



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:31 am GMT

PDB ID : 4A0F
Title : Structure of selenomethionine substituted bifunctional DAPA aminotransferase-dethiobiotin synthetase from *Arabidopsis thaliana* in its apo form.
Authors : Cobessi, D.; Dumas, R.; Pautre, V.; Meinguet, C.; Ferrer, J.L.; Alban, C.
Deposited on : 2011-09-09
Resolution : 2.71 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

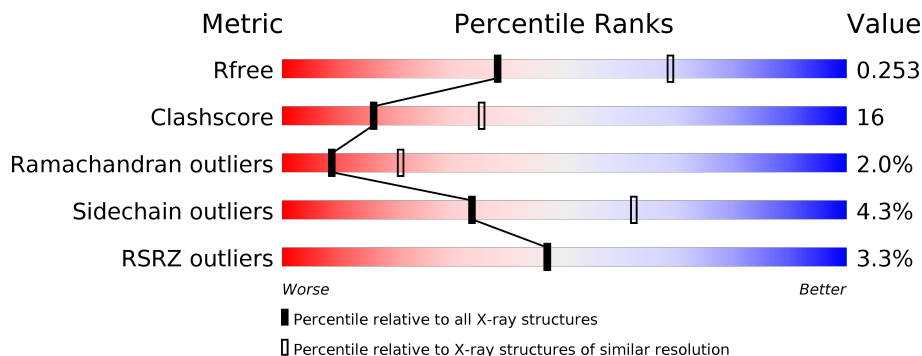
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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}	100719	2649 (2.74-2.70)
Clashscore	112137	2993 (2.74-2.70)
Ramachandran outliers	110173	2946 (2.74-2.70)
Sidechain outliers	110143	2947 (2.74-2.70)
RSRZ outliers	101464	2665 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>23%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	831	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>28%</div> <div>•</div> <div>10%</div> </div> </div>

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
3	SO4	A	1809	-	-	-	X
3	SO4	A	1810	-	-	-	X
3	SO4	B	1810	-	-	X	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11317 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	746	Total	C	N	O	S	Se	0	1	0
			5568	3562	937	1037	16	16			
1	B	750	Total	C	N	O	S	Se	0	0	0
			5619	3598	944	1046	16	15			

There are 42 discrepancies between the modelled and reference sequences:

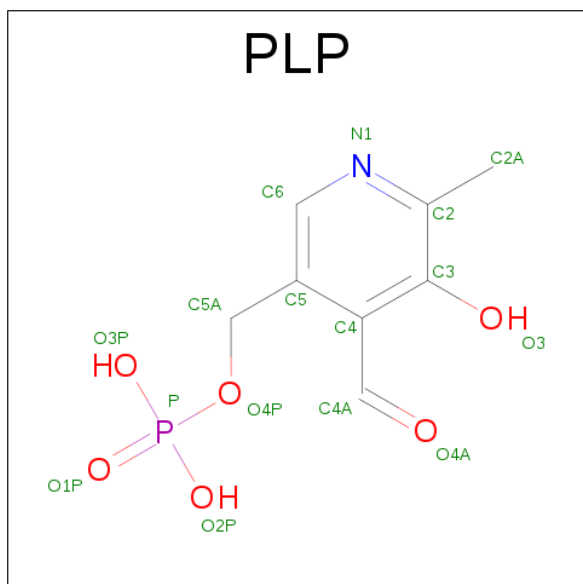
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	GLY	-	EXPRESSION TAG	UNP B0F481
A	-18	SER	-	EXPRESSION TAG	UNP B0F481
A	-17	SER	-	EXPRESSION TAG	UNP B0F481
A	-16	HIS	-	EXPRESSION TAG	UNP B0F481
A	-15	HIS	-	EXPRESSION TAG	UNP B0F481
A	-14	HIS	-	EXPRESSION TAG	UNP B0F481
A	-13	HIS	-	EXPRESSION TAG	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	MSE	-	EXPRESSION TAG	UNP B0F481
A	326	TYR	PHE	ENGINEERED MUTATION	UNP B0F481
B	-19	GLY	-	EXPRESSION TAG	UNP B0F481
B	-18	SER	-	EXPRESSION TAG	UNP B0F481
B	-17	SER	-	EXPRESSION TAG	UNP B0F481

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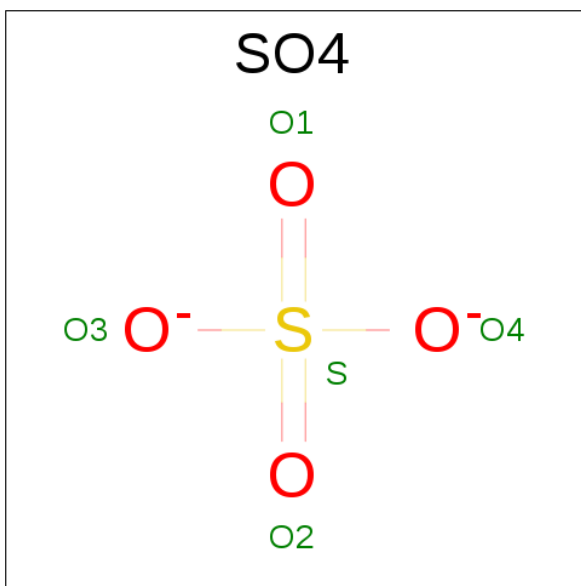
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	EXPRESSION TAG	UNP B0F481
B	-15	HIS	-	EXPRESSION TAG	UNP B0F481
B	-14	HIS	-	EXPRESSION TAG	UNP B0F481
B	-13	HIS	-	EXPRESSION TAG	UNP B0F481
B	-12	HIS	-	EXPRESSION TAG	UNP B0F481
B	-11	HIS	-	EXPRESSION TAG	UNP B0F481
B	-10	SER	-	EXPRESSION TAG	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	MSE	-	EXPRESSION TAG	UNP B0F481
B	326	TYR	PHE	ENGINEERED MUTATION	UNP B0F481

