



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:59 AM UTC

PDB ID : 4A0H / pdb_00004a0h
Title : Structure of bifunctional DAPA aminotransferase-DTB synthetase from *Arabidopsis thaliana* bound to 7-keto 8-amino pelargonic acid (KAPA)
Authors : Cobessi, D.; Dumas, R.; Pautre, V.; Meinguet, C.; Ferrer, J.L.; Alban, C.
Deposited on : 2011-09-09
Resolution : 2.81 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

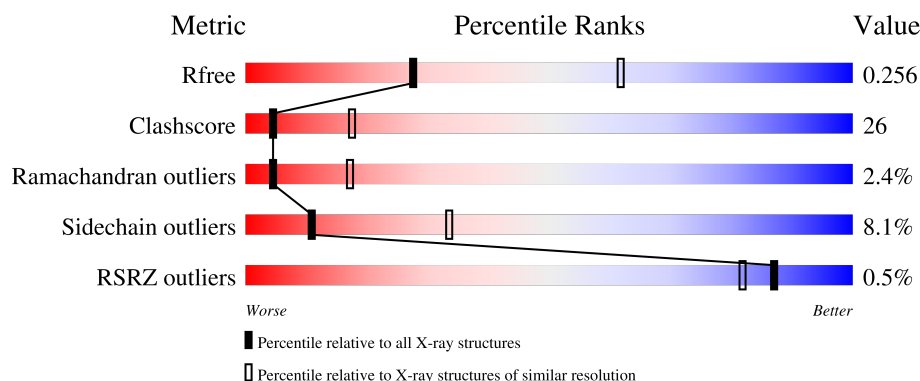
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	831	48% 36% 5% 10%
1	B	831	47% 36% 5% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TLA	A	1810	-	X	X	-
4	TLA	B	1810	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11459 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 ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	748	Total	C	N	O	S	0	1	0
			5732	3672	964	1065	31			
1	B	738	Total	C	N	O	S	0	1	0
			5625	3608	947	1039	31			

There are 40 discrepancies between the modelled and reference sequences:

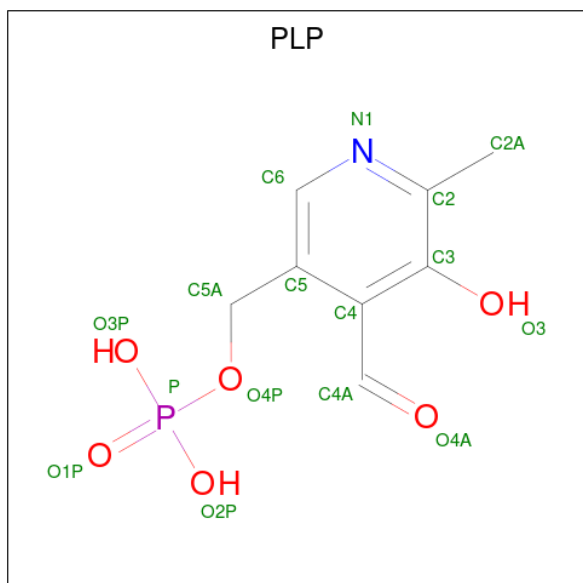
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	GLY	-	expression tag	UNP B0F481
A	-18	SER	-	expression tag	UNP B0F481
A	-17	SER	-	expression tag	UNP B0F481
A	-16	HIS	-	expression tag	UNP B0F481
A	-15	HIS	-	expression tag	UNP B0F481
A	-14	HIS	-	expression tag	UNP B0F481
A	-13	HIS	-	expression tag	UNP B0F481
A	-12	HIS	-	expression tag	UNP B0F481
A	-11	HIS	-	expression tag	UNP B0F481
A	-10	SER	-	expression tag	UNP B0F481
A	-9	SER	-	expression tag	UNP B0F481
A	-8	GLY	-	expression tag	UNP B0F481
A	-7	LEU	-	expression tag	UNP B0F481
A	-6	VAL	-	expression tag	UNP B0F481
A	-5	PRO	-	expression tag	UNP B0F481
A	-4	ARG	-	expression tag	UNP B0F481
A	-3	GLY	-	expression tag	UNP B0F481
A	-2	SER	-	expression tag	UNP B0F481
A	-1	HIS	-	expression tag	UNP B0F481
A	0	MET	-	expression tag	UNP B0F481
B	-19	GLY	-	expression tag	UNP B0F481
B	-18	SER	-	expression tag	UNP B0F481
B	-17	SER	-	expression tag	UNP B0F481
B	-16	HIS	-	expression tag	UNP B0F481

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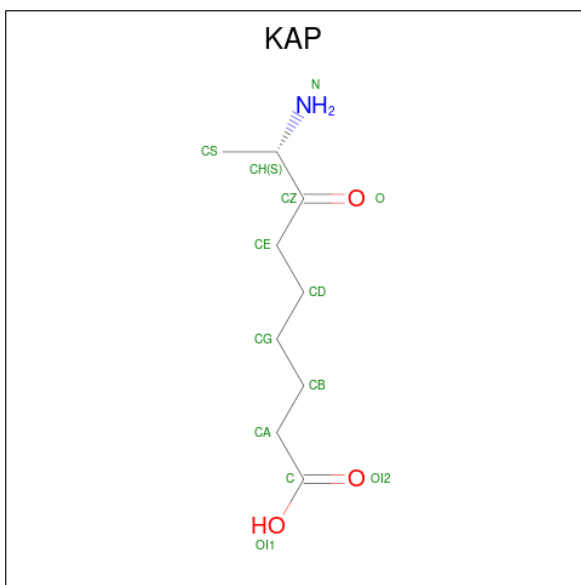
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP B0F481
B	-14	HIS	-	expression tag	UNP B0F481
B	-13	HIS	-	expression tag	UNP B0F481
B	-12	HIS	-	expression tag	UNP B0F481
B	-11	HIS	-	expression tag	UNP B0F481
B	-10	SER	-	expression tag	UNP B0F481
B	-9	SER	-	expression tag	UNP B0F481
B	-8	GLY	-	expression tag	UNP B0F481
B	-7	LEU	-	expression tag	UNP B0F481
B	-6	VAL	-	expression tag	UNP B0F481
B	-5	PRO	-	expression tag	UNP B0F481
B	-4	ARG	-	expression tag	UNP B0F481
B	-3	GLY	-	expression tag	UNP B0F481
B	-2	SER	-	expression tag	UNP B0F481
B	-1	HIS	-	expression tag	UNP B0F481
B	0	MET	-	expression tag	UNP B0F481

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



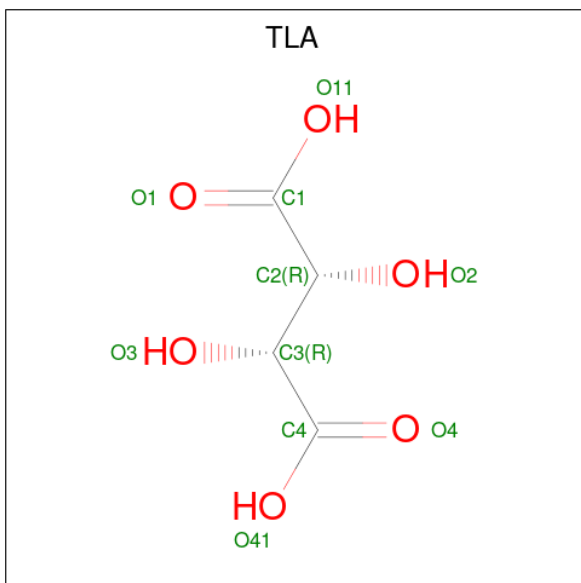
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 7-KETO-8-AMINOPELARGONIC ACID (CCD ID: KAP) (formula: $C_9H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	9	1	3		
3	A	1	Total	C	N	O	0	0
			13	9	1	3		
3	B	1	Total	C	N	O	0	0
			13	9	1	3		
3	B	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 4 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).

