Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 08:13 AM EDT

PDB ID	:	4H67
Title	:	Crystal structure of HMP synthase Thi5 from S. cerevisiae
Authors	:	Coquille, S.C.; Roux, C.; Fitzpatrick, T.; Thore, S.
Deposited on	:	2012-09-19
Resolution	:	2.70 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

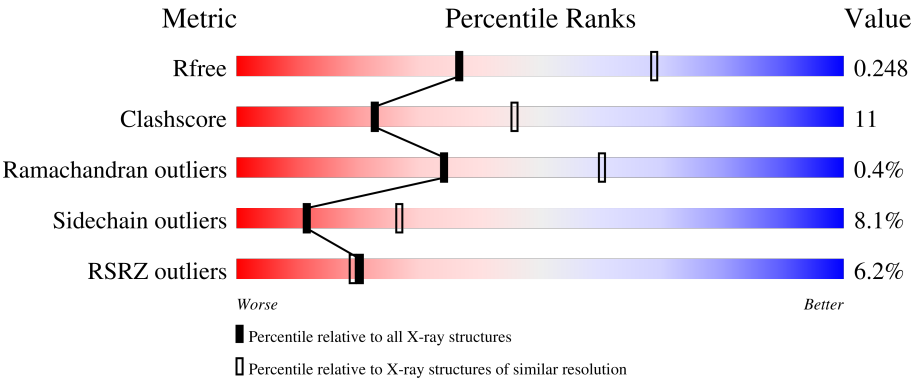
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	346	3% 73% 21%
1	B	346	5% 69% 16% 11%
1	C	346	8% 71% 23%
1	D	346	4% 74% 19%
1	E	346	5% 68% 17% 12%

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Mol	Chain	Length	Quality of chain
1	F	346	6% 73% 20%
1	G	346	6% 71% 19% 6%
1	H	346	9% 68% 16% 12%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	403	-	-	X	-
2	SO4	C	406	-	-	X	-
2	SO4	D	403	-	-	X	-
2	SO4	G	402	-	-	X	-
2	SO4	H	401	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20928 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 Pyrimidine precursor biosynthesis enzyme THI5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2701	1741	450	494	16			
1	B	307	Total	C	N	O	S	0	0	0
			2457	1592	399	452	14			
1	C	338	Total	C	N	O	S	0	0	0
			2696	1736	449	494	17			
1	D	335	Total	C	N	O	S	0	0	0
			2668	1720	438	492	18			
1	E	305	Total	C	N	O	S	0	0	0
			2440	1580	396	449	15			
1	F	335	Total	C	N	O	S	0	0	0
			2668	1720	438	492	18			
1	G	326	Total	C	N	O	S	0	0	0
			2609	1682	428	483	16			
1	H	305	Total	C	N	O	S	0	0	0
			2440	1580	396	450	14			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	SER	LYS	engineered mutation	UNP P43534
A	241	GLY	GLU	engineered mutation	UNP P43534
A	317	THR	GLN	engineered mutation	UNP P43534
A	341	HIS	-	expression tag	UNP P43534
A	342	HIS	-	expression tag	UNP P43534
A	343	HIS	-	expression tag	UNP P43534
A	344	HIS	-	expression tag	UNP P43534
A	345	HIS	-	expression tag	UNP P43534
A	346	HIS	-	expression tag	UNP P43534
B	240	SER	LYS	engineered mutation	UNP P43534
B	241	GLY	GLU	engineered mutation	UNP P43534
B	317	THR	GLN	engineered mutation	UNP P43534
B	341	HIS	-	expression tag	UNP P43534

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Chain	Residue	Modelled	Actual	Comment	Reference
B	342	HIS	-	expression tag	UNP P43534
B	343	HIS	-	expression tag	UNP P43534
B	344	HIS	-	expression tag	UNP P43534
B	345	HIS	-	expression tag	UNP P43534
B	346	HIS	-	expression tag	UNP P43534
C	240	SER	LYS	engineered mutation	UNP P43534
C	241	GLY	GLU	engineered mutation	UNP P43534
C	317	THR	GLN	engineered mutation	UNP P43534
C	341	HIS	-	expression tag	UNP P43534
C	342	HIS	-	expression tag	UNP P43534
C	343	HIS	-	expression tag	UNP P43534
C	344	HIS	-	expression tag	UNP P43534
C	345	HIS	-	expression tag	UNP P43534
C	346	HIS	-	expression tag	UNP P43534
D	240	SER	LYS	engineered mutation	UNP P43534
D	241	GLY	GLU	engineered mutation	UNP P43534
D	317	THR	GLN	engineered mutation	UNP P43534
D	341	HIS	-	expression tag	UNP P43534
D	342	HIS	-	expression tag	UNP P43534
D	343	HIS	-	expression tag	UNP P43534
D	344	HIS	-	expression tag	UNP P43534
D	345	HIS	-	expression tag	UNP P43534
D	346	HIS	-	expression tag	UNP P43534
E	240	SER	LYS	engineered mutation	UNP P43534
E	241	GLY	GLU	engineered mutation	UNP P43534
E	317	THR	GLN	engineered mutation	UNP P43534
E	341	HIS	-	expression tag	UNP P43534
E	342	HIS	-	expression tag	UNP P43534
E	343	HIS	-	expression tag	UNP P43534
E	344	HIS	-	expression tag	UNP P43534
E	345	HIS	-	expression tag	UNP P43534
E	346	HIS	-	expression tag	UNP P43534
F	240	SER	LYS	engineered mutation	UNP P43534
F	241	GLY	GLU	engineered mutation	UNP P43534
F	317	THR	GLN	engineered mutation	UNP P43534
F	341	HIS	-	expression tag	UNP P43534
F	342	HIS	-	expression tag	UNP P43534
F	343	HIS	-	expression tag	UNP P43534
F	344	HIS	-	expression tag	UNP P43534
F	345	HIS	-	expression tag	UNP P43534
F	346	HIS	-	expression tag	UNP P43534
G	240	SER	LYS	engineered mutation	UNP P43534

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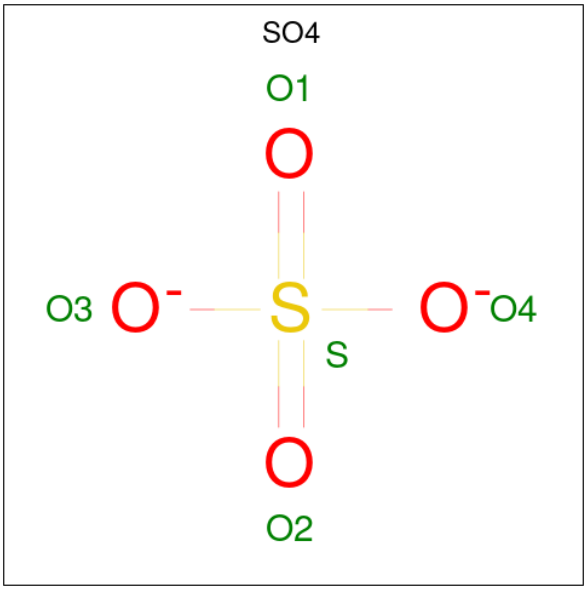
Chain	Residue	Modelled	Actual	Comment	Reference
G	241	GLY	GLU	engineered mutation	UNP P43534
G	317	THR	GLN	engineered mutation	UNP P43534
G	341	HIS	-	expression tag	UNP P43534
G	342	HIS	-	expression tag	UNP P43534
G	343	HIS	-	expression tag	UNP P43534
G	344	HIS	-	expression tag	UNP P43534
G	345	HIS	-	expression tag	UNP P43534
G	346	HIS	-	expression tag	UNP P43534
H	240	SER	LYS	engineered mutation	UNP P43534
H	241	GLY	GLU	engineered mutation	UNP P43534
H	317	THR	GLN	engineered mutation	UNP P43534
H	341	HIS	-	expression tag	UNP P43534
H	342	HIS	-	expression tag	UNP P43534
H	343	HIS	-	expression tag	UNP P43534
H	344	HIS	-	expression tag	UNP P43534
H	345	HIS	-	expression tag	UNP P43534
H	346	HIS	-	expression tag	UNP P43534

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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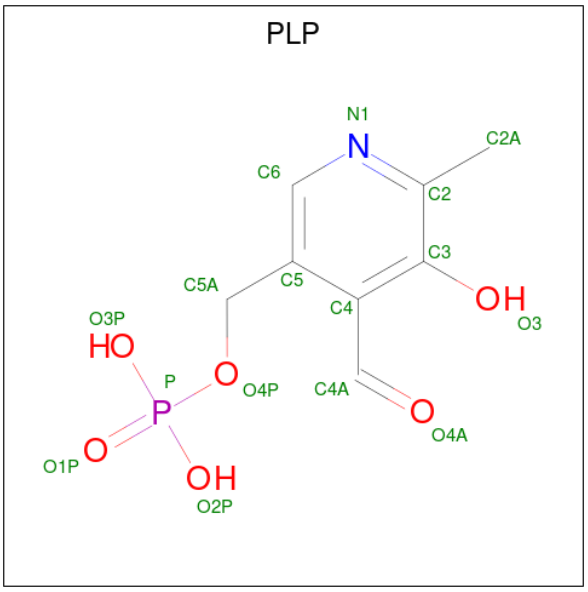
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0

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



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

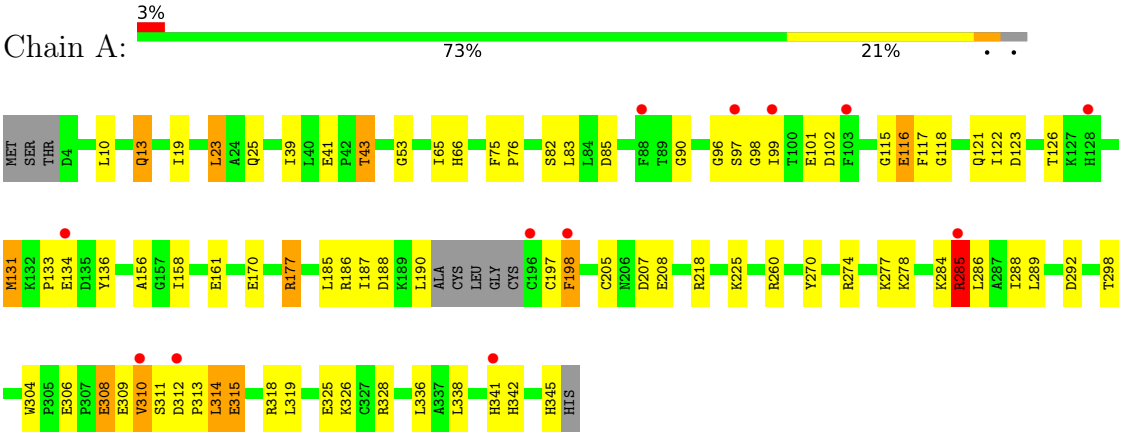
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	31	Total O 31 31	0	0
4	B	20	Total O 20 20	0	0
4	C	25	Total O 25 25	0	0
4	D	15	Total O 15 15	0	0
4	E	14	Total O 14 14	0	0
4	F	14	Total O 14 14	0	0
4	G	13	Total O 13 13	0	0
4	H	17	Total O 17 17	0	0

