



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:43 PM UTC

PDB ID : 1KL7 / pdb_00001kl7
Title : Crystal Structure of Threonine Synthase from Yeast
Authors : Garrido-Franco, M.; Ehlert, S.; Messerschmidt, A.; Marinkovic, S.; Huber, R.;
Laber, B.; Bourenkov, G.P.; Clausen, T.
Deposited on : 2001-12-11
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 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

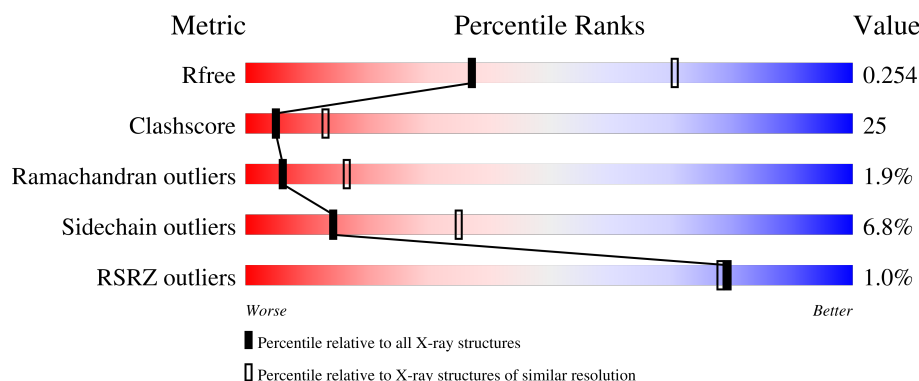
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	514	57% 36% 6% ..
1	B	514	60% 33% 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	1400	-	X	-	-
2	PLP	B	1400	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8294 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.

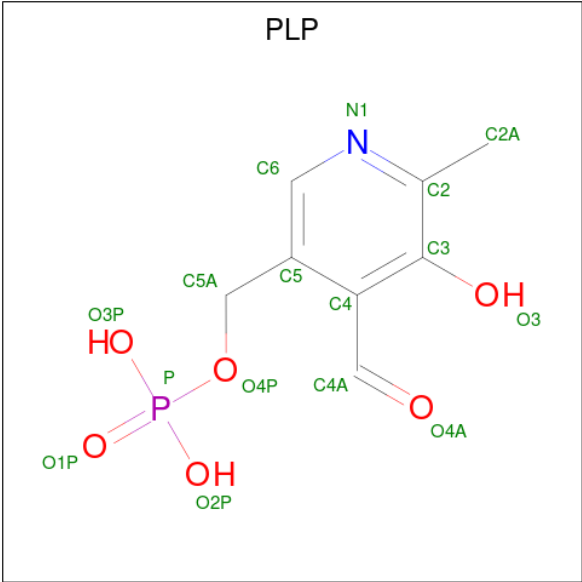
- Molecule 1 is a protein called Threonine Synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	Se	0	0	0
			3965	2532	656	769	2	6			
1	B	509	Total	C	N	O	S	Se	0	0	0
			3965	2532	656	769	2	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P16120
A	66	MSE	MET	modified residue	UNP P16120
A	197	MSE	MET	modified residue	UNP P16120
A	251	MSE	MET	modified residue	UNP P16120
A	291	MSE	MET	modified residue	UNP P16120
A	331	MSE	MET	modified residue	UNP P16120
A	512	MSE	MET	modified residue	UNP P16120
B	1	MSE	MET	modified residue	UNP P16120
B	66	MSE	MET	modified residue	UNP P16120
B	197	MSE	MET	modified residue	UNP P16120
B	251	MSE	MET	modified residue	UNP P16120
B	291	MSE	MET	modified residue	UNP P16120
B	331	MSE	MET	modified residue	UNP P16120
B	512	MSE	MET	modified residue	UNP P16120

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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		

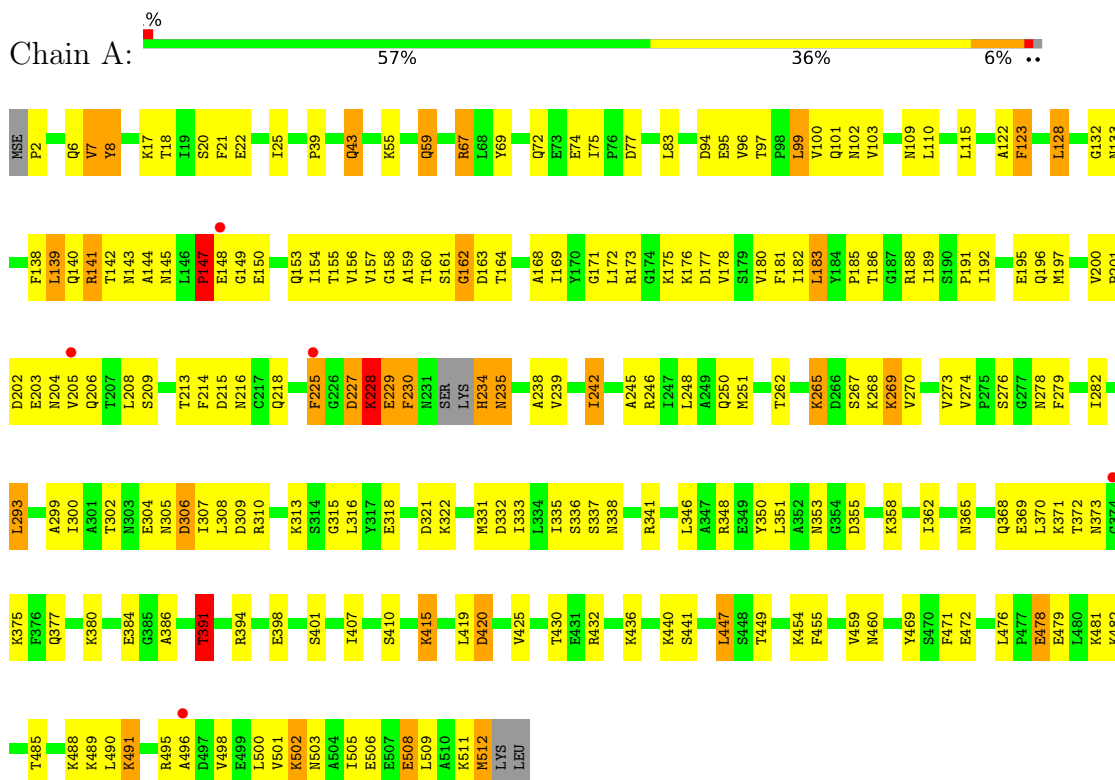
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	159	Total	O	0	0
			159	159		
3	B	175	Total	O	0	0
			175	175		

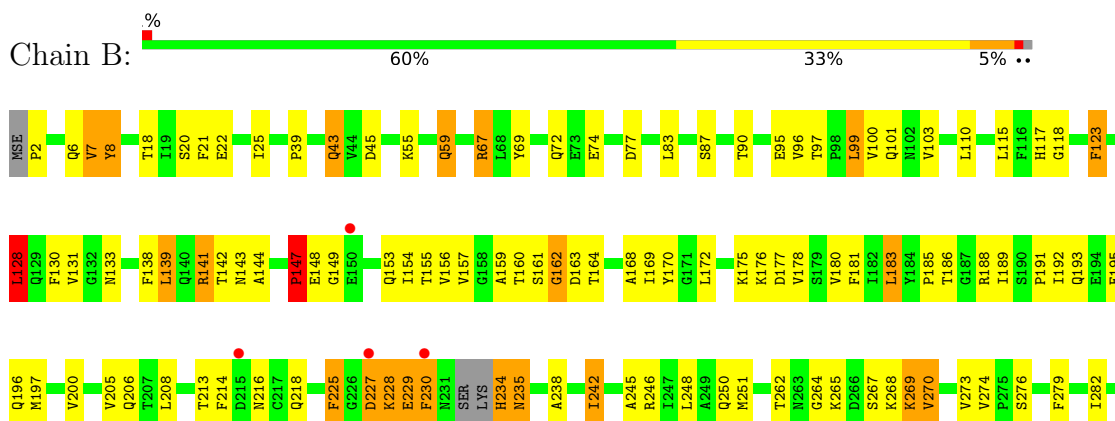
3 Residue-property plots

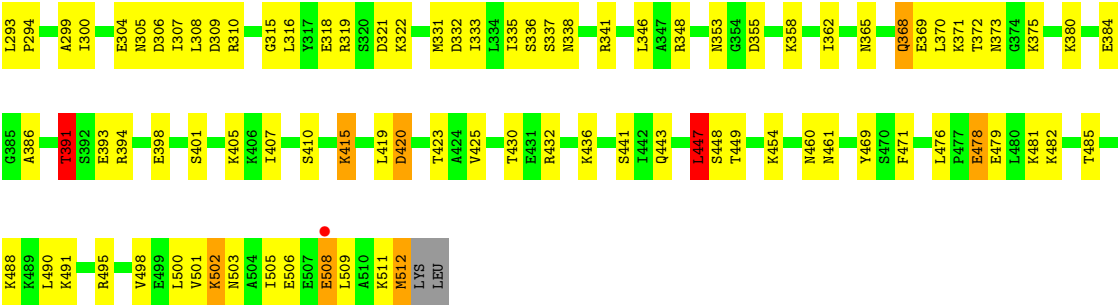
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Threonine Synthase



• Molecule 1: Threonine Synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.30Å 51.60Å 106.90Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.70) 99.1 (20.00-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.70Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.201 , 0.253 0.202 , 0.254	Depositor DCC
R_{free} test set	1381 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8294	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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

