



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:36 PM UTC

PDB ID : 2Z67 / pdb_00002z67
Title : Crystal structure of archaeal O-phosphoseryl-tRNA(Sec) selenium transferase (SepSecS)
Authors : Araiso, Y.; Ishitani, R.; Pailouer, S.; Oshikane, H.; Domae, N.; Soll, D.; Nureki, O.
Deposited on : 2007-07-23
Resolution : 2.50 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

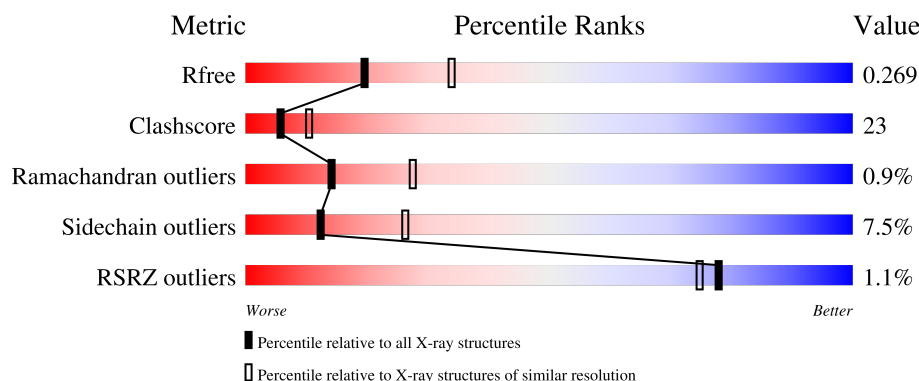
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	456	2% 65% 25% 5%
1	B	456	54% 34% 6% 5%
1	C	456	2% 52% 36% 7% 5%
1	D	456	2% 48% 41% 6% 5%

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	A	1001	-	-	X	-
2	PLP	B	1001	-	-	X	-
2	PLP	C	1001	-	-	X	-
2	PLP	D	1001	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13764 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 O-phosphoseryl-tRNA(Sec) selenium transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	Se	0	0	0
			3387	2156	569	646	6	10			
1	B	434	Total	C	N	O	S	Se	0	0	0
			3387	2156	569	646	6	10			
1	C	434	Total	C	N	O	S	Se	0	0	0
			3387	2156	569	646	6	10			
1	D	434	Total	C	N	O	S	Se	0	0	0
			3387	2156	569	646	6	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q6LZM9
A	-18	GLY	-	expression tag	UNP Q6LZM9
A	-17	SER	-	expression tag	UNP Q6LZM9
A	-16	SER	-	expression tag	UNP Q6LZM9
A	-15	HIS	-	expression tag	UNP Q6LZM9
A	-14	HIS	-	expression tag	UNP Q6LZM9
A	-13	HIS	-	expression tag	UNP Q6LZM9
A	-12	HIS	-	expression tag	UNP Q6LZM9
A	-11	HIS	-	expression tag	UNP Q6LZM9
A	-10	HIS	-	expression tag	UNP Q6LZM9
A	-9	SER	-	expression tag	UNP Q6LZM9
A	-8	SER	-	expression tag	UNP Q6LZM9
A	-7	GLY	-	expression tag	UNP Q6LZM9
A	-6	LEU	-	expression tag	UNP Q6LZM9
A	-5	VAL	-	expression tag	UNP Q6LZM9
A	-4	PRO	-	expression tag	UNP Q6LZM9
A	-3	ARG	-	expression tag	UNP Q6LZM9
A	-2	GLY	-	expression tag	UNP Q6LZM9
A	-1	SER	-	expression tag	UNP Q6LZM9
A	0	HIS	-	expression tag	UNP Q6LZM9
B	-19	MET	-	expression tag	UNP Q6LZM9

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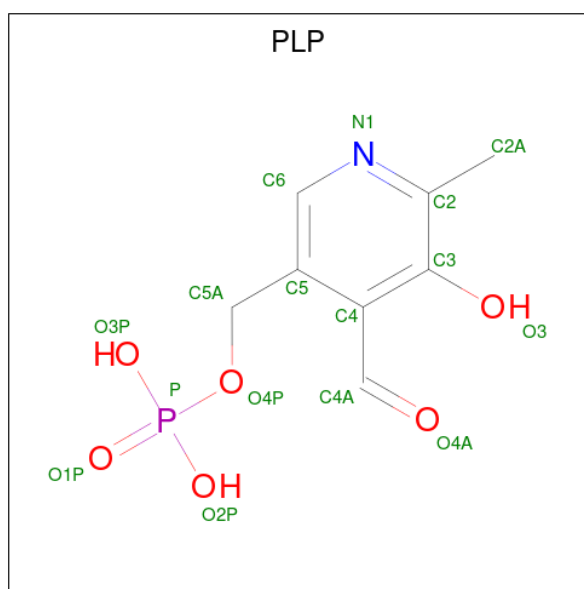
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q6LZM9
B	-17	SER	-	expression tag	UNP Q6LZM9
B	-16	SER	-	expression tag	UNP Q6LZM9
B	-15	HIS	-	expression tag	UNP Q6LZM9
B	-14	HIS	-	expression tag	UNP Q6LZM9
B	-13	HIS	-	expression tag	UNP Q6LZM9
B	-12	HIS	-	expression tag	UNP Q6LZM9
B	-11	HIS	-	expression tag	UNP Q6LZM9
B	-10	HIS	-	expression tag	UNP Q6LZM9
B	-9	SER	-	expression tag	UNP Q6LZM9
B	-8	SER	-	expression tag	UNP Q6LZM9
B	-7	GLY	-	expression tag	UNP Q6LZM9
B	-6	LEU	-	expression tag	UNP Q6LZM9
B	-5	VAL	-	expression tag	UNP Q6LZM9
B	-4	PRO	-	expression tag	UNP Q6LZM9
B	-3	ARG	-	expression tag	UNP Q6LZM9
B	-2	GLY	-	expression tag	UNP Q6LZM9
B	-1	SER	-	expression tag	UNP Q6LZM9
B	0	HIS	-	expression tag	UNP Q6LZM9
C	-19	MET	-	expression tag	UNP Q6LZM9
C	-18	GLY	-	expression tag	UNP Q6LZM9
C	-17	SER	-	expression tag	UNP Q6LZM9
C	-16	SER	-	expression tag	UNP Q6LZM9
C	-15	HIS	-	expression tag	UNP Q6LZM9
C	-14	HIS	-	expression tag	UNP Q6LZM9
C	-13	HIS	-	expression tag	UNP Q6LZM9
C	-12	HIS	-	expression tag	UNP Q6LZM9
C	-11	HIS	-	expression tag	UNP Q6LZM9
C	-10	HIS	-	expression tag	UNP Q6LZM9
C	-9	SER	-	expression tag	UNP Q6LZM9
C	-8	SER	-	expression tag	UNP Q6LZM9
C	-7	GLY	-	expression tag	UNP Q6LZM9
C	-6	LEU	-	expression tag	UNP Q6LZM9
C	-5	VAL	-	expression tag	UNP Q6LZM9
C	-4	PRO	-	expression tag	UNP Q6LZM9
C	-3	ARG	-	expression tag	UNP Q6LZM9
C	-2	GLY	-	expression tag	UNP Q6LZM9
C	-1	SER	-	expression tag	UNP Q6LZM9
C	0	HIS	-	expression tag	UNP Q6LZM9
D	-19	MET	-	expression tag	UNP Q6LZM9
D	-18	GLY	-	expression tag	UNP Q6LZM9
D	-17	SER	-	expression tag	UNP Q6LZM9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q6LZM9
D	-15	HIS	-	expression tag	UNP Q6LZM9
D	-14	HIS	-	expression tag	UNP Q6LZM9
D	-13	HIS	-	expression tag	UNP Q6LZM9
D	-12	HIS	-	expression tag	UNP Q6LZM9
D	-11	HIS	-	expression tag	UNP Q6LZM9
D	-10	HIS	-	expression tag	UNP Q6LZM9
D	-9	SER	-	expression tag	UNP Q6LZM9
D	-8	SER	-	expression tag	UNP Q6LZM9
D	-7	GLY	-	expression tag	UNP Q6LZM9
D	-6	LEU	-	expression tag	UNP Q6LZM9
D	-5	VAL	-	expression tag	UNP Q6LZM9
D	-4	PRO	-	expression tag	UNP Q6LZM9
D	-3	ARG	-	expression tag	UNP Q6LZM9
D	-2	GLY	-	expression tag	UNP Q6LZM9
D	-1	SER	-	expression tag	UNP Q6LZM9
D	0	HIS	-	expression tag	UNP Q6LZM9

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



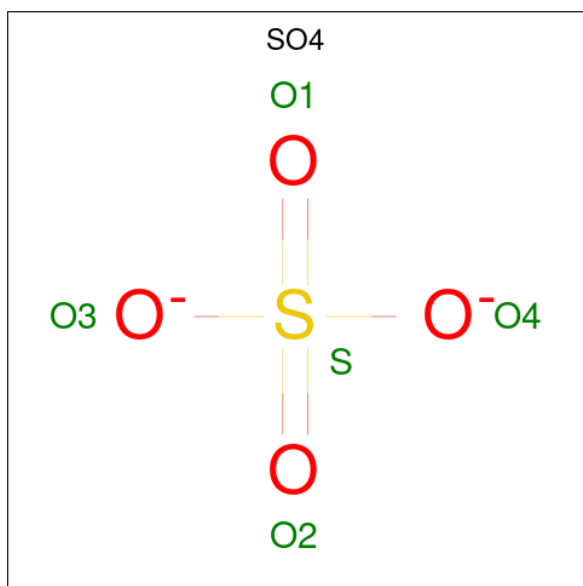
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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