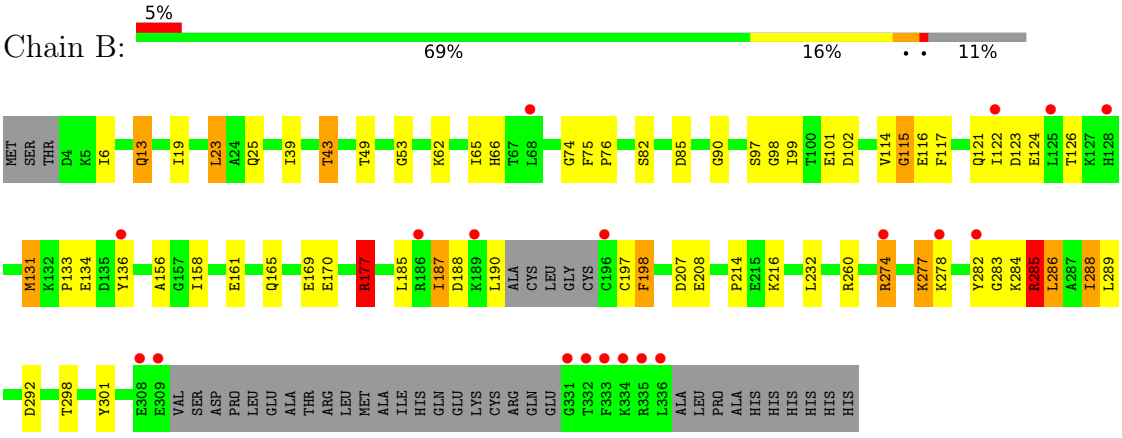
3 Residue-property plots (i)

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.

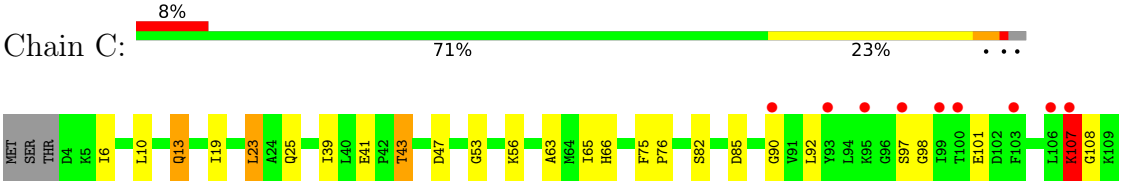
• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

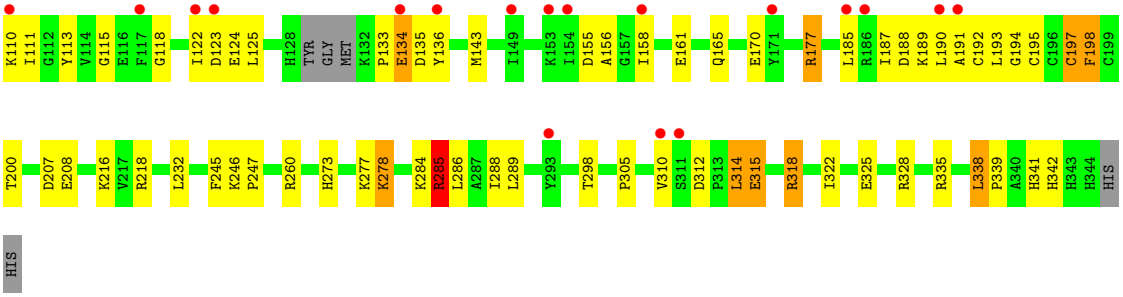


• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

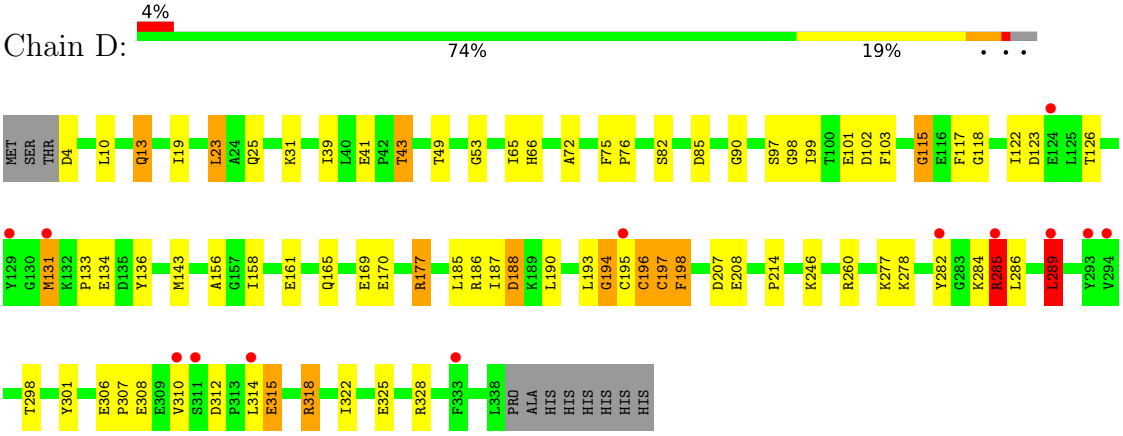


• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

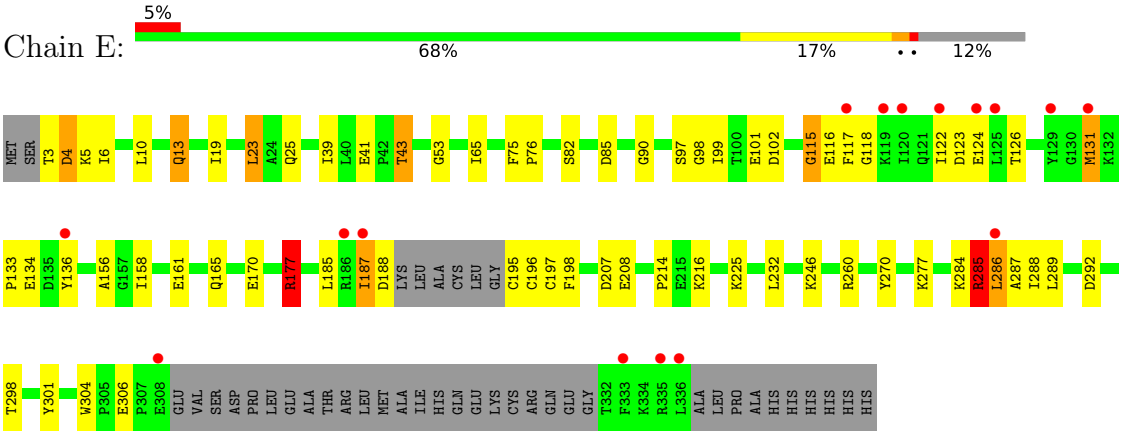




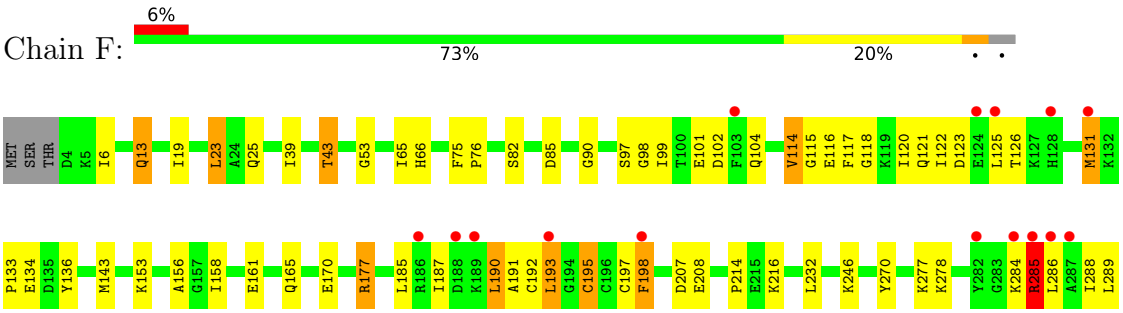
• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

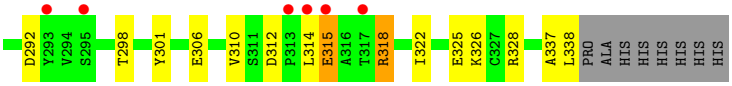


• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5



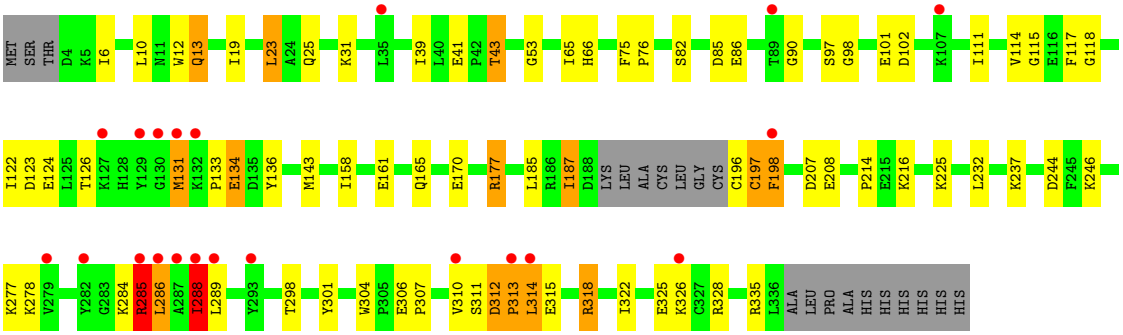
• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5





