Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:13 PM GMT

PDB ID	:	4O6Z
Title	:	Crystal structure of serine hydroxymethyltransferase with covalently bound PLP Schiff-base from Plasmodium falciparum
Authors	:	Chitnumsub, P.; Jaruwat, A.; Leartsakulpanich, U.
Deposited on	:	2013-12-24
Resolution	:	2.98 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

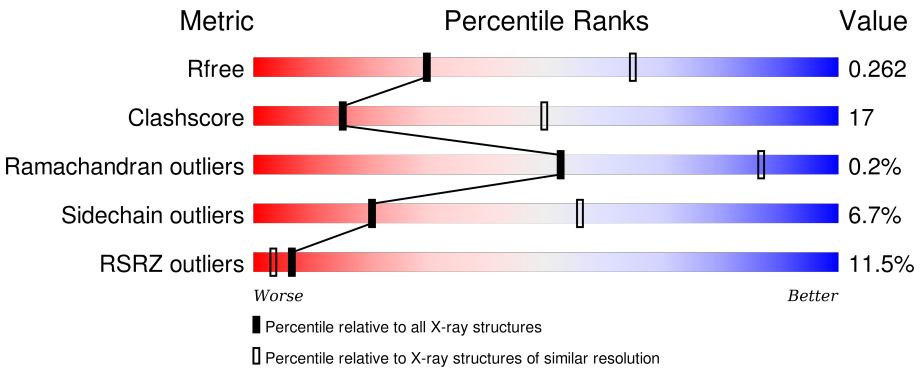
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.98 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}	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	480	% 63% 28% • 7%
1	B	480	% 59% 30% • 7%
1	C	480	5% 63% 27% • 8%
1	D	480	36% 58% 31% • 7%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	B	701	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14254 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 Serine hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	448	3544	2251	603	672	18	0	0	0
1	B	445	3516	2231	598	669	18	0	0	0
1	C	441	3490	2215	594	664	17	0	0	0
1	D	445	3516	2231	598	669	18	0	0	0

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-37	MET	-	EXPRESSION TAG	UNP Q8I566
A	-36	ARG	-	EXPRESSION TAG	UNP Q8I566
A	-35	GLY	-	EXPRESSION TAG	UNP Q8I566
A	-34	SER	-	EXPRESSION TAG	UNP Q8I566
A	-33	HIS	-	EXPRESSION TAG	UNP Q8I566
A	-32	HIS	-	EXPRESSION TAG	UNP Q8I566
A	-31	HIS	-	EXPRESSION TAG	UNP Q8I566
A	-30	HIS	-	EXPRESSION TAG	UNP Q8I566
A	-29	HIS	-	EXPRESSION TAG	UNP Q8I566
A	-28	HIS	-	EXPRESSION TAG	UNP Q8I566
A	-27	GLY	-	EXPRESSION TAG	UNP Q8I566
A	-26	MET	-	EXPRESSION TAG	UNP Q8I566
A	-25	ALA	-	EXPRESSION TAG	UNP Q8I566
A	-24	SER	-	EXPRESSION TAG	UNP Q8I566
A	-23	MET	-	EXPRESSION TAG	UNP Q8I566
A	-22	THR	-	EXPRESSION TAG	UNP Q8I566
A	-21	GLY	-	EXPRESSION TAG	UNP Q8I566
A	-20	GLY	-	EXPRESSION TAG	UNP Q8I566
A	-19	GLN	-	EXPRESSION TAG	UNP Q8I566
A	-18	GLN	-	EXPRESSION TAG	UNP Q8I566
A	-17	MET	-	EXPRESSION TAG	UNP Q8I566

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	GLY	-	EXPRESSION TAG	UNP Q8I566
A	-15	ARG	-	EXPRESSION TAG	UNP Q8I566
A	-14	ASP	-	EXPRESSION TAG	UNP Q8I566
A	-13	LEU	-	EXPRESSION TAG	UNP Q8I566
A	-12	TYR	-	EXPRESSION TAG	UNP Q8I566
A	-11	ASP	-	EXPRESSION TAG	UNP Q8I566
A	-10	ASP	-	EXPRESSION TAG	UNP Q8I566
A	-9	ASP	-	EXPRESSION TAG	UNP Q8I566
A	-8	ASP	-	EXPRESSION TAG	UNP Q8I566
A	-7	LYS	-	EXPRESSION TAG	UNP Q8I566
A	-6	ASP	-	EXPRESSION TAG	UNP Q8I566
A	-5	HIS	-	EXPRESSION TAG	UNP Q8I566
A	-4	PRO	-	EXPRESSION TAG	UNP Q8I566
A	-3	PHE	-	EXPRESSION TAG	UNP Q8I566
A	-2	THR	-	EXPRESSION TAG	UNP Q8I566
A	-1	PRO	-	EXPRESSION TAG	UNP Q8I566
A	0	GLY	-	EXPRESSION TAG	UNP Q8I566
A	292	GLU	PHE	ENGINEERED MUTATION	UNP Q8I566
B	-37	MET	-	EXPRESSION TAG	UNP Q8I566
B	-36	ARG	-	EXPRESSION TAG	UNP Q8I566
B	-35	GLY	-	EXPRESSION TAG	UNP Q8I566
B	-34	SER	-	EXPRESSION TAG	UNP Q8I566
B	-33	HIS	-	EXPRESSION TAG	UNP Q8I566
B	-32	HIS	-	EXPRESSION TAG	UNP Q8I566
B	-31	HIS	-	EXPRESSION TAG	UNP Q8I566
B	-30	HIS	-	EXPRESSION TAG	UNP Q8I566
B	-29	HIS	-	EXPRESSION TAG	UNP Q8I566
B	-28	HIS	-	EXPRESSION TAG	UNP Q8I566
B	-27	GLY	-	EXPRESSION TAG	UNP Q8I566
B	-26	MET	-	EXPRESSION TAG	UNP Q8I566
B	-25	ALA	-	EXPRESSION TAG	UNP Q8I566
B	-24	SER	-	EXPRESSION TAG	UNP Q8I566
B	-23	MET	-	EXPRESSION TAG	UNP Q8I566
B	-22	THR	-	EXPRESSION TAG	UNP Q8I566
B	-21	GLY	-	EXPRESSION TAG	UNP Q8I566
B	-20	GLY	-	EXPRESSION TAG	UNP Q8I566
B	-19	GLN	-	EXPRESSION TAG	UNP Q8I566
B	-18	GLN	-	EXPRESSION TAG	UNP Q8I566
B	-17	MET	-	EXPRESSION TAG	UNP Q8I566
B	-16	GLY	-	EXPRESSION TAG	UNP Q8I566
B	-15	ARG	-	EXPRESSION TAG	UNP Q8I566
B	-14	ASP	-	EXPRESSION TAG	UNP Q8I566

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	LEU	-	EXPRESSION TAG	UNP Q8I566
B	-12	TYR	-	EXPRESSION TAG	UNP Q8I566
B	-11	ASP	-	EXPRESSION TAG	UNP Q8I566
B	-10	ASP	-	EXPRESSION TAG	UNP Q8I566
B	-9	ASP	-	EXPRESSION TAG	UNP Q8I566
B	-8	ASP	-	EXPRESSION TAG	UNP Q8I566
B	-7	LYS	-	EXPRESSION TAG	UNP Q8I566
B	-6	ASP	-	EXPRESSION TAG	UNP Q8I566
B	-5	HIS	-	EXPRESSION TAG	UNP Q8I566
B	-4	PRO	-	EXPRESSION TAG	UNP Q8I566
B	-3	PHE	-	EXPRESSION TAG	UNP Q8I566
B	-2	THR	-	EXPRESSION TAG	UNP Q8I566
B	-1	PRO	-	EXPRESSION TAG	UNP Q8I566
B	0	GLY	-	EXPRESSION TAG	UNP Q8I566
B	292	GLU	PHE	ENGINEERED MUTATION	UNP Q8I566
C	-37	MET	-	EXPRESSION TAG	UNP Q8I566
C	-36	ARG	-	EXPRESSION TAG	UNP Q8I566
C	-35	GLY	-	EXPRESSION TAG	UNP Q8I566
C	-34	SER	-	EXPRESSION TAG	UNP Q8I566
C	-33	HIS	-	EXPRESSION TAG	UNP Q8I566
C	-32	HIS	-	EXPRESSION TAG	UNP Q8I566
C	-31	HIS	-	EXPRESSION TAG	UNP Q8I566
C	-30	HIS	-	EXPRESSION TAG	UNP Q8I566
C	-29	HIS	-	EXPRESSION TAG	UNP Q8I566
C	-28	HIS	-	EXPRESSION TAG	UNP Q8I566
C	-27	GLY	-	EXPRESSION TAG	UNP Q8I566
C	-26	MET	-	EXPRESSION TAG	UNP Q8I566
C	-25	ALA	-	EXPRESSION TAG	UNP Q8I566
C	-24	SER	-	EXPRESSION TAG	UNP Q8I566
C	-23	MET	-	EXPRESSION TAG	UNP Q8I566
C	-22	THR	-	EXPRESSION TAG	UNP Q8I566
C	-21	GLY	-	EXPRESSION TAG	UNP Q8I566
C	-20	GLY	-	EXPRESSION TAG	UNP Q8I566
C	-19	GLN	-	EXPRESSION TAG	UNP Q8I566
C	-18	GLN	-	EXPRESSION TAG	UNP Q8I566
C	-17	MET	-	EXPRESSION TAG	UNP Q8I566
C	-16	GLY	-	EXPRESSION TAG	UNP Q8I566
C	-15	ARG	-	EXPRESSION TAG	UNP Q8I566
C	-14	ASP	-	EXPRESSION TAG	UNP Q8I566
C	-13	LEU	-	EXPRESSION TAG	UNP Q8I566
C	-12	TYR	-	EXPRESSION TAG	UNP Q8I566
C	-11	ASP	-	EXPRESSION TAG	UNP Q8I566

Continued on next page...

Continued from previous page...

