



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 09:42 am GMT

PDB ID : 1C7N  
Title : CRYSTAL STRUCTURE OF CYSTALYSIN FROM TREPONEMA DENTICOLOA CONTAINS A PYRIDOXAL 5'-PHOSPHATE COFACTOR  
Authors : Krupka, H.I.; Huber, R.; Holt, S.C.; Clausen, T.  
Deposited on : 2000-03-16  
Resolution : 1.90 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

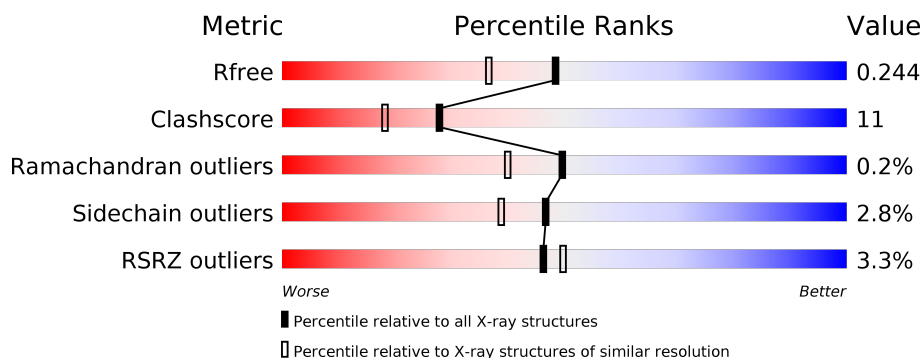
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (1.90-1.90)

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.

Mol	Chain	Length	Quality of chain
1	A	399	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>..</div> </div> </div>
1	B	399	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div> </div>
1	C	399	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>..</div> </div> </div>
1	D	399	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>..</div> </div> </div>
1	E	399	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>..</div> </div> </div>
1	F	399	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	399	<div><div></div><div>3%</div><div>76%</div><div>22%</div><div>••</div></div>
1	H	399	<div><div></div><div>6%</div><div>74%</div><div>23%</div><div>••</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28402 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 CRYSTALYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	B	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	C	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	D	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	E	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	F	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	G	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	H	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			

There are 24 discrepancies between the modelled and reference sequences:

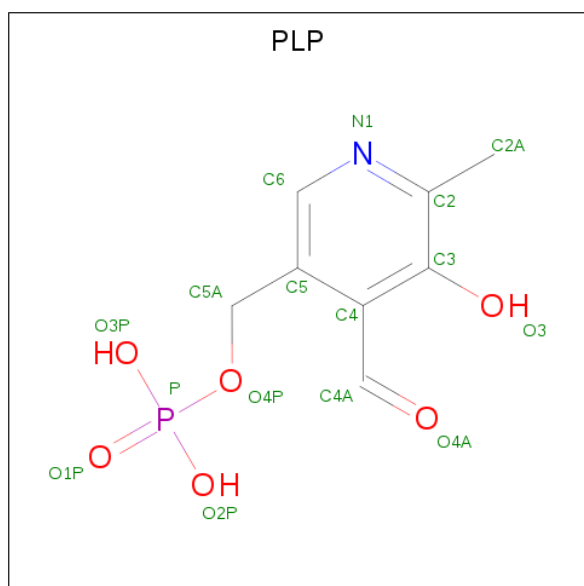
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	GLN	GLU	CONFLICT	UNP Q56257
A	154	GLN	GLU	CONFLICT	UNP Q56257
A	267	ALA	ILE	CONFLICT	UNP Q56257
B	88	GLN	GLU	CONFLICT	UNP Q56257
B	154	GLN	GLU	CONFLICT	UNP Q56257
B	267	ALA	ILE	CONFLICT	UNP Q56257
C	88	GLN	GLU	CONFLICT	UNP Q56257
C	154	GLN	GLU	CONFLICT	UNP Q56257
C	267	ALA	ILE	CONFLICT	UNP Q56257
D	88	GLN	GLU	CONFLICT	UNP Q56257
D	154	GLN	GLU	CONFLICT	UNP Q56257
D	267	ALA	ILE	CONFLICT	UNP Q56257
E	88	GLN	GLU	CONFLICT	UNP Q56257

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Chain	Residue	Modelled	Actual	Comment	Reference
E	154	GLN	GLU	CONFLICT	UNP Q56257
E	267	ALA	ILE	CONFLICT	UNP Q56257
F	88	GLN	GLU	CONFLICT	UNP Q56257
F	154	GLN	GLU	CONFLICT	UNP Q56257
F	267	ALA	ILE	CONFLICT	UNP Q56257
G	88	GLN	GLU	CONFLICT	UNP Q56257
G	154	GLN	GLU	CONFLICT	UNP Q56257
G	267	ALA	ILE	CONFLICT	UNP Q56257
H	88	GLN	GLU	CONFLICT	UNP Q56257
H	154	GLN	GLU	CONFLICT	UNP Q56257
H	267	ALA	ILE	CONFLICT	UNP Q56257

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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		
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		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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

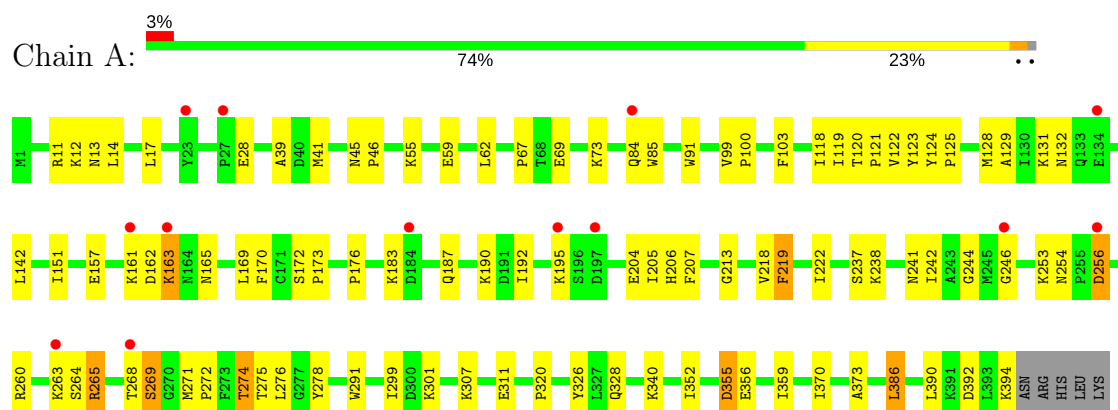
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	313	Total	O	0	0
			313	313		
3	B	269	Total	O	0	0
			269	269		
3	C	354	Total	O	0	0
			354	354		
3	D	379	Total	O	0	0
			379	379		
3	E	292	Total	O	0	0
			292	292		
3	F	380	Total	O	0	0
			380	380		
3	G	334	Total	O	0	0
			334	334		
3	H	305	Total	O	0	0
			305	305		

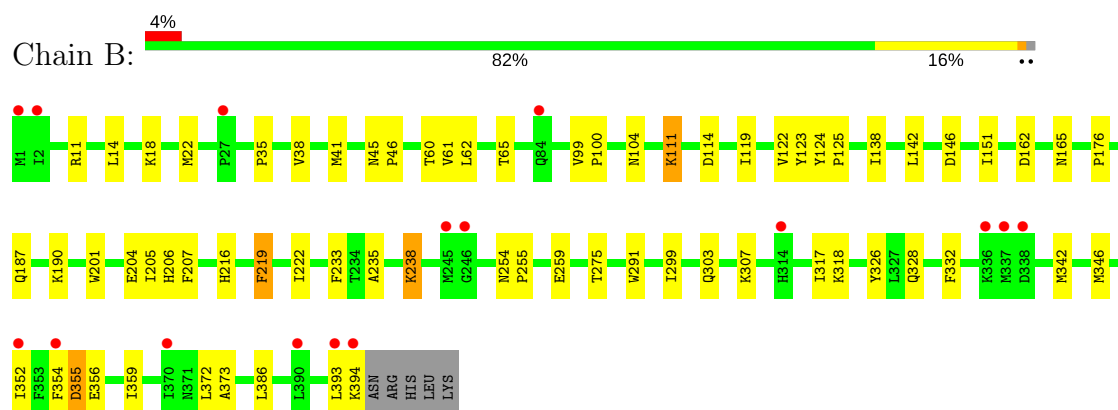
### 3 Residue-property plots [i](#)

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

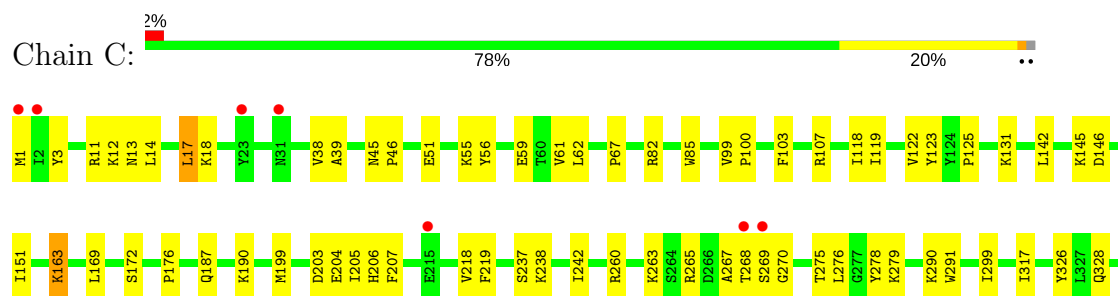
#### • Molecule 1: CYSTALYSIN



#### • Molecule 1: CYSTALYSIN

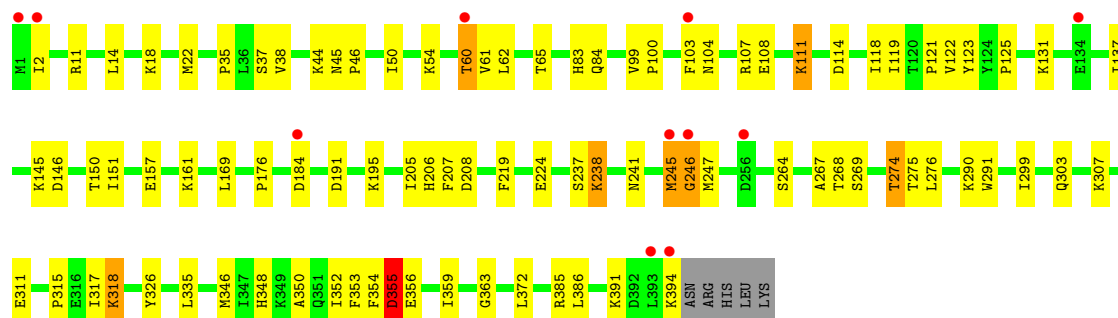
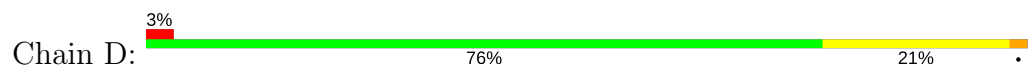


