



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:31 pm GMT

PDB ID : 1F2D  
Title : 1-AMINOCYCLOPROPANE-1-CARBOXYLATE DEAMINASE  
Authors : Yao, M.; Ose, T.; Sugimoto, H.; Horiuchi, A.; Nakagawa, A.; Yokoi, D.; Murakami, T.; Honma, M.; Wakatsuki, S.; Tanaka, I.  
Deposited on : 2000-05-24  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

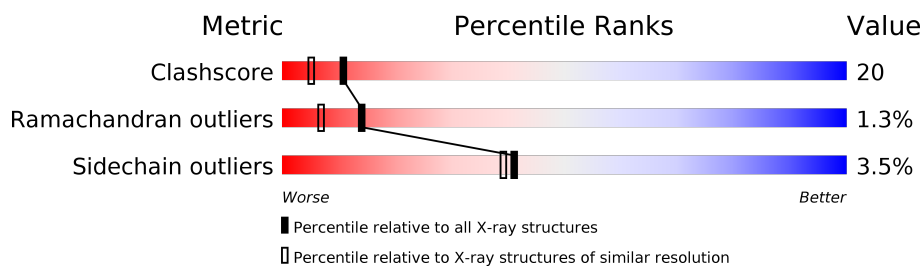
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	341	
1	B	341	
1	C	341	
1	D	341	

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	SO4	B	941	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11447 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 1-AMINOCYCLOPROPANE-1-CARBOXYLATE DEAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2607	1655	441	499	12			
1	B	341	Total	C	N	O	S	0	0	0
			2607	1655	441	499	12			
1	C	341	Total	C	N	O	S	0	0	0
			2607	1655	441	499	12			
1	D	341	Total	C	N	O	S	0	0	0
			2607	1655	441	499	12			

There are 4 discrepancies between the modelled and reference sequences:

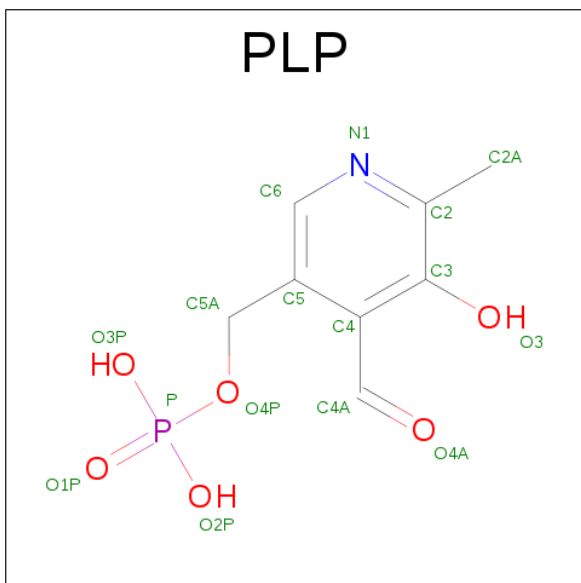
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	SER	cloning artifact	UNP Q7M523
B	1	ALA	SER	cloning artifact	UNP Q7M523
C	1	ALA	SER	cloning artifact	UNP Q7M523
D	1	ALA	SER	cloning artifact	UNP Q7M523

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



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.

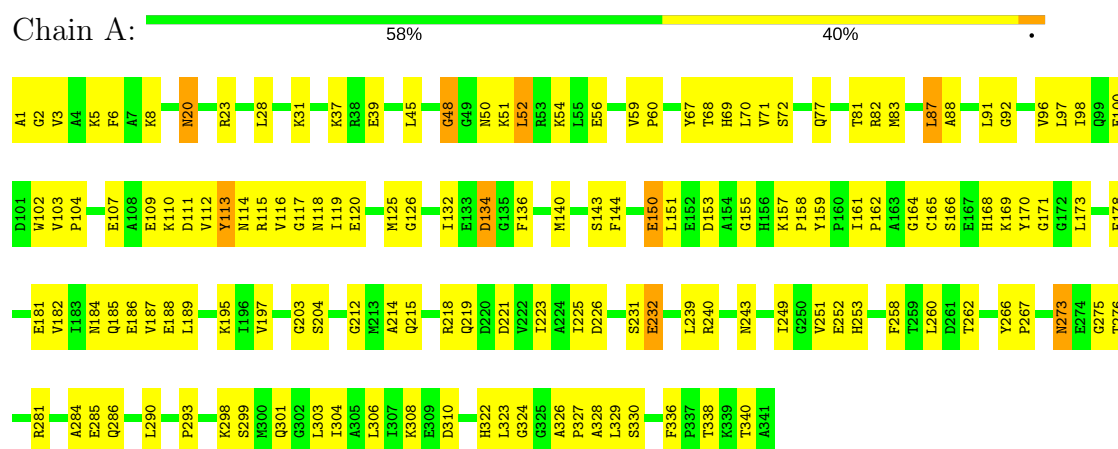
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	132	Total	O	0	0
			132	132		
4	B	121	Total	O	0	0
			121	121		
4	C	368	Total	O	0	0
			368	368		
4	D	318	Total	O	0	0
			318	318		

### 3 Residue-property plots

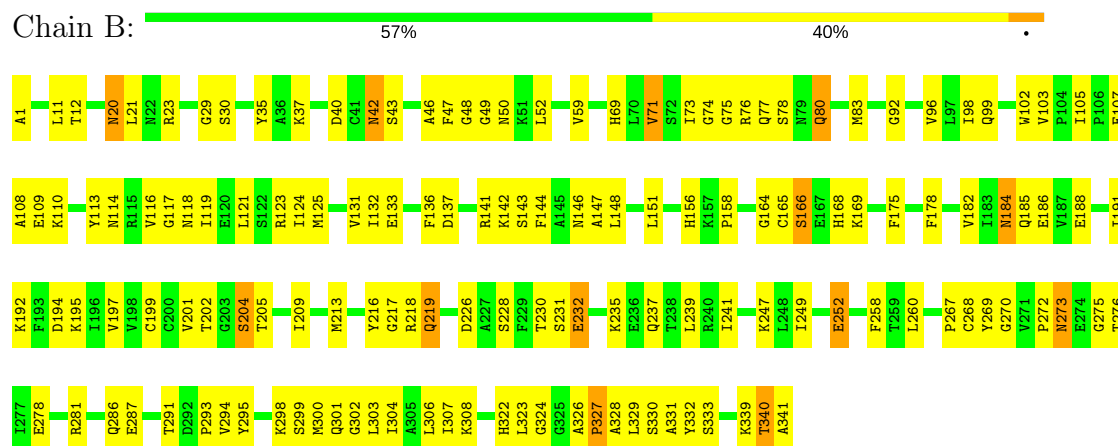
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