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	0.53	0/4037	1.01	19/5456 (0.3%)
1	B	0.55	0/4037	1.02	19/5456 (0.3%)
All	All	0.54	0/8074	1.02	38/10912 (0.3%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	GLU	N-CA-C	-8.70	102.80	113.15
1	A	229	GLU	N-CA-C	-8.59	102.92	113.15
1	A	508	GLU	N-CA-C	-7.49	102.38	112.94
1	B	508	GLU	N-CA-C	-7.39	102.52	113.61
1	A	315	GLY	N-CA-C	-6.76	105.89	115.43
1	B	315	GLY	N-CA-C	-6.69	106.00	115.43
1	B	276	SER	N-CA-C	6.54	120.34	109.95
1	B	420	ASP	N-CA-C	-6.46	100.69	110.39
1	A	337	SER	N-CA-C	6.07	121.38	111.37
1	A	420	ASP	N-CA-C	-5.99	101.41	110.39
1	A	276	SER	N-CA-C	5.98	119.29	109.72
1	A	147	PRO	N-CA-CB	5.92	109.46	103.25
1	B	242	ILE	N-CA-C	5.76	117.76	111.77
1	B	410	SER	N-CA-C	5.70	117.49	111.28
1	B	337	SER	N-CA-C	5.68	120.74	111.37
1	B	391	THR	N-CA-C	-5.60	100.84	109.52
1	A	391	THR	N-CA-C	-5.57	100.88	109.52
1	B	147	PRO	N-CA-CB	5.55	109.08	103.25
1	A	215	ASP	N-CA-C	-5.53	106.24	112.87
1	B	441	SER	N-CA-C	-5.48	106.10	112.89
1	A	128	LEU	N-CA-C	5.42	117.89	111.33
1	A	410	SER	N-CA-C	5.41	117.93	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ILE	N-CA-C	5.41	117.39	111.77
1	B	128	LEU	N-CA-C	5.31	117.75	111.33
1	A	8	TYR	N-CA-C	5.30	117.44	109.23
1	A	75	ILE	CA-C-N	5.26	125.55	119.92
1	A	75	ILE	C-N-CA	5.26	125.55	119.92
1	B	368	GLN	N-CA-C	-5.20	105.05	111.40
1	B	447	LEU	N-CA-C	5.18	117.17	109.25
1	B	118	GLY	CA-C-N	5.17	126.31	119.84
1	B	118	GLY	C-N-CA	5.17	126.31	119.84
1	A	306	ASP	N-CA-C	5.15	119.26	112.25
1	A	368	GLN	N-CA-C	-5.14	105.12	111.40
1	B	8	TYR	N-CA-C	5.11	117.16	109.23
1	B	200	VAL	CA-C-N	5.10	124.41	118.85
1	B	200	VAL	C-N-CA	5.10	124.41	118.85
1	A	441	SER	N-CA-C	-5.07	106.61	112.89
1	A	228	LYS	N-CA-C	-5.02	100.12	110.80

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	3965	0	3890	204	0
1	B	3965	0	3890	190	0
2	A	15	0	7	0	0
2	B	15	0	7	0	0
3	A	159	0	0	35	0
3	B	175	0	0	24	0
All	All	8294	0	7794	394	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 25.

All (394) 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:59:GLN:H	1:A:59:GLN:HE21	1.06	1.02
1:A:322:LYS:HD2	1:A:322:LYS:O	1.67	0.94
1:B:59:GLN:H	1:B:59:GLN:NE2	1.66	0.93
1:B:322:LYS:HD2	1:B:322:LYS:O	1.68	0.93
1:B:59:GLN:H	1:B:59:GLN:HE21	0.90	0.90
1:B:59:GLN:HE21	1:B:59:GLN:N	1.73	0.87
1:B:160:THR:HG22	1:B:162:GLY:H	1.40	0.86
1:A:147:PRO:C	1:A:149:GLY:H	1.82	0.86
1:B:147:PRO:C	1:B:149:GLY:H	1.83	0.86
1:A:160:THR:HG22	1:A:162:GLY:H	1.40	0.86