#### • Molecule 1: CYSTALYSIN

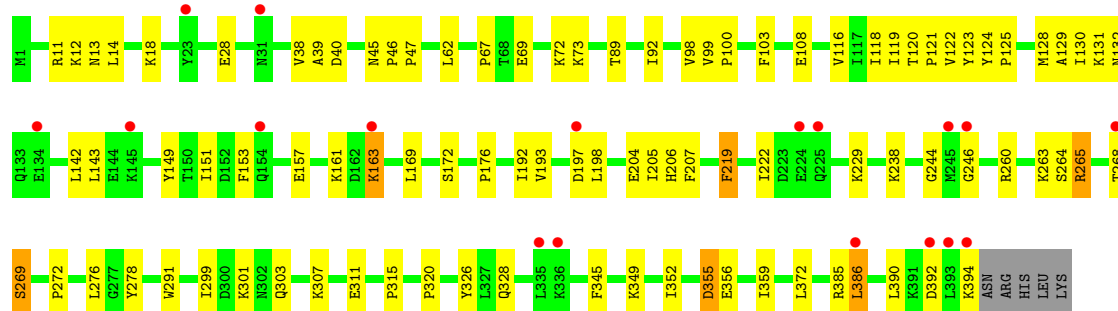




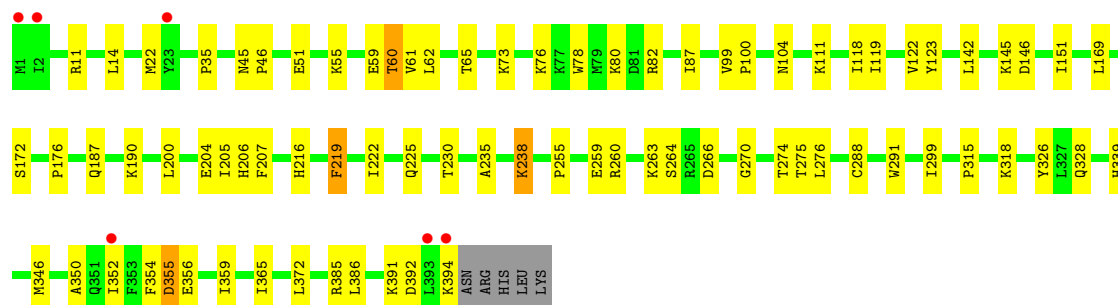
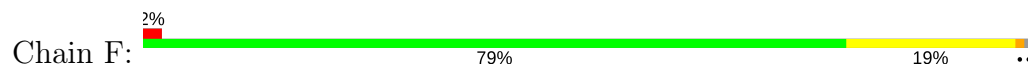
• Molecule 1: CYSTALYSIN



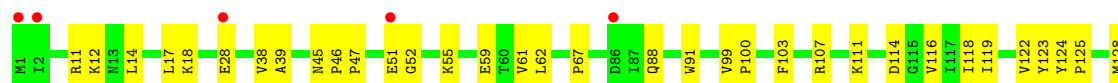
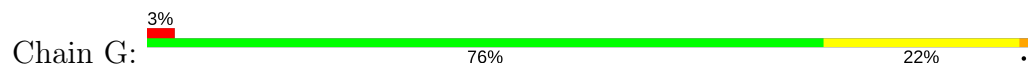
• Molecule 1: CYSTALYSIN



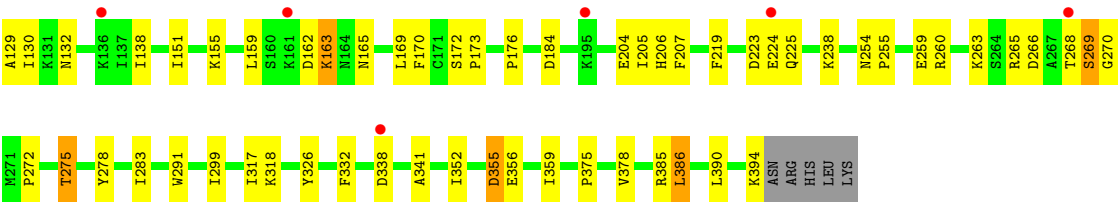
• Molecule 1: CYSTALYSIN



• Molecule 1: CYSTALYSIN







• Molecule 1: CYSTALYSIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.47Å 108.44Å 176.09Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	25.00 – 1.90 24.89 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.5 (25.00-1.90) 96.5 (24.89-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 1.90Å)	Xtriage
Refinement program	unknown	Depositor
R, $R_{free}$	0.208 , 0.247 0.205 , 0.244	Depositor DCC
$R_{free}$ test set	12711 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.6	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	28402	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.32	0/3283	0.62	1/4429 (0.0%)
1	B	0.31	0/3283	0.60	0/4429
1	C	0.35	0/3283	0.64	1/4429 (0.0%)
1	D	0.33	0/3283	0.63	2/4429 (0.0%)
1	E	0.32	0/3283	0.62	1/4429 (0.0%)
1	F	0.34	0/3283	0.64	1/4429 (0.0%)
1	G	0.33	0/3283	0.62	1/4429 (0.0%)
1	H	0.31	0/3283	0.62	1/4429 (0.0%)
All	All	0.33	0/26264	0.63	8/35432 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	355	ASP	N-CA-C	-6.32	93.94	111.00
1	G	355	ASP	N-CA-C	-6.15	94.39	111.00
1	C	355	ASP	N-CA-C	-5.91	95.05	111.00
1	F	355	ASP	N-CA-C	-5.90	95.07	111.00
1	E	355	ASP	N-CA-C	-5.62	95.81	111.00
1	H	355	ASP	N-CA-C	-5.46	96.27	111.00
1	A	355	ASP	N-CA-C	-5.45	96.29	111.00
1	D	246	GLY	N-CA-C	5.05	125.73	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	3207	0	3221	79	0
1	B	3207	0	3221	55	0
1	C	3207	0	3221	70	0
1	D	3207	0	3221	73	0
1	E	3207	0	3221	86	0
1	F	3207	0	3221	64	0
1	G	3207	0	3221	73	0
1	H	3207	0	3221	81	0
2	A	15	0	6	4	0
2	B	15	0	6	1	0
2	C	15	0	6	4	0
2	D	15	0	6	4	0
2	E	15	0	6	4	0
2	F	15	0	6	1	0
2	G	15	0	6	3	0
2	H	15	0	6	1	0
3	A	313	0	0	9	0
3	B	269	0	0	1	0
3	C	354	0	0	8	0
3	D	379	0	0	11	0
3	E	292	0	0	18	0
3	F	380	0	0	8	0
3	G	334	0	0	4	0
3	H	305	0	0	15	0
All	All	28402	0	25816	553	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 11.

