:GLN:HG3	2.06	0.56
1:A:25:LEU:HD23	1:B:433:THR:HG22	1.88	0.56
1:B:182:ALA:CB	1:B:185:LYS:HD2	2.36	0.56
1:A:303:THR:HG23	1:A:321:VAL:HG21	1.88	0.56
1:A:354:GLU:O	1:A:358:LYS:HE2	2.06	0.55
1:A:330:ASP:HA	1:A:338:GLN:HE21	1.70	0.55
1:B:318:PHE:HE1	1:B:442:MET:CE	2.19	0.55
1:A:15:ASP:HA	5:A:553:HOH:O	2.05	0.55
1:A:110:SER:HB2	1:A:159:LEU:HD23	1.87	0.55
1:A:270:GLY:HA3	1:A:336:CYS:HB2	1.89	0.55
1:B:208:ALA:HB2	1:B:258:LEU:HB3	1.89	0.54
1:A:4:MET:HG2	1:A:36:SER:HA	1.90	0.54
1:B:7:LEU:HD22	1:B:10:ARG:HE	1.72	0.54
1:A:63:ASN:OD1	1:A:68:ALA:HA	2.08	0.54
1:B:110:SER:HB2	1:B:159:LEU:HD23	1.90	0.53
1:B:11:ALA:HB2	1:B:71:PHE:HB3	1.90	0.53
1:A:214:THR:HG22	1:A:224:THR:HA	1.91	0.53
1:B:40:LYS:O	1:B:424:PRO:HB3	2.08	0.53
1:A:53:MET:HA	1:A:57:GLU:HG2	1.91	0.53
1:A:309:LEU:HA	1:A:312:LYS:HE2	1.90	0.53
1:A:182:ALA:HB1	1:A:184:GLU:CD	2.33	0.52
1:B:142:ALA:HB3	1:B:317:PHE:HB3	1.92	0.52
1:A:298:THR:OG1	1:A:301:GLN:HG3	2.08	0.52
1:A:318:PHE:HE1	1:A:442:MET:CE	2.22	0.52
1:A:391:ASN:HB3	5:A:640:HOH:O	2.09	0.52
1:B:236:LEU:HA	1:B:256:LEU:O	2.08	0.52
1:A:182:ALA:CB	1:A:185:LYS:HD2	2.39	0.52
1:B:331:HIS:CD2	1:B:372:HIS:HE2	2.27	0.52
1:B:83:GLN:HG3	5:B:657:HOH:O	2.10	0.52
1:A:148:THR:HG23	1:A:299:LEU:HD13	1.92	0.51
1:A:182:ALA:HB1	1:A:184:GLU:OE2	2.10	0.51
1:A:25:LEU:HD12	1:A:25:LEU:O	2.10	0.51
1:B:221:GLN:HB2	5:B:682:HOH:O	2.09	0.51
1:B:270:GLY:HA3	1:B:336:CYS:HB2	1.91	0.51
1:A:330:ASP:HA	1:A:338:GLN:NE2	2.26	0.51
1:B:214:THR:HG22	1:B:224:THR:CA	2.40	0.51
1:A:139:ALA:CB	1:A:448:LEU:HD21	2.40	0.51
1:B:213:GLU:O	1:B:224:THR:HA	2.11	0.50
1:B:47:LEU:HD11	1:B:49:ILE:HD11	1.93	0.50
1:B:363:LEU:HD13	1:B:424:PRO:O	2.11	0.50
1:A:337:GLY:O	1:A:341:GLU:HG2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ASN:OD1	1:B:68:ALA:HA	2.11	0.50
1:A:119:ALA:HB1	1:A:122:VAL:HG22	1.94	0.50
1:A:37:LEU:HD13	1:B:34:ARG:HG3	1.93	0.50
1:A:40:LYS:O	1:A:424:PRO:HB3	2.11	0.50
1:A:129:HIS:O	1:A:162:HIS:HE1	1.94	0.50
1:B:61:ALA:HA	1:B:339:ILE:HG23	1.93	0.50
1:B:306:ALA:O	1:B:310:LEU:HG	2.11	0.49