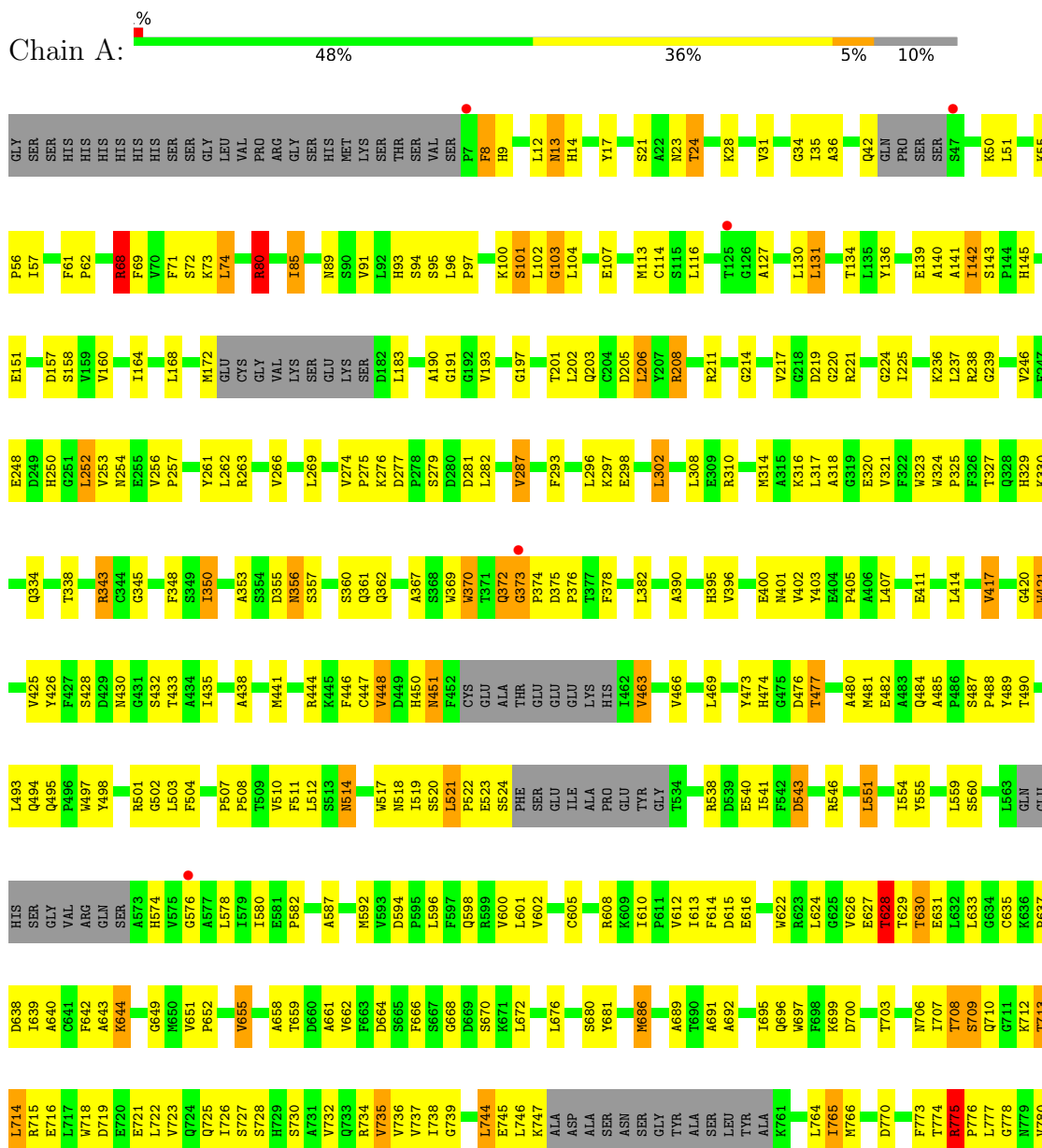


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	4	6		
4	B	1	Total	C	O	0	0
			10	4	6		

3 Residue-property plots

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.

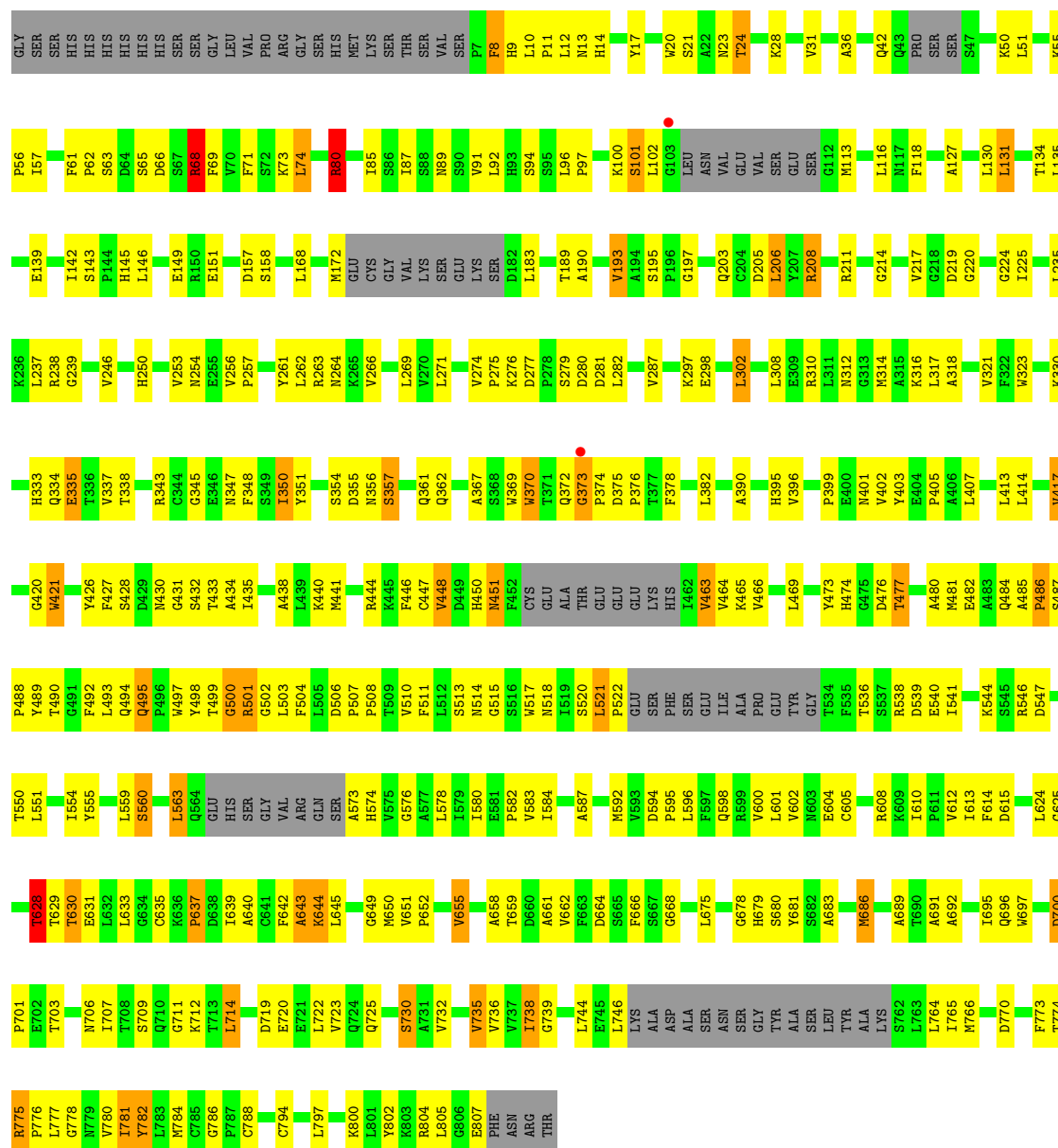
• Molecule 1: ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOATE AMINOTRANSFERASE





• Molecule 1: ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOATE AMINOTRANSFERASE

Chain B: 47% 36% 5% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	235.32Å 76.94Å 89.22Å 90.00° 109.89° 90.00°	Depositor
Resolution (Å)	44.57 – 2.81 44.57 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.57-2.81) 99.1 (44.57-2.81)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.193 , 0.262 0.185 , 0.256	Depositor DCC
R_{free} test set	1822 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11459	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: PLP, TLA, KAP

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	0.63	1/5866 (0.0%)	0.99	19/7975 (0.2%)
1	B	0.62	1/5757 (0.0%)	0.96	15/7832 (0.2%)
All	All	0.63	2/11623 (0.0%)	0.98	34/15807 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	628	THR	CB-CG2	-9.14	1.22	1.52
1	B	628	THR	CB-CG2	-7.19	1.28	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	628	THR	OG1-CB-CG2	-8.19	92.92	109.30
1	A	80	ARG	CD-NE-CZ	-7.86	113.39	124.40
1	B	80	ARG	CG-CD-NE	7.79	129.13	112.00
1	A	68	ARG	CG-CD-NE	7.11	127.64	112.00
1	A	628	THR	OG1-CB-CG2	-6.79	95.71	109.30
1	A	543	ASP	N-CA-C	6.41	118.57	110.24
1	B	700	ASP	CA-C-N	6.29	125.98	119.56
1	B	700	ASP	C-N-CA	6.29	125.98	119.56
1	A	80	ARG	NE-CZ-NH2	6.21	124.79	119.20
1	A	356	ASN	N-CA-C	-6.12	105.66	112.57
1	A	80	ARG	CG-CD-NE	6.10	125.42	112.00
1	A	628	THR	CB-CA-C	-5.89	97.72	109.79
1	B	280	ASP	N-CA-C	5.76	118.68	110.10
1	B	277	ASP	CA-C-N	5.75	125.42	119.56
1	B	277	ASP	C-N-CA	5.75	125.42	119.56
1	A	775	ARG	CB-CG-CD	5.62	124.22	111.30
1	A	197	GLY	CA-C-N	5.61	125.44	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	GLY	C-N-CA	5.61	125.44	119.28
1	A	782	TYR	N-CA-C	5.55	118.13	109.52
1	B	492	PHE	N-CA-C	-5.51	107.20	114.04
1	A	277	ASP	CA-C-N	5.48	125.15	119.56
1	A	277	ASP	C-N-CA	5.48	125.15	119.56
1	A	68	ARG	CB-CG-CD	5.37	123.64	111.30
1	B	782	TYR	N-CA-C	5.36	117.82	109.52
1	B	197	GLY	CA-C-N	5.33	125.14	119.28
1	B	197	GLY	C-N-CA	5.33	125.14	119.28
1	A	700	ASP	CA-C-N	5.31	124.98	119.56
1	A	700	ASP	C-N-CA	5.31	124.98	119.56
1	B	347	ASN	N-CA-C	5.14	117.34	109.07
1	B	271	LEU	CA-C-N	5.04	123.29	119.66
1	B	271	LEU	C-N-CA	5.04	123.29	119.66
1	A	551	LEU	N-CA-C	5.02	117.48	111.71
1	A	372	GLN	N-CA-C	5.02	117.91	110.48
1	B	68	ARG	CG-CD-NE	5.01	123.01	112.00

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	5732	0	5648	328	0
1	B	5625	0	5524	308	1
2	A	15	0	6	3	0
2	B	15	0	6	4	0
3	A	26	0	32	5	0
3	B	26	0	32	7	0
4	A	10	0	4	5	0
4	B	10	0	4	4	0
All	All	11459	0	11256	594	1

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 26.

