Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 03:56 PM EDT

PDB ID	:	2NV9
Title	:	The X-ray Crystal Structure of the Paramecium bursaria Chlorella virus arginine decarboxylase
Authors	:	Shah, R.H.; Akella, R.; Goldsmith, E.; Phillips, M.A.
Deposited on	:	2006-11-11
Resolution	:	1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

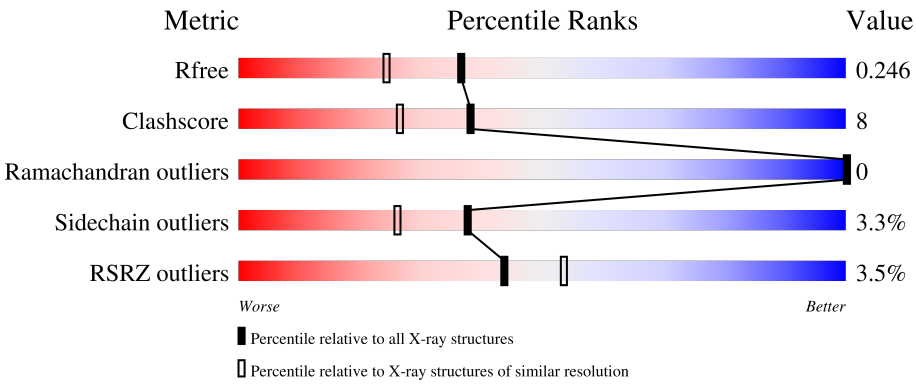
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	372	3% 87% 12% •
1	B	372	3% 87% 12% •
1	C	372	5% 85% 12% • •
1	D	372	4% 83% 14% • •
1	E	372	% 85% 13% • •

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Mol	Chain	Length	Quality of chain
1	F	372	2% 84% 15%
1	G	372	5% 81% 15%
1	H	372	3% 87% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	A	2001	-	-	X	-
2	PLP	B	2002	-	-	X	-
2	PLP	C	2003	-	-	X	-
2	PLP	D	2004	-	-	X	-
2	PLP	E	2005	-	-	X	-
2	PLP	F	2006	-	-	X	-
2	PLP	G	2007	-	-	X	-
2	PLP	H	2008	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24712 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.

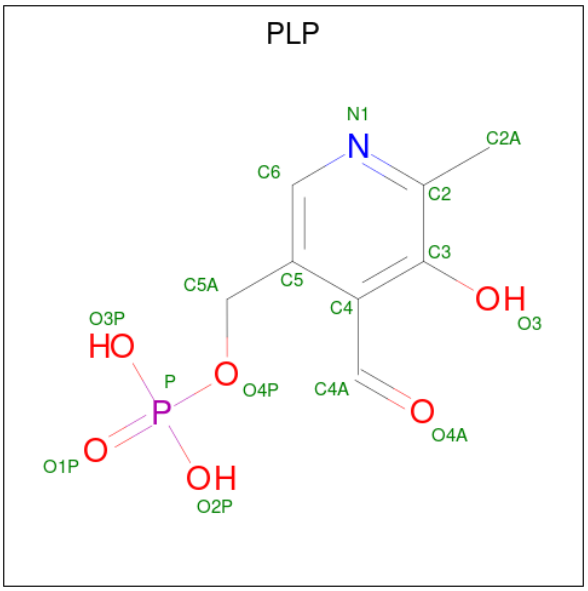
- Molecule 1 is a protein called A207R protein, arginine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	371	2955	1890	482	570	13	0	1	0
1	B	372	2962	1896	483	570	13	0	1	0
1	C	367	2925	1874	478	560	13	0	1	0
1	D	363	2890	1853	471	553	13	0	1	0
1	E	370	2945	1884	479	569	13	0	1	0
1	F	369	2936	1882	478	563	13	0	1	0
1	G	362	2885	1848	468	556	13	0	2	0
1	H	367	2915	1868	476	558	13	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	ALA	THR	engineered mutation	UNP Q84527
B	142	ALA	THR	engineered mutation	UNP Q84527
C	142	ALA	THR	engineered mutation	UNP Q84527
D	142	ALA	THR	engineered mutation	UNP Q84527
E	142	ALA	THR	engineered mutation	UNP Q84527
F	142	ALA	THR	engineered mutation	UNP Q84527
G	142	ALA	THR	engineered mutation	UNP Q84527
H	142	ALA	THR	engineered mutation	UNP Q84527

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	E	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	F	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	G	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	H	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	143	Total	O	0	0
			143	143		
3	B	146	Total	O	0	0
			146	146		
3	C	112	Total	O	0	0
			112	112		
3	D	128	Total	O	0	0
			128	128		

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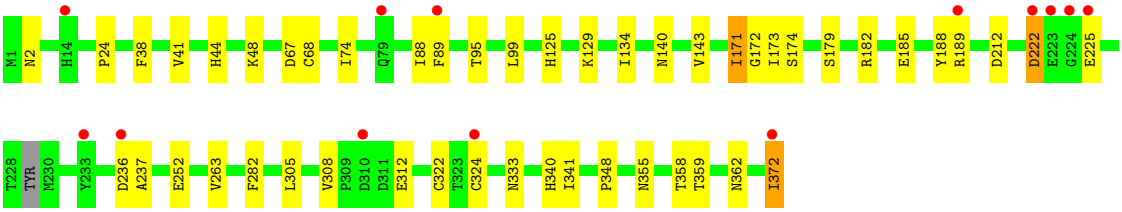
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	E	205	205	205	0	0
			Total	O		
3	F	137	137	137	0	0
			Total	O		
3	G	135	135	135	0	0
			Total	O		
3	H	165	165	165	0	0

3 Residue-property plots (i)

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

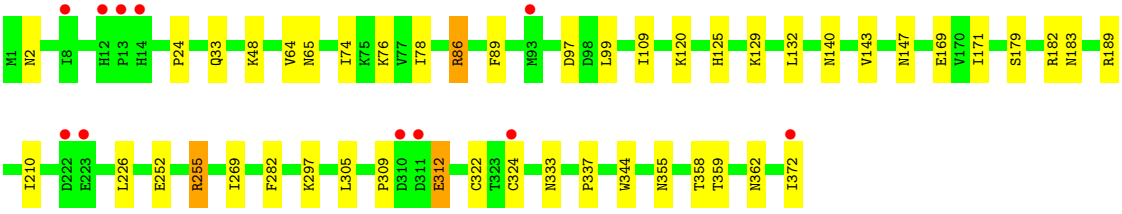
• Molecule 1: A207R protein, arginine decarboxylase

Chain A:



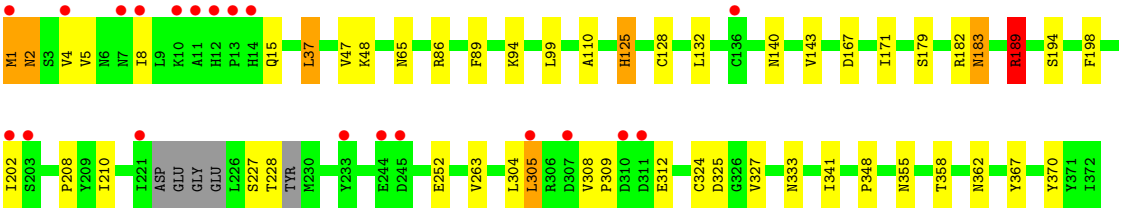
• Molecule 1: A207R protein, arginine decarboxylase

Chain B:



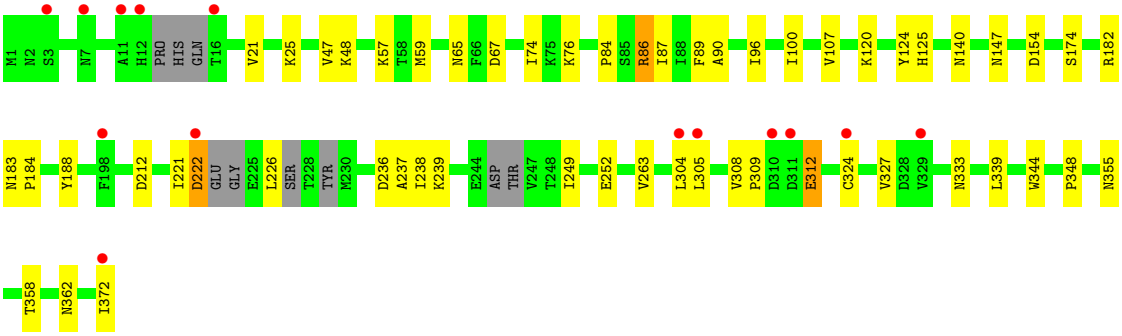
• Molecule 1: A207R protein, arginine decarboxylase

Chain C:



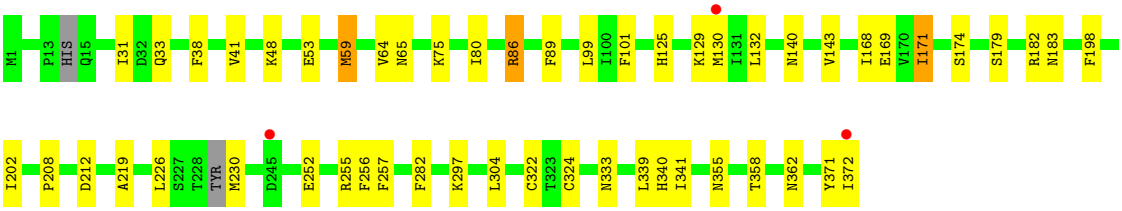
• Molecule 1: A207R protein, arginine decarboxylase

Chain D:



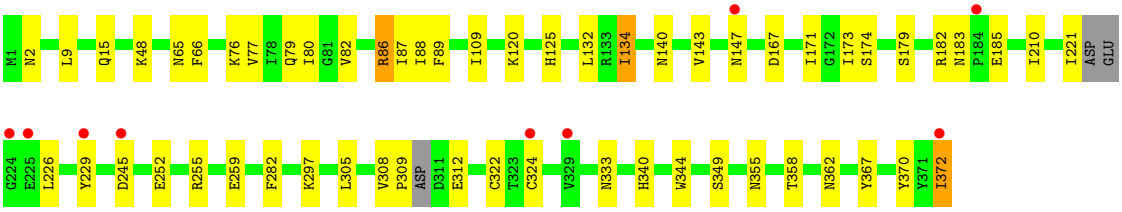
• Molecule 1: A207R protein, arginine decarboxylase

Chain E:



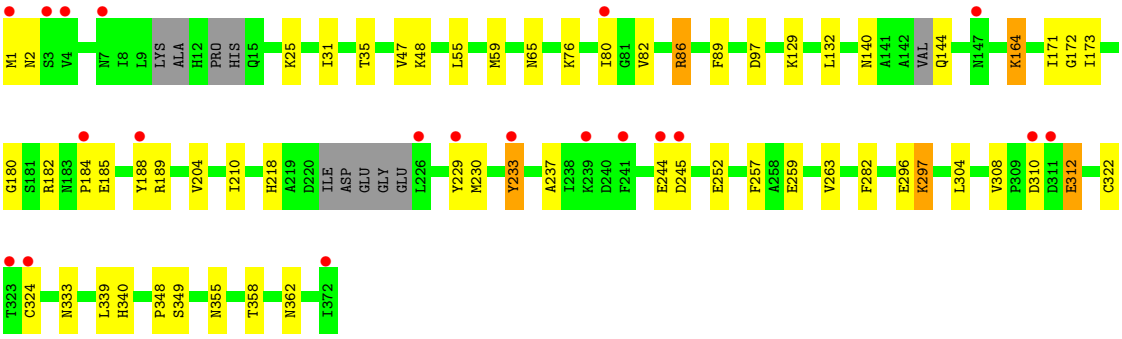
• Molecule 1: A207R protein, arginine decarboxylase

Chain F:



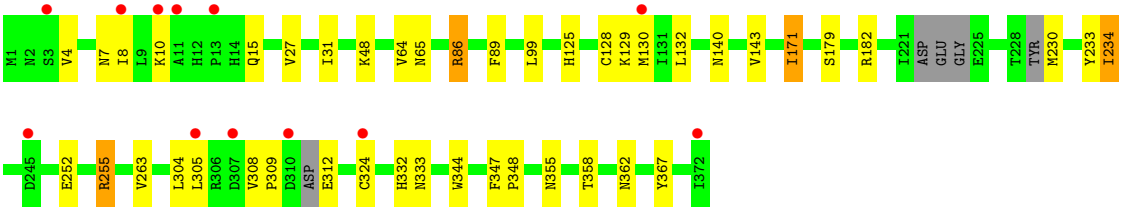
• Molecule 1: A207R protein, arginine decarboxylase

Chain G:



• Molecule 1: A207R protein, arginine decarboxylase

Chain H:


M1
N2
S3
V4
N7
I8
L9
K10
A11
H12
P13
H14
Q15
V27
I31
K48
V64
N65
R86
F89
L99
H125
C128
K129
M130
I131
L132
N140
V143
I171
S179
R182
I221
ASP
GLU
GLY
E225
T228
TYR
M230
Y233
I234
D245
E252
R255
V263
L304
L305
R306
D307
V308
P309
D310
ASP
E312
C324
H332
N333
W344
F347
P348
N355
T358
N362
Y367
I372

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.11Å 116.87Å 269.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 1.95 48.88 – 1.95	Depositor EDS
% Data completeness (in resolution range)	88.7 (48.91-1.95) 88.7 (48.88-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.242 0.225 , 0.246	Depositor DCC
R_{free} test set	1455 reflections (0.62%)	wwPDB-VP
Wilson B-factor (Å^2)	15.5	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	24712	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8352e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.81	0/3029	0.70	1/4115 (0.0%)
1	B	0.79	0/3038	0.71	3/4129 (0.1%)
1	C	0.75	0/2998	0.73	3/4072 (0.1%)
1	D	0.76	0/2958	0.73	2/4011 (0.0%)
1	E	0.80	0/3017	0.72	1/4097 (0.0%)
1	F	0.76	0/3009	0.71	3/4086 (0.1%)
1	G	0.78	0/2954	0.72	2/4008 (0.0%)
1	H	0.77	0/2986	0.72	4/4053 (0.1%)
All	All	0.78	0/23989	0.72	19/32571 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	189	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	F	86	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	E	86	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	H	86	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	B	86	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	H	255	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	F	86	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	B	255	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	255	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	G	86	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	G	245	ASP	CB-CG-OD2	5.87	123.58	118.30
1	D	86	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	C	189	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	H	86	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	H	255	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	F	255	ARG	NE-CZ-NH2	-5.46	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	325	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	67	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	154	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2955	0	2844	44	0
1	B	2962	0	2849	46	0
1	C	2925	0	2824	48	0
1	D	2890	0	2788	47	0
1	E	2945	0	2836	45	0
1	F	2936	0	2832	59	0
1	G	2885	0	2773	53	0
1	H	2915	0	2814	47	0
2	A	16	0	7	9	0
2	B	16	0	7	10	0
2	C	16	0	7	8	0
2	D	16	0	8	6	0
2	E	16	0	7	7	0
2	F	16	0	7	9	0
2	G	16	0	8	8	0
2	H	16	0	7	9	0
3	A	143	0	0	3	0
3	B	146	0	0	7	0
3	C	112	0	0	0	0
3	D	128	0	0	3	0
3	E	205	0	0	2	0
3	F	137	0	0	3	0
3	G	135	0	0	5	0
3	H	165	0	0	2	0
All	All	24712	0	22618	348	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 8.

