



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:34 PM UTC

PDB ID : 6S8W / pdb_00006s8w
Title : Aromatic aminotransferase AroH (Aro8) form *Aspergillus fumigatus* in complex with PLP (internal aldimine)
Authors : Giardina, G.; Mirco, D.; Spizzichino, S.; Zelante, T.; Cutruzzola, F.; Romani, L.; Cellini, B.
Deposited on : 2019-07-10
Resolution : 2.40 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

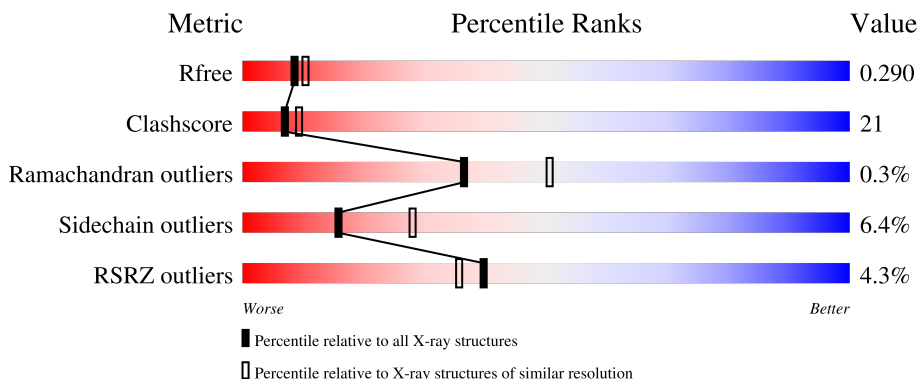
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	534	2% 63% 28% 8%
1	B	534	2% 63% 26% 8%
1	C	534	6% 60% 26% 12%
1	D	534	6% 56% 32% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	C	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14737 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 Aromatic aminotransferase Aro8, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3689	2360	629	686	14			
1	B	491	Total	C	N	O	S	0	0	0
			3721	2379	640	689	13			
1	C	470	Total	C	N	O	S	0	0	0
			3475	2219	604	638	14			
1	D	490	Total	C	N	O	S	0	0	0
			3620	2322	624	661	13			

There are 32 discrepancies between the modelled and reference sequences:

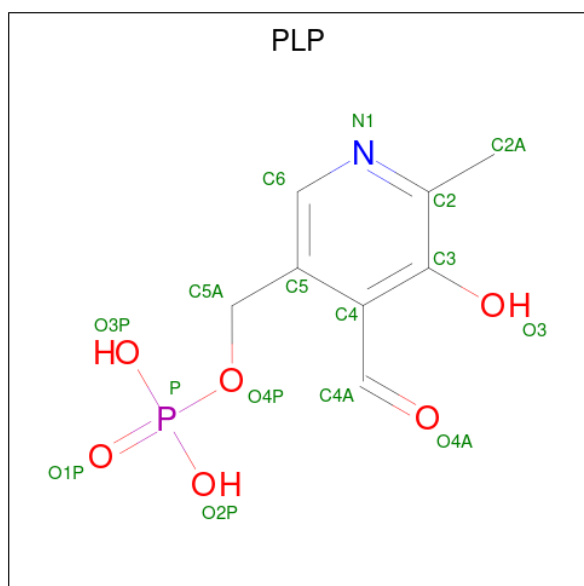
Chain	Residue	Modelled	Actual	Comment	Reference
A	527	LEU	-	expression tag	UNP Q4X0F7
A	528	GLU	-	expression tag	UNP Q4X0F7
A	529	HIS	-	expression tag	UNP Q4X0F7
A	530	HIS	-	expression tag	UNP Q4X0F7
A	531	HIS	-	expression tag	UNP Q4X0F7
A	532	HIS	-	expression tag	UNP Q4X0F7
A	533	HIS	-	expression tag	UNP Q4X0F7
A	534	HIS	-	expression tag	UNP Q4X0F7
B	527	LEU	-	expression tag	UNP Q4X0F7
B	528	GLU	-	expression tag	UNP Q4X0F7
B	529	HIS	-	expression tag	UNP Q4X0F7
B	530	HIS	-	expression tag	UNP Q4X0F7
B	531	HIS	-	expression tag	UNP Q4X0F7
B	532	HIS	-	expression tag	UNP Q4X0F7
B	533	HIS	-	expression tag	UNP Q4X0F7
B	534	HIS	-	expression tag	UNP Q4X0F7
C	527	LEU	-	expression tag	UNP Q4X0F7
C	528	GLU	-	expression tag	UNP Q4X0F7
C	529	HIS	-	expression tag	UNP Q4X0F7
C	530	HIS	-	expression tag	UNP Q4X0F7
C	531	HIS	-	expression tag	UNP Q4X0F7

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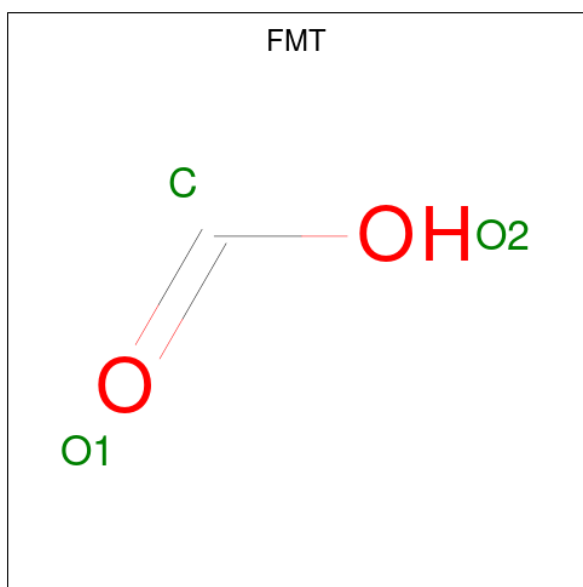
Chain	Residue	Modelled	Actual	Comment	Reference
C	532	HIS	-	expression tag	UNP Q4X0F7
C	533	HIS	-	expression tag	UNP Q4X0F7
C	534	HIS	-	expression tag	UNP Q4X0F7
D	527	LEU	-	expression tag	UNP Q4X0F7
D	528	GLU	-	expression tag	UNP Q4X0F7
D	529	HIS	-	expression tag	UNP Q4X0F7
D	530	HIS	-	expression tag	UNP Q4X0F7
D	531	HIS	-	expression tag	UNP Q4X0F7
D	532	HIS	-	expression tag	UNP Q4X0F7
D	533	HIS	-	expression tag	UNP Q4X0F7
D	534	HIS	-	expression tag	UNP Q4X0F7

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



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

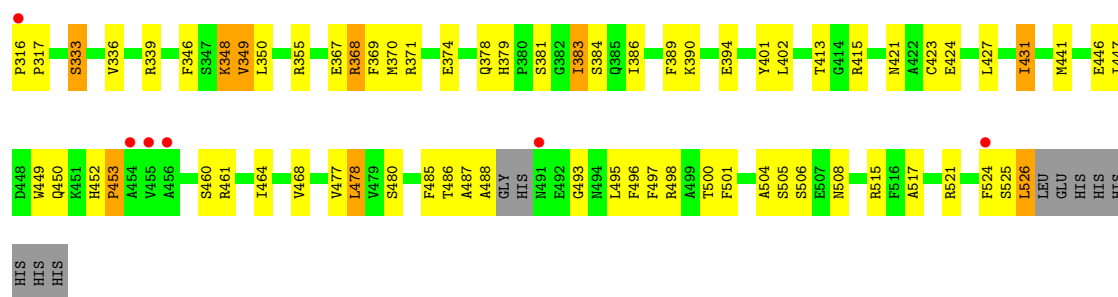
- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



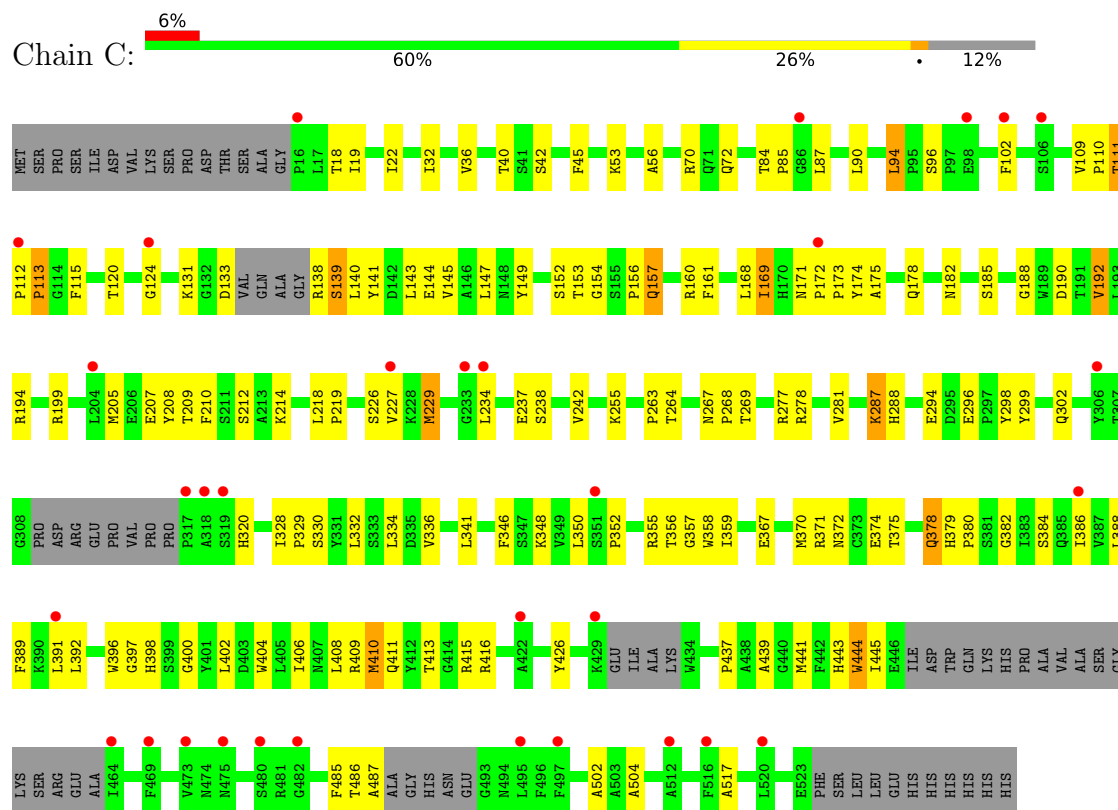
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		

- Molecule 4 is water.

