



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:03 AM UTC

PDB ID : 1C7G / pdb_00001c7g
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

<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

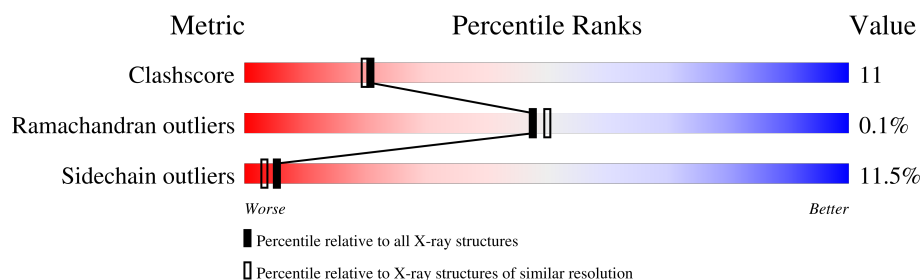
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 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	456	
1	B	456	
1	C	456	
1	D	456	

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 [i](#)

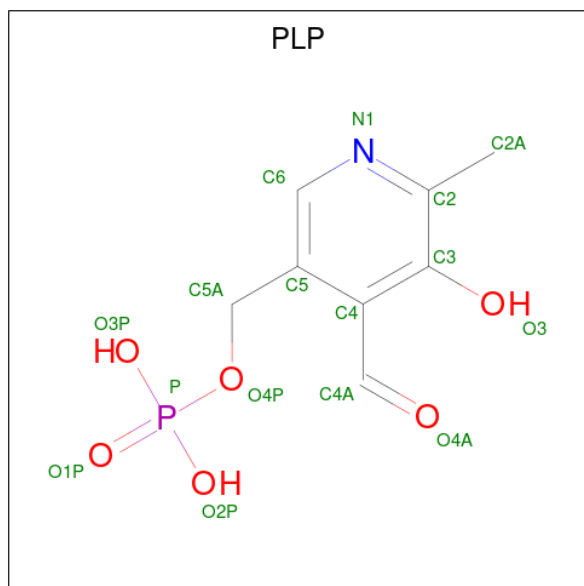
There are 3 unique types of molecules in this entry. The entry contains 14905 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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.

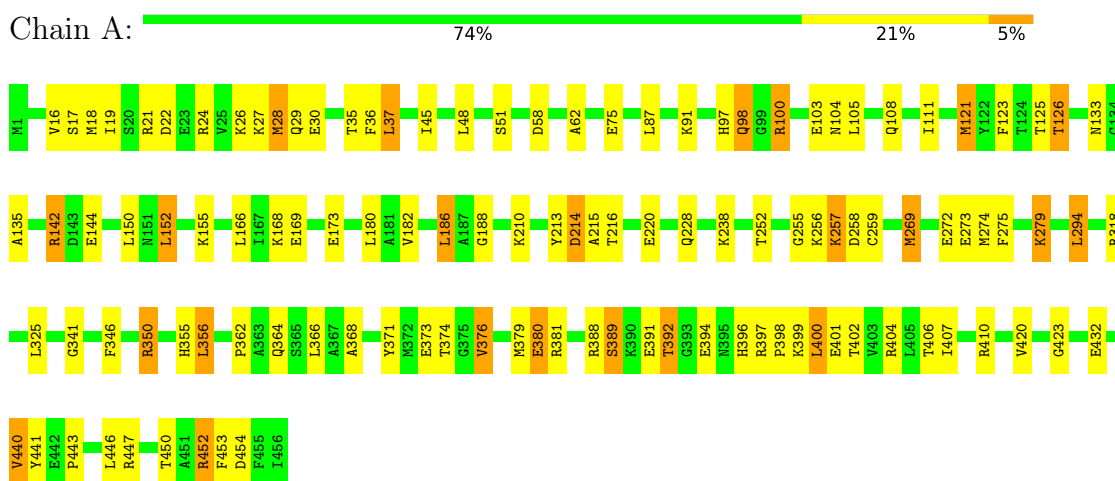
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	103	Total	O	0	0
			103	103		
3	B	77	Total	O	0	0
			77	77		
3	C	158	Total	O	0	0
			158	158		
3	D	87	Total	O	0	0
			87	87		

3 Residue-property plots

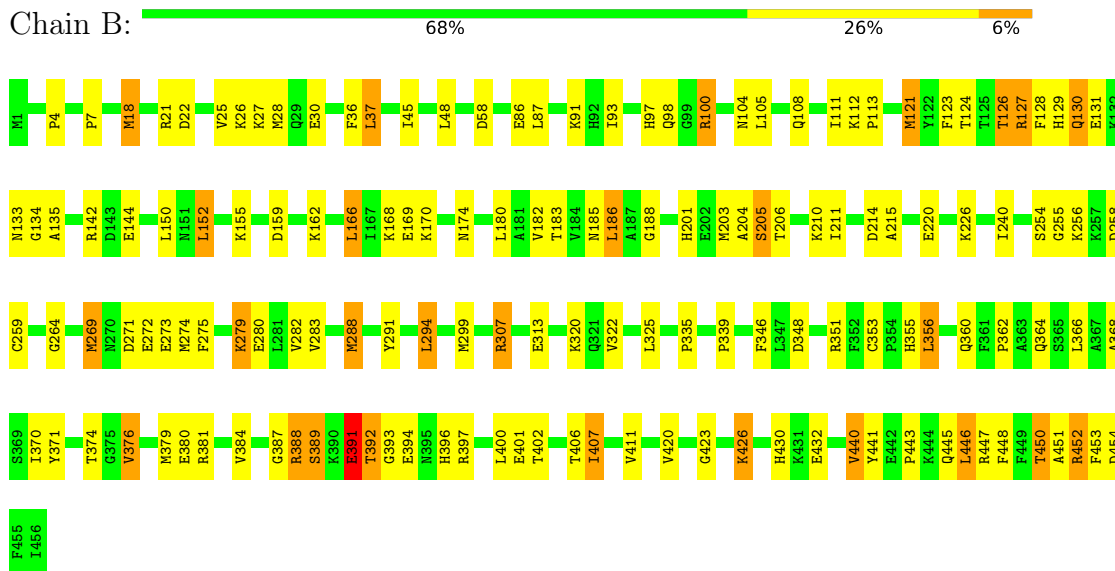
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