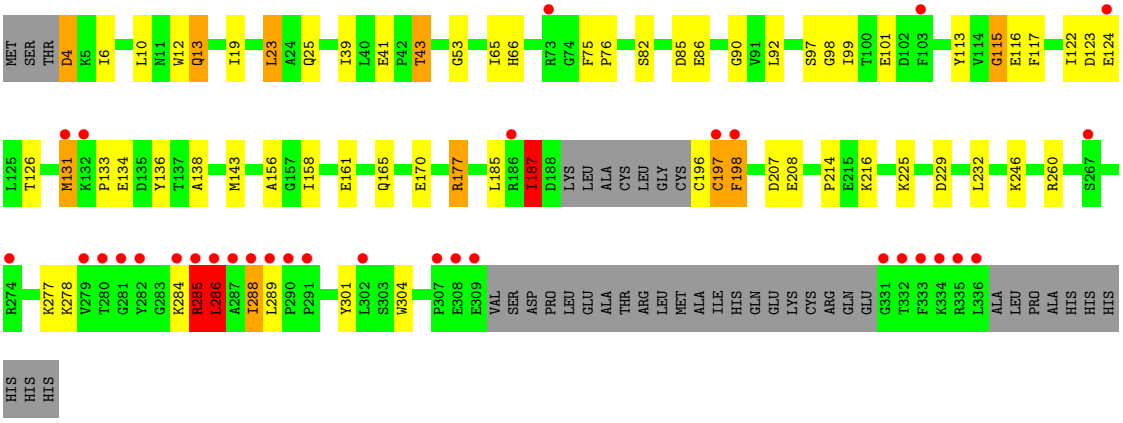
• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

Chain G:



• Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.79Å 188.46Å 101.67Å 90.00° 112.51° 90.00°	Depositor
Resolution (Å)	49.14 – 2.70 49.14 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.3 (49.14-2.70) 95.3 (49.14-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.207 , 0.247 0.207 , 0.248	Depositor DCC
R_{free} test set	2010 reflections (2.81%)	wwPDB-VP
Wilson B-factor (Å^2)	62.4	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.064 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20928	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.43% 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, 0.333 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: SO4, PLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.65	1/2768 (0.0%)	0.69	1/3739 (0.0%)
1	B	0.61	0/2515	0.89	6/3394 (0.2%)
1	C	0.60	0/2761	0.71	2/3730 (0.1%)
1	D	0.58	0/2730	0.70	3/3687 (0.1%)
1	E	0.58	0/2498	0.70	2/3373 (0.1%)
1	F	0.55	0/2730	0.70	4/3687 (0.1%)
1	G	0.57	0/2670	0.69	2/3605 (0.1%)
1	H	0.58	0/2498	0.67	2/3372 (0.1%)
All	All	0.59	1/21170 (0.0%)	0.72	22/28587 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
1	H	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	CYS	CB-SG	-6.62	1.71	1.82

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	274	ARG	NE-CZ-NH1	-23.03	108.79	120.30
1	B	274	ARG	NE-CZ-NH2	21.24	130.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	274	ARG	CD-NE-CZ	11.09	139.12	123.60
1	F	115	GLY	N-CA-C	9.30	136.36	113.10
1	B	285	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	E	285	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	D	285	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	H	285	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	C	285	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	F	285	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	C	107	LYS	CD-CE-NZ	6.58	126.83	111.70
1	A	285	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	G	285	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	H	286	LEU	CA-CB-CG	5.61	128.19	115.30
1	F	193	LEU	CA-CB-CG	5.55	128.07	115.30
1	D	194	GLY	N-CA-C	5.38	126.54	113.10
1	D	289	LEU	CB-CG-CD1	5.35	120.10	111.00
1	F	114	VAL	CB-CA-C	-5.17	101.58	111.40
1	B	286	LEU	CA-CB-CG	-5.17	103.41	115.30
1	E	177	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	177	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	G	288	ILE	CB-CA-C	5.00	121.61	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	288	ILE	Peptide
1	H	187	ILE	Peptide