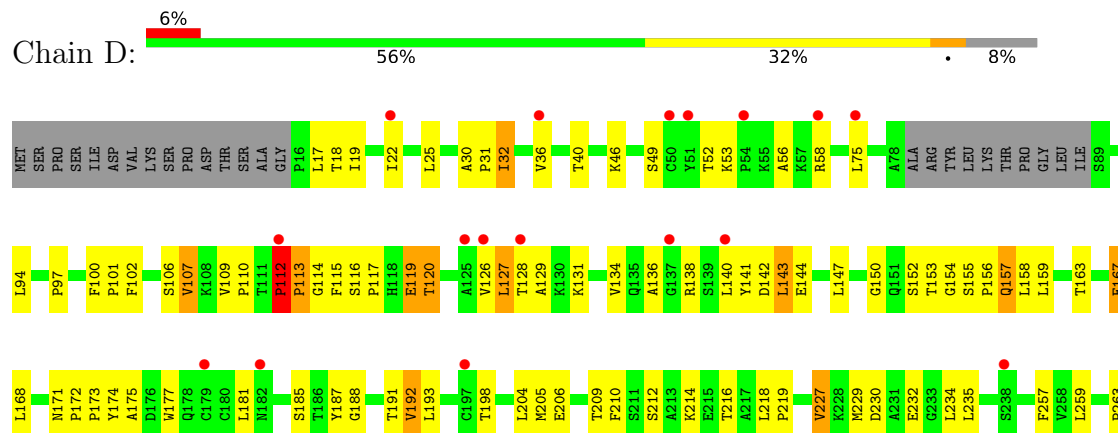
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	58	Total	O	0	0
			58	58		
4	C	28	Total	O	0	0
			28	28		
4	D	25	Total	O	0	0
			25	25		

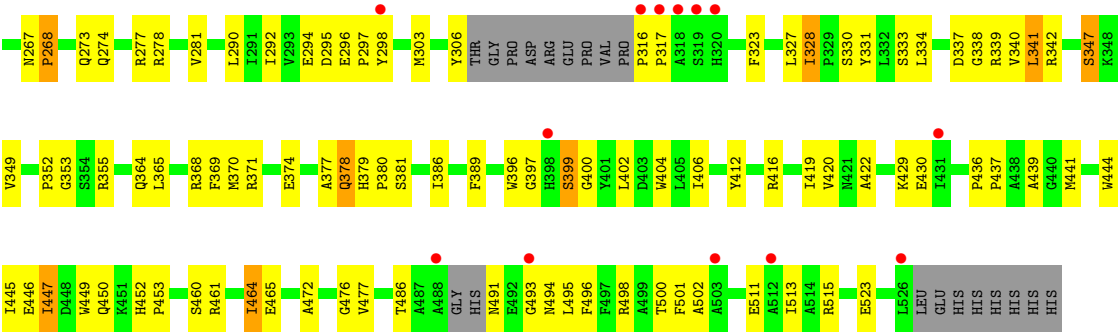


- Molecule 1: Aromatic aminotransferase Aro8, putative



- Molecule 1: Aromatic aminotransferase Aro8, putative





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.21Å 75.26Å 121.63Å 84.77° 87.51° 65.37°	Depositor
Resolution (Å)	47.20 – 2.40 47.20 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.2 (47.20-2.40) 97.2 (47.20-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.245 , 0.293 0.246 , 0.290	Depositor DCC
R_{free} test set	3871 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14737	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, 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	0.97	0/3791	1.41	4/5171 (0.1%)
1	B	0.98	0/3823	1.40	4/5212 (0.1%)
1	C	0.98	0/3566	1.44	5/4863 (0.1%)
1	D	0.98	0/3720	1.41	5/5082 (0.1%)
All	All	0.98	0/14900	1.41	18/20328 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ASN	CA-C-N	8.18	125.63	119.66
1	A	171	ASN	C-N-CA	8.18	125.63	119.66
1	B	112	PRO	N-CA-C	7.96	120.41	110.70
1	A	172	PRO	N-CA-C	7.71	117.88	110.47
1	D	112	PRO	N-CA-C	7.00	119.24	110.70
1	B	262	ILE	CA-C-N	6.72	126.98	119.32
1	B	262	ILE	C-N-CA	6.72	126.98	119.32
1	C	154	GLY	CA-C-O	-6.10	118.02	122.23
1	B	160	ARG	CG-CD-NE	6.04	125.28	112.00
1	C	329	PRO	N-CA-C	5.29	120.88	113.53
1	C	139	SER	O-C-N	5.20	128.49	122.25
1	D	328	ILE	CA-C-N	5.19	125.18	119.89
1	D	328	ILE	C-N-CA	5.19	125.18	119.89
1	D	349	VAL	N-CA-C	-5.18	108.79	113.71
1	D	154	GLY	CA-C-O	-5.16	117.82	122.57
1	C	444	TRP	CA-CB-CG	5.15	123.39	113.60
1	C	144	GLU	N-CA-C	-5.13	106.87	113.23
1	A	172	PRO	CB-CA-C	-5.10	106.60	111.39

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3689	0	3455	131	0
1	B	3721	0	3520	131	0
1	C	3475	0	3215	178	0
1	D	3620	0	3357	189	0
2	A	15	0	6	3	0
2	B	15	0	6	1	0
2	C	15	0	6	6	0
2	D	15	0	6	3	0
3	A	3	0	1	0	0
3	D	3	0	1	0	0
4	A	55	0	0	3	0
4	B	58	0	0	4	0
4	C	28	0	0	2	0
4	D	25	0	0	1	0
All	All	14737	0	13573	595	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 21.

