



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:41 AM UTC

PDB ID : 1PS6 / pdb_00001ps6
Title : Crystal structure of E.coli PdxA
Authors : Sivaraman, J.; Li, Y.; Banks, J.; Cane, D.E.; Matte, A.; Cygler, M.
Deposited on : 2003-06-20
Resolution : 2.25 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

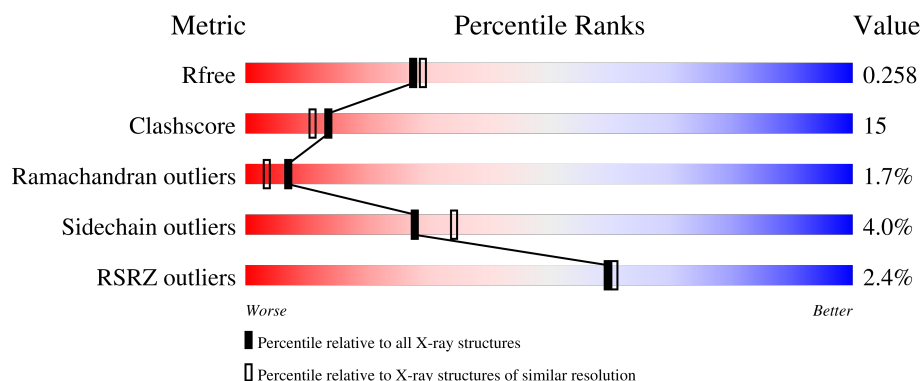
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	328	% 70% 25% .
1	B	328	4% 70% 26% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5007 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.

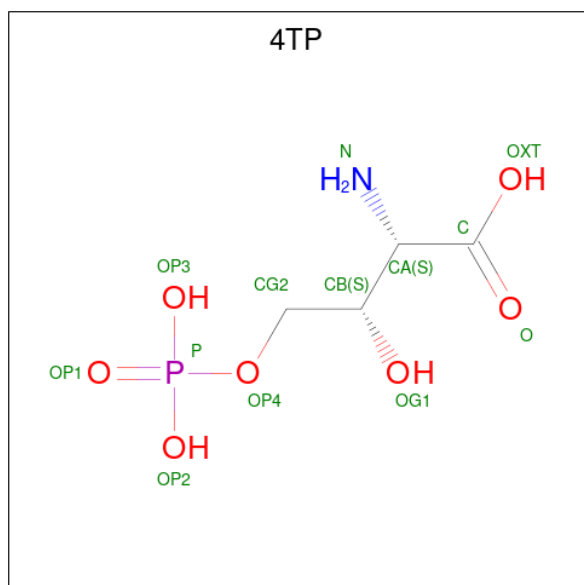
- Molecule 1 is a protein called 4-hydroxythreonine-4-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2402	1529	419	443	11			
1	B	328	Total	C	N	O	S	0	0	0
			2402	1529	422	440	11			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 4-HYDROXY-L-THREONINE-5-MONOPHOSPHATE (CCD ID: 4TP) (formula: C₄H₁₀NO₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			13	4	1	7	1		

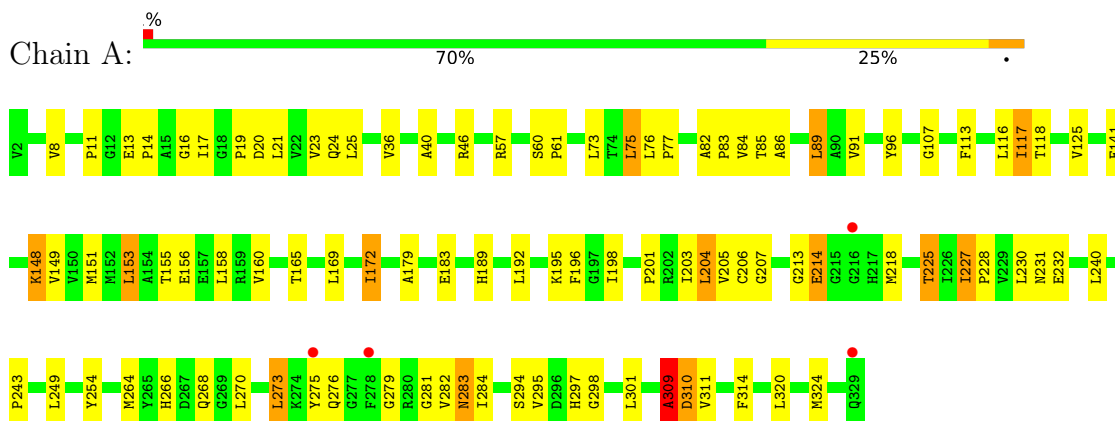
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total	O	0	0
			96	96		
4	B	92	Total	O	0	0
			92	92		