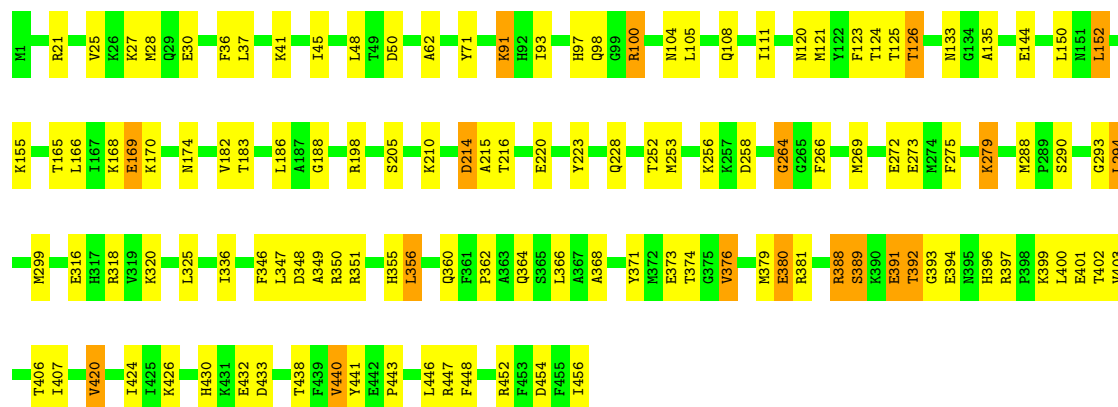


• Molecule 1: TYROSINE PHENOL-LYASE

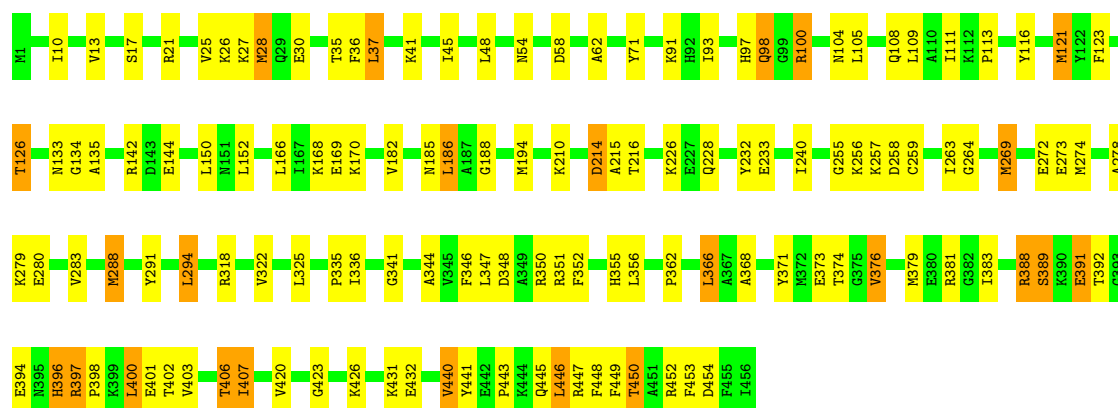


• Molecule 1: TYROSINE PHENOL-LYASE





● Molecule 1: TYROSINE PHENOL-LYASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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	0.43	0/3678	0.90	10/4955 (0.2%)
1	B	0.41	0/3678	0.90	13/4955 (0.3%)
1	C	0.46	0/3678	0.93	15/4955 (0.3%)
1	D	0.42	0/3678	0.91	12/4955 (0.2%)
All	All	0.43	0/14712	0.91	50/19820 (0.3%)