All (553) 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:163:LYS:HD3	1:C:163:LYS:H	1.06	1.13
1:A:163:LYS:HD3	1:A:163:LYS:H	1.07	1.09
1:E:163:LYS:HD3	1:E:163:LYS:H	1.07	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:LYS:HD3	1:G:163:LYS:H	1.15	1.04
1:E:45:ASN:HD21	1:F:62:LEU:H	1.15	0.94
1:E:62:LEU:H	1:F:45:ASN:HD21	1.16	0.90
1:C:163:LYS:H	1:C:163:LYS:CD	1.85	0.89
1:G:45:ASN:HD21	1:H:62:LEU:H	1.21	0.89
1:A:45:ASN:HD21	1:B:62:LEU:H	1.21	0.88
1:C:62:LEU:H	1:D:45:ASN:HD21	1.20	0.88
1:E:205:ILE:HD13	2:E:400:PLP:H5A1	1.54	0.87
1:C:163:LYS:HD3	1:C:163:LYS:N	1.90	0.87
1:H:60:THR:HG22	1:H:61:VAL:H	1.44	0.82
1:E:163:LYS:HD3	1:E:163:LYS:N	1.92	0.81
1:A:163:LYS:HD3	1:A:163:LYS:N	1.91	0.81
1:D:150:THR:HG23	3:D:575:HOH:O	1.81	0.81
1:D:346:MET:SD	1:D:352:ILE:HD11	2.21	0.81
1:D:65:THR:OG1	1:D:275:THR:HG22	1.80	0.80
1:G:163:LYS:CD	1:G:163:LYS:H	1.94	0.79
1:F:255:PRO:O	1:F:259:GLU:HG3	1.83	0.79
1:A:62:LEU:H	1:B:45:ASN:HD21	1.26	0.79
1:B:65:THR:OG1	1:B:275:THR:HG22	1.82	0.79
1:C:62:LEU:CD2	1:C:275:THR:HG21	2.14	0.78
1:F:11:ARG:HA	1:F:14:LEU:HD12	1.66	0.78
1:A:84:GLN:HG3	3:A:611:HOH:O	1.84	0.77
1:C:45:ASN:HD21	1:D:62:LEU:H	1.28	0.77
1:D:22:MET:SD	1:D:35:PRO:HG3	2.24	0.77
1:G:67:PRO:HG3	1:G:278:TYR:CE2	2.20	0.77
1:G:62:LEU:H	1:H:45:ASN:HD21	1.32	0.76
1:H:84:GLN:HG3	3:H:456:HOH:O	1.85	0.76
1:H:22:MET:SD	1:H:35:PRO:HG3	2.26	0.75
1:D:84:GLN:HG3	3:D:594:HOH:O	1.86	0.74
1:H:255:PRO:O	1:H:259:GLU:HG3	1.87	0.74
1:C:12:LYS:O	1:C:14:LEU:HD13	1.88	0.74
1:B:255:PRO:O	1:B:259:GLU:HG3	1.89	0.73
1:D:352:ILE:HD13	1:D:386:LEU:HD13	1.71	0.73
1:D:205:ILE:HD13	2:D:400:PLP:H5A1	1.71	0.72
1:C:62:LEU:HD23	1:C:275:THR:HG21	1.72	0.72
1:A:192:ILE:HA	1:A:195:LYS:HE3	1.70	0.72
1:E:46:PRO:HG3	1:E:291:TRP:CD2	2.25	0.72
1:D:315:PRO:O	1:D:318:LYS:HE2	1.89	0.71
1:H:205:ILE:CD1	1:H:235:ALA:HB3	2.19	0.71
1:A:119:ILE:HD13	1:A:151:ILE:HD12	1.73	0.71
1:D:60:THR:HG22	1:D:61:VAL:H	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ILE:HD13	2:C:400:PLP:H5A1	1.72	0.71
1:D:104:ASN:HD22	1:D:107:ARG:HH21	1.38	0.71
1:F:187:GLN:HE22	1:F:190:LYS:NZ	1.88	0.70
1:G:260:ARG:HA	1:G:263:LYS:HD3	1.73	0.70
1:B:346:MET:SD	1:B:352:ILE:HD11	2.31	0.70
1:C:386:LEU:HD22	1:C:390:LEU:HG	1.73	0.70
1:A:190:LYS:HE2	3:A:572:HOH:O	1.92	0.70
1:H:356:GLU:O	1:H:359:ILE:HG12	1.92	0.70
1:D:307:LYS:O	1:D:311:GLU:HG3	1.92	0.70
1:G:163:LYS:HD3	1:G:163:LYS:N	1.99	0.70
1:A:67:PRO:HG3	1:A:278:TYR:CE2	2.26	0.69
1:F:205:ILE:CD1	1:F:235:ALA:HB3	2.22	0.69
1:C:299:ILE:HD13	1:C:326:TYR:HB3	1.72	0.69
1:H:80:LYS:HE2	3:H:566:HOH:O	1.92	0.69
1:C:39:ALA:HB1	1:C:238:LYS:HE2	1.74	0.69
1:F:346:MET:SD	1:F:352:ILE:HD11	2.32	0.69
1:H:60:THR:HG23	3:H:513:HOH:O	1.92	0.69
1:E:67:PRO:HG3	1:E:278:TYR:CE2	2.29	0.68
1:G:119:ILE:HD13	1:G:151:ILE:HD12	1.75	0.68
1:D:157:GLU:HG2	1:D:161:LYS:NZ	2.08	0.68
1:B:11:ARG:HA	1:B:14:LEU:HD12	1.74	0.67
1:F:352:ILE:HD13	1:F:386:LEU:HD13	1.76	0.67
1:H:65:THR:OG1	1:H:275:THR:HG22	1.94	0.67
1:A:12:LYS:O	1:A:14:LEU:HD13	1.94	0.67
1:H:191:ASP:O	1:H:195:LYS:HE2	1.95	0.67
1:C:119:ILE:HD13	1:C:151:ILE:HD12	1.76	0.67
1:E:301:LYS:HG2	3:E:558:HOH:O	1.94	0.66
1:G:386:LEU:HD22	1:G:390:LEU:HG	1.75	0.66
1:H:65:THR:CB	1:H:275:THR:HG22	2.26	0.66
1:B:205:ILE:CD1	1:B:235:ALA:HB3	2.26	0.66
1:E:128:MET:O	1:E:132:ASN:HB2	1.96	0.65
1:H:346:MET:SD	1:H:352:ILE:HD11	2.36	0.65
1:B:187:GLN:HE22	1:B:190:LYS:NZ	1.94	0.65
1:B:18:LYS:HB2	1:B:38:VAL:HB	1.79	0.65
1:D:352:ILE:CD1	1:D:386:LEU:HD13	2.27	0.65
1:H:99:VAL:HB	1:H:100:PRO:HD3	1.77	0.65
1:H:191:ASP:O	1:H:195:LYS:HG3	1.97	0.65
1:H:299:ILE:HD13	1:H:326:TYR:HB3	1.78	0.65
1:F:46:PRO:HG3	1:F:291:TRP:CD2	2.32	0.64
1:A:46:PRO:HG3	1:A:291:TRP:CD2	2.32	0.64
1:C:55:LYS:HE2	1:C:59:GLU:OE2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:205:ILE:HD11	1:H:235:ALA:HB3	1.78	0.64
1:H:242:ILE:HB	1:H:245:MET:HB2	1.79	0.64
1:B:22:MET:SD	1:B:35:PRO:HG3	2.37	0.64
1:A:260:ARG:O	1:A:263:LYS:HG2	1.97	0.64
1:G:394:LYS:HB2	1:G:394:LYS:HZ2	1.61	0.64
1:A:205:ILE:CD1	2:A:400:PLP:H5A1	2.28	0.64
1:H:21:LEU:O	1:H:25:GLN:HG3	1.97	0.64
1:F:352:ILE:CD1	1:F:386:LEU:HD13	2.28	0.63
1:C:82:ARG:HD2	3:C:739:HOH:O	1.98	0.63
1:C:51:GLU:HG3	3:C:496:HOH:O	1.97	0.63
1:E:99:VAL:HB	1:E:100:PRO:HD3	1.81	0.63
1:E:386:LEU:HD22	1:E:390:LEU:HG	1.79	0.63
1:F:394:LYS:HD2	3:F:747:HOH:O	1.99	0.63
1:B:60:THR:HG22	1:B:61:VAL:H	1.64	0.62
1:D:119:ILE:HD13	1:D:151:ILE:HD12	1.81	0.62
1:E:92:ILE:HD12	3:E:433:HOH:O	1.99	0.62
1:F:22:MET:SD	1:F:35:PRO:HG3	2.39	0.62
1:F:55:LYS:HE2	1:F:59:GLU:OE2	1.99	0.62
1:D:2:ILE:HA	3:D:585:HOH:O	2.00	0.62
1:F:206:HIS:HE1	2:F:400:PLP:O3	1.83	0.62
1:G:46:PRO:HG3	1:G:291:TRP:CD2	2.35	0.62
1:H:352:ILE:CD1	1:H:386:LEU:HD13	2.30	0.62
1:G:299:ILE:HD13	1:G:326:TYR:HB3	1.82	0.62
1:B:46:PRO:HG3	1:B:291:TRP:CD2	2.36	0.61
1:B:356:GLU:O	1:B:359:ILE:HG12	1.99	0.61
1:A:118:ILE:HG22	1:A:169:LEU:HB3	1.81	0.61
1:F:65:THR:OG1	1:F:275:THR:HG22	2.00	0.61
1:A:39:ALA:CB	1:A:238:LYS:HE2	2.31	0.60
1:A:299:ILE:HD13	1:A:326:TYR:HB3	1.83	0.60
1:A:39:ALA:HB1	1:A:238:LYS:HE2	1.82	0.60
1:E:260:ARG:O	1:E:263:LYS:HG2	2.01	0.60
1:A:301:LYS:HD3	3:A:664:HOH:O	2.01	0.60
1:E:307:LYS:O	1:E:311:GLU:HG3	2.01	0.60
1:C:62:LEU:HD22	1:C:275:THR:HG21	1.82	0.60
1:B:352:ILE:CD1	1:B:386:LEU:HD13	2.31	0.60
1:F:260:ARG:O	1:F:263:LYS:HG2	2.01	0.59
1:F:299:ILE:HD13	1:F:326:TYR:HB3	1.85	0.59
1:A:263:LYS:HG3	1:A:264:SER:N	2.17	0.59
1:A:157:GLU:HG3	1:A:195:LYS:HE2	1.84	0.59
1:B:352:ILE:HD12	1:B:354:PHE:CE2	2.37	0.59
1:E:394:LYS:HB2	1:E:394:LYS:NZ	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:PRO:HG3	3:A:519:HOH:O	2.03	0.59
1:G:12:LYS:O	1:G:14:LEU:HD13	2.02	0.59
1:H:65:THR:HB	1:H:275:THR:HG22	1.84	0.59
1:H:60:THR:HG22	1:H:61:VAL:N	2.14	0.59
1:E:157:GLU:O	1:E:161:LYS:HD3	2.03	0.59
1:F:391:LYS:O	1:F:394:LYS:HG2	2.02	0.59
1:E:118:ILE:HG22	1:E:169:LEU:HB3	1.85	0.59
1:H:238:LYS:HD3	3:H:420:HOH:O	2.03	0.58
1:C:356:GLU:O	1:C:359:ILE:HG12	2.03	0.58
1:D:205:ILE:HD13	2:D:400:PLP:C5A	2.33	0.58
1:D:107:ARG:NE	1:D:268:THR:HG21	2.18	0.58
1:E:72:LYS:HB3	3:E:433:HOH:O	2.03	0.58
1:E:205:ILE:CD1	2:E:400:PLP:H5A1	2.29	0.58
1:G:255:PRO:O	1:G:259:GLU:HG3	2.03	0.58
