



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:52 PM 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 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/ValidationPDFNotes.html>

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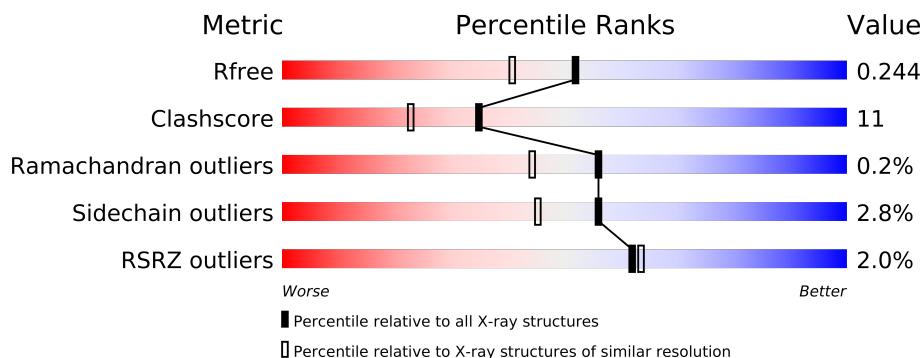
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	399	
1	B	399	
1	C	399	
1	D	399	
1	E	399	
1	F	399	
1	G	399	
1	H	399	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PLP	A	400	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	PLP	B	400	-	X
2	PLP	C	400	-	X
2	PLP	D	400	-	X
2	PLP	E	400	-	X
2	PLP	F	400	-	X
2	PLP	G	400	-	X
2	PLP	H	400	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28402 atoms, of which 0 are hydrogen and 0 are deuterium.

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:

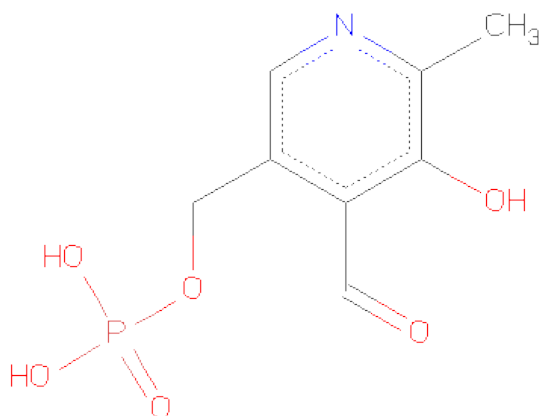
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	GLN	GLU	CONFLICT	UNP Q56257
A	154	GLN	GLU	CONFLICT	UNP Q56257
A	267	ALA	ILE	CONFLICT	UNP Q56257
B	88	GLN	GLU	CONFLICT	UNP Q56257
B	154	GLN	GLU	CONFLICT	UNP Q56257
B	267	ALA	ILE	CONFLICT	UNP Q56257
C	88	GLN	GLU	CONFLICT	UNP Q56257
C	154	GLN	GLU	CONFLICT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

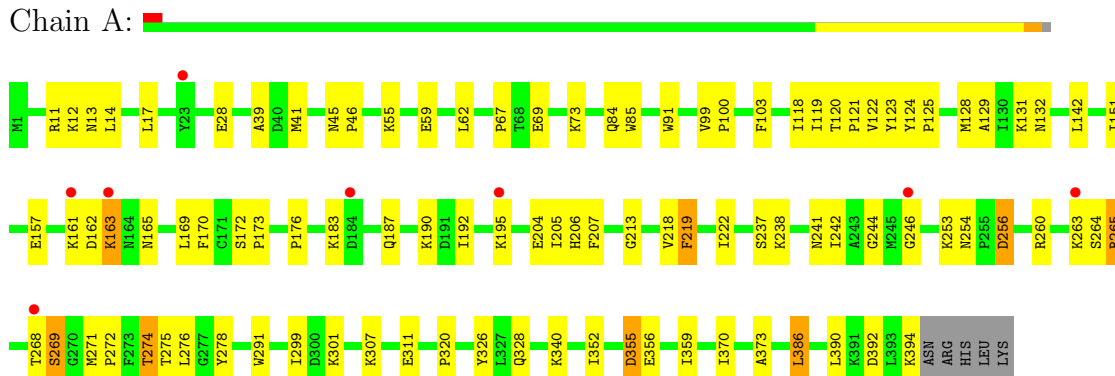
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	313	Total	O	0	0
			313	313		
3	B	269	Total	O	0	0
			269	269		
3	C	354	Total	O	0	0
			354	354		
3	D	379	Total	O	0	0
			379	379		
3	E	292	Total	O	0	0
			292	292		
3	F	380	Total	O	0	0
			380	380		
3	G	334	Total	O	0	0
			334	334		
3	H	305	Total	O	0	0
			305	305		

### 3 Residue-property plots

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

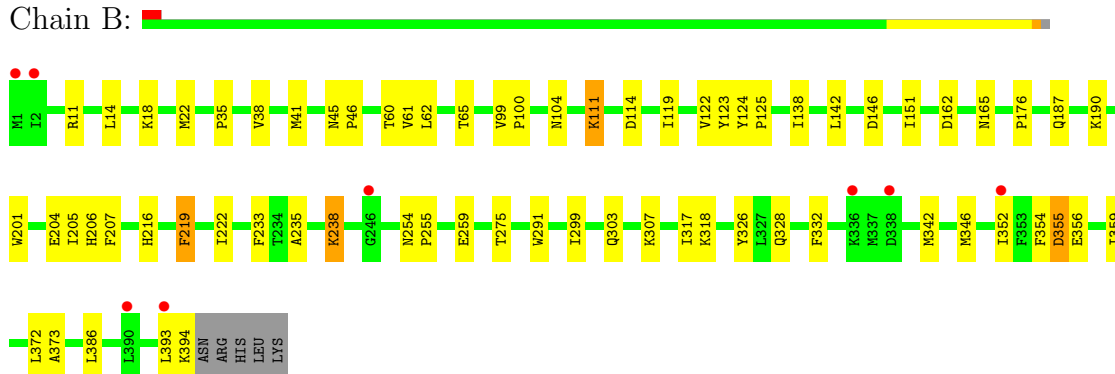
#### • Molecule 1: CYSTALYSIN

Chain A:



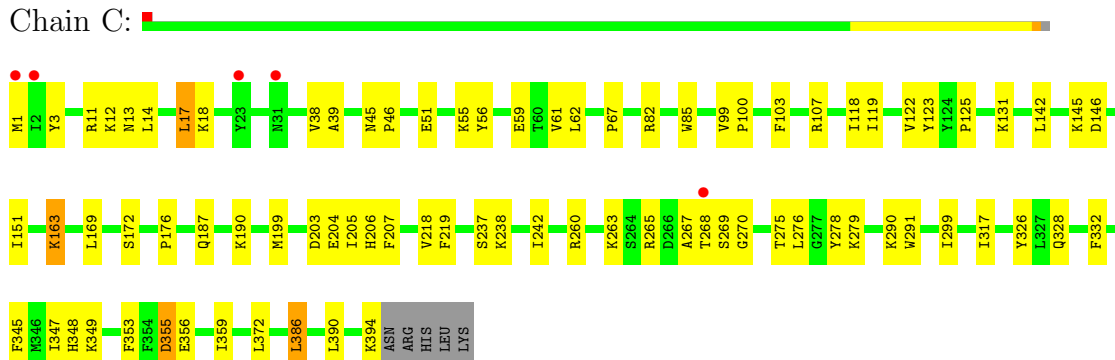
#### • Molecule 1: CYSTALYSIN

Chain B:



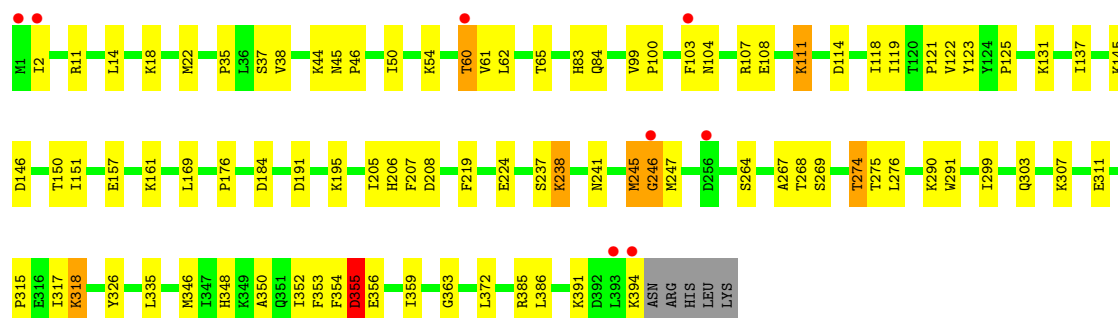
#### • Molecule 1: CYSTALYSIN

Chain C:



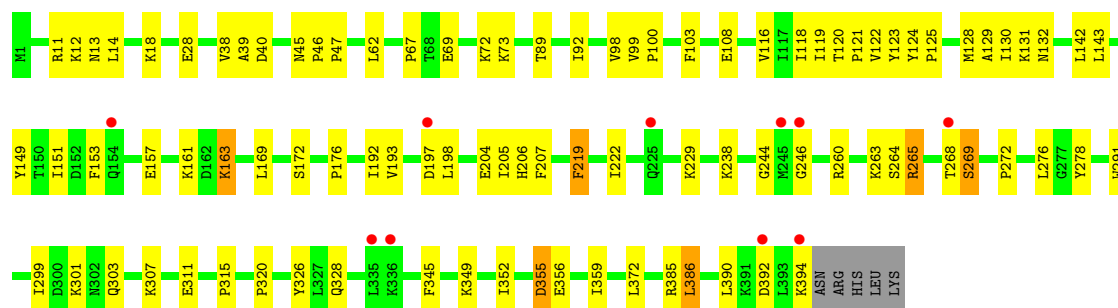
- Molecule 1: CYSTALYSIN

Chain D:



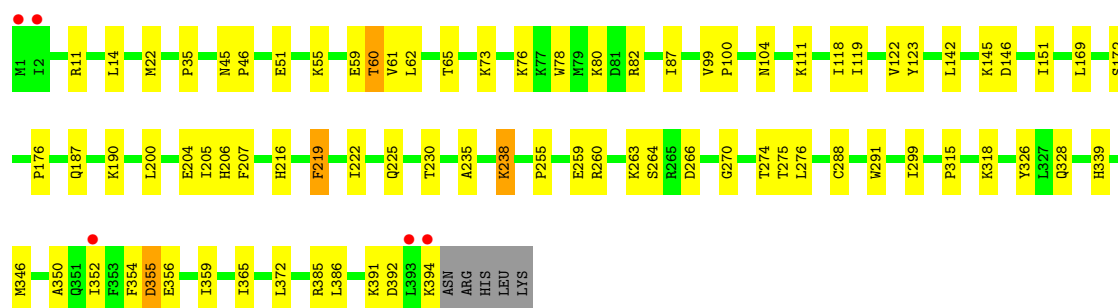
- Molecule 1: CYSTALYSIN

Chain E:



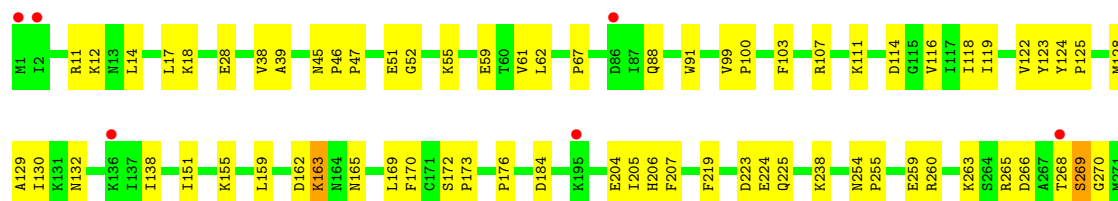
- Molecule 1: CYSTALYSIN

Chain F:



- Molecule 1: CYSTALYSIN

Chain G:

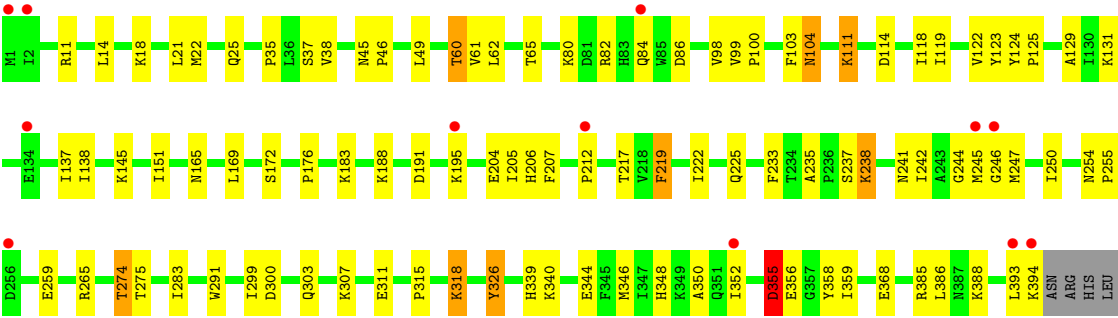






● Molecule 1: CYSTALYSIN

Chain H:



LYS

## 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 (5.25%)	DCC
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 , 35.1	EDS
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 254956 reflections (0.000%)	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.

## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (553) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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:D:60:THR:HG22	1:D:61:VAL:H	1.54	0.71
1:A:119:ILE:HD13	1:A:151:ILE:HD12	1.73	0.71
1:C:205:ILE:HD13	2:C:400:PLP:H5A1	1.72	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:F:205:ILE:CD1	1:F:235:ALA:HB3	2.22	0.69
1:A:67:PRO:HG3	1:A:278:TYR:CE2	2.26	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:F:346:MET:SD	1:F:352:ILE:HD11	2.32	0.69
1:C:39:ALA:HB1	1:C:238:LYS:HE2	1.74	0.69
1:H:60:THR:HG23	3:H:513:HOH:O	1.92	0.69
1:G:119:ILE:HD13	1:G:151:ILE:HD12	1.75	0.68
1:E:67:PRO:HG3	1:E:278:TYR:CE2	2.29	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:H:346:MET:SD	1:H:352:ILE:HD11	2.36	0.65
1:E:128:MET:O	1:E:132:ASN:HB2	1.96	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:H:242:ILE:HB	1:H:245:MET:HB2	1.79	0.64
1:H:205:ILE:HD11	1:H:235:ALA:HB3	1.78	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	Distance(Å)	Clash(Å)
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:386:LEU:HD22	1:E:390:LEU:HG	1.79	0.63
1:E:99:VAL:HB	1:E:100:PRO:HD3	1.81	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: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:E:92:ILE:HD12	3:E:433:HOH:O	1.99	0.62
1:D:2:ILE:HA	3:D:585:HOH:O	2.00	0.62
1:G:46:PRO:HG3	1:G:291:TRP:CD2	2.35	0.62
1:F:206:HIS:HE1	2:F:400:PLP:O3	1.83	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:356:GLU:O	1:B:359:ILE:HG12	1.99	0.61
1:B:46:PRO:HG3	1:B:291:TRP:CD2	2.36	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:E:260:ARG:O	1:E:263:LYS:HG2	2.01	0.60
1:A:299:ILE:HD13	1:A:326:TYR:HB3	1.83	0.60
1:A:39:ALA:CB	1:A:238:LYS:HE2	2.31	0.60
1:A:39:ALA:HB1	1:A:238:LYS:HE2	1.82	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
1:H:65:THR:HB	1:H:275:THR:HG22	1.84	0.59
1:G:12:LYS:O	1:G:14:LEU:HD13	2.02	0.59
1:A:320:PRO:HG3	3:A:519:HOH:O	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:60:THR:HG22	1:H:61:VAL:N	2.14	0.59
1:F:391:LYS:O	1:F:394:LYS:HG2	2.02	0.59
1:E:157:GLU:O	1:E:161:LYS:HD3	2.03	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:D:60:THR:HG23	3:D:441:HOH:O	2.03	0.56
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: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: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:B:122:VAL:HG22	1:B:123:TYR:N	2.19	0.56
1:H:46:PRO:HG3	1:H:291:TRP:CD2	2.40	0.56
1:A:128:MET:O	1:A:132:ASN:HB2	2.05	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
1:A:386:LEU:HD22	1:A:390:LEU:HG	1.86	0.55
1:G:394:LYS:NZ	1:G:394:LYS:HB2	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:391:LYS:O	1:F:394:LYS:HE2	2.07	0.55
1:A:268:THR:O	1:A:269:SER:HB2	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:E:198:LEU:HD12	3:E:598:HOH:O	2.07	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: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:206:HIS:HE1	2:E:400:PLP:O3	1.89	0.54
1:E:299:ILE:HD13	1:E:326:TYR:HB3	1.88	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:60:THR:HG22	1:D:61:VAL:N	2.22	0.54
1:D:264:SER:O	1:D:268:THR:HG23	2.07	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:B:111:LYS:HD2	1:B:114:ASP:OD2	2.08	0.54
1:A:99:VAL:HB	1:A:100:PRO:HD3	1.89	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:G:62:LEU:CD2	1:G:275:THR:HG21	2.38	0.53
1:C:206:HIS:HE1	2:C:400:PLP:O3	1.91	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:D:205:ILE:CD1	2:D:400:PLP:H5A1	2.38	0.53
1:C:67:PRO:HG3	1:C:278:TYR:CE2	2.42	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:E:163:LYS:CD	1:E:163:LYS:H	1.91	0.53
1:G:11:ARG:HA	1:G:14:LEU:HD22	1.89	0.53
1:E:268:THR:O	1:E:269:SER:HB2	2.08	0.53
1:D:50:ILE:O	1:D:54:LYS:HG3	2.09	0.53
1:D:191:ASP:O	1:D:195:LYS:HG3	2.08	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:D:206:HIS:HE1	2:D:400:PLP:O3	1.92	0.52
1:A:205:ILE:HD13	2:A:400:PLP:H5A1	1.92	0.52
1:E:311:GLU:O	1:E:315:PRO:HG3	2.10	0.52
1:C:145:LYS:HE3	1:C:146:ASP:OD1	2.09	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:H:11:ARG:HA	1:H:14:LEU:HD12	1.91	0.52
1:D:247:MET:HE2	1:D:274:THR:HG23	1.91	0.52
1:H:352:ILE:HD11	1:H:386:LEU:HD13	1.93	0.51
1:H:122:VAL:HG22	1:H:123:TYR:N	2.26	0.51
1:G:155:LYS:O	1:G:159:LEU:HG	2.09	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:D:18:LYS:HB2	1:D:38:VAL:HB	1.92	0.51
1:B:119:ILE:HD13	1:B:151:ILE:HD12	1.93	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
3:E:648:HOH:O	1:F:60:THR:HG21	2.11	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:F:352:ILE:HD12	1:F:354:PHE:CE2	2.46	0.50
1:B:99:VAL:HB	1:B:100:PRO:HD3	1.93	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
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
1:H:247:MET:CE	1:H:274:THR:HG23	2.41	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:E:151:ILE:HB	1:E:153:PHE:CE1	2.46	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:46:PRO:HG3	1:D:291:TRP:CD2	2.47	0.49
1:B:162:ASP:HB3	1:B:165:ASN:ND2	2.27	0.49
1:H:37:SER:HB2	1:H:355:ASP:OD1	2.11	0.49
1:G:47:PRO:O	1:G:51:GLU:HG3	2.13	0.49