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 (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	407	ILE	N-CA-C	9.49	116.95	107.55
1	A	440	VAL	N-CA-C	-9.40	103.97	113.47
1	D	440	VAL	N-CA-C	-9.39	103.99	113.47
1	A	407	ILE	N-CA-C	9.18	116.64	107.55
1	C	440	VAL	N-CA-C	-9.16	102.71	113.42
1	B	440	VAL	N-CA-C	-8.86	103.77	113.43
1	A	214	ASP	N-CA-C	-8.75	91.98	107.73
1	D	407	ILE	N-CA-C	8.00	115.47	107.55
1	B	407	ILE	N-CA-C	7.39	116.04	107.77
1	C	252	THR	N-CA-C	-7.30	97.51	109.40
1	D	214	ASP	N-CA-C	-7.23	94.71	107.73
1	C	214	ASP	N-CA-C	-7.20	92.86	107.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ASN	N-CA-C	6.82	118.37	111.07
1	C	62	ALA	N-CA-C	-6.64	104.12	111.36
1	C	50	ASP	N-CA-C	-6.48	105.33	112.72
1	D	185	ASN	N-CA-C	6.45	118.19	111.03
1	C	215	ALA	N-CA-C	6.36	120.53	113.21
1	C	258	ASP	N-CA-C	6.30	120.68	113.19
1	B	214	ASP	N-CA-C	-6.29	95.75	107.71
1	A	62	ALA	N-CA-C	-6.21	104.59	111.36
1	D	402	THR	N-CA-C	6.14	119.04	109.52
1	B	124	THR	N-CA-C	5.98	118.31	111.02
1	B	220	GLU	N-CA-C	-5.97	104.35	111.69
1	B	258	ASP	N-CA-C	5.95	120.27	113.19
1	C	403	VAL	N-CA-C	-5.86	99.69	108.12
1	D	62	ALA	N-CA-C	-5.82	105.02	111.36
1	A	252	THR	N-CA-C	-5.73	99.56	108.90
1	B	411	VAL	N-CA-C	5.71	116.53	111.90
1	A	220	GLU	N-CA-C	-5.66	105.19	111.36
1	C	228	GLN	N-CA-C	5.64	121.96	114.12
1	A	87	LEU	N-CA-C	5.62	118.61	111.69
1	C	220	GLU	N-CA-C	-5.60	105.17	111.28
1	D	258	ASP	N-CA-C	5.52	119.76	113.19
1	A	258	ASP	N-CA-C	5.50	119.74	113.19
1	D	396	HIS	N-CA-C	-5.50	102.34	110.48
1	C	396	HIS	N-CA-C	-5.33	101.79	110.20
1	B	360	GLN	N-CA-C	-5.32	106.02	112.88
1	C	402	THR	N-CA-C	5.30	117.93	109.81
1	B	299	MET	N-CA-C	-5.30	105.56	112.23
1	B	215	ALA	N-CA-C	5.29	119.44	113.15
1	B	87	LEU	N-CA-C	5.28	117.12	111.36
1	D	215	ALA	N-CA-C	5.26	119.26	113.21
1	C	299	MET	N-CA-C	-5.23	105.64	112.23
1	A	215	ALA	N-CA-C	5.22	119.21	113.21
1	C	264	GLY	N-CA-C	5.20	116.89	111.95
1	D	54	ASN	N-CA-C	5.10	117.28	110.35
1	A	228	GLN	N-CA-C	5.09	121.24	113.61
1	D	228	GLN	N-CA-C	5.08	121.18	114.12
1	B	402	THR	N-CA-C	5.08	117.39	109.52
1	D	383	ILE	N-CA-C	5.05	115.77	110.62

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 ⓘ

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	71	0
1	B	3605	0	3548	98	1
1	C	3605	0	3548	74	0
1	D	3605	0	3548	84	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	318	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 11.