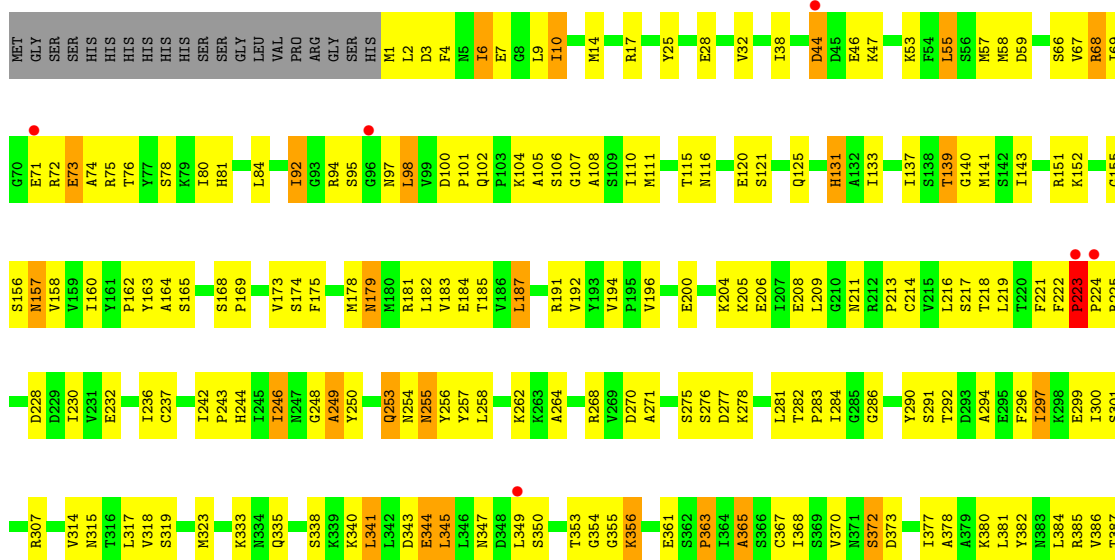
- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	38	Total	O	0	0
			38	38		
4	C	25	Total	O	0	0
			25	25		
4	D	30	Total	O	0	0
			30	30		





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.75Å 108.14Å 110.39Å 90.00° 96.50° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.50) 97.8 (50.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.208 , 0.270 0.207 , 0.269	Depositor DCC
R_{free} test set	3020 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13764	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: 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	0.48	0/3437	1.02	14/4626 (0.3%)
1	B	0.45	0/3437	1.04	23/4626 (0.5%)
1	C	0.43	0/3437	0.99	20/4626 (0.4%)
1	D	0.44	0/3437	0.99	20/4626 (0.4%)
All	All	0.45	0/13748	1.01	77/18504 (0.4%)

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	PHE	CA-C-N	10.09	130.78	120.38
1	A	222	PHE	C-N-CA	10.09	130.78	120.38
1	C	222	PHE	CA-C-N	10.09	130.77	120.38
1	C	222	PHE	C-N-CA	10.09	130.77	120.38
1	A	409	ASP	N-CA-C	-9.38	93.95	109.24
1	B	409	ASP	N-CA-C	-9.28	94.13	109.07
1	C	223	PRO	N-CA-C	9.21	121.94	110.70
1	A	223	PRO	N-CA-C	8.26	120.78	110.70
1	D	222	PHE	CA-C-N	7.17	127.77	120.38
1	D	222	PHE	C-N-CA	7.17	127.77	120.38
1	D	268	ARG	N-CA-C	6.97	120.33	107.99
1	C	409	ASP	N-CA-C	-6.86	97.33	108.52
1	C	38	ILE	N-CA-C	-6.72	102.37	108.95
1	D	253	GLN	N-CA-C	6.56	120.55	112.54
1	A	68	ARG	N-CA-C	6.45	119.33	107.99
1	B	253	GLN	N-CA-C	6.42	118.28	111.28
1	C	408	HIS	N-CA-C	6.32	118.46	108.79
1	B	392	ILE	N-CA-C	6.24	117.00	107.77
1	C	227	SER	N-CA-C	-6.09	101.46	110.48
1	D	223	PRO	N-CA-C	6.09	118.13	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	431	LEU	N-CA-C	-6.09	104.76	111.82
1	B	362	SER	N-CA-C	6.07	117.04	109.57
1	D	410	TYR	N-CA-C	6.03	117.74	109.18
1	D	409	ASP	N-CA-C	-5.96	97.44	107.99
1	B	223	PRO	N-CA-C	5.87	117.86	110.70
1	D	363	PRO	N-CA-C	-5.87	107.94	114.92
1	A	12	LYS	N-CA-C	5.83	118.11	111.11
1	B	7	GLU	N-CA-C	5.81	119.08	110.48
1	C	252	ILE	N-CA-C	5.81	116.55	110.62
1	D	131	HIS	N-CA-C	-5.81	99.77	109.24
1	C	7	GLU	N-CA-C	5.79	118.22	110.35
1	B	222	PHE	CA-C-N	5.77	126.32	120.38
1	B	222	PHE	C-N-CA	5.77	126.32	120.38
1	D	408	HIS	N-CA-C	5.76	117.72	109.14
1	B	12	LYS	N-CA-C	5.76	118.02	111.11
1	B	373	ASP	CA-C-N	5.74	125.10	118.85
1	B	373	ASP	C-N-CA	5.74	125.10	118.85
1	D	292	THR	N-CA-C	-5.73	106.33	113.38
1	C	350	SER	N-CA-C	-5.70	102.98	110.33
1	C	282	THR	CA-C-N	-5.69	114.40	120.03
1	C	282	THR	C-N-CA	-5.69	114.40	120.03
1	A	60	THR	N-CA-C	5.65	119.28	112.38
1	B	324	GLY	N-CA-C	-5.62	105.60	112.68
1	D	7	GLU	N-CA-C	5.60	117.96	110.35
1	C	45	ASP	N-CA-C	5.60	117.83	111.11
1	C	361	GLU	N-CA-C	5.59	117.46	111.36
1	B	130	VAL	N-CA-C	5.57	116.72	108.65
1	D	163	TYR	N-CA-C	5.55	118.85	110.64
1	D	255	ASN	N-CA-C	5.54	118.03	111.33
1	A	392	ILE	N-CA-C	5.45	115.80	108.17
1	D	68	ARG	N-CA-C	5.39	117.41	108.20
1	B	227	SER	N-CA-C	-5.36	103.45	110.53
1	B	126	LEU	N-CA-C	-5.34	106.15	113.30
1	B	246	ILE	N-CA-C	5.31	115.61	108.17
1	D	246	ILE	N-CA-C	5.29	115.58	108.17
1	C	311	THR	CA-C-N	-5.29	113.46	119.28
1	C	311	THR	C-N-CA	-5.29	113.46	119.28
1	B	135	THR	CA-C-N	5.29	126.45	119.84
1	B	135	THR	C-N-CA	5.29	126.45	119.84
1	A	268	ARG	N-CA-C	5.28	118.03	107.62
1	D	361	GLU	N-CA-C	5.26	117.10	111.36
1	C	98	LEU	N-CA-C	5.24	117.41	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	SER	N-CA-C	5.22	117.60	108.52
1	D	286	GLY	N-CA-C	5.20	118.73	111.14
1	C	246	ILE	N-CA-C	5.20	115.33	107.75
1	C	268	ARG	N-CA-C	5.17	117.16	108.73
1	A	212	ARG	CA-C-N	5.16	125.06	119.85
1	A	212	ARG	C-N-CA	5.16	125.06	119.85
1	C	92	ILE	N-CA-C	5.16	115.91	108.48
1	D	98	LEU	N-CA-C	5.12	116.55	110.97
1	B	68	ARG	N-CA-C	5.09	117.01	107.99
1	A	431	LEU	N-CA-C	-5.08	105.82	111.36
1	A	406	TYR	N-CA-C	-5.06	104.19	110.41
1	A	324	GLY	N-CA-C	-5.05	105.33	112.81
1	B	357	PHE	N-CA-C	-5.02	98.41	107.75
1	B	410	TYR	N-CA-C	5.01	116.42	108.96
1	D	365	ALA	N-CA-C	5.01	117.56	109.40

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	3387	0	3465	134	0
1	B	3387	0	3465	181	0
1	C	3387	0	3465	174	0
1	D	3387	0	3465	201	0
2	A	15	0	6	10	0
2	B	15	0	6	9	0
2	C	15	0	6	7	0
2	D	15	0	6	10	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
4	A	53	0	0	2	0
4	B	38	0	0	0	0
4	C	25	0	0	0	0
4	D	30	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13764	0	13884	633	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 23.