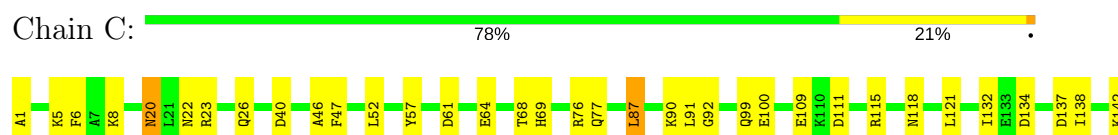
#### • Molecule 1: 1-AMINOCYCLOPROPANE-1-CARBOXYLATE DEAMINASE

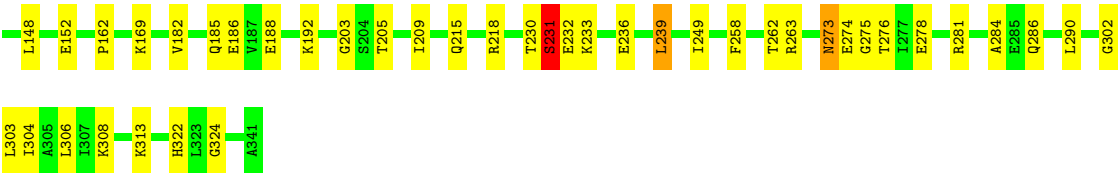


#### • Molecule 1: 1-AMINOCYCLOPROPANE-1-CARBOXYLATE DEAMINASE

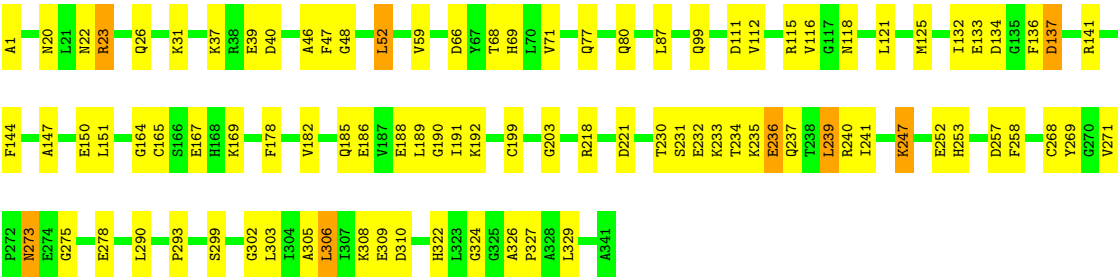


#### • Molecule 1: 1-AMINOCYCLOPROPANE-1-CARBOXYLATE DEAMINASE





● Molecule 1: 1-AMINOCYCLOPROPANE-1-CARBOXYLATE DEAMINASE





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.38Å 269.37Å 186.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00	Depositor
% Data completeness (in resolution range)	90.4 (15.00-2.00)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.221 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11447	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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: SO4, 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	0/2658	0.61	1/3594 (0.0%)
1	B	0.34	0/2658	0.60	0/3594
1	C	0.60	0/2658	0.74	1/3594 (0.0%)
1	D	0.53	0/2658	0.72	1/3594 (0.0%)
All	All	0.47	0/10632	0.67	3/14376 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	GLY	N-CA-C	6.87	130.28	113.10
1	A	203	GLY	N-CA-C	6.51	129.38	113.10
1	D	203	GLY	N-CA-C	6.27	128.79	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2607	0	2593	145	0
1	B	2607	0	2593	158	0
1	C	2607	0	2593	64	0
1	D	2607	0	2593	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	5	0	0	2	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	15	0	7	0	0
3	B	15	0	7	1	0
3	C	15	0	6	0	0
3	D	15	0	6	0	0
4	A	132	0	0	16	0
4	B	121	0	0	11	0
4	C	368	0	0	10	0
4	D	318	0	0	19	0
All	All	11447	0	10398	425	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 20.

