Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:44 PM GMT

PDB ID	:	1C7G
Title	:	TYROSINE PHENOL-LYASE FROM ERWINIA HERBICOLA
Authors	:	Mikami, B.; Yamamoto, Y.; Katayama, T.; Suzuki, H.
Deposited on	:	2000-02-18
Resolution	:	2.10 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 (i) symbol.

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

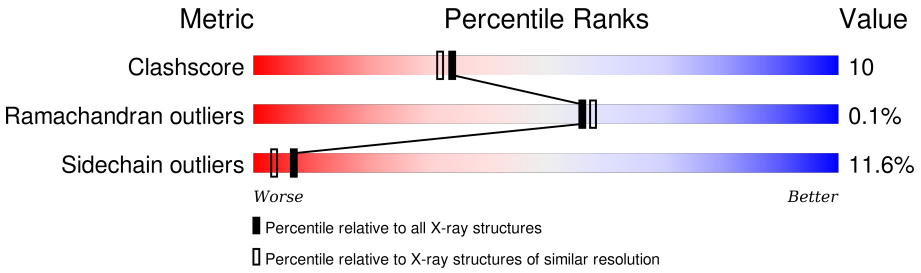
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	456	76% 21% .
1	B	456	70% 26% .
1	C	456	75% 21% .
1	D	456	73% 23% .

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
2	PLP	A	1000	-	X	-	-
2	PLP	B	1000	-	X	-	-
2	PLP	C	1000	-	X	-	-
2	PLP	D	1000	-	X	-	-

2 Entry composition

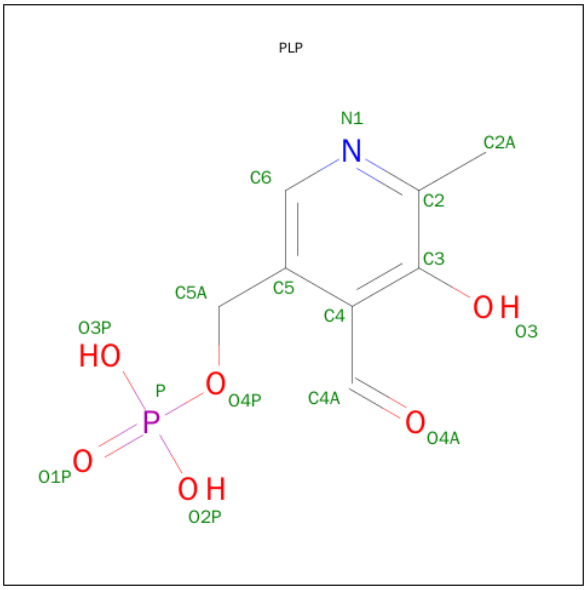
There are 3 unique types of molecules in this entry. The entry contains 14905 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TYROSINE PHENOL-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3605	2282	618	678	27			
1	B	456	Total	C	N	O	S	0	0	0
			3605	2282	618	678	27			
1	C	456	Total	C	N	O	S	0	0	0
			3605	2282	618	678	27			
1	D	456	Total	C	N	O	S	0	0	0
			3605	2282	618	678	27			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	103	Total	O	0	0
			103	103		
3	B	77	Total	O	0	0
			77	77		
3	C	158	Total	O	0	0
			158	158		
3	D	87	Total	O	0	0
			87	87		

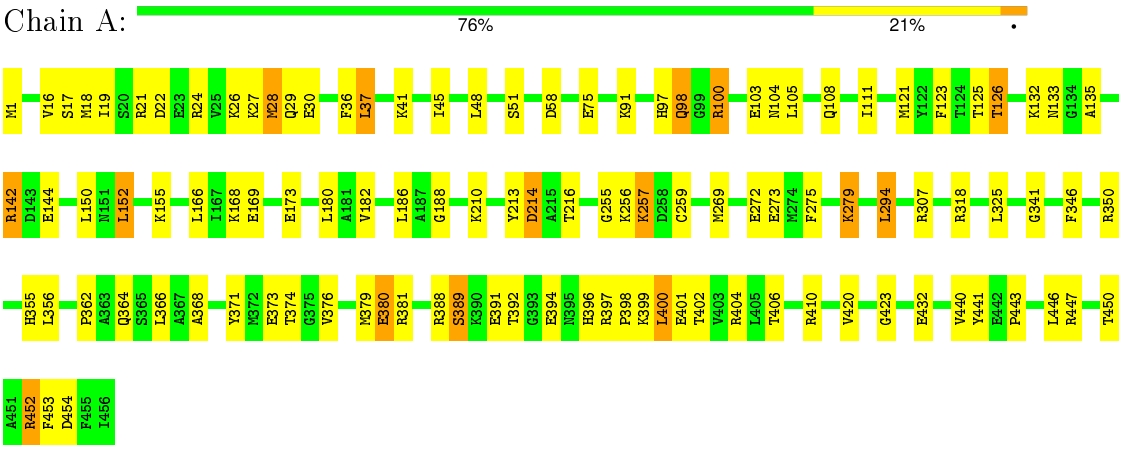
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

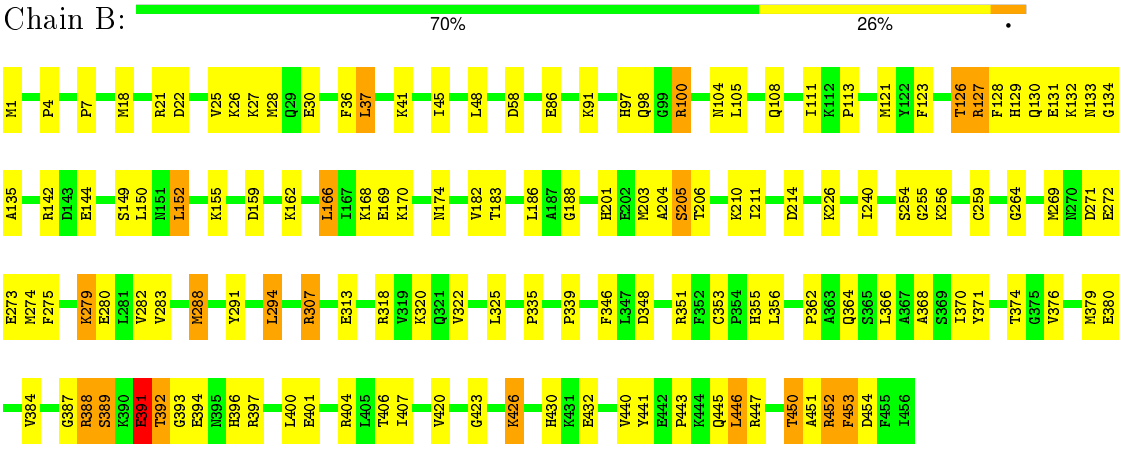
- Molecule 1: TYROSINE PHENOL-LYASE

Chain A:



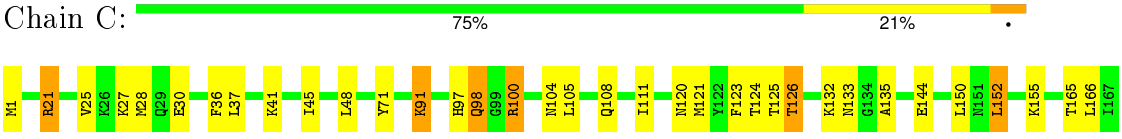
- Molecule 1: TYROSINE PHENOL-LYASE

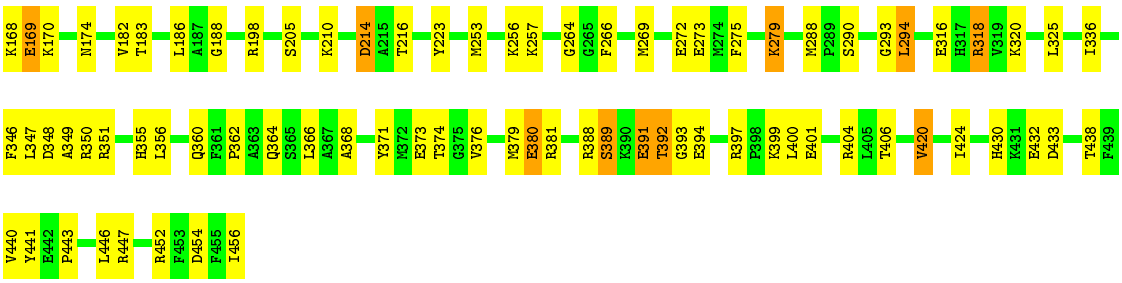
Chain B:



- Molecule 1: TYROSINE PHENOL-LYASE

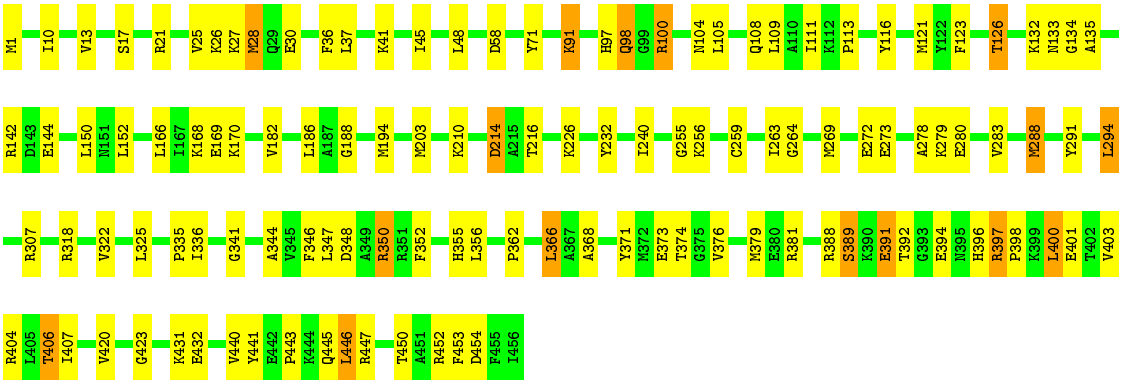
Chain C:





- Molecule 1: TYROSINE PHENOL-LYASE

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	163.49Å 113.04Å 101.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	78.6 (8.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.186 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14905	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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

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	0.35	0/3678	0.60	1/4955 (0.0%)
1	B	0.35	0/3678	0.59	1/4955 (0.0%)
1	C	0.36	0/3678	0.62	1/4955 (0.0%)
1	D	0.35	0/3678	0.59	1/4955 (0.0%)
All	All	0.35	0/14712	0.60	4/19820 (0.0%)

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	C	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	ASP	N-CA-C	-7.04	91.98	111.00
1	C	214	ASP	N-CA-C	-6.72	92.86	111.00
1	D	214	ASP	N-CA-C	-6.03	94.71	111.00
1	B	214	ASP	N-CA-C	-5.65	95.75	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	223	TYR	Sidechain

5.2 Too-close contacts (i)

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	3605	0	3548	67	0
1	B	3605	0	3548	87	1
1	C	3605	0	3548	70	0
1	D	3605	0	3548	73	0
2	A	15	0	6	1	0
2	B	15	0	6	1	0
2	C	15	0	6	2	0
2	D	15	0	6	1	0
3	A	103	0	0	2	0
3	B	77	0	0	3	0
3	C	158	0	0	3	0
3	D	87	0	0	0	0
All	All	14905	0	14216	289	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 10.