All (594) 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:80:ARG:NH1	1:A:287:VAL:HG21	1.66	1.11
1:A:659:THR:HG22	1:A:661:ALA:H	1.15	1.10
1:B:659:THR:HG22	1:B:661:ALA:H	1.18	1.04
1:B:65:SER:HB3	1:B:68:ARG:NH1	1.77	0.99
1:A:80:ARG:HH11	1:A:287:VAL:HG21	1.26	0.99
1:A:220:GLY:O	1:A:252[A]:LEU:HD21	1.63	0.97
1:A:252[A]:LEU:HD12	1:A:252[A]:LEU:H	1.28	0.95
1:B:446:PHE:CD2	1:B:576:GLY:HA2	2.02	0.94
1:A:446:PHE:CD2	1:A:576:GLY:HA2	2.05	0.92
1:B:208:ARG:HH12	1:B:211:ARG:HD3	1.31	0.92
1:A:493:LEU:HB3	1:B:444:ARG:HH21	1.36	0.91
1:A:55:LYS:NZ	4:A:1810:TLA:O4	2.04	0.90
1:A:208:ARG:HH12	1:A:211:ARG:HD3	1.36	0.89
1:B:68:ARG:HH11	1:B:68:ARG:HB3	1.35	0.88
1:A:521:LEU:N	1:A:521:LEU:CD1	2.35	0.88
1:B:560:SER:HA	1:B:563:LEU:HD12	1.56	0.88
1:A:708:THR:HG21	1:A:710:GLN:NE2	1.89	0.86
1:A:262:LEU:HD13	1:A:266:VAL:HB	1.59	0.85
1:A:510:VAL:HG11	1:A:541:ILE:HD13	1.59	0.85
1:B:521:LEU:H	1:B:521:LEU:HD12	1.41	0.84
1:A:401:ASN:OD1	1:B:338:THR:HB	1.79	0.83
1:A:417:VAL:HG22	1:A:628:THR:HG23	1.60	0.82
1:A:520:SER:C	1:A:521:LEU:HD12	2.05	0.80
1:A:497:TRP:HZ3	1:B:482:GLU:HB2	1.45	0.80
1:B:36:ALA:HA	1:B:51:LEU:HD13	1.64	0.79
1:A:446:PHE:HD2	1:A:576:GLY:HA2	1.48	0.79
1:A:103:GLY:O	1:A:104:LEU:HG	1.83	0.79
1:A:36:ALA:HA	1:A:51:LEU:HD13	1.65	0.79
1:B:28:LYS:NZ	4:B:1810:TLA:H2	1.98	0.78
1:B:101:SER:O	1:B:102:LEU:HD23	1.83	0.78
1:B:428:SER:HB2	1:B:433:THR:OG1	1.84	0.78
1:A:21:SER:HB2	1:A:28:LYS:HD3	1.66	0.78
1:A:338:THR:HB	1:B:401:ASN:OD1	1.85	0.77
1:A:325:PRO:O	1:A:327:THR:HG23	1.85	0.77
1:B:65:SER:HB3	1:B:68:ARG:HH12	1.47	0.77
1:B:446:PHE:HD2	1:B:576:GLY:HA2	1.44	0.77
1:A:521:LEU:N	1:A:521:LEU:HD12	1.98	0.77
1:B:262:LEU:HD13	1:B:266:VAL:HB	1.68	0.76
1:B:405:PRO:HB3	1:B:689:ALA:HB2	1.67	0.76
1:B:14:HIS:HB2	1:B:172:MET:HE3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:PHE:CE2	1:A:576:GLY:HA2	2.23	0.73
1:A:723:VAL:HG11	1:A:737:VAL:HG11	1.70	0.73
1:B:446:PHE:CE2	1:B:576:GLY:HA2	2.23	0.73
1:A:428:SER:HB2	1:A:433:THR:OG1	1.87	0.73
1:B:68:ARG:HH11	1:B:68:ARG:CB	2.00	0.73
1:B:21:SER:HB2	1:B:28:LYS:HD3	1.71	0.73
1:B:770:ASP:HB3	1:B:800:LYS:HD2	1.71	0.72
1:B:521:LEU:HD12	1:B:521:LEU:N	2.04	0.72
1:A:497:TRP:CZ3	1:B:482:GLU:HB2	2.23	0.72
1:B:608:ARG:HG3	1:B:608:ARG:HH11	1.54	0.72
1:A:373:GLY:H	1:A:374:PRO:CD	2.03	0.71
1:A:96:LEU:HB3	1:A:97:PRO:HD3	1.73	0.71
1:A:770:ASP:HB3	1:A:800:LYS:HD2	1.71	0.71
1:B:373:GLY:H	1:B:374:PRO:CD	2.04	0.71
1:A:726:ILE:HG12	1:A:802:TYR:HD1	1.55	0.71
1:A:14:HIS:HB2	1:A:172:MET:HE3	1.71	0.70
1:A:208:ARG:NH1	1:A:211:ARG:HD3	2.06	0.70
1:A:497:TRP:HB3	1:B:501:ARG:HE	1.56	0.69
1:A:708:THR:HG23	1:A:709:SER:N	2.07	0.69
1:A:608:ARG:HG3	1:A:608:ARG:HH11	1.56	0.69
3:A:1809:KAP:HA2	1:B:195:SER:OG	1.91	0.69
1:A:730:SER:O	1:A:747:LYS:HD2	1.93	0.69
1:A:8:PHE:CD1	1:A:8:PHE:C	2.71	0.69
1:A:8:PHE:CE2	1:A:361:GLN:HG3	2.29	0.68
1:B:8:PHE:CE2	1:B:361:GLN:HG3	2.27	0.68
1:B:208:ARG:NH1	1:B:211:ARG:HD3	2.06	0.68
1:A:8:PHE:CD2	1:A:361:GLN:HG3	2.28	0.68
1:B:485:ALA:HB2	1:B:504:PHE:CG	2.29	0.68
1:A:74:LEU:HD13	1:A:130:LEU:HD22	1.75	0.67
1:A:477:THR:HG21	1:B:477:THR:HG21	1.77	0.67
1:A:405:PRO:HB3	1:A:689:ALA:HB2	1.76	0.67
1:B:8:PHE:CD2	1:B:361:GLN:HG3	2.30	0.66
1:A:659:THR:HG22	1:A:661:ALA:N	2.00	0.66
1:B:8:PHE:C	1:B:8:PHE:CD1	2.73	0.65
1:B:578:LEU:HD23	1:B:612:VAL:HG13	1.77	0.65
1:B:766:MET:HE2	1:B:804:ARG:HB3	1.79	0.65
1:A:485:ALA:HB2	1:A:504:PHE:CG	2.32	0.65
1:A:101:SER:O	1:A:102:LEU:HD23	1.95	0.65
1:B:143:SER:HB3	1:B:145:HIS:ND1	2.10	0.65
1:A:28:LYS:HZ2	4:A:1810:TLA:H2	1.61	0.65
1:A:13:ASN:ND2	1:A:356:ASN:HB3	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:LEU:HA	1:B:554:ILE:HD12	1.79	0.65
1:B:539:ASP:C	1:B:541:ILE:H	2.04	0.64
1:A:481:MET:HE2	1:A:490:THR:HA	1.80	0.64
1:B:96:LEU:HB3	1:B:97:PRO:HD3	1.79	0.64
1:A:521:LEU:N	1:A:521:LEU:HD13	2.13	0.64
1:A:80:ARG:HH12	1:A:287:VAL:HG21	1.62	0.64
1:A:375:ASP:HB2	1:A:378:PHE:H	1.63	0.64
1:A:9:HIS:ND1	1:A:360:SER:HB3	2.13	0.63
1:A:220:GLY:C	1:A:252[A]:LEU:HD21	2.23	0.63
1:A:592:MET:HE2	1:A:736:VAL:HG13	1.81	0.63
1:B:430:ASN:HB2	2:B:1644:PLP:O3P	1.98	0.63
1:B:484:GLN:HE22	1:B:489:TYR:HB2	1.63	0.63
1:A:580:ILE:O	1:A:582:PRO:HD3	1.97	0.63
1:B:62:PRO:HG3	1:B:102:LEU:HD21	1.79	0.63
1:A:766:MET:HE2	1:A:804:ARG:HB3	1.81	0.62
1:B:474:HIS:O	1:B:480:ALA:HB1	1.99	0.62
1:A:100:LYS:C	1:A:102:LEU:H	2.08	0.62
1:A:191:GLY:H	4:A:1810:TLA:H3	1.64	0.62
1:B:61:PHE:O	1:B:139:GLU:HA	1.98	0.62
1:B:350:ILE:HD12	1:B:362:GLN:HB3	1.81	0.62
1:A:616:GLU:OE2	1:A:628:THR:HG22	2.00	0.62
1:B:446:PHE:C	1:B:446:PHE:CD1	2.77	0.62
1:A:546:ARG:NH2	1:A:596:LEU:HD23	2.15	0.61
1:B:692:ALA:O	1:B:696:GLN:HG3	2.00	0.61
1:A:321:VAL:HG13	1:B:414:LEU:CD1	2.30	0.61
1:A:367:ALA:HB1	1:A:372:GLN:HB2	1.82	0.61
1:A:718:TRP:CE3	1:A:794:CYS:HB3	2.34	0.61
1:B:373:GLY:H	1:B:374:PRO:HD3	1.65	0.61
1:B:580:ILE:O	1:B:582:PRO:HD3	2.00	0.61
1:A:484:GLN:HE22	1:A:489:TYR:HB2	1.66	0.61
1:B:390:ALA:HB2	1:B:686:MET:HE1	1.81	0.61
1:B:651:VAL:HG22	1:B:652:PRO:HD2	1.82	0.61
1:B:441:MET:HE2	1:B:639:ILE:HG12	1.80	0.61
1:B:517:TRP:CZ3	1:B:592:MET:HE1	2.36	0.61
1:B:310:ARG:O	1:B:314:MET:HG3	2.01	0.61
1:B:592:MET:HE2	1:B:736:VAL:HG13	1.83	0.61
1:B:601:LEU:O	1:B:601:LEU:HD12	2.00	0.60
1:B:94:SER:O	1:B:113:MET:HE3	2.01	0.60
1:A:252[A]:LEU:HD22	1:A:254:ASN:OD1	2.01	0.60
1:A:708:THR:HB	1:A:713:THR:O	2.02	0.60
1:B:143:SER:HB3	1:B:145:HIS:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:PRO:HG3	1:A:102:LEU:HD21	1.83	0.60
1:A:766:MET:HE3	1:A:807:GLU:OE1	2.01	0.60
1:B:74:LEU:HD13	1:B:130:LEU:HD22	1.84	0.60
1:B:546:ARG:NH2	1:B:596:LEU:HD23	2.17	0.59
1:A:692:ALA:O	1:A:696:GLN:HG3	2.02	0.59
1:B:65:SER:HB3	1:B:68:ARG:HH11	1.66	0.59
1:B:100:LYS:C	1:B:102:LEU:H	2.10	0.59
1:A:719:ASP:O	1:A:723:VAL:HG23	2.02	0.59
1:B:510:VAL:HG11	1:B:541:ILE:HD13	1.83	0.59
1:A:446:PHE:CD1	1:A:446:PHE:C	2.76	0.59
1:A:517:TRP:CZ3	1:A:592:MET:HE1	2.38	0.59
1:B:66:ASP:OD2	4:B:1810:TLA:O1	2.20	0.59
1:A:157:ASP:HB3	1:A:206:LEU:HD12	1.84	0.59
1:A:430:ASN:HB2	2:A:1644:PLP:O3P	2.03	0.59
1:A:497:TRP:CZ3	1:B:482:GLU:CB	2.85	0.59
1:A:310:ARG:O	1:A:314:MET:HG3	2.02	0.59
1:A:707:ILE:HD13	1:A:714:LEU:HD12	1.83	0.59
1:A:353:ALA:HA	1:A:357:SER:HA	1.85	0.59
1:B:485:ALA:HB2	1:B:504:PHE:CD1	2.37	0.59
1:B:659:THR:HG22	1:B:661:ALA:N	2.03	0.59
1:A:68:ARG:HH11	1:A:68:ARG:HB3	1.66	0.58
1:A:805:LEU:C	1:A:807:GLU:H	2.11	0.58
1:B:481:MET:HE2	1:B:490:THR:HA	1.85	0.58
1:B:539:ASP:C	1:B:541:ILE:N	2.59	0.58
1:A:578:LEU:HD23	1:A:612:VAL:HG13	1.84	0.58