1:D:356:GLU:O	1:D:359:ILE:HG12	2.13	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:G:62:LEU:HD22	1:G:275:THR:HG21	1.95	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:B:41:MET:HG2	1:B:373:ALA:CB	2.43	0.49
1:G:205:ILE:CD1	2:G:400:PLP:H5A1	2.42	0.49
1:D:104:ASN:ND2	1:D:107:ARG:HH21	2.07	0.49
1:B:41:MET:HG2	1:B:373:ALA:HB1	1.94	0.49
1:B:342:MET:O	1:B:346:MET:HG2	2.13	0.49
1:E:328:GLN:HB2	1:E:372:LEU:HD11	1.95	0.49
1:D:238:LYS:HD2	3:D:444:HOH:O	2.13	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:350:ALA:O	1:H:385:ARG:HD2	2.12	0.48
1:H:315:PRO:O	1:H:318:LYS:HE2	2.13	0.48
1:H:60:THR:CG2	1:H:61:VAL:H	2.22	0.48
1:G:17:LEU:HD12	3:G:702:HOH:O	2.13	0.48
1:D:303:GLN:HB3	1:D:372:LEU:HD13	1.95	0.48
1:A:122:VAL:HG22	1:A:123:TYR:N	2.28	0.48
1:E:172:SER:O	1:E:204:GLU:HA	2.14	0.48
1:G:205:ILE:HD13	2:G:400:PLP:H5A1	1.96	0.48
1:E:72:LYS:HE2	3:E:577:HOH:O	2.13	0.48
1:E:12:LYS:HG2	1:E:13:ASN:ND2	2.28	0.48
1:H:123:TYR:CG	1:H:125:PRO:HD2	2.48	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:A:62:LEU:H	1:B:45:ASN:ND2	2.02	0.48
1:G:275:THR:HG22	1:H:244:GLY:O	2.13	0.48
1:A:123:TYR:CZ	1:A:125:PRO:HG2	2.49	0.48
1:G:162:ASP:HB3	1:G:165:ASN:ND2	2.29	0.48
1:C:103:PHE:HD2	1:D:267:ALA:O	1.96	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:317:ILE:HD13	1:C:332:PHE:CE2	2.48	0.47
1:C:163:LYS:N	1:C:163:LYS:CD	2.64	0.47
1:B:187:GLN:HE22	1:B:190:LYS:HZ3	1.62	0.47
1:E:11:ARG:HD3	1:F:61:VAL:HB	1.96	0.47
1:F:356:GLU:O	1:F:359:ILE:HG12	2.14	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: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:A:69:GLU:O	1:A:73:LYS:HG3	2.15	0.47
1:F:187:GLN:NE2	1:F:190:LYS:NZ	2.61	0.47
1:C:118:ILE:HG22	1:C:169:LEU:HB3	1.95	0.47
1:B:119:ILE:HG22	1:B:142:LEU:HG	1.97	0.47
1:E:193:VAL:HA	3:E:598:HOH:O	2.15	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:A:162:ASP:HB3	1:A:165:ASN:ND2	2.30	0.47
1:E:116:VAL:HB	1:E:130:ILE:HD13	1.97	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:C:276:LEU:HD12	1:D:276:LEU:CD1	2.44	0.46
1:H:138:ILE:HG13	1:H:165:ASN:OD1	2.15	0.46
1:A:219:PHE:O	1:A:222:ILE:HG12	2.16	0.46
1:E:131:LYS:HE3	1:E:131:LYS:HB2	1.79	0.46
1:H:118:ILE:HG22	1:H:169:LEU:HB3	1.96	0.46
1:A:392:ASP:O	1:A:394:LYS:HG3	2.15	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: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:H:123:TYR:CZ	1:H:125:PRO:HG2	2.50	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:G:39:ALA:HB1	1:G:238:LYS:HE2	1.96	0.46
1:D:247:MET:CE	1:D:274:THR:HG23	2.46	0.46
1:E:352:ILE:HG23	1:E:352:ILE:O	2.14	0.46
1:G:51:GLU:HG2	3:G:573:HOH:O	2.16	0.46
1:G:206:HIS:HE1	2:G:400:PLP:O3	1.99	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:46:PRO:HG3	1:G:291:TRP:CE3	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:119:ILE:HD13	1:F:151:ILE:HD12	1.97	0.46
1:B:317:ILE:HD13	1:B:332:PHE:CE2	2.50	0.46
1:A:172:SER:O	1:A:204:GLU:HA	2.16	0.46
1:G:356:GLU:O	1:G:359:ILE:HG12	2.15	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:F:118:ILE:HG22	1:F:169:LEU:HB3	1.97	0.46
1:F:392:ASP:O	1:F:394:LYS:HG3	2.16	0.45
1:B:111:LYS:HD2	1:B:114:ASP:CG	2.37	0.45
1:A:41:MET:HG2	1:A:373:ALA:HB1	1.97	0.45
1:C:394:LYS:HB2	1:C:394:LYS:NZ	2.31	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:C:62:LEU:H	1:D:45:ASN:ND2	2.01	0.45
1:B:205:ILE:HD11	1:B:235:ALA:HB3	1.99	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:G:107:ARG:CZ	1:G:107:ARG:HB2	2.46	0.45
1:B:328:GLN:HB2	1:B:372:LEU:HD11	1.98	0.45
1:B:307:LYS:HE2	3:B:498:HOH:O	2.16	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
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:B:303:GLN:HB3	1:B:372:LEU:HD13	1.99	0.44
1:A:307:LYS:O	1:A:311:GLU:HG3	2.17	0.44
1:C:18:LYS:HB2	1:C:38:VAL:HB	1.99	0.44
1:F:315:PRO:O	1:F:318:LYS:HE3	2.17	0.44
1:F:145:LYS:HD3	3:F:574:HOH:O	2.16	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:205:ILE:HD13	2:E:400:PLP:C5A	2.36	0.44
1:D:352:ILE:HD12	1:D:354:PHE:CZ	2.53	0.44
1:A:119:ILE:HG22	1:A:142:LEU:HG	2.00	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:G:260:ARG:HA	1:G:263:LYS:CD	2.46	0.44
1:A:265:ARG:NH2	3:A:620:HOH:O	2.50	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:D:44:LYS:HD2	3:D:424:HOH:O	2.17	0.44
1:F:205:ILE:HD12	1:F:235:ALA:HB3	1.98	0.44
1:G:62:LEU:HD13	1:H:245:MET:CG	2.47	0.44
1:E:193:VAL:HG12	1:E:229:LYS:HE3	2.00	0.44
1:G:338:ASP:OD2	1:G:341:ALA:HB3	2.18	0.44
1:D:83:HIS:HE1	1:D:208:ASP:OD1	2.00	0.44
1:G:61:VAL:CG1	1:H:241:ASN:HD21	2.31	0.44
1:G:172:SER:O	1:G:204:GLU:HA	2.18	0.44
1:C:347:ILE:HG23	1:C:353:PHE:CE2	2.53	0.44
1:F:172:SER:O	1:F:204:GLU:HA	2.18	0.44
1:G:45:ASN:ND2	1:H:62:LEU:H	2.01	0.43
1:H:124:TYR:CD1	1:H:125:PRO:HD3	2.53	0.43
1:C:328:GLN:HB2	1:C:372:LEU:HD11	1.99	0.43
1:C:345:PHE:O	1:C:349:LYS:HB2	2.17	0.43
1:H:188:LYS:HG2	3:H:417:HOH:O	2.17	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:G:122:VAL:O	1:G:123:TYR:C	2.57	0.43
1:B:123:TYR:CZ	1:B:125:PRO:HG2	2.54	0.43
1:E:122:VAL:HG22	1:E:123:TYR:H	1.83	0.43
1:E:123:TYR:CZ	1:E:125:PRO:HG2	2.53	0.43
1:A:41:MET:HB2	1:A:241:ASN:ND2	2.33	0.43
1:D:157:GLU:HG2	1:D:161:LYS:HZ2	1.82	0.43
1:H:394:LYS:HD2	3:H:668:HOH:O	2.18	0.43
1:G:55:LYS:O	1:G:59:GLU:HG3	2.19	0.43
1:C:187:GLN:NE2	1:C:190:LYS:CE	2.81	0.43