All (318) 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:D:28:MET:HE3	1:D:368:ALA:HA	1.40	1.02
1:A:28:MET:HE3	1:A:368:ALA:HA	1.43	0.99
1:C:28:MET:HE3	1:C:368:ALA:HA	1.45	0.96
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	0.75
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
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:D:28:MET:HE2	1:D:371:TYR:HB3	1.71	0.71
1:A:28:MET:HE2	1:A:371:TYR:HB3	1.72	0.71
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:28:MET:HE3	1:C:368:ALA:CA	2.20	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:28:MET:HE3	1:D:368:ALA:CA	2.22	0.68
1:D:362:PRO:HG2	1:D:401:GLU:HG2	1.75	0.67
1:C:28:MET:HE2	1:C:371:TYR:HB3	1.76	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: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:28:MET:HE2	1:B:371:TYR:CD2	2.33	0.64
1:B:26:LYS:O	1:B:30:GLU:HG3	1.98	0.64
1:A:379:MET:HE3	1:A:381:ARG:CD	2.28	0.64
1:A:111:ILE:HG21	1:A:135:ALA:HB2	1.81	0.63
1:B:355:HIS:CD2	1:B:356:LEU:HD13	2.34	0.62
1:D:214:ASP:OD1	1:D:216:THR:HG23	1.98	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:C:98:GLN:HE21	1:C:100:ARG:HD2	1.65	0.62
1:D:30:GLU:O	1:D:452:ARG:NH2	2.33	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:B:159:ASP:CG	1:B:162:LYS:HG3	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:MET:HE3	1:D:449:PHE:CD1	2.36	0.60
1:D:389:SER:CB	1:D:392:THR:HG22	2.31	0.59
1:B:111:ILE:HG21	1:B:135:ALA:HB2	1.84	0.59
1:D:37:LEU:HD11	1:D:450:THR:HA	1.83	0.59
1:D:123:PHE:HB3	1:D:126:THR:HG23	1.83	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:D:121:MET:HE2	1:D:186:LEU:HB3	1.85	0.58
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: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:D:350:ARG:NH2	1:D:398:PRO:O	2.37	0.57
1:C:28:MET:CE	1:C:368:ALA:HA	2.29	0.57
1:D:28:MET:HE1	1:D:35:THR:HG22	1.87	0.57
1:B:379:MET:HE3	1:B:381:ARG:NE	2.20	0.57
1:B:113:PRO:HA	1:B:134:GLY:O	2.05	0.57
1:B:440:VAL:CG1	1:B:454:ASP:HB2	2.35	0.57
1:B:392:THR:HG23	1:B:394:GLU:HB2	1.87	0.56
1:B:389:SER:O	1:B:393:GLY:HA2	2.05	0.56
1:C:28:MET:CE	1:C:371:TYR:HB3	2.35	0.56
1:A:350:ARG:HH21	1:A:399:LYS:C	2.13	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:A:28:MET:HE1	1:A:35:THR:HG22	1.87	0.56
1:B:86:GLU:CD	1:B:307:ARG:HH22	2.14	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:A:188:GLY:HA2	1:A:346:PHE:CE1	2.42	0.55
1:C:440:VAL:HG22	1:C:452:ARG:O	2.06	0.55
1:D:441:TYR:HD2	1:D:452:ARG:HG3	1.71	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:A:121:MET:HE2	1:A:186:LEU:HB3	1.88	0.55
1:D:71:TYR:CE2	1:D:288:MET:HG2	2.42	0.55
1:D:188:GLY:HA2	1:D:346:PHE:CE1	2.42	0.55
1:B:441:TYR:CE2	1:B:443:PRO:HD3	2.42	0.55
1:A:214:ASP:OD1	1:A:216:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:GLU:O	1:C:452:ARG:NH2	2.39	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:A:144:GLU:HB3	1:A:150:LEU:HD23	1.90	0.54
1:B:362:PRO:HG2	1:B:401:GLU:CG	2.37	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:28:MET:HE2	1:B:371:TYR:HD2	1.73	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:B:152:LEU:HD23	1:B:155:LYS:HG2	1.91	0.53
1:D:111:ILE:HG21	1:D:135:ALA:HB2	1.90	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:B:275:PHE:CZ	1:B:279:LYS:HD2	2.44	0.52
1:C:98:GLN:NE2	1:C:100:ARG:HD2	2.24	0.52
1:C:108:GLN:HG2	1:C:133:ASN:HD21	1.74	0.52
1:A:22:ASP:O	1:A:26:LYS:HG3	2.09	0.51
1:B:353:CYS:HB3	1:B:355:HIS:CE1	2.44	0.51
1:B:104:ASN:O	1:B:108:GLN:HG3	2.11	0.51
1:B:430:HIS:HB2	3:B:886:HOH:O	2.10	0.51
1:D:98:GLN:HE21	1:D:100:ARG:HD2	1.75	0.51
1:B:108:GLN:HG2	1:B:133:ASN:HD21	1.76	0.51
1:D:400:LEU:H	1:D:400:LEU:HD12	1.76	0.51
1:C:355:HIS:CD2	1:C:356:LEU:HD13	2.46	0.51
1:A:255:GLY:HA2	1:A:259:CYS:HB2	1.93	0.51
1:C:45:ILE:O	1:C:376:VAL:HA	2.11	0.51