1:A:140:ALA:HB1	1:A:142:ILE:HD13	1.85	0.58
1:A:708:THR:CG2	1:A:710:GLN:CD	2.76	0.58
1:A:441:MET:HE1	1:A:658:ALA:HB2	1.86	0.58
1:A:519:ILE:HG12	1:A:521:LEU:CD1	2.33	0.58
4:A:1810:TLA:O41	3:B:1809:KAP:N	2.36	0.58
1:B:725:GLN:HB3	1:B:802:TYR:CE1	2.37	0.58
1:A:211:ARG:HD2	1:A:239:GLY:O	2.04	0.57
1:B:80:ARG:NH1	1:B:287:VAL:HG21	2.20	0.57
1:A:370:TRP:N	1:A:370:TRP:CD1	2.69	0.57
1:A:485:ALA:HB2	1:A:504:PHE:CD1	2.39	0.57
1:B:91:VAL:HG22	1:B:134:THR:HB	1.86	0.57
1:A:598:GLN:O	1:A:602:VAL:HG23	2.05	0.57
1:A:225:ILE:HD13	1:A:257:PRO:HG2	1.86	0.57
1:A:373:GLY:H	1:A:374:PRO:HD3	1.68	0.57
1:B:31:VAL:HG21	1:B:217:VAL:HG22	1.86	0.57
1:A:252[A]:LEU:HD22	1:A:254:ASN:CG	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335[B]:GLU:OE1	1:B:335[B]:GLU:HA	2.05	0.57
1:B:208:ARG:HH12	1:B:211:ARG:CD	2.11	0.57
1:B:508:PRO:HA	1:B:520:SER:O	2.05	0.57
1:A:220:GLY:O	1:A:250:HIS:HB2	2.05	0.56
1:A:61:PHE:O	1:A:139:GLU:HA	2.05	0.56
1:A:220:GLY:O	1:A:252[A]:LEU:CD2	2.47	0.56
1:A:473:TYR:OH	1:A:476:ASP:OD1	2.16	0.56
1:A:508:PRO:HA	1:A:520:SER:O	2.06	0.56
1:A:601:LEU:HD12	1:A:601:LEU:O	2.05	0.56
1:B:417:VAL:HG23	1:B:628:THR:HG22	1.86	0.56
1:B:466:VAL:HG12	1:B:502:GLY:HA3	1.87	0.56
1:B:651:VAL:CG2	1:B:652:PRO:HD2	2.36	0.56
1:B:732:VAL:HG22	1:B:744:LEU:HD22	1.87	0.56
1:A:708:THR:HG21	1:A:710:GLN:CD	2.31	0.56
1:A:719:ASP:HB3	1:A:722:LEU:HD12	1.87	0.56
1:A:323:TRP:HB3	1:B:426:TYR:HD2	1.71	0.56
1:B:446:PHE:C	1:B:446:PHE:HD1	2.14	0.56
1:A:493:LEU:HB3	1:B:444:ARG:NH2	2.14	0.56
1:A:706:ASN:HA	1:A:715:ARG:HE	1.71	0.55
1:B:370:TRP:CD1	1:B:370:TRP:N	2.70	0.55
1:A:417:VAL:CG2	1:A:628:THR:HG23	2.33	0.55
1:A:396:VAL:HG12	1:B:348:PHE:HE1	1.70	0.55
1:B:23:ASN:OD1	1:B:24:THR:N	2.32	0.55
1:B:644:LYS:NZ	2:B:1644:PLP:O3	2.40	0.55
1:A:441:MET:HE2	1:A:639:ILE:HG12	1.87	0.55
1:B:14:HIS:HB2	1:B:172:MET:CE	2.34	0.55
1:B:375:ASP:HB2	1:B:378:PHE:H	1.70	0.55
1:B:254:ASN:O	1:B:257:PRO:HD2	2.06	0.55
1:B:711:GLY:O	1:B:712:LYS:HB2	2.05	0.55
1:A:446:PHE:C	1:A:446:PHE:HD1	2.13	0.55
1:B:441:MET:HE1	1:B:658:ALA:HB2	1.88	0.55
1:A:551:LEU:HA	1:A:554:ILE:HD12	1.89	0.55
3:A:1808:KAP:H2	1:B:679:HIS:HA	1.72	0.55
1:A:414:LEU:CD1	1:B:321:VAL:HG13	2.35	0.55
1:A:723:VAL:CG1	1:A:737:VAL:HG11	2.36	0.55
1:B:432:SER:HB3	1:B:477:THR:OG1	2.07	0.55
1:A:512:LEU:HD23	1:A:727:SER:HB3	1.88	0.55
1:B:417:VAL:HG21	1:B:642:PHE:CE1	2.41	0.54
1:A:441:MET:CE	1:A:658:ALA:HB2	2.37	0.54
1:A:521:LEU:HD13	1:A:521:LEU:H	1.70	0.54
1:A:732:VAL:HG22	1:A:744:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PRO:HG2	1:A:151:GLU:HB3	1.90	0.54
2:A:1644:PLP:C4A	3:A:1808:KAP:O	2.56	0.54
1:B:628:THR:OG1	1:B:630:THR:HB	2.07	0.54
1:A:490:THR:HB	1:A:498:TYR:CE2	2.43	0.54
1:A:546:ARG:HB3	1:A:596:LEU:HD22	1.88	0.54
1:B:746:LEU:HD11	1:B:781:ILE:HD12	1.90	0.54
1:B:506:ASP:HB3	1:B:522:PRO:HG2	1.89	0.54
1:B:208:ARG:NH1	1:B:211:ARG:CD	2.71	0.54
1:A:100:LYS:O	1:A:102:LEU:N	2.40	0.54
1:B:719:ASP:HB3	1:B:722:LEU:HB2	1.90	0.54
1:B:12:LEU:O	1:B:308:LEU:HD11	2.08	0.53
1:A:190:ALA:O	1:A:203:GLN:NE2	2.42	0.53
1:A:330:LYS:HD3	1:B:668:GLY:O	2.07	0.53
1:A:446:PHE:C	1:A:448:VAL:H	2.16	0.53
1:A:474:HIS:O	1:A:480:ALA:HB1	2.08	0.53
1:B:28:LYS:HZ2	4:B:1810:TLA:H2	1.71	0.53
1:A:350:ILE:HD12	1:A:362:GLN:HB3	1.88	0.53
1:A:681:TYR:OH	1:B:649:GLY:HA2	2.09	0.53
1:B:446:PHE:C	1:B:448:VAL:H	2.16	0.53
1:B:473:TYR:C	1:B:474:HIS:CD2	2.87	0.53
1:B:625:GLY:HA2	1:B:714:LEU:HD12	1.91	0.53
1:A:746:LEU:HD11	1:A:781:ILE:HD12	1.90	0.53
1:A:622:TRP:CE3	1:A:714:LEU:HD13	2.44	0.52
1:A:668:GLY:O	1:B:330:LYS:HD3	2.10	0.52
1:B:473:TYR:OH	1:B:476:ASP:OD1	2.19	0.52
1:A:497:TRP:HE1	1:B:464:VAL:HG23	1.74	0.52
1:A:706:ASN:O	1:A:715:ARG:HG2	2.09	0.52
1:A:469:LEU:HD13	1:A:507:PRO:HB3	1.90	0.52
1:B:211:ARG:HD2	1:B:239:GLY:O	2.10	0.52
1:B:544:LYS:O	1:B:547:ASP:HB2	2.09	0.52
1:B:405:PRO:HB3	1:B:689:ALA:CB	2.39	0.52
2:B:1644:PLP:C4A	3:B:1808:KAP:O	2.58	0.52
1:A:432:SER:HB3	1:A:477:THR:OG1	2.09	0.52
1:A:644:LYS:NZ	2:A:1644:PLP:O3	2.43	0.51
1:B:225:ILE:HD13	1:B:257:PRO:HG2	1.92	0.51
1:A:91:VAL:HG22	1:A:134:THR:HB	1.91	0.51
1:A:396:VAL:HG12	1:B:348:PHE:CE1	2.45	0.51
1:A:71:PHE:CD2	1:A:89:ASN:HB2	2.45	0.51
1:A:473:TYR:C	1:A:474:HIS:CD2	2.88	0.51
1:B:487:SER:HB2	1:B:488:PRO:HD2	1.92	0.51
1:A:14:HIS:HB2	1:A:172:MET:CE	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:MET:HE2	1:A:136:TYR:HD1	1.75	0.51
1:A:208:ARG:NH1	1:A:211:ARG:CD	2.72	0.51
1:B:71:PHE:CD2	1:B:89:ASN:HB2	2.46	0.51
1:B:720:GLU:O	1:B:723:VAL:HG22	2.11	0.51
1:A:501:ARG:HD2	1:B:497:TRP:CD2	2.46	0.51
1:A:777:LEU:HB2	1:A:780:VAL:HB	1.91	0.51
1:A:321:VAL:HG13	1:B:414:LEU:HD12	1.93	0.51
1:A:514:ASN:HD22	1:A:728:SER:HA	1.75	0.51
1:B:298:GLU:O	1:B:302:LEU:HB2	2.09	0.51
1:A:68:ARG:HB3	1:A:68:ARG:NH1	2.25	0.51
1:A:256:VAL:HB	1:A:257:PRO:HD3	1.92	0.51
1:B:23:ASN:CG	1:B:24:THR:H	2.18	0.51
1:B:42:GLN:OE1	1:B:42:GLN:HA	2.10	0.51
1:B:441:MET:CE	1:B:658:ALA:HB2	2.40	0.51
1:A:511:PHE:CE1	1:A:518:ASN:HB2	2.46	0.50
1:B:85:ILE:HA	1:B:127:ALA:HB1	1.93	0.50
1:B:469:LEU:HD13	1:B:507:PRO:HB3	1.93	0.50
1:B:563:LEU:HD13	1:B:608:ARG:NH1	2.26	0.50
1:B:28:LYS:CE	4:B:1810:TLA:H2	2.40	0.50
1:B:605:CYS:HB3	1:B:610:ILE:HB	1.93	0.50
1:A:356:ASN:O	1:A:357:SER:HB2	2.12	0.50
1:A:482:GLU:HB3	1:A:501:ARG:HB3	1.94	0.50
1:B:80:ARG:HG3	1:B:80:ARG:HH11	1.77	0.50
1:A:321:VAL:HG13	1:B:414:LEU:HD11	1.94	0.50
1:B:608:ARG:HH11	1:B:608:ARG:CG	2.24	0.50
1:A:735:VAL:HG22	1:A:744:LEU:HB3	1.94	0.50
1:B:157:ASP:HB3	1:B:206:LEU:HD12	1.92	0.50
1:A:100:LYS:C	1:A:102:LEU:N	2.69	0.50
1:B:345:GLY:HA3	1:B:376:PRO:HD3	1.94	0.50
1:A:473:TYR:C	1:A:474:HIS:CG	2.90	0.50
1:B:367:ALA:HB1	1:B:372:GLN:HB2	1.92	0.50
1:A:93:HIS:HA	1:A:114:CYS:O	2.12	0.49
1:B:777:LEU:HB2	1:B:780:VAL:HB	1.94	0.49
1:A:85:ILE:HA	1:A:127:ALA:HB1	1.94	0.49
1:A:93:HIS:HB2	1:A:113:MET:HE2	1.93	0.49
1:A:766:MET:HE2	1:A:804:ARG:HD2	1.93	0.49
1:A:252[A]:LEU:H	1:A:252[A]:LEU:CD1	2.04	0.49
1:A:605:CYS:HB3	1:A:610:ILE:HB	1.94	0.49
1:B:633:LEU:HB3	1:B:635:CYS:SG	2.53	0.49
1:A:373:GLY:HA2	1:A:786:GLY:HA3	1.94	0.49
1:A:805:LEU:O	1:A:807:GLU:N	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:LEU:HD11	1:B:604:GLU:HB3	1.94	0.49
1:A:390:ALA:HB2	1:A:686:MET:HE1	1.95	0.49
1:B:190:ALA:O	1:B:203:GLN:NE2	2.43	0.49
1:A:8:PHE:C	1:A:8:PHE:HD1	2.21	0.49
1:A:766:MET:HB3	1:A:804:ARG:NE	2.27	0.49
1:B:438:ALA:HB1	1:B:613:ILE:HD13	1.93	0.49
1:B:511:PHE:CE1	1:B:518:ASN:HB2	2.48	0.49
1:B:633:LEU:C	1:B:635:CYS:H	2.20	0.49