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



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		
4	B	30	Total	O	0	0
			30	30		

Tyr	L645	L562	V464	G373	L262	E138	T49
Ala	M650	GLN	K465	P374	V266	E139	K50
S757	V651	GLU	V466	L382			L51
Y759	P652	HIS	I467	A383	L269	I142	
		SER	R470	K384			Q58
L763	T659	GLY	H474	E385	D277	H145	T59
L764	D660	VAL		K386	P278	L146	G60
L765	A661	ARG		G387	S279	R150	F61
H766	V662	GLN	L478	Y388	D280		P62
		SER	G479	Y388	D281	L168	S67
E769	F666	A573	A480	K392	L282		
	S667	H574	M481	K395	V287	M172	F71
T774	G668	V575	E482	Y396	GLY	CYS	S72
	D669	G576		K397	GLY	L74	K73
W779	S670	A577	A485	F398	F293		L79
	K671	L578	P486	S487	L296	VAL	
L783	L672	I580	P488	P399	K297	LYS	R80
						SER	
S790	L675	V583	G491	V402	M300	GLU	R81
		I584		V403	V301	LYS	
L797	S880				L302	SER	I85
L798	Y681	M590	W497	E411		D182	S86
					A315	L183	I87
L801	A685	H591	R501	L414	K316	L184	S88
	M686	M592			L317	C185	N89
R804	G687	V593	P508	V417	L186		S90
L805	C688	D594	T509		V187		V91
		P595	V510	S428	V321	L92	
		L596		D429		P196	
E807	T708	F597	S513	N430	P325	H93	S94
F808	S709	Q598	N514		Y326	L206	S95
ASN	Q710	R599	G515	T433	T327	Y207	L96
ARG		V600				R208	P97
THR	L714	L601	I519	T437	K330	P209	
		V602	S520	A438	H333	F210	S101
	L717					R211	
	W718						L104
	D719	I610	F525	N441	T336	G218	ASN
		P611	SER	A442	V337	D219	VAL
	V723	V612	GLU	F443		G220	GLU
	Q724	I613	ILE	R444		R221	VAL
		F614	ALA	K445	I340	L222	SER
	H729	D615	PRO	F446	F348	G223	E110
S730	S730	E616	GLU	C447	S349	G224	
A731	A731	V617	TYR	V448		I225	
			GLY	D449	K352		M113
	V737	W622	T534	H450	I229		C114
	I738	R623	F535	N451	D355		
		L624	T536	F452	N356	E233	R119
	L741		S537	CYS	S357		
			R538	GLU		A127	
	L746	T628		ALA	K236	P128	
	LYS	T629		THR	L237	E129	
	ALA			GLU	L130		
ASP	ASP	K636		GLU	D241		
ALA	ALA		S556	GLU	A367		
SER	SER	I639		LYS	S368		
ASN	ASN		L559	HIS	W369		
SER	SER	A643	S560		P257		
GLY	GLY	K644	K561	T462	Q372		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	233.67Å 75.97Å 88.63Å 90.00° 109.20° 90.00°	Depositor
Resolution (Å)	41.85 – 2.71 41.85 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.1 (41.85-2.71) 99.2 (41.85-2.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.73Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.200 , 0.261 0.189 , 0.253	Depositor DCC
R_{free} test set	1989 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11317	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 3.71% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PLP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/5681	0.60	1/7722 (0.0%)
1	B	0.45	0/5731	0.60	0/7787
All	All	0.45	0/11412	0.60	1/15509 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	PRO	N-CA-CB	6.07	110.59	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5568	0	5367	172	0
1	B	5619	0	5425	206	0
2	A	15	0	6	2	0
2	B	15	0	6	2	0
3	A	10	0	0	1	0
3	B	10	0	0	3	0
4	A	50	0	0	1	0
4	B	30	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11317	0	10804	355	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 16.