1:A:59:GLN:H	1:A:59:GLN:NE2	1.73	0.85
1:B:185:PRO:HB2	1:B:188:ARG:HG3	1.59	0.84
1:B:380:LYS:O	1:B:384:GLU:HG3	1.78	0.83
1:B:478:GLU:CD	1:B:478:GLU:H	1.86	0.82
1:A:478:GLU:H	1:A:478:GLU:CD	1.87	0.82
1:B:25:ILE:HD12	1:B:245:ALA:HB2	1.63	0.81
1:B:128:LEU:HD12	1:B:168:ALA:HA	1.62	0.81
1:A:185:PRO:HB2	1:A:188:ARG:HG3	1.61	0.81
1:A:380:LYS:O	1:A:384:GLU:HG3	1.81	0.79
1:A:128:LEU:HD12	1:A:168:ALA:HA	1.63	0.79
1:A:501:VAL:O	1:A:505:ILE:HG12	1.82	0.79
1:B:501:VAL:O	1:B:505:ILE:HG12	1.83	0.79
1:A:225:PHE:HZ	1:A:238:ALA:HA	1.51	0.76
1:A:169:ILE:HD12	1:A:197:MSE:HG2	1.69	0.74
1:B:169:ILE:HD12	1:B:197:MSE:HG2	1.68	0.74
1:A:25:ILE:HD12	1:A:245:ALA:HB2	1.68	0.74
1:A:299:ALA:HA	1:A:391:THR:HG23	1.68	0.74
1:A:230:PHE:HE2	1:A:502:LYS:HG3	1.53	0.74
1:B:225:PHE:HZ	1:B:238:ALA:HA	1.53	0.73
1:A:316:LEU:HD11	1:A:375:LYS:HE3	1.72	0.71
1:B:230:PHE:HE2	1:B:502:LYS:HG3	1.53	0.71
1:B:299:ALA:HA	1:B:391:THR:HG23	1.71	0.71
1:A:158:GLY:HA3	3:A:1420:HOH:O	1.91	0.70
1:A:213:THR:OG1	1:A:216:ASN:HB2	1.91	0.70
1:A:482:LYS:HD3	3:A:1426:HOH:O	1.90	0.70
1:B:305:ASN:ND2	1:B:332:ASP:HA	2.06	0.70
1:A:99:LEU:HD13	1:A:101:GLN:HG2	1.74	0.69
1:A:373:ASN:O	1:A:375:LYS:HG2	1.92	0.69
1:A:200:VAL:HG23	3:A:1494:HOH:O	1.93	0.69
1:A:377:GLN:HA	3:A:1509:HOH:O	1.92	0.69
1:A:115:LEU:HD11	1:A:447:LEU:HD13	1.74	0.68
1:A:185:PRO:HG2	1:A:188:ARG:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:PRO:HG2	1:B:188:ARG:HB2	1.76	0.68
1:A:440:LYS:HE2	3:A:1543:HOH:O	1.93	0.68
1:B:123:PHE:HE1	1:B:250:GLN:NE2	1.92	0.68
1:A:305:ASN:ND2	1:A:332:ASP:HA	2.10	0.67
1:B:213:THR:OG1	1:B:216:ASN:HB2	1.95	0.67
1:A:147:PRO:O	1:A:149:GLY:N	2.28	0.67
1:B:115:LEU:HD11	1:B:447:LEU:HD13	1.76	0.67
1:A:147:PRO:C	1:A:149:GLY:N	2.52	0.67
1:B:500:LEU:HA	1:B:503:ASN:HD22	1.60	0.67
1:A:265:LYS:HB3	3:A:1481:HOH:O	1.95	0.66
1:A:500:LEU:HA	1:A:503:ASN:HD22	1.61	0.66
1:B:99:LEU:HD13	1:B:101:GLN:HG2	1.79	0.65
1:A:316:LEU:HA	3:A:1509:HOH:O	1.96	0.65
1:B:147:PRO:O	1:B:149:GLY:N	2.30	0.65
1:A:230:PHE:CE2	1:A:502:LYS:HG3	2.32	0.64
1:A:59:GLN:HE21	1:A:59:GLN:N	1.87	0.64
1:A:372:THR:HG22	1:A:373:ASN:OD1	1.97	0.64
1:B:316:LEU:HD11	1:B:375:LYS:HE3	1.78	0.64
1:B:7:VAL:HG13	1:B:18:THR:HB	1.79	0.63
1:B:230:PHE:CE2	1:B:502:LYS:HG3	2.33	0.63
1:A:7:VAL:HG13	1:A:18:THR:HB	1.80	0.63
1:A:123:PHE:HE1	1:A:250:GLN:NE2	1.95	0.63
1:B:373:ASN:O	1:B:375:LYS:HG2	1.99	0.63
1:B:512:MSE:HA	1:B:512:MSE:HE3	1.78	0.63
1:B:147:PRO:C	1:B:149:GLY:N	2.53	0.62
1:A:228:LYS:C	1:A:230:PHE:H	2.08	0.62
1:B:228:LYS:C	1:B:230:PHE:H	2.07	0.62