1:A:519:ILE:HG12	1:A:521:LEU:HD12	1.94	0.49
1:B:97:PRO:HG2	1:B:151:GLU:HB3	1.93	0.49
1:B:101:SER:C	1:B:102:LEU:HD23	2.38	0.49
1:B:237:LEU:HD12	1:B:237:LEU:HA	1.57	0.49
1:B:473:TYR:C	1:B:474:HIS:CG	2.90	0.49
1:A:220:GLY:O	1:A:252[A]:LEU:HD11	2.13	0.49
1:A:254:ASN:O	1:A:257:PRO:HD2	2.12	0.49
1:B:100:LYS:C	1:B:102:LEU:N	2.71	0.49
1:A:407:LEU:HD11	1:B:317:LEU:HG	1.95	0.48
1:A:775:ARG:HG3	1:A:776:PRO:HD2	1.95	0.48
1:A:487:SER:HB2	1:A:488:PRO:HD2	1.94	0.48
1:B:356:ASN:O	1:B:357:SER:C	2.55	0.48
1:A:463:VAL:O	1:A:574:HIS:HB2	2.13	0.48
1:B:50:LYS:HE3	1:B:131:LEU:HD12	1.95	0.48
1:B:316:LYS:HB2	1:B:334:GLN:OE1	2.12	0.48
1:B:559:LEU:HD12	1:B:600:VAL:HG12	1.96	0.48
1:B:420:GLY:O	1:B:421:TRP:HB3	2.13	0.48
1:B:594:ASP:OD1	1:B:596:LEU:HB3	2.13	0.48
1:B:598:GLN:O	1:B:602:VAL:HG23	2.13	0.48
1:B:735:VAL:HG22	1:B:744:LEU:HB3	1.95	0.48
1:A:23:ASN:CG	1:A:24:THR:H	2.22	0.48
1:A:616:GLU:CD	1:A:628:THR:HG22	2.39	0.48
1:A:744:LEU:C	1:A:744:LEU:HD12	2.38	0.48
1:B:312:ASN:ND2	1:B:351:TYR:OH	2.46	0.48
1:B:446:PHE:HD2	1:B:576:GLY:CA	2.21	0.48
1:B:465:LYS:NZ	1:B:573:ALA:HB1	2.28	0.48
1:B:775:ARG:NE	3:B:1808:KAP:OI1	2.32	0.48
1:A:21:SER:CB	1:A:28:LYS:HD3	2.41	0.48
1:B:498:TYR:CE1	1:B:500:GLY:N	2.82	0.48
1:A:160:VAL:O	1:A:164:ILE:HG13	2.14	0.48
1:A:805:LEU:C	1:A:807:GLU:N	2.71	0.48
1:B:546:ARG:HB3	1:B:596:LEU:HD22	1.95	0.48
1:B:625:GLY:HA2	1:B:714:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ASN:OD1	1:A:24:THR:N	2.42	0.47
1:A:400:GLU:O	1:B:337:VAL:HA	2.13	0.47
1:A:261:TYR:CD1	1:A:261:TYR:C	2.91	0.47
1:A:608:ARG:HH11	1:A:608:ARG:CG	2.26	0.47
1:B:208:ARG:HH11	1:B:211:ARG:HG3	1.79	0.47
1:B:560:SER:CA	1:B:563:LEU:HD12	2.36	0.47
1:A:248:GLU:O	1:A:250:HIS:ND1	2.43	0.47
1:A:323:TRP:CG	1:B:426:TYR:HD2	2.33	0.47
1:B:614:PHE:O	1:B:640:ALA:HA	2.15	0.47
1:A:691:ALA:O	1:A:695:ILE:HG13	2.13	0.47
1:B:482:GLU:OE2	1:B:501:ARG:NH1	2.47	0.47
1:A:73:LYS:HD3	1:A:73:LYS:HA	1.66	0.47
1:A:140:ALA:O	1:A:142:ILE:N	2.43	0.47
1:A:414:LEU:HD11	1:B:321:VAL:HG13	1.96	0.47
1:A:629:THR:C	1:A:631:GLU:N	2.71	0.47
1:A:633:LEU:HB3	1:A:635:CYS:SG	2.54	0.47
1:B:68:ARG:NH1	1:B:68:ARG:HB3	2.16	0.47
1:B:94:SER:HB3	1:B:116:LEU:HD11	1.97	0.47
1:B:335[B]:GLU:OE1	1:B:335[B]:GLU:CA	2.63	0.47
1:A:555:TYR:O	1:A:559:LEU:HG	2.14	0.47
1:A:649:GLY:HA2	1:B:681:TYR:OH	2.15	0.47
1:A:806:GLY:O	1:A:807:GLU:CG	2.63	0.47
1:B:628:THR:HG1	1:B:630:THR:HB	1.79	0.47
1:A:143:SER:HG	1:A:145:HIS:CE1	2.23	0.47
1:A:343:ARG:NH1	1:B:395:HIS:O	2.46	0.47
1:A:345:GLY:HA3	1:A:376:PRO:HD3	1.97	0.47
1:A:781:ILE:O	1:A:781:ILE:HG22	2.15	0.47
1:A:722:LEU:HD13	1:A:798:LEU:HB2	1.97	0.46
1:B:403:TYR:HD2	1:B:405:PRO:HD2	1.80	0.46
1:B:659:THR:HB	1:B:662:VAL:HG23	1.96	0.46
1:A:318:ALA:HB2	1:B:402:VAL:HB	1.98	0.46
1:B:463:VAL:O	1:B:574:HIS:HB2	2.15	0.46
1:B:489:TYR:CE2	1:B:587:ALA:HB1	2.50	0.46
1:A:219:ASP:O	1:A:224:GLY:HA3	2.15	0.46
1:A:316:LYS:HB2	1:A:334:GLN:OE1	2.15	0.46
1:B:208:ARG:HD2	1:B:208:ARG:O	2.16	0.46
1:B:775:ARG:HH21	3:B:1808:KAP:C	2.28	0.46
1:A:35:ILE:HD11	1:A:296:LEU:CD2	2.46	0.46
1:A:95:SER:OG	1:A:151:GLU:OE1	2.32	0.46
1:A:411:GLU:OE2	1:B:317:LEU:HD21	2.16	0.46
1:A:806:GLY:O	1:A:807:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:O	1:A:308:LEU:HD11	2.15	0.46
1:A:444:ARG:HG3	1:A:666:PHE:CZ	2.50	0.46
1:A:444:ARG:HH21	1:B:493:LEU:HB3	1.81	0.46
1:A:766:MET:HB3	1:A:804:ARG:CD	2.45	0.46
1:A:55:LYS:HE3	1:A:57:ILE:O	2.16	0.46
1:B:183:LEU:HD23	1:B:183:LEU:C	2.40	0.46
1:B:220:GLY:O	1:B:250:HIS:HB2	2.16	0.46
1:B:629:THR:C	1:B:631:GLU:N	2.73	0.46
1:B:766:MET:HB3	1:B:804:ARG:CD	2.46	0.46
1:A:34:GLY:HA3	1:A:293:PHE:CE1	2.51	0.46
1:A:274:VAL:HG13	1:A:275:PRO:HD2	1.98	0.46
1:A:317:LEU:HG	1:B:407:LEU:HD11	1.97	0.46
1:A:651:VAL:HG22	1:A:652:PRO:HD2	1.98	0.46
1:B:744:LEU:HD12	1:B:744:LEU:C	2.41	0.46
1:A:62:PRO:HG3	1:A:102:LEU:CD2	2.45	0.46
1:B:369:TRP:CE2	3:B:1808:KAP:HS2	2.50	0.46
1:B:764:LEU:HD22	1:B:774:THR:HG23	1.98	0.46
1:B:766:MET:HB3	1:B:804:ARG:HD2	1.98	0.46
1:A:298:GLU:O	1:A:302:LEU:HB2	2.16	0.45
1:A:624:LEU:C	1:A:739:GLY:HA3	2.41	0.45
1:A:765:ILE:HG22	1:A:766:MET:N	2.30	0.45
1:B:773:PHE:CD1	1:B:773:PHE:C	2.93	0.45
1:A:205:ASP:OD1	1:A:238:ARG:NE	2.39	0.45
1:A:208:ARG:HH12	1:A:211:ARG:CD	2.16	0.45
1:A:794:CYS:O	1:A:797:LEU:HB2	2.16	0.45
1:A:446:PHE:CE1	1:A:450:HIS:ND1	2.84	0.45
1:A:708:THR:HG23	1:A:709:SER:H	1.79	0.45
1:A:31:VAL:HG21	1:A:217:VAL:HG22	1.97	0.45
1:B:17:TYR:HD2	1:B:214:GLY:HA2	1.80	0.45
1:B:766:MET:HE2	1:B:804:ARG:HD2	1.98	0.45
1:A:367:ALA:CB	1:A:372:GLN:HB2	2.46	0.45
1:A:473:TYR:C	1:A:473:TYR:CD1	2.95	0.45
1:A:722:LEU:O	1:A:725:GLN:HB2	2.17	0.45
1:A:782:TYR:CE2	1:A:784:MET:HE3	2.52	0.45
1:A:17:TYR:HD2	1:A:214:GLY:HA2	1.81	0.45
1:A:323:TRP:HB3	1:B:426:TYR:CD2	2.51	0.45
1:A:435:ILE:HD11	1:A:615:ASP:CG	2.42	0.45
1:A:495:GLN:HG2	1:B:440:LYS:HE2	1.99	0.45
1:B:10:LEU:HA	1:B:11:PRO:HD3	1.78	0.45
1:B:446:PHE:CE1	1:B:450:HIS:ND1	2.85	0.45
1:B:539:ASP:N	1:B:539:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:ASP:O	1:B:541:ILE:N	2.50	0.45
1:B:555:TYR:O	1:B:559:LEU:HG	2.17	0.45
1:A:614:PHE:O	1:A:640:ALA:HA	2.17	0.45
1:B:55:LYS:HE3	1:B:57:ILE:O	2.17	0.45
1:B:62:PRO:HG3	1:B:102:LEU:CD2	2.45	0.45
1:B:100:LYS:O	1:B:102:LEU:N	2.50	0.45
1:B:413:LEU:HD13	1:B:655:VAL:HG11	1.99	0.45
1:B:521:LEU:N	1:B:521:LEU:CD1	2.72	0.45
1:A:9:HIS:CE1	1:A:360:SER:HB3	2.52	0.45
1:B:274:VAL:HG13	1:B:275:PRO:HD2	1.99	0.45
1:A:426:TYR:HD2	1:B:323:TRP:HB3	1.81	0.44
1:A:466:VAL:HG12	1:A:502:GLY:HA3	1.99	0.44
1:B:517:TRP:HZ3	1:B:592:MET:HE1	1.82	0.44
1:B:521:LEU:H	1:B:521:LEU:CD1	2.20	0.44
1:A:438:ALA:HB1	1:A:613:ILE:HD13	1.99	0.44
3:A:1808:KAP:N	1:B:678:GLY:O	2.50	0.44
1:B:193:VAL:HG22	1:B:235:LEU:HD21	1.98	0.44
1:A:651:VAL:CG2	1:A:652:PRO:HD2	2.48	0.44
1:A:103:GLY:C	1:A:104:LEU:HG	2.42	0.44
1:B:297:LYS:HE2	1:B:297:LYS:HB3	1.60	0.44
1:A:348:PHE:HE1	1:B:396:VAL:HG12	1.83	0.44
1:A:414:LEU:HD12	1:B:321:VAL:HG13	1.98	0.44
1:A:420:GLY:O	1:A:421:TRP:HB3	2.18	0.44
1:B:71:PHE:CE2	1:B:87:ILE:HG13	2.53	0.44
1:B:446:PHE:HD1	1:B:446:PHE:O	2.01	0.44
1:B:764:LEU:HD11	1:B:776:PRO:HB3	1.99	0.44
1:B:794:CYS:O	1:B:797:LEU:HB2	2.17	0.44
1:B:168:LEU:HA	1:B:168:LEU:HD23	1.73	0.44
1:A:446:PHE:HD1	1:A:446:PHE:O	1.99	0.44
1:A:626:VAL:CG2	1:A:628:THR:O	2.65	0.44
1:B:261:TYR:CD1	1:B:261:TYR:C	2.96	0.44
1:B:707:ILE:HG22	1:B:712:LYS:HA	2.00	0.44
1:A:13:ASN:ND2	1:A:356:ASN:O	2.46	0.43
1:A:402:VAL:HB	1:B:318:ALA:HB2	1.99	0.43
1:B:20:TRP:CE3	1:B:189:THR:HG21	2.53	0.43