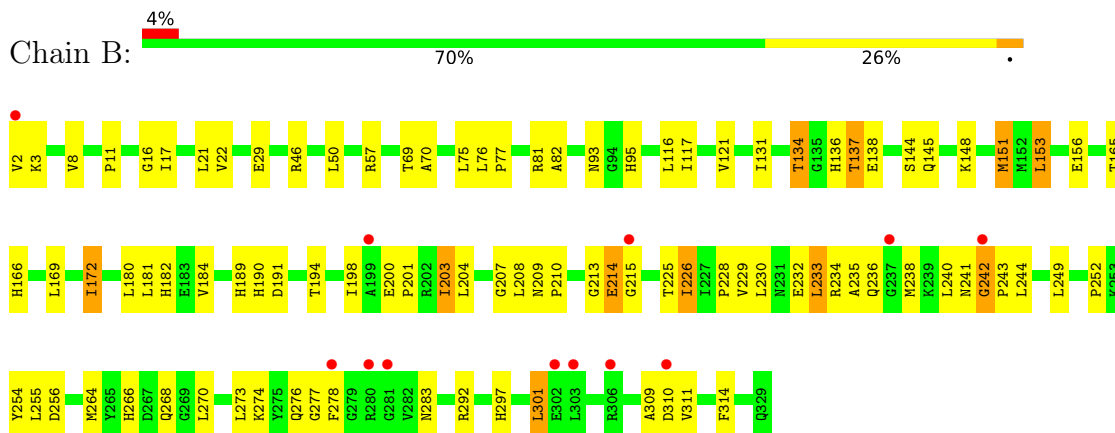
3 Residue-property plots

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 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: 4-hydroxythreonine-4-phosphate dehydrogenase



- Molecule 1: 4-hydroxythreonine-4-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.72Å 79.14Å 114.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 50.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	90.3 (50.00-2.25) 90.3 (50.00-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.258 0.207 , 0.258	Depositor DCC
R_{free} test set	2087 reflections (6.97%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.034 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5007	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: ZN, 4TP

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	0.45	0/2449	1.01	11/3347 (0.3%)
1	B	0.44	0/2450	1.02	11/3347 (0.3%)
All	All	0.45	0/4899	1.02	22/6694 (0.3%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	LEU	CA-C-N	7.84	128.30	119.83
1	B	76	LEU	C-N-CA	7.84	128.30	119.83
1	B	215	GLY	N-CA-C	-6.82	97.02	113.18
1	B	77	PRO	N-CA-C	6.63	121.23	111.03
1	A	75	LEU	N-CA-C	6.60	119.69	109.07
1	A	77	PRO	N-CA-C	6.40	120.89	111.03
1	B	172	ILE	N-CA-C	6.33	116.50	110.42
1	B	75	LEU	N-CA-C	6.14	118.96	109.07
1	B	203	ILE	N-CA-C	6.10	116.66	108.11
1	B	226	ILE	N-CA-C	6.07	116.24	110.42
1	A	205	VAL	N-CA-C	5.97	116.53	108.17
1	A	172	ILE	N-CA-C	5.96	116.14	110.42
1	B	165	THR	N-CA-C	5.88	117.47	108.30
1	A	282	VAL	N-CA-C	5.83	116.88	108.48
1	B	207	GLY	N-CA-C	-5.80	103.51	112.85
1	A	84	VAL	N-CA-C	5.75	116.86	108.53
1	A	232	GLU	N-CA-C	-5.69	105.16	111.36
1	A	309	ALA	N-CA-C	5.58	122.68	110.80
1	B	194	THR	N-CA-C	5.54	118.24	111.82
1	A	295	VAL	N-CA-C	-5.53	104.03	110.05
1	A	207	GLY	N-CA-C	-5.42	103.88	112.66
1	A	227	ILE	CB-CA-C	-5.07	108.89	113.70