1:D:26:LYS:O	1:D:30:GLU:HG3	2.10	0.51
1:A:18:MET:HG3	1:B:313:GLU:HG2	1.91	0.50
1:B:111:ILE:CG2	1:B:135:ALA:HB2	2.41	0.50
1:B:446:LEU:HD11	1:D:283:VAL:HG21	1.94	0.50
1:C:111:ILE:HG21	1:C:135:ALA:HB2	1.94	0.50
1:D:116:TYR:CE2	1:D:170:LYS:HD2	2.47	0.50
1:D:264:GLY:HA2	1:D:294:LEU:HD11	1.94	0.50
1:A:28:MET:HE3	1:A:368:ALA:CA	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:SER:HB2	3:C:716:HOH:O	2.12	0.49
1:D:182:VAL:O	1:D:182:VAL:HG23	2.12	0.49
1:B:269:MET:CE	1:B:274:MET:HE2	2.42	0.49
1:B:392:THR:O	1:B:394:GLU:HG3	2.12	0.49
1:C:91:LYS:HB3	1:C:91:LYS:NZ	2.27	0.49
1:C:100:ARG:HG2	1:C:125:THR:HG21	1.93	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:A:379:MET:HE3	1:A:381:ARG:NE	2.26	0.49
1:B:121:MET:HE2	1:B:186:LEU:HB3	1.93	0.49
1:D:194:MET:HG2	1:D:232:TYR:OH	2.13	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:D:28:MET:CE	1:D:371:TYR:HB3	2.43	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
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:A:269:MET:HE3	1:A:274:MET:HE2	1.94	0.48
1:C:98:GLN:HG3	1:C:256:LYS:HD2	1.96	0.48
1:A:75:GLU:OE2	1:C:41:LYS:HD3	2.13	0.48
1:B:98:GLN:HE21	1:B:100:ARG:HD2	1.78	0.48
1:B:440:VAL:HG22	1:B:452:ARG:C	2.39	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:388:ARG:HB2	1:B:394:GLU:C	2.38	0.47
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:B:445:GLN:HG2	1:D:280:GLU:OE1	2.14	0.47
1:C:182:VAL:HG23	1:C:182:VAL:O	2.15	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: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: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:B:387:GLY:HA2	1:B:447:ARG:NE	2.30	0.47
1:B:392:THR:CG2	1:B:394:GLU:HB2	2.45	0.47
1:D:28:MET:CE	1:D:368:ALA:HA	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ASP:OD1	1:A:58:ASP:N	2.48	0.47
1:B:348:ASP:CG	1:B:351:ARG:HG3	2.39	0.47
1:D:379:MET:HE3	1:D:381:ARG:CD	2.44	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:B:280:GLU:OE1	1:D:445:GLN:HG2	2.14	0.46
1:B:453:PHE:N	1:B:453:PHE:CD1	2.84	0.46
1:D:397:ARG:CG	1:D:397:ARG:HH11	2.29	0.46
1:A:355:HIS:CD2	1:A:356:LEU:HD13	2.50	0.46
1:D:381:ARG:HE	1:D:381:ARG:HA	1.81	0.46
1:B:28:MET:HE3	1:B:368:ALA:CA	2.42	0.46
1:B:28:MET:HE2	1:B:371:TYR:HB3	1.98	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:C:440:VAL:HG22	1:C:452:ARG:C	2.41	0.46
1:B:86:GLU:CD	1:B:307:ARG:NH2	2.74	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:HG23	1:B:182:VAL:O	2.16	0.46
1:B:269:MET:HE3	1:B:274:MET:HE2	1.97	0.46
1:D:111:ILE:CG2	1:D:135:ALA:HB2	2.46	0.46
1:B:170:LYS:O	1:B:174:ASN:ND2	2.48	0.46
1:C:253:MET:HG2	1:C:266:PHE:CZ	2.51	0.46
1:C:392:THR:HG23	1:C:394:GLU:HG3	1.98	0.46
1:A:19:ILE:HD11	1:A:24:ARG:HG2	1.97	0.45
1:A:142:ARG:HD3	1:A:144:GLU:OE1	2.17	0.45
1:B:204:ALA:HB3	1:B:211:ILE:HD11	1.98	0.45
1:B:389:SER:HA	1:B:396:HIS:NE2	2.31	0.45
1:C:318:ARG:HD3	1:C:318:ARG:C	2.41	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:A:152:LEU:HD23	1:A:155:LYS:HG2	1.98	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:C:28:MET:HE2	1:C:371:TYR:CD2	2.51	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:B:283:VAL:HG21	1:D:446:LEU:HD11	1.98	0.45
1:D:381:ARG:HA	1:D:381:ARG:NE	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:GLN:OE1	1:C:380:GLU:HG2	2.17	0.45
1:C:440:VAL:HG11	1:C:454:ASP:HB2	1.98	0.45
1:D:269:MET:CE	1:D:274:MET:HE2	2.47	0.45
1:B:364:GLN:OE1	1:B:384:VAL:HG11	2.16	0.45
1:D:45:ILE:O	1:D:376:VAL:HA	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: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:453:PHE:N	1:A:453:PHE:CD1	2.85	0.44
1:C:350:ARG:NH1	1:C:399:LYS:O	2.50	0.44
1:D:100:ARG:HD2	2:D:1000:PLP:O3P	2.18	0.44
1:C:349:ALA:HB3	1:C:401:GLU:HG3	2.00	0.44
1:D:374:THR:CG2	1:D:423:GLY:HA3	2.48	0.44
1:A:440:VAL:HG22	1:A:452:ARG:O	2.18	0.44