All (289) 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:28:MET:HE3	1:C:368:ALA:HA	1.43	1.01
1:C:97:HIS:HA	1:C:294:LEU:HD13	1.59	0.83
1:B:362:PRO:HG2	1:B:401:GLU:HG2	1.61	0.83
1:A:374:THR:OG1	1:A:376:VAL:HG13	1.79	0.82
1:B:374:THR:OG1	1:B:376:VAL:HG13	1.79	0.82
1:D:443:PRO:HG2	1:D:447:ARG:HA	1.61	0.82
1:B:389:SER:OG	1:B:392:THR:HG22	1.82	0.79
1:D:374:THR:OG1	1:D:376:VAL:HG13	1.83	0.78
1:B:123:PHE:HB3	1:B:126:THR:HG23	1.66	0.78
1:C:443:PRO:HG2	1:C:447:ARG:HA	1.66	0.77
1:D:97:HIS:HA	1:D:294:LEU:HD13	1.65	0.76
1:B:28:MET:HE3	1:B:368:ALA:HA	1.68	0.74
1:D:28:MET:HE3	1:D:368:ALA:HA	1.70	0.73
1:A:362:PRO:HG2	1:A:401:GLU:HG2	1.69	0.73
1:C:374:THR:OG1	1:C:376:VAL:HG13	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:THR:HG23	3:C:745:HOH:O	1.90	0.72
1:A:97:HIS:HA	1:A:294:LEU:HD13	1.72	0.72
1:B:97:HIS:HA	1:B:294:LEU:HD13	1.70	0.71
1:B:123:PHE:HB3	1:B:126:THR:CG2	2.21	0.70
1:A:443:PRO:HG2	1:A:447:ARG:HA	1.73	0.70
1:C:123:PHE:HB3	1:C:126:THR:HG23	1.74	0.70
1:B:426:LYS:HD3	3:B:826:HOH:O	1.92	0.69
1:C:389:SER:HB3	1:C:392:THR:HG22	1.74	0.69
1:B:443:PRO:HG2	1:B:447:ARG:HA	1.74	0.68
1:D:362:PRO:HG2	1:D:401:GLU:HG2	1.75	0.67
1:D:123:PHE:HB3	1:D:126:THR:CG2	2.24	0.67
1:C:389:SER:CB	1:C:392:THR:HG22	2.25	0.67
1:B:127:ARG:HD3	1:B:131:GLU:OE2	1.94	0.67
1:A:28:MET:HE3	1:A:368:ALA:HA	1.77	0.66
1:A:123:PHE:HB3	1:A:126:THR:HG23	1.77	0.65
1:D:108:GLN:HG2	1:D:133:ASN:HD21	1.62	0.64
1:B:26:LYS:O	1:B:30:GLU:HG3	1.98	0.64
1:D:28:MET:CE	1:D:368:ALA:HA	2.28	0.63
1:A:379:MET:HE2	1:A:404:ARG:CZ	2.29	0.63
1:A:111:ILE:HG21	1:A:135:ALA:HB2	1.81	0.63
1:D:214:ASP:OD1	1:D:216:THR:HG23	1.98	0.62
1:B:355:HIS:CD2	1:B:356:LEU:HD13	2.34	0.62
1:D:113:PRO:HA	1:D:134:GLY:O	1.98	0.62
1:C:123:PHE:HB3	1:C:126:THR:CG2	2.29	0.62
1:D:389:SER:OG	1:D:392:THR:HG22	2.00	0.62
1:D:30:GLU:O	1:D:452:ARG:NH2	2.33	0.62
1:C:98:GLN:HE21	1:C:100:ARG:HD2	1.65	0.62
1:A:392:THR:O	1:A:394:GLU:HG3	1.99	0.61
1:B:201:HIS:O	1:B:205:SER:HB3	2.00	0.61
1:A:389:SER:OG	1:A:392:THR:HG22	2.01	0.61
1:C:362:PRO:HG2	1:C:401:GLU:HG2	1.83	0.61
1:D:389:SER:CB	1:D:392:THR:HG22	2.31	0.59
1:D:123:PHE:HB3	1:D:126:THR:HG23	1.83	0.59
1:D:37:LEU:HD11	1:D:450:THR:HA	1.83	0.59
1:B:111:ILE:HG21	1:B:135:ALA:HB2	1.84	0.59
1:A:182:VAL:HG23	1:A:182:VAL:O	2.03	0.59
1:A:123:PHE:HB3	1:A:126:THR:CG2	2.32	0.59
1:A:441:TYR:HD2	1:A:452:ARG:HG3	1.67	0.59
1:B:440:VAL:HG11	1:B:454:ASP:HB2	1.85	0.58
1:C:170:LYS:O	1:C:174:ASN:ND2	2.36	0.58
1:D:379:MET:HE2	1:D:404:ARG:CZ	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:SER:CB	1:A:392:THR:HG22	2.33	0.58
1:C:389:SER:OG	1:C:392:THR:HG22	2.03	0.58
1:A:28:MET:CE	1:A:368:ALA:HA	2.33	0.58
1:D:350:ARG:NH2	1:D:398:PRO:O	2.37	0.57
1:B:440:VAL:CG1	1:B:454:ASP:HB2	2.35	0.57
1:B:113:PRO:HA	1:B:134:GLY:O	2.05	0.57
1:B:392:THR:HG23	1:B:394:GLU:HB2	1.87	0.56
1:C:28:MET:CE	1:C:371:TYR:HB3	2.35	0.56
1:B:389:SER:O	1:B:393:GLY:HA2	2.05	0.56
1:D:389:SER:HB3	1:D:392:THR:HG22	1.87	0.56
1:D:21:ARG:O	1:D:25:VAL:HG23	2.06	0.56
1:D:344:ALA:HB2	1:D:406:THR:HG23	1.87	0.56
1:B:159:ASP:CG	1:B:162:LYS:HG3	2.27	0.56
1:B:389:SER:CB	1:B:392:THR:HG22	2.36	0.56
1:A:100:ARG:HG2	1:A:125:THR:HG21	1.88	0.55
1:C:144:GLU:HB3	1:C:150:LEU:HD23	1.87	0.55
1:D:441:TYR:HD2	1:D:452:ARG:HG3	1.71	0.55
1:C:440:VAL:HG22	1:C:452:ARG:O	2.06	0.55
1:A:188:GLY:HA2	1:A:346:PHE:CE1	2.42	0.55
1:B:144:GLU:HB3	1:B:150:LEU:HD23	1.87	0.55
1:C:275:PHE:CZ	1:C:279:LYS:HD2	2.42	0.55
1:D:188:GLY:HA2	1:D:346:PHE:CE1	2.42	0.55
1:D:71:TYR:CE2	1:D:288:MET:HG2	2.42	0.55
1:B:441:TYR:CE2	1:B:443:PRO:HD3	2.42	0.55
1:C:30:GLU:O	1:C:452:ARG:NH2	2.39	0.55
1:A:214:ASP:OD1	1:A:216:THR:HG23	2.07	0.55
1:B:203:MET:O	1:B:206:THR:HB	2.07	0.54
1:B:441:TYR:HD2	1:B:452:ARG:HG3	1.71	0.54
1:B:362:PRO:HG2	1:B:401:GLU:CG	2.37	0.54
1:A:144:GLU:HB3	1:A:150:LEU:HD23	1.90	0.54
1:C:28:MET:CE	1:C:368:ALA:HA	2.29	0.54
1:A:51:SER:HB2	1:A:257:LYS:HE3	1.89	0.54
1:A:389:SER:HB3	1:A:392:THR:HG22	1.89	0.54
1:C:165:THR:O	1:C:169:GLU:HG2	2.07	0.54
1:C:198:ARG:NH1	3:C:710:HOH:O	2.40	0.54
1:C:420:VAL:HG23	1:C:424:ILE:HD12	1.89	0.54
1:A:275:PHE:CZ	1:A:279:LYS:HD2	2.42	0.54
1:A:440:VAL:HG11	1:A:454:ASP:HB2	1.90	0.53
1:B:279:LYS:O	1:B:282:VAL:HG12	2.09	0.53
1:A:98:GLN:HE21	1:A:100:ARG:HD2	1.74	0.53