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	2402	0	2430	76	0
1	B	2402	0	2434	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	13	0	5	2	0
4	A	96	0	0	3	0
4	B	92	0	0	3	0
All	All	5007	0	4869	141	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 15.

All (141) 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:24:GLN:HE22	1:A:309:ALA:HB2	1.32	0.90
1:B:301:LEU:HD22	1:B:301:LEU:H	1.36	0.90
1:A:24:GLN:HE22	1:A:309:ALA:CB	1.90	0.84
1:B:204:LEU:HD23	1:B:241:ASN:HB3	1.65	0.79
1:A:89:LEU:HD12	1:A:125:VAL:HB	1.65	0.79
1:A:264:MET:H	1:A:268:GLN:HE22	1.36	0.73
1:A:195:LYS:HB3	1:A:324:MET:CE	2.20	0.72
1:A:264:MET:H	1:A:268:GLN:NE2	1.88	0.72
1:B:29:GLU:OE1	1:B:69:THR:HA	1.92	0.69
1:B:234:ARG:NH2	1:B:242:GLY:HA2	2.11	0.66
1:B:301:LEU:H	1:B:301:LEU:CD2	2.08	0.66
1:A:117:ILE:HD12	1:A:117:ILE:N	2.11	0.65
1:A:155:THR:HG23	1:A:273:LEU:CD1	2.26	0.65
1:A:275:TYR:OH	1:B:276:GLN:NE2	2.30	0.64
1:B:198:ILE:O	1:B:201:PRO:HG3	1.97	0.64
1:A:151:MET:HE3	1:A:165:THR:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ALA:H	1:B:93:ASN:HD21	1.44	0.62
1:B:301:LEU:HD22	1:B:301:LEU:N	2.12	0.62
1:A:273:LEU:O	1:A:276:GLN:HB3	2.00	0.61
1:B:230:LEU:HD12	1:B:243:PRO:HD3	1.82	0.61
1:A:218:MET:SD	1:B:166:HIS:HB3	2.40	0.61
1:B:172:ILE:HD11	4:B:360:HOH:O	2.01	0.61
1:B:169:LEU:HD22	1:B:172:ILE:HD12	1.83	0.61
1:B:266:HIS:CE1	1:B:270:LEU:HD12	2.36	0.60
1:B:232:GLU:O	1:B:235:ALA:HB3	2.01	0.60
1:A:89:LEU:CD1	1:A:125:VAL:HB	2.31	0.59
1:B:11:PRO:HG3	1:B:22:VAL:HG21	1.83	0.59
1:A:204:LEU:HD11	1:A:254:TYR:HB3	1.85	0.58
1:A:284:ILE:HD11	1:A:320:LEU:HD21	1.84	0.58
1:A:11:PRO:HD2	4:A:345:HOH:O	2.04	0.58
1:A:169:LEU:HD12	1:A:172:ILE:HD12	1.86	0.58
1:A:179:ALA:O	1:A:183:GLU:HG3	2.04	0.58
1:A:189:HIS:CD2	1:A:201:PRO:HG2	2.40	0.57
1:A:195:LYS:HB3	1:A:324:MET:HE3	1.86	0.57
1:B:153:LEU:HD12	1:B:283:ASN:HA	1.87	0.57
1:B:311:VAL:HG22	1:B:311:VAL:O	2.04	0.57
1:B:180:LEU:O	1:B:184:VAL:HG23	2.05	0.57
1:B:200:GLU:N	1:B:201:PRO:HD3	2.20	0.56
1:B:189:HIS:HD2	4:B:457:HOH:O	1.89	0.56
1:A:82:ALA:HB1	1:A:83:PRO:HD2	1.87	0.56
1:B:153:LEU:HD22	1:B:270:LEU:HD22	1.86	0.56
1:A:14:PRO:HG3	1:A:96:TYR:CE2	2.42	0.55
1:B:241:ASN:O	1:B:242:GLY:O	2.24	0.55
1:A:151:MET:HE3	1:A:165:THR:CG2	2.35	0.55