All (633) 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:278:LYS:HZ1	2:C:1001:PLP:C4A	1.28	1.37
1:A:278:LYS:HZ2	2:A:1001:PLP:C4A	1.36	1.29
1:D:278:LYS:HZ1	2:D:1001:PLP:C4A	1.37	1.23
1:B:278:LYS:HZ1	2:B:1001:PLP:C4A	1.42	1.20
1:D:278:LYS:CE	2:D:1001:PLP:C4A	2.24	1.15
1:B:278:LYS:HZ2	2:B:1001:PLP:C4A	1.44	1.13
1:C:72:ARG:HD2	1:D:284:ILE:HD11	1.40	1.03
1:A:1:MSE:HE2	1:D:4:PHE:HB3	1.40	1.01
1:B:1:MSE:HE3	1:C:4:PHE:HB3	1.41	1.00
1:B:110:ILE:HD13	1:C:6:ILE:HD12	1.44	0.98
1:A:364:ILE:HD11	1:A:414:ASN:HD22	1.27	0.97
1:C:68:ARG:HB2	1:C:68:ARG:HH11	1.28	0.95
1:A:278:LYS:HZ1	2:A:1001:PLP:C4A	1.55	0.94
1:D:278:LYS:HZ2	2:D:1001:PLP:C4A	1.73	0.94
1:D:68:ARG:HB3	1:D:73:GLU:HG2	1.52	0.92
1:B:364:ILE:HD11	1:B:414:ASN:HD22	1.33	0.91
1:C:278:LYS:CE	2:C:1001:PLP:C4A	2.47	0.91
1:D:278:LYS:HE3	2:D:1001:PLP:C4A	1.98	0.91
1:C:278:LYS:HZ2	2:C:1001:PLP:C4A	1.69	0.90
1:A:278:LYS:HZ2	2:A:1001:PLP:C4	1.84	0.89
1:B:137:ILE:HD12	1:B:141:MSE:HG3	1.57	0.86
1:B:78:SER:H	1:B:81:HIS:CD2	1.95	0.84
1:C:78:SER:H	1:C:81:HIS:HD2	1.23	0.84
1:B:394:LYS:HB2	1:B:406:TYR:O	1.80	0.81
1:C:105:ALA:O	1:C:106:SER:HB2	1.79	0.81
1:B:63:ASP:HB3	1:B:66:SER:HB3	1.62	0.80
1:B:181:ARG:NH2	1:B:205:LYS:HD3	1.97	0.80
1:C:364:ILE:CD1	1:C:414:ASN:HD22	1.93	0.80
1:A:278:LYS:CE	2:A:1001:PLP:C4A	2.60	0.79
1:A:102:GLN:NE2	1:A:104:LYS:H	1.80	0.79
1:C:1:MSE:HE2	1:C:26:LEU:HD13	1.62	0.79
1:B:78:SER:H	1:B:81:HIS:HD2	1.27	0.79
1:D:151:ARG:HG3	1:D:178:MSE:HE2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:ILE:HD11	1:C:414:ASN:HD22	1.46	0.78
1:D:340:LYS:O	1:D:344:GLU:HG2	1.84	0.78
1:D:137:ILE:HD12	1:D:141:MSE:HG3	1.64	0.78
1:B:218:THR:HB	1:B:225:ARG:HH21	1.47	0.78
1:B:139:THR:CG2	2:B:1001:PLP:H5A2	2.14	0.78
1:B:364:ILE:HD11	1:B:414:ASN:ND2	1.98	0.77
1:A:106:SER:O	1:A:110:ILE:HG12	1.86	0.76
1:C:420:ARG:NH1	1:D:75:ARG:HH12	1.83	0.76
1:A:223:PRO:HG3	1:A:365:ALA:HB3	1.68	0.75
1:C:78:SER:H	1:C:81:HIS:CD2	2.04	0.75
1:B:10:ILE:HD11	1:B:14:MSE:HB3	1.68	0.74
1:D:407:THR:HG23	1:D:408:HIS:CD2	2.23	0.74
1:A:278:LYS:NZ	2:A:1001:PLP:C4	2.46	0.74
1:C:139:THR:HG21	1:C:275:SER:OG	1.87	0.74
1:B:139:THR:HG23	2:B:1001:PLP:H5A2	1.67	0.74
1:B:25:TYR:O	1:B:47:LYS:HE3	1.87	0.74
1:D:214:CYS:CB	1:D:243:PRO:HG2	2.17	0.73
1:C:54:PHE:HA	1:C:57:MSE:HE2	1.69	0.73
1:C:238:GLU:HG3	1:C:267:TYR:HB3	1.70	0.73
1:A:225:ARG:HD2	1:A:401:CYS:SG	2.29	0.73
1:D:345:LEU:HD22	1:D:428:VAL:HG11	1.72	0.72
1:C:94:ARG:HD3	1:C:103:PRO:HD2	1.72	0.72
1:D:157:ASN:ND2	1:D:158:VAL:HG12	2.04	0.72
1:D:157:ASN:HD22	1:D:158:VAL:N	1.86	0.72
1:A:102:GLN:HE21	1:A:104:LYS:H	1.37	0.71
1:A:377:ILE:HG21	1:A:411:ILE:HD11	1.71	0.71
1:B:24:GLU:HG3	1:C:64:PRO:HG2	1.72	0.71
1:D:214:CYS:HB2	1:D:243:PRO:HG2	1.73	0.71
1:B:158:VAL:HG13	1:B:213:PRO:HA	1.71	0.71
1:A:347:ASN:O	1:A:350:SER:HB3	1.90	0.70
1:A:71:GLU:HG2	1:B:222:PHE:HZ	1.57	0.70
1:A:6:ILE:HG12	1:D:110:ILE:HD13	1.74	0.70
1:A:213:PRO:O	1:A:242:ILE:HG13	1.92	0.69
1:C:158:VAL:HG13	1:C:213:PRO:HA	1.74	0.69
1:B:101:PRO:HB3	1:C:10:ILE:HD11	1.74	0.68
1:D:160:ILE:HD13	1:D:213:PRO:HB2	1.75	0.68
1:C:282:THR:OG1	1:C:315:ASN:HB3	1.94	0.68
1:C:137:ILE:HD12	1:C:141:MSE:HG3	1.76	0.68
1:D:97:ASN:ND2	1:D:100:ASP:HB2	2.08	0.67
1:D:349:LEU:HD23	1:D:432:GLU:HG2	1.75	0.67
1:D:372:SER:HB2	1:D:377:ILE:HD11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ASN:HD21	1:C:7:GLU:HG2	1.59	0.67
1:D:223:PRO:HG3	1:D:365:ALA:HB3	1.77	0.67
1:D:278:LYS:NZ	2:D:1001:PLP:C4	2.55	0.67
1:D:278:LYS:HZ2	2:D:1001:PLP:C4	2.07	0.67
1:A:171:LYS:HE3	1:B:96:GLY:HA3	1.76	0.67
1:B:137:ILE:HD12	1:B:141:MSE:CG	2.25	0.67
1:D:223:PRO:HB2	1:D:224:PRO:HD3	1.76	0.66
1:D:258:LEU:O	1:D:262:LYS:HG3	1.94	0.66
1:C:277:ASP:HA	1:C:282:THR:HG22	1.75	0.66
1:D:157:ASN:HD22	1:D:157:ASN:C	2.04	0.66
1:D:205:LYS:O	1:D:209:LEU:HD13	1.96	0.66
1:D:391:GLY:C	1:D:392:ILE:HD12	2.20	0.66
1:D:185:THR:HG22	1:D:194:VAL:HG22	1.76	0.66
1:A:6:ILE:HD11	1:D:110:ILE:HG21	1.78	0.66
1:C:278:LYS:HE3	2:C:1001:PLP:C4A	2.25	0.66
1:B:60:THR:HB	1:B:104:LYS:O	1.95	0.66
1:C:356:LYS:HB3	1:C:369:SER:OG	1.96	0.66
1:C:63:ASP:HB3	1:C:66:SER:HB3	1.77	0.66
1:C:125:GLN:HE21	1:C:125:GLN:HA	1.61	0.66
1:C:353:THR:HG23	1:C:355:GLY:H	1.61	0.65
1:C:230:ILE:HG22	1:C:264:ALA:HB2	1.78	0.65
1:D:380:LYS:HD2	1:D:434:ILE:HD13	1.79	0.65
1:A:68:ARG:HH11	1:A:68:ARG:HG2	1.62	0.65
1:D:102:GLN:OE1	1:D:104:LYS:HB2	1.97	0.65
1:A:116:ASN:O	1:A:120:GLU:HG3	1.97	0.65
1:A:110:ILE:HG21	1:D:6:ILE:HD11	1.78	0.64
1:A:389:PRO:HD3	1:B:69:ILE:HD11	1.79	0.64
1:B:10:ILE:HD11	1:B:14:MSE:HE2	1.80	0.64
1:C:383:ASN:O	1:C:384:LEU:HD23	1.98	0.64
1:A:69:ILE:HD13	1:B:413:MSE:HB3	1.79	0.64
1:B:218:THR:HB	1:B:225:ARG:NH2	2.13	0.64
1:B:235:LYS:HG2	1:B:267:TYR:CE2	2.33	0.64
1:B:55:LEU:HD13	1:B:111:MSE:HB3	1.80	0.64
1:B:109:SER:HB3	1:C:10:ILE:HD11	1.79	0.63
1:C:238:GLU:HG2	1:C:268:ARG:HB2	1.80	0.63
1:B:93:GLY:O	1:B:102:GLN:HG2	1.98	0.63
1:D:390:ARG:HB2	1:D:412:VAL:HG13	1.80	0.63
1:A:390:ARG:HB2	1:A:412:VAL:HB	1.80	0.63
1:C:370:VAL:HG21	1:C:377:ILE:CD1	2.28	0.63
1:D:55:LEU:HA	1:D:58:MSE:HE3	1.80	0.63
1:A:277:ASP:OD2	1:B:72:ARG:HD2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:THR:HG23	2:C:1001:PLP:O2P	1.99	0.62
1:D:223:PRO:HG2	1:D:412:VAL:HG21	1.81	0.62
1:B:278:LYS:CE	2:B:1001:PLP:C4A	2.74	0.62
1:D:392:ILE:HD12	1:D:392:ILE:N	2.14	0.62
1:C:377:ILE:HG21	1:C:411:ILE:HD11	1.82	0.62
1:B:341:LEU:HD22	1:B:345:LEU:HG	1.82	0.62
1:B:422:GLU:O	1:B:426:ASN:HB2	2.00	0.62
1:A:364:ILE:HD11	1:A:414:ASN:ND2	2.08	0.62
1:C:204:LYS:O	1:C:208:GLU:HG3	2.00	0.62
1:D:139:THR:HG21	1:D:275:SER:HB2	1.82	0.62
1:A:71:GLU:HG2	1:B:222:PHE:CZ	2.35	0.61
1:C:182:LEU:HD23	1:C:183:VAL:N	2.15	0.61
1:B:417:ILE:HG23	1:B:418:GLY:N	2.16	0.61
1:C:99:VAL:HG12	1:C:99:VAL:O	2.00	0.61
1:A:223:PRO:HG3	1:A:365:ALA:CB	2.29	0.61
1:D:373:ASP:O	1:D:377:ILE:HG13	2.01	0.61
1:B:356:LYS:HG3	1:B:358:LEU:HD23	1.81	0.61
1:B:364:ILE:C	1:B:364:ILE:HD12	2.26	0.61
1:B:96:GLY:O	1:B:302:LEU:HA	1.99	0.60
1:C:111:MSE:CE	1:C:314:VAL:HG22	2.30	0.60
1:A:206:GLU:HA	1:A:209:LEU:HD11	1.83	0.60
1:B:181:ARG:HH22	1:B:205:LYS:HD3	1.64	0.60
1:D:277:ASP:HA	1:D:282:THR:HG22	1.83	0.60
1:A:314:VAL:O	1:A:318:VAL:HG23	2.02	0.60
1:B:282:THR:HG23	1:B:283:PRO:O	2.02	0.60
1:D:185:THR:HB	1:D:192:VAL:HG13	1.84	0.59
1:D:100:ASP:OD2	1:D:101:PRO:HD2	2.01	0.59
1:B:94:ARG:HB3	3:B:1002:SO4:O1	2.02	0.59
1:B:112:TYR:CD1	1:B:313:VAL:HG11	2.37	0.59
1:B:139:THR:HG23	2:B:1001:PLP:O2P	2.03	0.59
1:C:68:ARG:HB2	1:C:68:ARG:NH1	2.09	0.59
1:A:69:ILE:HD12	1:A:69:ILE:O	2.03	0.59
1:B:213:PRO:HG2	1:B:242:ILE:HG12	1.85	0.59
1:D:152:LYS:HD2	1:D:299:GLU:OE1	2.03	0.59
1:C:139:THR:OG1	2:C:1001:PLP:H5A1	2.03	0.59
1:D:139:THR:OG1	2:D:1001:PLP:H5A1	2.02	0.58
1:B:276:SER:OG	1:B:282:THR:HG21	2.03	0.58
1:C:213:PRO:O	1:C:242:ILE:HG13	2.03	0.58
1:A:94:ARG:HG2	1:A:95:SER:H	1.68	0.58
1:A:94:ARG:HG2	1:A:95:SER:N	2.18	0.58
1:B:205:LYS:HA	1:B:208:GLU:OE1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ILE:HG12	1:C:310:ALA:HA	1.85	0.58