All (348) 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:F:48:LYS:NZ	2:F:2006:PLP:C4A	2.05	1.20
1:A:48:LYS:NZ	2:A:2001:PLP:C4A	2.11	1.14
1:C:48:LYS:NZ	2:C:2003:PLP:H4A	1.60	1.14
1:H:308:VAL:HB	1:H:312:GLU:HG3	1.29	1.12
1:A:308:VAL:HB	1:A:312:GLU:HG3	1.28	1.10
1:C:48:LYS:HZ3	2:C:2003:PLP:C4A	1.61	1.08
1:D:48:LYS:NZ	2:D:2004:PLP:C4A	2.18	1.07
1:F:48:LYS:HZ3	2:F:2006:PLP:C4A	1.63	1.06
1:G:48:LYS:NZ	2:G:2007:PLP:C4A	2.18	1.05
1:H:48:LYS:NZ	2:H:2008:PLP:C4A	2.21	1.04
1:A:48:LYS:HZ1	2:A:2001:PLP:C4A	1.72	1.03
1:F:48:LYS:NZ	2:F:2006:PLP:H4A	1.72	1.03
1:G:48:LYS:NZ	2:G:2007:PLP:H4A	1.74	1.02
1:E:48:LYS:NZ	2:E:2005:PLP:C4A	2.23	1.00
1:D:48:LYS:HZ3	2:D:2004:PLP:C4A	1.72	1.00
1:B:48:LYS:HZ1	2:B:2002:PLP:H4A	1.27	1.00
1:B:48:LYS:HZ3	2:B:2002:PLP:C4A	1.70	0.99
1:C:308:VAL:HB	1:C:312:GLU:HG3	1.42	0.98
1:G:48:LYS:HZ1	2:G:2007:PLP:C4A	1.74	0.98
1:F:333:ASN:HD21	1:H:333:ASN:HD21	1.13	0.96
1:G:48:LYS:HZ2	2:G:2007:PLP:H4A	1.27	0.95
1:C:48:LYS:HZ1	2:C:2003:PLP:H4A	1.16	0.95
1:G:324[B]:CYS:SG	1:H:48:LYS:NZ	2.38	0.95
1:C:1:MET:HG2	1:C:2:ASN:H	1.29	0.94
1:D:76:LYS:HE2	3:D:2113:HOH:O	1.69	0.93
1:H:48:LYS:HZ1	2:H:2008:PLP:C4A	1.80	0.93
1:F:48:LYS:HZ1	2:F:2006:PLP:H4A	1.33	0.92
1:E:48:LYS:NZ	1:F:324[B]:CYS:SG	2.44	0.90
1:B:372:ILE:HG12	3:B:2049:HOH:O	1.75	0.87
1:G:48:LYS:NZ	1:H:324[B]:CYS:SG	2.47	0.87
1:B:48:LYS:HZ1	2:B:2002:PLP:C4A	1.76	0.86
1:E:130:MET:O	1:E:171:ILE:HD13	1.73	0.86
1:E:371:TYR:O	1:E:372:ILE:HG12	1.77	0.85
1:C:48:LYS:HZ1	2:C:2003:PLP:C4A	1.76	0.85
1:E:48:LYS:HZ1	2:E:2005:PLP:C4A	1.85	0.84
1:G:244:GLU:OE2	1:G:244:GLU:HA	1.78	0.84
1:F:48:LYS:HZ1	2:F:2006:PLP:C4A	1.85	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:ASN:HD21	1:G:333:ASN:HD21	1.24	0.83
1:A:48:LYS:HZ3	2:A:2001:PLP:C4A	1.89	0.83
1:F:185:GLU:OE1	1:G:229:TYR:CD1	2.33	0.82
1:B:48:LYS:NZ	2:B:2002:PLP:H4A	1.86	0.81
1:D:48:LYS:HZ1	2:D:2004:PLP:H4A	1.45	0.81
1:H:48:LYS:HZ1	2:H:2008:PLP:H4A	1.43	0.81
1:H:309:PRO:HD2	1:H:312:GLU:HG2	1.63	0.80
1:F:308:VAL:HB	1:F:312:GLU:CG	2.12	0.80
1:H:332:HIS:HD2	3:H:2166:HOH:O	1.63	0.79
1:F:308:VAL:HB	1:F:312:GLU:HG3	1.63	0.79
1:A:48:LYS:HZ1	2:A:2001:PLP:H4A	1.48	0.79
1:D:48:LYS:HZ1	2:D:2004:PLP:C4A	1.96	0.79
1:H:31:ILE:HD12	1:H:64:VAL:HG21	1.66	0.77
1:A:48:LYS:NZ	2:A:2001:PLP:H4A	1.99	0.76
1:E:65:ASN:OD1	1:E:86:ARG:HD3	1.86	0.76
1:F:66:PHE:HB2	1:F:87:ILE:HD12	1.67	0.75
1:A:129:LYS:HB3	1:A:171:ILE:HD12	1.69	0.74
1:E:48:LYS:HZ3	2:E:2005:PLP:C4A	2.00	0.74
1:G:97:ASP:HB2	3:G:2132:HOH:O	1.88	0.74
1:G:296:GLU:O	1:G:297:LYS:HG2	1.87	0.74
1:B:372:ILE:HA	3:B:2092:HOH:O	1.86	0.73
1:H:48:LYS:NZ	2:H:2008:PLP:H4A	2.03	0.72
1:A:341:ILE:HD13	1:B:120:LYS:HD2	1.70	0.71
1:C:48:LYS:CE	2:C:2003:PLP:H4A	2.18	0.71
1:B:309:PRO:HD2	1:B:312:GLU:HG3	1.72	0.71
1:E:48:LYS:HZ1	2:E:2005:PLP:H4A	1.56	0.70
1:G:31:ILE:HD13	1:G:257:PHE:CE1	2.26	0.70
1:D:308:VAL:HB	1:D:312:GLU:HG3	1.73	0.70
1:F:182:ARG:HH11	1:G:140:ASN:HD21	1.40	0.70
1:B:333:ASN:HD21	1:C:333:ASN:HD21	1.40	0.69
1:H:48:LYS:HZ3	2:H:2008:PLP:C4A	2.02	0.68
1:D:355:ASN:O	1:D:358:THR:HG23	1.94	0.68
1:D:372:ILE:OXT	1:D:372:ILE:HG13	1.93	0.67
1:H:130:MET:O	1:H:171:ILE:HD13	1.94	0.67
1:F:305:LEU:HD12	1:F:344:TRP:CB	2.25	0.67
1:H:324[B]:CYS:H	1:H:362:ASN:HD21	1.43	0.67
1:B:109:ILE:HD11	3:B:2067:HOH:O	1.94	0.67
1:D:324[A]:CYS:H	1:D:362:ASN:HD21	1.41	0.67
1:A:333:ASN:HD21	1:D:333:ASN:HD21	1.43	0.67
1:D:221:ILE:HG12	1:D:226:LEU:HD23	1.77	0.66
1:H:230:MET:O	1:H:234:ILE:HD13	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:PRO:HD2	1:C:312:GLU:CG	2.26	0.66
1:G:76:LYS:HE2	3:G:2115:HOH:O	1.96	0.66
1:C:1:MET:HG2	1:C:2:ASN:N	2.04	0.65
1:G:129:LYS:HE3	1:G:171:ILE:HG21	1.77	0.65
1:E:31:ILE:HD13	1:E:257:PHE:CE1	2.32	0.65
1:F:48:LYS:CE	2:F:2006:PLP:H4A	2.26	0.65
1:F:324[B]:CYS:H	1:F:362:ASN:ND2	1.95	0.65
1:G:55:LEU:O	1:G:59:MET:HG3	1.97	0.65
1:H:324[B]:CYS:H	1:H:362:ASN:ND2	1.95	0.65
1:D:48:LYS:NZ	2:D:2004:PLP:H4A	2.01	0.65
1:C:309:PRO:HD2	1:C:312:GLU:HG2	1.78	0.64
1:E:129:LYS:HB3	1:E:171:ILE:HD12	1.78	0.64
1:A:324[A]:CYS:SG	1:B:48:LYS:NZ	2.65	0.64