1:A:225:THR:HG23	4:A:409:HOH:O	2.06	0.54
1:B:137:THR:HG22	1:B:292:ARG:HH12	1.72	0.54
1:B:234:ARG:NH2	1:B:242:GLY:CA	2.70	0.54
1:A:195:LYS:HB3	1:A:324:MET:HE2	1.89	0.54
1:A:89:LEU:HD21	1:A:301:LEU:HD11	1.90	0.54
1:A:213:GLY:O	1:A:214:GLU:C	2.50	0.53
1:B:117:ILE:HD12	1:B:117:ILE:N	2.24	0.53
1:B:203:ILE:HB	1:B:240:LEU:HD23	1.91	0.53
1:B:264:MET:H	1:B:268:GLN:NE2	2.06	0.53
1:A:266:HIS:CE1	1:A:270:LEU:HD12	2.44	0.53
1:B:17:ILE:HD11	1:B:297:HIS:CD2	2.44	0.52
1:B:234:ARG:HH22	1:B:242:GLY:HA2	1.74	0.52
1:B:249:LEU:C	1:B:249:LEU:HD23	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:CYS:SG	1:A:249:LEU:HD13	2.49	0.52
1:A:227:ILE:HB	1:A:228:PRO:HD3	1.92	0.52
1:A:301:LEU:H	1:A:301:LEU:HD22	1.75	0.52
1:A:160:VAL:CG2	1:A:273:LEU:HD23	2.40	0.52
1:A:158:LEU:HG	1:A:273:LEU:HD21	1.92	0.51
1:A:309:ALA:O	1:A:310:ASP:HB3	2.11	0.51
1:B:190:HIS:HD2	1:B:191:ASP:OD1	1.93	0.51
1:A:25:LEU:HD11	1:A:314:PHE:CD1	2.45	0.51
1:A:309:ALA:O	1:A:310:ASP:CB	2.58	0.51
1:A:24:GLN:NE2	1:A:309:ALA:CB	2.69	0.51
1:B:16:GLY:HA2	1:B:301:LEU:HD13	1.93	0.50
1:B:273:LEU:C	1:B:273:LEU:HD13	2.37	0.50
1:A:160:VAL:HG23	1:A:273:LEU:HD23	1.94	0.50
1:B:236:GLN:HE21	1:B:236:GLN:HA	1.77	0.49
1:B:81:ARG:H	1:B:93:ASN:ND2	2.10	0.49
1:B:137:THR:HG22	4:B:337:HOH:O	2.13	0.49
1:B:228:PRO:O	1:B:232:GLU:HG3	2.12	0.49
1:A:107:GLY:HA3	1:A:113:PHE:CE2	2.47	0.49
1:A:249:LEU:C	1:A:249:LEU:HD23	2.37	0.49
1:A:275:TYR:CE1	1:B:276:GLN:HG3	2.48	0.49
1:A:148:LYS:HG3	1:A:149:VAL:N	2.28	0.48
1:B:144:SER:O	1:B:145:GLN:HB2	2.13	0.48
1:A:189:HIS:NE2	1:A:201:PRO:HG2	2.28	0.48
1:A:155:THR:HG23	1:A:273:LEU:HD13	1.96	0.48
1:B:151:MET:O	1:B:151:MET:HG3	2.13	0.47
1:B:21:LEU:HD21	1:B:297:HIS:NE2	2.29	0.47
1:A:225:THR:CG2	4:A:409:HOH:O	2.61	0.47
1:A:19:PRO:O	1:A:23:VAL:HG23	2.14	0.47
1:A:40:ALA:HB2	1:A:75:LEU:CD2	2.44	0.47
1:B:17:ILE:O	1:B:21:LEU:HD13	2.15	0.47
1:B:225:THR:O	1:B:229:VAL:HG23	2.15	0.47
1:B:234:ARG:HH21	1:B:242:GLY:N	2.13	0.47
1:A:8:VAL:HG13	1:A:116:LEU:HD13	1.96	0.47
1:A:13:GLU:OE1	1:A:14:PRO:HD2	2.15	0.47
1:A:203:ILE:HB	1:A:240:LEU:HD23	1.96	0.47
1:A:158:LEU:HG	1:A:273:LEU:CD2	2.45	0.47
1:B:8:VAL:HG13	1:B:116:LEU:HD13	1.96	0.46
1:B:29:GLU:CD	1:B:70:ALA:H	2.24	0.46