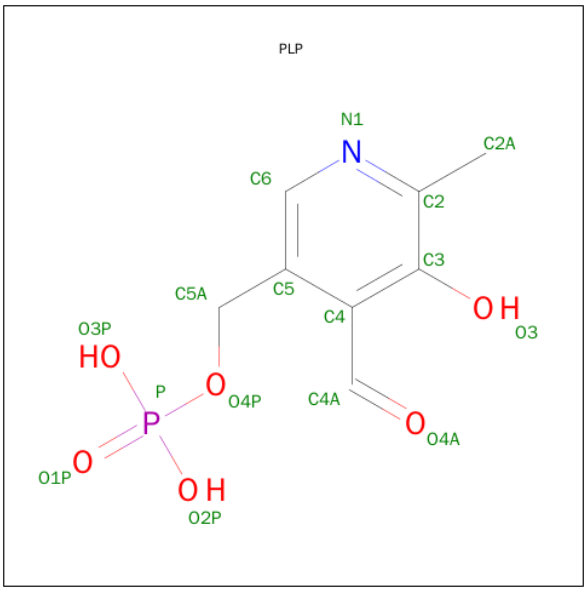
Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	ASP	-	EXPRESSION TAG	UNP Q8I566
C	-9	ASP	-	EXPRESSION TAG	UNP Q8I566
C	-8	ASP	-	EXPRESSION TAG	UNP Q8I566
C	-7	LYS	-	EXPRESSION TAG	UNP Q8I566
C	-6	ASP	-	EXPRESSION TAG	UNP Q8I566
C	-5	HIS	-	EXPRESSION TAG	UNP Q8I566
C	-4	PRO	-	EXPRESSION TAG	UNP Q8I566
C	-3	PHE	-	EXPRESSION TAG	UNP Q8I566
C	-2	THR	-	EXPRESSION TAG	UNP Q8I566
C	-1	PRO	-	EXPRESSION TAG	UNP Q8I566
C	0	GLY	-	EXPRESSION TAG	UNP Q8I566
C	292	GLU	PHE	ENGINEERED MUTATION	UNP Q8I566
D	-37	MET	-	EXPRESSION TAG	UNP Q8I566
D	-36	ARG	-	EXPRESSION TAG	UNP Q8I566
D	-35	GLY	-	EXPRESSION TAG	UNP Q8I566
D	-34	SER	-	EXPRESSION TAG	UNP Q8I566
D	-33	HIS	-	EXPRESSION TAG	UNP Q8I566
D	-32	HIS	-	EXPRESSION TAG	UNP Q8I566
D	-31	HIS	-	EXPRESSION TAG	UNP Q8I566
D	-30	HIS	-	EXPRESSION TAG	UNP Q8I566
D	-29	HIS	-	EXPRESSION TAG	UNP Q8I566
D	-28	HIS	-	EXPRESSION TAG	UNP Q8I566
D	-27	GLY	-	EXPRESSION TAG	UNP Q8I566
D	-26	MET	-	EXPRESSION TAG	UNP Q8I566
D	-25	ALA	-	EXPRESSION TAG	UNP Q8I566
D	-24	SER	-	EXPRESSION TAG	UNP Q8I566
D	-23	MET	-	EXPRESSION TAG	UNP Q8I566
D	-22	THR	-	EXPRESSION TAG	UNP Q8I566
D	-21	GLY	-	EXPRESSION TAG	UNP Q8I566
D	-20	GLY	-	EXPRESSION TAG	UNP Q8I566
D	-19	GLN	-	EXPRESSION TAG	UNP Q8I566
D	-18	GLN	-	EXPRESSION TAG	UNP Q8I566
D	-17	MET	-	EXPRESSION TAG	UNP Q8I566
D	-16	GLY	-	EXPRESSION TAG	UNP Q8I566
D	-15	ARG	-	EXPRESSION TAG	UNP Q8I566
D	-14	ASP	-	EXPRESSION TAG	UNP Q8I566
D	-13	LEU	-	EXPRESSION TAG	UNP Q8I566
D	-12	TYR	-	EXPRESSION TAG	UNP Q8I566
D	-11	ASP	-	EXPRESSION TAG	UNP Q8I566
D	-10	ASP	-	EXPRESSION TAG	UNP Q8I566
D	-9	ASP	-	EXPRESSION TAG	UNP Q8I566
D	-8	ASP	-	EXPRESSION TAG	UNP Q8I566

Continued on next page...

Continued from previous page...

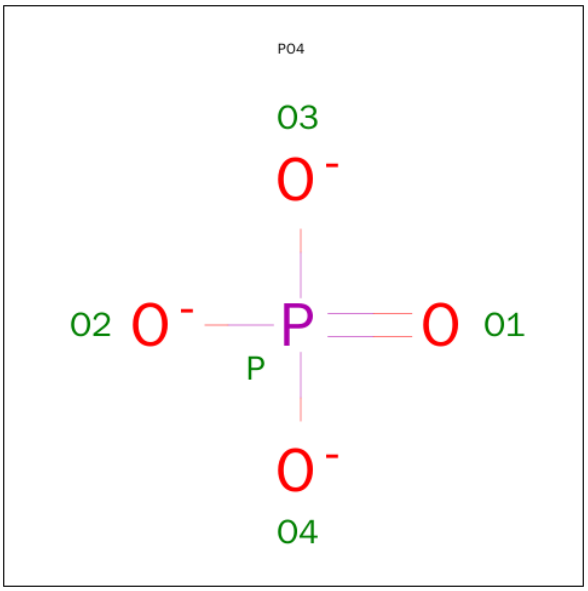
Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	LYS	-	EXPRESSION TAG	UNP Q8I566
D	-6	ASP	-	EXPRESSION TAG	UNP Q8I566
D	-5	HIS	-	EXPRESSION TAG	UNP Q8I566
D	-4	PRO	-	EXPRESSION TAG	UNP Q8I566
D	-3	PHE	-	EXPRESSION TAG	UNP Q8I566
D	-2	THR	-	EXPRESSION TAG	UNP Q8I566
D	-1	PRO	-	EXPRESSION TAG	UNP Q8I566
D	0	GLY	-	EXPRESSION TAG	UNP Q8I566
D	292	GLU	PHE	ENGINEERED MUTATION	UNP Q8I566

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



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

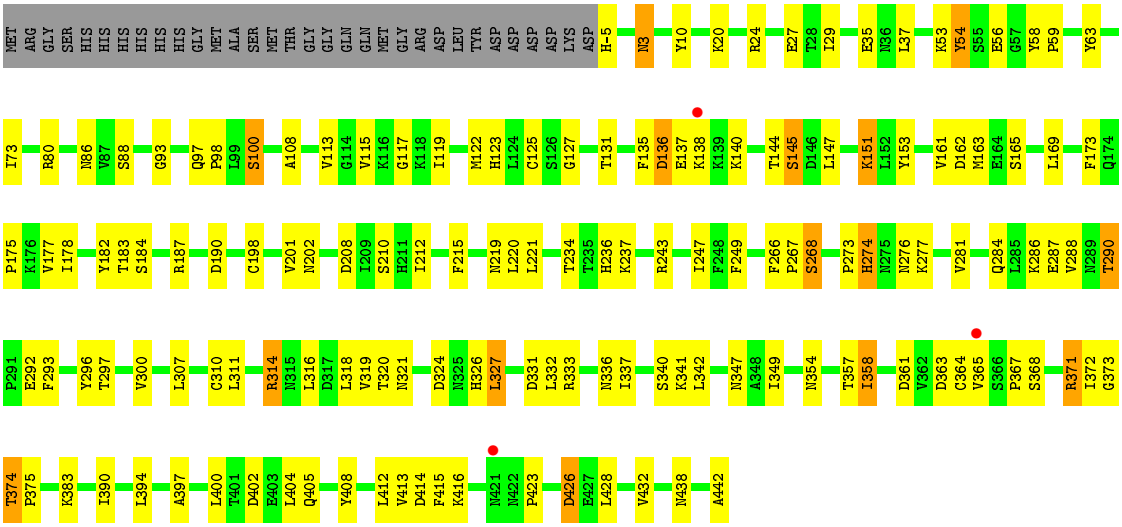
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	56	Total O 56 56	0	0
4	B	55	Total O 55 55	0	0
4	C	20	Total O 20 20	0	0
4	D	7	Total O 7 7	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

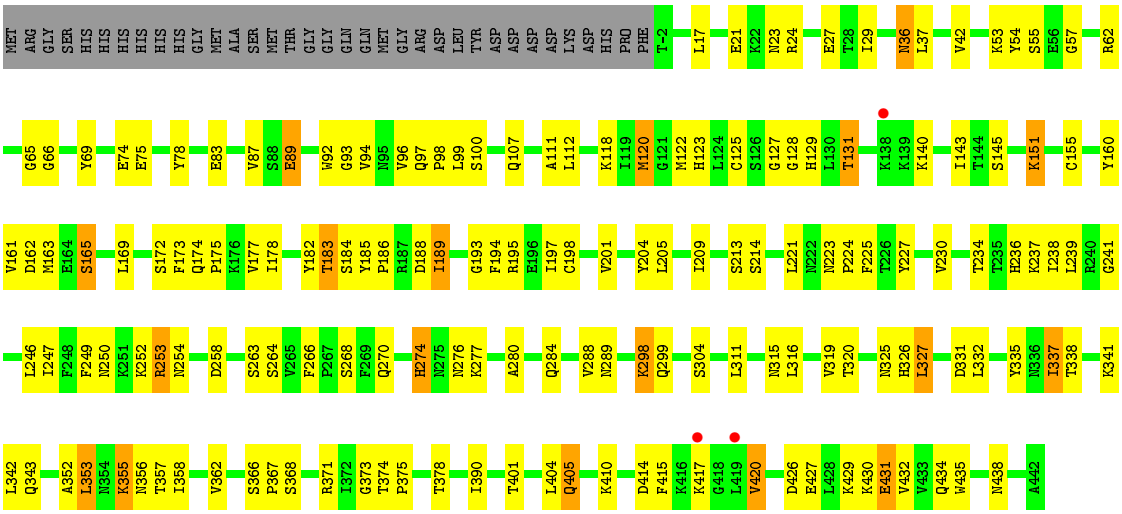
- Molecule 1: Serine hydroxymethyltransferase

Chain A:



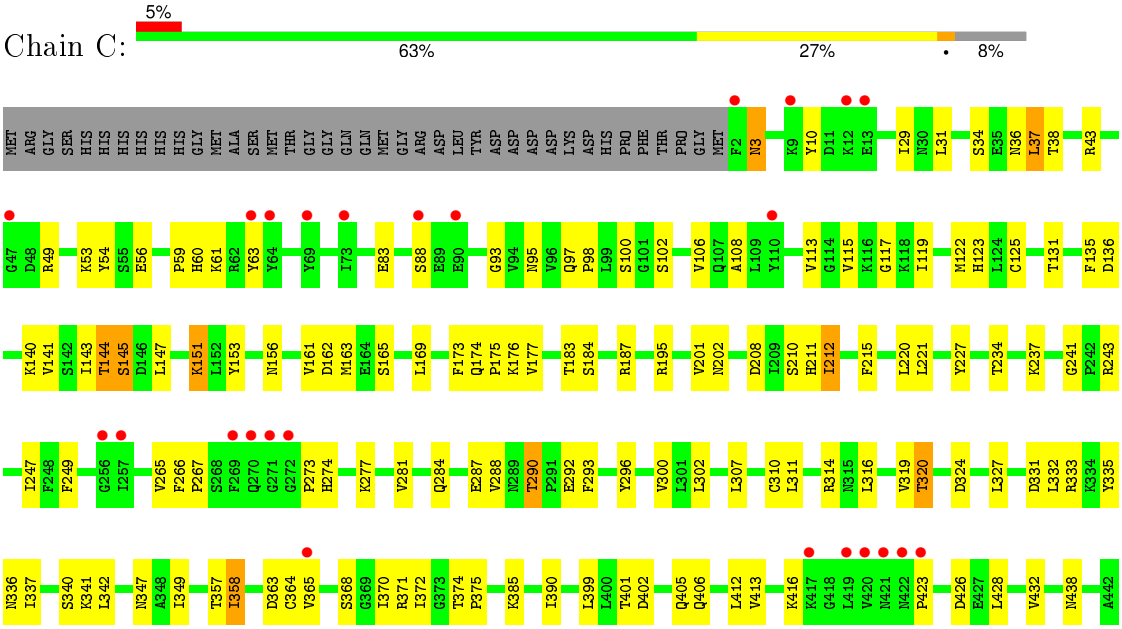
- Molecule 1: Serine hydroxymethyltransferase

Chain B:



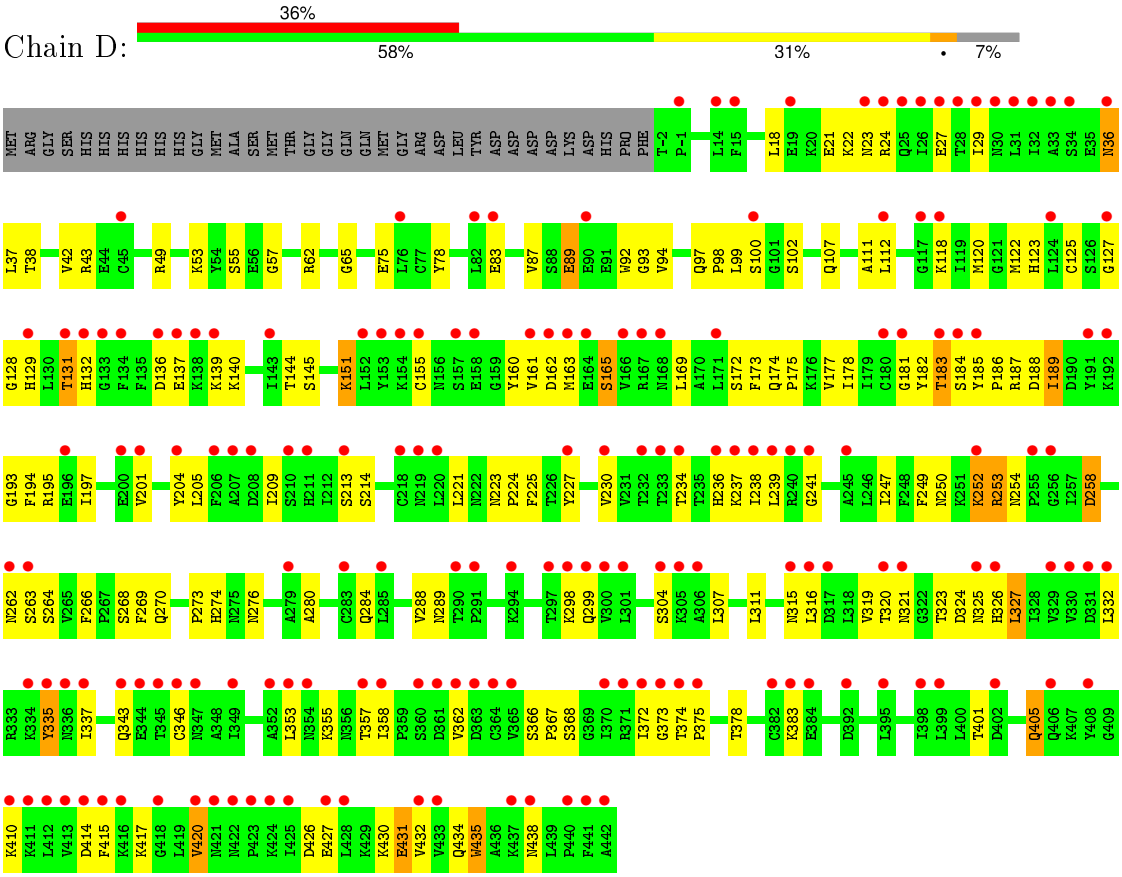
• Molecule 1: Serine hydroxymethyltransferase

Chain C:



• Molecule 1: Serine hydroxymethyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	254.95Å 254.95Å 61.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.85 – 2.98 29.85 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.85-2.98) 99.8 (29.85-2.98)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.03 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.224 , 0.270 0.216 , 0.262	Depositor DCC
R_{free} test set	4739 reflections (11.16%)	DCC
Wilson B-factor (Å^2)	63.6	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 64.9	EDS
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 47265 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14254	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4, 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	0.64	0/3612	0.79	2/4878 (0.0%)
1	B	0.66	0/3581	0.81	2/4835 (0.0%)
1	C	0.56	0/3554	0.74	1/4798 (0.0%)
1	D	0.51	1/3581 (0.0%)	0.69	0/4835
All	All	0.60	1/14328 (0.0%)	0.76	5/19346 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	435	TRP	CD2-CE2	5.54	1.48	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	353	LEU	CA-CB-CG	6.76	130.85	115.30
1	C	327	LEU	CA-CB-CG	5.90	128.88	115.30
1	B	327	LEU	CB-CG-CD1	-5.30	101.98	111.00
1	A	190	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	327	LEU	CA-CB-CG	5.25	127.37	115.30

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	3544	0	3558	131	0
1	B	3516	0	3537	134	0
1	C	3490	0	3508	115	0
1	D	3516	0	3539	136	0
2	A	15	0	6	2	0
2	B	15	0	7	1	0
2	C	15	0	6	2	0
3	D	5	0	0	1	0
4	A	56	0	0	6	0
4	B	55	0	0	2	0
4	C	20	0	0	3	0
4	D	7	0	0	1	0
All	All	14254	0	14161	492	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 17.