All (425) 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:23:ARG:HH11	1:D:23:ARG:HB3	1.06	1.07
1:D:23:ARG:HH11	1:D:23:ARG:CB	1.78	0.97
1:A:126:GLY:O	1:B:339:LYS:HE2	1.64	0.96
1:B:23:ARG:HH12	1:B:286:GLN:HA	1.28	0.95
1:B:76:ARG:NH1	1:B:131:VAL:HG13	1.82	0.93
1:B:185:GLN:HA	1:B:188:GLU:HG2	1.53	0.91
1:D:23:ARG:NH1	1:D:23:ARG:HB3	1.86	0.90
1:A:100:GLU:HA	1:A:132:ILE:HG23	1.56	0.88
1:A:273:ASN:HD22	1:A:275:GLY:H	1.22	0.87
1:B:77:GLN:HE22	1:B:118:ASN:H	1.25	0.85
1:A:23:ARG:NH1	1:A:286:GLN:HA	1.93	0.83
1:A:116:VAL:HG12	1:A:117:GLY:N	1.94	0.82
1:A:70:LEU:HB2	4:A:1013:HOH:O	1.79	0.82
1:B:273:ASN:HD22	1:B:275:GLY:H	1.28	0.82
1:B:40:ASP:HB3	1:B:324:GLY:HA2	1.62	0.81
1:C:230:THR:OG1	1:C:233:LYS:HE2	1.82	0.80
1:B:252:GLU:H	1:B:252:GLU:CD	1.84	0.80
1:B:219:GLN:NE2	1:B:219:GLN:H	1.80	0.79
1:A:240:ARG:HG3	4:A:1067:HOH:O	1.81	0.79
1:B:23:ARG:NH1	1:B:286:GLN:HA	1.97	0.79
1:D:230:THR:OG1	1:D:233:LYS:HE2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:SER:HA	1:A:204:SER:HB3	1.67	0.77
1:A:23:ARG:HH12	1:A:286:GLN:HA	1.50	0.77
1:B:304:ILE:O	1:B:308:LYS:HG2	1.85	0.77
1:B:205:THR:O	1:B:209:ILE:HG13	1.84	0.77
1:D:22:ASN:O	1:D:26:GLN:HG3	1.86	0.75
1:A:116:VAL:HG13	1:B:330:SER:HB3	1.69	0.75
1:B:228:SER:HB3	4:B:1006:HOH:O	1.87	0.74
1:B:76:ARG:HH12	1:B:131:VAL:HG13	1.51	0.74
1:C:185:GLN:HA	1:C:188:GLU:HG2	1.69	0.73
1:A:96:VAL:HG21	1:A:151:LEU:HD21	1.69	0.73
1:B:12:THR:HA	1:B:43:SER:HB3	1.71	0.73
1:A:116:VAL:HG12	1:A:117:GLY:H	1.53	0.73
1:D:308:LYS:HG3	4:D:1207:HOH:O	1.89	0.72
1:A:120:GLU:OE2	1:B:333:SER:HA	1.90	0.72
1:A:116:VAL:CG1	1:A:117:GLY:H	2.03	0.72
1:B:216:TYR:HB3	4:B:952:HOH:O	1.90	0.71
1:B:52:LEU:HD13	1:B:83:MET:SD	2.30	0.71
1:A:185:GLN:HA	1:A:188:GLU:HG2	1.72	0.71
1:C:77:GLN:HE22	1:C:118:ASN:H	1.38	0.71
1:B:141:ARG:HH11	1:B:141:ARG:HA	1.56	0.71
1:A:281:ARG:O	1:A:285:GLU:HG3	1.90	0.71
1:A:223:ILE:HD13	4:A:1023:HOH:O	1.89	0.70
1:B:184:ASN:HB3	4:B:1018:HOH:O	1.90	0.70
1:A:273:ASN:HD22	1:A:275:GLY:N	1.87	0.70
1:A:48:GLY:HA2	1:A:52:LEU:HD22	1.72	0.70
1:B:21:LEU:HD22	1:B:287:GLU:HG3	1.74	0.70
1:C:322:HIS:HD2	1:C:324:GLY:H	1.39	0.70
1:D:239:LEU:HD13	1:D:258:PHE:HD2	1.56	0.69
1:C:138:ILE:H	1:C:233:LYS:NZ	1.91	0.69
1:D:77:GLN:HE22	1:D:118:ASN:H	1.39	0.69
1:D:141:ARG:HB3	4:D:1245:HOH:O	1.92	0.69
1:A:116:VAL:CG1	1:A:117:GLY:N	2.56	0.69
1:A:77:GLN:HE22	1:A:118:ASN:H	1.40	0.68
1:A:68:THR:OG1	1:A:69:HIS:HD2	1.77	0.68
1:D:218:ARG:HD2	1:D:221:ASP:OD2	1.93	0.68
1:A:226:ASP:HB2	1:A:260:LEU:HD11	1.75	0.68
1:C:1:ALA:HA	1:C:249:ILE:O	1.94	0.68
1:B:281:ARG:HD3	4:B:1007:HOH:O	1.92	0.68
1:C:302:GLY:O	1:C:306:LEU:HD13	1.94	0.68
1:A:70:LEU:HD12	1:A:88:ALA:HB2	1.76	0.67
1:A:50:ASN:HD21	1:A:51:LYS:NZ	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:LYS:HD3	4:D:1161:HOH:O	1.94	0.67
1:C:23:ARG:HH12	1:C:286:GLN:HA	1.58	0.67
1:A:20:ASN:C	1:A:20:ASN:HD22	1.98	0.66
1:A:110:LYS:HB3	4:A:1029:HOH:O	1.95	0.66
1:C:23:ARG:NH1	1:C:286:GLN:O	2.28	0.66
1:A:118:ASN:ND2	1:A:328:ALA:HB2	2.10	0.66
1:B:37:LYS:HD3	1:B:178:PHE:CZ	2.32	0.65
1:C:239:LEU:HD13	1:C:258:PHE:HD2	1.62	0.65
1:D:271:VAL:HG23	4:D:1183:HOH:O	1.95	0.65
1:D:305:ALA:O	1:D:309:GLU:HG2	1.97	0.65
1:A:116:VAL:HG13	1:B:330:SER:CB	2.27	0.65
1:B:273:ASN:HD22	1:B:275:GLY:N	1.95	0.65
1:B:40:ASP:HB3	1:B:324:GLY:CA	2.26	0.65
1:A:126:GLY:C	1:B:339:LYS:HE2	2.17	0.64
1:C:239:LEU:HD13	1:C:258:PHE:CD2	2.33	0.64
1:A:112:VAL:HA	1:A:115:ARG:HG2	1.79	0.63
1:A:322:HIS:HD2	1:A:324:GLY:H	1.47	0.63
1:A:3:VAL:HG12	4:A:1036:HOH:O	1.98	0.63
1:B:40:ASP:CB	1:B:324:GLY:HA2	2.28	0.63
1:B:77:GLN:NE2	1:B:118:ASN:H	1.95	0.63
1:C:192:LYS:HG3	4:C:1136:HOH:O	1.97	0.63
1:D:132:ILE:HG22	1:D:133:GLU:H	1.63	0.63
1:D:66:ASP:HB2	4:D:1156:HOH:O	1.98	0.63
1:B:109:GLU:HG2	1:B:331:ALA:O	1.98	0.63
1:A:92:GLY:HA2	1:B:23:ARG:HH21	1.63	0.63
1:D:150:GLU:HG2	1:D:151:LEU:HD12	1.81	0.62
1:A:107:GLU:O	1:A:110:LYS:HG2	1.99	0.62
1:C:61:ASP:O	1:C:64:GLU:HB3	2.00	0.62
1:C:20:ASN:HD22	1:C:20:ASN:C	2.01	0.62
1:D:23:ARG:HH11	1:D:23:ARG:CG	2.11	0.62
1:C:273:ASN:HD22	1:C:275:GLY:H	1.47	0.61
1:D:239:LEU:HD13	1:D:258:PHE:CD2	2.35	0.61
1:D:271:VAL:N	4:D:1183:HOH:O	2.32	0.61
1:C:121:LEU:HD22	1:D:290:LEU:HD13	1.83	0.61
1:B:322:HIS:CD2	1:B:324:GLY:H	2.18	0.61
1:A:164:GLY:C	1:A:166:SER:H	2.04	0.61
1:B:119:ILE:HG22	4:B:1010:HOH:O	2.00	0.61
1:B:300:MET:O	1:B:304:ILE:HG13	2.01	0.61
1:B:322:HIS:HD2	1:B:324:GLY:H	1.47	0.61
1:C:138:ILE:H	1:C:233:LYS:HZ2	1.49	0.61
1:D:186:GLU:OE1	1:D:218:ARG:NH2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:VAL:CG2	1:B:270:GLY:HA3	2.31	0.61
1:A:23:ARG:NH2	1:B:92:GLY:HA2	2.17	0.60
1:B:201:VAL:HB	1:B:228:SER:HB2	1.83	0.60
1:A:304:ILE:O	1:A:308:LYS:HG2	2.01	0.60
1:D:185:GLN:HA	1:D:188:GLU:HG2	1.81	0.60
1:A:140:MET:HA	4:A:954:HOH:O	2.02	0.60
1:D:268:CYS:SG	4:D:1183:HOH:O	2.56	0.60
1:A:170:TYR:HB3	1:A:173:LEU:HD12	1.84	0.60
1:B:46:ALA:O	1:B:47:PHE:HB2	2.01	0.60
1:C:231:SER:HB2	4:C:1279:HOH:O	2.02	0.60
1:B:103:VAL:HG21	1:B:270:GLY:HA3	1.82	0.59
1:B:71:VAL:HG11	1:B:148:LEU:HD23	1.82	0.59
1:B:23:ARG:HH11	1:B:23:ARG:HG2	1.68	0.59
1:B:339:LYS:O	1:B:341:ALA:N	2.35	0.59
1:C:169:LYS:HA	4:C:1251:HOH:O	2.02	0.59
1:A:281:ARG:HD3	4:A:1020:HOH:O	2.03	0.58
1:B:226:ASP:HB2	1:B:260:LEU:HD11	1.85	0.58
1:C:182:VAL:O	1:C:186:GLU:HG3	2.04	0.58
1:A:8:LYS:HE3	1:A:56:GLU:OE1	2.02	0.58
1:B:217:GLY:C	1:B:219:GLN:NE2	2.56	0.58
1:A:52:LEU:HD13	1:A:83:MET:SD	2.44	0.58
1:B:116:VAL:C	4:B:1010:HOH:O	2.40	0.58
1:A:181:GLU:O	1:A:185:GLN:HG3	2.03	0.58
1:A:109:GLU:O	1:A:113:TYR:HB2	2.04	0.58
1:B:192:LYS:HD2	4:B:1048:HOH:O	2.04	0.58
1:A:212:GLY:O	1:A:215:GLN:HG3	2.04	0.58
1:D:278:GLU:HG2	4:D:1210:HOH:O	2.04	0.58
1:B:103:VAL:HG22	1:B:269:TYR:O	2.03	0.57
1:A:223:ILE:HG21	4:A:1023:HOH:O	2.05	0.57
1:A:195:LYS:HE2	4:A:958:HOH:O	2.02	0.57
1:D:167:GLU:HG3	4:D:1065:HOH:O	2.04	0.57
1:B:182:VAL:O	1:B:186:GLU:HG3	2.03	0.57
1:B:298:LYS:HA	1:B:301:GLN:HE21	1.70	0.57
1:B:303:LEU:O	1:B:307:ILE:HG13	2.05	0.57
1:A:82:ARG:O	1:A:125:MET:HE1	2.05	0.57
1:B:107:GLU:O	1:B:110:LYS:HG2	2.05	0.57
1:A:5:LYS:HG2	1:A:6:PHE:CD1	2.40	0.56
1:A:290:LEU:O	1:A:322:HIS:HE1	1.87	0.56
1:B:102:TRP:CD1	1:B:136:PHE:HA	2.41	0.56
1:C:109:GLU:HG3	4:C:1224:HOH:O	2.05	0.56