All (355) 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:21:SER:HB2	1:A:28:LYS:HD3	1.41	1.01
1:B:21:SER:HB2	1:B:28:LYS:HD3	1.41	1.00
1:A:510:VAL:HB	1:A:592:MSE:HE2	1.48	0.96
1:B:510:VAL:HB	1:B:592:MSE:HE2	1.51	0.91
1:B:766:MSE:HE2	1:B:804:ARG:HD2	1.57	0.86
1:A:766:MSE:HE2	1:A:804:ARG:HD2	1.58	0.84
1:A:397:MSE:HE3	1:A:397:MSE:HA	1.57	0.84
1:A:94:SER:N	1:A:113:MSE:HE1	1.92	0.84
1:A:628:THR:HG22	1:A:630:THR:H	1.43	0.83
1:B:628:THR:HG22	1:B:630:THR:H	1.43	0.82
1:B:113:MSE:HE2	1:B:136:TYR:HD1	1.43	0.81
1:A:93:HIS:HB3	1:A:113:MSE:CE	2.11	0.80
1:B:36:ALA:HA	1:B:51:LEU:HD13	1.64	0.79
1:B:397:MSE:HE3	1:B:397:MSE:HA	1.63	0.79
1:A:428:SER:HB2	1:A:433:THR:OG1	1.83	0.78
1:B:708:THR:HG22	1:B:709:SER:N	1.98	0.77
1:A:113:MSE:HE3	1:A:114:CYS:H	1.50	0.77
1:A:61:PHE:O	1:A:139:GLU:HA	1.84	0.76
1:B:428:SER:HB2	1:B:433:THR:OG1	1.85	0.75
1:B:437:ILE:O	1:B:441:MSE:HG3	1.87	0.75
1:A:36:ALA:HA	1:A:51:LEU:HD13	1.67	0.75
1:A:67:SER:HB3	1:A:89:ASN:OD1	1.85	0.75
1:A:538:ARG:NH2	1:A:716:GLU:OE2	2.16	0.74
1:B:237:LEU:HD21	1:B:384:ARG:HG2	1.68	0.73
1:A:590:MSE:HE2	1:A:741:LEU:HD21	1.69	0.73
1:B:590:MSE:HE2	1:B:741:LEU:HD21	1.69	0.73
1:A:237:LEU:HD21	1:A:384:ARG:HG2	1.70	0.72
1:A:515:GLY:HA2	1:A:724:GLN:OE1	1.90	0.71
1:A:321:VAL:HG22	1:B:414:LEU:HD12	1.72	0.70
1:A:221:ARG:O	1:A:222:LEU:HB2	1.91	0.70
1:A:93:HIS:HB3	1:A:113:MSE:HE2	1.73	0.69
1:B:67:SER:HB3	1:B:89:ASN:OD1	1.91	0.69
1:B:659:THR:HG22	1:B:662:VAL:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ILE:O	1:A:441:MSE:HG3	1.93	0.69
1:B:708:THR:CG2	1:B:709:SER:N	2.57	0.68
1:A:28:LYS:HE2	3:A:1809:SO4:O2	1.94	0.67
1:B:142:ILE:HD12	1:B:146:LEU:HB3	1.78	0.66
1:B:221:ARG:O	1:B:222:LEU:HB2	1.94	0.66
1:B:757:SER:O	1:B:759:TYR:N	2.28	0.66
1:B:42:GLN:HA	1:B:42:GLN:HE21	1.61	0.66
1:B:590:MSE:HE2	1:B:741:LEU:CD2	2.26	0.66
1:A:386:MSE:CE	1:A:686:MSE:HE1	2.24	0.66
1:A:103:GLY:O	1:A:104:LEU:C	2.34	0.65
1:B:333:HIS:O	1:B:336:THR:HG22	1.96	0.65
1:B:519:ILE:HD11	1:B:535:PHE:HZ	1.61	0.65
1:B:386:MSE:CE	1:B:686:MSE:HE1	2.26	0.65
1:A:659:THR:HG22	1:A:662:VAL:H	1.62	0.65
1:B:590:MSE:HA	1:B:590:MSE:HE3	1.79	0.65
1:A:590:MSE:HE2	1:A:741:LEU:CD2	2.27	0.65
1:A:686:MSE:C	1:A:686:MSE:HE3	2.18	0.64
1:A:590:MSE:HE3	1:A:590:MSE:HA	1.78	0.64
1:B:536:THR:HG23	1:B:537:SER:H	1.62	0.64
1:B:441:MSE:HE3	1:B:639:ILE:HG12	1.78	0.64
1:B:519:ILE:HD11	1:B:535:PHE:CZ	2.32	0.64
1:B:296:LEU:O	1:B:300:MSE:HG2	1.98	0.63
1:A:184:LEU:HD12	1:A:185:CYS:H	1.64	0.63
1:A:94:SER:H	1:A:113:MSE:HE1	1.61	0.63
1:A:386:MSE:HE2	1:A:686:MSE:HE1	1.80	0.63
1:A:369:TRP:HB2	1:B:397:MSE:HE1	1.80	0.63
1:B:764:LEU:HD22	1:B:774:THR:HG23	1.81	0.62
1:B:397:MSE:CE	1:B:397:MSE:HA	2.29	0.62
1:B:686:MSE:C	1:B:686:MSE:HE3	2.20	0.62
1:A:81:ARG:HH21	1:A:287:VAL:HG13	1.65	0.62
1:B:81:ARG:HH21	1:B:287:VAL:HG13	1.63	0.62
1:A:113:MSE:CE	1:A:114:CYS:H	2.13	0.62
1:A:699:LYS:NZ	4:A:2039:HOH:O	2.33	0.62
1:A:296:LEU:O	1:A:300:MSE:HG2	2.00	0.61
1:B:281:ASP:O	1:B:282:LEU:HB2	1.99	0.61
1:B:388:TYR:OH	1:B:392:ARG:NH1	2.33	0.61
1:A:397:MSE:HE2	1:A:399:PRO:HD2	1.82	0.61
1:A:397:MSE:CE	1:A:397:MSE:HA	2.29	0.61
1:B:397:MSE:HE2	1:B:399:PRO:HD2	1.82	0.61
1:A:510:VAL:HB	1:A:592:MSE:CE	2.27	0.61
1:B:225:ILE:HD13	1:B:257:PRO:HG2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:LEU:HD12	1:B:185:CYS:H	1.66	0.60
1:A:50:LYS:HG2	1:A:129:GLU:HB3	1.82	0.60
1:B:474:HIS:O	1:B:480:ALA:HB1	2.02	0.60
1:A:497:TRP:CD2	1:B:501:ARG:HD2	2.36	0.60
1:B:441:MSE:CE	1:B:639:ILE:HG23	2.32	0.60
1:B:386:MSE:HE2	1:B:686:MSE:HE1	1.83	0.60
1:A:356:ASN:O	1:A:357:SER:O	2.20	0.59
1:B:31:VAL:O	1:B:35:ILE:HG12	2.03	0.59
1:B:50:LYS:HG2	1:B:129:GLU:HB3	1.84	0.59
1:A:31:VAL:O	1:A:35:ILE:HG12	2.02	0.59
1:B:584:ILE:HG21	1:B:590:MSE:HE1	1.83	0.58
1:A:396:VAL:HG13	1:B:340:ILE:HD12	1.85	0.58
1:B:42:GLN:HA	1:B:42:GLN:NE2	2.18	0.58
1:B:575:VAL:HG12	1:B:610:ILE:HD13	1.86	0.57
1:B:515:GLY:HA2	1:B:724:GLN:OE1	2.04	0.57