1:A:16:GLY:O	1:A:19:PRO:HD2	2.15	0.46
1:B:182:HIS:CE1	1:B:233:LEU:HD11	2.51	0.45
1:B:225:THR:C	1:B:228:PRO:HD2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:MET:N	1:A:268:GLN:NE2	2.62	0.45
1:B:21:LEU:HD23	1:B:314:PHE:HD2	1.80	0.45
1:B:153:LEU:CD2	1:B:270:LEU:HD22	2.47	0.45
1:A:141:GLU:OE1	1:A:149:VAL:HG22	2.17	0.45
1:A:17:ILE:O	1:A:21:LEU:HG	2.16	0.45
1:B:95:HIS:ND1	1:B:131:ILE:HD11	2.32	0.44
1:A:275:TYR:HE2	1:B:255:LEU:CD1	2.31	0.44
1:B:204:LEU:HD11	1:B:254:TYR:HB3	2.00	0.44
1:A:276:GLN:O	1:A:276:GLN:HG3	2.17	0.43
1:B:204:LEU:HD23	1:B:241:ASN:CB	2.43	0.43
1:A:283:ASN:HD21	3:A:332:4TP:C	2.31	0.43
1:B:230:LEU:O	1:B:234:ARG:HG3	2.18	0.43
1:A:198:ILE:O	1:A:201:PRO:HD3	2.19	0.43
1:A:118:THR:OG1	1:A:294:SER:HB2	2.19	0.42
1:B:46:ARG:O	1:B:50:LEU:HD13	2.19	0.42
1:B:8:VAL:HG13	1:B:116:LEU:CD1	2.49	0.42
1:A:20:ASP:OD1	1:A:46:ARG:NH1	2.44	0.42
1:B:2:VAL:HB	1:B:3:LYS:H	1.57	0.42
1:A:297:HIS:HD2	1:A:298:GLY:O	2.03	0.42
1:A:192:LEU:O	1:A:196:PHE:HB2	2.20	0.41
1:B:252:PRO:O	1:B:256:ASP:HB2	2.20	0.41
1:A:60:SER:HA	1:A:61:PRO:HD2	1.91	0.41
1:B:134:THR:OG1	1:B:138:GLU:HG2	2.20	0.41
1:A:311:VAL:HG22	1:A:311:VAL:O	2.21	0.41
1:B:213:GLY:O	1:B:214:GLU:C	2.63	0.41
1:B:242:GLY:O	1:B:244:LEU:HG	2.20	0.41
1:A:85:THR:O	1:A:86:ALA:C	2.63	0.41
1:A:231:ASN:HD22	1:A:231:ASN:HA	1.76	0.41
1:A:36:VAL:HG21	1:A:73:LEU:HD13	2.03	0.41
1:A:40:ALA:HB2	1:A:75:LEU:HD21	2.02	0.41
1:B:209:ASN:HB3	1:B:210:PRO:HD2	2.03	0.41
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.88	0.41
1:B:252:PRO:C	1:B:254:TYR:N	2.78	0.41
1:A:153:LEU:HD21	1:A:283:ASN:ND2	2.36	0.40
1:A:279:GLY:C	1:A:281:GLY:H	2.29	0.40
1:A:283:ASN:ND2	3:A:332:4TP:O	2.54	0.40
1:A:284:ILE:CD1	1:A:320:LEU:HD21	2.51	0.40
1:B:181:LEU:HD11	1:B:226:ILE:HG12	2.03	0.40
1:B:189:HIS:CD2	1:B:238:MET:HG2	2.56	0.40
1:A:117:ILE:N	1:A:117:ILE:CD1	2.81	0.40
1:A:169:LEU:CD2	1:B:208:LEU:HD11	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HD12	1:A:243:PRO:HD3	2.04	0.40
1:B:121:VAL:HG22	1:B:136:HIS:ND1	2.36	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	326/328 (99%)	308 (94%)	14 (4%)	4 (1%)	10	7
1	B	326/328 (99%)	304 (93%)	15 (5%)	7 (2%)	5	2
All	All	652/656 (99%)	612 (94%)	29 (4%)	11 (2%)	7	3