1:C:175:PHE:CE1	1:D:175:PHE:HE1	2.21	0.58
1:C:364:ILE:HD12	1:C:364:ILE:C	2.29	0.58
1:D:139:THR:HG23	2:D:1001:PLP:O2P	2.04	0.58
1:A:1:MSE:HE2	1:D:4:PHE:CB	2.25	0.58
1:B:65:LYS:HG3	1:C:24:GLU:CD	2.28	0.58
1:A:5:ASN:C	1:A:5:ASN:HD22	2.11	0.58
1:A:55:LEU:HD23	1:A:58:MSE:CE	2.33	0.58
1:C:319:SER:O	1:C:323:MSE:HB2	2.03	0.58
1:D:282:THR:OG1	1:D:315:ASN:HB3	2.04	0.58
1:A:17:ARG:HG2	1:A:17:ARG:HH11	1.68	0.58
1:D:282:THR:HG23	1:D:283:PRO:O	2.04	0.58
1:C:263:LYS:O	1:C:266:LYS:HB2	2.03	0.58
1:D:115:THR:OG1	1:D:317:LEU:HB2	2.04	0.58
1:C:277:ASP:CA	1:C:282:THR:HG22	2.34	0.57
1:C:60:THR:HB	1:C:104:LYS:O	2.04	0.57
1:B:120:GLU:OE2	1:B:131:HIS:HA	2.05	0.57
1:D:341:LEU:HD22	1:D:345:LEU:HD12	1.87	0.57
1:A:391:GLY:C	1:A:392:ILE:HD12	2.29	0.57
1:B:232:GLU:OE2	1:B:232:GLU:HA	2.04	0.57
1:D:9:LEU:O	1:D:10:ILE:HD12	2.05	0.57
1:B:319:SER:O	1:B:323:MSE:HG3	2.05	0.57
1:C:291:SER:HB3	1:C:297:ILE:CD1	2.35	0.57
1:C:342:LEU:HD12	1:C:415:ALA:HB2	1.85	0.57
1:C:278:LYS:HZ2	2:C:1001:PLP:C4	2.17	0.57
1:D:230:ILE:HG22	1:D:264:ALA:CB	2.34	0.57
1:B:151:ARG:NH2	1:B:176:VAL:HG13	2.20	0.56
1:D:59:ASP:HA	1:D:105:ALA:O	2.06	0.56
1:C:347:ASN:O	1:C:350:SER:HB3	2.06	0.56
1:C:350:SER:O	1:C:351:LYS:HB2	2.06	0.56
1:A:181:ARG:HD2	1:A:206:GLU:OE2	2.05	0.56
1:C:40:GLU:HA	1:C:325:SER:OG	2.06	0.56
1:C:40:GLU:O	1:C:326:LYS:HB2	2.06	0.56
1:D:55:LEU:HD12	1:D:58:MSE:CE	2.35	0.56
1:A:330:GLU:O	1:A:330:GLU:HG3	2.05	0.56
1:B:230:ILE:HG22	1:B:264:ALA:CB	2.36	0.56
1:B:364:ILE:HD12	1:B:364:ILE:O	2.06	0.56
1:C:213:PRO:HG2	1:C:242:ILE:HG12	1.86	0.56
1:A:114:LEU:O	1:A:118:ILE:HG13	2.06	0.56
1:B:6:ILE:O	1:B:6:ILE:CG2	2.54	0.56
1:B:139:THR:HG23	2:B:1001:PLP:C5A	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:GLY:N	1:C:389:PRO:HD2	2.20	0.56
1:C:277:ASP:OD2	1:D:72:ARG:HD2	2.05	0.55
1:A:209:LEU:HD13	1:A:211:ASN:ND2	2.21	0.55
1:B:281:LEU:HD21	1:B:417:ILE:CG2	2.36	0.55
1:B:180:MSE:HE3	1:B:182:LEU:HB2	1.87	0.55
1:C:380:LYS:O	1:C:383:ASN:HB2	2.06	0.55
1:D:243:PRO:HA	1:D:270:ASP:OD2	2.07	0.55
1:B:223:PRO:O	1:B:224:PRO:C	2.50	0.55
1:D:116:ASN:O	1:D:120:GLU:HG3	2.05	0.55
1:A:284:ILE:HD13	1:B:90:HIS:HA	1.88	0.55
1:D:157:ASN:HD21	1:D:211:ASN:HB3	1.72	0.55
1:A:225:ARG:HH22	1:A:228:ASP:CG	2.15	0.55
1:C:358:LEU:HB2	1:C:367:CYS:HB2	1.89	0.55
1:A:364:ILE:HG13	1:A:365:ALA:N	2.21	0.55
1:A:5:ASN:HD22	1:A:6:ILE:N	2.05	0.55
1:A:69:ILE:HD11	1:B:389:PRO:HD3	1.88	0.54
1:A:390:ARG:HB3	1:A:392:ILE:CD1	2.37	0.54
1:B:222:PHE:C	1:B:224:PRO:HD2	2.32	0.54
1:C:151:ARG:HG3	1:C:178:MSE:HE2	1.87	0.54
1:C:44:ASP:OD1	1:C:46:GLU:HG2	2.07	0.54
1:B:116:ASN:O	1:B:120:GLU:HG3	2.08	0.54
1:A:60:THR:HB	1:A:104:LYS:O	2.07	0.54
1:C:79:LYS:HB3	1:C:79:LYS:NZ	2.22	0.54
1:B:293:ASP:OD1	1:B:295:GLU:HB2	2.07	0.54
1:C:157:ASN:HD21	1:C:211:ASN:HB3	1.72	0.54
1:A:392:ILE:HD12	1:A:392:ILE:N	2.23	0.54
1:B:384:LEU:C	1:B:385:ARG:HD3	2.32	0.54
1:A:102:GLN:NE2	1:A:104:LYS:HB2	2.22	0.54
1:A:353:THR:HG23	4:A:1021:HOH:O	2.07	0.54
1:C:348:ASP:O	1:C:350:SER:O	2.26	0.54
1:A:139:THR:HG23	2:A:1001:PLP:P	2.48	0.54
1:A:213:PRO:HG2	1:A:242:ILE:HG12	1.89	0.54
1:C:78:SER:O	1:C:81:HIS:HB2	2.08	0.54
1:C:293:ASP:OD1	1:C:295:GLU:HB3	2.08	0.54
1:D:214:CYS:HB3	1:D:243:PRO:HG2	1.87	0.54
1:A:364:ILE:HD11	1:A:414:ASN:HB3	1.90	0.54
1:B:78:SER:N	1:B:81:HIS:HD2	2.02	0.54
1:B:350:SER:O	1:B:355:GLY:HA2	2.07	0.54
1:C:97:ASN:ND2	1:C:100:ASP:HB2	2.23	0.54
1:A:432:GLU:C	1:A:434:ILE:H	2.16	0.53
1:B:10:ILE:HG23	1:B:15:GLU:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ARG:NH1	1:D:382:TYR:CE1	2.76	0.53
1:D:105:ALA:O	1:D:106:SER:HB3	2.09	0.53
1:D:157:ASN:ND2	1:D:157:ASN:C	2.67	0.53
1:A:205:LYS:O	1:A:208:GLU:HB3	2.08	0.53
1:B:326:LYS:HB2	1:B:326:LYS:NZ	2.23	0.53
1:C:94:ARG:HD3	1:C:103:PRO:CD	2.37	0.53
1:D:185:THR:HB	1:D:192:VAL:CG1	2.39	0.53
1:A:304:TYR:CE1	1:B:141:MSE:HE2	2.43	0.53
1:A:364:ILE:HD12	1:A:415:ALA:H	1.74	0.53
1:B:277:ASP:HA	1:B:282:THR:HG22	1.90	0.53
1:A:206:GLU:HA	1:A:209:LEU:CD1	2.40	0.53
1:B:356:LYS:HB3	1:B:369:SER:OG	2.08	0.53
1:D:278:LYS:NZ	2:D:1001:PLP:O3	2.41	0.53
1:B:54:PHE:CE2	1:C:2:LEU:HD11	2.44	0.52
1:B:256:TYR:CZ	1:B:260:LYS:HE2	2.45	0.52
1:B:6:ILE:O	1:B:6:ILE:HG22	2.08	0.52
1:D:196:VAL:HG11	1:D:232:GLU:HB3	1.91	0.52
1:A:110:ILE:HD12	1:D:6:ILE:HG13	1.91	0.52
1:B:271:ALA:HA	1:B:291:SER:HB3	1.92	0.52
1:B:387:THR:C	1:B:389:PRO:HD2	2.34	0.52
1:D:217:SER:OG	1:D:246:ILE:HG12	2.09	0.52
1:A:4:PHE:CE1	1:A:6:ILE:HD13	2.45	0.52
1:B:220:THR:HG22	1:B:257:TYR:CE1	2.45	0.52
1:B:222:PHE:HD2	1:B:223:PRO:HD2	1.75	0.52
1:D:219:LEU:HD13	1:D:230:ILE:HG13	1.92	0.52
1:A:187:LEU:HB2	1:A:402:TYR:CZ	2.44	0.52
1:B:182:LEU:C	1:B:182:LEU:HD23	2.34	0.52
1:C:10:ILE:HG13	1:C:11:PRO:HD2	1.92	0.52
1:C:73:GLU:HG2	1:C:75:ARG:HG3	1.91	0.52
1:D:55:LEU:HA	1:D:58:MSE:CE	2.40	0.52
1:B:92:ILE:CD1	1:B:313:VAL:HG21	2.40	0.52
1:C:390:ARG:HB2	1:C:412:VAL:CG1	2.40	0.52
1:D:157:ASN:HD21	1:D:158:VAL:HG12	1.73	0.52
1:B:131:HIS:NE2	1:B:294:ALA:HB2	2.24	0.52
1:B:204:LYS:O	1:B:208:GLU:HG3	2.09	0.52
1:C:238:GLU:HG2	1:C:268:ARG:CB	2.40	0.52
1:D:105:ALA:O	1:D:106:SER:CB	2.57	0.51
1:D:121:SER:O	1:D:125:GLN:HG2	2.10	0.51
1:D:204:LYS:O	1:D:208:GLU:HG3	2.09	0.51
1:D:277:ASP:CA	1:D:282:THR:HG22	2.40	0.51
1:A:282:THR:HG23	1:A:283:PRO:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LEU:HD22	1:B:4:PHE:CD2	2.45	0.51
1:C:385:ARG:HB3	1:D:66:SER:HA	1.90	0.51
1:B:163:TYR:HB3	1:B:185:THR:HG23	1.92	0.51
1:A:223:PRO:HG2	1:A:412:VAL:HG13	1.92	0.51
1:C:28:GLU:O	1:C:32:VAL:HG23	2.10	0.51
1:C:111:MSE:HE3	1:C:314:VAL:HG22	1.91	0.51
1:D:277:ASP:CG	1:D:284:ILE:HD13	2.35	0.51
1:B:374:PRO:CG	1:B:409:ASP:HB3	2.40	0.51
1:A:78:SER:H	1:A:81:HIS:CD2	2.27	0.51
1:D:225:ARG:HD2	1:D:401:CYS:SG	2.51	0.51
1:D:237:CYS:SG	1:D:244:HIS:HB2	2.51	0.51
1:B:101:PRO:HB2	1:C:14:MSE:HE1	1.93	0.51
1:C:390:ARG:HB2	1:C:412:VAL:HG12	1.93	0.51
1:A:68:ARG:HG2	1:A:68:ARG:NH1	2.25	0.51
1:A:206:GLU:O	1:A:209:LEU:HD12	2.11	0.51
1:B:55:LEU:O	1:B:107:GLY:HA3	2.10	0.51
1:B:281:LEU:HD21	1:B:417:ILE:HG21	1.93	0.51
1:C:73:GLU:HG3	1:C:75:ARG:CZ	2.41	0.51
1:A:139:THR:HG23	2:A:1001:PLP:O4P	2.11	0.50
1:A:182:LEU:N	1:A:182:LEU:HD12	2.25	0.50
1:C:282:THR:HG23	1:C:283:PRO:O	2.10	0.50
1:B:289:VAL:HG11	1:B:300:ILE:HD13	1.93	0.50
1:C:291:SER:HB3	1:C:297:ILE:HD11	1.93	0.50
1:D:349:LEU:HD13	1:D:349:LEU:O	2.10	0.50
1:A:54:PHE:HA	1:A:57:MSE:CE	2.41	0.50
1:A:78:SER:H	1:A:81:HIS:HD2	1.59	0.50
1:C:427:SER:OG	1:D:69:ILE:HD13	2.11	0.50
1:A:9:LEU:O	1:A:10:ILE:HD13	2.11	0.50
1:B:24:GLU:HG3	1:C:64:PRO:CG	2.38	0.50
1:B:235:LYS:HE2	1:B:267:TYR:CZ	2.46	0.50
1:D:223:PRO:HG2	1:D:412:VAL:CG2	2.41	0.50
1:D:355:GLY:O	1:D:356:LYS:HB3	2.11	0.50
1:A:10:ILE:HG23	1:A:11:PRO:HD2	1.93	0.50
1:A:6:ILE:CG1	1:D:110:ILE:HD13	2.40	0.49
1:B:422:GLU:CD	1:B:422:GLU:H	2.20	0.49
1:D:133:ILE:HD12	1:D:297:ILE:HG23	1.94	0.49
1:D:151:ARG:HB2	1:D:178:MSE:HE1	1.94	0.49
1:A:243:PRO:HA	1:A:270:ASP:OD2	2.11	0.49
1:A:377:ILE:HG21	1:A:411:ILE:CD1	2.39	0.49
