



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:57 am GMT

PDB ID : 1KH9
Title : E. COLI ALKALINE PHOSPHATASE MUTANT (D153GD330N) COM-
PLEX WITH PHOSPHATE
Authors : Le Du, M.H.; Lamoure, C.; Muller, B.H.; Bulgakov, O.V.; Lajeunesse, E.
Deposited on : 2001-11-29
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

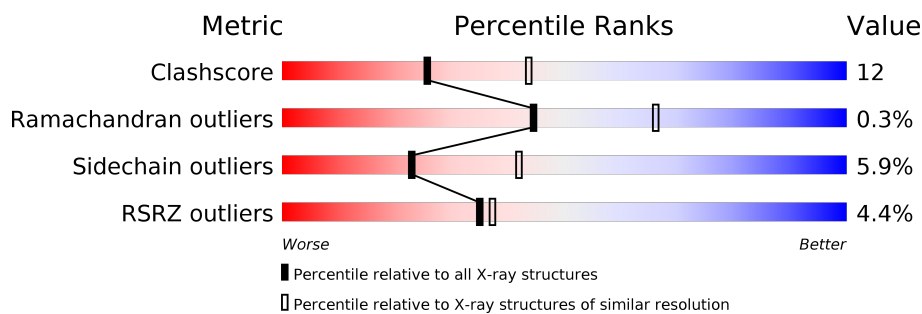
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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 $\leq 5\%$. 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	
1	B	449	

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	MG	A	452	-	-	-	X
4	PO4	B	453	-	X	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6665 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
			3252	2009	577	655	11			
1	B	444	Total	C	N	O	S	0	0	0
			3252	2009	577	655	11			

There are 12 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	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	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

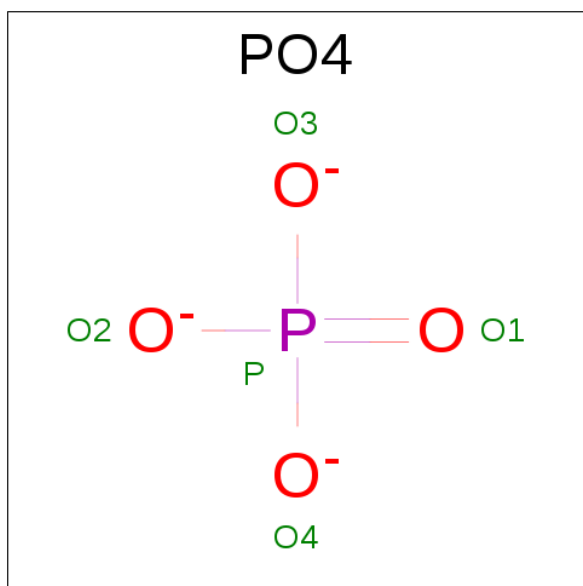
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			4	3	1		
4	B	1	Total	O	P	0	0
			5	4	1		

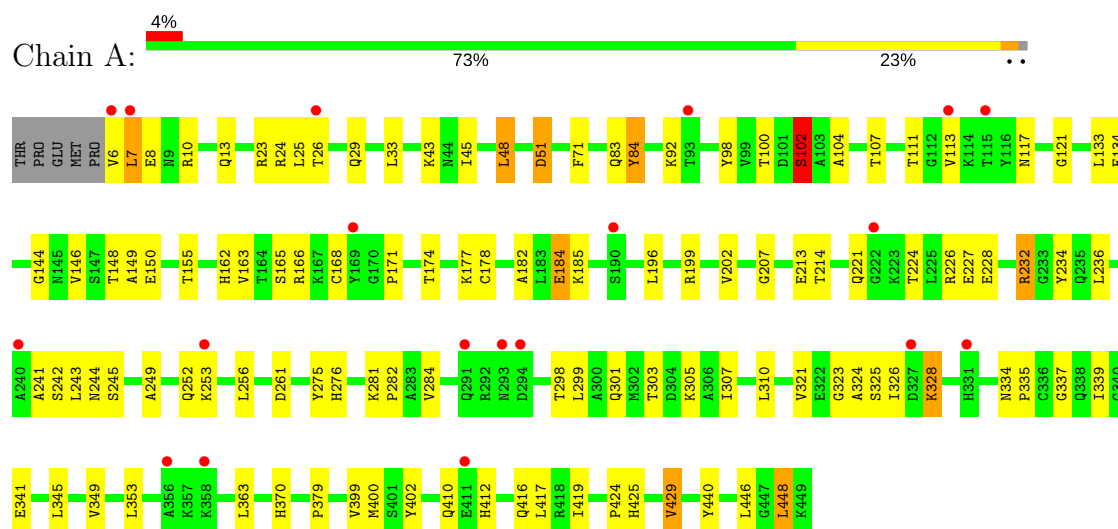
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	69	Total	O	0	0
			69	69		
5	B	78	Total	O	0	0
			78	78		