1:D:290:LYS:HG2	3:D:726:HOH:O	2.02	0.58
1:A:11:ARG:HA	1:A:14:LEU:HD22	1.84	0.58
1:H:119:ILE:HD13	1:H:151:ILE:HD12	1.84	0.58
1:A:244:GLY:HA3	1:B:275:THR:HG23	1.84	0.58
1:G:122:VAL:HG22	1:G:123:TYR:N	2.18	0.57
1:H:82:ARG:HD2	3:H:517:HOH:O	2.04	0.57
1:H:104:ASN:HD21	1:H:265:ARG:N	2.02	0.57
1:A:91:TRP:CZ2	1:A:253:LYS:HG3	2.39	0.57
1:E:244:GLY:HA3	1:F:275:THR:HG23	1.85	0.57
1:C:39:ALA:CB	1:C:238:LYS:HE2	2.34	0.57
1:E:392:ASP:C	1:E:394:LYS:H	2.07	0.57
1:F:352:ILE:HG13	1:F:352:ILE:O	2.03	0.57
1:B:352:ILE:HD13	1:B:386:LEU:HD13	1.86	0.56
1:D:99:VAL:HB	1:D:100:PRO:HD3	1.86	0.56
1:D:60:THR:HG23	3:D:441:HOH:O	2.03	0.56
1:E:98:VAL:HG21	1:E:205:ILE:HD12	1.87	0.56
1:E:89:THR:HG22	3:E:433:HOH:O	2.04	0.56
1:G:88:GLN:HB2	1:G:91:TRP:CD1	2.40	0.56
1:B:122:VAL:HG22	1:B:123:TYR:N	2.19	0.56
1:E:219:PHE:O	1:E:222:ILE:HG12	2.04	0.56
1:E:268:THR:O	1:E:269:SER:CB	2.54	0.56
1:A:128:MET:O	1:A:132:ASN:HB2	2.05	0.56
1:H:46:PRO:HG3	1:H:291:TRP:CD2	2.40	0.56
1:G:268:THR:O	1:G:269:SER:CB	2.53	0.56
1:A:340:LYS:HG2	3:A:499:HOH:O	2.05	0.56
1:D:118:ILE:HG22	1:D:169:LEU:HB3	1.88	0.56
1:F:80:LYS:HE2	3:F:611:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:LEU:HD22	1:A:390:LEU:HG	1.86	0.55
1:G:394:LYS:HB2	1:G:394:LYS:NZ	2.21	0.55
1:E:119:ILE:HD13	1:E:151:ILE:HD12	1.88	0.55
1:E:39:ALA:HB1	1:E:238:LYS:HE2	1.87	0.55
1:A:268:THR:O	1:A:269:SER:HB2	2.07	0.55
1:F:391:LYS:O	1:F:394:LYS:HE2	2.07	0.55
1:E:62:LEU:H	1:F:45:ASN:ND2	1.97	0.55
1:B:299:ILE:HD13	1:B:326:TYR:HB3	1.89	0.55
1:C:99:VAL:HB	1:C:100:PRO:HD3	1.89	0.55
1:D:317:ILE:HD11	1:D:335:LEU:HD11	1.88	0.55
1:E:198:LEU:HD12	3:E:598:HOH:O	2.07	0.55
1:F:187:GLN:HE22	1:F:190:LYS:HZ1	1.55	0.55
1:A:213:GLY:HA3	3:A:588:HOH:O	2.06	0.54
1:E:299:ILE:HD13	1:E:326:TYR:HB3	1.88	0.54
1:E:206:HIS:HE1	2:E:400:PLP:O3	1.89	0.54
1:F:328:GLN:HB2	1:F:372:LEU:HD11	1.89	0.54
1:H:225:GLN:HG2	3:H:618:HOH:O	2.07	0.54
1:D:264:SER:O	1:D:268:THR:HG23	2.07	0.54
1:D:60:THR:HG22	1:D:61:VAL:N	2.22	0.54
1:F:288:CYS:HA	3:F:571:HOH:O	2.06	0.54
1:G:99:VAL:HB	1:G:100:PRO:HD3	1.89	0.54
1:E:122:VAL:HG22	1:E:123:TYR:N	2.22	0.54
1:H:86:ASP:HB3	3:H:633:HOH:O	2.06	0.54
1:E:12:LYS:O	1:E:14:LEU:HD13	2.08	0.54
1:A:99:VAL:HB	1:A:100:PRO:HD3	1.89	0.54
1:B:111:LYS:HD2	1:B:114:ASP:OD2	2.08	0.54
1:C:275:THR:HG23	1:C:276:LEU:N	2.22	0.54
1:C:11:ARG:HA	1:C:14:LEU:HD22	1.90	0.54
1:G:375:PRO:HB2	1:G:378:VAL:HG23	1.90	0.54
1:A:268:THR:O	1:A:269:SER:CB	2.56	0.54
1:D:65:THR:CB	1:D:275:THR:HG22	2.37	0.53
1:C:206:HIS:HE1	2:C:400:PLP:O3	1.91	0.53
1:G:62:LEU:CD2	1:G:275:THR:HG21	2.38	0.53
1:B:60:THR:HG22	1:B:61:VAL:N	2.22	0.53
1:D:111:LYS:HE3	3:D:434:HOH:O	2.08	0.53
1:C:67:PRO:HG3	1:C:278:TYR:CE2	2.42	0.53
1:D:205:ILE:CD1	2:D:400:PLP:H5A1	2.38	0.53
1:E:320:PRO:HG3	3:E:565:HOH:O	2.09	0.53
1:B:206:HIS:HE1	2:B:400:PLP:O3	1.91	0.53
1:D:191:ASP:O	1:D:195:LYS:HG3	2.08	0.53
1:D:50:ILE:O	1:D:54:LYS:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:LYS:CD	1:E:163:LYS:H	1.91	0.53
1:E:268:THR:O	1:E:269:SER:HB2	2.08	0.53
1:G:11:ARG:HA	1:G:14:LEU:HD22	1.89	0.53
1:E:39:ALA:CB	1:E:238:LYS:HE2	2.39	0.53
1:A:163:LYS:CD	1:A:163:LYS:H	1.92	0.52
1:G:62:LEU:H	1:H:45:ASN:ND2	2.04	0.52
1:H:307:LYS:O	1:H:311:GLU:HG3	2.09	0.52
1:F:62:LEU:HA	1:F:275:THR:HG21	1.91	0.52
1:G:18:LYS:HB2	1:G:38:VAL:HB	1.91	0.52
1:A:394:LYS:NZ	1:A:394:LYS:HB2	2.23	0.52
1:H:388:LYS:HD2	3:H:623:HOH:O	2.10	0.52
1:A:205:ILE:HD13	2:A:400:PLP:H5A1	1.92	0.52
1:C:145:LYS:HE3	1:C:146:ASP:OD1	2.09	0.52
1:D:206:HIS:HE1	2:D:400:PLP:O3	1.92	0.52
1:E:311:GLU:O	1:E:315:PRO:HG3	2.10	0.52
1:G:238:LYS:HD3	3:H:569:HOH:O	2.09	0.52
1:B:65:THR:HG1	1:B:275:THR:HG22	1.73	0.52
1:D:65:THR:HG1	1:D:275:THR:HG22	1.74	0.52
1:F:99:VAL:HB	1:F:100:PRO:HD3	1.92	0.52
1:D:247:MET:HE2	1:D:274:THR:HG23	1.91	0.52
1:H:11:ARG:HA	1:H:14:LEU:HD12	1.91	0.52
1:H:352:ILE:HD11	1:H:386:LEU:HD13	1.93	0.51
1:G:155:LYS:O	1:G:159:LEU:HG	2.09	0.51
1:H:122:VAL:HG22	1:H:123:TYR:N	2.26	0.51
1:H:206:HIS:HE1	2:H:400:PLP:O3	1.94	0.51
1:H:352:ILE:HD13	1:H:386:LEU:HD13	1.93	0.51
1:D:352:ILE:HG13	1:D:352:ILE:O	2.10	0.51
1:B:119:ILE:HD13	1:B:151:ILE:HD12	1.93	0.51
1:D:18:LYS:HB2	1:D:38:VAL:HB	1.92	0.51
3:E:648:HOH:O	1:F:60:THR:HG21	2.11	0.51
1:F:80:LYS:CE	3:F:611:HOH:O	2.59	0.51
1:H:340:LYS:HG2	3:H:684:HOH:O	2.10	0.51
1:G:268:THR:O	1:G:269:SER:HB2	2.11	0.51
1:D:145:LYS:HG3	1:D:145:LYS:O	2.11	0.50
1:H:172:SER:O	1:H:204:GLU:HA	2.11	0.50
1:B:99:VAL:HB	1:B:100:PRO:HD3	1.93	0.50
1:F:352:ILE:HD12	1:F:354:PHE:CE2	2.46	0.50
1:D:299:ILE:HD13	1:D:326:TYR:HB3	1.93	0.50
1:F:219:PHE:O	1:F:222:ILE:HG12	2.11	0.50
1:H:212:PRO:HG2	3:H:427:HOH:O	2.10	0.50
1:A:11:ARG:HD3	1:B:61:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:67:PRO:HG3	1:G:278:TYR:HE2	1.74	0.50
1:E:108:GLU:OE2	1:E:260:ARG:HD2	2.11	0.50
3:E:415:HOH:O	1:F:238:LYS:HD3	2.12	0.50
1:G:118:ILE:HG22	1:G:169:LEU:HB3	1.93	0.50
1:H:247:MET:CE	1:H:274:THR:HG23	2.41	0.50
1:E:151:ILE:HB	1:E:153:PHE:CE1	2.46	0.49
1:B:162:ASP:HB3	1:B:165:ASN:ND2	2.27	0.49
1:D:356:GLU:O	1:D:359:ILE:HG12	2.13	0.49
1:D:46:PRO:HG3	1:D:291:TRP:CD2	2.47	0.49
1:G:47:PRO:O	1:G:51:GLU:HG3	2.13	0.49
1:H:37:SER:HB2	1:H:355:ASP:OD1	2.11	0.49
1:C:122:VAL:HG22	1:C:123:TYR:N	2.27	0.49
1:B:352:ILE:HG13	1:B:352:ILE:O	2.11	0.49
1:G:318:LYS:HD2	3:G:470:HOH:O	2.12	0.49
1:B:41:MET:HG2	1:B:373:ALA:CB	2.43	0.49
1:E:46:PRO:HG3	1:E:291:TRP:CE3	2.47	0.49
1:F:350:ALA:O	1:F:385:ARG:HD2	2.12	0.49
1:G:205:ILE:CD1	2:G:400:PLP:H5A1	2.42	0.49
1:G:62:LEU:HD22	1:G:275:THR:HG21	1.95	0.49
1:B:41:MET:HG2	1:B:373:ALA:HB1	1.94	0.49
1:D:104:ASN:ND2	1:D:107:ARG:HH21	2.07	0.49
1:B:342:MET:O	1:B:346:MET:HG2	2.13	0.49
1:D:238:LYS:HD2	3:D:444:HOH:O	2.13	0.49
1:E:328:GLN:HB2	1:E:372:LEU:HD11	1.95	0.49
1:E:392:ASP:C	1:E:394:LYS:N	2.66	0.48
1:E:385:ARG:HD3	3:E:583:HOH:O	2.12	0.48
1:H:315:PRO:O	1:H:318:LYS:HE2	2.13	0.48
1:H:350:ALA:O	1:H:385:ARG:HD2	2.12	0.48
1:H:60:THR:CG2	1:H:61:VAL:H	2.22	0.48
1:A:122:VAL:HG22	1:A:123:TYR:N	2.28	0.48
1:D:303:GLN:HB3	1:D:372:LEU:HD13	1.95	0.48
1:E:172:SER:O	1:E:204:GLU:HA	2.14	0.48
1:G:17:LEU:HD12	3:G:702:HOH:O	2.13	0.48