1:B:6:ILE:HG23	1:C:110:ILE:HD12	1.93	0.49
1:C:128:LEU:HD23	1:C:262:LYS:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:ARG:HB2	1:C:423:ASP:OD2	2.12	0.49
1:D:378:ALA:O	1:D:381:LEU:HB2	2.12	0.49
1:D:341:LEU:CD2	1:D:345:LEU:HD12	2.42	0.49
1:D:388:GLY:N	1:D:389:PRO:HD2	2.27	0.49
1:C:166:HIS:HB2	1:C:221:PHE:HE1	1.77	0.49
1:D:78:SER:H	1:D:81:HIS:CD2	2.29	0.49
1:A:289:VAL:HG11	1:A:300:ILE:HD13	1.94	0.49
1:B:277:ASP:CA	1:B:282:THR:HG22	2.42	0.49
1:D:184:GLU:CG	1:D:403:LEU:HD12	2.42	0.49
1:A:4:PHE:HB3	1:D:1:MSE:HE3	1.94	0.49
1:B:1:MSE:HE3	1:C:4:PHE:CB	2.29	0.49
1:C:230:ILE:HG22	1:C:264:ALA:CB	2.42	0.49
1:D:10:ILE:HG23	1:D:14:MSE:HB2	1.95	0.49
1:D:384:LEU:O	1:D:385:ARG:HB2	2.12	0.49
1:C:106:SER:O	1:C:110:ILE:HG12	2.13	0.49
1:C:165:SER:O	1:C:221:PHE:HZ	1.96	0.49
1:B:388:GLY:N	1:B:389:PRO:HD2	2.27	0.49
1:C:407:THR:HG23	1:C:408:HIS:CD2	2.48	0.49
1:B:68:ARG:HD2	1:B:73:GLU:HB3	1.95	0.49
1:B:100:ASP:OD2	1:B:101:PRO:HD2	2.13	0.49
1:A:195:PRO:O	1:A:198:ASP:HB2	2.13	0.48
1:C:55:LEU:O	1:C:107:GLY:HA3	2.12	0.48
1:C:137:ILE:HD12	1:C:141:MSE:CG	2.42	0.48
1:C:219:LEU:HD13	1:C:230:ILE:HG13	1.94	0.48
1:C:318:VAL:O	1:C:322:SER:HB3	2.14	0.48
1:D:182:LEU:HD12	1:D:182:LEU:H	1.78	0.48
1:D:335:GLN:HB3	4:D:1004:HOH:O	2.12	0.48
1:A:6:ILE:HG23	1:A:6:ILE:O	2.13	0.48
1:D:165:SER:HB2	1:D:398:PHE:CE1	2.49	0.48
1:D:181:ARG:CZ	1:D:206:GLU:OE2	2.61	0.48
1:A:133:ILE:HG22	1:A:289:VAL:HB	1.95	0.48
1:C:223:PRO:O	1:C:224:PRO:C	2.57	0.48
1:B:384:LEU:O	1:B:385:ARG:HB2	2.14	0.48
1:C:423:ASP:HA	1:D:67:VAL:HG13	1.95	0.48
1:A:96:GLY:HA2	1:A:304:TYR:O	2.13	0.48
1:D:165:SER:HB2	1:D:398:PHE:CD1	2.49	0.48
1:D:250:TYR:HB2	1:D:253:GLN:HE21	1.78	0.48
1:C:68:ARG:HH11	1:C:68:ARG:CB	2.14	0.48
1:D:92:ILE:HD12	1:D:108:ALA:HB1	1.96	0.48
1:D:179:ASN:HD22	1:D:179:ASN:HA	1.54	0.48
1:D:388:GLY:N	1:D:389:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:THR:HG21	2:B:1001:PLP:H5A2	1.92	0.48
1:C:377:ILE:HG21	1:C:411:ILE:CD1	2.44	0.48
1:D:343:ASP:C	1:D:345:LEU:H	2.22	0.48
1:B:382:TYR:HE2	1:D:17:ARG:NH2	2.12	0.48
1:B:54:PHE:HA	1:B:57:MSE:CE	2.43	0.47
1:B:296:PHE:O	1:B:300:ILE:HG13	2.14	0.47
1:C:220:THR:HG22	1:C:257:TYR:CZ	2.49	0.47
1:B:161:TYR:CE1	1:B:216:LEU:HD13	2.49	0.47
1:C:96:GLY:HA2	1:C:304:TYR:O	2.14	0.47
1:B:176:VAL:O	1:B:176:VAL:CG1	2.61	0.47
1:D:184:GLU:HG3	1:D:403:LEU:HD12	1.96	0.47
1:A:70:GLY:CA	1:B:388:GLY:HA3	2.44	0.47
1:B:181:ARG:NH1	1:B:206:GLU:HG2	2.30	0.47
1:D:394:LYS:HB2	1:D:406:TYR:O	2.14	0.47
1:A:248:GLY:O	1:A:249:ALA:C	2.57	0.47
1:C:105:ALA:O	1:C:106:SER:CB	2.53	0.47
1:A:342:LEU:HD13	1:A:366:SER:OG	2.15	0.47
1:A:364:ILE:CD1	1:A:414:ASN:HB3	2.44	0.47
1:B:123:PHE:CE2	1:B:252:ILE:HD12	2.50	0.47
1:C:187:LEU:HD23	1:C:188:ASP:N	2.29	0.47
1:C:277:ASP:HA	1:C:282:THR:H	1.80	0.47
1:C:339:LYS:HG3	1:C:363:PRO:O	2.15	0.47
1:C:392:ILE:HG21	1:C:400:ASN:OD1	2.14	0.47
1:B:364:ILE:CD1	1:B:414:ASN:HD22	2.16	0.47
1:C:133:ILE:HD13	1:C:297:ILE:HG21	1.96	0.47
1:D:80:ILE:O	1:D:84:LEU:HG	2.15	0.47
1:D:115:THR:OG1	1:D:317:LEU:HD22	2.14	0.47
1:D:341:LEU:O	1:D:345:LEU:HB2	2.13	0.47
1:B:417:ILE:CG2	1:B:418:GLY:N	2.77	0.47
1:B:235:LYS:HG2	1:B:267:TYR:CD2	2.51	0.46
1:B:263:LYS:HA	1:B:266:LYS:HE3	1.97	0.46
1:A:276:SER:O	1:A:282:THR:HB	2.14	0.46
1:D:133:ILE:CD1	1:D:297:ILE:HG23	2.45	0.46
1:D:432:GLU:C	1:D:434:ILE:H	2.24	0.46
1:C:69:ILE:HG12	1:D:413:MSE:HE2	1.96	0.46
1:C:392:ILE:N	1:C:392:ILE:HD12	2.30	0.46
1:D:164:ALA:HB1	1:D:221:PHE:CE1	2.50	0.46
1:C:382:TYR:C	1:C:384:LEU:H	2.23	0.46
1:D:394:LYS:HE3	1:D:409:ASP:OD2	2.15	0.46
1:A:252:ILE:HA	1:A:258:LEU:HD21	1.98	0.46
1:D:44:ASP:OD2	1:D:47:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:ARG:HG3	1:D:225:ARG:HH11	1.79	0.46
1:D:349:LEU:CD2	1:D:432:GLU:HG2	2.44	0.46
1:A:55:LEU:HA	1:A:58:MSE:CE	2.45	0.46
1:A:368:ILE:HG23	1:A:368:ILE:O	2.16	0.46
1:B:110:ILE:HD13	1:C:6:ILE:CD1	2.33	0.46
1:D:28:GLU:HG3	4:D:1024:HOH:O	2.15	0.46
1:A:53:LYS:HE2	1:D:46:GLU:OE1	2.15	0.46
1:B:131:HIS:CD2	1:B:294:ALA:HB2	2.50	0.46
1:D:53:LYS:O	1:D:57:MSE:HG3	2.16	0.46
1:D:140:GLY:HA3	1:D:168:SER:OG	2.15	0.46
1:D:187:LEU:HD23	1:D:191:ARG:O	2.16	0.46
1:C:133:ILE:HD13	1:C:297:ILE:CG2	2.46	0.46
1:B:223:PRO:N	1:B:224:PRO:HD2	2.30	0.45
1:D:139:THR:O	1:D:143:ILE:HG13	2.16	0.45
1:B:2:LEU:HD22	1:B:4:PHE:HD2	1.80	0.45
1:B:230:ILE:HG22	1:B:264:ALA:HB1	1.98	0.45
1:B:298:LYS:O	1:B:302:LEU:HG	2.16	0.45
1:C:187:LEU:HD23	1:C:189:GLY:H	1.81	0.45
1:D:155:GLY:O	1:D:156:SER:C	2.59	0.45
1:D:355:GLY:O	1:D:356:LYS:CB	2.64	0.45
1:B:181:ARG:HH22	1:B:205:LYS:CD	2.28	0.45
1:C:235:LYS:O	1:C:238:GLU:HB2	2.17	0.45
1:D:386:VAL:HG12	1:D:389:PRO:HD3	1.98	0.45
1:D:432:GLU:C	1:D:434:ILE:N	2.75	0.45
1:A:370:VAL:HG23	4:A:1015:HOH:O	2.16	0.45
1:C:200:GLU:O	1:C:203:ILE:HB	2.16	0.45
1:D:4:PHE:CD1	1:D:6:ILE:HD13	2.52	0.45
1:D:276:SER:C	1:D:282:THR:HG22	2.41	0.45
1:D:296:PHE:O	1:D:300:ILE:HG13	2.17	0.45
1:A:180:MSE:HE3	1:A:182:LEU:HG	1.99	0.45
1:B:53:LYS:O	1:B:57:MSE:HG3	2.16	0.45
1:B:101:PRO:HB3	1:C:10:ILE:CD1	2.43	0.45
1:B:368:ILE:HG23	1:B:368:ILE:O	2.17	0.45
1:B:374:PRO:HG3	1:B:409:ASP:HB3	1.97	0.45
1:C:385:ARG:HG2	1:C:385:ARG:HH11	1.82	0.45
1:D:10:ILE:CG2	1:D:14:MSE:HB2	2.47	0.45
1:D:68:ARG:HB3	1:D:73:GLU:CG	2.36	0.45
1:D:397:HIS:NE2	1:D:403:LEU:O	2.50	0.45
1:A:278:LYS:NZ	2:A:1001:PLP:C3	2.79	0.45
1:B:196:VAL:HG11	1:B:232:GLU:HB3	1.99	0.45
1:C:121:SER:O	1:C:125:GLN:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:LYS:HB2	1:B:434:ILE:HD13	1.97	0.45
1:A:238:GLU:HB2	1:A:268:ARG:HB2	1.99	0.45
1:C:125:GLN:HA	1:C:125:GLN:NE2	2.29	0.45
1:C:314:VAL:O	1:C:318:VAL:HG23	2.17	0.45
1:D:314:VAL:O	1:D:318:VAL:HG23	2.17	0.45
1:D:169:PRO:O	1:D:173:VAL:HG23	2.17	0.45
1:D:392:ILE:N	1:D:392:ILE:CD1	2.79	0.45
1:A:136:PRO:HA	1:A:312:PRO:HB2	1.99	0.44
1:A:223:PRO:HB2	1:A:224:PRO:HD3	1.99	0.44
1:C:167:LYS:HB2	1:D:95:SER:OG	2.17	0.44
1:C:189:GLY:O	1:C:407:THR:HG21	2.17	0.44
1:B:230:ILE:HG23	1:B:246:ILE:HD11	1.98	0.44
1:B:223:PRO:CG	1:B:365:ALA:HB3	2.47	0.44
1:D:181:ARG:HG2	1:D:181:ARG:HH11	1.83	0.44
1:D:278:LYS:NZ	2:D:1001:PLP:C3	2.80	0.44
1:D:373:ASP:OD2	1:D:393:LYS:HE2	2.17	0.44
1:A:17:ARG:HG2	1:A:17:ARG:NH1	2.29	0.44
1:B:235:LYS:HE2	1:B:267:TYR:OH	2.18	0.44
1:C:368:ILE:HG23	1:C:368:ILE:O	2.17	0.44
1:C:390:ARG:HB3	1:C:392:ILE:HD11	1.98	0.44
1:D:254:ASN:HD21	1:D:363:PRO:CG	2.30	0.44
1:A:225:ARG:HG2	1:A:226:ASN:O	2.18	0.44
1:D:370:VAL:HG21	1:D:377:ILE:HD13	1.98	0.44
1:B:54:PHE:HA	1:B:57:MSE:HE2	2.00	0.44
1:B:160:ILE:HA	1:B:181:ARG:HB3	2.00	0.44
1:B:323:MSE:HE2	1:B:331:LEU:HD11	1.99	0.44
1:B:380:LYS:HD2	1:B:434:ILE:HG23	1.99	0.44
1:C:304:TYR:CE2	1:C:308:ALA:HB2	2.53	0.44
1:D:94:ARG:HG3	1:D:102:GLN:HE21	1.82	0.44
1:D:353:THR:O	1:D:354:GLY:C	2.61	0.44
1:B:400:ASN:O	1:B:401:CYS:C	2.61	0.44
1:C:345:LEU:HD12	1:C:424:ILE:HG22	1.98	0.44
1:D:423:ASP:O	1:D:427:SER:HB3	2.17	0.44
1:B:22:LEU:HD12	1:B:22:LEU:O	2.18	0.44
1:B:184:GLU:H	1:B:184:GLU:HG2	1.54	0.44
1:C:187:LEU:HD23	1:C:187:LEU:C	2.43	0.44
1:D:248:GLY:O	1:D:249:ALA:C	2.61	0.44