1:F:263:LYS:HG3	1:F:264:SER:N	2.33	0.43
1:A:265:ARG:O	1:A:268:THR:O	2.36	0.43
1:H:247:MET:HE2	1:H:274:THR:HG23	1.99	0.43
1:D:391:LYS:O	1:D:394:LYS:HG3	2.18	0.43
1:D:11:ARG:HA	1:D:14:LEU:HD12	1.99	0.43
1:H:219:PHE:O	1:H:222:ILE:HG12	2.19	0.43
1:E:89:THR:HA	3:E:433:HOH:O	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:394:LYS:HB2	1:E:394:LYS:HZ3	1.81	0.43
1:C:267:ALA:HA	1:D:103:PHE:CE2	2.52	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:E:192:ILE:HG22	3:E:598:HOH:O	2.19	0.43
1:A:392:ASP:C	1:A:394:LYS:N	2.72	0.43
1:H:233:PHE:HD2	1:H:250:ILE:HD12	1.82	0.43
1:B:201:TRP:HB3	1:B:233:PHE:HE1	1.84	0.43
1:E:260:ARG:HA	1:E:263:LYS:HG2	1.99	0.43
1:C:265:ARG:HD3	1:C:270:GLY:C	2.39	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:C:206:HIS:HD2	3:C:415:HOH:O	2.02	0.43
1:G:119:ILE:HD12	1:G:170:PHE:CE1	2.54	0.43
1:A:124:TYR:CG	1:A:125:PRO:HD3	2.53	0.43
1:E:143:LEU:O	1:E:149:TYR:HA	2.19	0.43
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:E:11:ARG:NH2	1:E:40:ASP:OD2	2.48	0.42
1:C:123:TYR:CZ	1:C:125:PRO:HG2	2.54	0.42
1:F:274:THR:O	1:F:274:THR:HG23	2.19	0.42
1:G:123:TYR:CG	1:G:125:PRO:HD2	2.54	0.42
1:B:123:TYR:CG	1:B:125:PRO:HD2	2.54	0.42
1:F:350:ALA:O	1:F:385:ARG:CD	2.67	0.42
1:F:200:LEU:O	1:F:230:THR:HA	2.20	0.42
1:H:339:HIS:HB2	1:H:358:TYR:CD2	2.55	0.42
1:G:116:VAL:HB	1:G:130:ILE:HD13	2.01	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
1:C:103:PHE:CD2	1:D:267:ALA:O	2.73	0.42
1:C:46:PRO:HG3	1:C:291:TRP:CD2	2.55	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:H:254:ASN:HA	1:H:255:PRO:HD3	1.90	0.42
1:F:266:ASP:HA	1:F:270:GLY:HA2	2.01	0.42
1:C:263:LYS:HE3	1:C:263:LYS:HB2	1.87	0.42
1:B:393:LEU:O	1:B:394:LYS:HB2	2.19	0.42
1:E:265:ARG:NE	3:E:536:HOH:O	2.53	0.42
1:C:107:ARG:HD3	3:C:435:HOH:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:A:157:GLU:O	1:A:161:LYS:HD3	2.19	0.42
1:G:260:ARG:O	1:G:263:LYS:CG	2.67	0.42
1:H:122:VAL:O	1:H:123:TYR:C	2.59	0.42
1:B:355:ASP:O	1:B:356:GLU:C	2.57	0.42
1:H:393:LEU:O	1:H:394:LYS:C	2.58	0.42
1:C:187:GLN:NE2	1:C:190:LYS:HE3	2.35	0.42
1:A:237:SER:HA	1:A:242:ILE:HG13	2.01	0.42
1:H:111:LYS:HD2	1:H:114:ASP:CG	2.40	0.42
1:C:56:TYR:CD1	1:C:279:LYS:HG2	2.55	0.42
1:D:205:ILE:HD11	1:D:237:SER:OG	2.20	0.42
1:B:46:PRO:HG3	1:B:291:TRP:CE3	2.55	0.42
1:G:254:ASN:HA	1:G:255:PRO:HD3	1.91	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: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:G:124:TYR:CG	1:G:125:PRO:HD3	2.55	0.41
1:F:238:LYS:HD2	1:F:238:LYS:HA	1.95	0.41
1:E:272:PRO:HD3	3:E:536:HOH:O	2.18	0.41
1:E:103:PHE:CZ	1:E:129:ALA:HA	2.55	0.41
1:A:328:GLN:HB3	1:A:370:ILE:HG22	2.02	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
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:C:12:LYS:HE2	1:C:13:ASN:ND2	2.35	0.41
1:H:124:TYR:CE2	1:H:359:ILE:HD12	2.56	0.41
1:A:271:MET:HA	1:A:272:PRO:HD3	1.94	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:F:46:PRO:HG3	1:F:291:TRP:CE3	2.56	0.41
1:E:122:VAL:O	1:E:123:TYR:C	2.57	0.41
1:A:123:TYR:CG	1:A:125:PRO:HD2	2.54	0.41
1:G:172:SER:HA	1:G:173:PRO:C	2.41	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:124:TYR:CG	1:E:125:PRO:HD3	2.56	0.41
1:D:111:LYS:HD2	1:D:114:ASP:OD2	2.20	0.41
1:A:119:ILE:HD12	1:A:170:PHE:CE1	2.56	0.41
1:C:386:LEU:HD22	1:C:390:LEU:CG	2.47	0.41
1:C:290:LYS:HG2	3:C:626:HOH:O	2.21	0.41
1:B:204:GLU:OE1	1:B:216:HIS:HE1	2.04	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:E:163:LYS:CD	1:E:163:LYS:N	2.68	0.41
1:H:356:GLU:OE2	1:H:368:GLU:OE1	2.38	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:G:138:ILE:HG13	1:G:165:ASN:OD1	2.20	0.41
1:F:119:ILE:O	1:F:122:VAL:HB	2.21	0.41
1:F:51:GLU:HG2	3:F:758:HOH:O	2.20	0.41
1:E:69:GLU:O	1:E:73:LYS:HG3	2.20	0.41
1:A:275:THR:HG23	1:A:276:LEU:N	2.36	0.41
1:D:353:PHE:CD1	1:D:353:PHE:N	2.88	0.41
1:C:131:LYS:HE3	1:C:131:LYS:HB2	1.87	0.41
1:H:237:SER:HA	1:H:242:ILE:HG13	2.03	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:C:203:ASP:OD1	2:C:400:PLP:N1	2.54	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:HD2	1:H:318:LYS:N	2.36	0.40
1:A:122:VAL:O	1:A:123:TYR:C	2.60	0.40
1:H:394:LYS:HB2	3:H:668:HOH:O	2.21	0.40
1:C:85:TRP:CD2	1:C:218:VAL:HG11	2.56	0.40
1:D:121:PRO:HG3	1:D:363:GLY:HA3	2.03	0.40
1:C:172:SER:O	1:C:204:GLU:HA	2.21	0.40
1:A:103:PHE:CZ	1:A:129:ALA:HA	2.56	0.40
1:C:1:MET:HB3	1:C:3:TYR:CE2	2.56	0.40
1:G:260:ARG:HA	1:G:263:LYS:HG2	2.03	0.40
1:E:46:PRO:HG3	1:E:291:TRP:CE2	2.57	0.40
1:A:124:TYR:CD1	1:A:125:PRO:HD3	2.56	0.40
1:H:49:LEU:HA	1:H:283:ILE:HG21	2.03	0.40
1:F:225:GLN:HG2	3:F:667:HOH:O	2.21	0.40
1:E:46:PRO:HA	1:E:47:PRO:HD3	1.97	0.40
1:C:260:ARG:O	1:C:263:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:52:GLY:HA3	1:G:283:ILE:HD13	2.04	0.40
1:E:120:THR:HB	1:E:121:PRO:HA	2.03	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%)	38	23
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%)	50	37
1	E	392/399 (98%)	377 (96%)	14 (4%)	1 (0%)	50	37
1	F	392/399 (98%)	383 (98%)	9 (2%)	0	100	100
1	G	392/399 (98%)	384 (98%)	7 (2%)	1 (0%)	50	37
1	H	392/399 (98%)	376 (96%)	15 (4%)	1 (0%)	50	37
All	All	3136/3192 (98%)	3029 (97%)	101 (3%)	6 (0%)	56	44