1:G:205:ILE:HD13	2:G:400:PLP:H5A1	1.96	0.48
1:E:12:LYS:HG2	1:E:13:ASN:ND2	2.28	0.48
1:E:72:LYS:HE2	3:E:577:HOH:O	2.13	0.48
1:C:17:LEU:HD22	3:C:562:HOH:O	2.14	0.48
1:C:268:THR:O	1:C:269:SER:CB	2.60	0.48
1:H:123:TYR:CG	1:H:125:PRO:HD2	2.48	0.48
1:A:123:TYR:CZ	1:A:125:PRO:HG2	2.49	0.48
1:A:62:LEU:H	1:B:45:ASN:ND2	2.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:PHE:HD2	1:D:267:ALA:O	1.96	0.48
1:G:162:ASP:HB3	1:G:165:ASN:ND2	2.29	0.48
1:G:275:THR:HG22	1:H:244:GLY:O	2.13	0.48
1:E:18:LYS:HD3	1:E:38:VAL:HB	1.96	0.48
1:F:122:VAL:HG22	1:F:123:TYR:N	2.29	0.48
1:D:123:TYR:CG	1:D:125:PRO:HD2	2.49	0.47
1:E:246:GLY:HA2	3:E:530:HOH:O	2.13	0.47
1:C:317:ILE:HD13	1:C:332:PHE:CE2	2.48	0.47
1:B:187:GLN:HE22	1:B:190:LYS:HZ3	1.62	0.47
1:C:163:LYS:N	1:C:163:LYS:CD	2.64	0.47
1:F:356:GLU:O	1:F:359:ILE:HG12	2.14	0.47
1:E:11:ARG:HD3	1:F:61:VAL:HB	1.96	0.47
1:H:352:ILE:HG13	1:H:352:ILE:O	2.15	0.47
1:E:246:GLY:CA	3:E:530:HOH:O	2.62	0.47
1:H:18:LYS:HB2	1:H:38:VAL:HB	1.96	0.47
1:A:69:GLU:O	1:A:73:LYS:HG3	2.15	0.47
1:C:205:ILE:CD1	2:C:400:PLP:H5A1	2.41	0.47
1:E:263:LYS:HG3	1:E:264:SER:N	2.30	0.47
1:C:118:ILE:HG22	1:C:169:LEU:HB3	1.95	0.47
1:F:187:GLN:NE2	1:F:190:LYS:NZ	2.61	0.47
1:B:119:ILE:HG22	1:B:142:LEU:HG	1.97	0.47
1:A:162:ASP:HB3	1:A:165:ASN:ND2	2.30	0.47
1:D:122:VAL:HG22	1:D:123:TYR:N	2.28	0.47
1:D:123:TYR:CZ	1:D:125:PRO:HG2	2.50	0.47
1:E:116:VAL:HB	1:E:130:ILE:HD13	1.97	0.47
1:E:193:VAL:HA	3:E:598:HOH:O	2.15	0.47
1:C:123:TYR:CD2	1:C:125:PRO:HD2	2.49	0.47
1:G:352:ILE:O	1:G:352:ILE:HG23	2.15	0.47
1:A:219:PHE:O	1:A:222:ILE:HG12	2.16	0.46
1:C:276:LEU:HD12	1:D:276:LEU:CD1	2.44	0.46
1:E:131:LYS:HE3	1:E:131:LYS:HB2	1.79	0.46
1:H:138:ILE:HG13	1:H:165:ASN:OD1	2.15	0.46
1:H:118:ILE:HG22	1:H:169:LEU:HB3	1.96	0.46
1:A:120:THR:HB	1:A:121:PRO:HA	1.96	0.46
1:A:274:THR:HG21	3:A:697:HOH:O	2.15	0.46
1:A:392:ASP:O	1:A:394:LYS:HG3	2.15	0.46
1:G:317:ILE:HD13	1:G:332:PHE:CE2	2.49	0.46
1:A:254:ASN:OD1	1:A:256:ASP:HB2	2.16	0.46
1:B:205:ILE:HD12	1:B:235:ALA:HB3	1.96	0.46
1:D:195:LYS:HE2	3:D:708:HOH:O	2.16	0.46
1:D:247:MET:CE	1:D:274:THR:HG23	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:352:ILE:HG23	1:E:352:ILE:O	2.14	0.46
1:G:39:ALA:HB1	1:G:238:LYS:HE2	1.96	0.46
1:H:123:TYR:CZ	1:H:125:PRO:HG2	2.50	0.46
1:D:348:HIS:HD2	3:D:744:HOH:O	1.97	0.46
1:E:356:GLU:O	1:E:359:ILE:HG12	2.14	0.46
1:G:206:HIS:HE1	2:G:400:PLP:O3	1.99	0.46
1:G:51:GLU:HG2	3:G:573:HOH:O	2.16	0.46
1:A:172:SER:O	1:A:204:GLU:HA	2.16	0.46
1:B:317:ILE:HD13	1:B:332:PHE:CE2	2.50	0.46
1:F:119:ILE:HD13	1:F:151:ILE:HD12	1.97	0.46
1:G:46:PRO:HG3	1:G:291:TRP:CE3	2.50	0.46
1:F:73:LYS:HG2	3:F:612:HOH:O	2.15	0.46
1:F:78:TRP:CE2	1:F:82:ARG:HG3	2.51	0.46
1:G:224:GLU:OE1	1:G:224:GLU:HA	2.16	0.46
1:G:356:GLU:O	1:G:359:ILE:HG12	2.15	0.46
1:F:118:ILE:HG22	1:F:169:LEU:HB3	1.97	0.46
1:A:41:MET:HG2	1:A:373:ALA:HB1	1.97	0.45
1:B:111:LYS:HD2	1:B:114:ASP:CG	2.37	0.45
1:C:394:LYS:HB2	1:C:394:LYS:NZ	2.31	0.45
1:F:392:ASP:O	1:F:394:LYS:HG3	2.16	0.45
1:D:224:GLU:HG3	3:D:618:HOH:O	2.16	0.45
1:E:301:LYS:HG3	3:E:631:HOH:O	2.16	0.45
1:E:18:LYS:HB2	1:E:38:VAL:HB	1.97	0.45
1:C:237:SER:HA	1:C:242:ILE:HG13	1.98	0.45
1:A:260:ARG:O	1:A:263:LYS:CG	2.64	0.45
1:A:17:LEU:HD21	1:B:65:THR:C	2.37	0.45
1:A:67:PRO:HG3	1:A:278:TYR:HE2	1.79	0.45
1:C:123:TYR:CG	1:C:125:PRO:HD2	2.52	0.45
1:B:205:ILE:HD11	1:B:235:ALA:HB3	1.99	0.45
1:C:62:LEU:H	1:D:45:ASN:ND2	2.01	0.45
1:E:119:ILE:HG22	1:E:142:LEU:HG	1.99	0.45
1:F:119:ILE:HG22	1:F:142:LEU:HG	1.99	0.45
1:F:339:HIS:HB3	1:F:365:ILE:HG23	1.98	0.45
1:A:356:GLU:O	1:A:359:ILE:HG12	2.17	0.45
1:B:307:LYS:HE2	3:B:498:HOH:O	2.16	0.45
1:B:328:GLN:HB2	1:B:372:LEU:HD11	1.98	0.45
1:G:107:ARG:CZ	1:G:107:ARG:HB2	2.46	0.45
1:E:123:TYR:CG	1:E:125:PRO:HD2	2.51	0.45
1:D:108:GLU:HB2	1:D:264:SER:HB2	1.99	0.44
1:C:61:VAL:HG11	1:D:241:ASN:HD21	1.82	0.44
1:C:62:LEU:HD13	1:D:245:MET:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:344:GLU:OE2	1:H:348:HIS:ND1	2.50	0.44
1:A:172:SER:HA	1:A:173:PRO:C	2.36	0.44
1:A:307:LYS:O	1:A:311:GLU:HG3	2.17	0.44
1:B:303:GLN:HB3	1:B:372:LEU:HD13	1.99	0.44
1:C:18:LYS:HB2	1:C:38:VAL:HB	1.99	0.44
1:F:145:LYS:HD3	3:F:574:HOH:O	2.16	0.44
1:F:315:PRO:O	1:F:318:LYS:HE3	2.17	0.44
1:A:205:ILE:HD12	2:A:400:PLP:H5A1	1.98	0.44
1:C:145:LYS:HG2	3:C:686:HOH:O	2.16	0.44
1:A:119:ILE:HG22	1:A:142:LEU:HG	2.00	0.44
1:D:352:ILE:HD12	1:D:354:PHE:CZ	2.53	0.44
1:E:205:ILE:HD13	2:E:400:PLP:C5A	2.36	0.44
1:E:386:LEU:CD2	1:E:390:LEU:HG	2.45	0.44
1:F:76:LYS:HA	1:F:87:ILE:HD11	1.98	0.44
1:A:265:ARG:NH2	3:A:620:HOH:O	2.50	0.44
1:G:260:ARG:HA	1:G:263:LYS:CD	2.46	0.44
1:D:44:LYS:HD2	3:D:424:HOH:O	2.17	0.44
1:F:60:THR:HG22	1:F:61:VAL:H	1.81	0.44
1:G:128:MET:O	1:G:132:ASN:HB2	2.18	0.44
1:F:205:ILE:HD12	1:F:235:ALA:HB3	1.98	0.44
1:C:347:ILE:HG23	1:C:353:PHE:CE2	2.53	0.44
1:D:83:HIS:HE1	1:D:208:ASP:OD1	2.00	0.44
1:E:193:VAL:HG12	1:E:229:LYS:HE3	2.00	0.44
1:F:172:SER:O	1:F:204:GLU:HA	2.18	0.44
1:G:172:SER:O	1:G:204:GLU:HA	2.18	0.44
1:G:338:ASP:OD2	1:G:341:ALA:HB3	2.18	0.44
1:G:62:LEU:HD13	1:H:245:MET:CG	2.47	0.44
1:G:61:VAL:CG1	1:H:241:ASN:HD21	2.31	0.44
1:C:345:PHE:O	1:C:349:LYS:HB2	2.17	0.43
1:C:328:GLN:HB2	1:C:372:LEU:HD11	1.99	0.43
1:H:124:TYR:CD1	1:H:125:PRO:HD3	2.53	0.43
1:H:188:LYS:HG2	3:H:417:HOH:O	2.17	0.43
1:G:45:ASN:ND2	1:H:62:LEU:H	2.01	0.43
1:A:41:MET:HB2	1:A:241:ASN:ND2	2.33	0.43
1:B:123:TYR:CZ	1:B:125:PRO:HG2	2.54	0.43
1:B:352:ILE:HD11	1:B:386:LEU:HD13	1.99	0.43
1:C:119:ILE:HG22	1:C:142:LEU:HG	2.00	0.43
1:E:123:TYR:CZ	1:E:125:PRO:HG2	2.53	0.43
1:E:122:VAL:HG22	1:E:123:TYR:H	1.83	0.43
1:G:122:VAL:O	1:G:123:TYR:C	2.57	0.43
1:C:187:GLN:NE2	1:C:190:LYS:CE	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:GLU:HG2	1:D:161:LYS:HZ2	1.82	0.43
1:G:55:LYS:O	1:G:59:GLU:HG3	2.19	0.43
1:H:394:LYS:HD2	3:H:668:HOH:O	2.18	0.43
1:A:265:ARG:O	1:A:268:THR:O	2.36	0.43
1:D:11:ARG:HA	1:D:14:LEU:HD12	1.99	0.43
1:D:391:LYS:O	1:D:394:LYS:HG3	2.18	0.43
1:F:263:LYS:HG3	1:F:264:SER:N	2.33	0.43
1:H:219:PHE:O	1:H:222:ILE:HG12	2.19	0.43
1:H:247:MET:HE2	1:H:274:THR:HG23	1.99	0.43
1:C:267:ALA:HA	1:D:103:PHE:CE2	2.52	0.43