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	2701	0	2699	75	3
1	B	2457	0	2466	51	0
1	C	2696	0	2702	85	1
1	D	2668	0	2684	71	1
1	E	2440	0	2446	49	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2668	0	2684	59	0
1	G	2609	0	2614	65	0
1	H	2440	0	2444	45	0
2	A	15	0	0	3	0
2	C	30	0	0	6	0
2	D	15	0	0	3	0
2	E	5	0	0	1	0
2	F	5	0	0	1	0
2	G	10	0	0	3	0
2	H	5	0	0	2	0
3	B	15	0	6	5	0
4	A	31	0	0	1	0
4	B	20	0	0	2	0
4	C	25	0	0	5	0
4	D	15	0	0	1	0
4	E	14	0	0	0	0
4	F	14	0	0	1	0
4	G	13	0	0	1	0
4	H	17	0	0	3	0
All	All	20928	0	20745	477	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (477) 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:A:312:ASP:HB3	1:A:315:GLU:CB	1.64	1.27
1:A:274:ARG:NH2	1:A:310:VAL:HG11	1.58	1.16
1:D:118:GLY:N	2:D:403:SO4:O4	1.77	1.15
1:C:193:LEU:CG	1:C:194:GLY:H	1.55	1.13
1:C:115:GLY:N	2:C:406:SO4:O2	1.82	1.10
1:C:193:LEU:HD21	1:C:278:LYS:CE	1.81	1.09
1:G:312:ASP:HB3	1:G:315:GLU:HB2	1.10	1.09
1:G:312:ASP:CB	1:G:315:GLU:HB2	1.85	1.05
1:C:193:LEU:HG	1:C:194:GLY:N	1.70	1.02
1:C:193:LEU:HG	1:C:194:GLY:H	0.84	1.00
1:C:193:LEU:HD21	1:C:278:LYS:HE3	1.42	0.99
1:A:312:ASP:CB	1:A:315:GLU:HB2	1.92	0.99
1:A:274:ARG:HH22	1:A:310:VAL:HG11	1.18	0.98
1:A:274:ARG:HH22	1:A:310:VAL:CG1	1.76	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:LEU:HD11	1:C:195:CYS:SG	2.04	0.98
1:D:115:GLY:N	2:D:403:SO4:O1	1.98	0.97
1:A:274:ARG:NH2	1:A:310:VAL:CG1	2.28	0.97
1:F:125:LEU:HD13	1:F:190:LEU:HD11	1.45	0.96
1:B:66:HIS:HD2	1:B:117:PHE:CD2	1.83	0.96
1:G:312:ASP:HB3	1:G:315:GLU:CB	1.96	0.95
1:A:274:ARG:CZ	1:A:310:VAL:HG11	1.73	0.95
1:A:312:ASP:HB3	1:A:315:GLU:HB2	0.96	0.94
1:C:113:TYR:HE1	1:C:115:GLY:O	1.51	0.92
1:D:66:HIS:HD2	1:D:117:PHE:CD2	1.88	0.90
1:B:292:ASP:OD2	1:C:218:ARG:NH1	2.05	0.89
1:C:115:GLY:CA	2:C:406:SO4:O2	2.21	0.88
1:F:116:GLU:OE1	1:F:117:PHE:CZ	2.30	0.85
1:F:116:GLU:OE1	1:F:117:PHE:CE2	2.30	0.84
1:D:66:HIS:CD2	1:D:117:PHE:HD2	1.94	0.84
1:A:315:GLU:OE2	1:A:315:GLU:HA	1.75	0.84
1:C:110:LYS:O	4:C:504:HOH:O	1.94	0.84
1:B:115:GLY:N	3:B:400:PLP:O3P	2.11	0.83
1:A:315:GLU:O	1:A:318:ARG:HG2	1.78	0.83
1:B:66:HIS:CD2	1:B:117:PHE:CD2	2.66	0.83
1:B:277:LYS:NZ	4:B:514:HOH:O	2.07	0.83
1:D:195:CYS:SG	1:D:196:CYS:N	2.53	0.81
1:A:314:LEU:HD13	1:A:314:LEU:O	1.80	0.80
1:A:314:LEU:O	1:A:314:LEU:CD1	2.30	0.80
1:C:193:LEU:CD1	1:C:195:CYS:SG	2.70	0.80
1:A:315:GLU:OE2	1:A:318:ARG:CD	2.30	0.80
1:A:315:GLU:OE2	1:A:315:GLU:CA	2.30	0.79
1:C:156:ALA:N	4:C:504:HOH:O	2.16	0.79
1:D:66:HIS:HD2	1:D:117:PHE:HD2	1.29	0.78
1:C:125:LEU:HD21	1:C:191:ALA:HB2	1.66	0.78
1:C:113:TYR:CE1	1:C:115:GLY:O	2.36	0.78
1:A:312:ASP:CB	1:A:315:GLU:CB	2.53	0.78
1:C:193:LEU:CD2	1:C:278:LYS:HE3	2.13	0.78
1:C:177:ARG:HH11	1:C:177:ARG:HG2	1.50	0.77
1:G:66:HIS:HD2	1:G:117:PHE:HD2	1.33	0.76
1:F:192:CYS:HB3	1:F:195:CYS:SG	2.26	0.76
1:G:285:ARG:HD2	1:G:286:LEU:HD22	1.66	0.76
1:D:177:ARG:HG2	1:D:177:ARG:HH11	1.50	0.76
1:G:66:HIS:CD2	1:G:117:PHE:HD2	2.02	0.75
1:A:116:GLU:N	2:A:403:SO4:O2	2.19	0.74
1:G:66:HIS:NE2	2:G:402:SO4:O1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:HIS:CE1	2:A:403:SO4:O1	2.41	0.74
1:G:66:HIS:HD2	1:G:117:PHE:CD2	2.06	0.73
1:D:193:LEU:HB3	1:D:195:CYS:SG	2.27	0.73
1:C:193:LEU:HD21	1:C:278:LYS:HE2	1.70	0.72
1:G:315:GLU:OE2	1:G:318:ARG:NE	2.18	0.72
1:B:124:GLU:HG3	1:B:286:LEU:HG	1.72	0.72
1:A:312:ASP:HB3	1:A:315:GLU:HB3	1.69	0.72
1:A:177:ARG:HH11	1:A:177:ARG:HG2	1.55	0.72
1:G:177:ARG:HG2	1:G:177:ARG:HH11	1.55	0.71
1:H:66:HIS:CD2	1:H:117:PHE:CD2	2.78	0.71
1:G:312:ASP:O	1:G:313:PRO:C	2.28	0.71
1:C:338:LEU:HD22	1:C:339:PRO:HD2	1.71	0.71
1:E:124:GLU:HG3	1:E:286:LEU:HG	1.73	0.71
1:F:177:ARG:HG2	1:F:177:ARG:HH11	1.56	0.70
1:E:90:GLY:HA2	1:E:187:ILE:HG13	1.73	0.70
1:H:229:ASP:OD1	4:H:514:HOH:O	2.08	0.70
1:H:90:GLY:HA2	1:H:187:ILE:HG13	1.72	0.70
1:B:177:ARG:HG2	1:B:177:ARG:HH11	1.56	0.70
1:H:177:ARG:HH11	1:H:177:ARG:HG2	1.55	0.70
1:G:124:GLU:CD	1:G:286:LEU:HG	2.13	0.69
1:C:90:GLY:HA2	1:C:187:ILE:HG13	1.74	0.69
1:E:195:CYS:SG	1:E:196:CYS:N	2.66	0.69
1:G:90:GLY:HA2	1:G:187:ILE:HG13	1.73	0.69
1:B:190:LEU:HD22	1:B:282:TYR:HD1	1.58	0.68
1:B:90:GLY:HA2	1:B:187:ILE:HG13	1.75	0.68
1:D:66:HIS:CD2	1:D:117:PHE:CD2	2.71	0.68
1:G:312:ASP:O	1:G:315:GLU:N	2.27	0.68
1:D:90:GLY:HA2	1:D:187:ILE:HG13	1.76	0.68
1:C:312:ASP:HB3	1:C:315:GLU:HB2	1.75	0.68
1:C:315:GLU:OE2	1:C:318:ARG:NE	2.25	0.68
1:E:4:ASP:C	1:E:4:ASP:OD1	2.30	0.67
1:E:3:THR:O	1:E:4:ASP:CG	2.34	0.66
1:D:193:LEU:HD11	1:D:282:TYR:HB2	1.77	0.66
1:F:90:GLY:HA2	1:F:187:ILE:HG13	1.77	0.66
1:E:53:GLY:HA3	1:E:75:PHE:HB3	1.77	0.66
1:F:13:GLN:OE1	1:G:246:LYS:NZ	2.29	0.66
1:F:312:ASP:HB3	1:F:315:GLU:HB2	1.77	0.66
1:E:177:ARG:HG2	1:E:177:ARG:HH11	1.60	0.66
1:D:315:GLU:HA	1:D:315:GLU:OE2	1.96	0.66
1:D:193:LEU:HG	1:D:194:GLY:H	1.60	0.65
1:F:301:TYR:O	4:F:512:HOH:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:SER:HB3	1:A:341:HIS:HB2	1.79	0.65
1:A:315:GLU:OE2	1:A:318:ARG:NE	2.30	0.65
1:H:115:GLY:N	2:H:401:SO4:O1	2.29	0.65
1:B:66:HIS:CD2	1:B:117:PHE:HD2	2.13	0.64
1:F:246:LYS:NZ	1:G:13:GLN:OE1	2.31	0.64
1:F:284:LYS:HA	1:F:289:LEU:HB2	1.80	0.63
1:G:122:ILE:HD11	1:G:158:ILE:HD11	1.79	0.63
1:B:97:SER:N	1:B:98:GLY:HA2	2.12	0.63
1:D:13:GLN:HE21	1:D:13:GLN:HA	1.63	0.63
1:F:39:ILE:O	1:G:43:THR:HB	1.98	0.63
1:G:76:PRO:HB2	1:G:207:ASP:HB2	1.80	0.63
1:A:90:GLY:HA2	1:A:187:ILE:HG13	1.80	0.63
1:F:315:GLU:OE2	1:F:318:ARG:NE	2.23	0.63
1:C:43:THR:HB	1:E:39:ILE:O	1.98	0.62
1:C:97:SER:N	1:C:98:GLY:HA2	2.14	0.62
1:H:123:ASP:OD1	1:H:136:TYR:OH	2.17	0.62
1:A:97:SER:N	1:A:98:GLY:HA2	2.15	0.62
1:F:53:GLY:HA3	1:F:75:PHE:HB3	1.81	0.62
1:A:274:ARG:CZ	1:A:310:VAL:CG1	2.43	0.61
1:C:13:GLN:OE1	1:E:246:LYS:NZ	2.33	0.61
1:E:97:SER:N	1:E:98:GLY:HA2	2.15	0.61
1:H:53:GLY:HA3	1:H:75:PHE:HB3	1.81	0.61
1:A:284:LYS:HA	1:A:289:LEU:HB2	1.82	0.61
1:E:126:THR:HB	1:E:131:MET:HB2	1.82	0.61
1:A:122:ILE:HD11	1:A:158:ILE:HD11	1.83	0.61
1:A:315:GLU:OE2	1:A:318:ARG:CG	2.48	0.61
1:C:65:ILE:HG23	1:C:66:HIS:ND1	2.15	0.61
1:C:188:ASP:OD1	1:C:189:LYS:HG3	2.00	0.61
1:D:194:GLY:CA	1:D:278:LYS:HE2	2.31	0.61
1:A:315:GLU:O	1:A:318:ARG:CG	2.46	0.60
1:F:122:ILE:HD11	1:F:158:ILE:HD11	1.82	0.60
1:C:246:LYS:NZ	1:E:13:GLN:OE1	2.34	0.60
1:D:246:LYS:NZ	1:H:13:GLN:OE1	2.32	0.60
1:H:284:LYS:HA	1:H:289:LEU:HB2	1.83	0.60
1:G:13:GLN:HA	1:G:13:GLN:HE21	1.66	0.60
1:B:122:ILE:HD11	1:B:158:ILE:HD11	1.83	0.60
1:C:193:LEU:CG	1:C:194:GLY:N	2.30	0.60
1:D:13:GLN:OE1	1:H:246:LYS:NZ	2.34	0.60
1:C:122:ILE:HD11	1:C:158:ILE:HD11	1.84	0.60
1:D:43:THR:HB	1:H:39:ILE:O	2.01	0.60
1:H:97:SER:N	1:H:98:GLY:HA2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:13:GLN:HA	1:H:13:GLN:HE21	1.66	0.60
1:A:123:ASP:OD1	1:A:136:TYR:OH	2.21	0.59
1:B:53:GLY:HA3	1:B:75:PHE:HB3	1.84	0.59
1:E:76:PRO:HB2	1:E:207:ASP:HB2	1.83	0.59
1:H:126:THR:HB	1:H:131:MET:HB2	1.85	0.59
1:F:76:PRO:HB2	1:F:207:ASP:HB2	1.85	0.59
1:C:318:ARG:NH1	4:C:512:HOH:O	2.35	0.59
1:F:97:SER:N	1:F:98:GLY:HA2	2.17	0.59
1:F:123:ASP:OD1	1:F:136:TYR:OH	2.20	0.59
1:G:284:LYS:HA	1:G:289:LEU:HB2	1.84	0.59
1:B:74:GLY:O	1:C:305:PRO:HD3	2.03	0.58
1:G:97:SER:N	1:G:98:GLY:HA2	2.18	0.58
1:B:123:ASP:OD1	1:B:136:TYR:OH	2.22	0.58