1:D:111:ILE:HG21	1:D:135:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:HD23	1:B:155:LYS:HG2	1.91	0.53
1:A:350:ARG:NH2	1:A:398:PRO:O	2.41	0.53
1:B:28:MET:CE	1:B:371:TYR:HB3	2.39	0.53
1:A:108:GLN:HG2	1:A:133:ASN:HD21	1.74	0.52
1:C:98:GLN:NE2	1:C:100:ARG:HD2	2.24	0.52
1:B:275:PHE:CZ	1:B:279:LYS:HD2	2.44	0.52
1:C:91:LYS:HB3	1:C:91:LYS:HZ2	1.75	0.52
1:C:108:GLN:HG2	1:C:133:ASN:HD21	1.74	0.52
1:B:353:CYS:HB3	1:B:355:HIS:CE1	2.44	0.51
1:A:22:ASP:O	1:A:26:LYS:HG3	2.09	0.51
1:A:350:ARG:HH21	1:A:399:LYS:C	2.13	0.51
1:C:379:MET:HE2	1:C:404:ARG:CZ	2.40	0.51
1:B:104:ASN:O	1:B:108:GLN:HG3	2.11	0.51
1:D:98:GLN:HE21	1:D:100:ARG:HD2	1.75	0.51
1:B:430:HIS:HB2	3:B:886:HOH:O	2.10	0.51
1:B:108:GLN:HG2	1:B:133:ASN:HD21	1.76	0.51
1:D:400:LEU:HD12	1:D:400:LEU:H	1.76	0.51
1:B:86:GLU:CD	1:B:307:ARG:HH22	2.14	0.51
1:C:355:HIS:CD2	1:C:356:LEU:HD13	2.46	0.51
1:D:26:LYS:O	1:D:30:GLU:HG3	2.10	0.51
1:C:45:ILE:O	1:C:376:VAL:HA	2.11	0.51
1:A:255:GLY:HA2	1:A:259:CYS:HB2	1.93	0.51
1:B:111:ILE:CG2	1:B:135:ALA:HB2	2.41	0.50
1:A:18:MET:HG3	1:B:313:GLU:HG2	1.91	0.50
1:B:446:LEU:HD11	1:D:283:VAL:HG21	1.94	0.50
1:D:264:GLY:HA2	1:D:294:LEU:HD11	1.94	0.50
1:D:116:TYR:CE2	1:D:170:LYS:HD2	2.47	0.50
1:C:111:ILE:HG21	1:C:135:ALA:HB2	1.94	0.50
1:D:182:VAL:O	1:D:182:VAL:HG23	2.12	0.49
1:C:290:SER:HB2	3:C:716:HOH:O	2.12	0.49
1:B:392:THR:O	1:B:394:GLU:HG3	2.12	0.49
1:C:100:ARG:HG2	1:C:125:THR:HG21	1.93	0.49
1:C:91:LYS:HB3	1:C:91:LYS:NZ	2.27	0.49
1:D:355:HIS:CD2	1:D:356:LEU:HD13	2.48	0.49
1:A:111:ILE:CG2	1:A:135:ALA:HB2	2.42	0.49
1:D:194:MET:HG2	1:D:232:TYR:OH	2.13	0.49
1:D:28:MET:CE	1:D:371:TYR:HB3	2.43	0.49
1:B:98:GLN:HG3	1:B:256:LYS:HD2	1.95	0.49
1:B:255:GLY:HA2	1:B:259:CYS:HB2	1.95	0.49
1:B:37:LEU:HD11	1:B:450:THR:HA	1.94	0.49
1:C:316:GLU:HG2	1:C:320:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ARG:HG3	2:C:1000:PLP:O3P	2.13	0.48
1:A:255:GLY:CA	1:A:259:CYS:HB2	2.44	0.48
1:C:98:GLN:HG3	1:C:256:LYS:HD2	1.96	0.48
1:B:98:GLN:HE21	1:B:100:ARG:HD2	1.78	0.48
1:A:75:GLU:OE2	1:C:41:LYS:HD3	2.13	0.48
1:A:26:LYS:O	1:A:30:GLU:HG3	2.13	0.48
1:D:336:ILE:HG22	1:D:347:LEU:HD23	1.96	0.48
1:B:389:SER:N	1:B:394:GLU:O	2.44	0.47
1:A:37:LEU:HD11	1:A:450:THR:HA	1.96	0.47
1:C:182:VAL:O	1:C:182:VAL:HG23	2.15	0.47
1:B:445:GLN:HG2	1:D:280:GLU:OE1	2.14	0.47
1:D:144:GLU:HB3	1:D:150:LEU:HD23	1.95	0.47
1:D:391:GLU:H	1:D:391:GLU:HG2	1.47	0.47
1:A:103:GLU:OE2	2:A:1000:PLP:H6	2.13	0.47
1:D:440:VAL:HG11	1:D:454:ASP:HB2	1.95	0.47
1:B:264:GLY:HA2	1:B:294:LEU:HD11	1.96	0.47
1:B:288:MET:HB2	1:B:291:TYR:CE2	2.49	0.47
1:A:410:ARG:HA	3:A:612:HOH:O	2.14	0.47
1:B:188:GLY:HA2	1:B:346:PHE:CE1	2.50	0.47
1:B:392:THR:CG2	1:B:394:GLU:HB2	2.45	0.47
1:B:387:GLY:HA2	1:B:447:ARG:NE	2.30	0.47
1:A:58:ASP:N	1:A:58:ASP:OD1	2.48	0.47
1:A:98:GLN:OE1	1:C:293:GLY:HA2	2.15	0.46
1:A:389:SER:N	1:A:394:GLU:O	2.45	0.46
1:C:28:MET:HE1	1:C:371:TYR:HB3	1.97	0.46
1:B:280:GLU:OE1	1:D:445:GLN:HG2	2.14	0.46
1:D:397:ARG:CG	1:D:397:ARG:HH11	2.29	0.46
1:B:453:PHE:CD1	1:B:453:PHE:N	2.84	0.46
1:D:381:ARG:HA	1:D:381:ARG:HE	1.81	0.46
1:A:355:HIS:CD2	1:A:356:LEU:HD13	2.50	0.46
1:B:392:THR:HG23	1:B:394:GLU:CB	2.44	0.46
1:C:389:SER:N	1:C:394:GLU:O	2.44	0.46
1:B:271:ASP:HB3	1:B:274:MET:HB2	1.98	0.46
1:B:335:PRO:HB2	1:B:348:ASP:HB3	1.97	0.46
1:B:182:VAL:O	1:B:182:VAL:HG23	2.16	0.46
1:D:111:ILE:CG2	1:D:135:ALA:HB2	2.46	0.46
1:C:392:THR:HG23	1:C:394:GLU:HG3	1.98	0.46
1:C:253:MET:HG2	1:C:266:PHE:CZ	2.51	0.46
1:B:170:LYS:O	1:B:174:ASN:ND2	2.48	0.46
1:B:389:SER:HA	1:B:396:HIS:NE2	2.31	0.45
1:A:142:ARG:HD3	1:A:144:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ALA:HB3	1:B:211:ILE:HD11	1.98	0.45
1:A:19:ILE:HD11	1:A:24:ARG:HG2	1.97	0.45
1:D:263:ILE:HG13	1:D:264:GLY:N	2.31	0.45
1:B:443:PRO:HD2	1:B:451:ALA:HA	1.97	0.45
1:B:127:ARG:O	1:B:130:GLN:HB2	2.17	0.45
1:C:188:GLY:HA2	1:C:346:PHE:CE1	2.50	0.45
1:A:152:LEU:HD23	1:A:155:LYS:HG2	1.98	0.45
1:A:45:ILE:O	1:A:376:VAL:HA	2.17	0.45
1:A:188:GLY:O	1:A:341:GLY:HA3	2.16	0.45
1:D:381:ARG:NE	1:D:381:ARG:HA	2.31	0.45
1:B:283:VAL:HG21	1:D:446:LEU:HD11	1.98	0.45
1:C:21:ARG:O	1:C:25:VAL:HG23	2.17	0.45
1:A:374:THR:HG21	1:A:423:GLY:HA3	1.98	0.45
1:C:440:VAL:HG11	1:C:454:ASP:HB2	1.98	0.45