1:E:394:LYS:HB2	1:E:394:LYS:HZ3	1.81	0.43
1:E:89:THR:HA	3:E:433:HOH:O	2.17	0.43
1:D:107:ARG:HE	1:D:268:THR:HG21	1.84	0.43
1:D:37:SER:HB2	1:D:355:ASP:OD1	2.19	0.43
1:A:392:ASP:C	1:A:394:LYS:N	2.72	0.43
1:B:201:TRP:HB3	1:B:233:PHE:HE1	1.84	0.43
1:E:192:ILE:HG22	3:E:598:HOH:O	2.19	0.43
1:H:233:PHE:HD2	1:H:250:ILE:HD12	1.82	0.43
1:C:265:ARG:HD3	1:C:270:GLY:C	2.39	0.43
1:E:260:ARG:HA	1:E:263:LYS:HG2	1.99	0.43
1:F:204:GLU:OE1	1:F:216:HIS:HE1	2.02	0.43
1:H:183:LYS:HG2	1:H:217:THR:HG21	2.00	0.43
1:F:205:ILE:HD11	1:F:235:ALA:HB3	1.99	0.43
1:A:124:TYR:CG	1:A:125:PRO:HD3	2.53	0.43
1:C:206:HIS:HD2	3:C:415:HOH:O	2.02	0.43
1:E:143:LEU:O	1:E:149:TYR:HA	2.19	0.43
1:G:119:ILE:HD12	1:G:170:PHE:CE1	2.54	0.43
1:C:123:TYR:CZ	1:C:125:PRO:HG2	2.54	0.42
1:E:11:ARG:NH2	1:E:40:ASP:OD2	2.48	0.42
1:F:274:THR:O	1:F:274:THR:HG23	2.19	0.42
1:H:98:VAL:HG21	1:H:205:ILE:HD13	2.00	0.42
1:H:80:LYS:CE	3:H:566:HOH:O	2.62	0.42
1:B:123:TYR:CG	1:B:125:PRO:HD2	2.54	0.42
1:F:200:LEU:O	1:F:230:THR:HA	2.20	0.42
1:F:350:ALA:O	1:F:385:ARG:CD	2.67	0.42
1:G:123:TYR:CG	1:G:125:PRO:HD2	2.54	0.42
1:G:116:VAL:HB	1:G:130:ILE:HD13	2.01	0.42
1:H:339:HIS:HB2	1:H:358:TYR:CD2	2.55	0.42
1:A:183:LYS:O	1:A:187:GLN:HG2	2.20	0.42
1:A:394:LYS:HZ2	1:A:394:LYS:HB2	1.84	0.42
1:C:265:ARG:O	1:C:268:THR:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:PRO:HG3	1:C:291:TRP:CD2	2.55	0.42
1:C:103:PHE:CD2	1:D:267:ALA:O	2.73	0.42
1:D:350:ALA:O	1:D:385:ARG:HD2	2.18	0.42
1:C:348:HIS:HD2	3:C:657:HOH:O	2.01	0.42
1:H:145:LYS:HG3	1:H:145:LYS:O	2.20	0.42
1:B:393:LEU:O	1:B:394:LYS:HB2	2.19	0.42
1:C:107:ARG:HD3	3:C:435:HOH:O	2.20	0.42
1:C:263:LYS:HE3	1:C:263:LYS:HB2	1.87	0.42
1:E:265:ARG:NE	3:E:536:HOH:O	2.53	0.42
1:F:266:ASP:HA	1:F:270:GLY:HA2	2.01	0.42
1:H:254:ASN:HA	1:H:255:PRO:HD3	1.90	0.42
1:A:131:LYS:HB2	1:A:131:LYS:HE3	1.81	0.42
1:A:352:ILE:O	1:A:352:ILE:HG23	2.20	0.42
1:D:122:VAL:O	1:D:123:TYR:C	2.58	0.42
1:G:266:ASP:HA	1:G:270:GLY:HA2	2.01	0.42
1:G:272:PRO:HG3	3:G:557:HOH:O	2.20	0.42
1:A:157:GLU:O	1:A:161:LYS:HD3	2.19	0.42
1:A:237:SER:HA	1:A:242:ILE:HG13	2.01	0.42
1:B:355:ASP:O	1:B:356:GLU:C	2.57	0.42
1:C:187:GLN:NE2	1:C:190:LYS:HE3	2.35	0.42
1:C:56:TYR:CD1	1:C:279:LYS:HG2	2.55	0.42
1:G:260:ARG:O	1:G:263:LYS:CG	2.67	0.42
1:H:111:LYS:HD2	1:H:114:ASP:CG	2.40	0.42
1:H:122:VAL:O	1:H:123:TYR:C	2.59	0.42
1:H:393:LEU:O	1:H:394:LYS:C	2.58	0.42
1:B:46:PRO:HG3	1:B:291:TRP:CE3	2.55	0.42
1:D:205:ILE:HD11	1:D:237:SER:OG	2.20	0.42
1:E:11:ARG:NH2	1:E:18:LYS:HE2	2.35	0.42
1:E:303:GLN:HB3	1:E:372:LEU:HD13	2.00	0.42
1:G:254:ASN:HA	1:G:255:PRO:HD3	1.91	0.42
1:H:103:PHE:CZ	1:H:129:ALA:HA	2.55	0.42
1:A:85:TRP:CD2	1:A:218:VAL:HG11	2.55	0.41
1:B:219:PHE:O	1:B:222:ILE:HG12	2.19	0.41
1:A:17:LEU:H	1:A:17:LEU:HD22	1.85	0.41
1:A:328:GLN:HB3	1:A:370:ILE:HG22	2.02	0.41
1:E:103:PHE:CZ	1:E:129:ALA:HA	2.55	0.41
1:E:272:PRO:HD3	3:E:536:HOH:O	2.18	0.41
1:F:238:LYS:HD2	1:F:238:LYS:HA	1.95	0.41
1:G:124:TYR:CG	1:G:125:PRO:HD3	2.55	0.41
1:H:300:ASP:O	1:H:303:GLN:HG2	2.20	0.41
1:B:138:ILE:HG13	1:B:165:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:454:HOH:O	1:B:238:LYS:HD3	2.20	0.41
1:G:103:PHE:CZ	1:G:129:ALA:HA	2.56	0.41
1:G:223:ASP:OD1	1:G:225:GLN:HB2	2.20	0.41
1:A:271:MET:HA	1:A:272:PRO:HD3	1.94	0.41
1:C:12:LYS:HE2	1:C:13:ASN:ND2	2.35	0.41
1:D:131:LYS:HB2	1:D:137:ILE:HD11	2.02	0.41
1:G:111:LYS:HG2	1:G:114:ASP:OD1	2.20	0.41
1:H:124:TYR:CE2	1:H:359:ILE:HD12	2.56	0.41
1:A:123:TYR:CG	1:A:125:PRO:HD2	2.54	0.41
1:E:122:VAL:O	1:E:123:TYR:C	2.57	0.41
1:F:46:PRO:HG3	1:F:291:TRP:CE3	2.56	0.41
1:G:172:SER:HA	1:G:173:PRO:C	2.41	0.41
1:D:111:LYS:HD2	1:D:114:ASP:OD2	2.20	0.41
1:E:124:TYR:CG	1:E:125:PRO:HD3	2.56	0.41
1:A:119:ILE:HD12	1:A:170:PHE:CE1	2.56	0.41
1:B:204:GLU:OE1	1:B:216:HIS:HE1	2.04	0.41
1:C:290:LYS:HG2	3:C:626:HOH:O	2.21	0.41
1:C:386:LEU:HD22	1:C:390:LEU:CG	2.47	0.41
1:B:124:TYR:CG	1:B:125:PRO:HD3	2.55	0.41
1:G:338:ASP:OD2	1:G:341:ALA:CB	2.69	0.41
1:A:13:ASN:O	1:A:14:LEU:HD12	2.20	0.41
1:A:206:HIS:HE1	2:A:400:PLP:O3	2.04	0.41
1:C:268:THR:O	1:C:268:THR:OG1	2.35	0.41
1:E:163:LYS:CD	1:E:163:LYS:N	2.68	0.41
1:E:69:GLU:O	1:E:73:LYS:HG3	2.20	0.41
1:F:51:GLU:HG2	3:F:758:HOH:O	2.20	0.41
1:A:275:THR:HG23	1:A:276:LEU:N	2.36	0.41
1:C:131:LYS:HE3	1:C:131:LYS:HB2	1.87	0.41
1:D:353:PHE:CD1	1:D:353:PHE:N	2.88	0.41
1:F:119:ILE:O	1:F:122:VAL:HB	2.21	0.41
1:G:138:ILE:HG13	1:G:165:ASN:OD1	2.20	0.41
1:H:356:GLU:OE2	1:H:368:GLU:OE1	2.38	0.41
1:B:254:ASN:HA	1:B:255:PRO:HD3	1.93	0.41
1:E:345:PHE:O	1:E:349:LYS:HB2	2.20	0.41
1:H:131:LYS:HB2	1:H:137:ILE:HD11	2.03	0.41
1:H:237:SER:HA	1:H:242:ILE:HG13	2.03	0.41
1:A:122:VAL:O	1:A:123:TYR:C	2.60	0.40
1:A:103:PHE:CZ	1:A:129:ALA:HA	2.56	0.40
1:C:172:SER:O	1:C:204:GLU:HA	2.21	0.40
1:C:203:ASP:OD1	2:C:400:PLP:N1	2.54	0.40
1:C:85:TRP:CD2	1:C:218:VAL:HG11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HB3	1:C:3:TYR:CE2	2.56	0.40
1:D:121:PRO:HG3	1:D:363:GLY:HA3	2.03	0.40
1:G:122:VAL:CG2	1:G:123:TYR:N	2.84	0.40
1:G:124:TYR:CD1	1:G:125:PRO:HD3	2.56	0.40
1:H:318:LYS:N	1:H:318:LYS:HD2	2.36	0.40
1:H:394:LYS:HB2	3:H:668:HOH:O	2.21	0.40
1:G:260:ARG:HA	1:G:263:LYS:HG2	2.03	0.40
1:A:124:TYR:CD1	1:A:125:PRO:HD3	2.56	0.40
1:E:46:PRO:HG3	1:E:291:TRP:CE2	2.57	0.40
1:F:225:GLN:HG2	3:F:667:HOH:O	2.21	0.40
1:H:49:LEU:HA	1:H:283:ILE:HG21	2.03	0.40
1:C:260:ARG:O	1:C:263:LYS:HG2	2.21	0.40
1:E:120:THR:HB	1:E:121:PRO:HA	2.03	0.40
1:E:46:PRO:HA	1:E:47:PRO:HD3	1.97	0.40
1:G:52:GLY:HA3	1:G:283:ILE:HD13	2.04	0.40
1:A:55:LYS:O	1:A:59:GLU:HG3	2.21	0.40
1:E:276:LEU:CD1	1:F:276:LEU:HD12	2.52	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	392/399 (98%)	378 (96%)	12 (3%)	2 (0%)	31	20
1	B	392/399 (98%)	375 (96%)	17 (4%)	0	100	100
1	C	392/399 (98%)	378 (96%)	14 (4%)	0	100	100
1	D	392/399 (98%)	378 (96%)	13 (3%)	1 (0%)	43	33
1	E	392/399 (98%)	377 (96%)	14 (4%)	1 (0%)	43	33
1	F	392/399 (98%)	383 (98%)	9 (2%)	0	100	100
1	G	392/399 (98%)	384 (98%)	7 (2%)	1 (0%)	43	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	392/399 (98%)	376 (96%)	15 (4%)	1 (0%)	43	33
All	All	3136/3192 (98%)	3029 (97%)	101 (3%)	6 (0%)	49	40