1:F:43:THR:HB	1:G:39:ILE:O	2.03	0.58
1:G:312:ASP:O	1:G:314:LEU:N	2.35	0.58
1:D:126:THR:HB	1:D:131:MET:HB2	1.85	0.58
1:H:76:PRO:HB2	1:H:207:ASP:HB2	1.85	0.58
1:B:190:LEU:HD22	1:B:282:TYR:CD1	2.39	0.58
1:G:126:THR:HB	1:G:131:MET:HB2	1.86	0.58
1:D:97:SER:N	1:D:98:GLY:HA2	2.19	0.58
1:C:124:GLU:HG3	1:C:286:LEU:HD13	1.86	0.58
1:D:123:ASP:OD1	1:D:136:TYR:OH	2.21	0.57
1:F:13:GLN:HA	1:F:13:GLN:HE21	1.69	0.57
1:F:125:LEU:HD21	1:F:191:ALA:HB2	1.85	0.57
1:C:284:LYS:HA	1:C:289:LEU:HB2	1.86	0.57
1:G:123:ASP:OD1	1:G:136:TYR:OH	2.21	0.57
1:H:66:HIS:HD2	1:H:117:PHE:CD2	2.21	0.57
1:D:122:ILE:HD11	1:D:158:ILE:HD11	1.85	0.57
1:A:19:ILE:HG12	1:A:23:LEU:HD22	1.87	0.57
1:A:314:LEU:O	1:A:314:LEU:HD12	2.03	0.57
1:D:188:ASP:OD2	1:D:188:ASP:N	2.34	0.57
1:F:101:GLU:HA	1:F:185:LEU:HD21	1.87	0.57
1:F:126:THR:HB	1:F:131:MET:HB2	1.85	0.57
1:E:122:ILE:HD11	1:E:158:ILE:HD11	1.87	0.57
1:C:123:ASP:OD1	1:C:136:TYR:OH	2.23	0.56
1:E:123:ASP:OD1	1:E:136:TYR:OH	2.23	0.56
1:B:126:THR:HB	1:B:131:MET:HB2	1.86	0.56
1:B:76:PRO:HB2	1:B:207:ASP:HB2	1.86	0.56
1:D:194:GLY:HA2	1:D:278:LYS:HE2	1.86	0.56
1:H:122:ILE:HD11	1:H:158:ILE:HD11	1.87	0.56
1:A:314:LEU:CD1	1:A:314:LEU:C	2.72	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:GLN:HE21	1:C:13:GLN:HA	1.70	0.56
1:A:126:THR:HB	1:A:131:MET:HB2	1.86	0.56
1:A:53:GLY:HA3	1:A:75:PHE:HB3	1.86	0.56
1:A:76:PRO:HB2	1:A:207:ASP:HB2	1.88	0.56
1:D:76:PRO:HB2	1:D:207:ASP:HB2	1.86	0.56
1:C:76:PRO:HB2	1:C:207:ASP:HB2	1.88	0.55
1:A:308:GLU:OE2	1:A:308:GLU:HA	2.07	0.55
1:E:161:GLU:OE2	1:E:260:ARG:NH1	2.40	0.55
1:C:101:GLU:HA	1:C:185:LEU:HD21	1.88	0.55
1:F:116:GLU:HG3	1:F:117:PHE:CD2	2.40	0.55
1:A:315:GLU:OE2	1:A:318:ARG:HD3	2.07	0.55
1:D:72:ALA:HB2	1:D:289:LEU:HD12	1.88	0.55
1:B:284:LYS:HA	1:B:289:LEU:HB2	1.89	0.55
1:C:19:ILE:HG12	1:C:23:LEU:HD22	1.88	0.55
1:C:318:ARG:O	1:C:322:ILE:HG12	2.07	0.55
1:B:101:GLU:HA	1:B:185:LEU:HD21	1.88	0.55
1:C:47:ASP:OD2	1:E:5:LYS:NZ	2.35	0.55
1:C:285:ARG:HG3	1:C:285:ARG:HH11	1.72	0.55
1:D:101:GLU:HA	1:D:185:LEU:HD21	1.90	0.54
1:G:325:GLU:OE2	1:G:328:ARG:NH1	2.40	0.54
1:E:284:LYS:HA	1:E:289:LEU:HB2	1.89	0.54
1:G:19:ILE:HG12	1:G:23:LEU:HD22	1.89	0.54
1:A:101:GLU:HA	1:A:185:LEU:HD21	1.90	0.54
1:G:285:ARG:HG2	1:G:286:LEU:HD13	1.90	0.54
1:A:325:GLU:OE2	1:A:328:ARG:NH1	2.40	0.53
1:D:177:ARG:HH11	1:D:177:ARG:CG	2.21	0.53
1:A:13:GLN:HE21	1:A:13:GLN:HA	1.73	0.53
1:E:101:GLU:HA	1:E:185:LEU:HD21	1.89	0.53
1:G:285:ARG:HG3	1:G:285:ARG:HH11	1.72	0.53
1:A:312:ASP:O	1:A:313:PRO:C	2.43	0.53
1:C:193:LEU:HD21	1:C:278:LYS:CD	2.38	0.53
1:D:53:GLY:HA3	1:D:75:PHE:HB3	1.90	0.53
1:B:13:GLN:HE21	1:B:13:GLN:HA	1.74	0.53
1:C:325:GLU:OE2	1:C:328:ARG:NH1	2.41	0.53
1:D:193:LEU:C	1:D:195:CYS:HB2	2.29	0.53
1:G:101:GLU:HA	1:G:185:LEU:HD21	1.91	0.53
1:F:318:ARG:O	1:F:322:ILE:HG12	2.08	0.52
1:A:10:LEU:HD12	1:A:41:GLU:HG2	1.90	0.52
1:A:285:ARG:NH1	1:A:285:ARG:HB2	2.24	0.52
1:A:285:ARG:HH11	1:A:285:ARG:CG	2.22	0.52
1:B:292:ASP:CG	1:C:218:ARG:HH12	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:ARG:HH11	1:F:285:ARG:HG3	1.74	0.52
1:H:116:GLU:N	2:H:401:SO4:O3	2.35	0.52
1:A:286:LEU:HB2	1:A:288:ILE:HG13	1.91	0.52
1:A:315:GLU:CD	1:A:318:ARG:HE	2.12	0.52
1:C:53:GLY:HA3	1:C:75:PHE:HB3	1.91	0.52
1:D:318:ARG:O	1:D:322:ILE:HG12	2.10	0.52
1:E:19:ILE:HG12	1:E:23:LEU:HD22	1.91	0.52
1:A:285:ARG:HH11	1:A:285:ARG:HG3	1.73	0.52
1:C:177:ARG:HH11	1:C:177:ARG:CG	2.21	0.52
1:F:117:PHE:O	1:F:121:GLN:HG3	2.09	0.52
1:H:97:SER:OG	4:H:502:HOH:O	2.19	0.52
1:H:285:ARG:HG3	1:H:285:ARG:HH11	1.75	0.52
1:D:103:PHE:HD2	1:D:190:LEU:HD22	1.73	0.52
1:G:66:HIS:CD2	1:G:117:PHE:CD2	2.87	0.51
1:F:325:GLU:OE2	1:F:328:ARG:NH1	2.43	0.51
1:G:318:ARG:O	1:G:322:ILE:HG12	2.11	0.51
1:D:19:ILE:HG12	1:D:23:LEU:HD22	1.92	0.51
1:E:285:ARG:HB2	1:E:285:ARG:NH1	2.25	0.51
1:C:10:LEU:HD12	1:C:41:GLU:HG2	1.92	0.51
1:E:13:GLN:HE21	1:E:13:GLN:HA	1.74	0.51
1:A:117:PHE:O	1:A:121:GLN:HG3	2.10	0.51
1:A:186:ARG:HG2	1:A:188:ASP:HB2	1.93	0.51
1:A:312:ASP:CB	1:A:315:GLU:HB3	2.34	0.51
1:H:19:ILE:HG12	1:H:23:LEU:HD22	1.92	0.51
1:D:31:LYS:HB3	1:D:31:LYS:HZ3	1.74	0.51
1:G:53:GLY:HA3	1:G:75:PHE:HB3	1.92	0.51
1:F:114:VAL:HB	2:F:401:SO4:O1	2.11	0.51
1:G:285:ARG:HD2	1:G:286:LEU:CD2	2.38	0.51
1:H:161:GLU:OE2	1:H:260:ARG:NH1	2.44	0.51
1:C:335:ARG:NE	2:C:402:SO4:O2	2.44	0.50
1:G:285:ARG:HH11	1:G:285:ARG:CG	2.24	0.50
1:B:117:PHE:O	1:B:121:GLN:HG3	2.12	0.50
1:E:3:THR:O	1:E:4:ASP:OD1	2.29	0.50
1:E:3:THR:O	1:E:4:ASP:CB	2.60	0.50
1:E:214:PRO:HB3	1:E:301:TYR:HE1	1.75	0.50
1:A:315:GLU:OE2	1:A:315:GLU:O	2.30	0.50
1:H:4:ASP:N	4:H:503:HOH:O	2.44	0.50
1:A:65:ILE:HG23	1:A:66:HIS:ND1	2.27	0.50
1:F:19:ILE:HG12	1:F:23:LEU:HD22	1.93	0.50
1:C:115:GLY:HA3	2:C:406:SO4:O2	2.11	0.49
1:B:19:ILE:HG12	1:B:23:LEU:HD22	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ARG:HG3	1:D:285:ARG:HH11	1.76	0.49
1:F:125:LEU:CD1	1:F:190:LEU:HD11	2.32	0.49
1:G:177:ARG:HH11	1:G:177:ARG:CG	2.24	0.49
1:G:312:ASP:OD2	1:G:315:GLU:HB2	2.12	0.49
1:D:13:GLN:HG2	1:D:143:MET:SD	2.53	0.49
1:D:193:LEU:HD22	1:D:198:PHE:CE1	2.47	0.49
1:D:194:GLY:HA3	1:D:278:LYS:HE2	1.94	0.49
1:H:101:GLU:HA	1:H:185:LEU:HD21	1.93	0.49
1:D:284:LYS:HA	1:D:289:LEU:HB2	1.94	0.49
1:F:125:LEU:HD13	1:F:190:LEU:CD1	2.32	0.49
1:F:285:ARG:HH11	1:F:285:ARG:CG	2.26	0.49
1:A:274:ARG:HH22	1:A:310:VAL:HG12	1.70	0.49
1:A:312:ASP:O	1:A:315:GLU:N	2.46	0.48
1:B:285:ARG:NH1	1:B:285:ARG:HB2	2.28	0.48
1:D:195:CYS:C	1:D:197:CYS:H	2.17	0.48
1:G:117:PHE:O	1:G:118:GLY:C	2.50	0.48
1:H:214:PRO:HB3	1:H:301:TYR:HE1	1.78	0.48
1:C:118:GLY:N	2:C:406:SO4:O3	2.46	0.48
1:E:285:ARG:HG3	1:E:285:ARG:HH11	1.78	0.48
1:E:285:ARG:HH11	1:E:285:ARG:CG	2.25	0.48
1:D:285:ARG:NH1	1:D:285:ARG:HB2	2.29	0.48
1:B:49:THR:CG2	1:B:62:LYS:HG2	2.43	0.48
1:G:133:PRO:HA	1:G:134:GLU:HA	1.62	0.48
1:G:214:PRO:HB3	1:G:301:TYR:HE1	1.77	0.48
1:H:177:ARG:HH11	1:H:177:ARG:CG	2.26	0.48
1:A:285:ARG:HB2	1:A:285:ARG:HH11	1.78	0.48
1:B:177:ARG:HH11	1:B:177:ARG:CG	2.26	0.48
1:F:177:ARG:HH11	1:F:177:ARG:CG	2.25	0.48
1:A:66:HIS:NE2	2:A:403:SO4:O1	2.47	0.48
1:A:83:LEU:O	4:A:515:HOH:O	2.18	0.48
1:B:117:PHE:N	3:B:400:PLP:O1P	2.46	0.48
1:B:283:GLY:O	1:B:288:ILE:HG12	2.13	0.48
1:C:39:ILE:O	1:E:43:THR:HB	2.14	0.48
1:B:99:ILE:HD12	1:B:156:ALA:HB2	1.95	0.48
1:G:326:LYS:HA	1:G:326:LYS:HD3	1.73	0.48
1:G:312:ASP:CG	1:G:315:GLU:HB2	2.30	0.47
1:B:187:ILE:O	1:B:187:ILE:HG22	2.14	0.47
1:C:285:ARG:HH11	1:C:285:ARG:CG	2.27	0.47
1:D:193:LEU:CD1	1:D:282:TYR:HB2	2.42	0.47
1:D:308:GLU:HG2	1:E:134:GLU:CD	2.35	0.47
1:A:177:ARG:HH11	1:A:177:ARG:CG	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ARG:HH11	1:D:285:ARG:CG	2.27	0.47
1:D:312:ASP:HB3	1:D:315:GLU:HB2	1.96	0.47
1:E:117:PHE:O	1:E:118:GLY:C	2.53	0.47
1:E:286:LEU:HD13	1:E:286:LEU:HA	1.63	0.47
1:B:285:ARG:CG	1:B:285:ARG:HH11	2.27	0.47
1:H:86:GLU:HG2	1:H:197:CYS:HB3	1.97	0.47
1:C:187:ILE:HG22	1:C:187:ILE:O	2.14	0.47
1:D:39:ILE:O	1:H:43:THR:HB	2.14	0.47
1:E:285:ARG:HB2	1:E:285:ARG:HH11	1.79	0.47
1:H:187:ILE:HG22	1:H:187:ILE:O	2.14	0.47
1:C:107:LYS:HG3	1:C:135:ASP:HB3	1.96	0.47
1:H:285:ARG:HH11	1:H:285:ARG:CG	2.27	0.47
1:E:133:PRO:HA	1:E:134:GLU:HA	1.63	0.47
1:E:285:ARG:HD2	1:E:286:LEU:HD22	1.96	0.47