1:B:624:LEU:C	1:B:739:GLY:HA3	2.43	0.43
1:A:94:SER:HB3	1:A:116:LEU:HD11	2.00	0.43
1:A:633:LEU:C	1:A:635:CYS:H	2.25	0.43
1:B:8:PHE:C	1:B:8:PHE:HD1	2.23	0.43
1:B:370:TRP:CH2	3:B:1808:KAP:HE2	2.53	0.43
1:B:373:GLY:N	1:B:374:PRO:CD	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:VAL:HA	1:B:628:THR:CG2	2.49	0.43
1:B:559:LEU:HD13	1:B:601:LEU:HA	2.00	0.43
1:B:691:ALA:O	1:B:695:ILE:HG13	2.18	0.43
1:A:766:MET:HB3	1:A:804:ARG:HD2	2.00	0.43
1:B:666:PHE:CE2	1:B:675:LEU:HB2	2.53	0.43
1:B:766:MET:HB3	1:B:804:ARG:NE	2.32	0.43
1:A:446:PHE:CD1	1:A:450:HIS:ND1	2.87	0.43
1:A:686:MET:HB2	1:A:686:MET:HE2	1.63	0.43
1:A:773:PHE:CD1	1:A:773:PHE:C	2.97	0.43
1:B:486:PRO:HD3	1:B:498:TYR:OH	2.19	0.43
1:B:725:GLN:HB3	1:B:802:TYR:CZ	2.53	0.43
1:B:805:LEU:C	1:B:807:GLU:H	2.26	0.43
1:A:276:LYS:HA	1:A:276:LYS:HD3	1.68	0.43
1:A:719:ASP:OD2	1:A:722:LEU:HD12	2.17	0.43
1:B:12:LEU:HB3	1:B:308:LEU:HD21	2.00	0.43
1:B:444:ARG:HG3	1:B:666:PHE:CZ	2.53	0.43
1:A:638:ASP:C	1:A:639:ILE:HG13	2.43	0.43
1:B:435:ILE:HD11	1:B:615:ASP:CG	2.43	0.43
1:B:608:ARG:NH1	1:B:608:ARG:CG	2.81	0.43
1:B:786:GLY:C	1:B:788:CYS:H	2.27	0.43
1:A:221:ARG:HE	1:A:221:ARG:HB2	1.65	0.43
1:A:519:ILE:HG12	1:A:521:LEU:HD11	1.99	0.43
1:A:522:PRO:O	1:A:523:GLU:C	2.61	0.43
1:A:297:LYS:HB3	1:A:297:LYS:HE2	1.54	0.43
1:A:324:TRP:HB2	1:A:327:THR:OG1	2.18	0.43
1:A:608:ARG:HG3	1:A:608:ARG:NH1	2.30	0.43
1:A:664:ASP:C	1:A:666:PHE:H	2.27	0.43
1:A:764:LEU:HD13	1:A:776:PRO:HD3	2.00	0.43
1:B:378:PHE:CE1	1:B:382:LEU:HG	2.54	0.43
1:A:50:LYS:HE3	1:A:131:LEU:HD12	2.00	0.43
1:A:446:PHE:O	1:A:448:VAL:N	2.50	0.43
1:A:517:TRP:HZ3	1:A:592:MET:HE1	1.83	0.43
1:A:766:MET:CE	1:A:804:ARG:HD2	2.49	0.43
1:A:628:THR:HB	1:A:630:THR:H	1.83	0.43
1:B:550:THR:O	1:B:554:ILE:HG13	2.19	0.43
1:A:382:LEU:HD23	1:A:382:LEU:HA	1.92	0.42
1:A:782:TYR:CD2	1:A:784:MET:HE3	2.54	0.42
1:B:706:ASN:HB3	1:B:714:LEU:CD2	2.48	0.42
1:A:378:PHE:CE1	1:A:382:LEU:HG	2.55	0.42
1:A:403:TYR:HD2	1:A:405:PRO:HD2	1.84	0.42
1:A:784:MET:HE3	1:A:784:MET:HB2	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:SER:O	1:B:515:GLY:N	2.52	0.42
1:B:538:ARG:O	1:B:541:ILE:HG13	2.19	0.42
1:A:369:TRP:CH2	1:B:399:PRO:HG3	2.55	0.42
1:B:219:ASP:O	1:B:224:GLY:HA3	2.19	0.42
1:B:373:GLY:HA2	1:B:786:GLY:HA3	2.00	0.42
1:A:103:GLY:O	1:A:104:LEU:CG	2.61	0.42
1:B:486:PRO:HA	1:B:490:THR:OG1	2.19	0.42
1:A:594:ASP:OD1	1:A:594:ASP:C	2.62	0.42
1:A:659:THR:HB	1:A:662:VAL:HG23	2.01	0.42
1:B:143:SER:CB	1:B:145:HIS:ND1	2.80	0.42
1:B:697:TRP:CE2	1:B:703:THR:HB	2.55	0.42
1:A:697:TRP:CE2	1:A:703:THR:HB	2.55	0.42
1:A:770:ASP:CB	1:A:800:LYS:HD2	2.45	0.42
1:B:431:GLY:HA3	2:B:1644:PLP:O4P	2.20	0.42
1:B:625:GLY:HA2	1:B:714:LEU:CB	2.50	0.42
1:A:183:LEU:C	1:A:183:LEU:HD23	2.45	0.42
1:A:764:LEU:HD22	1:A:774:THR:HG23	2.02	0.42
1:B:700:ASP:HA	1:B:701:PRO:HD2	1.79	0.42
1:A:219:ASP:HB3	1:A:224:GLY:HA2	2.02	0.42
1:B:473:TYR:C	1:B:473:TYR:CD1	2.98	0.42
1:A:69:PHE:CD1	1:A:69:PHE:C	2.97	0.42
1:A:201:THR:O	1:A:202:LEU:C	2.63	0.42
1:A:237:LEU:HD11	1:B:237:LEU:HD11	2.02	0.42
1:A:707:ILE:HD13	1:A:707:ILE:HA	1.78	0.42
1:B:417:VAL:HA	1:B:628:THR:HG22	2.01	0.42
1:B:494:GLN:O	1:B:495:GLN:HB2	2.20	0.42
1:A:489:TYR:CE2	1:A:587:ALA:HB1	2.55	0.41
1:A:501:ARG:CD	1:B:497:TRP:CD2	3.03	0.41
1:A:786:GLY:C	1:A:788:CYS:H	2.28	0.41
1:B:435:ILE:HG13	1:B:474:HIS:HB3	2.02	0.41
1:A:140:ALA:CB	1:A:142:ILE:HD13	2.48	0.41
1:A:225:ILE:HB	3:A:1809:KAP:OI2	2.20	0.41
1:A:281:ASP:O	1:A:282:LEU:HB2	2.20	0.41
1:B:65:SER:CB	1:B:68:ARG:HH12	2.25	0.41
1:B:369:TRP:CD2	3:B:1808:KAP:HS2	2.56	0.41
1:B:446:PHE:CD1	1:B:450:HIS:ND1	2.88	0.41
1:B:643:ALA:O	1:B:645:LEU:N	2.52	0.41
1:A:435:ILE:HG13	1:A:474:HIS:HB3	2.03	0.41
1:A:594:ASP:OD1	1:A:596:LEU:HB3	2.20	0.41
1:A:627:GLU:OE2	1:A:699:LYS:HE2	2.19	0.41
1:B:219:ASP:HB3	1:B:224:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:ASP:C	1:B:666:PHE:H	2.28	0.41
1:A:321:VAL:O	1:A:321:VAL:HG12	2.19	0.41
1:A:670:SER:C	1:A:672:LEU:N	2.77	0.41
1:A:316:LYS:O	1:A:320:GLU:HG3	2.20	0.41
1:A:484:GLN:NE2	1:A:489:TYR:HB2	2.34	0.41
1:A:538:ARG:HH22	1:A:716:GLU:CD	2.28	0.41
1:B:92:LEU:HD12	1:B:135:LEU:CD2	2.51	0.41
1:A:208:ARG:HH11	1:A:211:ARG:HG3	1.84	0.41
1:A:734:ARG:HE	1:A:745:GLU:CD	2.28	0.41
1:B:69:PHE:CD1	1:B:69:PHE:C	2.99	0.41
1:B:256:VAL:HB	1:B:257:PRO:HD3	2.03	0.41
1:B:264:ASN:OD1	1:B:264:ASN:O	2.38	0.41
1:B:431:GLY:O	1:B:434:ALA:HB3	2.20	0.41
1:A:96:LEU:N	1:A:97:PRO:CD	2.84	0.41
1:A:425:VAL:HG13	1:A:655:VAL:HG22	2.02	0.41
1:A:426:TYR:HD2	1:B:323:TRP:CG	2.39	0.41
1:A:501:ARG:CD	1:B:497:TRP:CE2	3.03	0.41
1:A:642:PHE:HB2	1:A:655:VAL:HG12	2.03	0.41
1:A:676:LEU:HG	1:B:494:GLN:NE2	2.34	0.41
1:B:56:PRO:O	1:B:57:ILE:HD13	2.21	0.41
1:A:481:MET:HE1	1:A:494:GLN:HB3	2.02	0.41
1:A:719:ASP:CB	1:A:722:LEU:HD12	2.49	0.41
1:B:594:ASP:HA	1:B:595:PRO:HD2	1.95	0.41
1:B:722:LEU:HD23	1:B:722:LEU:HA	1.73	0.41
1:A:28:LYS:NZ	4:A:1810:TLA:H2	2.32	0.41
1:A:446:PHE:HD2	1:A:576:GLY:CA	2.23	0.41
1:B:36:ALA:HA	1:B:51:LEU:CD1	2.42	0.41
1:B:73:LYS:HA	1:B:73:LYS:HD3	1.68	0.41
1:B:246:VAL:HA	1:B:269:LEU:O	2.21	0.41
1:B:333:HIS:HB3	1:B:335[A]:GLU:OE2	2.21	0.41
1:B:490:THR:HB	1:B:498:TYR:CE2	2.56	0.41
1:B:624:LEU:HD22	1:B:738:ILE:HG23	2.03	0.41
1:B:764:LEU:HD13	1:B:776:PRO:HD3	2.03	0.41
1:B:782:TYR:CE2	1:B:784:MET:HE3	2.55	0.41
1:A:395:HIS:HB3	1:B:649:GLY:O	2.21	0.41
1:A:608:ARG:CG	1:A:608:ARG:NH1	2.83	0.41
1:B:205:ASP:OD1	1:B:238:ARG:NE	2.43	0.41
1:B:396:VAL:HG23	1:B:403:TYR:CE1	2.56	0.41
1:B:584:ILE:HD13	1:B:592:MET:HA	2.02	0.41
1:A:34:GLY:HA3	1:A:293:PHE:CZ	2.55	0.40
1:A:56:PRO:O	1:A:57:ILE:HD13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:TRP:H	1:A:329:HIS:CE1	2.39	0.40
1:B:276:LYS:HD3	1:B:276:LYS:HA	1.81	0.40
1:B:582:PRO:O	1:B:584:ILE:N	2.47	0.40
1:A:168:LEU:HD23	1:A:168:LEU:HA	1.86	0.40
1:A:246:VAL:HA	1:A:269:LEU:O	2.21	0.40
1:A:348:PHE:CE1	1:B:396:VAL:HG12	2.56	0.40
1:A:712:LYS:HE3	1:A:712:LYS:HB2	1.95	0.40
1:A:559:LEU:HD12	1:A:600:VAL:HG12	2.02	0.40
1:A:714:LEU:HD12	1:A:714:LEU:HA	1.92	0.40
1:B:146:LEU:HA	1:B:146:LEU:HD23	1.83	0.40
1:B:382:LEU:HD13	1:B:650:MET:HG3	2.04	0.40
1:B:484:GLN:NE2	1:B:489:TYR:HB2	2.32	0.40
1:B:614:PHE:CD2	1:B:637:PRO:HG3	2.56	0.40
1:A:74:LEU:HD13	1:A:130:LEU:CD2	2.48	0.40
1:A:236:LYS:HD2	1:A:236:LYS:HA	1.86	0.40
1:A:783:LEU:HD11	1:A:801:LEU:HD22	2.04	0.40
1:B:281:ASP:O	1:B:282:LEU:HB2	2.22	0.40
1:A:13:ASN:HD22	1:A:356:ASN:HB3	1.86	0.40
1:B:427:PHE:CD2	1:B:683:ALA:HB2	2.57	0.40
1:B:482:GLU:O	1:B:500:GLY:HA2	2.21	0.40