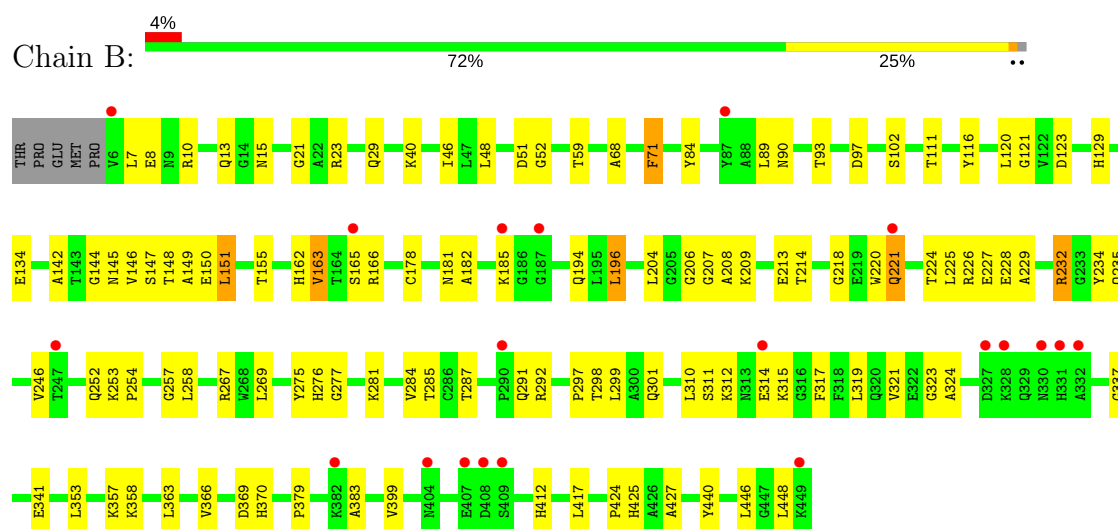
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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	164.01Å 164.01Å 138.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.50 19.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	83.4 (10.00-2.50) 83.4 (19.86-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.50Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.196 , 0.250 0.268 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6665	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: PO4, MG, 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	0.53	1/3305 (0.0%)	0.78	2/4486 (0.0%)
1	B	0.51	0/3305	0.76	2/4486 (0.0%)
All	All	0.52	1/6610 (0.0%)	0.77	4/8972 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	SER	CA-C	7.05	1.71	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	LEU	CA-CB-CG	6.36	129.94	115.30
1	B	97	ASP	N-CA-C	-5.88	95.12	111.00
1	A	323	GLY	N-CA-C	-5.25	99.98	113.10
1	B	323	GLY	N-CA-C	-5.13	100.29	113.10

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	3252	0	3189	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3252	0	3190	76	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
4	A	4	0	0	1	0
4	B	5	0	0	2	0
5	A	69	0	0	4	0
5	B	78	0	0	3	0
All	All	6665	0	6379	154	0

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 12.