1:B:622:TRP:HE3	1:B:714:LEU:HD13	1.68	0.57
1:A:93:HIS:HB3	1:A:113:MSE:HE1	1.85	0.57
1:B:74:LEU:HD12	1:B:130:LEU:HD22	1.85	0.57
1:A:547:ASP:CG	1:A:599:ARG:HH11	2.07	0.57
1:A:74:LEU:HD12	1:A:130:LEU:HD22	1.87	0.57
1:A:764:LEU:HD22	1:A:774:THR:HG23	1.87	0.57
1:A:584:ILE:HG21	1:A:590:MSE:HE1	1.86	0.57
1:B:93:HIS:HB3	1:B:113:MSE:HE3	1.87	0.57
1:A:269:LEU:HD12	1:A:296:LEU:HD13	1.87	0.56
1:B:719:ASP:O	1:B:723:VAL:HG23	2.05	0.56
1:A:113:MSE:HE3	1:A:114:CYS:N	2.19	0.56
1:A:325:PRO:O	1:A:327:THR:HG23	2.06	0.56
1:B:142:ILE:HD12	1:B:146:LEU:CB	2.35	0.56
1:A:143:SER:OG	1:A:145:HIS:ND1	2.35	0.55
1:A:652:PRO:HG3	1:B:681:TYR:CB	2.36	0.55
1:B:74:LEU:CD1	1:B:130:LEU:HD22	2.36	0.55
1:B:60:GLY:HA2	1:B:139:GLU:O	2.06	0.55
1:B:547:ASP:CG	1:B:599:ARG:HH11	2.10	0.55
1:B:325:PRO:O	1:B:327:THR:HG23	2.06	0.55
1:B:6:SER:HB3	1:B:7:PRO:HD2	1.89	0.55
1:B:91:VAL:HG22	1:B:134:THR:HB	1.89	0.55
1:A:225:ILE:HD13	1:A:257:PRO:HG2	1.88	0.55
1:A:474:HIS:O	1:A:480:ALA:HB1	2.07	0.54
1:A:651:VAL:HG22	1:A:652:PRO:HD2	1.89	0.54
1:B:510:VAL:HB	1:B:592:MSE:CE	2.31	0.54
1:B:27:GLY:CA	3:B:1810:SO4:O4	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:PHE:CE1	1:B:450:HIS:HD2	2.25	0.54
1:B:61:PHE:CD1	1:B:62:PRO:HA	2.43	0.54
1:B:446:PHE:CE1	1:B:450:HIS:CD2	2.95	0.54
1:B:487:SER:HB2	1:B:488:PRO:HD2	1.89	0.54
1:B:222:LEU:C	1:B:224:GLY:H	2.11	0.54
1:B:644:LYS:NZ	2:B:1644:PLP:O3	2.39	0.54
1:B:487:SER:HB2	1:B:488:PRO:CD	2.38	0.54
1:A:547:ASP:OD2	1:A:599:ARG:NH1	2.41	0.54
1:A:74:LEU:CD1	1:A:130:LEU:HD22	2.37	0.54
1:A:91:VAL:HG22	1:A:134:THR:HB	1.90	0.54
1:A:443:PHE:CD1	1:A:464:VAL:HG11	2.43	0.54
1:A:681:TYR:CB	1:B:652:PRO:HG3	2.36	0.53
1:A:446:PHE:CE1	1:A:450:HIS:CD2	2.96	0.53
1:B:710:GLN:OE1	1:B:710:GLN:HA	2.08	0.53
1:A:317:LEU:HD21	1:B:411:GLU:OE2	2.08	0.53
1:A:388:TYR:OH	1:A:392:ARG:NH1	2.39	0.53
1:A:407:LEU:HD21	1:B:317:LEU:HD23	1.90	0.53
1:A:222:LEU:C	1:A:224:GLY:H	2.11	0.53
1:A:27:GLY:O	1:A:30:LEU:N	2.42	0.53
1:A:708:THR:N	1:A:713:THR:O	2.34	0.53
1:A:584:ILE:HG21	1:A:590:MSE:CE	2.39	0.53
1:B:269:LEU:HD12	1:B:296:LEU:HD13	1.89	0.53
1:B:559:LEU:HD21	1:B:601:LEU:HD12	1.90	0.53
1:B:547:ASP:OD2	1:B:599:ARG:NH1	2.42	0.53
1:A:644:LYS:NZ	2:A:1644:PLP:O3	2.39	0.52
1:A:746:LEU:HD13	1:A:759:TYR:HD1	1.74	0.52
1:A:71:PHE:CE1	1:A:87:ILE:HG13	2.44	0.52
1:A:335:GLU:HA	1:A:335:GLU:OE1	2.09	0.52
1:B:221:ARG:O	1:B:252:LEU:HD12	2.09	0.52
1:A:446:PHE:CE1	1:A:450:HIS:HD2	2.26	0.52
1:B:8:PHE:CD1	1:B:8:PHE:C	2.83	0.52
1:A:487:SER:HB2	1:A:488:PRO:HD2	1.91	0.52
1:B:27:GLY:O	1:B:30:LEU:N	2.41	0.52
1:A:321:VAL:HG22	1:B:414:LEU:CD1	2.40	0.52
1:A:397:MSE:HE1	1:B:369:TRP:HB2	1.91	0.52
1:B:237:LEU:O	1:B:237:LEU:HG	2.10	0.52
1:A:441:MSE:HE3	1:A:639:ILE:HG12	1.91	0.51
1:B:211:ARG:NH2	1:B:241:ASP:OD2	2.44	0.51
1:A:113:MSE:HE3	1:A:113:MSE:CA	2.40	0.51
1:A:221:ARG:O	1:A:222:LEU:CB	2.58	0.51
1:B:729:HIS:O	1:B:731:ALA:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:MSE:CE	1:A:639:ILE:HG23	2.40	0.51
1:A:184:LEU:HD12	1:A:185:CYS:N	2.25	0.51
1:B:538:ARG:NH1	1:B:737:VAL:O	2.41	0.51
1:A:575:VAL:HG12	1:A:610:ILE:HD13	1.93	0.51
1:A:221:ARG:O	1:A:252:LEU:HD12	2.11	0.51
1:A:211:ARG:NH2	1:A:241:ASP:OD2	2.43	0.51
1:A:348:PHE:CE1	1:B:396:VAL:HG22	2.46	0.51
1:A:487:SER:HB2	1:A:488:PRO:CD	2.40	0.51
1:B:443:PHE:CD1	1:B:464:VAL:HG11	2.46	0.50
1:B:367:ALA:HB1	1:B:372:GLN:HB2	1.94	0.50
1:B:546:ARG:HG2	1:B:596:LEU:HD22	1.93	0.50
1:B:584:ILE:HG21	1:B:590:MSE:CE	2.41	0.50
1:B:470:ARG:HG3	1:B:485:ALA:CB	2.42	0.50
1:B:556:SER:O	1:B:560:SER:HB2	2.11	0.50
1:A:680:SER:HA	1:B:369:TRP:CG	2.47	0.50
1:A:501:ARG:HD2	1:B:497:TRP:CD2	2.47	0.49
1:B:478:LEU:O	1:B:482:GLU:HG2	2.13	0.49
1:B:35:ILE:HD12	1:B:300:MSE:SE	2.63	0.49
1:A:724:GLN:OE1	1:A:724:GLN:HA	2.12	0.49
1:A:652:PRO:HG3	1:B:681:TYR:HB3	1.94	0.49
1:A:168:LEU:O	1:A:172:MSE:HG2	2.13	0.49
1:A:681:TYR:HB3	1:B:652:PRO:HG3	1.94	0.49