1:B:372:THR:HG22	1:B:373:ASN:OD1	2.00	0.62
1:A:150:GLU:HA	3:A:1483:HOH:O	2.00	0.61
1:A:176:LYS:O	1:A:178:VAL:HG23	1.99	0.61
1:B:160:THR:HG22	1:B:162:GLY:N	2.14	0.61
1:A:370:LEU:HB3	3:A:1505:HOH:O	2.01	0.61
1:B:176:LYS:O	1:B:178:VAL:HG23	2.00	0.61
1:A:375:LYS:C	3:A:1411:HOH:O	2.43	0.61
1:A:512:MSE:HE3	1:A:512:MSE:HA	1.82	0.61
1:B:322:LYS:HD2	1:B:322:LYS:C	2.26	0.61
1:B:460:ASN:HD21	1:B:471:PHE:HB2	1.65	0.61
1:A:460:ASN:HD21	1:A:471:PHE:HB2	1.66	0.60
1:B:498:VAL:HG13	1:B:502:LYS:HZ2	1.66	0.60
1:A:322:LYS:HD2	1:A:322:LYS:C	2.26	0.60
1:A:160:THR:HG22	1:A:162:GLY:N	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:ASN:HD22	1:B:332:ASP:HA	1.63	0.60
1:B:322:LYS:HA	3:B:1458:HOH:O	2.00	0.60
1:A:316:LEU:HD13	3:A:1509:HOH:O	2.01	0.60
1:B:498:VAL:CG1	1:B:502:LYS:HZ2	2.13	0.59
1:A:55:LYS:HB2	3:A:1549:HOH:O	2.02	0.59
1:B:43:GLN:CA	1:B:43:GLN:HE21	2.16	0.59
1:B:394:ARG:NH1	3:B:1531:HOH:O	2.35	0.59
1:B:149:GLY:HA2	3:B:1505:HOH:O	2.02	0.59
1:A:161:SER:HB3	1:A:214:PHE:CE2	2.38	0.59
1:B:161:SER:HB3	1:B:214:PHE:CE2	2.38	0.59
1:A:496:ALA:HB2	3:A:1524:HOH:O	2.04	0.58
1:A:500:LEU:HA	1:A:503:ASN:ND2	2.18	0.58
1:A:20:SER:HB2	1:A:74:GLU:OE1	2.03	0.58
1:A:305:ASN:HD22	1:A:332:ASP:HA	1.68	0.58
1:B:478:GLU:HG3	3:B:1491:HOH:O	2.03	0.58
1:B:262:THR:HB	1:B:268:LYS:HD3	1.85	0.58
1:A:489:LYS:HB2	3:A:1423:HOH:O	2.03	0.58
1:B:365:ASN:O	1:B:369:GLU:HG3	2.04	0.58
1:A:269:LYS:NZ	1:A:269:LYS:HB3	2.19	0.58
1:A:498:VAL:HG13	1:A:502:LYS:NZ	2.19	0.58
1:B:20:SER:HB2	1:B:74:GLU:OE1	2.04	0.58
1:B:454:LYS:HE2	3:B:1511:HOH:O	2.04	0.58
1:B:498:VAL:HG13	1:B:502:LYS:NZ	2.19	0.57
1:B:500:LEU:HA	1:B:503:ASN:ND2	2.18	0.57
1:A:262:THR:HB	1:A:268:LYS:HD3	1.85	0.57
1:B:331:MSE:HE1	1:B:425:VAL:HG11	1.85	0.57
1:A:331:MSE:HE1	1:A:425:VAL:HG11	1.86	0.57
1:B:72:GLN:NE2	1:B:77:ASP:OD1	2.35	0.57
1:A:282:ILE:HD13	1:A:300:ILE:HG12	1.87	0.56
1:A:176:LYS:HE2	3:A:1523:HOH:O	2.05	0.56
1:B:346:LEU:HD11	1:B:386:ALA:HB2	1.87	0.56
1:A:498:VAL:CG1	1:A:502:LYS:HZ2	2.17	0.56
1:A:498:VAL:HG13	1:A:502:LYS:HZ2	1.69	0.56
1:A:100:VAL:HG12	1:A:103:VAL:HG22	1.88	0.55
1:B:154:ILE:HG22	1:B:155:THR:N	2.22	0.55
1:B:268:LYS:HE2	3:B:1467:HOH:O	2.06	0.55
1:A:225:PHE:CZ	1:A:238:ALA:HA	2.38	0.55
1:A:228:LYS:HG2	1:A:230:PHE:HB2	1.89	0.55
1:B:228:LYS:HG2	1:B:230:PHE:HB2	1.88	0.55
1:B:269:LYS:NZ	1:B:269:LYS:HB3	2.21	0.55
1:A:43:GLN:HE21	1:A:43:GLN:CA	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:LYS:HE3	1:B:502:LYS:N	2.21	0.55
1:A:346:LEU:HD11	1:A:386:ALA:HB2	1.88	0.55
1:A:128:LEU:HD21	1:A:246:ARG:HH21	1.72	0.54