1:A:23:ARG:HD2	1:B:440:TYR:CD1	2.47	0.49
1:B:168:CYS:O	1:B:191:ILE:HG13	2.12	0.49
1:B:84:TYR:CE2	1:B:435:GLN:HA	2.47	0.49
1:B:199:ARG:HA	1:B:234:TYR:OH	2.12	0.49
1:B:45:ILE:CD1	1:B:446:LEU:HG	2.34	0.49
1:B:337:GLY:O	1:B:341:GLU:HG2	2.12	0.49
1:B:354:GLU:O	1:B:358:LYS:HE2	2.12	0.49
1:A:139:ALA:HB2	1:A:448:LEU:HD21	1.95	0.49
1:A:443:LYS:HE2	1:A:449:LYS:HA	1.95	0.49
1:B:89:LEU:HD23	1:B:114:LYS:HB3	1.95	0.49
1:B:125:HIS:O	1:B:126:GLU:HB2	2.12	0.48
1:A:147:SER:O	1:A:205:GLY:HA2	2.13	0.48
1:A:433:THR:HG22	1:B:25:LEU:HD23	1.95	0.48
1:B:144:GLY:HA2	1:B:202:VAL:O	2.14	0.48
1:A:149:ALA:HB2	1:A:324:ALA:HB1	1.94	0.48
1:B:299:LEU:HD11	1:B:321:VAL:HG13	1.95	0.48
1:A:31:ALA:O	1:A:34:ARG:HB2	2.14	0.48
1:A:213:GLU:O	1:A:224:THR:HA	2.13	0.48
1:A:199:ARG:HA	1:A:234:TYR:OH	2.14	0.48
1:B:143:THR:OG1	1:B:200:ALA:HA	2.14	0.48
1:B:425:HIS:CE1	1:B:445:ALA:HA	2.49	0.48
1:A:426:ALA:O	1:A:429:VAL:HG22	2.13	0.48
1:B:379:PRO:HA	1:B:399:VAL:CG2	2.43	0.48
1:B:109:TRP:CD1	1:B:109:TRP:C	2.92	0.47
1:B:119:ALA:HB1	1:B:122:VAL:HG22	1.97	0.47
1:B:20:GLY:HA2	1:B:23:ARG:HG3	1.95	0.47
1:B:275:TYR:O	1:B:276:HIS:HB2	2.13	0.47
1:A:10:ARG:NH2	1:A:29:GLN:HG2	2.30	0.47
1:B:29:GLN:O	1:B:30:THR:C	2.58	0.47
1:B:223:LYS:HD2	1:B:227:GLU:HB3	1.96	0.47
1:A:171:PRO:HD3	1:A:225:LEU:HD11	1.97	0.47
1:B:182:ALA:HB1	1:B:184:GLU:OE2	2.15	0.47
1:A:268:TRP:HB2	1:A:336:CYS:O	2.14	0.46
1:A:114:LYS:HA	5:A:626:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:THR:OG1	1:A:200:ALA:HA	2.15	0.46
1:A:419:ILE:HD11	1:A:438:LEU:HD13	1.97	0.46
1:B:182:ALA:HB1	1:B:184:GLU:CD	2.40	0.46
1:B:215:ALA:HB3	1:B:221:GLN:HA	1.96	0.46
1:A:144:GLY:HA3	1:A:310:LEU:HD11	1.96	0.46
1:B:229:ALA:O	1:B:234:TYR:HB2	2.16	0.46
1:A:305:LYS:O	1:A:308:GLU:HB3	2.15	0.46
1:B:7:LEU:HB2	1:B:77:ALA:CA	2.45	0.46
1:B:268:TRP:HB2	1:B:336:CYS:O	2.15	0.46
1:A:188:LYS:HB2	1:A:188:LYS:NZ	2.30	0.46
1:A:211:PHE:HA	1:A:225:LEU:HB2	1.97	0.46
1:A:29:GLN:O	1:A:30:THR:C	2.58	0.46
1:B:292:ARG:HG3	1:B:292:ARG:HH11	1.80	0.46
1:A:90:ASN:HB3	1:A:93:THR:OG1	2.16	0.46
