



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:23 PM UTC

PDB ID : 1VE5 / pdb_00001ve5
Title : Crystal Structure of T.th. HB8 Threonine deaminase
Authors : Goto, M.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2004-03-27
Resolution : 2.15 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

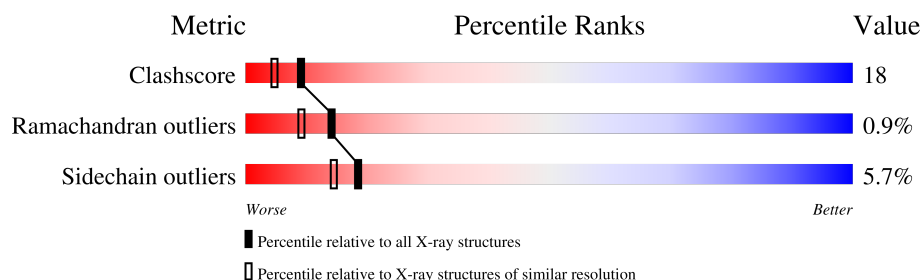
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)

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	311	68% 28% . .
1	B	311	66% 25% . 5%
1	C	311	60% 25% . 12%
1	D	311	63% 24% . 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8882 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 Threonine deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2279	1444	413	419	3			
1	B	297	Total	C	N	O	S	0	0	0
			2190	1389	398	400	3			
1	C	274	Total	C	N	O	S	0	0	0
			2024	1286	366	371	1			
1	D	280	Total	C	N	O	S	0	0	0
			2069	1315	375	377	2			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	B	87	Total	O	0	0
			87	87		
4	C	60	Total	O	0	0
			60	60		
4	D	50	Total	O	0	0
			50	50		

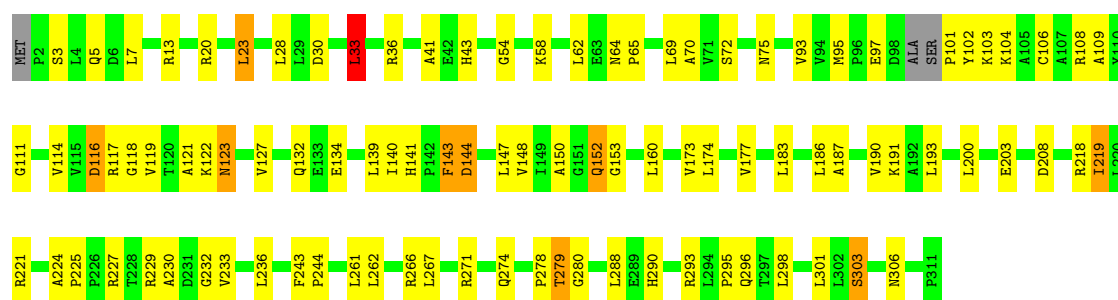
3 Residue-property plots

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.

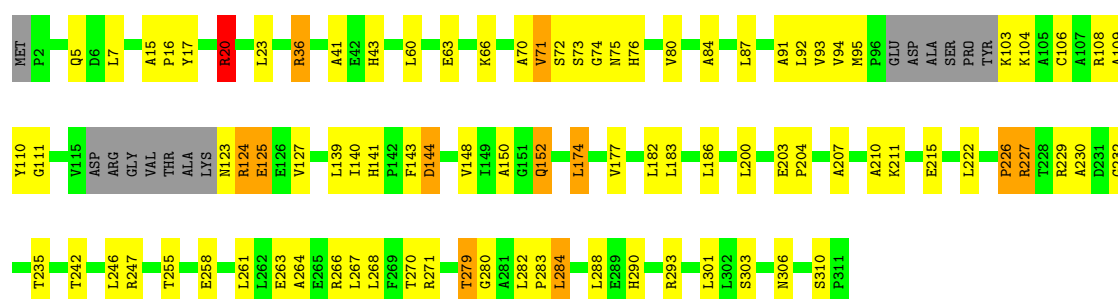
• Molecule 1: Threonine deaminase

Chain A: 



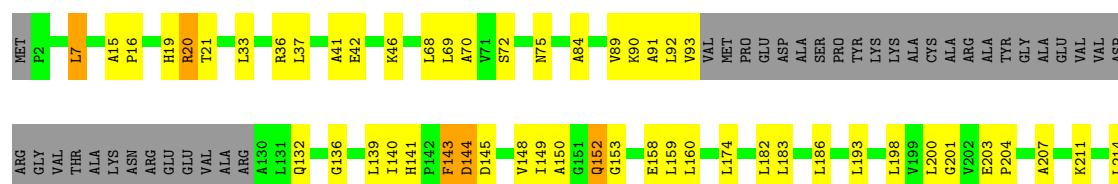
• Molecule 1: Threonine deaminase

Chain B: 