All (154) 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:102:SER:OG	4:B:453:PO4:P	2.03	1.17
1:B:102:SER:HG	4:B:453:PO4:P	1.93	0.92
1:B:178:CYS:HB3	1:B:181:ASN:HD22	1.36	0.89
1:A:7:LEU:HD13	1:A:7:LEU:H	1.44	0.82
1:A:334:ASN:HD22	1:A:337:GLY:H	1.30	0.77
1:A:325:SER:HA	1:A:328:LYS:HD2	1.69	0.75
1:B:208:ALA:HB2	1:B:258:LEU:HB3	1.69	0.74
1:A:335:PRO:HB3	1:A:400:MET:HE3	1.72	0.71
1:A:111:THR:CG2	1:A:113:VAL:HG12	2.21	0.71
1:A:168:CYS:SG	1:A:177:LYS:HB2	2.30	0.70
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.73	0.69
1:A:23:ARG:HD2	1:B:440:TYR:CE2	2.27	0.69
1:B:220:TRP:CZ2	1:B:232:ARG:HD3	2.27	0.69
1:A:6:VAL:N	1:A:29:GLN:HG2	2.08	0.68
1:A:48:LEU:HD13	1:A:321:VAL:HB	1.75	0.68
1:B:224:THR:OG1	1:B:227:GLU:HG3	1.93	0.68
1:A:174:THR:HG23	1:A:178:CYS:HB2	1.78	0.66
1:A:111:THR:HG22	1:A:113:VAL:HG12	1.77	0.66
1:B:267:ARG:HG2	1:B:267:ARG:HH21	1.62	0.65
1:A:249:ALA:HA	1:A:253:LYS:O	1.97	0.65
1:B:182:ALA:HB3	1:B:185:LYS:HD3	1.79	0.65
1:A:13:GLN:HG2	1:A:23:ARG:O	1.97	0.64
1:B:298:THR:OG1	1:B:301:GLN:HG3	1.99	0.62
1:A:107:THR:O	1:A:111:THR:HB	2.00	0.62
1:B:120:LEU:O	1:B:162:HIS:HA	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:HD22	1:A:10:ARG:HE	1.66	0.60
1:B:213:GLU:O	1:B:225:LEU:HD22	2.01	0.60
1:A:48:LEU:HG	1:A:349:VAL:HG22	1.83	0.60
1:A:163:VAL:HG12	1:A:165:SER:H	1.68	0.59
1:A:148:THR:HG23	1:A:299:LEU:HD13	1.84	0.59
1:A:144:GLY:HA2	1:A:202:VAL:O	2.03	0.59
1:A:146:VAL:HG22	1:A:321:VAL:HG13	1.86	0.58
1:B:363:LEU:HD13	1:B:424:PRO:O	2.02	0.58
1:B:120:LEU:HD12	1:B:166:ARG:HA	1.87	0.57
1:A:419:ILE:CD1	1:A:429:VAL:HG22	2.34	0.57
1:A:182:ALA:HB1	1:A:184:GLU:OE1	2.03	0.57
1:B:218:GLY:O	1:B:221:GLN:HG2	2.03	0.57
1:A:33:LEU:HD12	1:B:427:ALA:HB1	1.86	0.56
1:A:339:ILE:HD11	1:A:400:MET:HE1	1.88	0.56
1:A:303:THR:O	1:A:307:ILE:HG13	2.06	0.56
1:A:412:HIS:HE1	4:A:453:PO4:O1	1.71	0.56
1:B:48:LEU:HB2	1:B:366:VAL:HG22	1.87	0.56
1:B:121:GLY:O	1:B:162:HIS:HD2	1.89	0.55
1:A:419:ILE:HD11	1:A:429:VAL:HG22	1.89	0.55
1:B:353:LEU:O	1:B:357:LYS:HG3	2.06	0.55
1:A:334:ASN:ND2	1:A:337:GLY:H	1.99	0.54
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.89	0.54
1:A:182:ALA:HB3	1:A:185:LYS:HD3	1.90	0.54
1:A:134:GLU:OE2	1:A:162:HIS:HE1	1.91	0.54
1:A:7:LEU:CD1	1:A:7:LEU:H	2.19	0.53