1:C:364:GLN:OE1	1:C:380:GLU:HG2	2.17	0.45
1:D:45:ILE:O	1:D:376:VAL:HA	2.16	0.45
1:B:364:GLN:OE1	1:B:384:VAL:HG11	2.16	0.45
1:A:104:ASN:O	1:A:108:GLN:HG3	2.17	0.44
1:C:360:GLN:HG2	1:C:456:ILE:CD1	2.47	0.44
1:A:364:GLN:OE1	1:A:380:GLU:HG2	2.17	0.44
1:C:348:ASP:OD2	1:C:351:ARG:HG3	2.17	0.44
1:A:379:MET:HE3	1:A:381:ARG:CD	2.48	0.44
1:A:152:LEU:HD23	1:A:155:LYS:CG	2.47	0.44
1:B:45:ILE:O	1:B:376:VAL:HA	2.17	0.44
1:D:188:GLY:O	1:D:341:GLY:HA3	2.17	0.44
1:A:443:PRO:HG3	1:A:450:THR:OG1	2.17	0.44
1:A:379:MET:HE3	1:A:381:ARG:HG2	1.99	0.44
1:D:100:ARG:HD2	2:D:1000:PLP:O3P	2.18	0.44
1:C:350:ARG:NH1	1:C:399:LYS:O	2.50	0.44
1:A:453:PHE:CD1	1:A:453:PHE:N	2.85	0.44
1:D:374:THR:CG2	1:D:423:GLY:HA3	2.48	0.44
1:C:349:ALA:HB3	1:C:401:GLU:HG3	2.00	0.44
1:A:28:MET:CE	1:A:371:TYR:HB3	2.48	0.44
1:C:214:ASP:OD1	1:C:216:THR:HG23	2.18	0.44
1:A:440:VAL:HG22	1:A:452:ARG:O	2.18	0.44
1:A:350:ARG:NH2	1:A:399:LYS:O	2.39	0.43
1:C:389:SER:O	1:C:393:GLY:HA2	2.18	0.43
1:B:440:VAL:HG22	1:B:452:ARG:C	2.39	0.43
1:A:379:MET:CE	1:A:404:ARG:CZ	2.96	0.43
1:B:374:THR:CG2	1:B:423:GLY:HA3	2.48	0.43
1:C:336:ILE:HG22	1:C:347:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ARG:HB2	1:B:394:GLU:C	2.38	0.43
1:C:111:ILE:CG2	1:C:135:ALA:HB2	2.49	0.43
1:B:391:GLU:HG2	1:B:391:GLU:H	1.56	0.43
1:C:120:ASN:OD1	1:C:120:ASN:N	2.51	0.43
1:B:322:VAL:HG22	1:B:407:ILE:HG13	1.99	0.43
1:B:21:ARG:O	1:B:25:VAL:HG23	2.19	0.43
1:D:104:ASN:O	1:D:108:GLN:HG3	2.18	0.43
1:A:441:TYR:CD2	1:A:452:ARG:HG3	2.50	0.43
1:B:379:MET:HE2	1:B:404:ARG:CZ	2.49	0.43
1:D:335:PRO:HB2	1:D:348:ASP:HB3	2.01	0.43
1:D:453:PHE:N	1:D:453:PHE:CD1	2.87	0.43
1:D:366:LEU:HB3	1:D:403:VAL:HG21	2.01	0.43
1:B:166:LEU:CD2	1:B:170:LYS:HG3	2.49	0.42
1:A:98:GLN:HG3	1:A:256:LYS:HD2	2.01	0.42
1:D:109:LEU:HD11	1:D:278:ALA:HA	2.00	0.42
1:A:26:LYS:O	1:A:29:GLN:HB2	2.19	0.42
1:C:381:ARG:HE	1:C:381:ARG:HA	1.84	0.42
1:C:392:THR:O	1:C:394:GLU:HG3	2.20	0.42
1:B:254:SER:HB2	2:B:1000:PLP:H5A2	2.00	0.42
1:D:441:TYR:CE2	1:D:443:PRO:HD3	2.55	0.42
1:D:397:ARG:HG2	1:D:397:ARG:HH11	1.85	0.42
1:B:440:VAL:HG22	1:B:452:ARG:O	2.19	0.42
1:D:288:MET:HB2	1:D:291:TYR:CE2	2.55	0.42
1:B:348:ASP:CG	1:B:351:ARG:HG3	2.39	0.42
1:D:322:VAL:HG22	1:D:407:ILE:HG13	2.02	0.42
1:D:255:GLY:HA2	1:D:259:CYS:HB2	2.02	0.42
1:A:16:VAL:HG22	1:B:7:PRO:O	2.19	0.42
1:D:58:ASP:OD1	1:D:58:ASP:N	2.52	0.42
1:C:71:TYR:CE2	1:C:288:MET:HG2	2.55	0.42
1:B:4:PRO:HD3	1:B:320:LYS:HD3	2.02	0.42
1:B:226:LYS:HB2	1:B:240:ILE:CD1	2.50	0.42
1:B:18:MET:HG2	3:B:925:HOH:O	2.20	0.42
1:B:370:ILE:HG22	1:B:376:VAL:HG22	2.02	0.42
1:A:98:GLN:CG	1:A:256:LYS:HD2	2.50	0.42
1:D:389:SER:N	1:D:394:GLU:O	2.47	0.41
1:C:152:LEU:HD23	1:C:155:LYS:CG	2.49	0.41
1:D:374:THR:HG21	1:D:423:GLY:HA3	2.02	0.41
1:D:98:GLN:HG3	1:D:256:LYS:HD2	2.02	0.41
3:A:657:HOH:O	1:C:41:LYS:HG2	2.20	0.41
1:C:318:ARG:HD3	1:C:318:ARG:C	2.41	0.41
1:B:128:PHE:CD2	1:B:129:HIS:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:PHE:O	1:D:431:LYS:HD2	2.21	0.41
1:D:203:MET:HB2	1:D:203:MET:HE3	1.97	0.41
1:A:379:MET:HE1	1:A:381:ARG:HD2	2.02	0.41
1:D:226:LYS:HB2	1:D:240:ILE:CD1	2.51	0.41
1:C:441:TYR:HD2	1:C:452:ARG:HG3	1.86	0.41
1:C:182:VAL:HA	1:C:183:THR:HA	1.90	0.41
1:A:400:LEU:HB2	1:A:402:THR:HG23	2.03	0.41
1:C:216:THR:HG21	2:C:1000:PLP:C5	2.51	0.41
1:B:155:LYS:HD2	1:B:339:PRO:HD2	2.02	0.41
1:A:180:LEU:O	1:A:213:TYR:HA	2.21	0.41
1:D:28:MET:HE1	1:D:371:TYR:HB3	2.03	0.41
1:D:389:SER:HA	1:D:396:HIS:NE2	2.36	0.41
1:C:438:THR:HG22	1:C:454:ASP:O	2.21	0.41
1:C:440:VAL:HG22	1:C:452:ARG:C	2.41	0.40
1:B:86:GLU:CD	1:B:307:ARG:NH2	2.74	0.40
1:D:397:ARG:CG	1:D:397:ARG:NH1	2.84	0.40
1:C:430:HIS:O	1:C:433:ASP:HB2	2.21	0.40
1:B:182:VAL:HA	1:B:183:THR:HA	1.87	0.40
1:D:10:ILE:HG21	1:D:13:VAL:HG12	2.03	0.40
1:C:391:GLU:HG2	1:C:391:GLU:H	1.61	0.40
1:C:264:GLY:HA2	1:C:294:LEU:HD11	2.03	0.40
1:B:348:ASP:OD2	1:B:351:ARG:HG3	2.21	0.40
1:B:159:ASP:OD2	1:B:162:LYS:HG3	2.22	0.40
1:C:104:ASN:O	1:C:108:GLN:HG3	2.22	0.40
1:D:91:LYS:HB3	1:D:91:LYS:HZ2	1.86	0.40
1:A:389:SER:HA	1:A:396:HIS:NE2	2.36	0.40
1:D:440:VAL:CG1	1:D:454:ASP:HB2	2.51	0.40
1:B:58:ASP:OD1	1:B:58:ASP:N	2.54	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)
1:B:22:ASP:OD1	1:B:22:ASP:OD1[2_575]	1.80	0.40