All (1) 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:B:149:GLU:OE2	1:B:711:GLY:N[2_555]	2.14	0.06

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	735/831 (88%)	659 (90%)	62 (8%)	14 (2%)	6 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	723/831 (87%)	643 (89%)	59 (8%)	21 (3%)	3	13
All	All	1458/1662 (88%)	1302 (89%)	121 (8%)	35 (2%)	4	17

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	ASN
1	B	514	ASN
1	B	563	LEU
1	A	101	SER
1	A	103	GLY
1	A	141	ALA
1	A	421	TRP
1	A	451	ASN
1	A	644	LYS
1	B	101	SER
1	B	118	PHE
1	B	355	ASP
1	B	357	SER
1	B	421	TRP
1	B	447	CYS
1	B	451	ASN
1	A	355	ASP
1	A	373	GLY
1	A	643	ALA
1	A	778	GLY
1	B	373	GLY
1	B	644	LYS
1	A	447	CYS
1	B	354	SER
1	B	495	GLN
1	B	540	GLU
1	B	643	ALA
1	B	778	GLY
1	B	730	SER
1	A	806	GLY
1	B	486	PRO
1	B	500	GLY
1	B	637	PRO
1	A	637	PRO
1	B	583	VAL

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	615/704 (87%)	562 (91%)	53 (9%)	10	31
1	B	598/704 (85%)	551 (92%)	47 (8%)	11	35
All	All	1213/1408 (86%)	1113 (92%)	100 (8%)	11	33