1:C:68:THR:OG1	1:C:69:HIS:HD2	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:GLY:C	1:B:219:GLN:HE22	2.08	0.56
1:B:291:THR:HA	4:B:1033:HOH:O	2.05	0.56
1:D:112:VAL:HG12	1:D:116:VAL:HG22	1.87	0.56
1:A:37:LYS:HD3	1:A:178:PHE:CZ	2.41	0.56
1:B:23:ARG:NH1	1:B:286:GLN:O	2.39	0.56
1:C:137:ASP:HA	1:C:233:LYS:NZ	2.21	0.56
1:C:138:ILE:HG12	1:C:233:LYS:HE3	1.88	0.56
1:D:190:GLY:C	1:D:191:ILE:HD12	2.26	0.56
1:B:42:ASN:ND2	1:B:49:GLY:O	2.40	0.55
1:C:273:ASN:HD22	1:C:275:GLY:N	2.04	0.55
1:D:40:ASP:HB3	1:D:324:GLY:HA2	1.89	0.55
1:B:48:GLY:HA2	1:B:52:LEU:HD22	1.89	0.55
1:D:322:HIS:HD2	1:D:324:GLY:H	1.55	0.55
1:D:66:ASP:O	1:D:66:ASP:CG	2.43	0.55
1:D:230:THR:CB	1:D:233:LYS:HE2	2.36	0.55
1:B:37:LYS:HD3	1:B:178:PHE:CE1	2.42	0.55
1:A:273:ASN:ND2	1:A:275:GLY:H	2.00	0.55
1:A:1:ALA:HA	1:A:215:GLN:OE1	2.07	0.55
1:B:185:GLN:HA	1:B:188:GLU:CG	2.31	0.55
1:B:201:VAL:HG11	1:B:295:TYR:HE1	1.71	0.55
1:B:252:GLU:N	1:B:252:GLU:CD	2.59	0.55
1:B:166:SER:HA	1:B:204:SER:HB3	1.88	0.54
1:A:266:TYR:CD1	1:A:267:PRO:HA	2.42	0.54
1:B:199:CYS:HB2	1:B:299:SER:HB3	1.89	0.54
1:B:326:ALA:O	1:B:329:LEU:HB2	2.07	0.54
1:A:72:SER:HA	1:A:161:ILE:O	2.07	0.54
1:B:239:LEU:HD13	1:B:258:PHE:CD1	2.42	0.54
1:A:306:LEU:HD13	4:A:1023:HOH:O	2.07	0.54
1:B:116:VAL:HG12	1:B:117:GLY:N	2.23	0.54
1:A:100:GLU:HA	1:A:132:ILE:CG2	2.35	0.54
1:B:142:LYS:HG2	1:B:142:LYS:O	2.08	0.54
1:B:23:ARG:NH1	1:B:23:ARG:HG2	2.23	0.54
1:C:281:ARG:HD3	4:C:1194:HOH:O	2.07	0.54
1:B:71:VAL:HG22	1:B:144:PHE:CE1	2.43	0.54
1:D:68:THR:OG1	1:D:69:HIS:HD2	1.91	0.54
1:A:67:TYR:HA	1:A:157:LYS:HB3	1.88	0.54
1:D:199:CYS:HB2	1:D:299:SER:HB3	1.89	0.54
1:B:339:LYS:NZ	1:B:341:ALA:O	2.37	0.53
1:D:302:GLY:O	1:D:306:LEU:HD22	2.08	0.53
1:D:147:ALA:O	1:D:151:LEU:HD13	2.08	0.53
1:A:77:GLN:HE22	1:A:118:ASN:N	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:GLN:HE22	1:D:118:ASN:N	2.05	0.53
1:C:231:SER:OG	1:C:262:THR:HG21	2.09	0.53
1:B:197:VAL:HG21	1:B:303:LEU:HD23	1.91	0.53
1:B:23:ARG:NH1	1:B:286:GLN:CA	2.71	0.53
1:A:187:VAL:O	1:D:169:LYS:CE	2.57	0.53
1:D:191:ILE:HD12	1:D:191:ILE:N	2.22	0.53
1:D:31:LYS:HE3	1:D:310:ASP:OD1	2.09	0.53
1:A:284:ALA:HB1	1:B:125:MET:HG2	1.92	0.52
1:B:272:PRO:CG	1:B:293:PRO:HB3	2.39	0.52
1:A:273:ASN:ND2	1:A:276:THR:H	2.08	0.52
1:A:219:GLN:NE2	1:A:219:GLN:H	2.08	0.52
1:B:273:ASN:ND2	1:B:276:THR:H	2.07	0.52
1:D:132:ILE:HG22	1:D:133:GLU:N	2.24	0.52
1:B:74:GLY:HA2	1:B:102:TRP:CH2	2.45	0.52
1:B:293:PRO:HD3	1:B:329:LEU:HD13	1.91	0.52
1:C:22:ASN:O	1:C:26:GLN:HG3	2.09	0.52
1:D:253:HIS:HE1	4:D:1128:HOH:O	1.92	0.52
1:A:182:VAL:O	1:A:186:GLU:HG3	2.10	0.52
1:B:340:THR:O	1:B:341:ALA:HB3	2.10	0.52
1:A:214:ALA:HA	1:A:219:GLN:HE21	1.75	0.51
1:B:302:GLY:O	1:B:306:LEU:HD13	2.10	0.51
1:C:40:ASP:HB3	1:C:324:GLY:HA2	1.92	0.51
1:D:48:GLY:HA2	1:D:52:LEU:HD22	1.93	0.51
1:A:239:LEU:HD13	1:A:258:PHE:HD2	1.74	0.51
1:A:281:ARG:HH21	1:A:336:PHE:HA	1.75	0.51
1:B:235:LYS:HB2	1:B:260:LEU:HD23	1.91	0.51
1:C:274:GLU:O	1:C:278:GLU:HG3	2.10	0.51
1:A:219:GLN:CD	1:A:219:GLN:H	2.13	0.51
1:A:239:LEU:O	1:A:243:ASN:ND2	2.41	0.51
1:B:143:SER:HA	1:B:146:ASN:HD22	1.76	0.51
1:A:187:VAL:O	1:D:169:LYS:HE2	2.11	0.51
1:B:71:VAL:HG11	1:B:148:LEU:CD2	2.41	0.51
1:A:116:VAL:O	1:A:119:ILE:HG22	2.11	0.51
1:A:214:ALA:HB2	1:A:219:GLN:HG3	1.92	0.51
1:B:164:GLY:O	1:B:165:CYS:HB2	2.11	0.51
1:A:112:VAL:HG13	1:A:116:VAL:CG2	2.41	0.51
1:C:46:ALA:O	1:C:47:PHE:HB2	2.10	0.51
1:B:237:GLN:O	1:B:241:ILE:HG13	2.11	0.51
1:D:290:LEU:O	1:D:322:HIS:HE1	1.94	0.50
1:C:304:ILE:O	1:C:308:LYS:HG3	2.11	0.50
1:A:54:LYS:NZ	1:A:204:SER:OG	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ALA:N	1:A:327:PRO:CD	2.74	0.50
1:B:141:ARG:CA	1:B:141:ARG:HH11	2.25	0.50
1:D:273:ASN:HD22	1:D:275:GLY:H	1.58	0.50
1:A:115:ARG:HG3	1:A:116:VAL:HG23	1.92	0.50
1:A:338:THR:OG1	1:B:123:ARG:NE	2.45	0.50
1:B:218:ARG:N	1:B:219:GLN:NE2	2.60	0.50
1:B:30:SER:HA	4:B:1024:HOH:O	2.11	0.50
1:A:132:ILE:CD1	1:A:143:SER:HB3	2.41	0.50
1:B:278:GLU:HA	4:B:968:HOH:O	2.12	0.50
1:B:219:GLN:CD	1:B:219:GLN:H	2.10	0.50
1:B:23:ARG:NH1	1:B:286:GLN:OE1	2.45	0.50
1:C:239:LEU:CD1	1:C:258:PHE:HD2	2.23	0.50
1:C:322:HIS:CD2	1:C:324:GLY:H	2.25	0.50
1:B:235:LYS:O	1:B:239:LEU:HB2	2.11	0.50
1:B:293:PRO:HD3	1:B:329:LEU:CD1	2.42	0.50
1:B:272:PRO:HG3	1:B:293:PRO:HB3	1.92	0.49
1:B:270:GLY:HA2	1:B:294:VAL:HG13	1.94	0.49
1:B:11:LEU:HD11	1:B:59:VAL:HG21	1.95	0.49
1:B:77:GLN:HE22	1:B:118:ASN:N	2.02	0.49
1:A:290:LEU:HD13	1:B:121:LEU:HD22	1.94	0.49
1:D:46:ALA:O	1:D:47:PHE:HB2	2.12	0.49
1:D:308:LYS:HB3	4:D:1161:HOH:O	2.12	0.49
1:B:98:ILE:HD11	1:B:147:ALA:HB2	1.95	0.49
1:C:284:ALA:HB1	1:D:125:MET:HG2	1.94	0.49
1:A:290:LEU:O	1:A:322:HIS:CE1	2.67	0.48
1:D:192:LYS:HE3	4:D:1126:HOH:O	2.13	0.48
1:A:77:GLN:NE2	1:A:118:ASN:H	2.08	0.48
1:A:164:GLY:C	1:A:166:SER:N	2.66	0.48
1:C:263:ARG:NH2	1:C:306:LEU:HD12	2.29	0.48
1:C:8:LYS:HD3	1:C:57:TYR:CZ	2.48	0.48
1:D:182:VAL:O	1:D:186:GLU:HG3	2.13	0.48
1:B:73:ILE:HG12	1:B:74:GLY:N	2.27	0.48
1:B:20:ASN:HD22	1:B:20:ASN:C	2.16	0.48
1:B:219:GLN:HE21	1:B:219:GLN:H	1.57	0.48
1:C:273:ASN:ND2	1:C:276:THR:H	2.12	0.48
1:A:197:VAL:HG21	1:A:303:LEU:HD23	1.96	0.48
1:B:50:ASN:HB3	1:B:323:LEU:HD22	1.95	0.48
1:D:293:PRO:HD3	1:D:329:LEU:HD23	1.96	0.47
1:C:148:LEU:O	1:C:152:GLU:HG3	2.14	0.47
1:A:119:ILE:HG23	1:A:120:GLU:N	2.28	0.47
1:A:45:LEU:HB2	1:A:52:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ASP:O	1:B:195:LYS:HD3	2.12	0.47
1:C:5:LYS:HG3	1:C:6:PHE:CD1	2.49	0.47
1:B:273:ASN:ND2	1:B:275:GLY:H	2.03	0.47
1:D:269:TYR:O	4:D:1183:HOH:O	2.20	0.47
1:A:28:LEU:O	1:A:31:LYS:HG2	2.14	0.47
1:B:107:GLU:C	1:B:109:GLU:H	2.18	0.47
1:A:168:HIS:ND1	1:A:169:LYS:N	2.63	0.47
1:A:20:ASN:ND2	1:A:20:ASN:C	2.67	0.47
1:B:80:GLN:HB3	2:B:941:SO4:O2	2.15	0.47
1:A:98:ILE:CD1	1:A:144:PHE:HA	2.45	0.47
1:C:205:THR:O	1:C:209:ILE:HG13	2.15	0.47
1:A:87:LEU:O	1:A:87:LEU:HD22	2.15	0.47
1:B:239:LEU:HD13	1:B:258:PHE:HD1	1.79	0.47
1:B:267:PRO:O	1:B:268:CYS:HB3	2.15	0.47
1:B:96:VAL:HG21	1:B:151:LEU:HD11	1.96	0.46
1:A:23:ARG:HH21	1:B:92:GLY:HA2	1.80	0.46
1:B:141:ARG:NH1	1:B:141:ARG:HB3	2.29	0.46
1:B:69:HIS:CD2	1:B:156:HIS:HB3	2.50	0.46
1:D:1:ALA:HB3	4:D:1084:HOH:O	2.15	0.46
1:A:329:LEU:HD21	1:B:124:ILE:HD12	1.96	0.46