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	454/456 (100%)	437 (96%)	17 (4%)	0	100	100
1	B	454/456 (100%)	433 (95%)	20 (4%)	1 (0%)	52	53
1	C	454/456 (100%)	438 (96%)	16 (4%)	0	100	100
1	D	454/456 (100%)	433 (95%)	21 (5%)	0	100	100
All	All	1816/1824 (100%)	1741 (96%)	74 (4%)	1 (0%)	56	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	391	GLU

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	380/380 (100%)	334 (88%)	46 (12%)	6	3
1	B	380/380 (100%)	333 (88%)	47 (12%)	6	3
1	C	380/380 (100%)	339 (89%)	41 (11%)	8	4
1	D	380/380 (100%)	338 (89%)	42 (11%)	8	4
All	All	1520/1520 (100%)	1344 (88%)	176 (12%)	7	3

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	17	SER
1	A	21	ARG
1	A	27	LYS
1	A	28	MET
1	A	36	PHE
1	A	37	LEU
1	A	41	LYS
1	A	48	LEU
1	A	91	LYS
1	A	98	GLN
1	A	100	ARG
1	A	105	LEU
1	A	121	MET
1	A	126	THR
1	A	132	LYS
1	A	142	ARG
1	A	152	LEU
1	A	166	LEU
1	A	168	LYS
1	A	169	GLU
1	A	173	GLU
1	A	186	LEU
1	A	210	LYS
1	A	257	LYS
1	A	269	MET
1	A	272	GLU
1	A	273	GLU
1	A	279	LYS
1	A	294	LEU
1	A	307	ARG
1	A	318	ARG
1	A	325	LEU
1	A	366	LEU
1	A	373	GLU
1	A	380	GLU
1	A	388	ARG
1	A	389	SER
1	A	391	GLU
1	A	397	ARG
1	A	400	LEU
1	A	406	THR
1	A	420	VAL