1:A:333:ALA:O	1:A:335:PRO:HD3	2.16	0.46
1:A:37:LEU:HD13	1:B:34:ARG:CG	2.46	0.46
1:A:237:VAL:HG12	1:A:242:SER:HB3	1.98	0.46
1:A:31:ALA:O	1:A:34:ARG:N	2.49	0.46
1:A:45:ILE:CD1	1:A:446:LEU:HG	2.45	0.45
1:B:7:LEU:HB2	1:B:77:ALA:C	2.40	0.45
1:B:419:ILE:HD11	1:B:438:LEU:HD13	1.98	0.45
1:A:15:ASP:OD1	1:A:17:THR:HG23	2.16	0.45
1:A:237:VAL:CG2	1:A:255:LEU:HD11	2.46	0.45
1:A:267:ARG:NH1	1:A:267:ARG:HG3	2.31	0.45
1:B:176:GLU:HG3	1:B:177:LYS:N	2.31	0.45
1:B:147:SER:O	1:B:205:GLY:HA2	2.17	0.45
1:B:152:GLN:NE2	1:B:210:THR:HB	2.31	0.45
1:A:235:GLN:HE22	1:A:246:VAL:HG13	1.81	0.45
1:A:380:ASP:HA	5:A:600:HOH:O	2.17	0.45
1:B:7:LEU:HD23	1:B:7:LEU:HA	1.74	0.45
1:B:11:ALA:O	1:B:12:ALA:C	2.58	0.45
1:A:7:LEU:HA	1:A:7:LEU:HD23	1.60	0.45
1:A:245:SER:HB3	5:A:612:HOH:O	2.16	0.45
1:A:37:LEU:HD21	1:B:33:LEU:HD12	1.99	0.45
1:A:46:ILE:HG22	1:A:48:LEU:HD22	1.99	0.45
1:B:277:GLY:O	1:B:281:LYS:HB2	2.17	0.44
1:A:275:TYR:O	1:A:276:HIS:HB2	2.16	0.44
1:B:292:ARG:HH21	1:B:298:THR:HA	1.81	0.44
1:B:318:PHE:HE1	1:B:442:MET:HE2	1.82	0.44
1:A:10:ARG:NH1	1:B:433:THR:HG22	2.33	0.44
1:A:68:ALA:HB2	1:B:98:TYR:CE1	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:PRO:HD2	1:B:292:ARG:NH1	2.32	0.44
1:A:109:TRP:HB2	1:A:438:LEU:HD23	1.99	0.44
1:A:25:LEU:HG	1:B:437:ASP:OD1	2.17	0.44
1:A:237:VAL:HG21	1:A:255:LEU:HD11	1.99	0.44
1:A:10:ARG:HH21	1:A:29:GLN:HG2	1.83	0.44
1:A:98:TYR:HE1	1:B:68:ALA:HB2	1.82	0.44
1:B:15:ASP:O	1:B:17:THR:N	2.51	0.44
1:B:240:ALA:HA	1:B:297:PRO:HG3	2.00	0.44
1:B:289:ASN:HA	1:B:290:PRO:HD3	1.74	0.44
1:B:329:GLN:HE21	1:B:334:ASN:HB3	1.82	0.44
1:A:25:LEU:HD23	1:B:433:THR:CG2	2.47	0.44
1:A:98:TYR:CE1	1:B:68:ALA:HB2	2.52	0.44
1:A:176:GLU:HG3	1:A:177:LYS:N	2.32	0.44
1:A:269:LEU:HD13	1:A:290:PRO:HD2	1.99	0.44
1:B:53:MET:O	1:B:53:MET:HG2	2.18	0.44
1:B:116:TYR:HD1	1:B:124:ILE:HA	1.82	0.44
1:B:138:ALA:C	1:B:140:GLY:H	2.26	0.44
1:B:237:VAL:HG12	1:B:242:SER:HB3	1.99	0.44
1:B:332:ALA:O	1:B:333:ALA:HB3	2.17	0.43
1:B:45:ILE:HG12	1:B:363:LEU:HB3	2.00	0.43
1:A:284:VAL:HG12	1:A:285:THR:N	2.33	0.43