All (492) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:ILE:HD11	1:D:401:THR:HB	1.29	1.14
1:B:337:ILE:HD11	1:B:401:THR:HB	1.22	1.07
1:A:151:LYS:HE3	1:A:173:PHE:CD1	1.90	1.07
1:C:290:THR:HG22	1:C:293:PHE:H	1.20	1.06
1:A:290:THR:HG22	1:A:293:PHE:H	1.17	1.05
1:A:268:SER:HB2	4:A:836:HOH:O	1.58	1.04
1:C:122:MET:HE1	1:C:161:VAL:HG22	1.39	1.04
1:A:113:VAL:CG1	1:A:117:GLY:HA3	1.89	1.02
1:C:113:VAL:CG1	1:C:117:GLY:HA3	1.90	1.00
1:C:151:LYS:HE3	1:C:173:PHE:CD1	1.95	1.00
1:A:122:MET:HE1	1:A:161:VAL:HG22	1.44	0.96
1:D:346:CYS:SG	1:D:353:LEU:HD21	2.06	0.95
1:D:250:ASN:ND2	1:D:253:ARG:HD2	1.82	0.94
1:A:219:ASN:HB2	1:C:399:LEU:CD2	1.98	0.93
1:A:184:SER:HA	1:A:327:LEU:HD21	1.50	0.92
1:B:337:ILE:HD11	1:B:401:THR:CB	2.00	0.92
1:D:89:GLU:HG2	1:D:89:GLU:O	1.69	0.91
1:B:250:ASN:ND2	1:B:253:ARG:HD2	1.87	0.89
1:A:151:LYS:HE3	1:A:173:PHE:HD1	1.34	0.88
1:C:311:LEU:HD22	1:C:316:LEU:HD12	1.56	0.87
1:D:337:ILE:HD11	1:D:401:THR:CB	2.04	0.87
1:B:123:HIS:HD2	1:B:125:CYS:H	1.21	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ASP:OD1	2:C:701:PLP:H2A2	1.76	0.86
1:C:151:LYS:HE3	1:C:173:PHE:HD1	1.39	0.85
1:A:287:GLU:O	1:A:290:THR:HB	1.78	0.84
1:C:287:GLU:O	1:C:290:THR:HB	1.79	0.82
1:C:358:ILE:HD11	1:C:368:SER:HB2	1.60	0.82
1:A:311:LEU:HD22	1:A:316:LEU:HD12	1.60	0.81
1:A:122:MET:CE	1:A:161:VAL:HG22	2.09	0.81
1:D:177:VAL:HG22	1:D:204:TYR:HB2	1.61	0.81
1:B:89:GLU:O	1:B:89:GLU:HG2	1.75	0.81
1:B:316:LEU:HD23	1:B:335:TYR:OH	1.80	0.81
1:A:113:VAL:HG13	1:A:117:GLY:HA3	1.62	0.81
1:C:122:MET:CE	1:C:161:VAL:HG22	2.12	0.80
1:B:177:VAL:HG22	1:B:204:TYR:HB2	1.63	0.80
1:A:374:THR:N	1:A:375:PRO:HD3	1.98	0.79
1:D:123:HIS:HD2	1:D:125:CYS:H	1.27	0.79
1:B:36:ASN:HD22	1:B:37:LEU:H	1.31	0.79
1:B:414:ASP:O	1:B:417:LYS:HB3	1.84	0.78
1:D:316:LEU:HD23	1:D:335:TYR:OH	1.84	0.78
1:B:123:HIS:CD2	1:B:125:CYS:H	2.02	0.77
1:D:417:LYS:O	1:D:420:VAL:HG23	1.84	0.77
1:A:219:ASN:HB2	1:C:399:LEU:HD22	1.65	0.77
1:D:36:ASN:HD22	1:D:37:LEU:H	1.30	0.76
1:A:358:ILE:HD11	1:A:368:SER:HB2	1.66	0.76
1:B:358:ILE:CD1	1:B:368:SER:HB2	2.17	0.74
1:D:127:GLY:O	1:D:182:TYR:HB3	1.85	0.74
1:A:113:VAL:HG12	1:A:117:GLY:HA3	1.70	0.74
1:B:417:LYS:O	1:B:420:VAL:HG23	1.88	0.73
1:B:97:GLN:N	1:B:98:PRO:HD3	2.03	0.73
1:C:125:CYS:HB3	1:C:357:THR:HG21	1.68	0.73
1:B:332:LEU:HB3	1:B:337:ILE:HG22	1.70	0.73
1:C:113:VAL:HG13	1:C:117:GLY:HA3	1.69	0.73
1:D:89:GLU:CG	1:D:89:GLU:O	2.36	0.73
1:B:89:GLU:CG	1:B:89:GLU:O	2.36	0.72
1:C:113:VAL:HG12	1:C:117:GLY:HA3	1.69	0.72
1:D:250:ASN:HD22	1:D:253:ARG:HD2	1.52	0.72
1:D:414:ASP:O	1:D:417:LYS:HB3	1.89	0.72
1:D:97:GLN:N	1:D:98:PRO:HD3	2.06	0.71
1:B:319:VAL:HG12	1:B:320:THR:HG23	1.72	0.71
1:A:140:LYS:HB3	1:A:145:SER:OG	1.91	0.71
1:D:311:LEU:HD22	1:D:316:LEU:CD1	2.21	0.71
1:B:358:ILE:HD11	1:B:368:SER:HB2	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ILE:HG22	1:C:177:VAL:CG1	2.21	0.70
1:A:327:LEU:HD11	1:A:371:ARG:HD2	1.72	0.70
1:A:86:ASN:O	1:C:406:GLN:NE2	2.25	0.70
1:D:253:ARG:HH11	1:D:253:ARG:HG2	1.56	0.70
1:D:358:ILE:CD1	1:D:368:SER:HB2	2.22	0.70
1:B:127:GLY:O	1:B:182:TYR:HB3	1.91	0.69
1:A:423:PRO:HA	1:A:426:ASP:OD2	1.92	0.69
1:C:310:CYS:O	1:C:314:ARG:HD2	1.92	0.69
1:A:219:ASN:CB	1:C:399:LEU:CD2	2.70	0.69
1:D:319:VAL:HG12	1:D:320:THR:HG23	1.74	0.69
1:C:3:ASN:HB3	1:C:10:TYR:CE2	2.27	0.69
1:D:205:LEU:HD23	1:D:227:TYR:O	1.93	0.69
1:B:87:VAL:HB	1:B:92:TRP:CD1	2.28	0.68
1:A:371:ARG:HG3	1:A:371:ARG:HH11	1.58	0.68
1:D:93:GLY:HA3	1:D:249:PHE:CE1	2.30	0.67
1:D:123:HIS:CD2	1:D:125:CYS:H	2.10	0.67
1:C:119:ILE:HG22	1:C:177:VAL:HG12	1.77	0.67
1:C:371:ARG:HH11	1:C:371:ARG:HG3	1.59	0.67
1:C:108:ALA:HB2	1:C:247:ILE:HD13	1.76	0.67
1:C:140:LYS:HB3	1:C:145:SER:OG	1.95	0.67
1:C:290:THR:CG2	1:C:293:PHE:H	2.03	0.67
1:B:253:ARG:HH11	1:B:253:ARG:HG2	1.59	0.66
1:A:119:ILE:HG22	1:A:177:VAL:CG1	2.26	0.66
1:A:268:SER:O	1:B:143:ILE:HG22	1.95	0.66
1:D:120:MET:HE2	1:D:178:ILE:HG12	1.78	0.66
1:D:332:LEU:HB3	1:D:337:ILE:HG22	1.77	0.66
1:D:258:ASP:OD1	1:D:258:ASP:C	2.33	0.65
1:A:125:CYS:HB3	1:A:357:THR:HG21	1.78	0.65
1:D:87:VAL:HB	1:D:92:TRP:CD1	2.32	0.65
1:A:3:ASN:HB3	1:A:10:TYR:CE2	2.31	0.65
1:B:205:LEU:HD23	1:B:227:TYR:O	1.96	0.65
1:A:119:ILE:HG22	1:A:177:VAL:HG12	1.78	0.65
1:C:141:VAL:O	1:D:268:SER:HA	1.96	0.65
1:B:311:LEU:HD22	1:B:316:LEU:CD1	2.27	0.65
1:B:194:PHE:HB3	1:B:205:LEU:HD13	1.79	0.65
1:D:223:ASN:OD1	1:D:225:PHE:N	2.27	0.65
1:C:423:PRO:HA	1:C:426:ASP:OD2	1.96	0.65
1:A:363:ASP:CG	1:A:365:VAL:HB	2.18	0.64
1:D:326:HIS:O	1:D:373:GLY:HA2	1.97	0.64
1:C:3:ASN:CB	1:C:10:TYR:CE2	2.80	0.64
1:C:3:ASN:CB	1:C:10:TYR:HE2	2.11	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LEU:O	1:A:416:LYS:HB2	1.97	0.63
1:A:332:LEU:HB2	1:A:368:SER:O	1.98	0.63
1:A:290:THR:CG2	1:A:293:PHE:H	2.04	0.63
1:B:258:ASP:C	1:B:258:ASP:OD1	2.35	0.63
1:D:426:ASP:O	1:D:430:LYS:HG3	1.98	0.63
1:C:371:ARG:HG3	4:C:810:HOH:O	1.97	0.63
1:B:223:ASN:OD1	1:B:225:PHE:N	2.28	0.63
1:D:311:LEU:HB3	1:D:316:LEU:HD12	1.81	0.63
1:A:202:ASN:O	1:A:202:ASN:ND2	2.32	0.63
1:B:93:GLY:HA3	1:B:249:PHE:CE1	2.34	0.63
1:C:201:VAL:HG12	1:C:201:VAL:O	1.97	0.62
1:B:120:MET:CE	1:B:178:ILE:HG12	2.30	0.62
1:A:319:VAL:CG2	1:A:358:ILE:HG22	2.30	0.62
1:A:97:GLN:HG2	1:A:273:PRO:HB3	1.82	0.61
1:C:412:LEU:O	1:C:416:LYS:HB2	2.01	0.61
1:B:362:VAL:HG12	1:B:362:VAL:O	2.00	0.61
1:C:374:THR:N	1:C:375:PRO:HD3	2.15	0.61
1:A:290:THR:HG23	1:A:292:GLU:H	1.65	0.61
1:A:310:CYS:O	1:A:314:ARG:HD2	2.01	0.61