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Mol	Chain	Res	Type
1	A	432	GLU
1	A	446	LEU
1	A	452	ARG
1	B	1	MET
1	B	27	LYS
1	B	36	PHE
1	B	37	LEU
1	B	41	LYS
1	B	48	LEU
1	B	91	LYS
1	B	100	ARG
1	B	105	LEU
1	B	121	MET
1	B	126	THR
1	B	127	ARG
1	B	132	LYS
1	B	142	ARG
1	B	149	SER
1	B	152	LEU
1	B	166	LEU
1	B	168	LYS
1	B	169	GLU
1	B	186	LEU
1	B	205	SER
1	B	210	LYS
1	B	269	MET
1	B	272	GLU
1	B	273	GLU
1	B	279	LYS
1	B	288	MET
1	B	294	LEU
1	B	307	ARG
1	B	318	ARG
1	B	325	LEU
1	B	366	LEU
1	B	380	GLU
1	B	388	ARG
1	B	389	SER
1	B	391	GLU
1	B	392	THR
1	B	397	ARG
1	B	400	LEU

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Mol	Chain	Res	Type
1	B	406	THR
1	B	420	VAL
1	B	426	LYS
1	B	432	GLU
1	B	446	LEU
1	B	450	THR
1	B	452	ARG
1	B	453	PHE
1	C	1	MET
1	C	21	ARG
1	C	27	LYS
1	C	36	PHE
1	C	37	LEU
1	C	48	LEU
1	C	91	LYS
1	C	98	GLN
1	C	100	ARG
1	C	105	LEU
1	C	121	MET
1	C	126	THR
1	C	132	LYS
1	C	152	LEU
1	C	166	LEU
1	C	168	LYS
1	C	169	GLU
1	C	186	LEU
1	C	205	SER
1	C	210	LYS
1	C	257	LYS
1	C	269	MET
1	C	272	GLU
1	C	273	GLU
1	C	279	LYS
1	C	294	LEU
1	C	318	ARG
1	C	325	LEU
1	C	366	LEU
1	C	373	GLU
1	C	380	GLU
1	C	388	ARG
1	C	389	SER
1	C	391	GLU

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Mol	Chain	Res	Type
1	C	392	THR
1	C	397	ARG
1	C	400	LEU
1	C	406	THR
1	C	420	VAL
1	C	432	GLU
1	C	446	LEU
1	D	1	MET
1	D	17	SER
1	D	27	LYS
1	D	28	MET
1	D	36	PHE
1	D	41	LYS
1	D	48	LEU
1	D	91	LYS
1	D	98	GLN
1	D	100	ARG
1	D	105	LEU
1	D	121	MET
1	D	126	THR
1	D	132	LYS
1	D	142	ARG
1	D	152	LEU
1	D	166	LEU
1	D	168	LYS
1	D	169	GLU
1	D	186	LEU
1	D	210	LYS
1	D	269	MET
1	D	272	GLU
1	D	273	GLU
1	D	279	LYS
1	D	288	MET
1	D	294	LEU
1	D	307	ARG
1	D	318	ARG
1	D	325	LEU
1	D	350	ARG
1	D	366	LEU
1	D	373	GLU
1	D	388	ARG
1	D	389	SER

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Mol	Chain	Res	Type
1	D	391	GLU
1	D	397	ARG
1	D	400	LEU
1	D	406	THR
1	D	420	VAL
1	D	432	GLU
1	D	446	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	B	130	GLN
1	C	130	GLN
1	D	130	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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	$\#\|Z\|>2$
2	PLP	A	1000	1	15,15,16	3.68	6 (40%)	21,22,23	4.01	14 (66%)
2	PLP	B	1000	1	15,15,16	3.71	6 (40%)	21,22,23	4.00	14 (66%)
2	PLP	C	1000	1	15,15,16	3.66	5 (33%)	21,22,23	3.92	14 (66%)
2	PLP	D	1000	1	15,15,16	3.51	5 (33%)	21,22,23	3.94	14 (66%)