1:D:195:CYS:SG	1:D:198:PHE:CE2	3.09	0.46
1:F:288:ILE:O	1:F:289:LEU:HD23	2.14	0.46
1:G:314:LEU:HA	1:G:314:LEU:HD23	1.68	0.46
1:B:214:PRO:HB3	1:B:301:TYR:HE1	1.80	0.46
1:D:31:LYS:HE2	1:G:31:LYS:NZ	2.30	0.46
1:D:325:GLU:OE2	1:D:328:ARG:NH1	2.46	0.46
1:G:312:ASP:CB	1:G:315:GLU:CB	2.74	0.46
1:H:133:PRO:HA	1:H:134:GLU:HA	1.61	0.46
1:B:285:ARG:HH11	1:B:285:ARG:HG3	1.80	0.46
1:E:10:LEU:HD12	1:E:41:GLU:HG2	1.96	0.46
1:C:193:LEU:CD1	1:C:194:GLY:N	2.79	0.46
1:A:65:ILE:HB	1:A:198:PHE:HB3	1.98	0.46
1:B:116:GLU:N	3:B:400:PLP:O1P	2.44	0.46
1:B:133:PRO:HA	1:B:134:GLU:HA	1.62	0.46
1:D:214:PRO:HB3	1:D:301:TYR:HE1	1.80	0.46
1:E:177:ARG:HH11	1:E:177:ARG:CG	2.28	0.46
1:D:187:ILE:HG22	1:D:187:ILE:O	2.15	0.46
1:F:193:LEU:HD22	1:F:314:LEU:HD22	1.96	0.46
1:C:111:ILE:HD12	1:C:136:TYR:CD1	2.51	0.46
1:B:285:ARG:HB2	1:B:285:ARG:HH11	1.80	0.46
1:F:99:ILE:HD12	1:F:156:ALA:HB2	1.98	0.46
1:C:273:HIS:HE1	2:C:404:SO4:O2	1.97	0.45
1:D:186:ARG:HG2	1:D:188:ASP:OD2	2.16	0.45
1:G:187:ILE:O	1:G:187:ILE:HG22	2.15	0.45
1:G:335:ARG:NE	2:G:401:SO4:O3	2.47	0.45
1:A:338:LEU:HA	1:A:338:LEU:HD23	1.69	0.45
1:H:6:ILE:HD11	1:H:216:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:PRO:HA	1:F:134:GLU:HA	1.62	0.45
1:C:23:LEU:HD12	1:C:23:LEU:HA	1.77	0.45
1:F:214:PRO:HB3	1:F:301:TYR:HE1	1.81	0.45
1:A:318:ARG:HG3	1:A:319:LEU:N	2.31	0.45
1:F:13:GLN:HG2	1:F:143:MET:SD	2.56	0.45
1:F:326:LYS:HA	1:F:326:LYS:HD3	1.77	0.45
1:F:120:ILE:HG22	1:F:121:GLN:N	2.32	0.45
1:F:153:LYS:NZ	1:G:244:ASP:OD1	2.50	0.45
1:G:10:LEU:HD12	1:G:41:GLU:HG2	1.99	0.45
1:E:225:LYS:HB2	1:E:304:TRP:CH2	2.52	0.45
1:B:6:ILE:HD11	1:B:216:LYS:HD3	1.99	0.45
1:C:133:PRO:HA	1:C:134:GLU:HA	1.59	0.45
1:H:288:ILE:O	1:H:289:LEU:HD23	2.17	0.45
1:A:43:THR:HB	1:B:39:ILE:O	2.17	0.45
1:F:337:ALA:O	1:F:338:LEU:HG	2.17	0.45
1:A:39:ILE:O	1:B:43:THR:HB	2.17	0.44
1:A:161:GLU:OE2	1:A:260:ARG:NH1	2.50	0.44
1:D:99:ILE:HD12	1:D:156:ALA:HB2	2.00	0.44
1:D:133:PRO:HA	1:D:134:GLU:HA	1.61	0.44
1:F:116:GLU:HG3	1:F:117:PHE:CE2	2.53	0.44
1:A:118:GLY:O	1:A:122:ILE:HG13	2.17	0.44
1:C:113:TYR:HE1	1:C:115:GLY:C	2.19	0.44
1:C:155:ASP:HB2	4:C:504:HOH:O	2.16	0.44
1:B:292:ASP:CG	1:C:218:ARG:NH1	2.70	0.44
1:F:66:HIS:HD2	1:F:117:PHE:CD2	2.36	0.44
1:B:65:ILE:HB	1:B:198:PHE:HB3	2.00	0.44
1:D:65:ILE:HB	1:D:198:PHE:HB3	2.00	0.44
1:D:188:ASP:HA	1:D:195:CYS:SG	2.58	0.44
1:D:285:ARG:HH11	1:D:285:ARG:HB2	1.83	0.44
1:A:133:PRO:HA	1:A:134:GLU:HA	1.61	0.44
1:E:126:THR:OG1	1:E:133:PRO:HD3	2.17	0.44
1:G:86:GLU:HG2	1:G:197:CYS:HB3	1.99	0.44
1:G:114:VAL:HB	2:G:402:SO4:O4	2.17	0.44
1:B:169:GLU:OE1	1:B:260:ARG:NH2	2.51	0.44
1:B:232:LEU:HD23	1:B:232:LEU:HA	1.82	0.44
1:E:188:ASP:OD2	1:E:195:CYS:HA	2.17	0.44
1:F:161:GLU:O	1:F:165:GLN:HB3	2.18	0.44
1:A:186:ARG:O	1:A:190:LEU:HG	2.17	0.43
1:D:193:LEU:CG	1:D:194:GLY:H	2.30	0.43
1:F:187:ILE:HA	1:F:190:LEU:HD23	2.00	0.43
1:A:186:ARG:CD	1:A:188:ASP:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:THR:OG1	1:B:133:PRO:HD3	2.17	0.43
1:G:12:TRP:CZ2	1:G:143:MET:HG2	2.53	0.43
1:C:314:LEU:HD12	1:C:314:LEU:HA	1.80	0.43
1:D:66:HIS:NE2	2:D:403:SO4:O3	2.51	0.43
1:E:285:ARG:C	1:E:287:ALA:H	2.22	0.43
1:C:232:LEU:HD23	1:C:232:LEU:HA	1.82	0.43
1:F:187:ILE:HG22	1:F:187:ILE:O	2.19	0.43
1:C:56:LYS:O	4:C:515:HOH:O	2.21	0.43
1:C:65:ILE:HB	1:C:198:PHE:HB3	2.01	0.43
1:C:92:LEU:HD21	1:C:165:GLN:HB2	2.01	0.43
1:C:338:LEU:HD22	1:C:338:LEU:HA	1.83	0.43
1:C:338:LEU:HD13	1:C:339:PRO:HD2	2.00	0.43
1:D:10:LEU:HD12	1:D:41:GLU:HG2	2.00	0.43
1:H:65:ILE:HB	1:H:198:PHE:HB3	2.00	0.43
1:A:99:ILE:HD12	1:A:156:ALA:HB2	1.99	0.43
1:A:292:ASP:OD1	1:A:292:ASP:N	2.49	0.43
1:B:98:GLY:HA2	4:B:501:HOH:O	2.18	0.43
1:C:193:LEU:HD12	1:C:195:CYS:H	1.84	0.43
1:G:237:LYS:NZ	4:G:503:HOH:O	2.19	0.43
1:H:99:ILE:HD12	1:H:156:ALA:HB2	2.00	0.43
1:C:338:LEU:HD13	1:C:339:PRO:CD	2.48	0.43
1:G:161:GLU:O	1:G:165:GLN:HB3	2.18	0.43
1:G:285:ARG:HB2	1:G:285:ARG:NH1	2.34	0.43
1:H:161:GLU:O	1:H:165:GLN:HB3	2.19	0.43
1:D:103:PHE:CD2	1:D:190:LEU:HD22	2.54	0.42
1:H:126:THR:OG1	1:H:133:PRO:HD3	2.19	0.42
1:E:270:TYR:CE1	1:E:306:GLU:HB2	2.55	0.42
1:F:65:ILE:HB	1:F:198:PHE:HB3	2.00	0.42
1:H:12:TRP:CZ2	1:H:143:MET:HG2	2.55	0.42
1:A:315:GLU:OE2	1:A:315:GLU:C	2.57	0.42
1:G:306:GLU:HA	1:G:307:PRO:HD3	1.85	0.42
1:D:195:CYS:C	1:D:197:CYS:N	2.71	0.42
1:F:232:LEU:HD23	1:F:232:LEU:HA	1.80	0.42
1:G:23:LEU:HD12	1:G:23:LEU:HA	1.67	0.42
1:G:111:ILE:HD12	1:G:136:TYR:CD1	2.54	0.42
1:D:195:CYS:HG	1:D:196:CYS:H	1.61	0.42
1:F:270:TYR:CE1	1:F:306:GLU:HB2	2.54	0.42
1:D:117:PHE:O	1:D:118:GLY:C	2.57	0.42
1:E:99:ILE:HD12	1:E:156:ALA:HB2	2.01	0.42
1:H:225:LYS:HB2	1:H:304:TRP:CH2	2.55	0.42
1:A:326:LYS:HD3	1:A:326:LYS:HA	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:CYS:O	1:C:193:LEU:HB3	2.19	0.42
1:G:12:TRP:CE2	1:G:143:MET:HG2	2.55	0.42
1:H:113:TYR:CE2	1:H:138:ALA:HB1	2.54	0.42
1:C:75:PHE:HA	1:C:76:PRO:HD2	1.94	0.42
1:C:161:GLU:OE2	1:C:260:ARG:NH1	2.53	0.42
1:D:23:LEU:HD12	1:D:23:LEU:HA	1.66	0.42
1:E:23:LEU:HD12	1:E:23:LEU:HA	1.66	0.42
1:D:169:GLU:OE1	1:D:260:ARG:NH2	2.52	0.41
1:A:315:GLU:C	1:A:318:ARG:HG2	2.37	0.41
1:E:65:ILE:HB	1:E:198:PHE:HB3	2.02	0.41
1:E:6:ILE:HD11	1:E:216:LYS:HD3	2.03	0.41
1:F:292:ASP:OD1	1:F:292:ASP:N	2.52	0.41
1:G:65:ILE:HB	1:G:198:PHE:HB3	2.02	0.41
1:B:116:GLU:H	3:B:400:PLP:P	2.42	0.41
1:C:286:LEU:HB2	1:C:288:ILE:HG13	2.03	0.41
1:D:49:THR:HG21	4:D:515:HOH:O	2.19	0.41
1:C:108:GLY:N	1:C:135:ASP:O	2.22	0.41
1:C:161:GLU:O	1:C:165:GLN:HB3	2.20	0.41
1:D:306:GLU:HA	1:D:307:PRO:HD3	1.87	0.41
1:F:6:ILE:HD11	1:F:216:LYS:HD3	2.01	0.41
1:F:23:LEU:HD12	1:F:23:LEU:HA	1.65	0.41
1:F:118:GLY:O	1:F:122:ILE:HG13	2.20	0.41
1:G:6:ILE:HD11	1:G:216:LYS:HD3	2.01	0.41
1:C:13:GLN:HG2	1:C:143:MET:SD	2.60	0.41
1:E:286:LEU:O	1:E:288:ILE:HD12	2.21	0.41
1:H:232:LEU:HA	1:H:232:LEU:HD23	1.79	0.41
1:D:161:GLU:O	1:D:165:GLN:HB3	2.20	0.41
1:B:188:ASP:OD1	1:B:188:ASP:N	2.52	0.41
1:E:161:GLU:O	1:E:165:GLN:HB3	2.20	0.41
1:F:104:GLN:H	1:F:104:GLN:HG3	1.75	0.41
1:H:285:ARG:NH1	1:H:285:ARG:HB2	2.36	0.41
1:B:161:GLU:OE2	1:B:260:ARG:NH1	2.54	0.41
1:C:285:ARG:HB2	1:C:285:ARG:NH1	2.36	0.41
1:H:10:LEU:HD12	1:H:41:GLU:HG2	2.02	0.41
1:H:124:GLU:HG3	1:H:286:LEU:HD13	2.03	0.41
1:D:188:ASP:OD2	1:D:196:CYS:SG	2.71	0.41
1:A:270:TYR:CE1	1:A:306:GLU:HB2	2.56	0.40
1:C:245:PHE:O	1:C:247:PRO:HD3	2.21	0.40
1:F:126:THR:OG1	1:F:133:PRO:HD3	2.20	0.40
1:B:161:GLU:O	1:B:165:GLN:HB3	2.20	0.40
1:C:63:ALA:HA	1:C:200:THR:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:ARG:NH1	1:F:285:ARG:HB2	2.36	0.40
1:H:92:LEU:HD21	1:H:165:GLN:HB2	2.03	0.40
1:B:114:VAL:HB	3:B:400:PLP:O3P	2.20	0.40
1:C:195:CYS:C	1:C:197:CYS:N	2.75	0.40
1:D:31:LYS:HE2	1:G:31:LYS:HZ3	1.87	0.40
1:E:115:GLY:N	2:E:401:SO4:O4	2.37	0.40
1:E:232:LEU:HD23	1:E:232:LEU:HA	1.85	0.40
1:G:232:LEU:HD23	1:G:232:LEU:HA	1.92	0.40
1:A:225:LYS:HB2	1:A:304:TRP:CH2	2.56	0.40
1:C:6:ILE:HD11	1:C:216:LYS:HD3	2.02	0.40
1:C:193:LEU:HD11	1:C:195:CYS:HG	1.81	0.40
1:G:225:LYS:HB2	1:G:304:TRP:CH2	2.57	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ARG:NH1	1:D:314:LEU:CD2[1_455]	1.41	0.79
1:A:218:ARG:NH1	1:E:292:ASP:OD2[1_455]	1.94	0.26
1:A:96:GLY:O	1:C:107:LYS:O[2_656]	2.11	0.09