1:B:241:GLY:CA	1:B:284:GLN:HG2	2.31	0.61
1:A:108:ALA:HB2	1:A:247:ILE:HD13	1.83	0.61
1:B:337:ILE:CD1	1:B:401:THR:HB	2.14	0.60
1:A:374:THR:N	1:A:375:PRO:CD	2.63	0.60
1:A:201:VAL:O	1:A:201:VAL:HG12	2.00	0.60
1:B:311:LEU:HB3	1:B:316:LEU:HD12	1.81	0.60
1:D:241:GLY:CA	1:D:284:GLN:HG2	2.31	0.60
1:C:211:HIS:HD2	2:C:701:PLP:O3	1.84	0.59
1:D:236:HIS:O	1:D:237:LYS:HB2	2.02	0.59
1:B:250:ASN:HD22	1:B:253:ARG:HD2	1.65	0.59
1:D:183:THR:HG22	1:D:184:SER:HB3	1.83	0.59
1:C:363:ASP:C	1:C:365:VAL:H	2.05	0.59
1:A:113:VAL:CG1	1:A:117:GLY:CA	2.76	0.59
1:C:358:ILE:HD11	1:C:368:SER:CB	2.31	0.59
1:A:284:GLN:O	1:A:288:VAL:HG23	2.03	0.59
1:A:24:ARG:HH21	1:B:66:GLY:HA3	1.68	0.59
1:C:290:THR:HG23	1:C:292:GLU:H	1.68	0.58
1:B:29:ILE:HD12	1:B:432:VAL:HG13	1.85	0.58
1:B:182:TYR:CE2	1:B:189:ILE:HD13	2.37	0.58
1:D:435:TRP:O	1:D:438:ASN:HB3	2.04	0.58
1:B:36:ASN:ND2	1:B:37:LEU:H	2.02	0.58
1:D:337:ILE:HD11	1:D:401:THR:CG2	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:HIS:O	1:B:373:GLY:HA2	2.03	0.58
1:A:220:LEU:O	1:A:221:LEU:HD23	2.04	0.58
1:B:75:GLU:HA	1:B:78:TYR:CD2	2.38	0.58
1:D:129:HIS:ND1	1:D:131:THR:OG1	2.32	0.58
1:D:358:ILE:HD11	1:D:368:SER:HB2	1.85	0.57
1:D:362:VAL:HG12	1:D:362:VAL:O	2.02	0.57
1:B:97:GLN:N	1:B:98:PRO:CD	2.67	0.57
1:A:363:ASP:OD2	1:A:365:VAL:HB	2.03	0.57
1:C:374:THR:N	1:C:375:PRO:CD	2.67	0.57
1:B:161:VAL:HG11	1:B:163:MET:HE1	1.86	0.57
1:A:162:ASP:OD2	1:A:165:SER:N	2.37	0.57
1:B:29:ILE:CD1	1:B:432:VAL:HG13	2.34	0.57
1:D:311:LEU:HD22	1:D:316:LEU:HD12	1.87	0.57
1:B:371:ARG:HD3	4:B:823:HOH:O	2.04	0.57
1:D:311:LEU:HD22	1:D:316:LEU:HD11	1.87	0.57
1:D:75:GLU:HA	1:D:78:TYR:CD2	2.39	0.57
1:A:327:LEU:CD1	1:A:371:ARG:HD2	2.34	0.57
1:C:37:LEU:N	1:C:37:LEU:HD23	2.19	0.57
1:D:36:ASN:ND2	1:D:37:LEU:H	2.00	0.57
1:D:307:LEU:HD21	1:D:372:ILE:HD12	1.85	0.57
1:A:358:ILE:HD11	1:A:368:SER:CB	2.34	0.56
1:B:112:LEU:HD11	1:B:230:VAL:HG21	1.87	0.56
1:A:153:TYR:HB3	1:A:169:LEU:HD12	1.86	0.56
1:D:194:PHE:HB3	1:D:205:LEU:HD13	1.87	0.56
1:A:3:ASN:CB	1:A:10:TYR:CE2	2.89	0.56
1:B:21:GLU:OE2	1:B:24:ARG:NH1	2.39	0.56
1:C:202:ASN:ND2	1:C:202:ASN:O	2.38	0.56
1:B:357:THR:HG22	1:B:367:PRO:HB3	1.87	0.56
1:D:98:PRO:HA	1:D:270:GLN:HE22	1.69	0.56
1:D:343:GLN:OE1	1:D:355:LYS:HG2	2.06	0.56
1:A:162:ASP:HB3	1:A:165:SER:HB3	1.88	0.56
1:C:374:THR:H	1:C:375:PRO:HD3	1.71	0.56
1:C:113:VAL:CG1	1:C:117:GLY:CA	2.77	0.55
1:A:296:TYR:O	1:A:300:VAL:HG23	2.06	0.55
1:B:36:ASN:HD22	1:B:37:LEU:N	2.04	0.55
1:B:435:TRP:O	1:B:438:ASN:HB3	2.06	0.55
1:B:182:TYR:HE2	1:B:189:ILE:HD13	1.71	0.55
1:B:120:MET:HE2	1:B:178:ILE:HG12	1.87	0.55
1:A:37:LEU:HD23	1:A:442:ALA:H	1.72	0.55
1:C:162:ASP:OD2	1:C:165:SER:N	2.37	0.55
1:C:319:VAL:HG22	1:C:358:ILE:HG22	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PHE:HB3	1:A:145:SER:HB2	1.88	0.55
1:B:263:SER:HA	1:B:266:PHE:O	2.06	0.55
1:D:97:GLN:N	1:D:98:PRO:CD	2.70	0.55
1:B:431:GLU:O	1:B:434:GLN:HG2	2.07	0.55
1:D:337:ILE:CD1	1:D:401:THR:HB	2.19	0.55
1:A:319:VAL:HG22	1:A:358:ILE:HG22	1.88	0.55
1:B:57:GLY:O	1:B:62:ARG:NH1	2.40	0.55
1:B:123:HIS:HD2	1:B:125:CYS:N	2.00	0.55
1:C:153:TYR:HB3	1:C:169:LEU:HD12	1.87	0.55
1:C:284:GLN:O	1:C:288:VAL:HG23	2.07	0.55
1:B:140:LYS:HB3	1:B:145:SER:OG	2.07	0.55
1:B:284:GLN:O	1:B:288:VAL:HG23	2.07	0.54
1:A:97:GLN:N	1:A:98:PRO:CD	2.70	0.54
1:D:319:VAL:C	1:D:320:THR:HG23	2.28	0.54
1:B:23:ASN:O	1:B:27:GLU:HG3	2.07	0.54
1:A:210:SER:HB3	1:A:234:THR:OG1	2.07	0.54
1:B:98:PRO:HA	1:B:270:GLN:HE22	1.71	0.54
1:B:311:LEU:HD22	1:B:316:LEU:HD11	1.89	0.54
1:C:296:TYR:O	1:C:300:VAL:HG23	2.06	0.54
1:B:326:HIS:HB2	1:B:375:PRO:HD3	1.90	0.54
1:C:49:ARG:NH1	1:D:22:LYS:HE2	2.22	0.54
1:B:337:ILE:HD11	1:B:401:THR:CG2	2.37	0.54
1:D:111:ALA:HB2	1:D:264:SER:HB2	1.89	0.54
1:D:434:GLN:HG3	1:D:435:TRP:N	2.22	0.54
1:D:284:GLN:O	1:D:288:VAL:HG23	2.07	0.54
1:D:161:VAL:HG11	1:D:163:MET:HE1	1.90	0.53
1:D:120:MET:CE	1:D:178:ILE:HG12	2.38	0.53
1:D:112:LEU:HD11	1:D:230:VAL:HG21	1.89	0.53
1:C:220:LEU:O	1:C:221:LEU:HD23	2.07	0.53
1:A:371:ARG:NE	4:A:804:HOH:O	2.41	0.53
1:B:111:ALA:HB2	1:B:264:SER:HB2	1.89	0.53
1:D:21:GLU:OE2	1:D:24:ARG:NH1	2.42	0.53
1:D:299:GLN:HB3	1:D:378:THR:HG23	1.90	0.53
1:D:263:SER:HA	1:D:266:PHE:O	2.08	0.53
1:D:57:GLY:O	1:D:62:ARG:NH1	2.42	0.53
1:C:363:ASP:C	1:C:365:VAL:N	2.61	0.53
1:B:107:GLN:HE22	1:B:270:GLN:NE2	2.06	0.53
1:D:151:LYS:HA	1:D:151:LYS:NZ	2.24	0.53
1:C:135:PHE:HB3	1:C:145:SER:HB2	1.90	0.52
1:C:97:GLN:N	1:C:98:PRO:CD	2.72	0.52
1:D:362:VAL:O	1:D:362:VAL:CG1	2.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PHE:HB3	1:A:221:LEU:HG	1.91	0.52
1:A:337:ILE:HD11	1:A:402:ASP:CA	2.39	0.52
1:B:253:ARG:HH11	1:B:253:ARG:CG	2.21	0.52
1:B:343:GLN:OE1	1:B:355:LYS:HG2	2.09	0.52
1:D:29:ILE:HD12	1:D:432:VAL:HG13	1.92	0.52
1:B:213:SER:OG	1:B:239:LEU:HB2	2.08	0.52
1:B:122:MET:HG3	1:B:123:HIS:N	2.25	0.52
1:D:36:ASN:HD22	1:D:37:LEU:N	2.03	0.52
1:C:43:ARG:HH12	1:D:49:ARG:NH2	2.08	0.52
1:B:201:VAL:O	1:B:201:VAL:HG12	2.09	0.52
1:D:366:SER:N	1:D:367:PRO:HD3	2.25	0.52
1:D:188:ASP:OD2	1:D:221:LEU:HD22	2.10	0.52
1:B:223:ASN:OD1	1:B:225:PHE:HB2	2.10	0.51
1:C:337:ILE:HD11	1:C:402:ASP:CA	2.39	0.51
1:D:162:ASP:HB3	1:D:165:SER:HB3	1.91	0.51
1:D:29:ILE:CD1	1:D:432:VAL:HG13	2.40	0.51
1:D:366:SER:N	1:D:367:PRO:CD	2.72	0.51
1:C:332:LEU:HB2	1:C:368:SER:O	2.10	0.51
1:B:319:VAL:C	1:B:320:THR:HG23	2.30	0.51
1:A:35:GLU:HA	4:A:819:HOH:O	2.09	0.51
1:D:213:SER:OG	1:D:239:LEU:HB2	2.10	0.51