1:C:214:ASP:OD1	1:C:216:THR:HG23	2.18	0.44
1:A:350:ARG:NH2	1:A:399:LYS:O	2.39	0.43
1:A:379:MET:CE	1:A:404:ARG:CZ	2.96	0.43
1:C:389:SER:O	1:C:393:GLY:HA2	2.18	0.43
1:C:448:PHE:CD1	1:C:448:PHE:C	2.96	0.43
1:D:348:ASP:CG	1:D:351:ARG:HG3	2.43	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
1:D:388:ARG:HB2	1:D:394:GLU:C	2.44	0.43
1:B:203:MET:HE3	1:B:203:MET:HB2	1.93	0.43
1:B:391:GLU:H	1:B:391:GLU:HG2	1.56	0.43
1:C:111:ILE:CG2	1:C:135:ALA:HB2	2.49	0.43
1:C:120:ASN:OD1	1:C:120:ASN:N	2.51	0.43
1:B:21:ARG:O	1:B:25:VAL:HG23	2.19	0.43
1:B:322:VAL:HG22	1:B:407:ILE:HG13	1.99	0.43
1:D:255:GLY:C	1:D:257:LYS:H	2.27	0.43
1:A:441:TYR:CD2	1:A:452:ARG:HG3	2.50	0.43
1:D:104:ASN:O	1:D:108:GLN:HG3	2.18	0.43
1:D:335:PRO:HB2	1:D:348:ASP:HB3	2.01	0.43
1:D:366:LEU:HB3	1:D:403:VAL:HG21	2.01	0.43
1:D:453:PHE:CD1	1:D:453:PHE:N	2.87	0.43
1:B:166:LEU:CD2	1:B:170:LYS:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:254:SER:HB2	2:B:1000:PLP:H5A2	2.00	0.42
1:C:392:THR:O	1:C:394:GLU:HG3	2.20	0.42
1:D:397:ARG:HH11	1:D:397:ARG:HG2	1.85	0.42
1:D:441:TYR:CE2	1:D:443:PRO:HD3	2.55	0.42
1:B:440:VAL:HG22	1:B:452:ARG:O	2.19	0.42
1:C:379:MET:HE2	1:C:379:MET:HB3	1.77	0.42
1:C:379:MET:HE3	1:C:381:ARG:CD	2.50	0.42
1:D:233:GLU:CD	1:D:233:GLU:H	2.28	0.42
1:D:288:MET:HB2	1:D:291:TYR:CE2	2.55	0.42
1:D:322:VAL:HG22	1:D:407:ILE:HG13	2.02	0.42
1:A:16:VAL:HG22	1:B:7:PRO:O	2.19	0.42
1:C:71:TYR:CE2	1:C:288:MET:HG2	2.55	0.42
1:D:58:ASP:N	1:D:58:ASP:OD1	2.52	0.42
1:D:255:GLY:HA2	1:D:259:CYS:HB2	2.02	0.42
1:B:4:PRO:HD3	1:B:320:LYS:HD3	2.02	0.42
1:B:18:MET:HG2	3:B:925:HOH:O	2.20	0.42
1:B:226:LYS:HB2	1:B:240:ILE:CD1	2.50	0.42
1:A:98:GLN:CG	1:A:256:LYS:HD2	2.50	0.42
1:A:269:MET:CE	1:A:274:MET:HE2	2.50	0.42
1:B:370:ILE:HG22	1:B:376:VAL:HG22	2.02	0.42
1:D:255:GLY:C	1:D:257:LYS:N	2.77	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
3:A:657:HOH:O	1:C:41:LYS:HG2	2.20	0.41
1:D:98:GLN:HG3	1:D:256:LYS:HD2	2.02	0.41
1:D:318:ARG:C	1:D:318:ARG:HD3	2.45	0.41
1:D:374:THR:HG21	1:D:423:GLY:HA3	2.02	0.41
1:B:128:PHE:CD2	1:B:129:HIS:N	2.89	0.41
1:D:352:PHE:O	1:D:431:LYS:HD2	2.21	0.41
1:D:379:MET:HE3	1:D:381:ARG:NE	2.36	0.41
1:A:318:ARG:HD3	1:A:318:ARG:C	2.46	0.41
1:B:379:MET:HE3	1:B:381:ARG:CD	2.50	0.41
1:D:226:LYS:HB2	1:D:240:ILE:CD1	2.51	0.41
1:A:379:MET:HE3	1:A:381:ARG:CG	2.50	0.41
1:C:182:VAL:HA	1:C:183:THR:HA	1.90	0.41
1:C:441:TYR:HD2	1:C:452:ARG:HG3	1.86	0.41
1:A:400:LEU:HB2	1:A:402:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:PHE:CD1	1:D:448:PHE:C	2.98	0.41
1:A:180:LEU:O	1:A:213:TYR:HA	2.21	0.41
1:B:155:LYS:HD2	1:B:339:PRO:HD2	2.02	0.41
1:C:216:THR:HG21	2:C:1000:PLP:C5	2.51	0.41
1:C:438:THR:HG22	1:C:454:ASP:O	2.21	0.41
1:D:389:SER:HA	1:D:396:HIS:NE2	2.36	0.41
1:C:430:HIS:O	1:C:433:ASP:HB2	2.21	0.40
1:D:397:ARG:CG	1:D:397:ARG:NH1	2.84	0.40
1:B:182:VAL:HA	1:B:183:THR:HA	1.87	0.40
1:B:448:PHE:CD1	1:B:448:PHE:C	3.00	0.40
1:C:388:ARG:HB2	1:C:394:GLU:C	2.46	0.40
1:C:391:GLU:H	1:C:391:GLU:HG2	1.61	0.40
1:D:10:ILE:HG21	1:D:13:VAL:HG12	2.03	0.40
1:B:348:ASP:OD2	1:B:351:ARG:HG3	2.21	0.40
1:C:264:GLY:HA2	1:C:294:LEU:HD11	2.03	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:A:389:SER:HA	1:A:396:HIS:NE2	2.36	0.40
1:B:58:ASP:OD1	1:B:58:ASP:N	2.54	0.40
1:D:440:VAL:CG1	1:D:454:ASP:HB2	2.51	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	454/456 (100%)	433 (95%)	20 (4%)	1 (0%)	43	44
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%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	391	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	380/380 (100%)	334 (88%)	46 (12%)	5	3
1	B	380/380 (100%)	332 (87%)	48 (13%)	4	2
1	C	380/380 (100%)	341 (90%)	39 (10%)	7	4
1	D	380/380 (100%)	338 (89%)	42 (11%)	6	3
All	All	1520/1520 (100%)	1345 (88%)	175 (12%)	5	3