1:A:187:LEU:HD13	1:A:187:LEU:C	2.42	0.43
1:B:252:ILE:HB	1:B:279:ASN:HB3	2.00	0.43
1:D:98:LEU:HB2	1:D:301:SER:HB2	2.00	0.43
1:A:223:PRO:HG2	1:A:412:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLY:N	1:A:389:PRO:HD2	2.32	0.43
1:C:388:GLY:N	1:C:389:PRO:CD	2.81	0.43
1:D:158:VAL:HG13	1:D:213:PRO:HA	1.99	0.43
1:A:5:ASN:C	1:A:5:ASN:ND2	2.75	0.43
1:B:426:ASN:HD22	1:B:426:ASN:HA	1.63	0.43
1:C:111:MSE:HG3	1:C:112:TYR:N	2.34	0.43
1:C:349:LEU:CD2	1:C:431:LEU:HD13	2.47	0.43
1:C:432:GLU:C	1:C:434:ILE:H	2.26	0.43
1:A:228:ASP:O	1:A:230:ILE:N	2.50	0.43
1:A:392:ILE:HG23	1:A:396:ASP:HB3	1.99	0.43
1:B:17:ARG:O	1:B:21:VAL:HG23	2.18	0.43
1:B:278:LYS:NZ	2:B:1001:PLP:O3	2.51	0.43
1:C:84:LEU:HD12	1:D:315:ASN:OD1	2.18	0.43
1:C:138:SER:HB3	1:D:307:ARG:O	2.18	0.43
1:D:223:PRO:O	1:D:224:PRO:C	2.61	0.43
1:A:282:THR:CG2	1:A:283:PRO:O	2.66	0.43
1:A:354:GLY:O	1:A:355:GLY:O	2.36	0.43
1:A:390:ARG:HB3	1:A:392:ILE:HD11	1.99	0.43
1:B:252:ILE:HB	1:B:279:ASN:CG	2.44	0.43
1:C:143:ILE:O	1:C:147:LEU:HG	2.17	0.43
1:D:73:GLU:O	1:D:74:ALA:HB3	2.19	0.43
1:B:181:ARG:HH21	1:B:205:LYS:HD3	1.78	0.43
1:C:290:TYR:N	1:C:290:TYR:CD2	2.87	0.43
1:D:194:VAL:HG23	1:D:225:ARG:HH12	1.83	0.43
1:D:218:THR:HB	1:D:225:ARG:HH21	1.84	0.43
1:C:181:ARG:HG3	1:C:181:ARG:HH11	1.84	0.43
1:D:410:TYR:N	1:D:410:TYR:CD2	2.86	0.43
1:D:413:MSE:CE	1:D:427:SER:HB2	2.48	0.43
1:B:97:ASN:CG	1:B:100:ASP:HB2	2.44	0.43
1:D:200:GLU:HB2	1:D:236:ILE:HD13	2.01	0.43
1:B:10:ILE:HG12	1:B:14:MSE:HB2	2.00	0.43
1:B:223:PRO:HG3	1:B:365:ALA:HB3	1.99	0.43
1:B:232:GLU:OE2	1:B:235:LYS:HD2	2.19	0.43
1:C:200:GLU:HB2	1:C:236:ILE:HD13	2.00	0.43
1:D:349:LEU:HD12	1:D:368:ILE:CD1	2.48	0.43
1:D:367:CYS:SG	1:D:412:VAL:HB	2.58	0.43
1:A:28:GLU:O	1:A:32:VAL:HG23	2.19	0.42
1:B:211:ASN:HA	1:B:212:ARG:HH21	1.84	0.42
1:C:281:LEU:O	1:D:76:THR:HA	2.19	0.42
1:D:413:MSE:HE1	1:D:427:SER:HB2	2.02	0.42
1:A:10:ILE:HD12	1:D:101:PRO:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:HG12	1:A:301:SER:OG	2.19	0.42
1:A:181:ARG:NH2	1:A:205:LYS:NZ	2.67	0.42
2:A:1001:PLP:O3P	1:B:72:ARG:NH2	2.51	0.42
1:B:6:ILE:HD12	1:C:110:ILE:HG21	2.01	0.42
1:B:241:ASP:O	1:B:242:ILE:HD12	2.18	0.42
1:B:248:GLY:O	1:B:249:ALA:C	2.61	0.42
1:D:230:ILE:HG22	1:D:264:ALA:HB2	2.01	0.42
1:D:424:ILE:O	1:D:428:VAL:HG23	2.19	0.42
1:A:54:PHE:HA	1:A:57:MSE:HE2	2.01	0.42
1:A:55:LEU:HA	1:A:58:MSE:HE3	2.01	0.42
1:A:168:SER:HB3	1:A:169:PRO:CD	2.50	0.42
1:A:182:LEU:HD12	1:A:182:LEU:H	1.83	0.42
1:B:225:ARG:HG2	1:B:226:ASN:O	2.19	0.42
1:C:185:THR:HB	1:C:192:VAL:HG13	2.02	0.42
1:D:271:ALA:HA	1:D:291:SER:HB2	2.00	0.42
1:A:193:TYR:CE1	1:A:195:PRO:HG3	2.54	0.42
1:C:49:LYS:HB3	1:C:49:LYS:HE2	1.93	0.42
1:C:69:ILE:HD11	1:D:389:PRO:HD3	2.01	0.42
1:C:228:ASP:O	1:C:230:ILE:N	2.52	0.42
1:C:256:TYR:CD2	1:C:363:PRO:HG3	2.54	0.42
1:C:387:THR:C	1:C:389:PRO:HD2	2.44	0.42
1:D:255:ASN:O	1:D:256:TYR:C	2.62	0.42
1:B:10:ILE:CD1	1:B:14:MSE:HE2	2.48	0.42
1:C:63:ASP:OD2	1:D:385:ARG:NH1	2.52	0.42
1:C:190:ASP:OD2	1:C:358:LEU:HD22	2.18	0.42
1:C:305:PRO:HD2	1:D:141:MSE:HE2	2.00	0.42
1:A:161:TYR:CE1	1:A:216:LEU:HD13	2.55	0.42
1:A:81:HIS:HE1	1:B:315:ASN:O	2.02	0.42
1:B:6:ILE:HD13	1:B:6:ILE:HA	1.86	0.42
1:B:17:ARG:HD2	1:D:382:TYR:CE2	2.54	0.42
1:B:258:LEU:O	1:B:262:LYS:HG3	2.19	0.42
1:B:294:ALA:O	1:B:298:LYS:HG3	2.20	0.42
1:D:38:ILE:HG23	1:D:38:ILE:O	2.19	0.42
1:D:181:ARG:HG2	1:D:181:ARG:NH1	2.34	0.42
1:D:225:ARG:HH22	1:D:228:ASP:CG	2.27	0.42
1:A:385:ARG:HG2	1:A:385:ARG:HH11	1.85	0.42
1:B:253:GLN:HB2	1:B:417:ILE:HD13	2.01	0.42
1:B:358:LEU:HD21	1:B:408:HIS:CD2	2.55	0.42
1:C:162:PRO:HA	1:C:183:VAL:HB	2.02	0.42
1:C:353:THR:O	1:C:354:GLY:C	2.62	0.42
1:D:230:ILE:HG22	1:D:264:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:VAL:O	1:D:431:LEU:HB3	2.20	0.42
1:B:140:GLY:HA3	1:B:168:SER:OG	2.19	0.42
1:C:105:ALA:HB1	1:C:108:ALA:HB3	2.02	0.42
1:A:171:LYS:HD2	1:B:305:PRO:HA	2.01	0.42
1:B:180:MSE:CE	1:B:182:LEU:HB2	2.50	0.42
1:B:290:TYR:CD2	1:B:290:TYR:N	2.87	0.42
1:C:364:ILE:HD11	1:C:414:ASN:ND2	2.26	0.42
1:D:28:GLU:O	1:D:32:VAL:HG23	2.20	0.42
1:D:347:ASN:O	1:D:350:SER:HB2	2.20	0.42
1:A:1:MSE:CE	1:D:4:PHE:HB3	2.29	0.41
1:B:186:VAL:HG12	1:B:187:LEU:N	2.35	0.41
1:C:323:MSE:HE3	1:C:328:TYR:CD1	2.55	0.41
1:C:417:ILE:O	1:C:417:ILE:HG23	2.19	0.41
1:A:384:LEU:O	1:A:385:ARG:HB2	2.19	0.41
1:B:97:ASN:ND2	1:B:100:ASP:HB2	2.35	0.41
1:B:329:LEU:HD23	1:B:329:LEU:HA	1.92	0.41
1:C:9:LEU:O	1:C:10:ILE:HD12	2.20	0.41
1:D:338:SER:HB3	1:D:424:ILE:HD11	2.02	0.41
1:C:75:ARG:HB2	1:D:281:LEU:HD22	2.01	0.41
1:D:59:ASP:OD2	1:D:107:GLY:N	2.50	0.41
1:D:319:SER:HB3	1:D:323:MSE:HE2	2.02	0.41
1:D:160:ILE:CD1	1:D:213:PRO:HB2	2.48	0.41
1:D:162:PRO:HA	1:D:183:VAL:HB	2.03	0.41
1:A:171:LYS:HE3	1:B:96:GLY:CA	2.47	0.41
1:B:277:ASP:HA	1:B:282:THR:H	1.85	0.41
1:C:350:SER:O	1:C:351:LYS:CB	2.67	0.41
1:D:9:LEU:C	1:D:10:ILE:HD12	2.45	0.41
1:A:139:THR:HG22	2:A:1001:PLP:O2P	2.20	0.41
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.92	0.41
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.91	0.41
1:B:185:THR:HG22	1:B:194:VAL:HG22	2.03	0.41
1:D:181:ARG:NH2	1:D:206:GLU:OE2	2.54	0.41
1:A:4:PHE:CD1	1:A:6:ILE:HD13	2.55	0.41
1:A:63:ASP:HA	1:A:64:PRO:HD2	1.95	0.41
1:A:111:MSE:HG3	1:A:112:TYR:N	2.36	0.41
1:B:231:VAL:O	1:B:235:LYS:HG3	2.21	0.41
1:B:340:LYS:HB2	1:B:340:LYS:NZ	2.36	0.41
1:B:390:ARG:CZ	1:B:392:ILE:HD11	2.50	0.41
1:C:139:THR:HG22	1:C:275:SER:HA	2.02	0.41
1:C:220:THR:HG22	1:C:257:TYR:CE2	2.56	0.41
1:B:225:ARG:NH2	1:B:228:ASP:OD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:GLY:O	1:C:356:LYS:CB	2.69	0.41
1:D:168:SER:HB3	1:D:169:PRO:CD	2.51	0.41
1:D:394:LYS:HB3	1:D:408:HIS:O	2.21	0.41
1:A:388:GLY:N	1:A:389:PRO:CD	2.84	0.40
1:B:36:ARG:HG2	1:B:114:LEU:CD2	2.51	0.40
1:B:187:LEU:HB2	1:B:402:TYR:CZ	2.56	0.40
1:B:367:CYS:SG	1:B:412:VAL:HB	2.60	0.40
1:C:73:GLU:OE1	1:C:75:ARG:NH2	2.54	0.40
1:D:290:TYR:CD2	1:D:290:TYR:N	2.88	0.40
1:A:282:THR:HG23	1:A:283:PRO:N	2.37	0.40
1:C:51:PHE:HE2	1:C:317:LEU:HD21	1.86	0.40
1:C:60:THR:HG22	1:C:61:ASP:N	2.35	0.40
1:D:223:PRO:HB2	1:D:224:PRO:CD	2.48	0.40
1:C:59:ASP:HA	1:C:105:ALA:O	2.22	0.40
1:C:112:TYR:CD1	1:C:313:VAL:HG11	2.57	0.40
1:C:187:LEU:HD23	1:C:189:GLY:N	2.36	0.40
1:B:123:PHE:HE2	1:B:252:ILE:HD12	1.87	0.40
1:C:355:GLY:O	1:C:356:LYS:HB3	2.21	0.40
1:D:25:TYR:CZ	1:D:47:LYS:HE2	2.56	0.40
1:D:131:HIS:CD2	1:D:294:ALA:HB2	2.57	0.40
1:D:223:PRO:HG3	1:D:365:ALA:CB	2.50	0.40
1:D:225:ARG:NH2	1:D:228:ASP:OD2	2.54	0.40
1:D:349:LEU:HD12	1:D:368:ILE:HD13	2.03	0.40
1:D:390:ARG:O	1:D:411:ILE:HA	2.21	0.40
1:C:377:ILE:CG2	1:C:411:ILE:HD11	2.48	0.40
1:D:257:TYR:OH	1:D:363:PRO:HD2	2.21	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	432/456 (95%)	398 (92%)	31 (7%)	3 (1%)	18	34
1	B	432/456 (95%)	402 (93%)	26 (6%)	4 (1%)	14	27
1	C	432/456 (95%)	393 (91%)	36 (8%)	3 (1%)	18	34
1	D	432/456 (95%)	389 (90%)	38 (9%)	5 (1%)	10	20
All	All	1728/1824 (95%)	1582 (92%)	131 (8%)	15 (1%)	14	27