1:C:277:LYS:O	1:C:281:VAL:HG23	2.10	0.51
1:D:201:VAL:O	1:D:201:VAL:HG12	2.11	0.51
1:A:363:ASP:OD1	1:A:365:VAL:HB	2.11	0.51
1:A:234:THR:HB	1:A:236:HIS:CE1	2.46	0.51
1:A:243:ARG:O	1:A:277:LYS:HE3	2.10	0.51
1:A:331:ASP:OD1	1:A:333:ARG:HG2	2.11	0.51
1:D:323:THR:OG1	1:D:327:LEU:O	2.24	0.51
1:B:151:LYS:HA	1:B:151:LYS:NZ	2.25	0.51
1:D:107:GLN:HE22	1:D:270:GLN:NE2	2.08	0.50
1:B:183:THR:HG22	1:B:184:SER:HB3	1.93	0.50
1:C:162:ASP:HA	4:C:816:HOH:O	2.12	0.50
1:A:219:ASN:HB2	1:C:399:LEU:HD21	1.88	0.50
1:D:42:VAL:HG13	1:D:280:ALA:HB1	1.93	0.50
1:B:311:LEU:HD22	1:B:316:LEU:HD12	1.92	0.50
1:B:426:ASP:O	1:B:430:LYS:HG3	2.11	0.50
1:A:123:HIS:CD2	1:A:125:CYS:H	2.28	0.50
1:B:366:SER:N	1:B:367:PRO:HD3	2.26	0.50
1:A:336:ASN:O	1:A:337:ILE:HG13	2.10	0.50
1:C:349:ILE:HG21	1:C:428:LEU:HB2	1.92	0.50
1:B:129:HIS:ND1	1:B:131:THR:OG1	2.39	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:GLU:HG3	1:B:289:ASN:ND2	2.27	0.50
1:B:188:ASP:OD2	1:B:221:LEU:HD22	2.12	0.50
1:B:21:GLU:HA	1:B:21:GLU:OE1	2.12	0.49
1:D:140:LYS:HB3	1:D:145:SER:OG	2.13	0.49
1:C:131:THR:O	1:C:144:THR:HG21	2.11	0.49
1:C:341:LYS:HE2	1:C:405:GLN:HG3	1.93	0.49
1:C:135:PHE:C	1:C:135:PHE:CD1	2.85	0.49
1:B:366:SER:N	1:B:367:PRO:CD	2.74	0.49
1:D:374:THR:N	1:D:375:PRO:CD	2.74	0.49
1:B:162:ASP:HB3	1:B:165:SER:HB3	1.93	0.49
1:A:208:ASP:OD1	2:A:701:PLP:H2A2	2.11	0.49
1:A:80:ARG:NH2	1:A:286:LYS:HD3	2.27	0.49
1:B:120:MET:SD	1:B:169:LEU:HD23	2.53	0.49
1:A:277:LYS:O	1:A:281:VAL:HG23	2.11	0.49
1:A:29:ILE:HD12	1:A:432:VAL:HG13	1.94	0.49
1:C:358:ILE:CD1	1:C:368:SER:HB2	2.36	0.49
1:D:155:CYS:HB2	1:D:160:TYR:O	2.12	0.49
1:D:83:GLU:HG3	1:D:289:ASN:ND2	2.28	0.49
1:A:337:ILE:HD11	1:A:402:ASP:CB	2.43	0.49
1:B:174:GLN:N	1:B:175:PRO:CD	2.76	0.49
1:A:311:LEU:HD22	1:A:316:LEU:CD1	2.37	0.48
1:A:3:ASN:CB	1:A:10:TYR:HE2	2.26	0.48
1:D:326:HIS:HB2	1:D:375:PRO:HD3	1.94	0.48
1:C:97:GLN:HG2	1:C:273:PRO:HB3	1.95	0.48
1:C:210:SER:HB3	1:C:234:THR:OG1	2.12	0.48
1:A:187:ARG:HA	1:A:324:ASP:HB2	1.95	0.48
1:B:97:GLN:H	1:B:98:PRO:HD3	1.76	0.48
1:A:135:PHE:C	1:A:135:PHE:CD1	2.87	0.48
1:B:118:LYS:HB3	1:B:173:PHE:CE2	2.48	0.48
1:A:318:LEU:O	1:A:321:ASN:N	2.43	0.48
1:C:347:ASN:HD21	1:D:65:GLY:HA3	1.78	0.48
1:A:274:HIS:HD2	1:B:277:LYS:HZ3	1.60	0.48
1:D:405:GLN:HE21	1:D:410:LYS:HG3	1.78	0.48
1:C:161:VAL:CG1	1:C:163:MET:CE	2.92	0.48
1:D:97:GLN:HG2	1:D:273:PRO:HB3	1.96	0.48
1:B:332:LEU:HB3	1:B:337:ILE:CG2	2.41	0.48
1:D:21:GLU:OE1	1:D:21:GLU:HA	2.14	0.48
1:D:174:GLN:N	1:D:175:PRO:CD	2.77	0.48
1:A:173:PHE:CE2	1:A:175:PRO:HB3	2.49	0.47
1:D:99:LEU:H	1:D:270:GLN:HE22	1.61	0.47
1:A:123:HIS:HD2	1:A:125:CYS:H	1.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:ASN:O	1:C:337:ILE:HG13	2.14	0.47
1:A:365:VAL:O	1:A:367:PRO:HD3	2.14	0.47
1:D:23:ASN:O	1:D:27:GLU:HG3	2.13	0.47
1:A:131:THR:O	1:A:144:THR:HG21	2.14	0.47
1:A:375:PRO:HD2	4:A:848:HOH:O	2.14	0.47
1:C:195:ARG:HD3	1:C:227:TYR:O	2.15	0.47
1:A:73:ILE:HD11	1:B:17:LEU:HB3	1.96	0.47
1:A:93:GLY:HA3	1:A:249:PHE:CE1	2.50	0.47
1:C:319:VAL:HG12	1:C:320:THR:HG23	1.96	0.47
1:C:123:HIS:CD2	1:C:125:CYS:H	2.33	0.47
1:C:29:ILE:HD12	1:C:432:VAL:HG13	1.96	0.47
1:A:341:LYS:HE2	1:A:405:GLN:HG3	1.97	0.47
1:D:221:LEU:HB3	4:D:607:HOH:O	2.15	0.47
1:A:63:TYR:N	1:A:63:TYR:CD1	2.82	0.47
1:C:135:PHE:O	1:C:135:PHE:CD1	2.68	0.46
1:B:304:SER:OG	1:B:325:ASN:O	2.27	0.46
1:B:374:THR:N	1:B:375:PRO:CD	2.78	0.46
1:B:94:VAL:HA	1:B:247:ILE:O	2.16	0.46
1:C:331:ASP:OD1	1:C:333:ARG:HG2	2.14	0.46
1:B:276:ASN:OD1	1:B:276:ASN:N	2.48	0.46
1:A:219:ASN:CB	1:C:399:LEU:HD21	2.44	0.46
1:A:337:ILE:HD11	1:A:402:ASP:HB2	1.97	0.46
1:A:54:TYR:HA	4:A:829:HOH:O	2.15	0.46
1:B:401:THR:HG23	1:B:415:PHE:CZ	2.50	0.46
1:C:162:ASP:HB3	1:C:165:SER:HB3	1.97	0.46
1:A:326:HIS:O	1:A:373:GLY:HA2	2.16	0.46
1:D:401:THR:HG23	1:D:415:PHE:CZ	2.50	0.46
1:B:311:LEU:CB	1:B:316:LEU:HD12	2.45	0.46
1:A:307:LEU:HD11	1:A:390:ILE:HG22	1.98	0.46
1:D:182:TYR:HE2	1:D:189:ILE:HD13	1.81	0.46
1:D:258:ASP:OD1	1:D:262:ASN:ND2	2.46	0.46
1:A:332:LEU:HD11	1:A:342:LEU:HD22	1.98	0.46
1:C:187:ARG:HA	1:C:324:ASP:HB2	1.97	0.46
1:B:197:ILE:HG22	1:B:197:ILE:O	2.16	0.46
1:B:96:VAL:HG12	1:B:246:LEU:CD2	2.46	0.46
1:B:332:LEU:HD11	1:B:342:LEU:HD23	1.98	0.45
1:A:219:ASN:HB3	1:C:335:TYR:HE2	1.80	0.45
1:C:371:ARG:HH11	1:C:371:ARG:CG	2.28	0.45
1:C:115:VAL:HG23	1:C:147:LEU:HD12	1.98	0.45
1:A:219:ASN:HD22	1:C:399:LEU:HD23	1.82	0.45
1:C:319:VAL:CG2	1:C:358:ILE:HG22	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:TYR:CE2	1:D:189:ILE:HD13	2.51	0.45
1:B:99:LEU:H	1:B:270:GLN:HE22	1.64	0.45
1:B:87:VAL:HG11	1:B:225:PHE:CD1	2.51	0.45
1:A:63:TYR:N	1:A:63:TYR:HD1	2.14	0.45
1:B:193:GLY:O	1:B:197:ILE:HD12	2.16	0.45
1:C:162:ASP:OD2	1:C:165:SER:CB	2.63	0.45
1:D:36:ASN:C	1:D:37:LEU:HD12	2.37	0.45
1:D:118:LYS:HB3	1:D:173:PHE:CE2	2.52	0.45
1:B:178:ILE:HD12	1:B:198:CYS:SG	2.57	0.45
1:C:243:ARG:O	1:C:277:LYS:HE3	2.16	0.45
1:C:401:THR:O	1:C:405:GLN:HB2	2.17	0.45
1:A:100:SER:OG	1:B:274:HIS:HE1	2.00	0.45
1:B:42:VAL:HG13	1:B:280:ALA:HB1	1.98	0.45
1:D:223:ASN:OD1	1:D:225:PHE:HB2	2.16	0.45
1:B:155:CYS:HB2	1:B:160:TYR:O	2.17	0.45
1:A:347:ASN:ND2	1:B:65:GLY:HA3	2.32	0.45
1:D:237:LYS:HB3	1:D:238:ILE:H	1.65	0.45
1:C:215:PHE:HB3	1:C:221:LEU:HG	1.99	0.45
1:D:173:PHE:HB3	1:D:175:PRO:HD3	1.99	0.45
1:C:290:THR:HG23	1:C:292:GLU:N	2.32	0.45
1:A:371:ARG:CG	1:A:371:ARG:HH11	2.25	0.45
1:D:311:LEU:CB	1:D:316:LEU:HD12	2.45	0.44
1:D:94:VAL:HA	1:D:247:ILE:O	2.16	0.44