1:C:111:ASP:O	1:C:115:ARG:NE	2.41	0.46
1:C:192:LYS:HE2	1:C:218:ARG:NH2	2.30	0.46
1:B:209:ILE:O	1:B:213:MET:HG2	2.15	0.46
1:A:69:HIS:O	1:A:159:TYR:N	2.45	0.46
1:B:156:HIS:O	1:B:158:PRO:HD3	2.16	0.46
1:B:202:THR:OG1	3:B:342:PLP:O3P	2.20	0.46
1:A:102:TRP:CD1	1:A:136:PHE:HA	2.50	0.46
1:C:76:ARG:NH1	1:C:132:ILE:O	2.37	0.46
1:A:118:ASN:HD22	1:A:328:ALA:HB2	1.81	0.46
1:A:52:LEU:HD13	1:A:83:MET:CG	2.45	0.46
1:A:111:ASP:O	1:A:115:ARG:HD3	2.16	0.46
1:C:231:SER:N	4:C:1279:HOH:O	2.37	0.46
1:A:107:GLU:HA	4:A:1029:HOH:O	2.16	0.46
1:A:330:SER:HB3	1:B:116:VAL:CG1	2.44	0.46
1:A:20:ASN:ND2	4:A:952:HOH:O	2.49	0.45
1:C:23:ARG:CZ	4:D:1124:HOH:O	2.64	0.45
1:A:249:ILE:HG13	1:A:251:VAL:HG23	1.97	0.45
1:A:252:GLU:O	1:A:253:HIS:C	2.53	0.45
1:B:137:ASP:HB3	1:B:141:ARG:NE	2.32	0.45
1:B:201:VAL:HG11	1:B:295:TYR:CE1	2.50	0.45
1:A:116:VAL:HG11	1:A:330:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASN:ND2	1:B:328:ALA:HB2	2.32	0.45
1:C:230:THR:CB	1:C:233:LYS:HE2	2.47	0.45
1:A:186:GLU:OE1	1:A:218:ARG:NH2	2.45	0.45
1:A:273:ASN:ND2	1:A:275:GLY:N	2.60	0.45
1:B:76:ARG:NH1	1:B:99:GLN:O	2.49	0.45
1:D:59:VAL:HG22	1:D:87:LEU:HD21	1.99	0.45
1:A:150:GLU:O	1:A:153:ASP:HB2	2.17	0.45
1:A:310:ASP:HA	4:A:942:HOH:O	2.17	0.45
1:B:1:ALA:HA	1:B:249:ILE:O	2.17	0.45
1:A:164:GLY:O	1:A:166:SER:N	2.50	0.45
1:D:80:GLN:OE1	1:D:164:GLY:CA	2.65	0.45
1:C:92:GLY:HA2	1:D:23:ARG:HH21	1.82	0.45
1:B:75:GLY:O	1:B:78:SER:HB2	2.16	0.45
1:B:50:ASN:CB	1:B:323:LEU:HD22	2.47	0.45
1:C:142:LYS:HE2	4:C:1250:HOH:O	2.16	0.45
1:D:37:LYS:HD3	1:D:178:PHE:CE2	2.51	0.45
1:A:132:ILE:HG12	1:A:134:ASP:H	1.82	0.44
1:B:219:GLN:NE2	1:B:219:GLN:N	2.59	0.44
1:C:138:ILE:HG12	1:C:233:LYS:CE	2.48	0.44
1:D:77:GLN:NE2	1:D:118:ASN:H	2.11	0.44
1:D:237:GLN:O	1:D:241:ILE:HG13	2.16	0.44
1:B:201:VAL:HG22	1:B:202:THR:HG23	1.98	0.44
1:B:175:PHE:O	1:B:178:PHE:HB3	2.18	0.44
1:A:132:ILE:HD11	1:A:134:ASP:OD1	2.18	0.44
1:A:153:ASP:C	1:A:155:GLY:H	2.21	0.44
1:C:40:ASP:CB	1:C:324:GLY:HA2	2.48	0.44
1:C:76:ARG:NH1	1:C:99:GLN:O	2.51	0.44
1:D:136:PHE:O	1:D:137:ASP:HB2	2.18	0.44
1:D:240:ARG:HG2	1:D:240:ARG:HH11	1.83	0.44
1:A:103:VAL:HA	1:A:104:PRO:HD3	1.88	0.44
1:A:37:LYS:HD3	1:A:178:PHE:CE2	2.53	0.44
1:A:71:VAL:HG12	1:A:159:TYR:O	2.18	0.44
1:B:216:TYR:HA	4:D:1159:HOH:O	2.17	0.44
1:A:116:VAL:CG1	1:B:330:SER:HB3	2.45	0.44
1:B:35:TYR:OH	1:B:191:ILE:HD13	2.17	0.44
1:B:80:GLN:CB	2:B:941:SO4:O2	2.66	0.44
1:C:20:ASN:ND2	1:C:20:ASN:C	2.69	0.44
1:A:112:VAL:HA	1:A:115:ARG:CG	2.47	0.43
1:A:329:LEU:HD23	1:B:121:LEU:CD2	2.48	0.43
1:B:105:ILE:HD13	1:B:114:ASN:HD21	1.83	0.43
1:B:35:TYR:CZ	1:B:191:ILE:HD13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LYS:HE2	4:B:1015:HOH:O	2.18	0.43
1:D:111:ASP:O	1:D:115:ARG:NE	2.52	0.43
1:A:119:ILE:CG2	1:A:120:GLU:N	2.80	0.43
1:A:59:VAL:N	1:A:60:PRO:CD	2.81	0.43
1:C:162:PRO:HG3	4:C:1032:HOH:O	2.17	0.43
1:A:231:SER:OG	1:A:262:THR:HG21	2.18	0.43
1:D:80:GLN:OE1	1:D:164:GLY:HA2	2.18	0.43
1:D:236:GLU:HG3	1:D:237:GLN:N	2.33	0.43
1:A:169:LYS:HB3	1:A:169:LYS:NZ	2.33	0.43
1:D:186:GLU:CD	1:D:218:ARG:HH22	2.18	0.43
1:A:329:LEU:HD21	1:B:124:ILE:CD1	2.49	0.43
1:C:1:ALA:HB1	1:C:215:GLN:OE1	2.18	0.43
1:B:168:HIS:ND1	1:B:169:LYS:N	2.67	0.43
1:B:230:THR:O	1:B:232:GLU:N	2.52	0.43
1:B:235:LYS:HG3	1:B:258:PHE:CE1	2.54	0.43
1:D:192:LYS:HE2	1:D:218:ARG:CZ	2.49	0.43
1:D:290:LEU:O	1:D:322:HIS:CE1	2.72	0.42
1:C:1:ALA:CA	1:C:249:ILE:O	2.66	0.42
1:D:189:LEU:O	1:D:191:ILE:HD12	2.20	0.42
1:D:23:ARG:NH1	1:D:23:ARG:CG	2.75	0.42
1:A:171:GLY:O	1:A:204:SER:HB2	2.19	0.42
1:D:233:LYS:HG3	1:D:234:THR:N	2.33	0.42
1:A:70:LEU:HD12	1:A:88:ALA:CB	2.48	0.42
1:B:1:ALA:CB	4:D:1185:HOH:O	2.67	0.42
1:D:326:ALA:N	1:D:327:PRO:CD	2.82	0.42
1:B:326:ALA:N	1:B:327:PRO:CD	2.83	0.42
1:A:151:LEU:N	1:A:151:LEU:HD12	2.34	0.42
1:A:276:THR:OG1	1:A:301:GLN:NE2	2.53	0.42
1:A:225:ILE:HG21	1:A:299:SER:HA	2.00	0.42
1:A:81:THR:HB	1:A:97:LEU:HD13	2.01	0.42
1:B:20:ASN:ND2	1:B:20:ASN:C	2.72	0.42
1:A:298:LYS:HA	1:A:301:GLN:HG2	2.01	0.42
1:D:71:VAL:HG12	1:D:144:PHE:CE1	2.55	0.42
1:A:87:LEU:HD22	1:A:91:LEU:HG	2.02	0.42
1:B:164:GLY:C	1:B:166:SER:H	2.23	0.42
1:B:272:PRO:HG3	1:B:293:PRO:CB	2.50	0.42
1:C:115:ARG:NH1	4:C:1001:HOH:O	2.44	0.42
1:C:290:LEU:HD13	1:D:121:LEU:HD22	2.01	0.42
1:D:164:GLY:O	1:D:165:CYS:HB2	2.19	0.42
1:C:23:ARG:NH2	4:D:1124:HOH:O	2.52	0.42
1:D:192:LYS:HG3	4:D:1155:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:H	1:A:151:LEU:HD12	1.83	0.41
1:A:281:ARG:O	1:A:285:GLU:CG	2.66	0.41
1:A:59:VAL:HG22	1:A:87:LEU:HD11	2.02	0.41
1:C:90:LYS:HE3	4:C:1134:HOH:O	2.19	0.41
1:A:293:PRO:HD3	1:A:329:LEU:HD13	2.01	0.41
1:A:166:SER:HA	1:A:204:SER:CB	2.44	0.41
1:B:303:LEU:HD13	1:B:303:LEU:C	2.40	0.41
1:B:113:TYR:HE1	1:B:332:TYR:CE1	2.38	0.41
1:D:247:LYS:HB3	1:D:247:LYS:HE2	1.85	0.41
1:A:189:LEU:HD23	4:A:1066:HOH:O	2.18	0.41
1:B:247:LYS:HE2	1:B:247:LYS:HB3	1.92	0.41
1:A:232:GLU:HG2	4:A:1035:HOH:O	2.21	0.41
1:D:235:LYS:HD3	1:D:257:ASP:OD1	2.21	0.41
1:D:52:LEU:HD12	1:D:52:LEU:HA	1.89	0.41
1:B:132:ILE:HG22	1:B:133:GLU:N	2.36	0.41
1:A:151:LEU:HB2	1:A:158:PRO:HG2	2.03	0.41
1:B:219:GLN:N	1:B:219:GLN:CD	2.74	0.41
1:B:273:ASN:ND2	1:B:275:GLY:N	2.64	0.41
1:B:29:GLY:O	1:B:30:SER:HB2	2.21	0.41
1:A:82:ARG:NH1	1:A:83:MET:HG3	2.36	0.41
1:C:76:ARG:NH1	1:C:100:GLU:C	2.74	0.41
1:D:39:GLU:HB2	1:D:322:HIS:O	2.21	0.41
1:A:178:PHE:O	1:A:182:VAL:HG23	2.21	0.40
1:B:42:ASN:HD22	1:B:49:GLY:C	2.25	0.40
1:C:87:LEU:HD22	1:C:91:LEU:HG	2.01	0.40
1:B:144:PHE:O	1:B:148:LEU:HG	2.21	0.40
1:C:76:ARG:HH11	1:C:76:ARG:HD3	1.76	0.40
1:A:112:VAL:O	1:A:114:ASN:N	2.54	0.40
1:A:151:LEU:H	1:A:151:LEU:CD1	2.35	0.40
1:A:39:GLU:HB2	1:A:323:LEU:HA	2.03	0.40
1:A:340:THR:HG23	4:A:1030:HOH:O	2.21	0.40
1:B:166:SER:HA	1:B:204:SER:CB	2.50	0.40
1:B:218:ARG:N	1:B:219:GLN:HE21	2.20	0.40
1:C:100:GLU:HG2	1:C:132:ILE:HD11	2.03	0.40
1:D:112:VAL:HG12	1:D:116:VAL:CG2	2.50	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	339/341 (99%)	299 (88%)	34 (10%)	6 (2%)	10	4
1	B	339/341 (99%)	292 (86%)	38 (11%)	9 (3%)	6	2
1	C	339/341 (99%)	326 (96%)	12 (4%)	1 (0%)	44	40
1	D	339/341 (99%)	326 (96%)	11 (3%)	2 (1%)	28	21
All	All	1356/1364 (99%)	1243 (92%)	95 (7%)	18 (1%)	14	7