1:A:239:VAL:HB	3:A:1420:HOH:O	2.06	0.54
1:B:498:VAL:O	1:B:502:LYS:HD2	2.07	0.54
1:A:154:ILE:HG22	1:A:155:THR:N	2.21	0.54
1:A:371:LYS:O	1:A:371:LYS:HG2	2.08	0.54
1:A:502:LYS:N	1:A:502:LYS:HE3	2.22	0.54
1:B:77:ASP:HB2	3:B:1415:HOH:O	2.08	0.54
1:B:115:LEU:HD11	1:B:447:LEU:CD1	2.38	0.54
1:B:371:LYS:O	1:B:371:LYS:HG2	2.07	0.54
1:B:154:ILE:HD13	1:B:235:ASN:HB3	1.90	0.54
1:B:512:MSE:HA	1:B:512:MSE:CE	2.38	0.54
1:A:209:SER:N	3:A:1526:HOH:O	2.32	0.53
1:B:282:ILE:HD13	1:B:300:ILE:HG12	1.89	0.53
1:A:72:GLN:NE2	1:A:77:ASP:OD1	2.37	0.53
1:A:115:LEU:HD11	1:A:447:LEU:CD1	2.39	0.53
1:A:154:ILE:HD13	1:A:235:ASN:HB3	1.90	0.53
1:B:128:LEU:HD21	1:B:246:ARG:HH21	1.74	0.53
1:B:117:HIS:HD2	3:B:1432:HOH:O	1.92	0.53
1:A:153:GLN:HG2	1:A:177:ASP:HB3	1.91	0.52
1:A:139:LEU:HD22	1:A:143:ASN:ND2	2.25	0.52
1:B:153:GLN:HG2	1:B:177:ASP:HB3	1.92	0.52
1:B:488:LYS:HB3	1:B:490:LEU:CD1	2.40	0.52
1:B:175:LYS:NZ	3:B:1418:HOH:O	2.42	0.52
1:B:460:ASN:ND2	1:B:469:TYR:OH	2.42	0.52
1:A:141:ARG:HB2	3:A:1491:HOH:O	2.09	0.52
1:B:264:GLY:C	3:B:1459:HOH:O	2.51	0.52
1:B:432:ARG:O	1:B:436:LYS:HG2	2.10	0.52
1:B:185:PRO:HB2	1:B:188:ARG:CG	2.36	0.52
1:B:225:PHE:CZ	1:B:238:ALA:HA	2.40	0.52
1:A:365:ASN:O	1:A:369:GLU:HG3	2.10	0.52
1:A:488:LYS:HB3	1:A:490:LEU:CD1	2.40	0.52
1:B:162:GLY:HA2	1:B:189:ILE:HD12	1.92	0.52
1:A:398:GLU:CD	1:A:398:GLU:H	2.18	0.51
1:A:67:ARG:HA	1:A:67:ARG:NE	2.25	0.51
1:A:460:ASN:ND2	1:A:469:TYR:OH	2.43	0.51
1:B:141:ARG:HG3	1:B:142:THR:N	2.23	0.51
1:B:123:PHE:HE1	1:B:250:GLN:HE22	1.56	0.51
1:A:415:LYS:HB2	1:A:415:LYS:NZ	2.25	0.51
1:B:269:LYS:HA	3:B:1411:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:HD13	1:A:430:THR:HG21	1.92	0.51
1:A:333:ILE:O	1:A:333:ILE:HG13	2.11	0.51
1:B:139:LEU:HD22	1:B:143:ASN:ND2	2.26	0.51
1:A:498:VAL:CG1	1:A:502:LYS:NZ	2.74	0.51
1:A:498:VAL:O	1:A:502:LYS:HD2	2.11	0.51
1:A:141:ARG:HG3	1:A:142:THR:N	2.26	0.50
1:B:234:HIS:N	1:B:234:HIS:CD2	2.79	0.50
1:A:183:LEU:HD11	1:A:208:LEU:HD12	1.93	0.50
1:A:269:LYS:HB3	1:A:269:LYS:HZ3	1.74	0.50
1:B:67:ARG:HA	1:B:67:ARG:NE	2.27	0.50
1:A:169:ILE:HG23	1:A:205:VAL:HG11	1.94	0.50
1:A:302:THR:HG21	3:A:1415:HOH:O	2.12	0.50
1:A:157:VAL:HA	1:A:181:PHE:O	2.12	0.50
1:B:39:PRO:O	1:B:348:ARG:NH1	2.43	0.50
1:B:498:VAL:CG1	1:B:502:LYS:NZ	2.75	0.50
1:B:110:LEU:HD13	1:B:430:THR:HG21	1.92	0.50
1:B:355:ASP:CG	1:B:358:LYS:HG3	2.36	0.50
1:B:398:GLU:CD	1:B:398:GLU:H	2.20	0.50
1:A:228:LYS:C	1:A:230:PHE:N	2.70	0.50
1:B:509:LEU:N	3:B:1506:HOH:O	2.45	0.50
1:A:160:THR:CG2	1:A:162:GLY:H	2.19	0.49