All (595) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:TYR:H	1:C:229:MET:CE	1.42	1.31
1:B:306:TYR:OH	1:B:421:ASN:ND2	1.72	1.22
1:C:109:VAL:HG21	1:C:391:LEU:CD1	1.68	1.22
1:D:22:ILE:HD11	1:D:168:LEU:HD11	1.20	1.17
1:C:208:TYR:H	1:C:229:MET:HE1	1.07	1.17
1:C:32:ILE:HD11	1:C:160:ARG:NH1	1.59	1.17
1:D:22:ILE:CD1	1:D:168:LEU:HD11	1.74	1.17
1:C:40:THR:HG21	1:C:156:PRO:HB3	1.27	1.12
1:A:111:THR:HG22	1:A:112:PRO:HD2	1.22	1.12
1:A:265:GLY:H	1:A:272:THR:HG22	1.06	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:HIS:HB2	1:A:524:PHE:CD1	1.84	1.11
1:B:40:THR:HG21	1:B:156:PRO:HB3	1.33	1.11
1:C:109:VAL:HG21	1:C:391:LEU:HD13	1.17	1.09
1:D:110:PRO:HB3	1:D:120:THR:OG1	1.52	1.08
1:C:277:ARG:O	1:C:281:VAL:HG23	1.53	1.07
1:C:111:THR:OG1	1:C:112:PRO:CD	2.04	1.05
1:D:40:THR:HG21	1:D:156:PRO:HB3	1.39	1.05
1:C:409:ARG:HG2	1:C:410:MET:HE3	1.38	1.03
1:A:191:THR:HG23	1:A:372:ASN:HD22	1.19	1.03
1:B:153:THR:HG23	1:B:370:MET:SD	1.98	1.03
1:C:375:THR:HB	1:D:216:THR:HG22	1.37	1.03
1:A:383:ILE:HG22	1:B:383:ILE:HD11	1.40	1.03
1:B:209:THR:HG22	1:B:210:PHE:N	1.74	1.01
1:C:111:THR:OG1	1:C:112:PRO:HD3	1.61	1.00
1:C:208:TYR:N	1:C:229:MET:CE	2.24	1.00
1:A:111:THR:HG22	1:A:112:PRO:CD	1.92	1.00
1:A:452:HIS:CB	1:A:524:PHE:CD1	2.45	1.00
1:C:409:ARG:HG2	1:C:410:MET:CE	1.92	0.99
1:D:18:THR:O	1:D:22:ILE:HG13	1.64	0.98
1:B:207:GLU:HB2	1:B:229:MET:HE3	1.44	0.98
1:D:206:GLU:HB3	1:D:229:MET:HE1	1.42	0.98
1:A:167:GLU:O	1:A:171:ASN:HB2	1.62	0.97
1:A:265:GLY:H	1:A:272:THR:CG2	1.79	0.96
1:D:19:ILE:HA	1:D:22:ILE:HD12	1.48	0.95
1:C:237:GLU:CB	4:C:720:HOH:O	2.14	0.95
1:C:356:THR:HG21	1:C:388:LEU:HD11	1.46	0.94
1:D:153:THR:HG23	1:D:370:MET:HE3	1.46	0.94
1:D:206:GLU:HB3	1:D:229:MET:CE	1.97	0.94
1:A:265:GLY:N	1:A:272:THR:HG22	1.83	0.94
1:D:134:VAL:HG23	1:D:142:ASP:HB2	1.47	0.94
1:D:209:THR:HG22	1:D:210:PHE:N	1.81	0.93
1:A:272:THR:HG21	1:A:439:ALA:HB3	1.49	0.93
1:D:274:GLN:OE1	1:D:328:ILE:HD13	1.67	0.93
1:C:112:PRO:HB2	1:C:113:PRO:HD3	1.52	0.92
1:B:17:LEU:HD11	1:B:22:ILE:HD13	1.52	0.91
1:C:109:VAL:CG2	1:C:391:LEU:HD13	2.01	0.90
1:D:32:ILE:HG21	1:D:140:LEU:HD13	1.53	0.90
1:C:410:MET:HE2	1:C:410:MET:HA	1.52	0.90
1:D:152:SER:OG	1:D:374:GLU:HG2	1.70	0.90
1:B:423:CYS:O	1:B:427:LEU:HB2	1.72	0.89
1:C:32:ILE:CD1	1:C:160:ARG:NH1	2.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ILE:HD12	1:B:497:PHE:CE1	2.07	0.89
1:C:72:GLN:HG3	1:C:371:ARG:NH2	1.87	0.89
1:C:207:GLU:HB3	1:C:229:MET:HE3	1.51	0.89
1:D:153:THR:HG23	1:D:370:MET:CE	2.03	0.89
1:C:109:VAL:CG2	1:C:391:LEU:CD1	2.51	0.89
1:D:22:ILE:HD11	1:D:168:LEU:CD1	2.02	0.89
1:A:40:THR:HG21	1:A:156:PRO:HB3	1.55	0.87
1:C:207:GLU:HB3	1:C:229:MET:CE	2.04	0.87
1:C:208:TYR:N	1:C:229:MET:HE1	1.86	0.86
1:A:452:HIS:HB2	1:A:524:PHE:HD1	1.35	0.85
1:B:209:THR:HG22	1:B:210:PHE:H	1.36	0.84
1:A:87:LEU:HD13	1:A:87:LEU:C	2.02	0.84
1:D:134:VAL:CG2	1:D:142:ASP:HB2	2.06	0.84
1:D:209:THR:HG22	1:D:210:PHE:H	1.43	0.84
1:C:356:THR:HG21	1:C:388:LEU:CD1	2.08	0.84
1:B:390:LYS:NZ	1:B:394:GLU:OE2	2.11	0.84
1:D:227:VAL:CG2	1:D:234:LEU:HD11	2.08	0.83
1:A:17:LEU:HD23	1:A:167:GLU:HB3	1.59	0.83
1:B:209:THR:CG2	1:B:210:PHE:H	1.91	0.82
1:C:115:PHE:CD1	1:C:404:TRP:HE3	1.97	0.82
1:C:53:LYS:CD	1:C:173:PRO:O	2.26	0.82
1:B:449:TRP:NE1	1:B:493:GLY:O	2.12	0.82
1:B:209:THR:CG2	1:B:210:PHE:N	2.42	0.82
4:A:750:HOH:O	1:B:120:THR:HG21	1.79	0.82
1:B:446:GLU:HG3	1:B:496:PHE:CE2	2.15	0.81
1:B:208:TYR:H	1:B:229:MET:HE1	1.46	0.81
1:D:446:GLU:HG2	1:D:494:ASN:HD22	1.45	0.81
1:C:208:TYR:H	1:C:229:MET:HE2	1.44	0.80
1:D:274:GLN:OE1	1:D:328:ILE:CD1	2.29	0.80
1:C:207:GLU:N	1:C:229:MET:HE2	1.95	0.80
1:B:187:TYR:O	1:B:191:THR:HG22	1.80	0.80
1:D:205:MET:HE2	1:D:209:THR:HG21	1.64	0.80
1:C:111:THR:OG1	1:C:112:PRO:HD2	1.80	0.79
1:B:446:GLU:CG	1:B:496:PHE:CE2	2.66	0.79
1:D:112:PRO:HB2	1:D:113:PRO:HD3	1.64	0.78
1:B:205:MET:HE2	1:B:209:THR:HG21	1.66	0.78
1:D:209:THR:CG2	1:D:210:PHE:H	1.96	0.78
1:D:227:VAL:HG22	1:D:234:LEU:HD11	1.66	0.77
1:C:32:ILE:HD11	1:C:160:ARG:CZ	2.14	0.77
1:D:292:ILE:HB	1:D:340:VAL:HG22	1.66	0.77
1:B:114:GLY:HA2	4:B:709:HOH:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ASN:O	1:A:380:PRO:HG3	1.85	0.76
1:C:410:MET:HE2	1:C:410:MET:CA	2.15	0.76
1:D:212:SER:O	1:D:216:THR:HG23	1.85	0.76
1:D:110:PRO:CB	1:D:120:THR:OG1	2.31	0.76
1:D:230:ASP:OD1	1:D:277:ARG:NH1	2.18	0.76
1:C:110:PRO:HG2	1:C:396:TRP:HZ2	1.51	0.75
1:B:349:VAL:HG12	1:B:350:LEU:HG	1.65	0.75
1:D:294:GLU:OE1	1:D:342:ARG:NH1	2.18	0.75
1:A:383:ILE:HG22	1:B:383:ILE:CD1	2.16	0.75
1:D:232:GLU:HB3	1:D:277:ARG:HD2	1.68	0.74
1:B:208:TYR:H	1:B:229:MET:CE	2.00	0.74
1:D:227:VAL:HG22	1:D:234:LEU:CD1	2.16	0.74
1:D:419:ILE:HG13	1:D:513:ILE:HD11	1.68	0.74
1:B:187:TYR:O	1:B:191:THR:CG2	2.35	0.74
1:D:114:GLY:HA2	1:D:119:GLU:OE2	1.88	0.73
1:D:22:ILE:HD13	1:D:168:LEU:HD11	1.68	0.73
1:B:298:TYR:OH	2:B:601:PLP:O3	2.06	0.73
1:D:216:THR:HG21	4:D:701:HOH:O	1.87	0.73
1:C:172:PRO:HG3	1:C:332:LEU:HG	1.71	0.72
1:A:111:THR:CG2	1:A:112:PRO:CD	2.68	0.72
1:D:209:THR:CG2	1:D:210:PHE:N	2.48	0.72
1:D:227:VAL:CG2	1:D:234:LEU:CD1	2.67	0.71
1:B:207:GLU:HB2	1:B:229:MET:CE	2.20	0.71
1:A:316:PRO:N	1:A:317:PRO:CD	2.52	0.71
1:A:91:GLY:O	1:B:498:ARG:NH2	2.23	0.71
1:C:409:ARG:CG	1:C:410:MET:HE3	2.18	0.71
1:C:22:ILE:HD11	1:C:168:LEU:HD11	1.72	0.71
1:B:486:THR:HG22	1:B:488:ALA:H	1.53	0.71
1:A:167:GLU:O	1:A:171:ASN:CB	2.38	0.70
1:D:273:GLN:CD	1:D:331:TYR:HH	1.99	0.70
1:A:111:THR:CG2	1:A:112:PRO:HD2	2.14	0.70
1:C:22:ILE:HD13	1:C:398:HIS:CD2	2.26	0.70
1:C:110:PRO:HG3	1:D:101:PRO:HB3	1.74	0.70
1:D:449:TRP:HB3	1:D:495:LEU:HD12	1.74	0.70
1:A:300:PHE:CD1	1:A:405:LEU:HD13	2.27	0.69
1:C:140:LEU:HD12	1:C:140:LEU:O	1.92	0.69
1:B:386:ILE:O	1:B:390:LYS:HG2	1.92	0.69
1:C:32:ILE:CD1	1:C:160:ARG:HH12	2.05	0.69
1:B:446:GLU:HG3	1:B:496:PHE:HE2	1.56	0.69
1:C:53:LYS:HD2	1:C:173:PRO:O	1.91	0.69
1:D:303:MET:HE1	1:D:416:ARG:HG3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:SER:OG	1:B:368:ARG:HG2	1.93	0.68
1:B:207:GLU:CB	1:B:229:MET:HE3	2.20	0.68
1:A:498:ARG:NH2	1:B:91:GLY:O	2.26	0.68
1:C:94:LEU:HD12	1:C:94:LEU:N	2.08	0.68
1:D:32:ILE:CG2	1:D:140:LEU:HD13	2.24	0.67
1:D:107:VAL:CG1	1:D:109:VAL:HG13	2.24	0.67
1:D:419:ILE:CG1	1:D:513:ILE:HD11	2.24	0.67
1:C:111:THR:HG23	1:C:113:PRO:HD2	1.77	0.67
1:D:46:LYS:NZ	1:D:175:ALA:O	2.27	0.67
1:A:476:GLY:O	1:A:515:ARG:NH1	2.27	0.67
1:A:22:ILE:HD11	1:A:168:LEU:HD11	1.77	0.66
1:C:87:LEU:HD22	1:D:476:GLY:HA2	1.76	0.66
1:B:154:GLY:HA3	1:B:181:LEU:HD12	1.77	0.66
1:A:191:THR:HG23	1:A:372:ASN:ND2	2.03	0.66
1:B:316:PRO:N	1:B:317:PRO:CD	2.59	0.66
1:C:53:LYS:HD3	1:C:173:PRO:O	1.95	0.66