1:C:95:ASN:ND2	1:C:265:VAL:HG21	2.32	0.44
1:D:185:TYR:HA	1:D:186:PRO:HD3	1.84	0.44
1:C:93:GLY:HA3	1:C:249:PHE:CE1	2.52	0.44
1:D:123:HIS:HD2	1:D:125:CYS:N	2.05	0.44
1:D:122:MET:HG3	1:D:123:HIS:N	2.33	0.44
1:B:173:PHE:HB3	1:B:175:PRO:HD3	1.99	0.44
1:A:347:ASN:HD21	1:B:65:GLY:HA3	1.83	0.44
1:C:36:ASN:C	1:C:37:LEU:HD23	2.38	0.44
1:A:161:VAL:CG1	1:A:163:MET:CE	2.96	0.44
1:C:358:ILE:H	1:C:358:ILE:HG12	1.63	0.44
1:D:183:THR:HG22	1:D:184:SER:N	2.33	0.44
1:C:102:SER:HA	1:C:131:THR:HG21	1.99	0.44
1:B:331:ASP:C	1:B:331:ASP:OD1	2.57	0.44
1:D:223:ASN:C	1:D:223:ASN:OD1	2.56	0.44
1:C:201:VAL:CG1	1:C:201:VAL:O	2.65	0.44
1:C:363:ASP:O	1:C:365:VAL:N	2.51	0.43
1:A:331:ASP:OD1	1:A:331:ASP:C	2.54	0.43
1:B:183:THR:HG22	1:B:184:SER:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ILE:HG12	1:D:269:PHE:CE1	2.53	0.43
1:D:332:LEU:HB3	1:D:337:ILE:CG2	2.47	0.43
1:C:174:GLN:HG3	1:C:201:VAL:HG13	1.99	0.43
1:C:63:TYR:N	1:C:63:TYR:CD1	2.86	0.43
1:C:173:PHE:CE2	1:C:175:PRO:HB3	2.53	0.43
1:A:274:HIS:CD2	1:B:277:LYS:NZ	2.86	0.43
1:D:276:ASN:N	1:D:276:ASN:OD1	2.50	0.43
1:B:404:LEU:HA	1:B:404:LEU:HD23	1.77	0.43
1:D:187:ARG:NH2	1:D:320:THR:O	2.46	0.43
1:B:223:ASN:OD1	1:B:223:ASN:C	2.55	0.43
1:B:338:THR:OG1	1:B:341:LYS:HG3	2.19	0.43
1:A:394:LEU:O	1:A:397:ALA:HB3	2.17	0.43
1:D:252:LYS:HB2	1:D:252:LYS:HE2	1.70	0.43
1:D:97:GLN:H	1:D:98:PRO:HD3	1.81	0.43
1:D:38:THR:O	1:D:43:ARG:NH2	2.38	0.43
1:B:209:ILE:HG21	1:B:224:PRO:HG3	2.01	0.43
1:C:31:LEU:HB3	1:C:372:ILE:HG22	2.01	0.43
1:D:431:GLU:O	1:D:434:GLN:HG2	2.19	0.43
1:A:290:THR:HG23	1:A:292:GLU:N	2.32	0.43
1:D:136:ASP:OD1	1:D:137:GLU:N	2.49	0.43
1:B:214:SER:OG	1:B:239:LEU:HA	2.19	0.42
1:A:115:VAL:HG23	1:A:147:LEU:HD12	2.01	0.42
1:A:136:ASP:OD2	1:A:136:ASP:O	2.37	0.42
1:A:404:LEU:HB2	1:A:415:PHE:HE1	1.84	0.42
1:D:241:GLY:HA2	1:D:284:GLN:HG2	2.01	0.42
1:C:347:ASN:ND2	1:D:65:GLY:HA3	2.35	0.42
1:C:342:LEU:HD23	1:C:370:ILE:HD13	2.00	0.42
1:C:163:MET:N	4:C:816:HOH:O	2.52	0.42
1:A:161:VAL:HG12	1:A:163:MET:CE	2.49	0.42
1:D:253:ARG:HH11	1:D:253:ARG:CG	2.28	0.42
1:A:374:THR:H	1:A:375:PRO:HD3	1.79	0.42
1:B:36:ASN:C	1:B:37:LEU:HD12	2.40	0.42
1:B:362:VAL:CG1	1:B:362:VAL:O	2.65	0.42
1:A:201:VAL:O	1:A:201:VAL:CG1	2.67	0.42
1:D:140:LYS:HA	1:D:140:LYS:HD2	1.94	0.42
1:C:102:SER:O	1:C:106:VAL:HG23	2.18	0.42
1:B:298:LYS:HB3	1:B:298:LYS:HE2	1.76	0.42
1:B:74:GLU:HG2	1:B:78:TYR:CZ	2.54	0.42
1:D:187:ARG:HA	1:D:324:ASP:HB2	2.00	0.42
1:A:408:TYR:O	1:A:414:ASP:HB3	2.19	0.42
1:A:237:LYS:NZ	2:A:701:PLP:O3	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PHE:CD1	1:A:267:PRO:HA	2.54	0.42
1:A:178:ILE:HD12	1:A:198:CYS:SG	2.59	0.42
1:A:162:ASP:OD2	1:A:165:SER:CB	2.67	0.42
1:D:122:MET:O	1:D:128:GLY:HA3	2.20	0.42
1:B:236:HIS:O	1:B:237:LYS:HB2	2.18	0.42
1:A:404:LEU:HB2	1:A:415:PHE:CE1	2.55	0.42
1:A:183:THR:HG22	1:A:184:SER:HB3	2.02	0.41
1:A:357:THR:HG23	1:A:361:ASP:HB2	2.01	0.41
1:B:241:GLY:HA2	1:B:284:GLN:HG2	2.02	0.41
1:D:214:SER:OG	1:D:239:LEU:HA	2.20	0.41
1:D:107:GLN:HE22	1:D:270:GLN:HE21	1.67	0.41
1:A:220:LEU:HD12	1:A:297:THR:HG22	2.02	0.41
1:D:357:THR:HG22	1:D:367:PRO:HB3	2.02	0.41
1:B:122:MET:O	1:B:128:GLY:HA3	2.19	0.41
1:D:195:ARG:HD2	1:D:227:TYR:O	2.20	0.41
1:B:356:ASN:ND2	4:B:823:HOH:O	2.53	0.41
1:B:118:LYS:HE3	1:B:174:GLN:O	2.20	0.41
1:A:383:LYS:HE2	4:A:803:HOH:O	2.19	0.41
1:C:56:GLU:HB3	1:C:266:PHE:CZ	2.56	0.41
1:A:86:ASN:HB3	1:C:406:GLN:OE1	2.20	0.41
1:D:132:HIS:HE1	1:D:181:GLY:O	2.04	0.41
1:D:335:TYR:N	1:D:335:TYR:CD1	2.88	0.41
1:A:276:ASN:N	1:A:276:ASN:OD1	2.52	0.41
1:C:60:HIS:O	1:C:61:LYS:HG3	2.21	0.41
1:D:120:MET:SD	1:D:169:LEU:HD23	2.61	0.41
1:D:258:ASP:OD1	1:D:258:ASP:O	2.37	0.41
1:C:34:SER:HB2	1:C:237:LYS:HD3	2.03	0.41
1:A:58:TYR:HB3	1:A:59:PRO:HD2	2.03	0.41
1:C:183:THR:HG22	1:C:184:SER:HB3	2.02	0.41
1:C:212:ILE:CG1	1:C:212:ILE:O	2.69	0.41
1:A:349:ILE:HG21	1:A:428:LEU:HB2	2.02	0.41
1:C:266:PHE:CD1	1:C:267:PRO:HA	2.55	0.41
1:C:59:PRO:O	1:C:60:HIS:HB2	2.21	0.41
1:B:405:GLN:HE21	1:B:410:LYS:HG3	1.84	0.41
1:B:107:GLN:HE22	1:B:270:GLN:HE21	1.67	0.41
1:C:302:LEU:HD23	1:C:302:LEU:HA	1.78	0.41
1:D:209:ILE:HG21	1:D:224:PRO:HG3	2.03	0.41
1:A:358:ILE:CD1	1:A:368:SER:HB2	2.42	0.41
1:B:264:SER:O	1:B:268:SER:HB2	2.21	0.41
1:D:18:LEU:O	1:D:21:GLU:HB3	2.20	0.41
1:A:20:LYS:HD3	1:B:69:TYR:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:GLY:O	1:D:197:ILE:HD12	2.21	0.41
1:C:307:LEU:HD11	1:C:390:ILE:HG22	2.03	0.41
1:B:195:ARG:HD2	1:B:227:TYR:O	2.21	0.41
1:B:352:ALA:O	1:B:353:LEU:HB3	2.20	0.41
1:D:304:SER:OG	1:D:325:ASN:O	2.24	0.41
1:B:299:GLN:HB3	1:B:378:THR:HG23	2.03	0.41
1:A:202:ASN:O	1:A:202:ASN:CG	2.60	0.40
1:B:237:LYS:HB3	1:B:238:ILE:H	1.67	0.40
1:A:137:GLU:HB3	1:A:138:LYS:H	1.48	0.40
1:C:241:GLY:CA	1:C:284:GLN:HG2	2.51	0.40
1:D:102:SER:N	3:D:501:PO4:O3	2.54	0.40
1:D:98:PRO:HA	1:D:270:GLN:NE2	2.36	0.40
1:B:185:TYR:HA	1:B:186:PRO:HD3	1.83	0.40
1:C:176:LYS:HG3	1:C:176:LYS:O	2.21	0.40
1:A:127:GLY:O	1:A:182:TYR:HB3	2.20	0.40
1:A:56:GLU:H	1:A:56:GLU:HG3	1.70	0.40
1:D:163:MET:HE1	1:D:194:PHE:CE2	2.56	0.40
1:D:264:SER:O	1:D:268:SER:HB2	2.21	0.40
1:B:237:LYS:NZ	2:B:701:PLP:O3	2.54	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	446/480 (93%)	422 (95%)	23 (5%)	1 (0%)	52 87
1	B	443/480 (92%)	426 (96%)	17 (4%)	0	100 100
1	C	439/480 (92%)	415 (94%)	22 (5%)	2 (0%)	34 75
1	D	443/480 (92%)	428 (97%)	15 (3%)	0	100 100
All	All	1771/1920 (92%)	1691 (96%)	77 (4%)	3 (0%)	52 87