1:A:447:LEU:N	1:A:447:LEU:HD23	2.27	0.49
1:A:162:GLY:HA2	1:A:189:ILE:HD12	1.94	0.49
1:A:183:LEU:CD1	1:A:208:LEU:HD12	2.43	0.49
1:B:228:LYS:HG3	1:B:229:GLU:N	2.27	0.49
1:B:502:LYS:O	1:B:506:GLU:HG2	2.12	0.49
1:A:234:HIS:N	1:A:234:HIS:CD2	2.80	0.49
1:A:17:LYS:HD2	3:A:1532:HOH:O	2.11	0.49
1:B:153:GLN:O	1:B:235:ASN:HB2	2.13	0.49
1:A:154:ILE:CD1	1:A:235:ASN:HB3	2.43	0.49
1:B:476:LEU:HD23	1:B:481:LYS:HD3	1.94	0.49
1:A:508:GLU:HB3	1:A:512:MSE:HB2	1.94	0.49
1:B:169:ILE:HG23	1:B:205:VAL:HG11	1.93	0.49
1:B:186:THR:C	1:B:188:ARG:H	2.21	0.49
1:B:447:LEU:HD23	1:B:447:LEU:N	2.27	0.49
1:A:186:THR:C	1:A:188:ARG:H	2.21	0.49
1:A:248:LEU:HA	1:A:251:MSE:HE3	1.95	0.48
1:B:228:LYS:C	1:B:230:PHE:N	2.68	0.48
1:A:512:MSE:HA	1:A:512:MSE:CE	2.42	0.48
1:A:128:LEU:HD21	1:A:246:ARG:NH2	2.28	0.48
1:B:67:ARG:HA	1:B:67:ARG:HE	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:GLU:HB3	1:B:512:MSE:HB2	1.95	0.48
1:A:141:ARG:NE	3:A:1491:HOH:O	2.35	0.48
1:A:173:ARG:HG2	3:A:1538:HOH:O	2.12	0.48
1:B:274:VAL:HG22	1:B:447:LEU:HG	1.95	0.48
1:A:173:ARG:NH2	3:A:1494:HOH:O	2.37	0.48
1:A:358:LYS:O	1:A:362:ILE:HG13	2.14	0.48
1:A:370:LEU:HA	3:A:1411:HOH:O	2.14	0.48
1:B:228:LYS:CG	1:B:230:PHE:HB2	2.44	0.48
1:A:338:ASN:OD1	1:A:341:ARG:NH1	2.46	0.48
1:B:163:ASP:O	1:B:164:THR:C	2.57	0.48
1:A:407:ILE:HG13	1:A:419:LEU:HD11	1.96	0.48
1:B:415:LYS:NZ	1:B:415:LYS:HB2	2.29	0.48
1:A:502:LYS:O	1:A:506:GLU:HG2	2.14	0.47
1:B:333:ILE:HD12	1:B:335:ILE:C	2.39	0.47
1:A:67:ARG:HA	1:A:67:ARG:HE	1.78	0.47
1:A:159:ALA:HA	1:A:183:LEU:O	2.13	0.47
1:A:228:LYS:CG	1:A:230:PHE:HB2	2.45	0.47
1:B:338:ASN:OD1	1:B:341:ARG:NH1	2.47	0.47
1:A:273:VAL:HA	1:A:299:ALA:HB3	1.97	0.47
1:B:96:VAL:HG12	1:B:97:THR:HG23	1.95	0.47
1:B:123:PHE:CD2	1:B:449:THR:HB	2.49	0.47
1:A:153:GLN:O	1:A:235:ASN:HB2	2.15	0.47
1:A:479:GLU:O	1:A:482:LYS:HG2	2.15	0.47
1:B:509:LEU:CD1	1:B:511:LYS:HB2	2.45	0.47
1:B:128:LEU:HD21	1:B:246:ARG:NH2	2.29	0.47
1:B:306:ASP:HB2	1:B:309:ASP:HB3	1.97	0.47
1:B:353:ASN:CG	1:B:353:ASN:O	2.58	0.47
1:A:308:LEU:HB2	3:A:1415:HOH:O	2.13	0.47
1:B:159:ALA:HA	1:B:183:LEU:O	2.14	0.47
1:A:196:GLN:NE2	1:A:454:LYS:HE3	2.30	0.47
1:B:43:GLN:CA	1:B:43:GLN:NE2	2.76	0.47
1:B:157:VAL:HA	1:B:181:PHE:O	2.14	0.47
1:B:225:PHE:C	1:B:227:ASP:N	2.70	0.47
1:B:154:ILE:CD1	1:B:235:ASN:HB3	2.45	0.47
1:B:509:LEU:C	1:B:511:LYS:H	2.23	0.47
1:A:228:LYS:HG3	1:A:229:GLU:N	2.30	0.46
1:B:160:THR:CG2	1:B:162:GLY:H	2.19	0.46
1:B:407:ILE:HG13	1:B:419:LEU:HD11	1.97	0.46
1:B:488:LYS:HB3	1:B:490:LEU:HD13	1.97	0.46
1:A:138:PHE:O	1:A:141:ARG:HG2	2.15	0.46