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%)	56	45
1	B	353/358 (99%)	344 (98%)	9 (2%)	60	50
1	C	353/358 (99%)	345 (98%)	8 (2%)	63	55
1	D	353/358 (99%)	340 (96%)	13 (4%)	45	32
1	E	353/358 (99%)	344 (98%)	9 (2%)	60	50
1	F	353/358 (99%)	344 (98%)	9 (2%)	60	50
1	G	353/358 (99%)	342 (97%)	11 (3%)	52	41
1	H	353/358 (99%)	342 (97%)	11 (3%)	52	41
All	All	2824/2864 (99%)	2744 (97%)	80 (3%)	56	45

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

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 chains 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	14,15,16	3.22	4 (28%)	20,22,23	2.73	8 (40%)
2	PLP	B	400	1	14,15,16	3.20	4 (28%)	20,22,23	2.19	5 (25%)
2	PLP	C	400	1	14,15,16	3.21	4 (28%)	20,22,23	2.42	8 (40%)
2	PLP	D	400	1	14,15,16	3.25	3 (21%)	20,22,23	2.66	9 (45%)
2	PLP	E	400	1	14,15,16	3.22	4 (28%)	20,22,23	2.55	8 (40%)
2	PLP	F	400	1	14,15,16	3.17	4 (28%)	20,22,23	2.28	6 (30%)
2	PLP	G	400	1	14,15,16	3.02	3 (21%)	20,22,23	2.22	7 (35%)
2	PLP	H	400	1	14,15,16	3.15	4 (28%)	20,22,23	2.32	7 (35%)

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 (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	PLP	C3-C2	9.16	1.47	1.40
2	B	400	PLP	C3-C2	8.97	1.47	1.40
2	E	400	PLP	C3-C2	8.84	1.47	1.40
2	F	400	PLP	C3-C2	8.75	1.47	1.40
2	D	400	PLP	C3-C2	8.66	1.47	1.40
2	A	400	PLP	C3-C2	8.63	1.47	1.40
2	H	400	PLP	C3-C2	8.63	1.46	1.40
2	G	400	PLP	C3-C2	8.37	1.46	1.40
2	F	400	PLP	C4-C5	6.35	1.50	1.39
2	E	400	PLP	C4-C5	6.28	1.50	1.39
2	A	400	PLP	C4-C5	6.26	1.50	1.39
2	D	400	PLP	C4-C5	6.25	1.50	1.39
2	B	400	PLP	C4-C5	6.20	1.50	1.39
2	G	400	PLP	C4-C5	5.99	1.49	1.39
2	H	400	PLP	C4-C5	5.97	1.49	1.39
2	C	400	PLP	C4-C5	5.92	1.49	1.39
2	D	400	PLP	C2-N1	4.46	1.42	1.33
2	A	400	PLP	C2-N1	4.01	1.41	1.33
2	B	400	PLP	C2-N1	3.77	1.40	1.33
2	C	400	PLP	C2-N1	3.67	1.40	1.33
2	H	400	PLP	C2-N1	3.64	1.40	1.33
2	E	400	PLP	C2-N1	3.45	1.40	1.33
2	G	400	PLP	C2-N1	3.26	1.39	1.33
2	F	400	PLP	C2-N1	3.22	1.39	1.33
2	B	400	PLP	P-O3P	-2.33	1.46	1.54
2	E	400	PLP	P-O3P	-2.23	1.46	1.54
2	C	400	PLP	P-O3P	-2.22	1.46	1.54
2	F	400	PLP	P-O3P	-2.14	1.46	1.54
2	A	400	PLP	P-O3P	-2.08	1.47	1.54
2	H	400	PLP	P-O3P	-2.05	1.47	1.54