1:D:58:ARG:HA	1:D:364:GLN:OE1	1.95	0.66
1:D:127:LEU:HD23	1:D:127:LEU:N	2.10	0.66
1:A:452:HIS:HB3	1:A:524:PHE:CD1	2.30	0.65
1:C:320:HIS:HB3	1:C:402:LEU:HD13	1.76	0.65
1:A:232:GLU:OE1	1:A:274:GLN:HG2	1.95	0.65
1:C:188:GLY:O	1:C:192:VAL:HG13	1.96	0.65
1:A:367:GLU:OE1	1:A:371:ARG:NH1	2.30	0.65
1:B:153:THR:CG2	1:B:370:MET:SD	2.81	0.65
1:C:207:GLU:CA	1:C:229:MET:HE2	2.27	0.65
1:D:173:PRO:HG3	1:D:333:SER:O	1.97	0.65
1:C:115:PHE:CD1	1:C:404:TRP:CE3	2.82	0.65
1:A:191:THR:CG2	1:A:372:ASN:HD22	2.02	0.64
1:C:355:ARG:HH22	2:C:601:PLP:P	2.20	0.64
1:C:227:VAL:HG23	1:C:234:LEU:CD1	2.26	0.64
1:D:227:VAL:HG21	1:D:234:LEU:HD11	1.77	0.64
1:C:298:TYR:OH	2:C:601:PLP:O3	2.12	0.64
1:D:153:THR:HG23	1:D:370:MET:SD	2.37	0.64
1:D:355:ARG:HH22	2:D:602:PLP:P	2.20	0.64
1:D:131:LYS:HD2	1:D:144:GLU:CG	2.27	0.64
1:B:32:ILE:HD11	1:B:160:ARG:HD3	1.79	0.64
1:A:316:PRO:N	1:A:317:PRO:HD3	2.11	0.64
1:D:230:ASP:CG	1:D:235:LEU:HD21	2.22	0.64
1:D:188:GLY:O	1:D:192:VAL:HG13	1.98	0.63
1:B:70:ARG:NH2	4:B:703:HOH:O	2.30	0.63
1:C:182:ASN:OD1	1:C:357:GLY:C	2.40	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ARG:NH1	1:C:504:ALA:O	2.30	0.63
1:A:149:TYR:OH	1:B:348:LYS:HE3	1.97	0.63
1:C:141:TYR:HE2	1:C:386:ILE:HA	1.62	0.63
1:A:275:LEU:HD13	1:A:329:PRO:HG2	1.81	0.63
1:C:102:PHE:HB2	1:C:147:LEU:HD11	1.81	0.63
1:C:110:PRO:HA	1:C:120:THR:OG1	1.99	0.62
1:C:110:PRO:HG3	1:D:101:PRO:CB	2.30	0.62
1:A:514:ALA:O	1:A:518:THR:HG23	1.99	0.62
1:D:316:PRO:HB2	1:D:317:PRO:CD	2.29	0.62
1:D:187:TYR:CE1	1:D:377:ALA:HB2	2.34	0.62
1:D:155:SER:HB2	1:D:157:GLN:HE21	1.64	0.62
1:C:346:PHE:HD2	1:C:356:THR:HG23	1.65	0.62
1:C:375:THR:CB	1:D:216:THR:HG22	2.21	0.62
1:A:500:THR:HG21	1:B:92:GLY:O	1.99	0.61
1:B:446:GLU:HG2	1:B:496:PHE:CE2	2.34	0.61
1:C:367:GLU:O	1:C:371:ARG:HD3	2.00	0.61
1:A:452:HIS:CB	1:A:524:PHE:CE1	2.84	0.61
1:A:87:LEU:C	1:A:87:LEU:CD1	2.73	0.61
1:C:207:GLU:CB	1:C:229:MET:HE2	2.31	0.61
1:D:19:ILE:HA	1:D:22:ILE:CD1	2.26	0.61
1:A:298:TYR:OH	2:A:601:PLP:O3	2.17	0.60
1:B:447:ILE:HD12	1:B:497:PHE:CD1	2.36	0.60
1:C:278:ARG:NH1	1:C:330:SER:HA	2.15	0.60
1:C:391:LEU:HD22	1:D:102:PHE:CE1	2.36	0.60
1:C:210:PHE:CD2	2:C:601:PLP:H2A3	2.36	0.60
1:C:226:SER:HB3	1:C:487:ALA:HB3	1.83	0.60
1:C:278:ARG:HH11	1:C:330:SER:HA	1.67	0.60
1:A:42:SER:HB2	1:A:178:GLN:HG2	1.82	0.60
1:D:126:VAL:HG12	1:D:126:VAL:O	2.01	0.60
1:D:461:ARG:HD2	1:D:493:GLY:O	2.01	0.60
1:A:105:ILE:HG12	1:B:107:VAL:HG12	1.83	0.60
1:B:349:VAL:HG11	1:B:401:TYR:OH	2.02	0.60
1:D:298:TYR:OH	2:D:602:PLP:O3	2.14	0.60
1:A:452:HIS:HB3	1:A:524:PHE:CE1	2.37	0.59
1:C:109:VAL:CG2	1:C:110:PRO:HD2	2.32	0.59
1:C:120:THR:O	1:C:124:GLY:HA3	2.02	0.59
1:C:207:GLU:CB	1:C:229:MET:CE	2.80	0.59
1:A:19:ILE:HD11	1:A:402:LEU:HD12	1.82	0.59
1:A:100:PHE:O	1:A:131:LYS:NZ	2.35	0.59
1:B:211:SER:O	1:B:215:GLU:HG3	2.01	0.59
1:B:431:ILE:HD12	1:B:524:PHE:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ILE:HD12	1:B:497:PHE:HE1	1.60	0.59
1:D:355:ARG:NH2	2:D:602:PLP:O2P	2.30	0.59
1:C:207:GLU:HB3	1:C:229:MET:HE2	1.84	0.59
1:D:277:ARG:O	1:D:281:VAL:HG23	2.03	0.59
1:D:230:ASP:CG	1:D:277:ARG:HH12	2.10	0.59
1:D:116:SER:HB3	1:D:117:PRO:HD2	1.85	0.58
1:C:411:GLN:HG3	4:C:721:HOH:O	2.02	0.58
1:D:206:GLU:HB3	1:D:229:MET:HE3	1.84	0.58
1:D:334:LEU:HD12	1:D:334:LEU:N	2.18	0.58
1:C:111:THR:HG1	1:C:112:PRO:HD3	1.65	0.58
1:A:42:SER:O	1:A:46:LYS:HG3	2.03	0.58
1:C:56:ALA:HB2	1:C:174:TYR:CD2	2.39	0.58
1:D:446:GLU:HG2	1:D:494:ASN:ND2	2.17	0.58
1:D:107:VAL:HG12	1:D:109:VAL:HG13	1.84	0.58
1:B:480:SER:HB2	1:B:498:ARG:HB3	1.86	0.58
1:B:447:ILE:HB	1:B:495:LEU:CG	2.34	0.57
1:B:188:GLY:O	1:B:192:VAL:HG13	2.03	0.57
1:A:112:PRO:N	1:A:113:PRO:HD2	2.20	0.57
1:B:452:HIS:CD2	1:B:453:PRO:HD2	2.38	0.57
1:C:214:LYS:O	1:C:218:LEU:HD12	2.05	0.57
1:B:104:GLU:HG2	1:B:130:LYS:HG2	1.86	0.57
1:C:141:TYR:CE2	1:C:386:ILE:HA	2.39	0.56
1:C:396:TRP:HB3	1:C:400:GLY:HA3	1.87	0.56
1:D:206:GLU:CB	1:D:229:MET:CE	2.80	0.56
1:D:17:LEU:HG	1:D:168:LEU:HD21	1.88	0.56
1:D:416:ARG:HD2	1:D:416:ARG:C	2.30	0.56
1:B:460:SER:O	1:B:464:ILE:HD12	2.05	0.56
1:C:110:PRO:HG2	1:C:396:TRP:CZ2	2.39	0.56
1:C:152:SER:OG	1:C:370:MET:CG	2.53	0.56
1:D:330:SER:HB2	1:D:342:ARG:HH11	1.71	0.56
1:A:74:THR:HG23	1:B:215:GLU:OE2	2.06	0.55
1:D:420:VAL:HG11	1:D:436:PRO:HB3	1.88	0.55
1:A:182:ASN:OD1	1:A:369:PHE:HZ	1.90	0.55
1:C:152:SER:OG	1:C:370:MET:HG2	2.07	0.55
1:C:111:THR:CB	1:C:112:PRO:CD	2.84	0.55
1:A:70:ARG:NH2	1:A:375:THR:OG1	2.39	0.55
1:C:112:PRO:HB2	1:C:113:PRO:CD	2.33	0.55
1:C:264:THR:HG21	1:C:302:GLN:HG3	1.89	0.55
1:B:67:SER:OG	1:B:368:ARG:CG	2.54	0.55
1:C:185:SER:N	2:C:601:PLP:O3P	2.38	0.55
1:A:475:ASN:O	1:A:515:ARG:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:PRO:HG3	1:B:485:PHE:CG	2.42	0.55
1:A:378:GLN:HE21	1:B:355:ARG:NH1	2.05	0.55
1:A:139:SER:HB2	1:A:394:GLU:OE2	2.07	0.54
1:B:182:ASN:HD21	1:B:369:PHE:HE1	1.51	0.54
1:C:234:LEU:O	1:C:277:ARG:NH1	2.38	0.54
1:A:32:ILE:HG21	1:A:140:LEU:HD13	1.88	0.54
1:B:54:PRO:HG2	4:B:722:HOH:O	2.07	0.54
1:C:112:PRO:CB	1:C:113:PRO:HD3	2.32	0.54
1:B:415:ARG:HD3	1:B:501:PHE:O	2.08	0.53
1:C:384:SER:OG	1:D:381:SER:OG	2.26	0.53
1:D:134:VAL:HG23	1:D:142:ASP:CB	2.30	0.53
1:D:347:SER:OG	1:D:352:PRO:HA	2.07	0.53
1:B:306:TYR:CZ	1:B:421:ASN:ND2	2.73	0.53
1:B:452:HIS:HB2	1:B:524:PHE:CE2	2.43	0.53
1:C:115:PHE:HD1	1:C:404:TRP:HE3	1.53	0.53
1:D:316:PRO:HB2	1:D:317:PRO:HD3	1.90	0.53
1:A:210:PHE:CD2	2:A:601:PLP:H2A3	2.43	0.53
1:D:290:LEU:O	1:D:339:ARG:HD3	2.09	0.53
1:A:22:ILE:HD13	1:A:398:HIS:CD2	2.43	0.53
1:C:426:TYR:O	1:C:517:ALA:HB1	2.08	0.53
1:B:449:TRP:CD2	1:B:461:ARG:HG3	2.43	0.53
1:C:53:LYS:O	1:C:175:ALA:HB2	2.08	0.53
1:D:446:GLU:HG3	1:D:496:PHE:CE1	2.44	0.53
1:C:133:ASP:OD1	1:C:133:ASP:N	2.38	0.53
1:D:396:TRP:HB3	1:D:400:GLY:C	2.34	0.53
1:B:40:THR:HG21	1:B:156:PRO:CB	2.24	0.53
1:C:94:LEU:N	1:C:94:LEU:CD1	2.72	0.53
1:D:257:PHE:HA	1:D:290:LEU:HD23	1.91	0.53
1:C:410:MET:CE	1:C:410:MET:N	2.72	0.52
1:D:214:LYS:HE2	1:D:218:LEU:HD11	1.90	0.52
1:D:303:MET:HE2	1:D:439:ALA:HA	1.92	0.52
1:D:334:LEU:N	1:D:334:LEU:CD1	2.72	0.52
1:D:491:ASN:C	1:D:491:ASN:HD22	2.16	0.52
1:A:415:ARG:NH1	1:B:99:TYR:OH	2.40	0.52
1:D:274:GLN:CD	1:D:328:ILE:HD13	2.32	0.52
1:A:167:GLU:O	1:A:171:ASN:CA	2.58	0.52
1:C:346:PHE:CD1	1:C:350:LEU:HD12	2.43	0.52
1:D:187:TYR:CZ	1:D:377:ALA:HB2	2.45	0.52
1:A:294:GLU:O	1:A:294:GLU:HG3	2.10	0.52
1:C:352:PRO:HD2	1:D:147:LEU:O	2.10	0.52
1:A:150:GLY:H	1:A:379:HIS:CE1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:GLU:OE1	1:A:274:GLN:CG	2.57	0.52
1:A:367:GLU:CD	1:A:368:ARG:HH21	2.17	0.52
1:B:298:TYR:HB3	1:B:301:LEU:HD12	1.92	0.52