1:B:714:LEU:HD23	1:B:717:LEU:HD11	1.94	0.49
1:A:556:SER:O	1:A:560:SER:HB2	2.13	0.49
1:A:145:HIS:HB3	1:A:196:PRO:HB2	1.93	0.49
1:B:184:LEU:HD12	1:B:185:CYS:N	2.28	0.49
1:B:536:THR:HG23	1:B:537:SER:N	2.26	0.49
1:B:616:GLU:OE2	1:B:628:THR:HG23	2.12	0.49
1:B:622:TRP:CE3	1:B:714:LEU:HD13	2.47	0.48
1:B:622:TRP:CE3	1:B:714:LEU:CD1	2.96	0.48
1:B:746:LEU:HD13	1:B:759:TYR:HD1	1.77	0.48
1:B:221:ARG:O	1:B:222:LEU:CB	2.59	0.48
1:A:6:SER:HB3	1:A:7:PRO:HD2	1.96	0.48
1:B:61:PHE:CG	1:B:62:PRO:HA	2.48	0.48
1:B:9:HIS:CE1	1:B:360:SER:HB3	2.49	0.48
1:A:602:VAL:HG13	1:A:612:VAL:HG21	1.95	0.48
1:B:610:ILE:HD11	4:B:2020:HOH:O	2.12	0.48
1:A:546:ARG:HG2	1:A:596:LEU:HD22	1.96	0.48
1:A:113:MSE:HB3	1:A:113:MSE:HE2	1.60	0.48
1:A:94:SER:HA	1:A:137:ALA:O	2.14	0.48
1:A:466:VAL:HG22	1:A:467:ILE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PHE:CD1	1:A:62:PRO:HA	2.49	0.48
1:B:168:LEU:O	1:B:172:MSE:HG2	2.13	0.48
1:B:373:GLY:H	1:B:374:PRO:CD	2.27	0.48
1:B:382:LEU:HD13	1:B:650:MSE:HG3	1.95	0.48
1:B:659:THR:HG23	1:B:661:ALA:H	1.79	0.48
1:B:386:MSE:HE3	1:B:686:MSE:HE1	1.95	0.48
1:A:801:LEU:O	1:A:805:LEU:HB2	2.14	0.47
1:A:444:ARG:HG3	1:A:666:PHE:CZ	2.49	0.47
1:A:616:GLU:OE2	1:A:628:THR:HG23	2.14	0.47
1:A:113:MSE:HA	1:A:113:MSE:HE3	1.94	0.47
1:A:397:MSE:HE1	1:B:369:TRP:HE3	1.80	0.47
1:A:8:PHE:C	1:A:8:PHE:CD1	2.87	0.47
1:A:617:VAL:HG13	1:A:643:ALA:HB3	1.96	0.47
1:B:757:SER:N	1:B:779:ASN:OD1	2.47	0.47
1:B:764:LEU:CD2	1:B:774:THR:HG23	2.44	0.47
1:B:470:ARG:HG3	1:B:485:ALA:HB3	1.96	0.47
1:B:645:LEU:HB2	4:B:2024:HOH:O	2.14	0.47
1:B:18:LEU:HD23	1:B:187:VAL:HB	1.97	0.47
1:A:369:TRP:CG	1:B:680:SER:HA	2.50	0.47
1:B:708:THR:CG2	1:B:709:SER:H	2.27	0.47
1:B:94:SER:HA	1:B:137:ALA:O	2.15	0.47
1:B:519:ILE:HG12	1:B:535:PHE:HE2	1.79	0.46
1:B:801:LEU:O	1:B:805:LEU:HB2	2.15	0.46
1:A:222:LEU:C	1:A:224:GLY:N	2.67	0.46
1:A:333:HIS:O	1:A:336:THR:HG22	2.16	0.46
1:A:470:ARG:HG3	1:A:485:ALA:CB	2.44	0.46
1:A:477:THR:O	1:A:481[B]:MSE:HG3	2.15	0.46
1:A:373:GLY:H	1:A:374:PRO:CD	2.28	0.46
1:B:229:ILE:O	1:B:233:GLU:HG3	2.15	0.46
1:B:352:LYS:O	1:B:357:SER:HA	2.15	0.46
1:B:466:VAL:HG22	1:B:467:ILE:N	2.31	0.46
1:B:71:PHE:CE1	1:B:87:ILE:HG13	2.51	0.46
1:A:229:ILE:O	1:A:233:GLU:HG3	2.15	0.46
1:B:222:LEU:C	1:B:224:GLY:N	2.68	0.46
1:B:729:HIS:C	1:B:731:ALA:H	2.19	0.46
1:B:783:LEU:HD13	1:B:797:LEU:HB3	1.98	0.46
1:A:470:ARG:HG3	1:A:485:ALA:HB3	1.98	0.46
1:B:651:VAL:HG22	1:B:652:PRO:HD2	1.97	0.46
1:B:559:LEU:HD11	1:B:601:LEU:HB2	1.98	0.45
1:A:237:LEU:O	1:A:237:LEU:HG	2.16	0.45
1:A:262:LEU:HD13	1:A:266:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:LEU:HA	1:A:763:LEU:HD23	1.77	0.45
1:B:636:LYS:HE2	1:B:636:LYS:HB2	1.73	0.45
1:A:14:HIS:HB2	1:A:172:MSE:CE	2.46	0.45
1:A:579:ILE:O	1:A:579:ILE:HG23	2.16	0.45
1:B:444:ARG:HG3	1:B:666:PHE:CZ	2.51	0.45
1:A:369:TRP:HE3	1:B:397:MSE:HE1	1.82	0.45
1:A:386:MSE:HE3	1:A:686:MSE:HE1	1.97	0.45
1:B:559:LEU:HD21	1:B:601:LEU:CD1	2.46	0.45
1:A:113:MSE:CE	1:A:114:CYS:N	2.79	0.45
1:A:352:LYS:O	1:A:357:SER:HA	2.17	0.45
1:A:11:PRO:HB2	1:A:172:MSE:HE2	1.98	0.45
1:A:508:PRO:HD2	1:A:597:PHE:CD2	2.52	0.45
1:A:649:GLY:O	1:B:395:HIS:HB3	2.16	0.45
1:B:145:HIS:HB3	1:B:196:PRO:HB2	1.98	0.45
1:B:602:VAL:HG13	1:B:612:VAL:HG21	1.99	0.45
1:B:96:LEU:CB	1:B:97:PRO:HD3	2.47	0.45
1:A:442:ALA:O	1:A:611:PRO:HG2	2.17	0.44
1:B:442:ALA:O	1:B:611:PRO:HG2	2.18	0.44
1:A:42:GLN:OE1	1:A:42:GLN:HA	2.16	0.44
1:A:478:LEU:O	1:A:482:GLU:HG2	2.17	0.44
1:B:236:LYS:HA	1:B:236:LYS:HD2	1.45	0.44
1:B:27:GLY:C	3:B:1810:SO4:O4	2.55	0.44
1:A:340:ILE:HD12	1:B:396:VAL:HG13	2.00	0.44
1:A:8:PHE:CZ	1:A:361:GLN:HG3	2.53	0.44
1:B:763:LEU:HD23	1:B:763:LEU:HA	1.76	0.44
1:B:26:LEU:HD13	1:B:218:GLY:O	2.17	0.44
1:A:466:VAL:HG23	1:A:577:ALA:O	2.17	0.44
1:B:14:HIS:HB2	1:B:172:MSE:CE	2.48	0.44
1:B:8:PHE:CZ	1:B:361:GLN:HG3	2.53	0.44
1:A:140:ALA:HB1	1:A:142:ILE:HD13	1.99	0.44