1:H:324[A]:CYS:H	1:H:362:ASN:HD21	1.44	0.64
1:H:332:HIS:CD2	3:H:2166:HOH:O	2.42	0.64
1:B:109:ILE:CD1	3:B:2067:HOH:O	2.47	0.63
1:H:27:VAL:O	1:H:31:ILE:HG12	1.98	0.63
1:A:95:THR:HG22	1:B:269:ILE:HD12	1.81	0.63
1:A:182:ARG:HH11	1:C:140:ASN:HD21	1.44	0.63
1:A:48:LYS:NZ	1:B:324[B]:CYS:SG	2.63	0.62
1:E:48:LYS:HZ2	1:F:324[B]:CYS:CB	2.11	0.62
1:D:324[B]:CYS:H	1:D:362:ASN:HD21	1.44	0.62
1:C:183:ASN:C	1:C:183:ASN:HD22	2.02	0.62
1:C:324[B]:CYS:H	1:C:362:ASN:HD21	1.46	0.61
1:F:171:ILE:HD12	1:F:210:ILE:HD12	1.81	0.61
1:C:355:ASN:O	1:C:358:THR:HG23	2.00	0.61
1:D:327:VAL:HB	3:D:2130:HOH:O	1.99	0.61
1:D:304:LEU:HD21	1:D:339:LEU:HD21	1.83	0.61
1:C:48:LYS:CE	2:C:2003:PLP:C4A	2.79	0.61
1:A:355:ASN:O	1:A:358:THR:HG23	2.01	0.61
1:F:305:LEU:HD12	1:F:344:TRP:HB3	1.81	0.60
1:B:305:LEU:HD12	1:B:344:TRP:HB3	1.83	0.60
1:H:324[A]:CYS:H	1:H:362:ASN:ND2	1.99	0.60
1:F:134:ILE:HD13	1:F:174:SER:O	2.01	0.60
1:H:309:PRO:HD2	1:H:312:GLU:CG	2.30	0.60
1:D:238:ILE:HD12	1:D:249:ILE:HD13	1.83	0.60
1:D:263:VAL:HG12	1:D:348:PRO:HA	1.83	0.60
1:H:129:LYS:HB3	1:H:171:ILE:HD12	1.84	0.60
1:F:308:VAL:HB	1:F:312:GLU:HG2	1.84	0.60
1:B:255:ARG:HD2	2:B:2002:PLP:O1P	2.02	0.60
1:A:324[B]:CYS:H	1:A:362:ASN:HD21	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:324[B]:CYS:H	1:F:362:ASN:HD21	1.49	0.59
1:A:24:PRO:HD2	1:A:372:ILE:CG1	2.32	0.59
1:A:324[A]:CYS:H	1:A:362:ASN:HD21	1.49	0.59
1:B:305:LEU:HD12	1:B:344:TRP:CB	2.32	0.59
1:A:324[A]:CYS:H	1:A:362:ASN:ND2	2.00	0.59
1:E:65:ASN:OD1	1:E:86:ARG:CD	2.51	0.59
1:F:77:VAL:HG11	1:F:87:ILE:HD11	1.85	0.59
1:A:225:GLU:OE1	1:A:225:GLU:HA	2.01	0.59
1:G:48:LYS:HZ2	2:G:2007:PLP:C4A	1.99	0.59
1:D:372:ILE:OXT	1:D:372:ILE:CG1	2.51	0.58
1:B:324[B]:CYS:H	1:B:362:ASN:HD21	1.51	0.58
1:D:324[A]:CYS:H	1:D:362:ASN:ND2	2.01	0.58
1:D:96:ILE:HD11	1:D:120:LYS:HG2	1.84	0.58
1:F:65:ASN:OD1	1:F:86:ARG:HD2	2.03	0.58
1:F:229:TYR:CD2	1:G:185:GLU:OE1	2.57	0.58
1:G:144:GLN:N	3:G:2100:HOH:O	2.37	0.58
1:F:185:GLU:OE1	1:G:229:TYR:HD1	1.86	0.57
1:F:355:ASN:O	1:F:358:THR:HG23	2.04	0.57
1:C:324[A]:CYS:H	1:C:362:ASN:HD21	1.49	0.57
1:A:48:LYS:CE	2:A:2001:PLP:C4A	2.83	0.57
1:A:48:LYS:CE	2:A:2001:PLP:H4A	2.34	0.57
1:E:324[A]:CYS:H	1:E:362:ASN:HD21	1.53	0.57
1:C:48:LYS:NZ	1:D:324[A]:CYS:SG	2.67	0.57
1:F:309:PRO:HD2	1:F:312:GLU:HG2	1.85	0.56
1:H:355:ASN:O	1:H:358:THR:HG23	2.04	0.56
1:A:143:VAL:HB	1:A:179:SER:HB3	1.87	0.56
1:C:171:ILE:HD12	1:C:210:ILE:HD12	1.87	0.56
1:C:1:MET:CG	1:C:2:ASN:H	2.10	0.56
1:E:48:LYS:NZ	2:E:2005:PLP:H4A	2.13	0.56
1:E:129:LYS:HE3	1:E:169:GLU:OE2	2.05	0.56
1:F:182:ARG:HH11	1:G:140:ASN:ND2	2.02	0.55
1:F:76:LYS:O	1:F:80:ILE:HD12	2.06	0.55
1:C:252:GLU:O	2:C:2003:PLP:H6	2.07	0.55
1:G:164:LYS:HG3	1:G:204:VAL:HG12	1.88	0.55
1:A:372:ILE:HG22	3:A:2089:HOH:O	2.06	0.55
1:B:282:PHE:O	1:B:322:CYS:HB3	2.07	0.55
1:E:324[A]:CYS:H	1:E:362:ASN:ND2	2.05	0.55
1:A:324[B]:CYS:H	1:A:362:ASN:ND2	2.04	0.55
1:B:324[A]:CYS:H	1:B:362:ASN:HD21	1.53	0.55
1:F:324[A]:CYS:H	1:F:362:ASN:HD21	1.54	0.54
1:G:355:ASN:O	1:G:358:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:PRO:HD2	1:B:372:ILE:HG13	1.88	0.54
1:B:312:GLU:OE1	1:B:337:PRO:HB3	2.07	0.54
1:C:324[B]:CYS:H	1:C:362:ASN:ND2	2.06	0.54
1:F:229:TYR:HD2	1:G:185:GLU:OE1	1.90	0.54
1:G:324[A]:CYS:H	1:G:362:ASN:HD21	1.53	0.54
1:E:324[A]:CYS:SG	1:F:48:LYS:NZ	2.69	0.54
1:H:125:HIS:CE1	1:H:128:CYS:HB2	2.42	0.54
1:B:140:ASN:HD21	1:D:182:ARG:HH11	1.56	0.54
1:C:1:MET:O	1:C:5:VAL:HG23	2.08	0.54
1:E:371:TYR:O	1:E:372:ILE:CG1	2.52	0.54
1:G:65:ASN:OD1	1:G:86:ARG:CD	2.56	0.54
1:B:324[B]:CYS:H	1:B:362:ASN:ND2	2.05	0.53
1:D:324[B]:CYS:H	1:D:362:ASN:ND2	2.06	0.53
1:G:171:ILE:HD12	1:G:210:ILE:HD12	1.89	0.53
1:F:48:LYS:HZ3	2:F:2006:PLP:C4	2.20	0.52
1:F:324[A]:CYS:H	1:F:362:ASN:ND2	2.06	0.52
1:H:255:ARG:HD2	2:H:2008:PLP:O1P	2.09	0.52
1:A:222:ASP:HB3	1:C:189:ARG:HH11	1.74	0.52
1:F:221:ILE:HG12	1:F:226:LEU:HD23	1.91	0.52
1:C:324[A]:CYS:H	1:C:362:ASN:ND2	2.07	0.52
1:D:305:LEU:HD12	1:D:344:TRP:CB	2.40	0.52
1:H:48:LYS:CE	2:H:2008:PLP:C4A	2.87	0.52
1:A:188:TYR:CD1	1:A:237:ALA:HB2	2.44	0.52