1:C:161:PHE:CZ	1:C:392:LEU:HB3	2.45	0.52
1:D:153:THR:CG2	1:D:370:MET:SD	2.97	0.52
1:D:159:LEU:O	1:D:163:THR:OG1	2.13	0.52
1:D:396:TRP:HB3	1:D:400:GLY:HA3	1.91	0.52
1:C:53:LYS:HB3	1:C:173:PRO:O	2.10	0.52
1:C:190:ASP:O	1:C:194:ARG:HG3	2.10	0.52
1:C:355:ARG:NH1	1:D:378:GLN:NE2	2.58	0.52
1:D:371:ARG:NH1	1:D:374:GLU:OE1	2.42	0.52
1:C:109:VAL:CG2	1:C:391:LEU:HD11	2.37	0.51
1:C:153:THR:CG2	1:C:370:MET:SD	2.99	0.51
1:D:416:ARG:NH1	1:D:437:PRO:O	2.40	0.51
1:C:355:ARG:HH12	1:D:378:GLN:NE2	2.08	0.51
1:A:25:LEU:HD23	1:A:25:LEU:O	2.10	0.51
1:B:316:PRO:N	1:B:317:PRO:HD2	2.24	0.51
1:C:141:TYR:HB2	1:C:157:GLN:HG2	1.91	0.51
1:C:379:HIS:HB2	1:C:380:PRO:HD2	1.93	0.51
1:A:152:SER:OG	1:A:373:CYS:HB2	2.10	0.51
1:D:341:LEU:HD21	1:D:365:LEU:HD13	1.92	0.51
1:C:115:PHE:HD1	1:C:404:TRP:CE3	2.28	0.51
1:D:445:ILE:HG22	1:D:447:ILE:HD12	1.93	0.51
1:A:218:LEU:N	1:A:219:PRO:HD2	2.26	0.51
1:B:218:LEU:HB2	1:B:219:PRO:CD	2.41	0.51
1:C:210:PHE:CZ	1:C:212:SER:HB3	2.46	0.51
1:A:452:HIS:O	1:A:453:PRO:C	2.54	0.51
1:A:32:ILE:HD11	1:A:157:GLN:HA	1.92	0.51
1:B:427:LEU:HD12	1:B:517:ALA:HB2	1.93	0.51
1:C:367:GLU:O	1:C:371:ARG:CD	2.59	0.50
1:D:227:VAL:HG22	1:D:234:LEU:HD12	1.93	0.50
1:C:264:THR:HG21	1:C:302:GLN:CG	2.41	0.50
1:A:154:GLY:HA3	1:A:181:LEU:HD12	1.93	0.50
1:A:182:ASN:HB2	1:A:357:GLY:C	2.37	0.50
1:C:45:PHE:CD1	1:C:160:ARG:HG3	2.46	0.50
1:C:410:MET:CE	1:C:410:MET:CA	2.86	0.50
1:D:56:ALA:HB1	1:D:338:GLY:HA3	1.92	0.50
1:C:227:VAL:HG23	1:C:234:LEU:HD13	1.94	0.50
1:C:355:ARG:HH12	1:D:378:GLN:HE21	1.60	0.50
1:A:152:SER:HA	1:A:378:GLN:O	2.12	0.50
1:B:50:CYS:SG	1:B:167:GLU:OE2	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PRO:C	1:A:87:LEU:H	2.20	0.50
1:A:165:HIS:O	1:A:169:ILE:HG12	2.12	0.50
1:A:272:THR:CG2	1:A:439:ALA:HB3	2.31	0.50
1:D:141:TYR:HB2	1:D:389:PHE:CE2	2.47	0.49
1:D:187:TYR:CZ	1:D:377:ALA:CB	2.95	0.49
1:B:105:ILE:O	1:B:105:ILE:HG23	2.12	0.49
1:B:452:HIS:HB2	1:B:524:PHE:CD2	2.47	0.49
1:B:468:VAL:CG1	1:B:497:PHE:CZ	2.95	0.49
1:C:208:TYR:N	1:C:229:MET:HE2	2.13	0.49
1:A:202:TYR:HA	1:A:223:LYS:O	2.12	0.49
1:B:97:PRO:HA	1:B:100:PHE:CD2	2.47	0.49
1:B:206:GLU:HG3	1:B:234:LEU:HD23	1.93	0.49
1:C:227:VAL:CG2	1:C:234:LEU:CD1	2.89	0.49
1:D:449:TRP:CE2	1:D:461:ARG:HG3	2.47	0.49
1:B:116:SER:O	1:B:120:THR:HG22	2.12	0.49
1:B:207:GLU:N	1:B:229:MET:CE	2.75	0.49
1:D:323:PHE:CZ	1:D:327:LEU:HD11	2.48	0.49
1:C:53:LYS:CB	1:C:173:PRO:O	2.61	0.49
1:C:406:ILE:O	1:C:410:MET:HG2	2.13	0.49
1:D:370:MET:O	1:D:374:GLU:HG3	2.13	0.49
1:A:210:PHE:CD2	2:A:601:PLP:C2A	2.96	0.49
1:A:157:GLN:HB3	1:A:389:PHE:CD1	2.48	0.49
1:A:227:VAL:HG23	1:A:234:LEU:CD1	2.42	0.49
1:D:106:SER:OG	1:D:128:THR:HG22	2.13	0.49
1:A:431:ILE:O	1:A:447:ILE:HA	2.13	0.49
1:C:90:LEU:C	1:D:500:THR:HG22	2.38	0.49
1:C:199:ARG:NH2	1:C:219:PRO:O	2.46	0.49
1:D:274:GLN:HE22	1:D:328:ILE:HD11	1.78	0.49
1:A:157:GLN:HB3	1:A:389:PHE:CE1	2.48	0.48
1:A:346:PHE:CD1	1:A:350:LEU:HD12	2.48	0.48
1:A:468:VAL:HG11	1:A:497:PHE:CE2	2.48	0.48
1:B:208:TYR:N	1:B:229:MET:HE1	2.22	0.48
1:D:115:PHE:CE2	1:D:404:TRP:HA	2.48	0.48
1:A:182:ASN:OD1	1:A:369:PHE:CZ	2.66	0.48
1:C:143:LEU:HD12	1:C:143:LEU:O	2.13	0.48
1:C:149:TYR:CD2	1:D:352:PRO:HB3	2.49	0.48
1:C:441:MET:HB2	1:C:502:ALA:HB2	1.94	0.48
1:C:36:VAL:HA	1:C:145:VAL:HG13	1.95	0.48
1:D:17:LEU:HG	1:D:168:LEU:CD2	2.43	0.48
1:D:157:GLN:HB3	1:D:389:PHE:CD1	2.48	0.48
1:A:110:PRO:HG3	1:A:120:THR:OG1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLN:O	1:A:278:ARG:HG3	2.13	0.48
1:A:290:LEU:O	1:A:339:ARG:HD3	2.12	0.48
1:A:227:VAL:HG21	1:A:234:LEU:HD11	1.96	0.48
1:B:106:SER:HA	1:B:127:LEU:O	2.13	0.48
1:B:182:ASN:HB3	1:B:184:GLY:H	1.78	0.48
1:D:116:SER:HB3	1:D:117:PRO:CD	2.44	0.48
1:D:141:TYR:CD1	1:D:386:ILE:HD12	2.49	0.48
1:B:117:PRO:HA	1:B:120:THR:CG2	2.44	0.48
1:B:17:LEU:HD11	1:B:22:ILE:CD1	2.33	0.48
1:C:109:VAL:HG22	1:C:110:PRO:HD2	1.95	0.48
1:D:460:SER:O	1:D:464:ILE:HG12	2.13	0.48
1:D:412:TYR:HE1	1:D:502:ALA:HB2	1.79	0.47
1:A:227:VAL:CG2	1:A:234:LEU:CD1	2.91	0.47
1:C:153:THR:HG23	1:C:370:MET:HE3	1.96	0.47
1:B:200:GLY:O	1:B:253:SER:OG	2.22	0.47
1:C:372:ASN:O	1:C:372:ASN:ND2	2.44	0.47
1:D:294:GLU:HG2	1:D:296:GLU:HG3	1.96	0.47
1:D:422:ALA:HB3	1:D:513:ILE:HD12	1.96	0.47
1:C:268:PRO:HG3	1:C:485:PHE:CG	2.50	0.47
1:B:316:PRO:HG2	1:B:317:PRO:HD3	1.97	0.47
1:D:263:PRO:HG2	1:D:294:GLU:HG3	1.95	0.47
1:D:491:ASN:C	1:D:491:ASN:ND2	2.73	0.47
1:B:152:SER:HA	1:B:378:GLN:O	2.15	0.47
1:B:415:ARG:NH1	1:B:504:ALA:O	2.40	0.47
1:C:152:SER:OG	1:C:370:MET:HG3	2.15	0.47
1:C:218:LEU:N	1:C:219:PRO:CD	2.77	0.47
1:D:134:VAL:HG21	1:D:142:ASP:HB2	1.95	0.47
1:A:243:LEU:HD11	1:A:290:LEU:HD11	1.97	0.47
1:B:182:ASN:ND2	1:B:369:PHE:CE1	2.75	0.47
1:B:290:LEU:O	1:B:339:ARG:NH1	2.43	0.47
1:C:171:ASN:N	1:C:172:PRO:HD3	2.30	0.47
1:A:112:PRO:HD2	1:A:113:PRO:HD2	1.97	0.46
1:A:503:ALA:HA	1:B:96:SER:HB2	1.97	0.46
1:C:410:MET:HE2	1:C:410:MET:N	2.30	0.46
1:B:277:ARG:O	1:B:281:VAL:HG23	2.16	0.46
1:A:304:GLN:HE22	1:A:316:PRO:HB2	1.79	0.46
1:A:406:ILE:O	1:A:409:ARG:HB3	2.16	0.46
1:D:341:LEU:HD21	1:D:365:LEU:CD1	2.46	0.46
1:A:91:GLY:HA3	1:B:478:LEU:HD12	1.98	0.46
1:D:396:TRP:HB3	1:D:400:GLY:CA	2.45	0.46
1:B:187:TYR:O	1:B:191:THR:HG23	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:THR:CG2	1:D:370:MET:CE	2.85	0.46
1:A:227:VAL:CG2	1:A:234:LEU:HD11	2.45	0.46
1:A:268:PRO:CB	1:A:498:ARG:HD3	2.45	0.46
1:D:136:ALA:HB3	1:D:138:ARG:HG3	1.97	0.46
1:D:267:ASN:HA	1:D:268:PRO:HA	1.78	0.46
1:C:341:LEU:HD22	1:C:359:ILE:HD11	1.97	0.46
1:C:416:ARG:HG2	1:C:437:PRO:HG2	1.97	0.46
1:C:110:PRO:CG	1:D:101:PRO:HB2	2.46	0.46
1:A:112:PRO:CD	1:A:113:PRO:HD2	2.45	0.46
1:D:155:SER:HB2	1:D:157:GLN:NE2	2.31	0.46
1:A:115:PHE:CD1	1:A:404:TRP:HE3	2.34	0.46
1:B:116:SER:HG	1:B:119:GLU:CD	2.21	0.46
1:D:94:LEU:N	1:D:94:LEU:CD1	2.79	0.46
1:B:224:VAL:HG11	1:B:487:ALA:HB1	1.98	0.45
1:C:182:ASN:OD1	1:C:358:TRP:N	2.48	0.45
1:A:109:VAL:HG21	1:A:391:LEU:HD13	1.98	0.45
1:A:208:TYR:O	1:A:266:GLN:NE2	2.46	0.45
1:A:243:LEU:CD1	1:A:290:LEU:HD11	2.46	0.45
1:C:157:GLN:HB3	1:C:389:PHE:CE1	2.52	0.45
1:D:173:PRO:CG	1:D:333:SER:O	2.65	0.45
1:D:268:PRO:HG2	1:D:444:TRP:CZ3	2.51	0.45
1:B:87:LEU:HD12	1:B:87:LEU:C	2.41	0.45
1:C:268:PRO:HG3	1:C:485:PHE:CB	2.47	0.45
1:D:294:GLU:HG2	1:D:296:GLU:CG	2.47	0.45
1:A:19:ILE:HD11	1:A:402:LEU:CD1	2.46	0.45
1:D:110:PRO:CA	1:D:120:THR:OG1	2.64	0.45
1:B:266:GLN:O	1:B:270:GLY:N	2.42	0.45
1:C:157:GLN:HB3	1:C:389:PHE:CD1	2.52	0.45
1:A:91:GLY:HA3	1:B:478:LEU:CD1	2.46	0.45
1:C:169:ILE:N	1:C:169:ILE:HD13	2.32	0.45
1:C:214:LYS:O	1:C:218:LEU:CD1	2.65	0.45
1:A:19:ILE:HA	1:A:22:ILE:HD12	1.99	0.45