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	333/346 (96%)	324 (97%)	8 (2%)	1 (0%)	41 66
1	B	301/346 (87%)	290 (96%)	9 (3%)	2 (1%)	22 46
1	C	334/346 (96%)	320 (96%)	14 (4%)	0	100 100
1	D	333/346 (96%)	323 (97%)	9 (3%)	1 (0%)	41 66
1	E	299/346 (86%)	290 (97%)	7 (2%)	2 (1%)	22 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	333/346 (96%)	322 (97%)	11 (3%)	0	100 100
1	G	322/346 (93%)	312 (97%)	7 (2%)	3 (1%)	17 40
1	H	299/346 (86%)	286 (96%)	11 (4%)	2 (1%)	22 46
All	All	2554/2768 (92%)	2467 (97%)	76 (3%)	11 (0%)	34 60

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLY
1	B	115	GLY
1	E	115	GLY
1	B	187	ILE
1	G	115	GLY
1	H	115	GLY
1	D	115	GLY
1	E	187	ILE
1	H	187	ILE
1	G	187	ILE
1	G	313	PRO

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	291/298 (98%)	265 (91%)	26 (9%)	9 22
1	B	265/298 (89%)	246 (93%)	19 (7%)	14 34
1	C	291/298 (98%)	266 (91%)	25 (9%)	10 24
1	D	288/298 (97%)	264 (92%)	24 (8%)	11 25
1	E	264/298 (89%)	246 (93%)	18 (7%)	16 36
1	F	288/298 (97%)	265 (92%)	23 (8%)	12 27
1	G	282/298 (95%)	256 (91%)	26 (9%)	9 21
1	H	263/298 (88%)	244 (93%)	19 (7%)	14 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2232/2384 (94%)	2052 (92%)	180 (8%)	11 27

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	23	LEU
1	A	25	GLN
1	A	43	THR
1	A	82	SER
1	A	85	ASP
1	A	102	ASP
1	A	116	GLU
1	A	131	MET
1	A	170	GLU
1	A	177	ARG
1	A	197	CYS
1	A	198	PHE
1	A	208	GLU
1	A	277	LYS
1	A	278	LYS
1	A	285	ARG
1	A	298	THR
1	A	308	GLU
1	A	309	GLU
1	A	310	VAL
1	A	314	LEU
1	A	315	GLU
1	A	336	LEU
1	A	342	HIS
1	A	345	HIS
1	B	13	GLN
1	B	23	LEU
1	B	25	GLN
1	B	43	THR
1	B	82	SER
1	B	85	ASP
1	B	102	ASP
1	B	131	MET
1	B	170	GLU
1	B	177	ARG
1	B	197	CYS

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Mol	Chain	Res	Type
1	B	198	PHE
1	B	208	GLU
1	B	274	ARG
1	B	277	LYS
1	B	278	LYS
1	B	285	ARG
1	B	288	ILE
1	B	298	THR
1	C	13	GLN
1	C	23	LEU
1	C	25	GLN
1	C	43	THR
1	C	82	SER
1	C	85	ASP
1	C	107	LYS
1	C	134	GLU
1	C	170	GLU
1	C	177	ARG
1	C	190	LEU
1	C	197	CYS
1	C	198	PHE
1	C	208	GLU
1	C	277	LYS
1	C	278	LYS
1	C	285	ARG
1	C	298	THR
1	C	310	VAL
1	C	314	LEU
1	C	315	GLU
1	C	318	ARG
1	C	338	LEU
1	C	341	HIS
1	C	342	HIS
1	D	4	ASP
1	D	13	GLN
1	D	23	LEU
1	D	25	GLN
1	D	43	THR
1	D	82	SER
1	D	85	ASP
1	D	102	ASP
1	D	131	MET

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Mol	Chain	Res	Type
1	D	170	GLU
1	D	177	ARG
1	D	188	ASP
1	D	196	CYS
1	D	197	CYS
1	D	198	PHE
1	D	208	GLU
1	D	277	LYS
1	D	285	ARG
1	D	286	LEU
1	D	289	LEU
1	D	298	THR
1	D	310	VAL
1	D	315	GLU
1	D	318	ARG
1	E	4	ASP
1	E	13	GLN
1	E	23	LEU
1	E	25	GLN
1	E	43	THR
1	E	82	SER
1	E	85	ASP
1	E	102	ASP
1	E	116	GLU
1	E	131	MET
1	E	170	GLU
1	E	177	ARG
1	E	197	CYS
1	E	208	GLU
1	E	277	LYS
1	E	285	ARG
1	E	286	LEU
1	E	298	THR
1	F	13	GLN
1	F	23	LEU
1	F	25	GLN
1	F	43	THR
1	F	82	SER
1	F	85	ASP
1	F	102	ASP
1	F	131	MET
1	F	170	GLU

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Mol	Chain	Res	Type
1	F	177	ARG
1	F	190	LEU
1	F	195	CYS
1	F	197	CYS
1	F	198	PHE
1	F	208	GLU
1	F	277	LYS
1	F	278	LYS
1	F	285	ARG
1	F	286	LEU
1	F	298	THR
1	F	310	VAL
1	F	315	GLU
1	F	318	ARG
1	G	13	GLN
1	G	23	LEU
1	G	25	GLN
1	G	43	THR
1	G	82	SER
1	G	85	ASP
1	G	102	ASP
1	G	131	MET
1	G	134	GLU
1	G	170	GLU
1	G	177	ARG
1	G	196	CYS
1	G	197	CYS
1	G	198	PHE
1	G	208	GLU
1	G	277	LYS
1	G	278	LYS
1	G	285	ARG
1	G	286	LEU
1	G	288	ILE
1	G	298	THR
1	G	310	VAL
1	G	311	SER
1	G	312	ASP
1	G	314	LEU
1	G	318	ARG
1	H	4	ASP
1	H	13	GLN

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Mol	Chain	Res	Type
1	H	23	LEU
1	H	25	GLN
1	H	43	THR
1	H	82	SER
1	H	85	ASP
1	H	131	MET
1	H	170	GLU
1	H	177	ARG
1	H	196	CYS
1	H	197	CYS
1	H	198	PHE
1	H	208	GLU
1	H	277	LYS
1	H	278	LYS
1	H	285	ARG
1	H	286	LEU
1	H	288	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	HIS
1	D	66	HIS
1	H	66	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