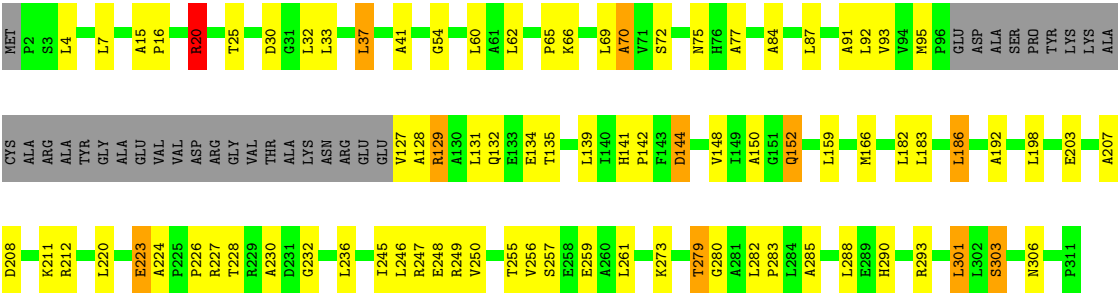
• Molecule 1: Threonine deaminase

Chain C: 





● Molecule 1: Threonine deaminase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.59Å 158.19Å 80.30Å 90.00° 108.52° 90.00°	Depositor
Resolution (Å)	10.00 – 2.15	Depositor
% Data completeness (in resolution range)	95.5 (10.00-2.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8882	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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: PLP, CA

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	0.41	0/2314	0.95	9/3138 (0.3%)
1	B	0.45	0/2222	0.93	7/3012 (0.2%)
1	C	0.39	0/2055	0.88	4/2788 (0.1%)
1	D	0.40	0/2101	0.93	5/2851 (0.2%)
All	All	0.42	0/8692	0.93	25/11789 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	303	SER	N-CA-C	8.88	122.12	111.82
1	A	303	SER	N-CA-C	7.44	119.39	111.28
1	A	41	ALA	N-CA-C	6.73	121.13	110.70
1	A	33	LEU	N-CA-C	-6.69	102.18	110.41
1	B	41	ALA	N-CA-C	6.51	119.73	109.39
1	C	303	SER	N-CA-C	6.26	120.02	112.38
1	D	41	ALA	N-CA-C	6.05	120.08	110.70
1	D	303	SER	N-CA-C	6.03	118.63	111.33
1	A	20	ARG	N-CA-C	-5.88	96.92	107.98
1	C	41	ALA	N-CA-C	5.75	118.54	109.39
1	D	20	ARG	N-CA-C	-5.72	97.22	107.98
1	B	20	ARG	N-CA-C	-5.65	97.35	107.98
1	C	270	THR	N-CA-C	5.56	118.27	111.82
1	B	43	HIS	N-CA-C	-5.37	105.98	112.54
1	A	134	GLU	N-CA-C	5.37	117.21	111.36
1	A	190	VAL	N-CA-C	5.34	115.54	110.42
1	D	70	ALA	N-CA-C	5.33	117.18	109.07
1	A	102	TYR	N-CA-C	-5.09	107.12	113.38
1	B	204	PRO	N-CA-C	-5.08	103.21	111.19
1	D	37	LEU	N-CA-C	5.05	117.48	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	201	GLY	N-CA-C	-5.05	104.99	113.02
1	A	75	ASN	N-CA-C	5.03	117.50	111.71
1	A	296	GLN	N-CA-C	5.03	116.85	111.36
1	B	270	THR	N-CA-C	5.02	118.56	112.23
1	B	280	GLY	N-CA-C	-5.00	108.77	115.32

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	2279	0	2375	79	0
1	B	2190	0	2287	84	0
1	C	2024	0	2120	85	0
1	D	2069	0	2172	76	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	15	0	7	0	0
3	B	15	0	7	0	0
3	C	15	0	7	0	0
3	D	15	0	7	0	0
4	A	59	0	0	3	0
4	B	87	0	0	5	0
4	C	60	0	0	2	0
4	D	50	0	0	1	0
All	All	8882	0	8982	322	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 18.