1:B:228:GLU:HB2	5:B:1103:HOH:O	2.07	0.53
1:A:7:LEU:HD21	1:A:25:LEU:HA	1.91	0.53
1:A:10:ARG:O	1:A:24:ARG:HD3	2.09	0.53
1:A:111:THR:HG21	1:A:113:VAL:HG12	1.90	0.53
1:A:7:LEU:HG	1:A:26:THR:OG1	2.09	0.52
1:B:10:ARG:NH2	1:B:29:GLN:OE1	2.42	0.52
1:B:148:THR:HG23	1:B:299:LEU:HD13	1.91	0.51
1:B:163:VAL:HG23	1:B:194:GLN:NE2	2.25	0.51
1:B:310:LEU:HD23	1:B:317:PHE:CD1	2.46	0.51
1:A:298:THR:OG1	1:A:301:GLN:HG3	2.11	0.50
1:B:235:GLN:HE22	1:B:246:VAL:HG13	1.76	0.50
1:B:267:ARG:NH2	1:B:267:ARG:HG2	2.26	0.50
1:A:202:VAL:HB	1:A:310:LEU:HD11	1.94	0.50
1:B:89:LEU:O	1:B:116:TYR:HA	2.11	0.50
1:A:102:SER:CB	1:A:166:ARG:HH12	2.24	0.50
1:A:199:ARG:NH2	1:A:232:ARG:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:HD22	1:A:10:ARG:NE	2.28	0.49
1:B:253:LYS:N	1:B:254:PRO:HD3	2.28	0.49
1:A:104:ALA:HB2	1:A:117:ASN:HA	1.95	0.49
1:A:275:TYR:O	1:A:276:HIS:HB2	2.12	0.49
1:B:383:ALA:HB1	5:B:1092:HOH:O	2.12	0.48
1:A:51:ASP:O	1:A:326:ILE:HB	2.13	0.48
1:B:370:HIS:CE1	1:B:412:HIS:CD2	3.01	0.48
1:A:121:GLY:O	1:A:162:HIS:HD2	1.96	0.48
1:B:13:GLN:HG2	1:B:23:ARG:O	2.13	0.48
1:B:369:ASP:N	1:B:369:ASP:OD1	2.47	0.48
1:A:199:ARG:HA	1:A:234:TYR:OH	2.14	0.48
1:A:402:TYR:HB3	1:A:410:GLN:HG3	1.96	0.48
1:B:370:HIS:CE1	1:B:412:HIS:CG	3.01	0.48
1:A:281:LYS:CG	1:A:282:PRO:HD2	2.44	0.48
1:A:440:TYR:CD2	1:B:23:ARG:HD3	2.48	0.48
1:A:424:PRO:O	1:A:425:HIS:HB2	2.13	0.47
1:A:23:ARG:HD2	1:B:440:TYR:CD2	2.48	0.47
1:A:146:VAL:CG2	1:A:321:VAL:HG13	2.44	0.47
1:B:145:ASN:ND2	5:B:1033:HOH:O	2.47	0.47
1:A:149:ALA:HB2	1:A:324:ALA:CB	2.45	0.47
1:B:204:LEU:HD23	1:B:257:GLY:HA3	1.96	0.47
1:B:150:GLU:HG2	1:B:207:GLY:HA2	1.96	0.46
1:A:149:ALA:HB2	1:A:324:ALA:HB1	1.97	0.46
1:A:102:SER:HB2	1:A:166:ARG:HH12	1.79	0.46
1:A:100:THR:HG22	5:A:1080:HOH:O	2.14	0.46
1:B:46:ILE:HG22	1:B:48:LEU:HD22	1.98	0.46
1:B:299:LEU:HD11	1:B:321:VAL:HG13	1.97	0.45
1:A:276:HIS:HA	5:A:1121:HOH:O	2.16	0.45
1:A:325:SER:HA	1:A:328:LYS:HB2	1.98	0.45
1:A:334:ASN:ND2	5:A:1047:HOH:O	2.50	0.45
1:B:446:LEU:HB3	1:B:448:LEU:HD13	1.99	0.45
1:A:337:GLY:O	1:A:341:GLU:HG2	2.16	0.45
1:B:90:ASN:HB3	1:B:93:THR:OG1	2.16	0.45
1:A:224:THR:OG1	1:A:227:GLU:HG3	2.16	0.45
1:A:84:TYR:HD1	1:A:84:TYR:O	1.99	0.45
1:B:142:ALA:HB3	1:B:317:PHE:HB3	1.99	0.45