1:C:183:ASN:C	1:C:183:ASN:ND2	2.63	0.52
1:A:222:ASP:HB3	1:C:189:ARG:NH1	2.24	0.52
1:C:341:ILE:HD13	1:D:120:LYS:HD2	1.92	0.52
1:D:21:VAL:HG12	1:D:372:ILE:HD13	1.91	0.52
1:G:296:GLU:O	1:G:297:LYS:HE2	2.09	0.52
1:H:358:THR:HG21	1:H:367:TYR:HE2	1.75	0.52
1:B:48:LYS:CE	2:B:2002:PLP:C4A	2.86	0.52
1:D:67:ASP:OD2	1:D:90:ALA:HB3	2.10	0.52
1:E:324[B]:CYS:H	1:E:362:ASN:HD21	1.56	0.51
1:D:76:LYS:HD3	3:D:2105:HOH:O	2.08	0.51
1:E:182:ARG:HH11	1:H:140:ASN:HD21	1.58	0.51
1:D:96:ILE:CD1	1:D:120:LYS:HG2	2.40	0.51
1:F:333:ASN:HD21	1:H:333:ASN:ND2	1.95	0.51
1:D:305:LEU:HD12	1:D:344:TRP:HB3	1.93	0.51
1:F:48:LYS:CE	2:F:2006:PLP:C4A	2.86	0.51
1:G:324[B]:CYS:H	1:G:362:ASN:HD21	1.57	0.51
1:E:143:VAL:HB	1:E:179:SER:HB3	1.93	0.51
1:G:229:TYR:CE2	1:G:230:MET:SD	3.04	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:65:ASN:OD1	1:H:86:ARG:CD	2.59	0.51
1:B:74:ILE:HG22	1:B:78:ILE:HD12	1.92	0.51
1:E:202:ILE:HD13	1:E:208:PRO:HD2	1.93	0.50
1:H:305:LEU:HD12	1:H:344:TRP:CB	2.41	0.50
1:E:59:MET:HE2	1:E:64:VAL:HG11	1.93	0.50
1:B:109:ILE:N	1:B:109:ILE:HD12	2.26	0.50
1:A:140:ASN:HD21	1:C:182:ARG:HH11	1.59	0.50
1:E:48:LYS:CE	2:E:2005:PLP:C4A	2.90	0.50
1:F:305:LEU:HD12	1:F:344:TRP:HB2	1.93	0.50
1:B:48:LYS:HZ3	2:B:2002:PLP:C4	2.24	0.50
1:F:143:VAL:HB	1:F:179:SER:HB3	1.94	0.50
1:G:1:MET:HG3	1:G:2:ASN:N	2.26	0.49
1:D:74:ILE:HD12	1:D:107:VAL:HG21	1.94	0.49
1:G:188:TYR:CD1	1:G:237:ALA:HB2	2.47	0.49
1:C:143:VAL:HB	1:C:179:SER:HB3	1.94	0.49
1:E:252:GLU:O	2:E:2005:PLP:H6	2.13	0.49
1:G:308:VAL:HB	1:G:312:GLU:HG3	1.95	0.49
1:H:308:VAL:CB	1:H:312:GLU:HG3	2.20	0.49
1:G:144:GLN:N	3:G:2048:HOH:O	2.45	0.49
1:E:130:MET:O	1:E:171:ILE:CD1	2.55	0.49
1:H:305:LEU:HD12	1:H:344:TRP:HB3	1.94	0.49
1:B:189:ARG:NH2	1:D:222:ASP:HB3	2.28	0.48
1:F:65:ASN:OD1	1:F:86:ARG:CD	2.61	0.48
1:D:188:TYR:CD1	1:D:237:ALA:HB2	2.48	0.48
1:E:140:ASN:HD21	1:H:182:ARG:HH11	1.60	0.48
1:G:48:LYS:CE	2:G:2007:PLP:H4A	2.42	0.48
1:H:125:HIS:CG	1:H:128:CYS:HB2	2.47	0.48
1:H:125:HIS:ND1	1:H:128:CYS:HB2	2.28	0.48
1:B:143:VAL:HB	1:B:179:SER:HB3	1.95	0.48
1:F:140:ASN:ND2	1:G:182:ARG:HE	2.11	0.48
1:B:324[A]:CYS:H	1:B:362:ASN:ND2	2.11	0.48
1:F:340:HIS:HD2	3:F:2010:HOH:O	1.97	0.48
1:G:244:GLU:OE2	1:G:244:GLU:CA	2.55	0.48
1:H:48:LYS:CE	2:H:2008:PLP:H4A	2.44	0.47
1:A:282:PHE:O	1:A:322:CYS:HB3	2.14	0.47
1:G:185:GLU:HG2	1:G:189:ARG:HE	1.78	0.47
1:G:129:LYS:CE	1:G:171:ILE:HG21	2.43	0.47
1:G:304:LEU:HD11	1:G:339:LEU:HD21	1.96	0.47
1:A:48:LYS:HZ3	2:A:2001:PLP:C4	2.26	0.47
1:A:185:GLU:OE1	1:C:227:SER:OG	2.30	0.47
1:E:324[B]:CYS:H	1:E:362:ASN:ND2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4:VAL:O	1:H:8:ILE:HG12	2.15	0.47
1:A:359:THR:HG22	1:B:359:THR:HG22	1.97	0.47
1:A:340:HIS:HD2	3:A:2012:HOH:O	1.97	0.47
1:C:358:THR:HG21	1:C:367:TYR:CE2	2.50	0.47
1:E:355:ASN:O	1:E:358:THR:HG23	2.15	0.47
1:G:55:LEU:O	1:G:59:MET:CG	2.62	0.47
1:G:263:VAL:HG12	1:G:348:PRO:HA	1.96	0.47
1:H:358:THR:HG21	1:H:367:TYR:CE2	2.50	0.47
1:B:252:GLU:O	2:B:2002:PLP:H6	2.15	0.46
1:E:341:ILE:HD13	1:F:120:LYS:HD2	1.97	0.46
1:F:252:GLU:O	2:F:2006:PLP:H6	2.15	0.46
1:H:263:VAL:HG12	1:H:348:PRO:HA	1.96	0.46
1:H:143:VAL:HB	1:H:179:SER:HB3	1.95	0.46
1:E:48:LYS:NZ	1:F:324[B]:CYS:CB	2.77	0.46
3:B:2115:HOH:O	1:E:33:GLN:NE2	2.46	0.46
1:E:182:ARG:HH11	1:H:140:ASN:ND2	2.14	0.46
1:A:38:PHE:HB3	1:A:41:VAL:HB	1.97	0.46
1:D:304:LEU:HD11	1:D:339:LEU:HD22	1.96	0.46
1:E:340:HIS:HD2	3:E:2036:HOH:O	1.98	0.46
1:C:358:THR:HG21	1:C:367:TYR:HE2	1.81	0.46
1:D:65:ASN:OD1	1:D:86:ARG:CD	2.64	0.46
1:B:147:ASN:HB3	3:B:2140:HOH:O	2.15	0.46
1:B:355:ASN:O	1:B:358:THR:HG23	2.15	0.45
1:G:282:PHE:O	1:G:322:CYS:HB3	2.16	0.45
1:A:174:SER:HB3	1:A:212:ASP:HB3	1.97	0.45
1:C:263:VAL:HG12	1:C:348:PRO:HA	1.99	0.45
1:F:308:VAL:CB	1:F:312:GLU:HG3	2.39	0.45
1:E:53:GLU:HG3	1:E:80:ILE:HD11	1.98	0.45
1:G:172:GLY:C	1:G:173:ILE:HD12	2.37	0.45
1:G:252:GLU:O	2:G:2007:PLP:H6	2.17	0.45
1:C:15:GLN:NE2	1:C:370:TYR:OH	2.49	0.45
1:F:282:PHE:O	1:F:322:CYS:HB3	2.17	0.45
1:B:182:ARG:HH11	1:D:140:ASN:HD21	1.63	0.45
1:C:48:LYS:HZ3	2:C:2003:PLP:C4	2.29	0.45