All (322) 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:C:20:ARG:HH11	1:C:20:ARG:HA	1.07	1.11
1:B:182:LEU:HD11	1:B:301:LEU:HD21	1.48	0.94
1:A:141:HIS:HD2	1:A:144:ASP:H	1.16	0.92
1:C:20:ARG:HA	1:C:20:ARG:NH1	1.87	0.88
1:D:232:GLY:H	1:D:279:THR:HG21	1.40	0.84
1:D:223:GLU:CD	1:D:223:GLU:H	1.85	0.84
1:C:141:HIS:HD2	1:C:144:ASP:H	1.25	0.84
1:B:182:LEU:HD21	1:B:301:LEU:HD23	1.61	0.82
1:D:129:ARG:H	1:D:129:ARG:HE	1.25	0.82
1:B:232:GLY:H	1:B:279:THR:HG21	1.43	0.82
1:A:141:HIS:CD2	1:A:144:ASP:H	1.98	0.82
1:C:20:ARG:HH11	1:C:20:ARG:CA	1.92	0.82
1:C:89:VAL:HG12	1:C:90:LYS:H	1.44	0.81
1:C:33:LEU:HD12	1:C:37:LEU:HD11	1.63	0.80
1:C:141:HIS:CD2	1:C:144:ASP:H	2.02	0.77
1:D:141:HIS:HD2	1:D:144:ASP:H	1.32	0.77
1:B:152:GLN:HE21	1:B:152:GLN:HA	1.48	0.77
1:C:200:LEU:HD23	1:C:254:LEU:HD11	1.66	0.76
1:B:141:HIS:CD2	1:B:144:ASP:H	2.04	0.76
1:A:221:ARG:HH21	1:A:236:LEU:HD12	1.52	0.74
1:C:182:LEU:HD21	1:C:301:LEU:HD22	1.68	0.73
1:B:141:HIS:HD2	1:B:144:ASP:H	1.36	0.73
1:B:174:LEU:HD13	1:B:200:LEU:HB2	1.70	0.73
1:A:101:PRO:HB2	1:A:103:LYS:HG2	1.71	0.73
1:A:152:GLN:HA	1:A:152:GLN:HE21	1.55	0.72
1:C:290:HIS:CD2	1:C:293:ARG:HH22	2.08	0.70
1:D:69:LEU:HD21	1:D:128:ALA:HB1	1.73	0.70
1:C:290:HIS:HD2	1:C:293:ARG:HH22	1.40	0.70
1:D:141:HIS:CD2	1:D:144:ASP:H	2.11	0.69
1:C:266:ARG:HG2	1:C:266:ARG:HH11	1.57	0.69
1:C:139:LEU:HD23	1:C:140:ILE:N	2.07	0.69
1:D:33:LEU:HD12	1:D:37:LEU:HD11	1.74	0.69
1:C:186:LEU:HD21	1:C:301:LEU:HD13	1.75	0.68
1:A:97:GLU:HA	1:A:116:ASP:OD1	1.93	0.68
1:C:229:ARG:HH11	1:C:229:ARG:HB3	1.58	0.68
1:A:290:HIS:HD2	1:A:293:ARG:HH21	1.39	0.68
1:A:7:LEU:HD11	1:A:153:GLY:HA3	1.75	0.68
1:C:89:VAL:HG12	1:C:90:LYS:N	2.09	0.68
1:A:33:LEU:HD22	1:A:33:LEU:H	1.58	0.67
1:C:198:LEU:HB3	1:C:200:LEU:HD11	1.77	0.67
1:B:15:ALA:HA	1:B:20:ARG:NH2	2.10	0.67
1:B:152:GLN:HE21	1:B:152:GLN:CA	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:GLN:HE21	1:C:152:GLN:HA	1.60	0.67
1:D:152:GLN:HE21	1:D:152:GLN:HA	1.58	0.67
1:B:230:ALA:HB1	1:B:279:THR:HB	1.76	0.66
1:D:152:GLN:HE21	1:D:152:GLN:CA	2.09	0.66
1:B:72:SER:O	1:B:73:SER:HB3	1.95	0.65
1:B:104:LYS:HD3	1:B:104:LYS:C	2.21	0.65
1:A:72:SER:O	1:A:95:MET:HG2	1.97	0.65
1:A:108:ARG:HH11	1:A:114:VAL:HB	1.61	0.65
1:A:104:LYS:O	1:A:108:ARG:HG3	1.97	0.65
1:C:229:ARG:HB3	1:C:229:ARG:NH1	2.12	0.65
1:A:290:HIS:CD2	1:A:293:ARG:HH21	2.14	0.64
1:B:186:LEU:CD2	1:B:301:LEU:HD22	2.26	0.64
1:B:232:GLY:N	1:B:279:THR:HG21	2.12	0.64
1:D:261:LEU:HD23	1:D:261:LEU:C	2.23	0.64
1:B:72:SER:HB2	1:B:95:MET:HA	1.80	0.64
1:A:108:ARG:HH12	1:A:114:VAL:H	1.43	0.63
1:D:54:GLY:H	1:D:152:GLN:HE22	1.47	0.63
1:D:256:VAL:HG11	1:D:285:ALA:HB1	1.81	0.63
1:B:93:VAL:HG12	1:B:95:MET:HG3	1.81	0.62
1:C:72:SER:HB2	1:C:93:VAL:HG12	1.81	0.62
1:C:152:GLN:HE21	1:C:152:GLN:CA	2.12	0.62
1:B:226:PRO:O	1:B:227:ARG:HB2	1.97	0.62
1:D:62:LEU:CB	1:D:65:PRO:HG3	2.29	0.62
1:D:127:VAL:HB	1:D:129:ARG:NH2	2.15	0.62
1:D:232:GLY:N	1:D:279:THR:HG21	2.15	0.61
1:A:227:ARG:HG3	1:A:227:ARG:O	2.00	0.61
1:B:84:ALA:HB2	1:B:91:ALA:HB2	1.80	0.61
1:B:75:ASN:ND2	1:B:103:LYS:HE3	2.15	0.61
1:D:30:ASP:O	1:D:33:LEU:O	2.19	0.61
1:A:108:ARG:NH1	1:A:114:VAL:HB	2.15	0.61
1:D:69:LEU:O	1:D:139:LEU:HA	2.00	0.61
1:B:177:VAL:HG21	1:B:183:LEU:HD22	1.83	0.60
1:D:186:LEU:HD21	1:D:301:LEU:HD13	1.83	0.60
1:D:128:ALA:H	1:D:129:ARG:HH21	1.49	0.60
1:A:152:GLN:HE21	1:A:152:GLN:CA	2.13	0.60
1:A:230:ALA:HB1	1:A:279:THR:HB	1.84	0.60
1:A:229:ARG:HG2	1:A:229:ARG:HH11	1.66	0.60