1:A:783:LEU:HD13	1:A:797:LEU:HB3	2.00	0.44
1:A:85:ILE:HA	1:A:127:ALA:HB1	2.00	0.43
1:B:11:PRO:HB2	1:B:172:MSE:HE2	1.99	0.43
1:A:438:ALA:HA	1:A:441:MSE:HE2	2.00	0.43
1:B:85:ILE:HA	1:B:127:ALA:HB1	1.99	0.43
1:A:24:THR:O	1:A:25:SER:HB2	2.19	0.43
1:A:269:LEU:CD1	1:A:296:LEU:HB2	2.49	0.43
1:B:281:ASP:O	1:B:282:LEU:CB	2.66	0.43
1:A:686:MSE:O	1:A:686:MSE:HE3	2.19	0.43
1:A:96:LEU:CB	1:A:97:PRO:HD3	2.49	0.43
1:A:315:ALA:HA	1:A:337:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ALA:HB1	1:A:639:ILE:HG21	2.00	0.43
1:A:92:LEU:O	1:A:115:SER:HA	2.19	0.43
1:B:11:PRO:HG3	1:B:172:MSE:HG3	2.00	0.43
1:B:280:ASP:OD1	1:B:282:LEU:N	2.49	0.43
1:B:146:LEU:HD13	1:B:150:ARG:NH2	2.33	0.42
1:B:262:LEU:HD13	1:B:266:VAL:HB	2.01	0.42
1:B:277:ASP:HA	1:B:278:PRO:HD3	1.80	0.42
1:B:96:LEU:HD23	1:B:114:CYS:SG	2.59	0.42
1:A:430:ASN:HB2	2:A:1644:PLP:O3P	2.18	0.42
1:B:508:PRO:HD2	1:B:597:PHE:CD2	2.54	0.42
1:B:546:ARG:HH22	1:B:594:ASP:CG	2.22	0.42
1:A:11:PRO:HG3	1:A:172:MSE:HG3	2.01	0.42
1:A:367:ALA:HB1	1:A:372:GLN:HB2	2.00	0.42
1:A:546:ARG:O	1:A:549:SER:OG	2.29	0.42
1:B:24:THR:O	1:B:25:SER:HB2	2.18	0.42
1:B:580:ILE:HD11	1:B:614:PHE:CE1	2.54	0.42
1:A:27:GLY:O	1:A:30:LEU:HB2	2.19	0.42
1:B:221:ARG:O	1:B:252:LEU:CD1	2.67	0.42
1:B:73:LYS:CE	1:B:281:ASP:O	2.67	0.42
1:B:58:GLN:O	1:B:137:ALA:HA	2.19	0.42
1:B:430:ASN:HB2	2:B:1644:PLP:O3P	2.19	0.42
1:B:466:VAL:HG23	1:B:577:ALA:O	2.19	0.42
1:B:766:MSE:HE1	1:B:807:GLU:CB	2.50	0.42
1:A:722:LEU:O	1:A:726:ILE:HG13	2.20	0.42
1:B:13:ASN:OD1	1:B:172:MSE:HE3	2.19	0.42
1:B:34:GLY:HA3	1:B:293:PHE:CZ	2.55	0.42
1:B:519:ILE:CG1	1:B:535:PHE:CE2	3.02	0.42
1:A:433:THR:O	1:A:437:ILE:HD12	2.20	0.42
1:A:546:ARG:NH1	1:A:596:LEU:HB3	2.35	0.42
1:B:11:PRO:CG	1:B:172:MSE:HG3	2.50	0.42
1:B:659:THR:CG2	1:B:661:ALA:H	2.32	0.42
1:A:378:PHE:CE1	1:A:382:LEU:HG	2.55	0.41
1:B:27:GLY:O	1:B:30:LEU:HB2	2.20	0.41
1:B:208:ARG:N	1:B:209:PRO:CD	2.84	0.41
1:B:315:ALA:HA	1:B:337:VAL:HG11	2.02	0.41
1:B:396:VAL:HG12	1:B:403:TYR:CE1	2.55	0.41
1:B:397:MSE:HE2	1:B:398:PHE:H	1.85	0.41
1:B:41:LEU:O	1:B:42:GLN:NE2	2.47	0.41
1:B:438:ALA:HB1	1:B:639:ILE:HG21	2.02	0.41
1:B:670:SER:C	1:B:672:LEU:H	2.23	0.41
1:A:297:LYS:O	1:A:301:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD23	1:A:187:VAL:HB	2.03	0.41
1:A:414:LEU:HA	1:A:414:LEU:HD23	1.87	0.41
1:A:61:PHE:CG	1:A:62:PRO:HA	2.56	0.41
1:B:617:VAL:HG13	1:B:643:ALA:HB3	2.03	0.41
1:B:718:TRP:HB3	1:B:798:LEU:HD11	2.01	0.41
1:A:14:HIS:O	1:A:172:MSE:HE1	2.21	0.41
1:A:297:LYS:HE2	1:A:297:LYS:HB3	1.76	0.41
1:A:89:ASN:O	1:A:119:ARG:HA	2.21	0.41
1:A:277:ASP:HA	1:A:278:PRO:HD3	1.79	0.41
1:A:396:VAL:HG12	1:A:403:TYR:CE1	2.55	0.41
1:A:396:VAL:HG22	1:B:348:PHE:CE1	2.56	0.41
1:B:146:LEU:O	1:B:150:ARG:HG3	2.21	0.41
1:B:559:LEU:HD11	1:B:601:LEU:HA	2.02	0.41
1:B:579:ILE:O	1:B:579:ILE:HG23	2.19	0.41
1:B:26:LEU:HD23	1:B:26:LEU:HA	1.80	0.41
1:A:766:MSE:O	1:A:769:GLU:HB2	2.21	0.41
1:B:47:SER:C	1:B:49:THR:H	2.23	0.41
1:B:219:ASP:OD1	1:B:221:ARG:HB2	2.21	0.41
1:A:14:HIS:HB2	1:A:172:MSE:HE3	2.03	0.41
1:B:297:LYS:O	1:B:301:VAL:HG23	2.21	0.41
1:B:766:MSE:O	1:B:769:GLU:HB2	2.21	0.41
1:A:314:MSE:HE2	1:B:402:VAL:HG22	2.03	0.40
1:B:27:GLY:HA2	3:B:1810:SO4:O4	2.20	0.40
1:B:89:ASN:O	1:B:119:ARG:HA	2.21	0.40
1:A:669:ASP:OD1	1:B:330:LYS:HD3	2.21	0.40
1:B:519:ILE:HG22	1:B:520:SER:N	2.36	0.40
1:B:113:MSE:HE2	1:B:136:TYR:CD1	2.35	0.40
1:A:744:LEU:C	1:A:744:LEU:HD12	2.41	0.40
1:B:96:LEU:N	1:B:97:PRO:CD	2.85	0.40
1:A:35:ILE:HD12	1:A:300:MSE:SE	2.72	0.40
1:A:659:THR:HG23	1:A:661:ALA:H	1.86	0.40
1:B:93:HIS:CB	1:B:113:MSE:HE3	2.50	0.40
1:B:430:ASN:OD1	1:B:433:THR:HG23	2.22	0.40
1:B:441:MSE:CE	1:B:639:ILE:CG2	2.99	0.40
1:B:806:GLY:C	1:B:808:PHE:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	733/831 (88%)	669 (91%)	50 (7%)	14 (2%)	9	22
1	B	734/831 (88%)	672 (92%)	46 (6%)	16 (2%)	8	19
All	All	1467/1662 (88%)	1341 (91%)	96 (6%)	30 (2%)	9	21