1:H:65:ASN:OD1	1:H:86:ARG:HD2	2.17	0.45
1:C:1:MET:CG	1:C:2:ASN:N	2.72	0.44
1:G:48:LYS:CE	2:G:2007:PLP:C4A	2.93	0.44
1:A:182:ARG:HH11	1:C:140:ASN:ND2	2.13	0.44
1:A:340:HIS:HE1	3:A:2062:HOH:O	1.99	0.44
1:D:309:PRO:HD2	1:D:312:GLU:HG3	1.99	0.44
1:F:77:VAL:HG12	1:F:82:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:358:THR:HG21	1:F:367:TYR:CE2	2.52	0.44
1:H:31:ILE:HD12	1:H:64:VAL:CG2	2.44	0.44
1:A:44:HIS:ND1	1:A:88:ILE:HG12	2.31	0.44
1:E:282:PHE:O	1:E:322:CYS:HB3	2.17	0.44
1:H:252:GLU:O	2:H:2008:PLP:H6	2.17	0.44
1:C:194:SER:O	1:C:198:PHE:HB2	2.18	0.44
1:G:65:ASN:OD1	1:G:86:ARG:HD3	2.18	0.44
1:E:255:ARG:O	1:E:256:PHE:C	2.57	0.43
1:E:304:LEU:HD11	1:E:339:LEU:HD21	2.00	0.43
1:A:68:CYS:CB	1:A:74:ILE:HD13	2.48	0.43
1:B:76:LYS:CE	3:B:2051:HOH:O	2.67	0.43
1:F:333:ASN:ND2	1:H:333:ASN:HD21	1.96	0.43
1:G:259:GLU:HG2	1:G:349:SER:HB3	1.99	0.43
1:A:263:VAL:HG12	1:A:348:PRO:HA	2.01	0.43
1:B:24:PRO:HD2	1:B:372:ILE:CG1	2.47	0.43
1:C:4:VAL:O	1:C:8:ILE:HG12	2.18	0.43
1:C:65:ASN:OD1	1:C:86:ARG:HD2	2.18	0.43
1:A:252:GLU:O	2:A:2001:PLP:H6	2.19	0.43
1:E:174:SER:HB3	1:E:212:ASP:HB3	2.01	0.43
1:E:230:MET:N	3:E:2126:HOH:O	2.51	0.43
1:A:172:GLY:C	1:A:173:ILE:HD12	2.40	0.43
1:C:309:PRO:HD2	1:C:312:GLU:HG3	1.98	0.43
1:D:96:ILE:HD12	1:D:124:TYR:CD2	2.54	0.43
1:F:372:ILE:HA	3:F:2027:HOH:O	2.19	0.43
1:B:182:ARG:HH11	1:D:140:ASN:ND2	2.17	0.42
1:F:324[B]:CYS:HB3	1:F:362:ASN:HD21	1.84	0.42
1:F:340:HIS:HE1	3:F:2073:HOH:O	2.02	0.42
1:C:202:ILE:HD13	1:C:208:PRO:HD2	2.01	0.42
1:B:171:ILE:HD12	1:B:210:ILE:HD12	2.01	0.42
1:D:183:ASN:HA	1:D:184:PRO:HD2	1.94	0.42
1:D:65:ASN:HB3	1:D:86:ARG:O	2.19	0.42
1:G:80:ILE:HG13	1:G:82:VAL:HG23	2.00	0.42
1:E:38:PHE:HB3	1:E:41:VAL:HB	2.02	0.42
1:F:88:ILE:HD12	1:F:109:ILE:HB	2.01	0.42
1:F:259:GLU:HG2	1:F:349:SER:HB3	2.02	0.42
1:B:48:LYS:CE	2:B:2002:PLP:H4A	2.49	0.42
1:C:125:HIS:CG	1:C:128:CYS:HB2	2.55	0.42
1:D:84:PRO:HA	1:D:87:ILE:HD12	2.02	0.42
1:G:180:GLY:HA2	1:G:218:HIS:CE1	2.55	0.42
1:D:100:ILE:HD11	1:D:124:TYR:CD1	2.55	0.41
1:E:75:LYS:HG3	1:E:101:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:SER:CB	1:D:212:ASP:HB3	2.50	0.41
1:F:134:ILE:HD12	1:F:173:ILE:CG2	2.50	0.41
1:D:252:GLU:O	2:D:2004:PLP:H6	2.20	0.41
1:B:33:GLN:HB3	1:B:226:LEU:HD12	2.01	0.41
1:C:305:LEU:HD13	1:C:305:LEU:HA	1.80	0.41
1:G:340:HIS:HD2	3:G:2021:HOH:O	2.02	0.41
1:A:185:GLU:O	1:A:189:ARG:HG3	2.21	0.41
1:F:15:GLN:NE2	1:F:370:TYR:OH	2.53	0.41
1:B:129:LYS:HE3	1:B:169:GLU:OE2	2.21	0.41
1:D:65:ASN:OD1	1:D:86:ARG:HD3	2.21	0.41
1:D:174:SER:HB3	1:D:212:ASP:HB3	2.03	0.41
1:E:130:MET:HG2	1:E:168:ILE:HG22	2.03	0.41
1:H:347:PHE:HA	1:H:348:PRO:HD3	1.91	0.41
1:F:9:LEU:HD11	1:F:305:LEU:HD13	2.03	0.41
1:F:358:THR:HG21	1:F:367:TYR:HE2	1.84	0.41
1:B:297:LYS:HA	1:B:297:LYS:HD2	1.90	0.40
1:C:37:LEU:HD11	1:C:228:THR:HG22	2.02	0.40
1:G:184:PRO:HB2	1:G:233:TYR:CD2	2.57	0.40
1:A:222:ASP:CB	1:C:189:ARG:NH1	2.85	0.40
1:B:48:LYS:NZ	2:B:2002:PLP:C4	2.82	0.40
1:B:65:ASN:OD1	1:B:86:ARG:CD	2.70	0.40
1:E:219:ALA:HB1	1:E:226:LEU:HD21	2.02	0.40
1:G:324[A]:CYS:H	1:G:362:ASN:ND2	2.18	0.40
1:C:94:LYS:HE3	1:C:110:ALA:HB1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	368/372 (99%)	354 (96%)	14 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	371/372 (100%)	362 (98%)	9 (2%)	0	100	100
1	C	362/372 (97%)	351 (97%)	11 (3%)	0	100	100
1	D	353/372 (95%)	340 (96%)	13 (4%)	0	100	100
1	E	365/372 (98%)	355 (97%)	10 (3%)	0	100	100
1	F	364/372 (98%)	353 (97%)	11 (3%)	0	100	100
1	G	354/372 (95%)	344 (97%)	10 (3%)	0	100	100
1	H	360/372 (97%)	349 (97%)	11 (3%)	0	100	100
All	All	2897/2976 (97%)	2808 (97%)	89 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	328/328 (100%)	318 (97%)	10 (3%)	41	30
1	B	328/328 (100%)	319 (97%)	9 (3%)	44	34
1	C	325/328 (99%)	311 (96%)	14 (4%)	29	16
1	D	320/328 (98%)	309 (97%)	11 (3%)	37	25
1	E	327/328 (100%)	318 (97%)	9 (3%)	43	33
1	F	325/328 (99%)	313 (96%)	12 (4%)	34	22
1	G	320/328 (98%)	310 (97%)	10 (3%)	40	28
1	H	323/328 (98%)	313 (97%)	10 (3%)	40	28
All	All	2596/2624 (99%)	2511 (97%)	85 (3%)	38	26