1:A:333:ILE:HD12	1:A:335:ILE:C	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:LEU:CD1	1:A:511:LYS:HB2	2.46	0.46
1:A:122:ALA:HB1	3:A:1548:HOH:O	2.15	0.46
1:A:488:LYS:C	3:A:1423:HOH:O	2.58	0.46
1:B:333:ILE:HG13	1:B:333:ILE:O	2.11	0.46
1:A:94:ASP:HB2	3:A:1501:HOH:O	2.16	0.46
1:A:99:LEU:HD13	1:A:101:GLN:CG	2.45	0.46
1:B:273:VAL:HA	1:B:299:ALA:HB3	1.97	0.46
1:A:234:HIS:O	1:A:235:ASN:C	2.58	0.46
1:A:306:ASP:HB2	1:A:309:ASP:HB3	1.98	0.46
1:B:7:VAL:HG13	1:B:18:THR:CB	2.45	0.46
1:B:45:ASP:OD2	1:B:45:ASP:C	2.59	0.46
1:B:183:LEU:HD11	1:B:208:LEU:HD12	1.97	0.46
1:A:432:ARG:O	1:A:436:LYS:HG2	2.15	0.46
1:B:21:PHE:CE1	1:B:25:ILE:HD11	2.51	0.46
1:A:133:ASN:HD21	1:A:175:LYS:HE2	1.81	0.46
1:B:447:LEU:CD1	3:B:1558:HOH:O	2.64	0.46
1:A:43:GLN:CA	1:A:43:GLN:NE2	2.79	0.46
1:A:196:GLN:HE22	1:A:454:LYS:HE3	1.81	0.46
1:A:225:PHE:C	1:A:227:ASP:N	2.71	0.46
1:A:269:LYS:NZ	1:A:269:LYS:CB	2.79	0.46
1:B:335:ILE:HG13	1:B:335:ILE:O	2.16	0.45
1:B:405:LYS:HE3	3:B:1504:HOH:O	2.16	0.45
1:A:21:PHE:CE1	1:A:25:ILE:HD11	2.52	0.45
1:A:141:ARG:O	1:A:144:ALA:HB3	2.16	0.45
1:B:170:TYR:HB3	3:B:1562:HOH:O	2.17	0.45
1:A:203:GLU:O	1:A:512:MSE:HE2	2.16	0.45
1:A:95:GLU:O	1:A:96:VAL:HB	2.16	0.45
1:B:172:LEU:HB2	1:B:180:VAL:HG21	1.98	0.45
1:B:508:GLU:O	1:B:509:LEU:HG	2.17	0.45
1:A:8:TYR:OH	1:A:69:TYR:HB3	2.17	0.45
1:A:313:LYS:HB2	1:A:313:LYS:HE3	1.77	0.45
1:A:476:LEU:HD23	1:A:481:LYS:HD3	1.99	0.45
1:A:161:SER:HB3	1:A:214:PHE:CZ	2.51	0.45
1:B:183:LEU:CD1	1:B:208:LEU:HD12	2.47	0.45
1:B:358:LYS:O	1:B:362:ILE:HG13	2.16	0.45
1:A:488:LYS:HB3	1:A:490:LEU:HD13	1.97	0.45
1:A:267:SER:OG	1:A:269:LYS:HG3	2.16	0.45
1:A:201:PRO:HG2	3:A:1494:HOH:O	2.17	0.45
1:A:335:ILE:O	1:A:335:ILE:HG13	2.17	0.45
1:A:185:PRO:HB2	1:A:188:ARG:CG	2.39	0.44
1:A:491:LYS:HD2	3:A:1447:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:SER:HB3	1:B:214:PHE:CZ	2.52	0.44
1:B:461:ASN:OD1	3:B:1454:HOH:O	2.21	0.44
1:A:123:PHE:HE1	1:A:250:GLN:HE22	1.65	0.44
1:A:123:PHE:CD2	1:A:449:THR:HB	2.52	0.44
1:A:478:GLU:CD	1:A:478:GLU:N	2.67	0.44
1:B:83:LEU:HD23	1:B:133:ASN:HB3	1.99	0.44
1:A:132:GLY:HA3	1:A:171:GLY:O	2.18	0.44
1:A:307:ILE:HG23	1:A:308:LEU:N	2.33	0.44
1:B:176:LYS:NZ	3:B:1484:HOH:O	2.51	0.44
1:B:267:SER:HB3	3:B:1425:HOH:O	2.17	0.44
1:A:7:VAL:HG13	1:A:18:THR:CB	2.47	0.44
1:A:377:GLN:CA	3:A:1509:HOH:O	2.59	0.44
1:B:242:ILE:C	1:B:242:ILE:HD12	2.42	0.44
1:B:368:GLN:NE2	3:B:1538:HOH:O	2.49	0.44
1:A:83:LEU:HD23	1:A:133:ASN:HB3	2.00	0.44
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.85	0.44