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	TYR
1	B	204	SER
1	B	232	GLU
1	B	340	THR
1	B	108	ALA
1	B	231	SER
1	A	2	GLY
1	B	166	SER
1	D	137	ASP
1	D	231	SER
1	A	150	GLU
1	A	162	PRO
1	A	165	CYS
1	B	42	ASN
1	B	80	GLN
1	C	231	SER
1	B	327	PRO
1	A	48	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	275/275 (100%)	267 (97%)	8 (3%)	48	47
1	B	275/275 (100%)	269 (98%)	6 (2%)	57	60
1	C	275/275 (100%)	264 (96%)	11 (4%)	36	32
1	D	275/275 (100%)	262 (95%)	13 (5%)	30	26
All	All	1100/1100 (100%)	1062 (96%)	38 (4%)	41	39

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	52	LEU
1	A	87	LEU
1	A	134	ASP
1	A	184	ASN
1	A	221	ASP
1	A	232	GLU
1	A	273	ASN
1	B	20	ASN
1	B	71	VAL
1	B	184	ASN
1	B	219	GLN
1	B	252	GLU
1	B	273	ASN
1	C	20	ASN
1	C	52	LEU
1	C	87	LEU
1	C	134	ASP
1	C	231	SER
1	C	232	GLU
1	C	236	GLU
1	C	239	LEU
1	C	273	ASN
1	C	303	LEU