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	89	PHE

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Mol	Chain	Res	Type
1	A	99	LEU
1	A	125	HIS
1	A	134	ILE
1	A	171	ILE
1	A	222	ASP
1	A	236	ASP
1	A	305	LEU
1	A	372	ILE
1	B	2	ASN
1	B	64	VAL
1	B	89	PHE
1	B	97	ASP
1	B	99	LEU
1	B	125	HIS
1	B	132	LEU
1	B	183	ASN
1	B	312	GLU
1	C	1	MET
1	C	2	ASN
1	C	37	LEU
1	C	47	VAL
1	C	89	PHE
1	C	99	LEU
1	C	125	HIS
1	C	132	LEU
1	C	167	ASP
1	C	183	ASN
1	C	189	ARG
1	C	304	LEU
1	C	305	LEU
1	C	327	VAL
1	D	25	LYS
1	D	47	VAL
1	D	57	LYS
1	D	59	MET
1	D	89	PHE
1	D	125	HIS
1	D	147	ASN
1	D	222	ASP
1	D	236	ASP
1	D	239	LYS
1	D	312	GLU

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Mol	Chain	Res	Type
1	E	59	MET
1	E	89	PHE
1	E	99	LEU
1	E	125	HIS
1	E	132	LEU
1	E	171	ILE
1	E	183	ASN
1	E	198	PHE
1	E	297	LYS
1	F	2	ASN
1	F	79	GLN
1	F	89	PHE
1	F	125	HIS
1	F	132	LEU
1	F	134	ILE
1	F	147	ASN
1	F	167	ASP
1	F	183	ASN
1	F	245	ASP
1	F	297	LYS
1	F	372	ILE
1	G	25	LYS
1	G	35	THR
1	G	47	VAL
1	G	89	PHE
1	G	132	LEU
1	G	164	LYS
1	G	233	TYR
1	G	297	LYS
1	G	310	ASP
1	G	312	GLU
1	H	7	ASN
1	H	10	LYS
1	H	15	GLN
1	H	89	PHE
1	H	99	LEU
1	H	132	LEU
1	H	171	ILE
1	H	233	TYR
1	H	234	ILE
1	H	304	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	15	GLN
1	A	79	GLN
1	A	127	ASN
1	A	140	ASN
1	A	218	HIS
1	A	340	HIS
1	A	362	ASN
1	B	6	ASN
1	B	7	ASN
1	B	140	ASN
1	B	183	ASN
1	B	218	HIS
1	B	362	ASN
1	C	7	ASN
1	C	15	GLN
1	C	79	GLN
1	C	140	ASN
1	C	183	ASN
1	C	218	HIS
1	C	333	ASN
1	C	362	ASN
1	D	6	ASN
1	D	33	GLN
1	D	140	ASN
1	D	165	GLN
1	D	218	HIS
1	D	332	HIS
1	D	333	ASN
1	D	340	HIS
1	D	362	ASN
1	E	7	ASN
1	E	33	GLN
1	E	140	ASN
1	E	144	GLN
1	E	183	ASN
1	E	218	HIS
1	E	340	HIS
1	E	362	ASN
1	F	7	ASN
1	F	15	GLN
1	F	140	ASN

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Mol	Chain	Res	Type
1	F	165	GLN
1	F	183	ASN
1	F	218	HIS
1	F	340	HIS
1	F	362	ASN
1	G	7	ASN
1	G	33	GLN
1	G	140	ASN
1	G	218	HIS
1	G	333	ASN
1	G	340	HIS
1	G	362	ASN
1	H	15	GLN
1	H	127	ASN
1	H	140	ASN
1	H	218	HIS
1	H	332	HIS
1	H	333	ASN
1	H	340	HIS
1	H	362	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PLP	E	2005	-	16,16,16	1.66	2 (12%)	20,23,23	1.55	4 (20%)
2	PLP	D	2004	-	16,16,16	1.68	1 (6%)	20,23,23	1.27	2 (10%)
2	PLP	G	2007	-	16,16,16	1.59	2 (12%)	20,23,23	1.23	4 (20%)
2	PLP	C	2003	1	16,16,16	1.63	3 (18%)	20,23,23	1.07	0
2	PLP	F	2006	-	16,16,16	1.93	2 (12%)	20,23,23	0.99	1 (5%)
2	PLP	B	2002	1	16,16,16	1.74	3 (18%)	20,23,23	1.09	0
2	PLP	H	2008	-	16,16,16	1.75	1 (6%)	20,23,23	0.93	1 (5%)
2	PLP	A	2001	-	16,16,16	1.79	3 (18%)	20,23,23	1.16	2 (10%)

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	E	2005	-	-	2/8/8/8	0/1/1/1
2	PLP	D	2004	-	-	2/8/8/8	0/1/1/1
2	PLP	G	2007	-	-	2/8/8/8	0/1/1/1
2	PLP	C	2003	1	-	2/8/8/8	0/1/1/1
2	PLP	F	2006	-	-	2/8/8/8	0/1/1/1
2	PLP	B	2002	1	-	2/8/8/8	0/1/1/1
2	PLP	H	2008	-	-	2/8/8/8	0/1/1/1
2	PLP	A	2001	-	-	2/8/8/8	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2006	PLP	C4-C4A	5.97	1.60	1.46
2	H	2008	PLP	C4-C4A	5.57	1.59	1.46
2	A	2001	PLP	C4-C4A	5.35	1.58	1.46
2	D	2004	PLP	C4-C4A	5.26	1.58	1.46
2	E	2005	PLP	C4-C4A	5.18	1.58	1.46
2	B	2002	PLP	C4-C4A	5.15	1.58	1.46
2	G	2007	PLP	C4-C4A	4.85	1.57	1.46
2	C	2003	PLP	C4-C4A	4.81	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2002	PLP	C2A-C2	2.87	1.55	1.50
2	G	2007	PLP	C2A-C2	2.40	1.54	1.50
2	A	2001	PLP	P-O3P	2.38	1.64	1.54
2	A	2001	PLP	C2A-C2	2.29	1.54	1.50
2	E	2005	PLP	C2A-C2	2.19	1.54	1.50
2	C	2003	PLP	O4A-C4A	2.17	1.29	1.21
2	F	2006	PLP	O4A-C4A	2.10	1.28	1.21
2	B	2002	PLP	P-O3P	2.09	1.62	1.54
2	C	2003	PLP	C2A-C2	2.02	1.53	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2005	PLP	C5A-C5-C6	-4.19	112.48	119.37
2	A	2001	PLP	C5A-C5-C6	-2.66	115.00	119.37
2	D	2004	PLP	O3P-P-O4P	2.54	113.48	106.73
2	E	2005	PLP	O2P-P-O4P	2.41	113.15	106.73
2	E	2005	PLP	C5-C6-N1	-2.39	119.83	123.82
2	F	2006	PLP	C4-C3-C2	2.26	121.59	120.19
2	G	2007	PLP	C5A-C5-C6	-2.24	115.69	119.37
2	H	2008	PLP	C5A-C5-C6	-2.20	115.75	119.37
2	D	2004	PLP	C2A-C2-C3	-2.18	118.19	120.89
2	G	2007	PLP	O3-C3-C2	2.15	122.18	117.49
2	G	2007	PLP	C5-C6-N1	-2.08	120.35	123.82
2	G	2007	PLP	O3P-P-O4P	2.05	112.19	106.73
2	A	2001	PLP	C4-C3-C2	2.04	121.45	120.19
2	E	2005	PLP	C2A-C2-N1	2.00	121.58	117.67