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	GLU
1	A	309	ALA
1	A	310	ASP
1	B	242	GLY
1	B	278	PHE
1	B	309	ALA
1	B	310	ASP
1	B	214	GLU
1	B	277	GLY
1	B	156	GLU
1	A	214	GLU

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	248/261 (95%)	237 (96%)	11 (4%)	25	29
1	B	249/261 (95%)	240 (96%)	9 (4%)	31	39
All	All	497/522 (95%)	477 (96%)	20 (4%)	28	34

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	76	LEU
1	A	89	LEU
1	A	91	VAL
1	A	117	ILE
1	A	148	LYS
1	A	153	LEU
1	A	204	LEU
1	A	225	THR
1	A	273	LEU
1	A	283	ASN
1	B	57	ARG
1	B	134	THR
1	B	137	THR
1	B	148	LYS
1	B	151	MET
1	B	153	LEU
1	B	233	LEU
1	B	274	LYS
1	B	301	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	27	GLN

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Mol	Chain	Res	Type
1	A	45	ASN
1	A	110	ASN
1	A	231	ASN
1	A	268	GLN
1	A	283	ASN
1	A	297	HIS
1	B	27	GLN
1	B	88	GLN
1	B	93	ASN
1	B	127	ASN
1	B	182	HIS
1	B	189	HIS
1	B	190	HIS
1	B	231	ASN
1	B	236	GLN
1	B	241	ASN
1	B	268	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	4TP	A	332	2	11,12,12	1.41	3 (27%)	13,17,17	1.22	1 (7%)

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	4TP	A	332	2	-	7/14/14/14	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	332	4TP	CG2-CB	3.07	1.56	1.51
3	A	332	4TP	OP4-CG2	2.44	1.53	1.44
3	A	332	4TP	OXT-C	-2.05	1.24	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	332	4TP	OP3-P-OP4	2.09	112.11	106.67

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	332	4TP	N-CA-CB-OG1
3	A	332	4TP	N-CA-CB-CG2
3	A	332	4TP	O-C-CA-CB
3	A	332	4TP	OXT-C-CA-CB
3	A	332	4TP	C-CA-CB-OG1
3	A	332	4TP	C-CA-CB-CG2
3	A	332	4TP	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	332	4TP	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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(Å ²)	Q<0.9
1	A	328/328 (100%)	-0.14	4 (1%) 76 77	19, 30, 44, 59	0
1	B	328/328 (100%)	0.04	12 (3%) 45 45	20, 32, 52, 62	0
All	All	656/656 (100%)	-0.05	16 (2%) 59 61	19, 31, 49, 62	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	GLY	3.9
1	B	278	PHE	3.8
1	A	275	TYR	3.8
1	B	242	GLY	3.4
1	A	278	PHE	3.2
1	B	306	ARG	2.9
1	A	329	GLN	2.9
1	B	237	GLY	2.9
1	B	310	ASP	2.6
1	B	215	GLY	2.6
1	B	2	VAL	2.4
1	A	216	GLY	2.4
1	B	303	LEU	2.3
1	B	199	ALA	2.3
1	B	280	ARG	2.3
1	B	302	GLU	2.2

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	4TP	A	332	13/13	0.82	0.17	37,41,47,48	0
2	ZN	B	331	1/1	0.98	0.04	37,37,37,37	0
2	ZN	A	330	1/1	0.99	0.03	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.