1:B:141:HIS:HD2	1:B:143:PHE:H	1.49	0.60
1:B:182:LEU:HD11	1:B:301:LEU:CD2	2.27	0.60
1:B:84:ALA:CB	1:B:91:ALA:HB2	2.32	0.59
1:D:72:SER:OG	1:D:95:MET:HE3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ARG:HG2	1:C:266:ARG:NH1	2.16	0.59
1:B:15:ALA:HA	1:B:20:ARG:HH22	1.68	0.59
1:B:242:THR:O	1:B:246:LEU:HG	2.03	0.59
1:D:212:ARG:HB3	1:D:220:LEU:HD12	1.84	0.59
1:C:7:LEU:HD22	1:C:150:ALA:HA	1.84	0.59
1:D:290:HIS:HA	1:D:293:ARG:HH21	1.67	0.58
1:C:256:VAL:HG11	1:C:285:ALA:HB1	1.84	0.58
1:C:256:VAL:HG13	1:C:260:ALA:HB3	1.84	0.58
1:C:267:LEU:O	1:C:271:ARG:HB2	2.03	0.58
1:B:15:ALA:O	1:B:20:ARG:NH2	2.37	0.58
1:D:32:LEU:O	1:D:32:LEU:HD23	2.04	0.58
1:D:69:LEU:HD23	1:D:70:ALA:N	2.19	0.58
1:D:72:SER:OG	1:D:95:MET:HG2	2.04	0.57
1:A:7:LEU:HD13	1:A:150:ALA:O	2.04	0.57
1:A:233:VAL:HB	4:A:1231:HOH:O	2.05	0.57
1:B:109:ALA:C	1:B:111:GLY:H	2.13	0.57
1:B:229:ARG:HG2	1:B:258:GLU:OE1	2.05	0.57
1:C:247:ARG:HH11	1:C:247:ARG:HB3	1.70	0.57
1:D:259:GLU:HG3	4:D:1058:HOH:O	2.05	0.57
1:D:232:GLY:H	1:D:279:THR:CG2	2.15	0.56
1:B:263:GLU:HG2	4:B:1112:HOH:O	2.05	0.56
1:A:54:GLY:H	1:A:152:GLN:HE22	1.53	0.56
1:A:95:MET:HE1	1:A:104:LYS:HA	1.86	0.56
1:A:148:VAL:O	1:A:152:GLN:HG2	2.06	0.56
1:A:5:GLN:HG3	4:A:1191:HOH:O	2.05	0.56
1:A:121:ALA:C	1:A:123:ASN:H	2.14	0.56
1:C:221:ARG:NH1	1:C:237:SER:OG	2.39	0.56
1:D:129:ARG:H	1:D:129:ARG:NE	2.02	0.56
1:D:62:LEU:HB3	1:D:65:PRO:HG3	1.87	0.56
1:A:266:ARG:HH12	1:A:271:ARG:HH12	1.54	0.55
1:A:36:ARG:HG2	1:A:36:ARG:HH11	1.70	0.55
1:C:214:LEU:HD12	1:C:253:ILE:HG12	1.89	0.55
1:A:33:LEU:HD22	1:A:33:LEU:N	2.22	0.55
1:B:177:VAL:CG2	1:B:183:LEU:HD22	2.36	0.55
1:D:208:ASP:O	1:D:212:ARG:HD3	2.07	0.55
1:B:186:LEU:HD21	1:B:301:LEU:HD22	1.86	0.55
1:D:66:LYS:HD2	1:D:135:THR:O	2.06	0.55
1:D:223:GLU:CD	1:D:223:GLU:N	2.61	0.55
1:D:248:GLU:HG2	1:D:249:ARG:HG3	1.89	0.54
1:A:54:GLY:H	1:A:152:GLN:NE2	2.06	0.54
1:C:19:HIS:O	1:C:20:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HD11	1:A:288:LEU:HD12	1.89	0.54
1:A:177:VAL:HG22	1:A:183:LEU:HD22	1.90	0.54
1:B:186:LEU:HD22	1:B:301:LEU:HD22	1.90	0.54
1:B:63:GLU:O	1:B:63:GLU:HG3	2.07	0.54
1:C:159:LEU:C	1:C:159:LEU:HD23	2.33	0.54
1:A:224:ALA:HB1	1:A:225:PRO:HD2	1.89	0.54
1:D:148:VAL:O	1:D:152:GLN:HG2	2.08	0.54
1:C:250:VAL:HG12	1:C:252:GLY:H	1.72	0.53
1:D:62:LEU:HB2	1:D:65:PRO:HG3	1.90	0.53
1:A:160:LEU:HD12	1:A:193:LEU:HD12	1.89	0.53
1:B:290:HIS:CD2	1:B:293:ARG:HH21	2.26	0.53
1:D:211:LYS:HD2	1:D:255:THR:HG23	1.91	0.53
1:B:60:LEU:HD23	1:B:87:LEU:HD21	1.91	0.53
1:C:254:LEU:N	1:C:254:LEU:HD12	2.22	0.53
1:D:230:ALA:CA	1:D:279:THR:HG22	2.38	0.52
1:C:84:ALA:CB	1:C:91:ALA:HB2	2.39	0.52
1:D:7:LEU:HD22	1:D:150:ALA:HA	1.90	0.52
1:D:230:ALA:HA	1:D:279:THR:HG22	1.92	0.52
1:B:71:VAL:O	1:B:94:VAL:O	2.27	0.52
1:B:109:ALA:O	1:B:111:GLY:N	2.43	0.52
1:D:54:GLY:H	1:D:152:GLN:NE2	2.06	0.52
1:A:93:VAL:HG12	1:A:95:MET:HG3	1.92	0.52
1:A:108:ARG:NH1	1:A:114:VAL:H	2.07	0.52
1:C:247:ARG:NH1	1:C:247:ARG:CB	2.72	0.52
1:C:20:ARG:NH1	1:C:158:GLU:OE2	2.44	0.51
1:C:20:ARG:CZ	4:C:1104:HOH:O	2.58	0.51
1:A:58:LYS:HD2	1:A:147:LEU:HD12	1.93	0.51
1:A:117:ARG:O	1:A:119:VAL:HG23	2.11	0.51
1:A:224:ALA:HB1	1:A:225:PRO:CD	2.40	0.51
1:C:7:LEU:HD13	1:C:153:GLY:HA3	1.93	0.51
1:C:200:LEU:N	1:C:200:LEU:HD12	2.26	0.51
1:B:5:GLN:HG3	4:B:1066:HOH:O	2.11	0.51
1:A:219:ILE:HG22	4:A:1145:HOH:O	2.10	0.51
1:B:266:ARG:HH12	1:B:271:ARG:HH12	1.59	0.51
1:B:72:SER:OG	1:B:95:MET:HG2	2.10	0.51
1:B:124:ARG:O	1:B:127:VAL:N	2.42	0.51