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	269	SER
1	G	269	SER
1	H	246	GLY
1	A	269	SER
1	D	246	GLY
1	A	246	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	353/358 (99%)	343 (97%)	10 (3%)	47	39
1	B	353/358 (99%)	344 (98%)	9 (2%)	50	43
1	C	353/358 (99%)	345 (98%)	8 (2%)	53	47
1	D	353/358 (99%)	340 (96%)	13 (4%)	37	27
1	E	353/358 (99%)	344 (98%)	9 (2%)	50	43
1	F	353/358 (99%)	344 (98%)	9 (2%)	50	43
1	G	353/358 (99%)	342 (97%)	11 (3%)	43	34
1	H	353/358 (99%)	342 (97%)	11 (3%)	43	34
All	All	2824/2864 (99%)	2744 (97%)	80 (3%)	47	39

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	163	LYS

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Mol	Chain	Res	Type
1	A	176	PRO
1	A	207	PHE
1	A	219	PHE
1	A	256	ASP
1	A	265	ARG
1	A	274	THR
1	A	355	ASP
1	A	386	LEU
1	B	104	ASN
1	B	111	LYS
1	B	146	ASP
1	B	176	PRO
1	B	207	PHE
1	B	219	PHE
1	B	238	LYS
1	B	318	LYS
1	B	355	ASP
1	C	17	LEU
1	C	163	LYS
1	C	176	PRO
1	C	199	MET
1	C	207	PHE
1	C	219	PHE
1	C	355	ASP
1	C	386	LEU
1	D	60	THR
1	D	111	LYS
1	D	146	ASP
1	D	176	PRO
1	D	184	ASP
1	D	207	PHE
1	D	219	PHE
1	D	238	LYS
1	D	245	MET
1	D	269	SER
1	D	274	THR
1	D	318	LYS
1	D	355	ASP
1	E	28	GLU
1	E	163	LYS
1	E	176	PRO
1	E	197	ASP

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Mol	Chain	Res	Type
1	E	207	PHE
1	E	219	PHE
1	E	265	ARG
1	E	355	ASP
1	E	386	LEU
1	F	60	THR
1	F	104	ASN
1	F	111	LYS
1	F	146	ASP
1	F	176	PRO
1	F	207	PHE
1	F	219	PHE
1	F	238	LYS
1	F	355	ASP
1	G	28	GLU
1	G	163	LYS
1	G	176	PRO
1	G	184	ASP
1	G	207	PHE
1	G	219	PHE
1	G	265	ARG
1	G	275	THR
1	G	355	ASP
1	G	385	ARG
1	G	386	LEU
1	H	60	THR
1	H	104	ASN
1	H	111	LYS
1	H	176	PRO
1	H	207	PHE
1	H	219	PHE
1	H	238	LYS
1	H	274	THR
1	H	318	LYS
1	H	326	TYR
1	H	355	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	45	ASN

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Mol	Chain	Res	Type
1	A	187	GLN
1	A	206	HIS
1	A	216	HIS
1	B	25	GLN
1	B	45	ASN
1	B	104	ASN
1	B	187	GLN
1	B	206	HIS
1	B	216	HIS
1	C	13	ASN
1	C	25	GLN
1	C	45	ASN
1	C	83	HIS
1	C	187	GLN
1	C	206	HIS
1	C	216	HIS
1	C	348	HIS
1	D	25	GLN
1	D	45	ASN
1	D	83	HIS
1	D	104	ASN
1	D	187	GLN
1	D	206	HIS
1	D	216	HIS
1	D	348	HIS
1	E	13	ASN
1	E	25	GLN
1	E	45	ASN
1	E	187	GLN
1	E	206	HIS
1	E	216	HIS
1	F	25	GLN
1	F	45	ASN
1	F	104	ASN
1	F	187	GLN
1	F	206	HIS
1	F	216	HIS
1	G	25	GLN
1	G	45	ASN
1	G	83	HIS
1	G	187	GLN
1	G	206	HIS

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Mol	Chain	Res	Type
1	G	216	HIS
1	H	45	ASN
1	H	83	HIS
1	H	104	ASN
1	H	187	GLN
1	H	206	HIS
1	H	216	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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
2	PLP	A	400	1	15,15,16	3.52	4 (26%)	20,22,23	2.88	8 (40%)
2	PLP	B	400	1	15,15,16	3.50	5 (33%)	20,22,23	2.39	9 (45%)
2	PLP	C	400	1	15,15,16	3.46	5 (33%)	20,22,23	2.59	10 (50%)
2	PLP	D	400	1	15,15,16	3.54	5 (33%)	20,22,23	2.83	10 (50%)
2	PLP	E	400	1	15,15,16	3.52	5 (33%)	20,22,23	2.70	9 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PLP	F	400	1	15,15,16	3.49	4 (26%)	20,22,23	2.45	8 (40%)
2	PLP	G	400	1	15,15,16	3.31	4 (26%)	20,22,23	2.41	8 (40%)
2	PLP	H	400	1	15,15,16	3.43	5 (33%)	20,22,23	2.48	8 (40%)

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	400	1	-	0/6/6/8	0/1/1/1
2	PLP	B	400	1	-	0/6/6/8	0/1/1/1
2	PLP	C	400	1	-	0/6/6/8	0/1/1/1
2	PLP	D	400	1	-	0/6/6/8	0/1/1/1
2	PLP	E	400	1	-	0/6/6/8	0/1/1/1
2	PLP	F	400	1	-	0/6/6/8	0/1/1/1
2	PLP	G	400	1	-	0/6/6/8	0/1/1/1
2	PLP	H	400	1	-	0/6/6/8	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	PLP	C4A-C4	-2.48	1.46	1.51
2	A	400	PLP	C4A-C4	-2.46	1.46	1.51
2	H	400	PLP	C4A-C4	-2.45	1.46	1.51
2	E	400	PLP	C4A-C4	-2.38	1.46	1.51
2	D	400	PLP	C4A-C4	-2.37	1.46	1.51
2	D	400	PLP	O4P-C5A	-2.29	1.36	1.44
2	B	400	PLP	P-O3P	-2.15	1.46	1.54
2	F	400	PLP	C4A-C4	-2.10	1.47	1.51
2	G	400	PLP	C4A-C4	-2.10	1.47	1.51
2	C	400	PLP	C4A-C4	-2.08	1.47	1.51
2	E	400	PLP	P-O3P	-2.06	1.46	1.54
2	C	400	PLP	P-O3P	-2.05	1.46	1.54
2	H	400	PLP	C6-N1	2.02	1.38	1.34
2	F	400	PLP	C2-N1	2.97	1.39	1.33
2	G	400	PLP	C2-N1	3.01	1.39	1.33
2	E	400	PLP	C2-N1	3.18	1.40	1.33
2	H	400	PLP	C2-N1	3.36	1.40	1.33
2	C	400	PLP	C2-N1	3.39	1.40	1.33
2	B	400	PLP	C2-N1	3.48	1.40	1.33
2	A	400	PLP	C2-N1	3.70	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	PLP	C2-N1	4.12	1.42	1.33
2	C	400	PLP	C5-C4	7.83	1.49	1.40
2	H	400	PLP	C5-C4	7.91	1.49	1.40
2	G	400	PLP	C5-C4	7.94	1.49	1.40
2	B	400	PLP	C5-C4	8.26	1.50	1.40
2	D	400	PLP	C5-C4	8.33	1.50	1.40
2	A	400	PLP	C5-C4	8.35	1.50	1.40
2	E	400	PLP	C5-C4	8.37	1.50	1.40
2	F	400	PLP	C5-C4	8.48	1.50	1.40
2	G	400	PLP	C3-C2	8.67	1.46	1.40
2	H	400	PLP	C3-C2	8.94	1.46	1.40
2	A	400	PLP	C3-C2	8.95	1.47	1.40
2	D	400	PLP	C3-C2	8.98	1.47	1.40
2	F	400	PLP	C3-C2	9.07	1.47	1.40
2	E	400	PLP	C3-C2	9.16	1.47	1.40
2	B	400	PLP	C3-C2	9.29	1.47	1.40
2	C	400	PLP	C3-C2	9.49	1.47	1.40