1:B:112:PRO:N	1:B:113:PRO:HD2	2.32	0.45
1:C:210:PHE:CE2	1:C:212:SER:HB3	2.51	0.45
1:C:294:GLU:HG3	1:C:294:GLU:O	2.15	0.45
1:C:391:LEU:HD22	1:D:102:PHE:CZ	2.52	0.45
1:B:207:GLU:CD	1:B:228:LYS:HA	2.41	0.45
1:C:172:PRO:HA	1:C:173:PRO:HD3	1.85	0.45
1:D:97:PRO:HA	1:D:100:PHE:CE2	2.52	0.45
1:A:297:PRO:HB2	1:A:348:LYS:HE3	1.98	0.44
1:B:19:ILE:HD11	1:B:402:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:VAL:HG21	1:D:234:LEU:CD1	2.42	0.44
1:A:78:ALA:O	1:A:81:TYR:HB2	2.17	0.44
1:C:174:TYR:HD1	1:C:174:TYR:H	1.64	0.44
1:D:30:ALA:HB1	1:D:31:PRO:HD2	1.98	0.44
1:B:172:PRO:HA	1:B:173:PRO:HD3	1.82	0.44
1:B:173:PRO:HG3	1:B:333:SER:O	2.17	0.44
1:B:247:ASP:OD1	1:B:247:ASP:N	2.49	0.44
1:D:511:GLU:O	1:D:515:ARG:HG3	2.17	0.44
1:A:230:ASP:CG	1:A:277:ARG:HH22	2.25	0.44
1:C:70:ARG:HG2	1:D:219:PRO:HB3	1.99	0.44
1:D:17:LEU:HD22	1:D:167:GLU:CD	2.42	0.44
1:A:33:PRO:HG2	1:A:156:PRO:HG3	2.00	0.44
1:A:67:SER:HB2	1:A:195:MET:HA	2.00	0.44
1:A:111:THR:HG22	1:A:113:PRO:HD2	2.00	0.44
1:C:32:ILE:CG1	1:C:160:ARG:NH1	2.81	0.44
1:D:441:MET:HA	1:D:501:PHE:CZ	2.53	0.44
1:B:486:THR:HG22	1:B:488:ALA:N	2.27	0.44
1:C:110:PRO:HD2	1:D:101:PRO:O	2.18	0.44
1:D:206:GLU:CB	1:D:229:MET:HE1	2.30	0.44
1:A:70:ARG:HG2	1:B:219:PRO:HB3	2.00	0.43
1:A:355:ARG:HA	1:A:355:ARG:NE	2.32	0.43
1:C:84:THR:HB	1:C:85:PRO:HD2	1.99	0.43
1:A:306:TYR:CE2	1:A:420:VAL:HG11	2.54	0.43
1:C:152:SER:HB3	1:C:374:GLU:HG3	2.01	0.43
1:A:120:THR:O	1:A:124:GLY:HA3	2.19	0.43
1:C:208:TYR:HA	1:C:485:PHE:O	2.17	0.43
1:D:227:VAL:CG2	1:D:234:LEU:HD12	2.47	0.43
1:D:46:LYS:HD3	1:D:177:TRP:CE2	2.54	0.43
1:D:274:GLN:O	1:D:278:ARG:CG	2.67	0.43
1:A:58:ARG:HA	1:A:364:GLN:HE22	1.83	0.43
1:B:521:ARG:O	1:B:525:SER:HB3	2.18	0.43
1:C:267:ASN:HA	1:C:268:PRO:HA	1.76	0.43
1:D:49:SER:O	1:D:52:THR:HG22	2.19	0.43
1:D:472:ALA:O	1:D:477:VAL:HG12	2.18	0.43
1:B:308:GLY:N	1:B:309:PRO:HD2	2.34	0.43
1:C:227:VAL:HG12	1:C:242:VAL:HG21	2.00	0.43
1:C:382:GLY:N	1:D:353:GLY:O	2.48	0.43
1:D:191:THR:OG1	1:D:369:PHE:CE2	2.71	0.43
1:D:205:MET:O	1:D:227:VAL:HG13	2.19	0.43
1:B:140:LEU:HA	1:B:140:LEU:HD23	1.75	0.43
1:B:157:GLN:HB3	1:B:389:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:LEU:HD12	1:C:408:LEU:HA	1.86	0.43
1:A:193:LEU:O	1:A:197:CYS:HB2	2.19	0.43
1:A:380:PRO:O	1:A:381:SER:C	2.61	0.43
1:B:26:ARG:HD3	1:B:160:ARG:NH2	2.34	0.43
1:C:210:PHE:CG	2:C:601:PLP:H2A3	2.54	0.43
1:C:263:PRO:HD2	1:C:296:GLU:HG2	2.00	0.43
1:C:392:LEU:O	1:C:397:GLY:N	2.52	0.43
1:D:449:TRP:CD2	1:D:461:ARG:HG3	2.54	0.43
1:B:526:LEU:HD12	1:B:526:LEU:O	2.18	0.42
1:D:214:LYS:CE	1:D:218:LEU:HD11	2.49	0.42
1:D:412:TYR:HE1	1:D:502:ALA:CB	2.32	0.42
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.86	0.42
1:B:477:VAL:CG2	1:B:515:ARG:HB2	2.49	0.42
1:C:205:MET:HB3	1:C:209:THR:HG21	2.01	0.42
1:D:204:LEU:HB2	1:D:259:LEU:HA	2.01	0.42
1:B:203:ILE:HD12	1:B:205:MET:HG3	2.01	0.42
1:D:268:PRO:HB3	1:D:498:ARG:HD3	2.00	0.42
1:C:141:TYR:CE2	1:C:386:ILE:CG1	3.03	0.42
1:C:152:SER:HA	1:C:378:GLN:O	2.19	0.42
1:A:133:ASP:N	1:A:142:ASP:OD2	2.52	0.42
1:B:248:GLU:HA	1:B:253:SER:O	2.20	0.42
1:C:409:ARG:O	1:C:413:THR:OG1	2.36	0.42
1:B:207:GLU:N	1:B:229:MET:HE2	2.34	0.42
1:B:367:GLU:OE2	1:B:371:ARG:NH1	2.53	0.42
1:B:449:TRP:CE2	1:B:450:GLN:HG3	2.54	0.42
1:D:174:TYR:CE2	1:D:177:TRP:HB3	2.54	0.42
1:A:269:THR:HA	1:A:444:TRP:CG	2.54	0.42
1:B:234:LEU:HD13	1:B:235:LEU:N	2.35	0.42
1:C:161:PHE:CE2	1:C:392:LEU:HB3	2.55	0.42
1:C:269:THR:HA	1:C:444:TRP:CD2	2.55	0.42
1:D:330:SER:O	1:D:334:LEU:HD13	2.19	0.42
1:D:397:GLY:C	1:D:399:SER:H	2.27	0.42
1:B:182:ASN:ND2	1:B:369:PHE:HE1	2.15	0.42
1:B:295:ASP:C	1:B:297:PRO:HD3	2.45	0.42
1:B:99:TYR:HB2	4:B:746:HOH:O	2.19	0.42
1:B:447:ILE:CD1	1:B:497:PHE:CE1	2.93	0.42
1:D:295:ASP:C	1:D:297:PRO:HD3	2.45	0.42
1:D:397:GLY:C	1:D:399:SER:N	2.77	0.42
1:A:37:ALA:N	1:A:38:PRO:HD3	2.35	0.41
1:A:391:LEU:HD11	1:A:396:TRP:CE2	2.55	0.41
1:B:441:MET:O	1:B:500:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:TYR:OH	1:C:328:ILE:O	2.27	0.41
1:D:464:ILE:HG12	1:D:464:ILE:H	1.75	0.41
1:D:465:GLU:HG3	1:D:495:LEU:HD22	2.02	0.41
1:A:70:ARG:NH2	4:A:703:HOH:O	2.37	0.41
1:A:87:LEU:HD13	1:A:88:ILE:N	2.32	0.41
1:C:208:TYR:CA	1:C:229:MET:HE1	2.51	0.41
1:C:437:PRO:HD3	1:C:443:HIS:ND1	2.35	0.41
1:A:344:GLU:CB	1:A:358:TRP:CE2	3.03	0.41
1:D:129:ALA:O	1:D:143:LEU:HD22	2.19	0.41
1:D:452:HIS:HA	1:D:453:PRO:HD2	1.82	0.41
1:A:88:ILE:HD13	1:B:508:ASN:HB3	2.02	0.41
1:D:22:ILE:HD11	1:D:168:LEU:HD21	2.03	0.41
1:A:267:ASN:HA	1:A:268:PRO:HA	1.81	0.41
1:B:370:MET:O	1:B:374:GLU:HG3	2.20	0.41
1:D:232:GLU:HB3	1:D:277:ARG:CD	2.43	0.41
1:C:341:LEU:HD23	1:C:341:LEU:HA	1.87	0.41
1:A:246:TRP:CE2	1:A:256:PRO:HD3	2.56	0.41
1:C:22:ILE:CD1	1:C:398:HIS:CD2	3.02	0.41
1:C:141:TYR:HE2	1:C:386:ILE:CA	2.33	0.41
1:D:274:GLN:CD	1:D:328:ILE:CD1	2.92	0.41
1:B:229:MET:HB2	1:B:233:GLY:C	2.46	0.41
1:B:449:TRP:CD1	1:B:493:GLY:O	2.72	0.41
1:C:147:LEU:HD23	1:C:147:LEU:HA	1.88	0.41
1:C:264:THR:HG22	1:C:439:ALA:HB1	2.03	0.41
1:C:355:ARG:NH2	2:C:601:PLP:O2P	2.53	0.41
1:D:94:LEU:N	1:D:94:LEU:HD12	2.36	0.41
1:D:171:ASN:N	1:D:172:PRO:HD3	2.36	0.41
1:D:234:LEU:HD12	1:D:234:LEU:HA	1.80	0.41
1:A:57:LYS:HD2	1:A:337:ASP:HB3	2.03	0.41
1:A:120:THR:HA	4:A:735:HOH:O	2.21	0.41
1:A:285:ALA:CB	1:A:292:ILE:HD11	2.51	0.41
1:C:102:PHE:O	1:C:131:LYS:HE3	2.21	0.41
1:C:269:THR:HG22	1:C:444:TRP:CE2	2.56	0.41
1:D:150:GLY:H	1:D:379:HIS:CE1	2.39	0.41
1:C:287:LYS:HD3	1:C:288:HIS:NE2	2.35	0.40
1:D:56:ALA:HB2	1:D:174:TYR:CD2	2.56	0.40
1:D:306:TYR:HB3	1:D:436:PRO:HB2	2.03	0.40
1:D:511:GLU:OE2	1:D:515:ARG:NE	2.52	0.40
1:B:346:PHE:CD1	1:B:350:LEU:HD12	2.57	0.40
1:D:380:PRO:O	1:D:381:SER:C	2.65	0.40
1:D:441:MET:HA	1:D:501:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:ILE:O	1:C:445:ILE:CG1	2.69	0.40
1:D:429:LYS:O	1:D:430:GLU:C	2.64	0.40
1:A:110:PRO:CB	1:A:120:THR:OG1	2.69	0.40
1:A:179:CYS:SG	1:A:360:VAL:HG22	2.61	0.40
1:B:150:GLY:H	1:B:379:HIS:CE1	2.40	0.40
1:D:75:LEU:HD13	1:D:75:LEU:HA	1.91	0.40
1:D:110:PRO:HB3	1:D:120:THR:HG1	1.73	0.40
1:D:337:ASP:N	1:D:337:ASP:OD1	2.54	0.40
1:B:478:LEU:HD22	1:B:478:LEU:HA	1.84	0.40
1:C:42:SER:HB2	1:C:178:GLN:HG2	2.03	0.40
1:C:110:PRO:CG	1:D:101:PRO:CB	2.98	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	481/534 (90%)	455 (95%)	26 (5%)	0	100	100
1	B	483/534 (90%)	457 (95%)	25 (5%)	1 (0%)	43	58
1	C	458/534 (86%)	432 (94%)	23 (5%)	3 (1%)	18	28
1	D	482/534 (90%)	455 (94%)	25 (5%)	2 (0%)	30	43
All	All	1904/2136 (89%)	1799 (94%)	99 (5%)	6 (0%)	36	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	378	GLN
1	B	453	PRO
1	D	113	PRO
1	C	111	THR