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	48	LEU
1	A	91	LYS
1	A	98	GLN
1	A	100	ARG

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Mol	Chain	Res	Type
1	A	105	LEU
1	A	121	MET
1	A	126	THR
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	238	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	325	LEU
1	A	350	ARG
1	A	356	LEU
1	A	366	LEU
1	A	373	GLU
1	A	376	VAL
1	A	380	GLU
1	A	388	ARG
1	A	389	SER
1	A	391	GLU
1	A	392	THR
1	A	397	ARG
1	A	400	LEU
1	A	406	THR
1	A	420	VAL
1	A	432	GLU
1	A	446	LEU
1	A	452	ARG
1	B	18	MET
1	B	27	LYS
1	B	36	PHE
1	B	37	LEU
1	B	48	LEU
1	B	91	LYS

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Mol	Chain	Res	Type
1	B	93	ILE
1	B	100	ARG
1	B	105	LEU
1	B	112	LYS
1	B	121	MET
1	B	126	THR
1	B	127	ARG
1	B	130	GLN
1	B	142	ARG
1	B	152	LEU
1	B	166	LEU
1	B	168	LYS
1	B	169	GLU
1	B	180	LEU
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	325	LEU
1	B	356	LEU
1	B	366	LEU
1	B	376	VAL
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
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

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Mol	Chain	Res	Type
1	C	27	LYS
1	C	36	PHE
1	C	37	LEU
1	C	48	LEU
1	C	91	LYS
1	C	93	ILE
1	C	100	ARG
1	C	105	LEU
1	C	121	MET
1	C	126	THR
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	269	MET
1	C	272	GLU
1	C	273	GLU
1	C	279	LYS
1	C	294	LEU
1	C	325	LEU
1	C	356	LEU
1	C	366	LEU
1	C	373	GLU
1	C	376	VAL
1	C	380	GLU
1	C	388	ARG
1	C	389	SER
1	C	391	GLU
1	C	392	THR
1	C	397	ARG
1	C	400	LEU
1	C	406	THR
1	C	420	VAL
1	C	426	LYS
1	C	432	GLU
1	C	446	LEU
1	D	17	SER
1	D	27	LYS
1	D	28	MET

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Mol	Chain	Res	Type
1	D	36	PHE
1	D	37	LEU
1	D	41	LYS
1	D	48	LEU
1	D	91	LYS
1	D	93	ILE
1	D	98	GLN
1	D	100	ARG
1	D	105	LEU
1	D	121	MET
1	D	126	THR
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	325	LEU
1	D	366	LEU
1	D	373	GLU
1	D	376	VAL
1	D	388	ARG
1	D	389	SER
1	D	391	GLU
1	D	397	ARG
1	D	400	LEU
1	D	406	THR
1	D	420	VAL
1	D	426	LYS
1	D	432	GLU
1	D	446	LEU
1	D	450	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	161	ASN
1	A	185	ASN
1	B	130	GLN
1	B	161	ASN
1	B	185	ASN
1	C	161	ASN
1	C	228	GLN
1	C	234	ASN
1	C	321	GLN
1	D	98	GLN
1	D	130	GLN
1	D	161	ASN
1	D	185	ASN
1	D	343	HIS
1	D	445	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	D	1000	1	15,15,16	3.40	6 (40%)	21,22,23	4.01	14 (66%)
2	PLP	A	1000	1	15,15,16	3.64	6 (40%)	21,22,23	4.09	14 (66%)
2	PLP	B	1000	1	15,15,16	3.60	6 (40%)	21,22,23	4.09	14 (66%)
2	PLP	C	1000	1	15,15,16	3.59	6 (40%)	21,22,23	4.02	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	D	1000	1	-	4/6/6/8	0/1/1/1
2	PLP	A	1000	1	-	4/6/6/8	0/1/1/1
2	PLP	B	1000	1	-	4/6/6/8	0/1/1/1
2	PLP	C	1000	1	-	4/6/6/8	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	PLP	C5-C4	12.23	1.54	1.40
2	C	1000	PLP	C5-C4	11.88	1.53	1.40
2	B	1000	PLP	C5-C4	11.78	1.53	1.40
2	D	1000	PLP	C5-C4	10.80	1.52	1.40
2	B	1000	PLP	C3-C2	4.22	1.45	1.41
2	D	1000	PLP	C3-C2	4.01	1.45	1.41
2	C	1000	PLP	C3-C2	3.74	1.44	1.41
2	A	1000	PLP	C3-C2	3.39	1.44	1.41
2	A	1000	PLP	C2-N1	3.29	1.39	1.33
2	B	1000	PLP	C2-N1	3.10	1.39	1.33
2	D	1000	PLP	C2-N1	3.04	1.39	1.33
2	C	1000	PLP	C2-N1	2.86	1.38	1.33
2	B	1000	PLP	C2A-C2	2.65	1.54	1.50
2	D	1000	PLP	C4A-C4	-2.42	1.46	1.51
2	C	1000	PLP	P-O3P	-2.35	1.46	1.54
2	C	1000	PLP	C4A-C4	-2.35	1.46	1.51
2	D	1000	PLP	P-O3P	-2.23	1.46	1.54
2	C	1000	PLP	C2A-C2	2.23	1.53	1.50
2	D	1000	PLP	C2A-C2	2.21	1.53	1.50
2	A	1000	PLP	P-O3P	-2.16	1.46	1.54
2	B	1000	PLP	P-O3P	-2.13	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	PLP	C4A-C4	-2.09	1.47	1.51
2	A	1000	PLP	C2A-C2	2.07	1.53	1.50
2	B	1000	PLP	C4A-C4	-2.04	1.47	1.51