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	364	CYS
1	C	156	ASN
1	A	374	THR

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	395/421 (94%)	369 (93%)	26 (7%)	21	56
1	B	392/421 (93%)	363 (93%)	29 (7%)	17	50
1	C	389/421 (92%)	368 (95%)	21 (5%)	27	65
1	D	392/421 (93%)	363 (93%)	29 (7%)	17	50
All	All	1568/1684 (93%)	1463 (93%)	105 (7%)	20	56

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	HIS
1	A	3	ASN
1	A	27	GLU
1	A	53	LYS
1	A	54	TYR
1	A	88	SER
1	A	100	SER
1	A	136	ASP
1	A	145	SER
1	A	151	LYS
1	A	212	ILE
1	A	268	SER
1	A	274	HIS
1	A	290	THR
1	A	314	ARG
1	A	320	THR
1	A	340	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	354	ASN
1	A	358	ILE
1	A	364	CYS
1	A	371	ARG
1	A	372	ILE
1	A	400	LEU
1	A	413	VAL
1	A	426	ASP
1	A	438	ASN
1	B	36	ASN
1	B	53	LYS
1	B	54	TYR
1	B	55	SER
1	B	89	GLU
1	B	100	SER
1	B	120	MET
1	B	131	THR
1	B	151	LYS
1	B	165	SER
1	B	172	SER
1	B	183	THR
1	B	189	ILE
1	B	234	THR
1	B	252	LYS
1	B	253	ARG
1	B	254	ASN
1	B	274	HIS
1	B	298	LYS
1	B	315	ASN
1	B	327	LEU
1	B	337	ILE
1	B	355	LYS
1	B	390	ILE
1	B	405	GLN
1	B	420	VAL
1	B	427	GLU
1	B	429	LYS
1	B	431	GLU
1	C	3	ASN
1	C	37	LEU
1	C	38	THR
1	C	53	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	54	TYR
1	C	83	GLU
1	C	88	SER
1	C	100	SER
1	C	136	ASP
1	C	144	THR
1	C	145	SER
1	C	151	LYS
1	C	212	ILE
1	C	274	HIS
1	C	290	THR
1	C	320	THR
1	C	340	SER
1	C	358	ILE
1	C	385	LYS
1	C	413	VAL
1	C	438	ASN
1	D	36	ASN
1	D	53	LYS
1	D	55	SER
1	D	89	GLU
1	D	100	SER
1	D	131	THR
1	D	139	LYS
1	D	144	THR
1	D	151	LYS
1	D	165	SER
1	D	172	SER
1	D	183	THR
1	D	189	ILE
1	D	234	THR
1	D	252	LYS
1	D	253	ARG
1	D	254	ASN
1	D	258	ASP
1	D	274	HIS
1	D	298	LYS
1	D	315	ASN
1	D	321	ASN
1	D	327	LEU
1	D	335	TYR
1	D	383	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	405	GLN
1	D	420	VAL
1	D	427	GLU
1	D	431	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	123	HIS
1	A	202	ASN
1	A	274	HIS
1	B	36	ASN
1	B	123	HIS
1	B	270	GLN
1	B	274	HIS
1	B	289	ASN
1	B	321	ASN
1	B	356	ASN
1	B	405	GLN
1	C	3	ASN
1	C	202	ASN
1	C	274	HIS
1	D	36	ASN
1	D	123	HIS
1	D	132	HIS
1	D	270	GLN
1	D	274	HIS
1	D	289	ASN
1	D	321	ASN
1	D	356	ASN
1	D	405	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PLP	A	701	1	15,15,16	0.97	1 (6%)	21,22,23	2.04	8 (38%)
2	PLP	B	701	1	15,15,16	1.57	1 (6%)	21,22,23	2.06	6 (28%)
2	PLP	C	701	1	15,15,16	0.74	0	21,22,23	1.56	4 (19%)
3	PO4	D	501	-	4,4,4	0.29	0	6,6,6	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	701	1	-	0/6/6/8	0/1/1/1
2	PLP	B	701	1	-	0/6/6/8	0/1/1/1
2	PLP	C	701	1	-	0/6/6/8	0/1/1/1
3	PO4	D	501	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	PLP	C3-C2	-5.61	1.36	1.40
2	A	701	PLP	C3-C2	-3.37	1.38	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	PLP	C4A-C4-C3	-2.85	115.19	120.36
2	C	701	PLP	O2P-P-O4P	-2.71	98.76	106.56
2	A	701	PLP	O4P-P-O1P	-2.50	100.78	107.14
2	B	701	PLP	C5A-C5-C6	-2.41	114.71	119.28
2	C	701	PLP	C5-C6-N1	-2.07	120.27	123.86
2	B	701	PLP	C4A-C4-C3	-2.06	116.63	120.36
2	A	701	PLP	O2P-P-O4P	-2.03	100.71	106.56
2	B	701	PLP	C4A-C4-C5	2.20	123.18	120.88
2	A	701	PLP	O3P-P-O2P	2.28	116.05	107.38
2	B	701	PLP	O3P-P-O2P	2.65	117.45	107.38
2	A	701	PLP	O3-C3-C2	2.71	122.37	117.66
2	C	701	PLP	O3P-P-O2P	2.81	118.07	107.38
2	A	701	PLP	O4P-C5A-C5	2.91	113.81	108.99
2	C	701	PLP	O4P-C5A-C5	3.29	114.43	108.99
2	A	701	PLP	C5A-C5-C4	3.57	126.38	121.65
2	A	701	PLP	C4A-C4-C5	4.83	125.91	120.88
2	B	701	PLP	O4P-C5A-C5	4.92	117.12	108.99
2	B	701	PLP	C5A-C5-C4	5.14	128.46	121.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	PLP	2	0
2	B	701	PLP	1	0
2	C	701	PLP	2	0
3	D	501	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	448/480 (93%)	-0.34	3 (0%)	89	75	24, 46, 88, 108	0
1	B	445/480 (92%)	-0.44	3 (0%)	89	75	25, 42, 73, 112	0
1	C	441/480 (91%)	0.35	25 (5%)	27	14	31, 77, 119, 120	0
1	D	445/480 (92%)	1.79	174 (39%)	0	0	55, 116, 120, 120	0
All	All	1779/1920 (92%)	0.34	205 (11%)	6	3	24, 63, 120, 120	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	364	CYS	8.3
1	D	441	PHE	6.4
1	D	315	ASN	6.0
1	D	345	THR	6.0
1	D	360	SER	5.9
1	D	306	ALA	5.9
1	D	211	HIS	5.8
1	D	210	SER	5.7
1	D	406	GLN	5.6
1	C	63	TYR	5.3
1	D	325	ASN	5.2
1	D	425	ILE	5.0
1	D	399	LEU	4.9
1	D	416	LYS	4.8
1	D	442	ALA	4.8
1	D	23	ASN	4.7
1	D	420	VAL	4.7
1	D	411	LYS	4.7
1	D	421	ASN	4.5
1	D	363	ASP	4.5
1	D	326	HIS	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	240	ARG	4.4
1	D	424	LYS	4.4
1	D	305	LYS	4.4
1	D	263	SER	4.3
1	D	233	THR	4.3
1	D	32	ILE	4.3
1	D	118	LYS	4.3
1	D	334	LYS	4.2
1	D	408	TYR	4.2
1	D	428	LEU	4.2
1	D	29	ILE	4.1
1	D	192	LYS	4.1
1	D	157	SER	4.1
1	D	45	CYS	4.1
1	D	237	LYS	4.0
1	D	208	ASP	4.0
1	D	255	PRO	4.0
1	C	69	TYR	3.9
1	D	185	TYR	3.9
1	D	201	VAL	3.9
1	D	82	LEU	3.8
1	D	298	LYS	3.8
1	D	373	GLY	3.7
1	D	413	VAL	3.7
1	C	419	LEU	3.7
1	D	371	ARG	3.7
1	D	26	ILE	3.6
1	D	218	CYS	3.6
1	D	239	LEU	3.6
1	C	417	LYS	3.6
1	D	432	VAL	3.5
1	D	414	ASP	3.5
1	D	34	SER	3.5
1	D	153	TYR	3.5
1	D	200	GLU	3.5
1	D	365	VAL	3.5
1	D	158	GLU	3.5
1	D	234	THR	3.5
1	D	262	ASN	3.5
1	D	415	PHE	3.5
1	D	352	ALA	3.5
1	D	353	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	419	LEU	3.4
1	D	196	GLU	3.4
1	D	241	GLY	3.4
1	D	331	ASP	3.4
1	D	133	GLY	3.3
1	D	167	ARG	3.3
1	D	219	ASN	3.3
1	D	227	TYR	3.3
1	D	412	LEU	3.3
1	D	168	ASN	3.2
1	D	36	ASN	3.2
1	C	73	ILE	3.2
1	C	271	GLY	3.2
1	D	76	LEU	3.2
1	D	164	GLU	3.1
1	D	161	VAL	3.1
1	D	358	ILE	3.1
1	D	304	SER	3.1
1	D	320	THR	3.0
1	D	321	ASN	3.0
1	D	25	GLN	3.0
1	D	139	LYS	3.0
1	D	181	GLY	3.0
1	D	336	ASN	3.0
1	D	14	LEU	3.0
1	D	100	SER	3.0
1	D	346	CYS	3.0
1	D	438	ASN	3.0
1	D	143	ILE	3.0
1	D	410	LYS	3.0
1	D	137	GLU	2.9
1	D	362	VAL	2.9
1	D	418	GLY	2.9
1	D	285	LEU	2.9
1	D	290	THR	2.9
1	D	152	LEU	2.9
1	D	163	MET	2.9
1	D	207	ALA	2.9
1	D	433	VAL	2.9
1	C	2	PHE	2.9
1	D	279	ALA	2.9
1	D	134	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	191	TYR	2.9
1	D	155	CYS	2.9
1	C	421	ASN	2.9
1	D	440	PRO	2.8
1	D	256	GLY	2.8
1	D	335	TYR	2.8
1	D	337	ILE	2.8
1	D	154	LYS	2.8
1	A	365	VAL	2.8
1	C	365	VAL	2.8
1	D	184	SER	2.8
1	D	423	PRO	2.8
1	D	132	HIS	2.8
1	D	344	GLU	2.8
1	C	90	GLU	2.7
1	D	392	ASP	2.7
1	D	30	ASN	2.7
1	C	9	LYS	2.7
1	C	269	PHE	2.7
1	D	27	GLU	2.7
1	D	427	GLU	2.7
1	D	129	HIS	2.7
1	D	162	ASP	2.6
1	D	232	THR	2.6
1	A	138	LYS	2.6
1	D	283	CYS	2.6
1	D	117	GLY	2.6
1	D	299	GLN	2.6
1	D	422	ASN	2.6
1	D	252	LYS	2.6
1	D	343	GLN	2.6
1	C	272	GLY	2.6
1	D	354	ASN	2.6
1	D	15	PHE	2.6
1	D	131	THR	2.6
1	D	329	VAL	2.6
1	D	220	LEU	2.5
1	D	138	LYS	2.5
1	D	361	ASP	2.5
1	C	110	TYR	2.5
1	D	330	VAL	2.5
1	D	370	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	213	SER	2.5
1	D	19	GLU	2.5
1	C	423	PRO	2.5
1	D	127	GLY	2.5
1	A	421	ASN	2.5
1	B	138	LYS	2.5
1	D	375	PRO	2.5
1	D	166	VAL	2.5
1	D	180	CYS	2.5
1	D	402	ASP	2.4
1	C	12	LYS	2.4
1	D	382	CYS	2.4
1	D	204	TYR	2.4
1	C	88	SER	2.4
1	D	395	LEU	2.4
1	C	420	VAL	2.4
1	D	238	ILE	2.3
1	D	206	PHE	2.3
1	D	357	THR	2.3
1	D	297	THR	2.3
1	D	437	LYS	2.3
1	D	28	THR	2.3
1	D	112	LEU	2.3
1	D	24	ARG	2.3
1	D	347	ASN	2.3
1	D	300	VAL	2.3
1	D	294	LYS	2.3
1	D	301	LEU	2.3
1	D	83	GLU	2.2
1	D	136	ASP	2.2
1	D	383	LYS	2.2
1	D	398	ILE	2.2
1	C	270	GLN	2.2
1	D	317	ASP	2.2
1	B	417	LYS	2.2
1	D	-1	PRO	2.2
1	D	316	LEU	2.2
1	C	257	ILE	2.2
1	D	90	GLU	2.2
1	D	349	ILE	2.2
1	D	124	LEU	2.2
1	D	374	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	171	LEU	2.1
1	C	64	TYR	2.1
1	D	291	PRO	2.1
1	D	384	GLU	2.1
1	D	236	HIS	2.1
1	D	372	ILE	2.1
1	D	332	LEU	2.1
1	C	47	GLY	2.1
1	C	422	ASN	2.1
1	D	245	ALA	2.1
1	C	256	GLY	2.1
1	D	33	ALA	2.0
1	D	31	LEU	2.0
1	D	183	THR	2.0
1	D	230	VAL	2.0
1	C	13	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	PLP	B	701	15/16	0.99	0.26	2.52	26,28,29,29	0
2	PLP	C	701	15/16	0.92	0.24	0.23	73,79,89,90	0
2	PLP	A	701	15/16	0.97	0.19	-0.01	26,31,33,36	0
3	PO4	D	501	5/5	0.91	0.25	-1.16	67,73,88,88	0

6.5 Other polymers (i)

There are no such residues in this entry.