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Mol	Chain	Res	Type
1	C	378	GLN
1	C	113	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/449 (82%)	355 (96%)	13 (4%)	32	53
1	B	376/449 (84%)	347 (92%)	29 (8%)	12	20
1	C	334/449 (74%)	316 (95%)	18 (5%)	20	35
1	D	349/449 (78%)	318 (91%)	31 (9%)	9	15
All	All	1427/1796 (80%)	1336 (94%)	91 (6%)	16	28

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	72	GLN
1	A	87	LEU
1	A	192	VAL
1	A	209	THR
1	A	238	SER
1	A	264	THR
1	A	268	PRO
1	A	336	VAL
1	A	348	LYS
1	A	452	HIS
1	A	506	SER
1	A	522	THR
1	B	19	ILE
1	B	32	ILE
1	B	105	ILE
1	B	120	THR
1	B	152	SER
1	B	153	THR

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Mol	Chain	Res	Type
1	B	191	THR
1	B	192	VAL
1	B	227	VAL
1	B	234	LEU
1	B	237	GLU
1	B	238	SER
1	B	272	THR
1	B	286	GLN
1	B	333	SER
1	B	336	VAL
1	B	348	LYS
1	B	349	VAL
1	B	368	ARG
1	B	381	SER
1	B	383	ILE
1	B	384	SER
1	B	413	THR
1	B	424	GLU
1	B	431	ILE
1	B	478	LEU
1	B	505	SER
1	B	506	SER
1	B	526	LEU
1	C	18	THR
1	C	19	ILE
1	C	94	LEU
1	C	96	SER
1	C	138	ARG
1	C	139	SER
1	C	157	GLN
1	C	169	ILE
1	C	192	VAL
1	C	229	MET
1	C	238	SER
1	C	255	LYS
1	C	287	LYS
1	C	334	LEU
1	C	336	VAL
1	C	348	LYS
1	C	410	MET
1	C	486	THR
1	D	25	LEU