1:A:4:MET:HG2	1:A:35:ASP:O	2.19	0.43
1:A:318:PHE:HE1	1:A:442:MET:HE2	1.82	0.43
1:A:327:ASP:OD1	1:A:370:HIS:HE1	2.01	0.43
1:A:412:HIS:N	5:A:643:HOH:O	2.51	0.43
1:A:415:SER:HB2	5:B:616:HOH:O	2.18	0.43
1:A:61:ALA:HA	1:A:339:ILE:HG23	2.00	0.43
1:A:80:LEU:HD12	1:A:426:ALA:HB3	2.01	0.43
1:A:415:SER:OG	1:B:56:SER:HA	2.18	0.43
1:A:237:VAL:HG23	1:A:257:GLY:HA2	2.01	0.43
1:A:267:ARG:CG	1:A:267:ARG:HH11	2.32	0.43
1:A:33:LEU:HD12	1:B:37:LEU:HD21	2.00	0.42
1:A:83:GLN:NE2	1:B:418:ARG:HG3	2.34	0.42
1:B:148:THR:O	1:B:264:MET:HB2	2.19	0.42
1:A:412:HIS:CD2	1:A:412:HIS:H	2.38	0.42
1:A:11:ALA:O	1:A:12:ALA:C	2.63	0.42
1:A:387:THR:HA	1:A:400:MET:O	2.19	0.42
1:A:139:ALA:HB2	1:A:448:LEU:CD2	2.50	0.42
1:A:109:TRP:CD1	1:A:109:TRP:C	2.97	0.42
1:A:425:HIS:CE1	1:A:445:ALA:HA	2.54	0.42
1:A:24:ARG:HG3	1:B:434:ASP:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:PHE:HE1	1:B:442:MET:HE1	1.83	0.42
1:A:269:LEU:HA	5:A:676:HOH:O	2.19	0.42
1:B:238:SER:HB2	5:B:659:HOH:O	2.19	0.42
1:B:246:VAL:HG21	1:B:255:LEU:CD1	2.45	0.42
1:B:142:ALA:HB3	1:B:317:PHE:CB	2.50	0.41
1:B:176:GLU:HG3	1:B:177:LYS:H	1.85	0.41
1:A:230:GLN:HG3	1:A:236:LEU:HD13	2.01	0.41
1:B:153:ASP:O	1:B:156:PRO:HG2	2.20	0.41
1:A:45:ILE:HG12	1:A:363:LEU:HB3	2.03	0.41
1:A:418:ARG:CG	1:A:419:ILE:N	2.83	0.41
1:B:4:MET:HG2	1:B:36:SER:CA	2.48	0.41
1:B:199:ARG:O	1:B:199:ARG:HG2	2.20	0.41
1:A:246:VAL:HG21	1:A:255:LEU:CD1	2.48	0.41
1:B:90:ASN:OD1	1:B:93:THR:HG23	2.21	0.41
1:B:236:LEU:HG	1:B:256:LEU:HD23	2.03	0.41
1:B:418:ARG:HG2	1:B:419:ILE:H	1.86	0.41
1:A:356:ALA:HB2	1:A:364:VAL:CG2	2.50	0.41
1:B:64:TYR:CE2	1:B:268:TRP:CZ3	3.09	0.41
1:B:155:THR:HB	1:B:156:PRO:CD	2.51	0.41
1:A:84:TYR:CE2	1:A:435:GLN:HA	2.56	0.41
1:A:68:ALA:HB2	1:B:98:TYR:HE1	1.86	0.41
1:A:4:MET:HB3	1:A:36:SER:HA	2.03	0.41
1:A:7:LEU:HB2	1:A:77:ALA:C	2.45	0.41
1:B:220:TRP:CG	1:B:228:GLN:HG3	2.56	0.41
1:B:265:PRO:HD2	1:B:292:ARG:HH12	1.86	0.40
1:B:436:THR:O	1:B:439:PHE:HB3	2.21	0.40
1:A:144:GLY:O	1:A:319:LEU:HA	2.21	0.40
1:B:129:HIS:O	1:B:162:HIS:HE1	2.05	0.40