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Mol	Chain	Res	Type
1	C	313	LYS
1	D	20	ASN
1	D	23	ARG
1	D	52	LEU
1	D	99	GLN
1	D	134	ASP
1	D	232	GLU
1	D	236	GLU
1	D	239	LEU
1	D	247	LYS
1	D	252	GLU
1	D	273	ASN
1	D	303	LEU
1	D	306	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	50	ASN
1	A	69	HIS
1	A	77	GLN
1	A	99	GLN
1	A	156	HIS
1	A	184	ASN
1	A	219	GLN
1	A	273	ASN
1	A	301	GLN
1	A	322	HIS
1	B	20	ASN
1	B	69	HIS
1	B	77	GLN
1	B	146	ASN
1	B	219	GLN
1	B	273	ASN
1	B	301	GLN
1	B	322	HIS
1	C	20	ASN
1	C	69	HIS
1	C	77	GLN
1	C	149	GLN
1	C	253	HIS

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Mol	Chain	Res	Type
1	C	273	ASN
1	C	301	GLN
1	C	322	HIS
1	D	20	ASN
1	D	69	HIS
1	D	77	GLN
1	D	273	ASN
1	D	301	GLN
1	D	322	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	$\# Z  > 2$
3	PLP	A	342	1	15,15,16	1.62	2 (13%)	20,22,23	1.89	3 (15%)
2	SO4	A	940	-	4,4,4	0.37	0	6,6,6	0.13	0
3	PLP	B	342	1	15,15,16	1.67	5 (33%)	20,22,23	1.79	5 (25%)
2	SO4	B	941	-	4,4,4	0.27	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PLP	C	342	1	15,15,16	1.79	4 (26%)	20,22,23	1.71	3 (15%)
2	SO4	C	942	-	4,4,4	0.34	0	6,6,6	0.31	0
3	PLP	D	342	1	15,15,16	2.11	5 (33%)	20,22,23	1.81	3 (15%)
2	SO4	D	943	-	4,4,4	0.25	0	6,6,6	0.25	0