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	PLP	O4P-C5A-C5	6.69	122.87	109.26
2	C	400	PLP	C2A-C2-C3	6.18	128.53	121.02
2	A	400	PLP	C2A-C2-C3	6.17	128.52	121.02
2	E	400	PLP	C2A-C2-C3	6.17	128.51	121.02
2	B	400	PLP	C2A-C2-C3	6.13	128.47	121.02
2	F	400	PLP	C2A-C2-C3	6.06	128.39	121.02
2	G	400	PLP	C2A-C2-C3	6.01	128.32	121.02
2	H	400	PLP	C2A-C2-C3	5.96	128.27	121.02
2	D	400	PLP	O4P-C5A-C5	5.65	120.75	109.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	PLP	C2A-C2-C3	5.57	127.79	121.02
2	E	400	PLP	O4P-C5A-C5	4.94	119.31	109.26
2	H	400	PLP	O4P-C5A-C5	4.15	117.70	109.26
2	C	400	PLP	O4P-C5A-C5	3.87	117.12	109.26
2	D	400	PLP	O4P-P-O1P	-3.43	96.67	106.71
2	E	400	PLP	C5-C6-N1	-3.42	117.69	123.86
2	A	400	PLP	C6-N1-C2	3.29	126.33	119.28
2	E	400	PLP	C6-N1-C2	3.26	126.27	119.28
2	D	400	PLP	C5-C6-N1	-3.25	117.99	123.86
2	A	400	PLP	C3-C2-N1	-3.22	116.24	120.66
2	F	400	PLP	C6-N1-C2	3.19	126.12	119.28
2	A	400	PLP	C5-C6-N1	-3.14	118.19	123.86
2	G	400	PLP	C6-N1-C2	3.11	125.95	119.28
2	B	400	PLP	C6-N1-C2	3.10	125.93	119.28
2	H	400	PLP	C3-C2-N1	-3.10	116.42	120.66
2	G	400	PLP	O3-C3-C2	-3.10	112.10	117.61
2	H	400	PLP	C5-C6-N1	-3.07	118.33	123.86
2	F	400	PLP	C5-C6-N1	-3.06	118.33	123.86
2	D	400	PLP	C6-N1-C2	3.06	125.84	119.28
2	D	400	PLP	C3-C2-N1	-3.05	116.47	120.66
2	D	400	PLP	O3P-P-O4P	3.04	115.03	106.65
2	C	400	PLP	C5-C6-N1	-3.02	118.41	123.86
2	C	400	PLP	C6-N1-C2	2.99	125.69	119.28
2	H	400	PLP	C6-N1-C2	2.98	125.66	119.28
2	F	400	PLP	C3-C2-N1	-2.97	116.58	120.66
2	G	400	PLP	C3-C2-N1	-2.96	116.60	120.66
2	B	400	PLP	C3-C2-N1	-2.93	116.64	120.66
2	B	400	PLP	C5-C6-N1	-2.92	118.58	123.86
2	E	400	PLP	C3-C2-N1	-2.90	116.69	120.66
2	F	400	PLP	O4P-C5A-C5	2.79	114.93	109.26
2	C	400	PLP	C3-C2-N1	-2.78	116.84	120.66
2	G	400	PLP	C5-C6-N1	-2.75	118.90	123.86
2	C	400	PLP	O3-C3-C2	-2.62	112.94	117.61
2	G	400	PLP	O4P-C5A-C5	2.61	114.57	109.26
2	F	400	PLP	O3-C3-C2	-2.56	113.05	117.61
2	C	400	PLP	O4P-P-O1P	-2.52	99.31	106.71
2	E	400	PLP	O4P-P-O1P	-2.51	99.33	106.71
2	A	400	PLP	O3-C3-C2	-2.50	113.17	117.61
2	C	400	PLP	O3P-P-O1P	2.48	118.56	110.44
2	E	400	PLP	O3-C3-C2	-2.48	113.20	117.61
2	B	400	PLP	O3-C3-C2	-2.42	113.30	117.61
2	A	400	PLP	C5A-C5-C4	-2.42	115.78	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	PLP	P-O4P-C5A	-2.39	112.61	121.22
2	D	400	PLP	O3-C3-C2	-2.39	113.36	117.61
2	H	400	PLP	O3-C3-C2	-2.35	113.43	117.61
2	D	400	PLP	C5A-C5-C4	-2.18	116.33	121.41
2	E	400	PLP	C5A-C5-C4	-2.14	116.43	121.41
2	H	400	PLP	C5A-C5-C4	-2.07	116.59	121.41
2	G	400	PLP	O3-C3-C4	2.02	127.56	120.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

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%)	0.20	8 (2%) 62 63	9, 17, 28, 39	0
1	B	394/399 (98%)	0.30	8 (2%) 62 63	10, 18, 32, 49	0
1	C	394/399 (98%)	0.05	5 (1%) 74 75	6, 11, 22, 44	0
1	D	394/399 (98%)	0.18	8 (2%) 62 63	8, 14, 26, 51	0
1	E	394/399 (98%)	0.26	10 (2%) 54 56	7, 17, 31, 50	0
1	F	394/399 (98%)	0.03	5 (1%) 74 75	5, 12, 23, 47	0
1	G	394/399 (98%)	0.20	6 (1%) 70 72	8, 16, 28, 47	0
1	H	394/399 (98%)	0.35	12 (3%) 48 49	10, 18, 31, 50	0
All	All	3152/3192 (98%)	0.20	62 (1%) 62 63	5, 16, 29, 51	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	ILE	9.2
1	H	2	ILE	9.2
1	G	1	MET	8.5
1	G	2	ILE	7.2
1	F	1	MET	6.8
1	H	195	LYS	6.8
1	C	1	MET	5.1
1	D	1	MET	4.9
1	B	2	ILE	4.8
1	E	246	GLY	4.5
1	F	2	ILE	4.3
1	D	393	LEU	4.2
1	H	1	MET	4.1
1	A	23	TYR	3.9
1	B	246	GLY	3.8
1	C	2	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	393	LEU	3.7
1	B	1	MET	3.5
1	E	268	THR	3.3
1	H	246	GLY	3.3
1	A	163	LYS	3.2
1	D	394	LYS	3.2
1	D	256	ASP	3.2
1	F	394	LYS	2.8
1	H	394	LYS	2.8
1	C	31	ASN	2.7
1	D	103	PHE	2.7
1	E	392	ASP	2.6
1	E	197	ASP	2.6
1	H	84	GLN	2.6
1	B	336	LYS	2.6
1	B	390	LEU	2.6
1	A	246	GLY	2.5
1	B	352	ILE	2.5
1	H	212	PRO	2.4
1	D	246	GLY	2.4
1	A	263	LYS	2.4
1	E	394	LYS	2.4
1	F	393	LEU	2.4
1	B	338	ASP	2.4
1	A	161	LYS	2.4
1	A	184	ASP	2.4
1	H	352	ILE	2.3
1	E	154	GLN	2.3
1	H	256	ASP	2.3
1	F	352	ILE	2.3
1	H	393	LEU	2.3
1	E	335	LEU	2.3
1	A	268	THR	2.3
1	C	268	THR	2.3
1	C	23	TYR	2.3
1	E	336	LYS	2.3
1	G	268	THR	2.2
1	E	245	MET	2.2
1	H	134	GLU	2.1
1	E	225	GLN	2.1
1	H	245	MET	2.1
1	G	195	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	86	ASP	2.1
1	G	136	LYS	2.0
1	D	60	THR	2.0
1	A	195	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PLP	H	400	15/16	0.19	4.34	17,20,34,35	0
2	PLP	C	400	15/16	0.16	3.79	10,14,23,26	0
2	PLP	F	400	15/16	0.17	3.37	9,14,24,26	0
2	PLP	D	400	15/16	0.15	2.79	16,18,26,27	0
2	PLP	A	400	15/16	0.15	2.78	17,20,29,32	0
2	PLP	E	400	15/16	0.17	2.66	16,18,28,30	0
2	PLP	B	400	15/16	0.17	2.64	15,19,26,28	0
2	PLP	G	400	15/16	0.15	2.35	14,17,25,28	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.