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	400	PLP	C5-C6-N1	-3.63	117.69	123.83
2	D	400	PLP	O4P-P-O1P	-3.50	96.67	106.47
2	D	400	PLP	C5-C6-N1	-3.45	117.99	123.83
2	A	400	PLP	C3-C2-N1	-3.43	116.24	120.75
2	A	400	PLP	C5-C6-N1	-3.33	118.19	123.83
2	H	400	PLP	C3-C2-N1	-3.30	116.42	120.75
2	D	400	PLP	C3-C2-N1	-3.26	116.47	120.75
2	H	400	PLP	C5-C6-N1	-3.25	118.33	123.83
2	F	400	PLP	C5-C6-N1	-3.25	118.33	123.83
2	C	400	PLP	C5-C6-N1	-3.20	118.41	123.83
2	F	400	PLP	C3-C2-N1	-3.17	116.58	120.75
2	G	400	PLP	C3-C2-N1	-3.16	116.60	120.75
2	B	400	PLP	C3-C2-N1	-3.13	116.64	120.75
2	B	400	PLP	C5-C6-N1	-3.10	118.58	123.83
2	E	400	PLP	C3-C2-N1	-3.09	116.69	120.75
2	C	400	PLP	C3-C2-N1	-2.97	116.84	120.75
2	G	400	PLP	C5-C6-N1	-2.91	118.90	123.83
2	G	400	PLP	O3-C3-C2	-2.71	112.10	117.78
2	C	400	PLP	O4P-P-O1P	-2.56	99.31	106.47
2	E	400	PLP	O4P-P-O1P	-2.55	99.33	106.47
2	C	400	PLP	O3-C3-C2	-2.31	112.94	117.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	400	PLP	O3-C3-C2	-2.26	113.05	117.78
2	A	400	PLP	O3-C3-C2	-2.20	113.17	117.78
2	E	400	PLP	O3-C3-C2	-2.19	113.20	117.78
2	B	400	PLP	O3-C3-C2	-2.14	113.30	117.78
2	D	400	PLP	O3-C3-C2	-2.11	113.36	117.78
2	H	400	PLP	O3-C3-C2	-2.08	113.43	117.78
2	B	400	PLP	O4P-P-O1P	-2.01	100.84	106.47
2	B	400	PLP	O4P-C5A-C5	2.00	113.25	109.39
2	C	400	PLP	O3P-P-O1P	2.04	118.56	110.60
2	G	400	PLP	O4P-C5A-C5	2.69	114.57	109.39
2	F	400	PLP	O4P-C5A-C5	2.88	114.93	109.39
2	G	400	PLP	C6-C5-C4	2.89	120.53	118.19
2	H	400	PLP	O3-C3-C4	2.96	126.19	118.14
2	H	400	PLP	C6-C5-C4	3.09	120.69	118.19
2	D	400	PLP	O3P-P-O4P	3.12	115.03	106.73
2	F	400	PLP	O3-C3-C4	3.14	126.67	118.14
2	D	400	PLP	O3-C3-C4	3.15	126.70	118.14
2	F	400	PLP	C6-C5-C4	3.18	120.77	118.19
2	E	400	PLP	O3-C3-C4	3.21	126.87	118.14
2	B	400	PLP	O3-C3-C4	3.25	126.99	118.14
2	A	400	PLP	O3-C3-C4	3.30	127.12	118.14
2	H	400	PLP	C6-N1-C2	3.36	125.66	119.19
2	C	400	PLP	C6-N1-C2	3.37	125.69	119.19
2	B	400	PLP	C6-C5-C4	3.37	120.92	118.19
2	C	400	PLP	O3-C3-C4	3.39	127.37	118.14
2	D	400	PLP	C6-N1-C2	3.45	125.84	119.19
2	G	400	PLP	O3-C3-C4	3.47	127.56	118.14
2	B	400	PLP	C6-N1-C2	3.50	125.93	119.19
2	G	400	PLP	C6-N1-C2	3.51	125.95	119.19
2	E	400	PLP	C6-C5-C4	3.53	121.05	118.19
2	D	400	PLP	C6-C5-C4	3.58	121.09	118.19
2	F	400	PLP	C6-N1-C2	3.59	126.12	119.19
2	A	400	PLP	C6-C5-C4	3.59	121.10	118.19
2	E	400	PLP	C6-N1-C2	3.67	126.27	119.19
2	C	400	PLP	C6-C5-C4	3.69	121.18	118.19
2	A	400	PLP	C6-N1-C2	3.70	126.33	119.19
2	C	400	PLP	O4P-C5A-C5	4.02	117.12	109.39
2	H	400	PLP	O4P-C5A-C5	4.32	117.70	109.39
2	E	400	PLP	O4P-C5A-C5	5.16	119.31	109.39
2	D	400	PLP	C2A-C2-C3	5.72	127.79	120.96
2	D	400	PLP	O4P-C5A-C5	5.91	120.75	109.39
2	H	400	PLP	C2A-C2-C3	6.13	128.27	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	400	PLP	C2A-C2-C3	6.17	128.32	120.96
2	F	400	PLP	C2A-C2-C3	6.23	128.39	120.96
2	B	400	PLP	C2A-C2-C3	6.29	128.47	120.96
2	E	400	PLP	C2A-C2-C3	6.33	128.51	120.96
2	A	400	PLP	C2A-C2-C3	6.33	128.52	120.96
2	C	400	PLP	C2A-C2-C3	6.35	128.53	120.96
2	A	400	PLP	O4P-C5A-C5	7.01	122.87	109.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	PLP	4	0
2	B	400	PLP	1	0
2	C	400	PLP	4	0
2	D	400	PLP	4	0
2	E	400	PLP	4	0
2	F	400	PLP	1	0
2	G	400	PLP	3	0
2	H	400	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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	394/399 (98%)	0.32	13 (3%)	46	50	9, 17, 28, 39	0
1	B	394/399 (98%)	0.43	16 (4%)	37	41	10, 18, 32, 49	0
1	C	394/399 (98%)	0.17	8 (2%)	65	68	6, 11, 22, 44	0
1	D	394/399 (98%)	0.30	11 (2%)	53	56	8, 14, 26, 51	0
1	E	394/399 (98%)	0.39	18 (4%)	32	36	7, 17, 31, 50	0
1	F	394/399 (98%)	0.13	6 (1%)	73	76	5, 12, 23, 47	0
1	G	394/399 (98%)	0.32	11 (2%)	53	56	8, 16, 28, 47	0
1	H	394/399 (98%)	0.50	22 (5%)	24	28	10, 18, 31, 50	0
All	All	3152/3192 (98%)	0.32	105 (3%)	46	50	5, 16, 29, 51	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1	MET	11.2
1	H	2	ILE	10.5
1	D	2	ILE	10.2
1	F	1	MET	8.4
1	G	2	ILE	7.9
1	H	195	LYS	7.6
1	D	1	MET	5.9
1	C	1	MET	5.6
1	D	393	LEU	5.3
1	E	246	GLY	5.1
1	F	2	ILE	5.1
1	B	1	MET	4.8
1	B	2	ILE	4.7
1	B	393	LEU	4.6
1	H	1	MET	4.5
1	A	23	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	246	GLY	4.3
1	E	268	THR	3.9
1	H	246	GLY	3.7
1	D	256	ASP	3.6
1	A	163	LYS	3.4
1	E	335	LEU	3.4
1	C	2	ILE	3.4
1	B	390	LEU	3.4
1	C	31	ASN	3.3
1	D	394	LYS	3.3
1	F	393	LEU	3.3
1	E	392	ASP	3.2
1	F	394	LYS	3.2
1	B	336	LYS	3.1
1	D	103	PHE	3.1
1	G	268	THR	3.0
1	E	197	ASP	3.0
1	H	394	LYS	3.0
1	B	352	ILE	3.0
1	A	246	GLY	3.0
1	E	225	GLN	3.0
1	H	393	LEU	2.9
1	H	256	ASP	2.9
1	A	184	ASP	2.9
1	A	263	LYS	2.9
1	E	394	LYS	2.8
1	H	212	PRO	2.8
1	E	245	MET	2.8
1	H	392	ASP	2.7
1	C	268	THR	2.7
1	A	161	LYS	2.7
1	C	23	TYR	2.7
1	E	336	LYS	2.7
1	E	393	LEU	2.6
1	B	338	ASP	2.6
1	H	134	GLU	2.6
1	H	352	ILE	2.6
1	A	27	PRO	2.5
1	A	268	THR	2.5
1	H	84	GLN	2.5
1	E	154	GLN	2.5
1	H	107	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	23	TYR	2.4
1	E	163	LYS	2.4
1	G	195	LYS	2.4
1	H	245	MET	2.4
1	H	111	LYS	2.4
1	H	169	LEU	2.4
1	C	338	ASP	2.3
1	A	195	LYS	2.3
1	F	352	ILE	2.3
1	G	51	GLU	2.3
1	H	128	MET	2.3
1	E	134	GLU	2.3
1	G	86	ASP	2.3
1	A	84	GLN	2.3
1	E	31	ASN	2.3
1	H	213	GLY	2.3
1	D	60	THR	2.3
1	G	338	ASP	2.3
1	H	270	GLY	2.3
1	D	184	ASP	2.3
1	E	23	TYR	2.2
1	D	134	GLU	2.2
1	B	370	ILE	2.2
1	E	145	LYS	2.2
1	A	134	GLU	2.2
1	B	354	PHE	2.2
1	E	224	GLU	2.2
1	B	84	GLN	2.2
1	H	225	GLN	2.2
1	D	246	GLY	2.2
1	G	136	LYS	2.2
1	B	337	MET	2.1
1	E	386	LEU	2.1
1	G	161	LYS	2.1
1	C	269	SER	2.1
1	A	197	ASP	2.1
1	B	394	LYS	2.1
1	A	256	ASP	2.0
1	C	215	GLU	2.0
1	G	224	GLU	2.0
1	B	245	MET	2.0
1	D	245	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	314	HIS	2.0
1	B	27	PRO	2.0
1	G	28	GLU	2.0
1	H	146	ASP	2.0
1	H	194	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PLP	B	400	15/16	0.80	0.18	15,19,26,28	0
2	PLP	C	400	15/16	0.82	0.17	10,14,23,26	0
2	PLP	F	400	15/16	0.82	0.17	9,14,24,26	0
2	PLP	G	400	15/16	0.83	0.15	14,17,25,28	0
2	PLP	H	400	15/16	0.85	0.20	17,20,34,35	0
2	PLP	E	400	15/16	0.86	0.17	16,18,28,30	0
2	PLP	D	400	15/16	0.88	0.15	16,18,26,27	0
2	PLP	A	400	15/16	0.89	0.16	17,20,29,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.