1:D:92:LEU:HD21	1:D:131:LEU:HD13	1.93	0.51
1:C:20:ARG:NE	4:C:1104:HOH:O	2.43	0.51
1:D:15:ALA:HB3	1:D:16:PRO:HD3	1.94	0.50
1:D:75:ASN:ND2	1:D:306:ASN:HD22	2.09	0.50
1:A:290:HIS:HD2	1:A:293:ARG:NH2	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ARG:NH1	1:C:20:ARG:CA	2.61	0.50
1:D:207:ALA:HB2	1:D:226:PRO:CB	2.42	0.50
1:A:295:PRO:HG2	1:A:298:LEU:CD2	2.42	0.50
1:C:203:GLU:OE2	1:C:253:ILE:HG21	2.11	0.50
1:D:84:ALA:CB	1:D:91:ALA:HB2	2.41	0.50
1:B:232:GLY:H	1:B:279:THR:CG2	2.18	0.50
1:A:139:LEU:C	1:A:139:LEU:HD23	2.36	0.50
1:A:203:GLU:CD	1:A:208:ASP:HA	2.37	0.50
1:B:290:HIS:HD2	1:B:293:ARG:HH21	1.59	0.50
1:B:7:LEU:HD22	1:B:150:ALA:HA	1.94	0.49
1:B:36:ARG:HD3	1:B:36:ARG:C	2.36	0.49
1:B:264:ALA:HB1	1:B:284:LEU:HB3	1.94	0.49
1:D:4:LEU:HD22	1:D:192:ALA:HB1	1.93	0.49
1:D:129:ARG:O	1:D:132:GLN:HB3	2.11	0.49
1:D:256:VAL:HG12	1:D:257:SER:O	2.11	0.49
1:D:261:LEU:HD23	1:D:261:LEU:O	2.12	0.49
1:D:236:LEU:N	1:D:236:LEU:HD22	2.26	0.49
1:C:221:ARG:HG2	1:C:237:SER:HB3	1.93	0.49
1:D:139:LEU:C	1:D:139:LEU:HD23	2.37	0.49
1:A:64:ASN:N	1:A:65:PRO:HD3	2.27	0.49
1:A:174:LEU:HD13	1:A:200:LEU:HB2	1.93	0.49
1:D:72:SER:CB	1:D:95:MET:HG2	2.42	0.49
1:B:226:PRO:O	1:B:227:ARG:CB	2.60	0.49
1:C:92:LEU:C	1:C:92:LEU:HD23	2.37	0.49
1:C:148:VAL:O	1:C:152:GLN:HG2	2.12	0.49
1:A:69:LEU:HD23	1:A:70:ALA:N	2.26	0.49
1:C:246:LEU:HD22	1:C:250:VAL:HG21	1.94	0.49
1:A:160:LEU:CD1	1:A:193:LEU:HD12	2.43	0.49
1:B:267:LEU:O	1:B:271:ARG:HB2	2.13	0.49
1:C:132:GLN:O	1:C:136:GLY:N	2.42	0.49
1:A:101:PRO:HB2	1:A:103:LYS:HZ2	1.78	0.48
1:D:182:LEU:HD21	1:D:301:LEU:HD22	1.95	0.48
1:B:70:ALA:HB2	1:B:80:VAL:HG21	1.93	0.48
1:B:203:GLU:O	1:B:255:THR:HA	2.14	0.48
1:C:33:LEU:HD11	1:C:284:LEU:HD21	1.95	0.48
1:C:89:VAL:CG1	1:C:90:LYS:H	2.21	0.48
1:C:139:LEU:HD23	1:C:139:LEU:C	2.39	0.48
1:C:221:ARG:HG2	1:C:237:SER:CB	2.44	0.48
1:A:62:LEU:CB	1:A:65:PRO:HG3	2.44	0.48
1:B:73:SER:HB3	1:B:76:HIS:HB3	1.96	0.48
1:B:108:ARG:HG3	1:B:108:ARG:HH11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ALA:N	1:C:16:PRO:HD2	2.29	0.47
1:A:132:GLN:NE2	1:A:139:LEU:HB2	2.30	0.47
1:A:139:LEU:HD23	1:A:140:ILE:N	2.29	0.47
1:C:19:HIS:NE2	1:C:46:LYS:HE2	2.29	0.47
1:C:229:ARG:HD2	1:C:265:GLU:OE2	2.13	0.47
1:A:13:ARG:NH2	1:A:147:LEU:HD22	2.29	0.47
1:B:222:LEU:HD13	1:B:226:PRO:HG3	1.97	0.47
1:C:72:SER:HB2	1:C:93:VAL:CG1	2.44	0.47
1:C:257:SER:OG	1:C:259:GLU:HG2	2.15	0.47
1:A:3:SER:O	1:A:7:LEU:HD23	2.15	0.47
1:B:74:GLY:HA2	1:B:95:MET:CE	2.45	0.47
1:C:19:HIS:C	1:C:20:ARG:NH1	2.73	0.47
1:B:268:LEU:HG	1:B:284:LEU:HD12	1.97	0.46
1:A:62:LEU:HB3	1:A:65:PRO:HG3	1.97	0.46
1:A:123:ASN:OD1	1:A:123:ASN:C	2.58	0.46
1:B:211:LYS:O	1:B:215:GLU:HG3	2.14	0.46
1:B:148:VAL:O	1:B:152:GLN:HG2	2.15	0.46
1:B:279:THR:CG2	4:B:1221:HOH:O	2.63	0.46
1:C:204:PRO:HG2	1:C:207:ALA:HB3	1.96	0.46
1:A:295:PRO:HG2	1:A:298:LEU:HD23	1.97	0.46
1:B:123:ASN:O	1:B:124:ARG:C	2.58	0.46
1:A:106:CYS:O	1:A:109:ALA:HB3	2.16	0.46
1:C:75:ASN:ND2	1:C:306:ASN:HD22	2.13	0.46
1:D:203:GLU:CD	1:D:208:ASP:HA	2.41	0.46
1:A:132:GLN:HE22	1:A:139:LEU:HB2	1.80	0.45
1:C:293:ARG:HB2	1:C:293:ARG:NH1	2.31	0.45
1:B:207:ALA:HB2	1:B:226:PRO:HB3	1.99	0.45
1:D:282:LEU:N	1:D:283:PRO:HD2	2.32	0.45
1:D:92:LEU:CD2	1:D:131:LEU:HD13	2.47	0.45
1:A:33:LEU:H	1:A:33:LEU:CD2	2.29	0.45
1:B:74:GLY:HA2	1:B:95:MET:HE1	1.97	0.45
1:C:229:ARG:NH1	1:C:229:ARG:CB	2.78	0.45
1:D:261:LEU:C	1:D:261:LEU:CD2	2.89	0.45
1:C:141:HIS:HD2	1:C:143:PHE:H	1.64	0.45
1:A:187:ALA:O	1:A:191:LYS:HB2	2.17	0.45