18 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	SO4	C	402	-	4,4,4	0.12	0	6,6,6	0.28	0
2	SO4	H	401	-	4,4,4	1.90	1 (25%)	6,6,6	0.93	0
3	PLP	B	400	1	15,15,16	1.88	4 (26%)	20,22,23	2.21	6 (30%)
2	SO4	F	401	-	4,4,4	0.64	0	6,6,6	0.61	0
2	SO4	D	401	-	4,4,4	0.14	0	6,6,6	0.29	0
2	SO4	A	402	-	4,4,4	0.21	0	6,6,6	0.37	0
2	SO4	A	403	-	4,4,4	0.61	0	6,6,6	0.55	0
2	SO4	A	401	-	4,4,4	0.10	0	6,6,6	0.64	0
2	SO4	C	401	-	4,4,4	0.23	0	6,6,6	0.61	0
2	SO4	C	404	-	4,4,4	0.21	0	6,6,6	0.30	0
2	SO4	C	405	-	4,4,4	0.17	0	6,6,6	0.28	0
2	SO4	C	406	-	4,4,4	0.58	0	6,6,6	0.90	0
2	SO4	D	402	-	4,4,4	0.20	0	6,6,6	0.46	0
2	SO4	C	403	-	4,4,4	0.29	0	6,6,6	0.38	0
2	SO4	D	403	-	4,4,4	0.64	0	6,6,6	0.63	0
2	SO4	G	401	-	4,4,4	0.13	0	6,6,6	0.28	0
2	SO4	G	402	-	4,4,4	0.64	0	6,6,6	0.38	0
2	SO4	E	401	-	4,4,4	0.55	0	6,6,6	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	B	400	1	-	3/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	PLP	O3-C3	-5.17	1.25	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	PLP	C2-N1	2.56	1.38	1.33
2	H	401	SO4	O2-S	2.30	1.58	1.46
3	B	400	PLP	P-O3P	-2.14	1.46	1.54
3	B	400	PLP	C3-C4	2.08	1.44	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	400	PLP	C4A-C4-C5	-6.79	113.94	120.94
3	B	400	PLP	C4A-C4-C3	3.64	126.66	120.50
3	B	400	PLP	O3-C3-C4	2.44	124.54	118.10
3	B	400	PLP	C2A-C2-C3	2.31	123.75	120.89
3	B	400	PLP	O2P-P-O1P	2.27	119.56	110.68
3	B	400	PLP	C5A-C5-C6	-2.18	115.79	119.37

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	400	PLP	C5A-O4P-P-O1P
3	B	400	PLP	C5A-O4P-P-O2P
3	B	400	PLP	C5A-O4P-P-O3P

There are no ring outliers.

11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	402	SO4	1	0
2	H	401	SO4	2	0
3	B	400	PLP	5	0
2	F	401	SO4	1	0
2	A	403	SO4	3	0
2	C	404	SO4	1	0
2	C	406	SO4	4	0
2	D	403	SO4	3	0
2	G	401	SO4	1	0
2	G	402	SO4	2	0
2	E	401	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	337/346 (97%)	0.38	12 (3%)	42	42	41, 65, 118, 135	0
1	B	307/346 (88%)	0.43	19 (6%)	20	19	40, 64, 113, 138	0
1	C	338/346 (97%)	0.58	27 (7%)	12	10	43, 66, 123, 142	0
1	D	335/346 (96%)	0.24	13 (3%)	39	38	42, 65, 124, 135	0
1	E	305/346 (88%)	0.39	16 (5%)	27	25	41, 66, 113, 134	0
1	F	335/346 (96%)	0.38	21 (6%)	20	19	44, 67, 126, 144	0
1	G	326/346 (94%)	0.29	21 (6%)	19	18	40, 68, 126, 143	0
1	H	305/346 (88%)	0.53	32 (10%)	6	4	45, 68, 115, 136	0
All	All	2588/2768 (93%)	0.40	161 (6%)	20	19	40, 66, 122, 144	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	LEU	8.6
1	F	314	LEU	7.6
1	B	333	PHE	7.6
1	G	286	LEU	6.9
1	H	285	ARG	6.4
1	E	336	LEU	6.1
1	B	334	LYS	6.0
1	F	193	LEU	5.5
1	C	103	PHE	5.5
1	E	122	ILE	5.2
1	H	336	LEU	5.0
1	H	334	LYS	4.9
1	H	282	TYR	4.8
1	E	125	LEU	4.7
1	C	99	ILE	4.7
1	H	333	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	311	SER	4.6
1	B	309	GLU	4.5
1	C	134	GLU	4.4
1	H	280	THR	4.4
1	E	186	ARG	4.4
1	E	333	PHE	4.3
1	G	287	ALA	4.3
1	H	331	GLY	4.3
1	F	286	LEU	4.3
1	B	335	ARG	4.3
1	E	124	GLU	4.3
1	H	198	PHE	4.2
1	H	309	GLU	4.1
1	F	287	ALA	4.1
1	D	311	SER	4.0
1	G	130	GLY	4.0
1	F	282	TYR	4.0
1	H	290	PRO	3.9
1	E	335	ARG	3.9
1	H	332	THR	3.7
1	F	131	MET	3.7
1	H	289	LEU	3.7
1	H	124	GLU	3.7
1	G	131	MET	3.6
1	E	120	ILE	3.6
1	B	332	THR	3.6
1	G	288	ILE	3.6
1	C	90	GLY	3.5
1	F	128	HIS	3.5
1	G	289	LEU	3.5
1	A	134	GLU	3.5
1	F	317	THR	3.5
1	C	107	LYS	3.4
1	F	285	ARG	3.4
1	D	314	LEU	3.4
1	E	187	ILE	3.4
1	H	308	GLU	3.4
1	F	124	GLU	3.4
1	E	129	TYR	3.3
1	B	331	GLY	3.3
1	G	313	PRO	3.3
1	H	302	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	97	SER	3.2
1	F	313	PRO	3.2
1	H	186	ARG	3.2
1	F	189	LYS	3.2
1	H	281	GLY	3.1
1	H	286	LEU	3.1
1	D	293	TYR	3.0
1	B	125	LEU	3.0
1	B	274	ARG	3.0
1	H	103	PHE	3.0
1	G	127	LYS	3.0
1	C	185	LEU	3.0
1	H	291	PRO	3.0
1	G	282	TYR	3.0
1	C	110	LYS	3.0
1	G	326	LYS	3.0
1	G	198	PHE	3.0
1	C	95	LYS	3.0
1	C	154	ILE	2.9
1	G	310	VAL	2.9
1	A	196	CYS	2.9
1	H	288	ILE	2.9
1	D	131	MET	2.9
1	B	282	TYR	2.9
1	F	315	GLU	2.9
1	F	186	ARG	2.9
1	E	286	LEU	2.9
1	D	289	LEU	2.8
1	B	278	LYS	2.8
1	H	284	LYS	2.8
1	G	314	LEU	2.8
1	C	122	ILE	2.8
1	H	131	MET	2.7
1	G	293	TYR	2.7
1	D	310	VAL	2.7
1	D	294	VAL	2.7
1	C	149	ILE	2.7
1	B	122	ILE	2.6
1	C	190	LEU	2.6
1	B	189	LYS	2.6
1	F	188	ASP	2.6
1	A	198	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	117	PHE	2.5
1	C	100	THR	2.5
1	D	129	TYR	2.5
1	H	335	ARG	2.5
1	D	124	GLU	2.5
1	A	128	HIS	2.5
1	C	106	LEU	2.5
1	G	107	LYS	2.5
1	H	274	ARG	2.5
1	H	287	ALA	2.5
1	F	284	LYS	2.5
1	C	171	TYR	2.5
1	C	158	ILE	2.4
1	H	279	VAL	2.4
1	D	282	TYR	2.4
1	G	35	LEU	2.4
1	A	88	PHE	2.4
1	A	310	VAL	2.4
1	G	132	LYS	2.4
1	C	293	TYR	2.4
1	H	307	PRO	2.4
1	C	191	ALA	2.4
1	A	99	ILE	2.4
1	A	103	PHE	2.4
1	H	73	ARG	2.4
1	C	136	TYR	2.4
1	C	186	ARG	2.4
1	G	89	THR	2.3
1	C	153	LYS	2.3
1	B	186	ARG	2.3
1	C	310	VAL	2.3
1	H	197	CYS	2.3
1	G	279	VAL	2.3
1	B	308	GLU	2.2
1	D	333	PHE	2.2
1	F	293	TYR	2.2
1	G	129	TYR	2.2
1	G	285	ARG	2.2
1	H	267	SER	2.2
1	A	312	ASP	2.2
1	D	195	CYS	2.2
1	D	285	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	341	HIS	2.1
1	E	136	TYR	2.1
1	H	132	LYS	2.1
1	B	68	LEU	2.1
1	E	131	MET	2.1
1	F	198	PHE	2.1
1	C	123	ASP	2.1
1	A	97	SER	2.1
1	C	117	PHE	2.1
1	B	128	HIS	2.1
1	E	308	GLU	2.1
1	B	136	TYR	2.1
1	C	93	TYR	2.0
1	E	119	LYS	2.0
1	F	103	PHE	2.0
1	F	125	LEU	2.0
1	F	295	SER	2.0
1	B	196	CYS	2.0
1	A	285	ARG	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, 95^{th} 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	SO4	C	403	5/5	0.69	0.20	91,95,140,159	0
3	PLP	B	400	15/16	0.82	0.25	56,81,103,112	0
2	SO4	C	405	5/5	0.84	0.22	102,106,139,147	0
2	SO4	E	401	5/5	0.87	0.16	54,96,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	C	406	5/5	0.87	0.17	85,95,107,115	0
2	SO4	A	402	5/5	0.89	0.17	65,109,111,125	0
2	SO4	G	402	5/5	0.90	0.16	68,88,95,111	0
2	SO4	F	401	5/5	0.90	0.15	66,75,111,112	0
2	SO4	C	404	5/5	0.92	0.12	60,87,142,158	0
2	SO4	D	403	5/5	0.92	0.22	61,73,105,132	0
2	SO4	C	401	5/5	0.92	0.17	59,92,104,110	0
2	SO4	D	402	5/5	0.93	0.12	68,70,85,92	0
2	SO4	D	401	5/5	0.93	0.17	74,86,112,122	0
2	SO4	A	403	5/5	0.94	0.11	77,80,93,100	0
2	SO4	H	401	5/5	0.95	0.12	85,87,96,99	0
2	SO4	G	401	5/5	0.95	0.13	51,95,108,113	0
2	SO4	A	401	5/5	0.96	0.15	55,66,77,103	0
2	SO4	C	402	5/5	0.97	0.16	54,55,80,94	0

6.5 Other polymers (i)

There are no such residues in this entry.