1:B:226:ARG:O	1:B:229:ALA:HB3	2.17	0.45
1:B:229:ALA:O	1:B:234:TYR:HD1	2.00	0.45
1:A:448:LEU:HD12	1:A:448:LEU:HA	1.57	0.44
1:B:134:GLU:OE2	1:B:162:HIS:HE1	2.00	0.44
1:B:358:LYS:HE3	1:B:358:LYS:HB2	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:HD13	1:A:424:PRO:O	2.18	0.44
1:A:370:HIS:CE1	1:A:412:HIS:CE1	3.06	0.44
1:B:284:VAL:HG12	1:B:285:THR:N	2.33	0.44
1:B:40:LYS:O	1:B:424:PRO:HB3	2.18	0.44
1:A:48:LEU:HD12	1:A:345:LEU:HD11	1.99	0.44
1:B:151:LEU:HD22	1:B:206:GLY:O	2.17	0.44
1:A:207:GLY:HA2	1:A:261:ASP:O	2.18	0.43
1:A:133:LEU:HD23	1:A:133:LEU:C	2.37	0.43
1:A:163:VAL:HG13	1:A:178:CYS:SG	2.59	0.43
1:B:111:THR:HG21	1:B:129:HIS:HB2	2.01	0.43
1:B:52:GLY:HA2	1:B:370:HIS:O	2.19	0.43
1:A:150:GLU:HG2	1:A:150:GLU:H	1.60	0.43
1:B:310:LEU:C	1:B:312:LYS:H	2.22	0.43
1:B:8:GLU:O	1:B:71:PHE:CZ	2.71	0.43
1:A:45:ILE:HD12	1:A:446:LEU:HG	2.00	0.42
1:B:275:TYR:O	1:B:276:HIS:HB2	2.18	0.42
1:B:144:GLY:O	1:B:319:LEU:HA	2.20	0.42
1:A:171:PRO:HG2	1:A:213:GLU:HB3	2.00	0.42
1:A:345:LEU:O	1:A:349:VAL:HG23	2.19	0.42
1:B:379:PRO:HA	1:B:399:VAL:HG21	2.01	0.42
1:B:277:GLY:O	1:B:281:LYS:HB2	2.19	0.42
1:A:236:LEU:HA	1:A:256:LEU:O	2.20	0.42
1:B:292:ARG:NH2	1:B:297:PRO:O	2.52	0.42
1:A:228:GLU:O	1:A:232:ARG:HG3	2.20	0.42
1:B:214:THR:HA	1:B:224:THR:HA	2.02	0.42
1:A:243:LEU:O	1:A:305:LYS:HE2	2.20	0.41
1:A:242:SER:O	1:A:245:SER:HB3	2.20	0.41
1:B:146:VAL:HG13	1:B:319:LEU:HD11	2.02	0.41
1:A:98:TYR:CE1	1:B:68:ALA:HB2	2.55	0.41
1:A:244:ASN:HA	1:A:305:LYS:HZ3	1.85	0.41
5:A:1007:HOH:O	1:B:123:ASP:HB2	2.20	0.41
1:B:424:PRO:O	1:B:425:HIS:HB2	2.21	0.41
1:B:178:CYS:HB3	1:B:181:ASN:ND2	2.19	0.41
1:B:337:GLY:O	1:B:341:GLU:HG2	2.20	0.41
1:A:98:TYR:HE1	1:B:68:ALA:HB2	1.86	0.41
1:B:196:LEU:HD12	1:B:196:LEU:HA	1.89	0.41
1:B:149:ALA:HB2	1:B:324:ALA:CB	2.50	0.41
1:B:15:ASN:O	1:B:21:GLY:HA3	2.20	0.41
1:B:10:ARG:HB2	1:B:71:PHE:CD1	2.56	0.40
1:B:48:LEU:O	1:B:366:VAL:HA	2.21	0.40
1:A:102:SER:HB2	1:A:166:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:HG2	1:A:199:ARG:O	2.21	0.40
1:A:48:LEU:HD12	1:A:345:LEU:CD1	2.50	0.40
1:B:165:SER:HB3	1:B:178:CYS:SG	2.62	0.40
1:B:7:LEU:HB2	1:B:10:ARG:HE	1.86	0.40
1:A:226:ARG:NH1	1:A:236:LEU:HD23	2.36	0.40
1:A:416:GLN:HG2	1:B:59:THR:OG1	2.21	0.40