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	GLY
1	C	106	SER
1	D	356	LYS
1	C	356	LYS
1	D	372	SER
1	B	223	PRO
1	B	356	LYS
1	C	223	PRO
1	D	249	ALA
1	D	344	GLU
1	A	97	ASN
1	A	223	PRO
1	D	223	PRO
1	B	354	GLY
1	B	417	ILE

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	382/391 (98%)	354 (93%)	28 (7%)	13	27
1	B	382/391 (98%)	354 (93%)	28 (7%)	13	27
1	C	382/391 (98%)	347 (91%)	35 (9%)	8	19
1	D	382/391 (98%)	359 (94%)	23 (6%)	17	36
All	All	1528/1564 (98%)	1414 (92%)	114 (8%)	12	26

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	17	ARG
1	A	19	GLU
1	A	60	THR
1	A	76	THR
1	A	102	GLN
1	A	111	MSE
1	A	137	ILE
1	A	139	THR
1	A	145	LEU
1	A	184	GLU
1	A	209	LEU
1	A	216	LEU
1	A	223	PRO
1	A	230	ILE
1	A	242	ILE
1	A	275	SER
1	A	282	THR
1	A	291	SER
1	A	330	GLU
1	A	335	GLN
1	A	342	LEU
1	A	353	THR
1	A	364	ILE
1	A	367	CYS
1	A	385	ARG
1	A	394	LYS
1	A	431	LEU
1	B	2	LEU
1	B	60	THR
1	B	69	ILE
1	B	72	ARG
1	B	102	GLN
1	B	139	THR
1	B	145	LEU
1	B	176	VAL
1	B	184	GLU
1	B	187	LEU
1	B	212	ARG
1	B	216	LEU
1	B	223	PRO
1	B	242	ILE