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2004	PLP	C3-C4-C4A-O4A
2	A	2001	PLP	C3-C4-C4A-O4A
2	B	2002	PLP	C3-C4-C4A-O4A
2	C	2003	PLP	C3-C4-C4A-O4A
2	E	2005	PLP	C3-C4-C4A-O4A
2	F	2006	PLP	C3-C4-C4A-O4A
2	H	2008	PLP	C3-C4-C4A-O4A
2	C	2003	PLP	C5-C4-C4A-O4A
2	F	2006	PLP	C5-C4-C4A-O4A
2	G	2007	PLP	C5-C4-C4A-O4A

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Mol	Chain	Res	Type	Atoms
2	G	2007	PLP	C3-C4-C4A-O4A
2	B	2002	PLP	C5-C4-C4A-O4A
2	E	2005	PLP	C5-C4-C4A-O4A
2	A	2001	PLP	C5-C4-C4A-O4A
2	H	2008	PLP	C5-C4-C4A-O4A
2	D	2004	PLP	C5-C4-C4A-O4A

There are no ring outliers.

8 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2005	PLP	7	0
2	D	2004	PLP	6	0
2	G	2007	PLP	8	0
2	C	2003	PLP	8	0
2	F	2006	PLP	9	0
2	B	2002	PLP	10	0
2	H	2008	PLP	9	0
2	A	2001	PLP	9	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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^2)	Q<0.9
1	A	371/372 (99%)	0.44	13 (3%)	44	53	9, 12, 16, 24	0
1	B	372/372 (100%)	0.38	11 (2%)	50	59	8, 12, 16, 23	0
1	C	367/372 (98%)	0.34	20 (5%)	25	34	7, 12, 17, 22	0
1	D	363/372 (97%)	0.30	14 (3%)	39	49	7, 12, 17, 24	0
1	E	370/372 (99%)	0.35	3 (0%)	86	90	9, 12, 16, 20	0
1	F	369/372 (99%)	0.34	9 (2%)	59	68	8, 12, 16, 21	0
1	G	362/372 (97%)	0.43	20 (5%)	25	34	7, 12, 16, 25	1 (0%)
1	H	367/372 (98%)	0.30	12 (3%)	46	56	9, 12, 16, 21	0
All	All	2941/2976 (98%)	0.36	102 (3%)	44	53	7, 12, 16, 25	1 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	323[A]	THR	9.0
1	G	229	TYR	5.7
1	E	372	ILE	5.6
1	F	372	ILE	5.3
1	B	14	HIS	4.8
1	C	14	HIS	4.4
1	C	1	MET	4.4
1	A	224	GLY	4.3
1	D	11	ALA	4.3
1	D	222	ASP	4.1
1	F	229	TYR	4.0
1	A	372	ILE	4.0
1	B	372	ILE	3.9
1	H	245	ASP	3.7
1	C	233	TYR	3.6
1	D	372	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	225	GLU	3.4
1	G	244	GLU	3.4
1	C	245	ASP	3.3
1	G	7	ASN	3.3
1	F	245	ASP	3.3
1	G	226	LEU	3.3
1	A	223	GLU	3.1
1	G	324[A]	CYS	3.1
1	D	310	ASP	3.1
1	G	245	ASP	3.0
1	B	223	GLU	3.0
1	G	4	VAL	3.0
1	B	13	PRO	3.0
1	A	14	HIS	3.0
1	H	305	LEU	3.0
1	A	222	ASP	2.9
1	G	372	ILE	2.9
1	H	10	LYS	2.8
1	B	8	ILE	2.8
1	D	12	HIS	2.8
1	F	225	GLU	2.8
1	H	307	ASP	2.8
1	C	305	LEU	2.8
1	H	3	SER	2.7
1	H	130	MET	2.7
1	D	324[A]	CYS	2.7
1	G	188	TYR	2.7
1	E	130	MET	2.7
1	A	89	PHE	2.7
1	C	4	VAL	2.7
1	D	304	LEU	2.7
1	F	224	GLY	2.7
1	A	310	ASP	2.6
1	H	310	ASP	2.6
1	C	202	ILE	2.6
1	C	10	LYS	2.6
1	B	311	ASP	2.6
1	F	324[A]	CYS	2.5
1	D	16	THR	2.5
1	H	8	ILE	2.5
1	C	221	ILE	2.5
1	A	236	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	3	SER	2.5
1	F	184	PRO	2.4
1	B	222	ASP	2.4
1	H	11	ALA	2.4
1	G	184	PRO	2.4
1	G	1	MET	2.4
1	D	305	LEU	2.4
1	G	147	ASN	2.4
1	C	13	PRO	2.4
1	H	324[A]	CYS	2.4
1	C	307	ASP	2.3
1	F	329	VAL	2.3
1	G	310	ASP	2.3
1	B	310	ASP	2.3
1	D	311	ASP	2.3
1	F	147	ASN	2.3
1	G	80	ILE	2.2
1	E	245	ASP	2.2
1	C	310	ASP	2.2
1	B	93	MET	2.2
1	G	241	PHE	2.2
1	C	8	ILE	2.2
1	H	13	PRO	2.2
1	D	7	ASN	2.2
1	A	324[A]	CYS	2.2
1	A	79	GLN	2.2
1	D	3	SER	2.1
1	C	12	HIS	2.1
1	G	233	TYR	2.1
1	B	12	HIS	2.1
1	G	239	LYS	2.1
1	B	324[A]	CYS	2.1
1	C	11	ALA	2.1
1	H	372	ILE	2.1
1	G	311	ASP	2.1
1	D	329	VAL	2.1
1	A	189	ARG	2.0
1	C	311	ASP	2.0
1	C	7	ASN	2.0
1	A	233	TYR	2.0
1	D	198	PHE	2.0
1	C	203	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	136	CYS	2.0
1	C	244	GLU	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 monosaccharides 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, 95th 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(Å^2)	Q<0.9
2	PLP	C	2003	16/16	0.95	0.14	11,12,13,16	0
2	PLP	F	2006	16/16	0.95	0.14	9,12,15,15	0
2	PLP	H	2008	16/16	0.95	0.13	8,11,14,15	0
2	PLP	E	2005	16/16	0.96	0.13	8,11,14,16	0
2	PLP	B	2002	16/16	0.96	0.12	8,10,13,16	0
2	PLP	G	2007	16/16	0.96	0.13	10,13,14,16	0
2	PLP	A	2001	16/16	0.96	0.14	9,12,14,15	0
2	PLP	D	2004	16/16	0.97	0.11	11,12,15,17	0

6.5 Other polymers (i)

There are no such residues in this entry.