There are no symmetry-related clashes.

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%)	422 (96%)	18 (4%)	2 (0%)	32	53
1	B	442/449 (98%)	414 (94%)	27 (6%)	1 (0%)	51	73
All	All	884/898 (98%)	836 (95%)	45 (5%)	3 (0%)	44	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	ALA
1	A	8	GLU
1	B	311	SER

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	331/340 (97%)	310 (94%)	21 (6%)	21	38
1	B	331/340 (97%)	313 (95%)	18 (5%)	26	47
All	All	662/680 (97%)	623 (94%)	39 (6%)	23	42

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	43	LYS
1	A	51	ASP
1	A	71	PHE
1	A	83	GLN
1	A	84	TYR
1	A	92	LYS
1	A	102	SER
1	A	155	THR
1	A	184	GLU
1	A	196	LEU
1	A	214	THR
1	A	221	GLN
1	A	232	ARG
1	A	252	GLN
1	A	284	VAL
1	A	328	LYS
1	A	353	LEU
1	A	417	LEU
1	A	429	VAL
1	A	448	LEU
1	B	51	ASP
1	B	71	PHE
1	B	84	TYR
1	B	147	SER
1	B	151	LEU
1	B	155	THR
1	B	163	VAL
1	B	196	LEU
1	B	209	LYS
1	B	221	GLN
1	B	232	ARG
1	B	252	GLN
1	B	269	LEU
1	B	287	THR

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Mol	Chain	Res	Type
1	B	291	GLN
1	B	314	GLU
1	B	315	LYS
1	B	417	LEU

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

Mol	Chain	Res	Type
1	A	13	GLN
1	A	15	ASN
1	A	83	GLN
1	A	162	HIS
1	A	235	GLN
1	A	244	ASN
1	A	263	ASN
1	A	334	ASN
1	A	388	GLN
1	B	9	ASN
1	B	83	GLN
1	B	145	ASN
1	B	162	HIS
1	B	181	ASN
1	B	235	GLN
1	B	263	ASN
1	B	334	ASN
1	B	375	GLN
1	B	410	GLN
1	B	435	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 5 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	1,2	0,3,4	0.00	-	0,3,6	0.00	-
4	PO4	B	453	2	4,4,4	1.52	1 (25%)	6,6,6	3.67	5 (83%)

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
4	PO4	A	453	1,2	-	0/0/0/0	0/0/0/0
4	PO4	B	453	2	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	453	PO4	P-O4	-2.91	1.44	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	453	PO4	O2-P-O1	-4.25	92.86	110.97
4	B	453	PO4	O4-P-O1	-4.14	93.36	110.97
4	B	453	PO4	O3-P-O1	-3.57	95.78	110.97
4	B	453	PO4	O3-P-O2	3.47	120.64	107.90
4	B	453	PO4	O4-P-O2	4.20	123.34	107.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	453	PO4	1	0
4	B	453	PO4	2	0

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%)	0.53	19 (4%) 36 38	3, 18, 46, 83	0
1	B	444/449 (98%)	0.34	20 (4%) 34 36	2, 18, 45, 65	0
All	All	888/898 (98%)	0.43	39 (4%) 35 37	2, 18, 46, 83	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	ASP	7.6
1	A	6	VAL	5.8
1	B	331	HIS	4.9
1	A	7	LEU	3.8
1	B	6	VAL	3.5
1	A	240	ALA	3.4
1	B	408	ASP	3.4
1	A	293	ASN	3.2
1	B	221	GLN	2.9
1	A	253	LYS	2.8
1	B	404	ASN	2.7
1	B	165	SER	2.7
1	A	327	ASP	2.6
1	A	294	ASP	2.6
1	B	314	GLU	2.6
1	A	190	SER	2.6
1	A	331	HIS	2.5
1	A	222	GLY	2.5
1	A	93	THR	2.5
1	B	449	LYS	2.4
1	B	87	TYR	2.4
1	B	247	THR	2.4
1	A	411	GLU	2.3
1	B	330	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	187	GLY	2.3
1	B	290	PRO	2.2
1	B	328	LYS	2.2
1	B	332	ALA	2.2
1	A	26	THR	2.1
1	A	115	THR	2.1
1	A	291	GLN	2.1
1	A	358	LYS	2.1
1	A	113	VAL	2.1
1	B	409	SER	2.1
1	B	382	LYS	2.0
1	A	169	TYR	2.0
1	B	407	GLU	2.0
1	A	356	ALA	2.0
1	B	185	LYS	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	MG	A	452	1/1	0.88	0.47	6.18	38,38,38,38	0
2	ZN	A	451	1/1	0.91	0.32	1.57	49,49,49,49	0
4	PO4	B	453	5/5	0.57	0.46	1.07	51,58,61,62	0
2	ZN	B	450	1/1	0.80	0.33	0.05	35,35,35,35	0
2	ZN	B	451	1/1	0.91	0.24	-0.02	56,56,56,56	0
4	PO4	A	453	4/5	0.88	0.17	-1.10	63,64,65,66	0
2	ZN	A	450	1/1	0.75	0.13	-1.84	32,32,32,32	0

6.5 Other polymers ⓘ

There are no such residues in this entry.