1:B:434:ASP:O	1:B:437:ASP:HB2	2.21	0.40
1:A:116:TYR:HD1	1:A:124:ILE:HA	1.87	0.40
1:A:37:LEU:HD11	1:B:37:LEU:HD11	2.03	0.40
1:A:181:ASN:C	1:A:187:GLY:HA3	2.47	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)
5:B:512:HOH:O	5:B:512:HOH:O[10_665]	0.58	1.62

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	447/449 (100%)	407 (91%)	34 (8%)	6 (1%)	9	31
1	B	447/449 (100%)	408 (91%)	32 (7%)	7 (2%)	7	27
All	All	894/898 (100%)	815 (91%)	66 (7%)	13 (2%)	8	28

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ASP
1	A	169	TYR
1	B	16	ILE
1	A	158	ALA
1	B	409	SER
1	A	16	ILE
1	B	23	ARG
1	B	169	TYR
1	A	154	ALA
1	B	8	GLU
1	A	8	GLU
1	B	77	ALA
1	B	154	ALA

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	340/340 (100%)	319 (94%)	21 (6%)	16	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	340/340 (100%)	318 (94%)	22 (6%)	15	43
All	All	680/680 (100%)	637 (94%)	43 (6%)	16	45

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	3	GLU
1	A	4	MET
1	A	13	GLN
1	A	17	THR
1	A	33	LEU
1	A	48	LEU
1	A	56	SER
1	A	84	TYR
1	A	89	LEU
1	A	113	VAL
1	A	122	VAL
1	A	155	THR
1	A	193	GLU
1	A	253	LYS
1	A	274	THR
1	A	279	ILE
1	A	379	PRO
1	A	382	LYS
1	A	413	THR
1	A	417	LEU
1	B	1	THR
1	B	3	GLU
1	B	4	MET
1	B	13	GLN
1	B	33	LEU
1	B	48	LEU
1	B	84	TYR
1	B	89	LEU
1	B	109	TRP
1	B	113	VAL
1	B	122	VAL
1	B	171	PRO
1	B	193	GLU
1	B	253	LYS
1	B	261	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	274	THR
1	B	279	ILE
1	B	343	VAL
1	B	351	ARG
1	B	382	LYS
1	B	413	THR
1	B	417	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	162	HIS
1	A	181	ASN
1	A	228	GLN
1	A	235	GLN
1	A	293	ASN
1	A	320	GLN
1	A	329	GLN
1	A	338	GLN
1	A	361	ASN
1	A	391	ASN
1	A	425	HIS
1	A	435	GLN
1	B	181	ASN
1	B	235	GLN
1	B	291	GLN
1	B	329	GLN
1	B	338	GLN
1	B	391	ASN
1	B	425	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 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	$\# Z > 2$
4	PO4	A	453	2	4,4,4	1.10	0	6,6,6	0.84	0
4	PO4	B	453	2	4,4,4	1.17	0	6,6,6	0.25	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.