1:C:198:LEU:HB3	1:C:200:LEU:CD1	2.44	0.45
1:B:139:LEU:HD23	1:B:140:ILE:N	2.32	0.44
1:A:267:LEU:O	1:A:271:ARG:HB2	2.17	0.44
1:B:106:CYS:O	1:B:109:ALA:HB3	2.18	0.44
1:B:15:ALA:CA	1:B:20:ARG:NH2	2.79	0.44
1:B:255:THR:O	1:B:290:HIS:HE1	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ALA:C	1:A:111:GLY:H	2.24	0.44
1:A:232:GLY:H	1:A:279:THR:HG21	1.83	0.44
1:B:109:ALA:C	1:B:111:GLY:N	2.75	0.44
1:C:15:ALA:HA	1:C:20:ARG:HH21	1.82	0.43
1:D:159:LEU:HD23	1:D:159:LEU:C	2.43	0.43
1:C:256:VAL:HG12	1:C:257:SER:O	2.18	0.43
1:A:30:ASP:O	1:A:33:LEU:O	2.35	0.43
1:D:54:GLY:N	1:D:152:GLN:NE2	2.66	0.43
1:D:245:ILE:HG23	1:D:249:ARG:HD2	1.99	0.43
1:D:15:ALA:O	1:D:20:ARG:NH2	2.51	0.43
1:A:23:LEU:HD23	1:A:23:LEU:HA	1.90	0.43
1:B:124:ARG:O	1:B:125:GLU:C	2.61	0.43
1:B:282:LEU:HB2	1:B:283:PRO:HD3	2.01	0.43
1:B:182:LEU:HD21	1:B:301:LEU:CD2	2.42	0.43
1:C:247:ARG:HB3	1:C:247:ARG:NH1	2.31	0.43
1:C:247:ARG:HB2	1:C:247:ARG:CZ	2.48	0.43
1:B:75:ASN:HD21	1:B:103:LYS:HE3	1.80	0.43
1:D:127:VAL:N	1:D:129:ARG:NE	2.66	0.43
1:C:69:LEU:HD12	1:C:92:LEU:O	2.19	0.42
1:C:243:PHE:N	1:C:244:PRO:HD2	2.33	0.42
1:A:280:GLY:HA2	1:A:303:SER:OG	2.19	0.42
1:B:279:THR:HG23	4:B:1221:HOH:O	2.19	0.42
1:C:68:LEU:HD22	1:C:140:ILE:HD11	2.00	0.42
1:C:70:ALA:HB3	1:C:93:VAL:HG22	2.01	0.42
1:A:218:ARG:HG2	1:A:218:ARG:HH11	1.83	0.42
1:A:218:ARG:HG2	1:A:218:ARG:NH1	2.34	0.42
1:B:16:PRO:HG2	1:B:17:TYR:CE1	2.54	0.42
1:B:152:GLN:CA	1:B:152:GLN:NE2	2.81	0.42
1:B:284:LEU:HD23	1:B:284:LEU:O	2.20	0.42
1:C:42:GLU:HB2	1:C:302:LEU:O	2.19	0.42
1:D:246:LEU:HD22	1:D:250:VAL:HG21	2.00	0.42
1:B:232:GLY:CA	1:B:279:THR:HG21	2.50	0.42
1:D:25:THR:HG21	1:D:166:MET:HE1	2.02	0.42
1:B:104:LYS:C	1:B:104:LYS:CD	2.92	0.42
1:C:145:ASP:O	1:C:149:ILE:HG13	2.20	0.42
1:D:7:LEU:CD2	1:D:150:ALA:HA	2.50	0.42
1:D:230:ALA:C	1:D:279:THR:HG22	2.45	0.42
1:B:7:LEU:CD2	1:B:150:ALA:HA	2.50	0.41
1:B:66:LYS:HD2	4:B:1204:HOH:O	2.19	0.41
1:C:211:LYS:HD2	1:C:255:THR:HG23	2.02	0.41
1:D:141:HIS:CG	1:D:142:PRO:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:HIS:HE1	1:A:274:GLN:OE1	2.02	0.41
1:C:36:ARG:NH1	1:C:36:ARG:HG3	2.35	0.41
1:C:247:ARG:HH11	1:C:247:ARG:CB	2.31	0.41
1:C:266:ARG:HH12	1:C:271:ARG:HH12	1.68	0.41
1:A:243:PHE:N	1:A:244:PRO:HD2	2.35	0.41
1:D:223:GLU:O	1:D:224:ALA:HB2	2.20	0.41
1:A:173:VAL:C	1:A:174:LEU:HD22	2.45	0.41
1:B:203:GLU:CD	1:B:210:ALA:HB3	2.45	0.41
1:B:203:GLU:OE1	1:B:210:ALA:HB3	2.21	0.41
1:B:75:ASN:ND2	1:B:306:ASN:HD22	2.18	0.41
1:C:174:LEU:HD12	1:C:174:LEU:N	2.36	0.41
1:C:266:ARG:HH12	1:C:271:ARG:NH1	2.18	0.41
1:C:268:LEU:HG	1:C:284:LEU:HD12	2.02	0.41
1:D:77:ALA:HB1	1:D:93:VAL:HG11	2.02	0.41
1:C:217:GLY:HA2	1:C:247:ARG:HD3	2.01	0.41
1:D:207:ALA:HB2	1:D:226:PRO:HB2	2.03	0.41
1:A:28:LEU:HD13	1:A:271:ARG:HG3	2.03	0.41
1:A:123:ASN:O	1:A:127:VAL:HG23	2.21	0.41
1:A:261:LEU:HD11	1:A:278:PRO:O	2.21	0.41
1:A:306:ASN:HD22	1:D:273:LYS:NZ	2.18	0.41
1:C:277:GLU:HG2	1:C:304:GLY:O	2.21	0.41
1:D:280:GLY:HA2	1:D:303:SER:OG	2.21	0.41
1:C:160:LEU:CD1	1:C:193:LEU:HD12	2.51	0.41
1:A:36:ARG:HH11	1:A:36:ARG:CG	2.34	0.40
1:A:229:ARG:HG2	1:A:229:ARG:NH1	2.36	0.40
1:B:20:ARG:HD3	1:B:20:ARG:HA	1.84	0.40
1:B:141:HIS:CD2	1:B:143:PHE:H	2.33	0.40
1:B:310:SER:OG	1:C:310:SER:OG	2.37	0.40
1:D:20:ARG:HD3	1:D:20:ARG:HA	1.82	0.40
1:A:141:HIS:HD2	1:A:143:PHE:H	1.70	0.40
1:D:60:LEU:HD23	1:D:87:LEU:HD21	2.03	0.40
1:D:69:LEU:HD23	1:D:69:LEU:C	2.47	0.40
1:D:128:ALA:H	1:D:129:ARG:NH2	2.16	0.40
1:C:247:ARG:NH1	1:C:247:ARG:HB2	2.36	0.40