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
2	PLP	A	1000	1	-	0/6/6/8	0/1/1/1
2	PLP	B	1000	1	-	0/6/6/8	0/1/1/1
2	PLP	C	1000	1	-	0/6/6/8	0/1/1/1
2	PLP	D	1000	1	-	0/6/6/8	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1000	PLP	P-O3P	-2.41	1.46	1.54
2	D	1000	PLP	C4A-C4	-2.40	1.46	1.51
2	C	1000	PLP	C4A-C4	-2.32	1.46	1.51
2	D	1000	PLP	P-O3P	-2.28	1.46	1.54
2	A	1000	PLP	P-O3P	-2.21	1.46	1.54
2	B	1000	PLP	P-O3P	-2.17	1.46	1.54
2	A	1000	PLP	P-O1P	-2.08	1.44	1.51
2	A	1000	PLP	C4A-C4	-2.08	1.47	1.51
2	B	1000	PLP	C4A-C4	-2.03	1.47	1.51
2	B	1000	PLP	C2A-C2	2.12	1.54	1.50
2	C	1000	PLP	C2-N1	2.30	1.38	1.34
2	D	1000	PLP	C2-N1	2.45	1.39	1.34
2	B	1000	PLP	C2-N1	2.50	1.39	1.34
2	A	1000	PLP	C2-N1	2.66	1.39	1.34
2	A	1000	PLP	C3-C2	5.37	1.44	1.40
2	C	1000	PLP	C3-C2	5.90	1.44	1.40
2	D	1000	PLP	C3-C2	6.30	1.45	1.40
2	B	1000	PLP	C3-C2	6.63	1.45	1.40
2	D	1000	PLP	C5-C4	10.51	1.52	1.40
2	B	1000	PLP	C5-C4	11.46	1.53	1.40
2	C	1000	PLP	C5-C4	11.56	1.53	1.40
2	A	1000	PLP	C5-C4	11.90	1.54	1.40

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1000	PLP	O3P-P-O4P	-8.76	81.34	106.56
2	B	1000	PLP	O3P-P-O4P	-8.72	81.45	106.56
2	C	1000	PLP	O3P-P-O4P	-8.54	81.96	106.56
2	D	1000	PLP	O3P-P-O4P	-8.47	82.16	106.56
2	C	1000	PLP	O3P-P-O1P	-6.71	88.98	110.58
2	D	1000	PLP	O3P-P-O1P	-6.60	89.32	110.58
2	B	1000	PLP	O3P-P-O1P	-6.60	89.33	110.58
2	D	1000	PLP	O3P-P-O2P	-6.54	82.49	107.38
2	C	1000	PLP	O3P-P-O2P	-6.51	82.58	107.38
2	B	1000	PLP	O3P-P-O2P	-6.49	82.66	107.38
2	A	1000	PLP	O3P-P-O2P	-6.43	82.88	107.38
2	A	1000	PLP	O3P-P-O1P	-6.40	89.98	110.58
2	D	1000	PLP	O3-C3-C2	-3.30	111.92	117.66
2	B	1000	PLP	O3-C3-C2	-3.20	112.10	117.66
2	C	1000	PLP	C3-C2-N1	-3.18	116.22	120.61
2	A	1000	PLP	O3-C3-C2	-3.15	112.18	117.66
2	B	1000	PLP	C3-C2-N1	-3.13	116.29	120.61
2	C	1000	PLP	O3-C3-C2	-3.09	112.29	117.66
2	D	1000	PLP	C3-C2-N1	-3.08	116.35	120.61
2	A	1000	PLP	C3-C2-N1	-2.93	116.56	120.61
2	A	1000	PLP	C5-C6-N1	-2.68	119.20	123.86
2	D	1000	PLP	C5-C6-N1	-2.63	119.30	123.86
2	B	1000	PLP	C5-C6-N1	-2.63	119.30	123.86
2	C	1000	PLP	C5-C6-N1	-2.60	119.35	123.86
2	D	1000	PLP	C4A-C4-C5	2.22	123.19	120.88
2	A	1000	PLP	O2P-P-O1P	2.98	120.19	110.58
2	B	1000	PLP	O2P-P-O1P	3.09	120.51	110.58
2	A	1000	PLP	O3-C3-C4	3.09	126.81	118.12
2	C	1000	PLP	O3-C3-C4	3.11	126.87	118.12
2	D	1000	PLP	O2P-P-O1P	3.12	120.61	110.58
2	B	1000	PLP	O3-C3-C4	3.22	127.18	118.12
2	C	1000	PLP	O2P-P-O1P	3.24	121.00	110.58
2	D	1000	PLP	O3-C3-C4	3.25	127.26	118.12
2	C	1000	PLP	O4P-C5A-C5	3.28	114.41	108.99
2	C	1000	PLP	C4A-C4-C5	3.41	124.44	120.88
2	B	1000	PLP	C4A-C4-C5	3.52	124.55	120.88
2	D	1000	PLP	C6-N1-C2	3.59	126.60	119.28
2	A	1000	PLP	C6-N1-C2	3.60	126.63	119.28
2	B	1000	PLP	C6-N1-C2	3.73	126.89	119.28
2	C	1000	PLP	C6-N1-C2	3.76	126.95	119.28
2	C	1000	PLP	O4P-P-O1P	3.95	117.19	107.14
2	A	1000	PLP	O4P-P-O1P	3.99	117.31	107.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1000	PLP	C4A-C4-C5	4.14	125.19	120.88
2	B	1000	PLP	O2P-P-O4P	4.19	118.63	106.56
2	D	1000	PLP	O4P-P-O1P	4.25	117.96	107.14
2	D	1000	PLP	O2P-P-O4P	4.27	118.85	106.56
2	B	1000	PLP	O4P-P-O1P	4.31	118.12	107.14
2	C	1000	PLP	O2P-P-O4P	4.35	119.09	106.56
2	B	1000	PLP	O4P-C5A-C5	4.44	116.33	108.99
2	A	1000	PLP	O2P-P-O4P	4.66	119.98	106.56
2	D	1000	PLP	O4P-C5A-C5	4.68	116.73	108.99
2	A	1000	PLP	O4P-C5A-C5	5.12	117.46	108.99
2	A	1000	PLP	C2A-C2-C3	5.72	127.94	121.04
2	D	1000	PLP	C2A-C2-C3	6.06	128.34	121.04
2	B	1000	PLP	C2A-C2-C3	6.15	128.46	121.04
2	C	1000	PLP	C2A-C2-C3	6.18	128.49	121.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	PLP	1	0
2	B	1000	PLP	1	0
2	C	1000	PLP	2	0
2	D	1000	PLP	1	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.