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	A	342	1	-	0/6/6/8	0/1/1/1
2	SO4	A	940	-	-	0/0/0/0	0/0/0/0
3	PLP	B	342	1	-	0/6/6/8	0/1/1/1
2	SO4	B	941	-	-	0/0/0/0	0/0/0/0
3	PLP	C	342	1	-	0/6/6/8	0/1/1/1
2	SO4	C	942	-	-	0/0/0/0	0/0/0/0
3	PLP	D	342	1	-	0/6/6/8	0/1/1/1
2	SO4	D	943	-	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	342	PLP	C3-C2	-4.24	1.37	1.40
3	C	342	PLP	C3-C2	-2.59	1.38	1.40
3	B	342	PLP	C3-C2	-2.35	1.39	1.40
3	B	342	PLP	P-O3P	-2.04	1.46	1.54
3	B	342	PLP	C4A-C4	2.08	1.55	1.51
3	D	342	PLP	C6-N1	2.26	1.39	1.34
3	D	342	PLP	C2-N1	2.49	1.39	1.33
3	B	342	PLP	C2-N1	2.53	1.39	1.33
3	A	342	PLP	C2-N1	2.58	1.39	1.33
3	C	342	PLP	C2A-C2	2.58	1.55	1.50
3	C	342	PLP	C5-C4	2.66	1.43	1.40
3	D	342	PLP	C4A-C4	3.30	1.58	1.51
3	C	342	PLP	C2-N1	3.56	1.41	1.33
3	A	342	PLP	C5-C4	3.65	1.44	1.40
3	B	342	PLP	C5-C4	3.66	1.44	1.40
3	D	342	PLP	C5-C4	4.09	1.45	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	342	PLP	C5-C6-N1	-2.93	118.92	123.87
3	C	342	PLP	O2P-P-O4P	-2.86	99.11	106.73
3	C	342	PLP	C5-C6-N1	-2.74	119.23	123.87
3	A	342	PLP	C5-C6-N1	-2.61	119.46	123.87
3	B	342	PLP	C5-C6-N1	-2.40	119.82	123.87
3	D	342	PLP	O2P-P-O4P	-2.11	101.13	106.73
3	B	342	PLP	O2P-P-O4P	-2.05	101.28	106.73
3	B	342	PLP	C5A-C5-C6	-2.03	115.84	119.33
3	A	342	PLP	C4A-C4-C5	2.01	122.89	120.86
3	B	342	PLP	C4A-C4-C5	2.08	122.96	120.86
3	C	342	PLP	O4P-C5A-C5	3.75	116.85	109.32
3	D	342	PLP	O4P-C5A-C5	5.21	119.80	109.32
3	B	342	PLP	O4P-C5A-C5	5.31	119.99	109.32
3	A	342	PLP	O4P-C5A-C5	6.11	121.60	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	342	PLP	1	0
2	B	941	SO4	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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.