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Mol	Chain	Res	Type
1	D	32	ILE
1	D	36	VAL
1	D	53	LYS
1	D	107	VAL
1	D	112	PRO
1	D	119	GLU
1	D	120	THR
1	D	127	LEU
1	D	143	LEU
1	D	157	GLN
1	D	158	LEU
1	D	167	GLU
1	D	181	LEU
1	D	185	SER
1	D	192	VAL
1	D	193	LEU
1	D	198	THR
1	D	227	VAL
1	D	268	PRO
1	D	341	LEU
1	D	347	SER
1	D	368	ARG
1	D	399	SER
1	D	402	LEU
1	D	406	ILE
1	D	447	ILE
1	D	450	GLN
1	D	464	ILE
1	D	486	THR
1	D	523	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	A	304	GLN
1	A	364	GLN
1	A	378	GLN
1	A	379	HIS
1	A	475	ASN
1	B	71	GLN
1	B	151	GLN

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Mol	Chain	Res	Type
1	B	379	HIS
1	B	395	HIS
1	B	407	ASN
1	B	411	GLN
1	B	421	ASN
1	B	452	HIS
1	B	494	ASN
1	C	121	GLN
1	C	157	GLN
1	C	171	ASN
1	C	320	HIS
1	C	372	ASN
1	D	72	GLN
1	D	157	GLN
1	D	165	HIS
1	D	378	GLN
1	D	379	HIS
1	D	407	ASN
1	D	435	ASN
1	D	443	HIS
1	D	475	ASN
1	D	491	ASN
1	D	494	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	$\# Z > 2$
3	FMT	A	602	-	2,2,2	0.24	0	1,1,1	0.16	0
2	PLP	A	601	1	15,15,16	0.94	1 (6%)	21,22,23	0.55	0
2	PLP	D	602	1	15,15,16	0.88	1 (6%)	21,22,23	0.58	0
2	PLP	B	601	1	15,15,16	0.81	1 (6%)	21,22,23	0.57	0
2	PLP	C	601	1	15,15,16	0.81	1 (6%)	21,22,23	0.83	1 (4%)
3	FMT	D	601	-	2,2,2	0.23	0	1,1,1	0.16	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	B	601	1	-	3/6/6/8	0/1/1/1
2	PLP	C	601	1	-	2/6/6/8	0/1/1/1
2	PLP	A	601	1	-	3/6/6/8	0/1/1/1
2	PLP	D	602	1	-	3/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	PLP	C4A-C4	-2.65	1.46	1.51
2	C	601	PLP	C4A-C4	-2.63	1.46	1.51
2	A	601	PLP	C4A-C4	-2.59	1.46	1.51
2	D	602	PLP	C4A-C4	-2.49	1.46	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	PLP	O4P-C5A-C5	2.64	114.31	109.36

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	PLP	C5A-O4P-P-O1P
2	A	601	PLP	C5A-O4P-P-O2P
2	B	601	PLP	C5A-O4P-P-O2P
2	B	601	PLP	C5A-O4P-P-O3P
2	D	602	PLP	C5A-O4P-P-O2P
2	D	602	PLP	C5A-O4P-P-O3P
2	D	602	PLP	C5A-O4P-P-O1P
2	C	601	PLP	C6-C5-C5A-O4P
2	A	601	PLP	C5A-O4P-P-O3P
2	B	601	PLP	C5A-O4P-P-O1P
2	C	601	PLP	C4-C5-C5A-O4P

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PLP	3	0
2	D	602	PLP	3	0
2	B	601	PLP	1	0
2	C	601	PLP	6	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, 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	489/534 (91%)	0.47	11 (2%) 62 58	32, 48, 77, 102	0
1	B	491/534 (91%)	0.45	10 (2%) 65 60	30, 50, 71, 96	0
1	C	470/534 (88%)	0.82	32 (6%) 23 20	40, 62, 95, 105	0
1	D	490/534 (91%)	0.87	30 (6%) 27 23	39, 68, 91, 119	0
All	All	1940/2136 (90%)	0.65	83 (4%) 40 36	30, 57, 89, 119	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	520	LEU	4.5
1	C	317	PRO	3.9
1	A	464	ILE	3.8
1	B	524	PHE	3.7
1	C	306	TYR	3.7
1	D	125	ALA	3.4
1	C	469	PHE	3.3
1	B	491	ASN	3.1
1	A	112	PRO	3.1
1	A	448	ASP	3.1
1	C	464	ILE	3.0
1	C	234	LEU	3.0
1	D	112	PRO	3.0
1	D	36	VAL	2.9
1	A	111	THR	2.9
1	C	497	PHE	2.9
1	D	319	SER	2.9
1	C	319	SER	2.8
1	C	422	ALA	2.8
1	D	503	ALA	2.7
1	D	75	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	126	VAL	2.7
1	D	488	ALA	2.7
1	C	516	PHE	2.6
1	C	512	ALA	2.6
1	D	51	TYR	2.6
1	A	113	PRO	2.6
1	D	54	PRO	2.6
1	D	197	CYS	2.6
1	D	512	ALA	2.6
1	C	204	LEU	2.5
1	C	106	SER	2.5
1	D	50	CYS	2.5
1	D	179	CYS	2.5
1	B	456	ALA	2.5
1	C	318	ALA	2.5
1	B	309	PRO	2.4
1	C	112	PRO	2.4
1	C	86	GLY	2.4
1	D	493	GLY	2.4
1	C	16	PRO	2.4
1	D	398	HIS	2.4
1	B	455	VAL	2.4
1	B	316	PRO	2.3
1	C	391	LEU	2.3
1	C	473	VAL	2.3
1	D	318	ALA	2.3
1	D	317	PRO	2.3
1	B	454	ALA	2.2
1	C	480	SER	2.2
1	D	431	ILE	2.2
1	C	172	PRO	2.2
1	D	58	ARG	2.2
1	C	124	GLY	2.2
1	A	453	PRO	2.2
1	D	316	PRO	2.2
1	C	429	LYS	2.2
1	C	495	LEU	2.2
1	D	140	LEU	2.2
1	D	22	ILE	2.2
1	A	524	PHE	2.2
1	B	86	GLY	2.2
1	C	98	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	102	PHE	2.2
1	C	475	ASN	2.1
1	B	88	ILE	2.1
1	D	238	SER	2.1
1	D	526	LEU	2.1
1	A	434	TRP	2.1
1	A	495	LEU	2.1
1	B	182	ASN	2.1
1	D	182	ASN	2.1
1	C	233	GLY	2.1
1	D	298	TYR	2.1
1	D	320	HIS	2.1
1	C	227	VAL	2.0
1	C	482	GLY	2.0
1	D	137	GLY	2.0
1	C	386	ILE	2.0
1	D	128	THR	2.0
1	A	51	TYR	2.0
1	C	351	SER	2.0
1	A	520	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLP	C	601	15/16	0.87	0.13	69,71,73,73	0
3	FMT	D	601	3/3	0.88	0.12	47,47,47,48	0
3	FMT	A	602	3/3	0.91	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLP	A	601	15/16	0.95	0.09	44,46,46,46	0
2	PLP	D	602	15/16	0.95	0.10	57,60,60,61	0
2	PLP	B	601	15/16	0.96	0.08	45,48,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.