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	LEU
1	A	357	SER
1	B	222	LEU
1	B	357	SER
1	B	730	SER
1	B	758	LEU
1	A	355	ASP
1	A	644	LYS
1	B	355	ASP
1	B	644	LYS
1	A	104	LEU
1	A	451	ASN
1	A	643	ALA
1	B	451	ASN
1	B	643	ALA
1	A	397	MSE
1	A	738	ILE
1	B	397	MSE
1	B	491	GLY
1	B	48	ALA
1	B	447	CYS
1	A	28	LYS
1	A	373	GLY
1	A	447	CYS
1	B	583	VAL

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Mol	Chain	Res	Type
1	B	738	ILE
1	A	583	VAL
1	A	491	GLY
1	B	373	GLY
1	B	417	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	575/688 (84%)	552 (96%)	23 (4%)	36	65
1	B	583/688 (85%)	556 (95%)	27 (5%)	31	60
All	All	1158/1376 (84%)	1108 (96%)	50 (4%)	33	62

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	96	LEU
1	A	113	MSE
1	A	115	SER
1	A	131	LEU
1	A	142	ILE
1	A	183	LEU
1	A	206	LEU
1	A	236	LYS
1	A	321	VAL
1	A	327	THR
1	A	369	TRP
1	A	396	VAL
1	A	397	MSE
1	A	417	VAL
1	A	428	SER
1	A	513	SER
1	A	659	THR