There are no symmetry-related clashes.

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	304/311 (98%)	287 (94%)	15 (5%)	2 (1%)	18	13
1	B	291/311 (94%)	275 (94%)	10 (3%)	6 (2%)	5	1
1	C	270/311 (87%)	257 (95%)	12 (4%)	1 (0%)	30	26
1	D	276/311 (89%)	260 (94%)	15 (5%)	1 (0%)	30	26
All	All	1141/1244 (92%)	1079 (95%)	52 (5%)	10 (1%)	14	9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	71	VAL
1	B	110	TYR
1	B	124	ARG
1	B	226	PRO
1	B	227	ARG
1	B	125	GLU
1	D	227	ARG
1	A	143	PHE
1	C	143	PHE
1	A	118	GLY

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	230/234 (98%)	218 (95%)	12 (5%)	21	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	220/234 (94%)	207 (94%)	13 (6%)	18	13
1	C	205/234 (88%)	195 (95%)	10 (5%)	22	19
1	D	210/234 (90%)	196 (93%)	14 (7%)	15	10
All	All	865/936 (92%)	816 (94%)	49 (6%)	18	14

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	33	LEU
1	A	116	ASP
1	A	122	LYS
1	A	123	ASN
1	A	144	ASP
1	A	152	GLN
1	A	186	LEU
1	A	219	ILE
1	A	262	LEU
1	A	279	THR
1	A	301	LEU
1	B	20	ARG
1	B	23	LEU
1	B	36	ARG
1	B	92	LEU
1	B	144	ASP
1	B	152	GLN
1	B	174	LEU
1	B	235	THR
1	B	247	ARG
1	B	261	LEU
1	B	279	THR
1	B	284	LEU
1	B	288	LEU
1	C	7	LEU
1	C	20	ARG
1	C	21	THR
1	C	144	ASP
1	C	152	GLN
1	C	183	LEU
1	C	259	GLU
1	C	261	LEU