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	PLP	O3P-P-O4P	-9.71	81.34	106.67
2	B	1000	PLP	O3P-P-O4P	-9.67	81.45	106.67
2	C	1000	PLP	O3P-P-O4P	-9.48	81.96	106.67
2	D	1000	PLP	O3P-P-O4P	-9.40	82.16	106.67
2	D	1000	PLP	O3P-P-O2P	-6.75	82.49	107.80
2	C	1000	PLP	O3P-P-O2P	-6.73	82.58	107.80
2	B	1000	PLP	O3P-P-O2P	-6.71	82.66	107.80
2	A	1000	PLP	O3P-P-O2P	-6.65	82.88	107.80
2	C	1000	PLP	C2A-C2-C3	6.58	128.49	120.80
2	B	1000	PLP	C2A-C2-C3	6.54	128.46	120.80
2	D	1000	PLP	C2A-C2-C3	6.45	128.34	120.80
2	A	1000	PLP	C2A-C2-C3	6.10	127.94	120.80
2	C	1000	PLP	O3P-P-O1P	-5.61	88.98	110.83
2	D	1000	PLP	O3P-P-O1P	-5.52	89.32	110.83
2	B	1000	PLP	O3P-P-O1P	-5.52	89.33	110.83
2	A	1000	PLP	O3P-P-O1P	-5.35	89.98	110.83
2	A	1000	PLP	O2P-P-O4P	5.11	119.98	106.67
2	C	1000	PLP	O2P-P-O4P	4.76	119.09	106.67
2	D	1000	PLP	O2P-P-O4P	4.67	118.85	106.67
2	B	1000	PLP	O2P-P-O4P	4.59	118.63	106.67
2	A	1000	PLP	O4P-C5A-C5	4.32	117.46	109.36
2	B	1000	PLP	O4P-P-O1P	4.32	118.12	106.44
2	C	1000	PLP	C6-N1-C2	4.28	126.95	119.20
2	D	1000	PLP	O4P-P-O1P	4.26	117.96	106.44
2	B	1000	PLP	C6-N1-C2	4.24	126.89	119.20
2	A	1000	PLP	C4A-C4-C5	4.12	125.19	120.94
2	A	1000	PLP	C6-N1-C2	4.10	126.63	119.20
2	D	1000	PLP	C6-N1-C2	4.08	126.60	119.20
2	A	1000	PLP	O4P-P-O1P	4.02	117.31	106.44
2	C	1000	PLP	O4P-P-O1P	3.98	117.19	106.44
2	D	1000	PLP	O4P-C5A-C5	3.93	116.73	109.36
2	C	1000	PLP	C3-C2-N1	-3.75	116.22	120.96
2	B	1000	PLP	O4P-C5A-C5	3.72	116.33	109.36
2	B	1000	PLP	C3-C2-N1	-3.70	116.29	120.96
2	D	1000	PLP	C3-C2-N1	-3.65	116.35	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1000	PLP	O3-C3-C4	3.51	127.26	118.10
2	B	1000	PLP	C4A-C4-C5	3.50	124.55	120.94
2	A	1000	PLP	C3-C2-N1	-3.49	116.56	120.96
2	B	1000	PLP	O3-C3-C4	3.48	127.18	118.10
2	C	1000	PLP	C4A-C4-C5	3.39	124.44	120.94
2	C	1000	PLP	O3-C3-C4	3.36	126.87	118.10
2	A	1000	PLP	O3-C3-C4	3.34	126.81	118.10
2	A	1000	PLP	C5-C6-N1	-2.85	119.20	123.83
2	D	1000	PLP	C5-C6-N1	-2.79	119.30	123.83
2	B	1000	PLP	C5-C6-N1	-2.79	119.30	123.83
2	C	1000	PLP	C5-C6-N1	-2.75	119.35	123.83
2	D	1000	PLP	O3-C3-C2	-2.73	111.92	117.58
2	C	1000	PLP	O4P-C5A-C5	2.70	114.41	109.36
2	B	1000	PLP	O3-C3-C2	-2.65	112.10	117.58
2	C	1000	PLP	O2P-P-O1P	2.61	121.00	110.83
2	A	1000	PLP	O3-C3-C2	-2.60	112.18	117.58
2	C	1000	PLP	O3-C3-C2	-2.55	112.29	117.58
2	D	1000	PLP	O2P-P-O1P	2.51	120.61	110.83
2	B	1000	PLP	O2P-P-O1P	2.48	120.51	110.83
2	A	1000	PLP	O2P-P-O1P	2.40	120.19	110.83
2	D	1000	PLP	C4A-C4-C5	2.18	123.19	120.94

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	PLP	C4-C5-C5A-O4P
2	A	1000	PLP	C6-C5-C5A-O4P
2	A	1000	PLP	C5A-O4P-P-O2P
2	A	1000	PLP	C5A-O4P-P-O3P
2	B	1000	PLP	C4-C5-C5A-O4P
2	B	1000	PLP	C6-C5-C5A-O4P
2	B	1000	PLP	C5A-O4P-P-O2P
2	B	1000	PLP	C5A-O4P-P-O3P
2	C	1000	PLP	C4-C5-C5A-O4P
2	C	1000	PLP	C6-C5-C5A-O4P
2	C	1000	PLP	C5A-O4P-P-O2P
2	C	1000	PLP	C5A-O4P-P-O3P
2	D	1000	PLP	C4-C5-C5A-O4P
2	D	1000	PLP	C6-C5-C5A-O4P
2	D	1000	PLP	C5A-O4P-P-O2P
2	D	1000	PLP	C5A-O4P-P-O3P

There are no ring outliers.

4 monomers are involved in 5 short contacts:

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

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.