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Mol	Chain	Res	Type
1	A	667	SER
1	A	675	LEU
1	A	680	SER
1	A	686	MSE
1	A	790	SER
1	B	9	HIS
1	B	51	LEU
1	B	67	SER
1	B	96	LEU
1	B	131	LEU
1	B	183	LEU
1	B	206	LEU
1	B	236	LYS
1	B	302	LEU
1	B	321	VAL
1	B	327	THR
1	B	349	SER
1	B	356	ASN
1	B	369	TRP
1	B	396	VAL
1	B	397	MSE
1	B	417	VAL
1	B	428	SER
1	B	513	SER
1	B	624	LEU
1	B	659	THR
1	B	667	SER
1	B	675	LEU
1	B	680	SER
1	B	686	MSE
1	B	709	SER
1	B	790	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	HIS
1	B	450	HIS
1	B	484	GLN
1	B	574	HIS

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 carbohydrates 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$
2	PLP	A	1644	1	15,15,16	1.78	2 (13%)	20,22,23	1.77	5 (25%)
3	SO4	A	1809	-	4,4,4	0.28	0	6,6,6	0.29	0
3	SO4	A	1810	-	4,4,4	0.18	0	6,6,6	0.41	0
2	PLP	B	1644	1	15,15,16	1.82	3 (20%)	20,22,23	1.68	4 (20%)
3	SO4	B	1809	-	4,4,4	0.30	0	6,6,6	0.17	0
3	SO4	B	1810	-	4,4,4	0.30	0	6,6,6	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	1644	1	-	0/6/6/8	0/1/1/1
3	SO4	A	1809	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1810	-	-	0/0/0/0	0/0/0/0
2	PLP	B	1644	1	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	1809	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1810	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1644	PLP	O3-C3	-5.67	1.23	1.37
2	B	1644	PLP	O3-C3	-5.44	1.24	1.37
2	A	1644	PLP	C2-N1	2.07	1.38	1.33
2	B	1644	PLP	C6-N1	2.34	1.39	1.34
2	B	1644	PLP	C2-N1	2.54	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1644	PLP	O3P-P-O4P	-2.62	99.77	106.73
2	A	1644	PLP	O3P-P-O4P	-2.56	99.91	106.73
2	A	1644	PLP	C5-C6-N1	-2.32	119.95	123.87
2	B	1644	PLP	O3P-P-O2P	2.00	115.69	107.61
2	A	1644	PLP	O3P-P-O2P	2.05	115.88	107.61
2	A	1644	PLP	C6-C5-C4	2.43	120.21	118.18
2	B	1644	PLP	C6-C5-C4	2.50	120.27	118.18
2	B	1644	PLP	O4P-C5A-C5	5.39	120.16	109.32
2	A	1644	PLP	O4P-C5A-C5	5.73	120.84	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1644	PLP	2	0
3	A	1809	SO4	1	0
2	B	1644	PLP	2	0
3	B	1810	SO4	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	731/831 (87%)	-0.03	30 (4%) 38 37	28, 54, 95, 119	0
1	B	735/831 (88%)	-0.06	18 (2%) 59 60	27, 56, 89, 114	0
All	All	1466/1662 (88%)	-0.04	48 (3%) 47 47	27, 55, 92, 119	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	551	LEU	5.8
1	A	449	ASP	4.6
1	A	574	HIS	4.2
1	A	762	SER	4.2
1	A	512	LEU	4.1
1	A	759	TYR	3.9
1	B	448	VAL	3.8
1	B	79	LEU	3.8
1	A	547	ASP	3.5
1	A	450	HIS	3.5
1	A	493	LEU	3.5
1	A	552	ALA	3.4
1	A	448	VAL	3.3
1	A	521	LEU	3.2
1	B	805	LEU	3.2
1	A	555	TYR	3.1
1	B	746	LEU	2.9
1	A	758	LEU	2.8
1	A	605	CYS	2.7
1	A	669	ASP	2.6
1	B	279	SER	2.6
1	B	446	PHE	2.6
1	A	428	SER	2.5
1	A	604	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	449	ASP	2.5
1	A	576	GLY	2.4
1	A	451	ASN	2.4
1	A	805	LEU	2.4
1	B	779	ASN	2.3
1	A	463	VAL	2.3
1	A	806	GLY	2.3
1	B	81	ARG	2.3
1	B	685	ALA	2.3
1	A	600	VAL	2.3
1	B	96	LEU	2.2
1	B	652	PRO	2.2
1	B	513	SER	2.2
1	A	746	LEU	2.1
1	B	688	CYS	2.1
1	A	744	LEU	2.1
1	B	450	HIS	2.1
1	A	607	ASN	2.1
1	A	545	SER	2.1
1	B	101	SER	2.1
1	B	49	THR	2.1
1	B	668	GLY	2.0
1	A	802	TYR	2.0
1	A	447	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	A	1809	5/5	0.93	0.22	3.36	48,57,85,89	5
3	SO4	B	1810	5/5	0.89	0.25	3.14	57,64,91,114	5
3	SO4	A	1810	5/5	0.96	0.21	2.76	31,34,44,57	5
3	SO4	B	1809	5/5	0.95	0.17	1.53	52,63,81,83	5
2	PLP	B	1644	15/16	0.97	0.21	0.37	34,47,56,60	0
2	PLP	A	1644	15/16	0.98	0.20	0.19	44,48,58,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.