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	13	ASN
1	A	24	THR
1	A	42	GLN
1	A	68	ARG
1	A	72	SER
1	A	74	LEU
1	A	80	ARG
1	A	85	ILE
1	A	107	GLU
1	A	131	LEU
1	A	142	ILE
1	A	158	SER
1	A	193	VAL
1	A	206	LEU
1	A	208	ARG
1	A	252[A]	LEU
1	A	252[B]	LEU
1	A	253	VAL
1	A	263	ARG
1	A	279	SER
1	A	287	VAL
1	A	302	LEU
1	A	343	ARG
1	A	350	ILE
1	A	370	TRP
1	A	417	VAL

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Mol	Chain	Res	Type
1	A	448	VAL
1	A	451	ASN
1	A	463	VAL
1	A	477	THR
1	A	503	LEU
1	A	521	LEU
1	A	524	SER
1	A	540	GLU
1	A	543	ASP
1	A	560	SER
1	A	628	THR
1	A	630	THR
1	A	655	VAL
1	A	680	SER
1	A	686	MET
1	A	708	THR
1	A	709	SER
1	A	713	THR
1	A	714	LEU
1	A	721	GLU
1	A	735	VAL
1	A	738	ILE
1	A	744	LEU
1	A	765	ILE
1	A	775	ARG
1	A	781	ILE
1	B	8	PHE
1	B	9	HIS
1	B	13	ASN
1	B	24	THR
1	B	63	SER
1	B	68	ARG
1	B	74	LEU
1	B	80	ARG
1	B	131	LEU
1	B	142	ILE
1	B	158	SER
1	B	193	VAL
1	B	206	LEU
1	B	208	ARG
1	B	253	VAL
1	B	263	ARG

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Mol	Chain	Res	Type
1	B	279	SER
1	B	302	LEU
1	B	335[A]	GLU
1	B	335[B]	GLU
1	B	343	ARG
1	B	350	ILE
1	B	370	TRP
1	B	417	VAL
1	B	448	VAL
1	B	451	ASN
1	B	463	VAL
1	B	477	THR
1	B	499	THR
1	B	501	ARG
1	B	503	LEU
1	B	521	LEU
1	B	536	THR
1	B	560	SER
1	B	628	THR
1	B	630	THR
1	B	655	VAL
1	B	680	SER
1	B	686	MET
1	B	709	SER
1	B	714	LEU
1	B	730	SER
1	B	735	VAL
1	B	738	ILE
1	B	765	ILE
1	B	775	ARG
1	B	781	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	312	ASN
1	A	329	HIS
1	A	334	GLN
1	A	395	HIS
1	A	484	GLN
1	A	495	GLN

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Mol	Chain	Res	Type
1	A	514	ASN
1	A	518	ASN
1	A	591	HIS
1	A	733	GLN
1	B	13	ASN
1	B	14	HIS
1	B	162	GLN
1	B	312	ASN
1	B	334	GLN
1	B	484	GLN
1	B	518	ASN
1	B	591	HIS
1	B	725	GLN
1	B	733	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	A	1644	1	15,15,16	1.85	2 (13%)	21,22,23	2.01	1 (4%)
4	TLA	B	1810	-	9,9,9	1.63	1 (11%)	12,12,12	2.67	7 (58%)
4	TLA	A	1810	-	9,9,9	1.63	2 (22%)	12,12,12	2.23	8 (66%)
3	KAP	B	1808	-	11,12,12	0.79	0	11,14,14	1.20	2 (18%)
3	KAP	A	1808	-	11,12,12	0.80	0	11,14,14	1.15	0
3	KAP	B	1809	-	11,12,12	0.88	0	11,14,14	2.31	5 (45%)
3	KAP	A	1809	-	11,12,12	1.20	1 (9%)	11,14,14	2.41	3 (27%)
2	PLP	B	1644	1	15,15,16	1.75	2 (13%)	21,22,23	2.16	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	1644	1	-	0/6/6/8	0/1/1/1
4	TLA	B	1810	-	-	3/12/12/12	-
4	TLA	A	1810	-	-	4/12/12/12	-
3	KAP	B	1808	-	-	8/10/12/12	-
3	KAP	A	1808	-	-	4/10/12/12	-
3	KAP	B	1809	-	-	4/10/12/12	-
3	KAP	A	1809	-	-	5/10/12/12	-
2	PLP	B	1644	1	-	0/6/6/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1644	PLP	O3-C3	-5.70	1.23	1.36
2	B	1644	PLP	O3-C3	-5.10	1.25	1.36
3	A	1809	KAP	CE-CZ	3.08	1.55	1.51
4	B	1810	TLA	C3-C2	-2.92	1.44	1.53
2	B	1644	PLP	C2-N1	2.84	1.38	1.33
4	A	1810	TLA	O3-C3	-2.66	1.37	1.42
2	A	1644	PLP	C2-N1	2.35	1.38	1.33
4	A	1810	TLA	O41-C4	-2.10	1.24	1.30

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1644	PLP	O4P-C5A-C5	8.07	124.48	109.36
2	A	1644	PLP	O4P-C5A-C5	7.77	123.92	109.36
3	A	1809	KAP	CD-CE-CZ	5.83	125.22	114.50
3	B	1809	KAP	CS-CH-CZ	5.62	117.79	109.67
4	B	1810	TLA	C3-C2-C1	-5.26	98.17	109.82
3	A	1809	KAP	CS-CH-CZ	3.51	114.74	109.67
4	B	1810	TLA	O1-C1-C2	-3.41	112.53	121.62
4	A	1810	TLA	C3-C2-C1	-3.10	102.95	109.82
4	B	1810	TLA	O2-C2-C1	3.04	117.20	110.69
4	A	1810	TLA	O4-C4-C3	-3.01	113.61	121.62
4	A	1810	TLA	C2-C3-C4	-2.95	103.28	109.82
4	B	1810	TLA	O11-C1-C2	2.95	121.51	113.31
4	A	1810	TLA	O41-C4-C3	2.80	121.09	113.31
4	A	1810	TLA	O1-C1-C2	-2.66	114.53	121.62
4	B	1810	TLA	O3-C3-C2	-2.44	105.19	110.17
4	A	1810	TLA	O11-C1-C2	2.41	120.02	113.31
3	B	1809	KAP	O-CZ-CE	-2.41	117.60	121.68
4	B	1810	TLA	C2-C3-C4	-2.40	104.49	109.82
3	B	1809	KAP	O11-C-CA	2.36	121.47	114.00
3	B	1809	KAP	O11-C-O12	-2.36	117.27	123.33
4	B	1810	TLA	O4-C4-C3	-2.26	115.58	121.62
4	A	1810	TLA	O3-C3-C4	2.14	115.27	110.69
3	B	1809	KAP	CG-CB-CA	2.12	120.92	113.13
2	B	1644	PLP	O4P-P-O1P	-2.12	100.72	106.44
2	B	1644	PLP	C6-C5-C4	2.10	119.82	118.10
4	A	1810	TLA	O2-C2-C1	2.08	115.14	110.69
3	B	1808	KAP	CB-CA-C	2.07	119.92	114.51
3	A	1809	KAP	O-CZ-CE	2.06	125.17	121.68
3	B	1808	KAP	O11-C-CA	2.04	120.43	114.00

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1810	TLA	C1-C2-C3-O3
3	B	1809	KAP	C-CA-CB-CG
4	A	1810	TLA	O2-C2-C3-C4
3	B	1808	KAP	CG-CD-CE-CZ
4	A	1810	TLA	O2-C2-C3-O3
3	B	1809	KAP	CA-CB-CG-CD
3	B	1808	KAP	CD-CE-CZ-O
4	A	1810	TLA	C1-C2-C3-C4
4	B	1810	TLA	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	1808	KAP	CE-CD-CG-CB
3	B	1808	KAP	CD-CE-CZ-CH
4	B	1810	TLA	O11-C1-C2-C3
3	A	1809	KAP	CE-CD-CG-CB
3	A	1808	KAP	CS-CH-CZ-O
3	B	1808	KAP	CS-CH-CZ-O
3	A	1808	KAP	CS-CH-CZ-CE
3	B	1808	KAP	CS-CH-CZ-CE
3	A	1808	KAP	OI2-C-CA-CB
3	A	1808	KAP	OI1-C-CA-CB
3	B	1808	KAP	OI1-C-CA-CB
3	B	1808	KAP	OI2-C-CA-CB
3	B	1809	KAP	OI1-C-CA-CB
4	B	1810	TLA	O1-C1-C2-O2
3	B	1809	KAP	OI2-C-CA-CB
3	A	1809	KAP	CG-CD-CE-CZ
3	A	1809	KAP	OI2-C-CA-CB
3	A	1809	KAP	CA-CB-CG-CD
3	A	1809	KAP	OI1-C-CA-CB

There are no ring outliers.

8 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1644	PLP	3	0
4	B	1810	TLA	4	0
4	A	1810	TLA	5	0
3	B	1808	KAP	6	0
3	A	1808	KAP	3	0
3	B	1809	KAP	1	0
3	A	1809	KAP	2	0
2	B	1644	PLP	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	748/831 (90%)	-0.30	5 (0%)	84 77	35, 62, 96, 134	1 (0%)
1	B	738/831 (88%)	-0.31	2 (0%)	90 86	35, 64, 99, 127	1 (0%)
All	All	1486/1662 (89%)	-0.30	7 (0%)	87 82	35, 63, 98, 134	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	373	GLY	3.7
1	A	47	SER	2.9
1	B	103	GLY	2.8
1	A	576	GLY	2.5
1	A	125	THR	2.3
1	A	7	PRO	2.3
1	A	373	GLY	2.2

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($\text{\AA}^2$)	Q<0.9
3	KAP	A	1808	13/13	0.90	0.11	40,56,81,85	0
3	KAP	A	1809	13/13	0.90	0.13	30,52,71,84	0
3	KAP	B	1808	13/13	0.91	0.12	46,61,84,92	0
4	TLA	B	1810	10/10	0.91	0.09	28,55,72,85	10
4	TLA	A	1810	10/10	0.92	0.08	49,57,76,92	0
3	KAP	B	1809	13/13	0.93	0.10	28,46,73,78	0
2	PLP	A	1644	15/16	0.94	0.08	32,52,71,74	0
2	PLP	B	1644	15/16	0.95	0.07	41,49,72,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.