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Mol	Chain	Res	Type
1	C	284	LEU
1	C	301	LEU
1	D	20	ARG
1	D	129	ARG
1	D	134	GLU
1	D	144	ASP
1	D	152	GLN
1	D	183	LEU
1	D	186	LEU
1	D	198	LEU
1	D	223	GLU
1	D	228	THR
1	D	247	ARG
1	D	279	THR
1	D	288	LEU
1	D	301	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	75	ASN
1	A	85	GLN
1	A	132	GLN
1	A	141	HIS
1	A	152	GLN
1	A	290	HIS
1	A	296	GLN
1	A	306	ASN
1	B	43	HIS
1	B	64	ASN
1	B	75	ASN
1	B	132	GLN
1	B	141	HIS
1	B	152	GLN
1	B	290	HIS
1	B	296	GLN
1	C	43	HIS
1	C	75	ASN
1	C	85	GLN
1	C	132	GLN
1	C	141	HIS

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Mol	Chain	Res	Type
1	C	152	GLN
1	C	290	HIS
1	D	43	HIS
1	D	75	ASN
1	D	141	HIS
1	D	152	GLN
1	D	290	HIS

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	PLP	C	1413	1	15,15,16	1.73	3 (20%)	21,22,23	1.86	6 (28%)
3	PLP	A	413	1	15,15,16	1.50	2 (13%)	21,22,23	1.47	5 (23%)
3	PLP	B	913	1	15,15,16	1.69	4 (26%)	21,22,23	1.91	4 (19%)
3	PLP	D	1913	1	15,15,16	1.47	3 (20%)	21,22,23	1.49	3 (14%)

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	PLP	C	1413	1	-	0/6/6/8	0/1/1/1
3	PLP	A	413	1	-	0/6/6/8	0/1/1/1
3	PLP	B	913	1	-	1/6/6/8	0/1/1/1
3	PLP	D	1913	1	-	1/6/6/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	913	PLP	C3-C2	-4.13	1.36	1.41
3	A	413	PLP	C2A-C2	4.03	1.56	1.50
3	C	1413	PLP	C3-C2	-3.86	1.37	1.41
3	C	1413	PLP	C2A-C2	3.39	1.55	1.50
3	B	913	PLP	C2A-C2	3.00	1.55	1.50
3	D	1913	PLP	C2A-C2	2.98	1.55	1.50
3	A	413	PLP	C4A-C4	2.51	1.56	1.51
3	D	1913	PLP	C2-N1	2.28	1.37	1.33
3	B	913	PLP	P-O3P	-2.23	1.46	1.54
3	D	1913	PLP	C4A-C4	2.20	1.56	1.51
3	B	913	PLP	C2-N1	2.15	1.37	1.33
3	C	1413	PLP	C6-C5	-2.04	1.33	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	913	PLP	O4P-C5A-C5	5.39	119.47	109.36
3	C	1413	PLP	O4P-C5A-C5	4.68	118.14	109.36
3	D	1913	PLP	O4P-C5A-C5	3.85	116.57	109.36
3	B	913	PLP	O3P-P-O4P	3.56	115.96	106.67
3	C	1413	PLP	O2P-P-O4P	-3.55	97.40	106.67
3	B	913	PLP	O2P-P-O4P	-3.50	97.55	106.67
3	D	1913	PLP	O2P-P-O4P	-3.12	98.52	106.67
3	A	413	PLP	O3P-P-O1P	2.74	121.51	110.83
3	A	413	PLP	O2P-P-O4P	-2.73	99.56	106.67
3	A	413	PLP	O4P-C5A-C5	2.66	114.35	109.36
3	C	1413	PLP	C5A-C5-C6	-2.48	115.32	119.36
3	A	413	PLP	C4A-C4-C5	2.43	123.44	120.94
3	C	1413	PLP	O3P-P-O1P	2.41	120.21	110.83
3	D	1913	PLP	O3P-P-O1P	2.37	120.08	110.83
3	C	1413	PLP	O3P-P-O4P	2.31	112.69	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1413	PLP	C4A-C4-C5	2.27	123.28	120.94
3	B	913	PLP	O3P-P-O1P	2.19	119.36	110.83
3	A	413	PLP	C5A-C5-C6	-2.15	115.85	119.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	913	PLP	C5A-O4P-P-O1P
3	D	1913	PLP	C5A-O4P-P-O1P

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.