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Mol	Chain	Res	Type
1	B	275	SER
1	B	282	THR
1	B	297	ILE
1	B	326	LYS
1	B	340	LYS
1	B	341	LEU
1	B	342	LEU
1	B	353	THR
1	B	364	ILE
1	B	407	THR
1	B	412	VAL
1	B	422	GLU
1	B	426	ASN
1	B	431	LEU
1	C	2	LEU
1	C	6	ILE
1	C	10	ILE
1	C	20	LEU
1	C	27	LYS
1	C	46	GLU
1	C	60	THR
1	C	68	ARG
1	C	69	ILE
1	C	71	GLU
1	C	73	GLU
1	C	98	LEU
1	C	106	SER
1	C	111	MSE
1	C	133	ILE
1	C	137	ILE
1	C	139	THR
1	C	145	LEU
1	C	153	LYS
1	C	157	ASN
1	C	190	ASP
1	C	192	VAL
1	C	201	ASN
1	C	216	LEU
1	C	223	PRO
1	C	238	GLU
1	C	242	ILE
1	C	255	ASN

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Mol	Chain	Res	Type
1	C	290	TYR
1	C	330	GLU
1	C	335	GLN
1	C	342	LEU
1	C	348	ASP
1	C	364	ILE
1	C	431	LEU
1	D	2	LEU
1	D	3	ASP
1	D	6	ILE
1	D	10	ILE
1	D	44	ASP
1	D	55	LEU
1	D	71	GLU
1	D	73	GLU
1	D	92	ILE
1	D	111	MSE
1	D	139	THR
1	D	157	ASN
1	D	174	SER
1	D	179	ASN
1	D	187	LEU
1	D	216	LEU
1	D	242	ILE
1	D	297	ILE
1	D	333	LYS
1	D	341	LEU
1	D	345	LEU
1	D	387	THR
1	D	412	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	23	ASN
1	A	81	HIS
1	A	97	ASN
1	A	102	GLN
1	A	179	ASN
1	A	211	ASN
1	A	315	ASN

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Mol	Chain	Res	Type
1	A	337	ASN
1	A	371	ASN
1	A	383	ASN
1	A	414	ASN
1	B	5	ASN
1	B	41	ASN
1	B	81	HIS
1	B	129	ASN
1	B	179	ASN
1	B	201	ASN
1	B	255	ASN
1	B	327	ASN
1	B	397	HIS
1	B	414	ASN
1	B	426	ASN
1	C	5	ASN
1	C	41	ASN
1	C	81	HIS
1	C	125	GLN
1	C	157	ASN
1	C	226	ASN
1	C	327	ASN
1	C	334	ASN
1	C	371	ASN
1	C	408	HIS
1	C	414	ASN
1	C	426	ASN
1	D	81	HIS
1	D	157	ASN
1	D	179	ASN
1	D	254	ASN
1	D	327	ASN
1	D	383	ASN
1	D	408	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 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	SO4	B	1002	-	4,4,4	1.02	0	6,6,6	1.32	1 (16%)
2	PLP	B	1001	1	15,15,16	1.08	0	21,22,23	1.12	2 (9%)
3	SO4	C	1002	-	4,4,4	1.10	0	6,6,6	1.30	1 (16%)
2	PLP	C	1001	1	15,15,16	1.08	0	21,22,23	1.01	2 (9%)
2	PLP	A	1001	1	15,15,16	1.08	0	21,22,23	0.94	1 (4%)
2	PLP	D	1001	1	15,15,16	1.07	0	21,22,23	0.99	1 (4%)

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	C	1001	1	-	3/6/6/8	0/1/1/1
2	PLP	B	1001	1	-	0/6/6/8	0/1/1/1
2	PLP	A	1001	1	-	3/6/6/8	0/1/1/1
2	PLP	D	1001	1	-	2/6/6/8	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	PLP	O4P-C5A-C5	2.95	114.89	109.36
3	B	1002	SO4	O4-S-O3	2.89	124.47	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	SO4	O4-S-O3	2.86	124.32	108.54
2	A	1001	PLP	O4P-P-O1P	2.21	112.40	106.44
2	B	1001	PLP	O4P-P-O1P	2.19	112.37	106.44
2	C	1001	PLP	O4P-P-O1P	2.18	112.34	106.44
2	D	1001	PLP	O4P-P-O1P	2.18	112.32	106.44
2	C	1001	PLP	O4P-C5A-C5	2.13	113.36	109.36

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	PLP	C5A-O4P-P-O2P
2	C	1001	PLP	C5A-O4P-P-O1P
2	C	1001	PLP	C5A-O4P-P-O3P
2	A	1001	PLP	C5A-O4P-P-O1P
2	D	1001	PLP	C5A-O4P-P-O1P
2	A	1001	PLP	C5A-O4P-P-O3P
2	C	1001	PLP	C4-C5-C5A-O4P
2	D	1001	PLP	C5A-O4P-P-O3P

There are no ring outliers.

5 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	SO4	1	0
2	B	1001	PLP	9	0
2	C	1001	PLP	7	0
2	A	1001	PLP	10	0
2	D	1001	PLP	10	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	424/456 (92%)	-0.23	3 (0%) 84 81	18, 34, 50, 59	0
1	B	424/456 (92%)	-0.16	2 (0%) 87 85	18, 37, 51, 65	0
1	C	424/456 (92%)	-0.03	5 (1%) 76 73	21, 39, 58, 70	0
1	D	424/456 (92%)	0.02	8 (1%) 66 62	21, 39, 62, 78	0
All	All	1696/1824 (92%)	-0.10	18 (1%) 78 75	18, 37, 56, 78	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	434	ILE	3.9
1	A	223	PRO	3.3
1	D	44	ASP	3.2
1	C	10	ILE	2.6
1	B	10	ILE	2.6
1	C	434	ILE	2.6
1	A	355	GLY	2.5
1	D	349	LEU	2.4
1	B	6	ILE	2.4
1	D	411	ILE	2.3
1	D	223	PRO	2.3
1	D	71	GLU	2.3
1	C	224	PRO	2.3
1	C	259	GLU	2.2
1	D	224	PRO	2.1
1	D	96	GLY	2.1
1	A	353	THR	2.1
1	C	385	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	SO4	C	1002	5/5	0.90	0.10	71,71,72,73	0
3	SO4	B	1002	5/5	0.93	0.08	61,61,63,63	0
2	PLP	D	1001	15/16	0.95	0.08	32,35,37,37	0
2	PLP	C	1001	15/16	0.96	0.08	31,36,38,41	0
2	PLP	A	1001	15/16	0.96	0.09	25,35,36,38	0
2	PLP	B	1001	15/16	0.97	0.07	22,31,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.