1:A:350:TYR:O	1:A:351:LEU:HD23	2.18	0.44
1:B:43:GLN:NE2	1:B:43:GLN:HA	2.32	0.44
1:B:234:HIS:O	1:B:235:ASN:C	2.59	0.44
1:A:509:LEU:C	1:A:511:LYS:H	2.25	0.44
1:B:371:LYS:C	3:B:1438:HOH:O	2.60	0.44
1:A:310:ARG:NH2	1:A:318:GLU:O	2.50	0.44
1:B:156:VAL:HG21	1:B:172:LEU:HD13	2.00	0.44
1:B:230:PHE:HE1	1:B:234:HIS:HE2	1.65	0.43
1:A:489:LYS:O	1:A:489:LYS:HG2	2.18	0.43
1:B:131:VAL:HG22	1:B:245:ALA:CB	2.48	0.43
1:B:196:GLN:NE2	1:B:454:LYS:HE3	2.33	0.43
1:A:163:ASP:O	1:A:164:THR:C	2.60	0.43
1:A:242:ILE:HD12	1:A:242:ILE:C	2.43	0.43
1:B:183:LEU:CD1	1:B:183:LEU:N	2.81	0.43
1:B:248:LEU:HA	1:B:251:MSE:HE3	1.99	0.43
1:B:447:LEU:N	1:B:447:LEU:CD2	2.81	0.43
1:B:133:ASN:HD21	1:B:175:LYS:HE2	1.83	0.43
1:A:508:GLU:O	1:A:509:LEU:HG	2.19	0.43
1:B:95:GLU:O	1:B:96:VAL:HB	2.18	0.43
1:B:141:ARG:O	1:B:144:ALA:HB3	2.19	0.43
1:B:269:LYS:NZ	1:B:269:LYS:CB	2.81	0.43
1:A:96:VAL:HG12	1:A:97:THR:HG23	2.00	0.43
1:B:192:ILE:O	1:B:196:GLN:HG3	2.19	0.43
1:A:225:PHE:HD2	1:A:225:PHE:HA	1.69	0.43
1:A:355:ASP:CG	1:A:358:LYS:HG3	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:SER:OG	1:B:130:PHE:HA	2.18	0.43
1:A:482:LYS:HD2	3:A:1503:HOH:O	2.19	0.43
1:B:225:PHE:HD2	1:B:225:PHE:HA	1.69	0.43
1:A:183:LEU:CD1	1:A:183:LEU:N	2.83	0.42
1:A:186:THR:O	1:A:188:ARG:HG2	2.19	0.42
1:A:306:ASP:OD1	1:A:394:ARG:HD2	2.18	0.42
1:A:455:PHE:O	1:A:459:VAL:HG23	2.19	0.42
1:B:294:PRO:HG2	3:B:1456:HOH:O	2.18	0.42
1:A:22:GLU:HG3	1:A:138:PHE:CG	2.54	0.42
1:B:279:PHE:HB2	1:B:336:SER:OG	2.18	0.42
1:B:479:GLU:O	1:B:482:LYS:HG2	2.19	0.42
1:B:133:ASN:ND2	1:B:175:LYS:NZ	2.67	0.42
1:B:196:GLN:HE22	1:B:454:LYS:HE3	1.84	0.42
1:B:319:ARG:HH11	1:B:319:ARG:HB2	1.85	0.42
1:A:133:ASN:ND2	1:A:175:LYS:NZ	2.68	0.42
1:A:318:GLU:OE2	1:A:375:LYS:HD2	2.19	0.42
1:A:181:PHE:HE1	3:A:1552:HOH:O	2.02	0.42
1:B:55:LYS:NZ	3:B:1435:HOH:O	2.49	0.42
1:B:100:VAL:HG12	1:B:103:VAL:HG22	2.01	0.42
1:A:133:ASN:ND2	1:A:175:LYS:HE2	2.35	0.42
1:A:172:LEU:HB2	1:A:180:VAL:HG21	2.01	0.42
1:B:90:THR:HA	3:B:1492:HOH:O	2.19	0.42
1:A:274:VAL:HG22	1:A:447:LEU:HG	2.01	0.42
1:B:306:ASP:O	1:B:307:ILE:C	2.63	0.42
1:A:509:LEU:HD12	1:A:511:LYS:HB2	2.02	0.41
1:B:423:THR:HG23	1:B:448:SER:HA	2.02	0.41
1:A:191:PRO:O	1:A:195:GLU:HG3	2.20	0.41
1:A:353:ASN:CG	1:A:353:ASN:O	2.64	0.41
1:B:123:PHE:HD2	1:B:449:THR:HB	1.85	0.41
1:B:270:VAL:HB	1:B:443:GLN:HB2	2.02	0.41
1:B:318:GLU:OE2	1:B:375:LYS:HD2	2.20	0.41
1:B:123:PHE:HB3	1:B:449:THR:HA	2.02	0.41
1:A:133:ASN:HD22	1:A:133:ASN:HA	1.67	0.41
1:A:143:ASN:C	1:A:145:ASN:H	2.29	0.41
1:B:138:PHE:O	1:B:141:ARG:HG2	2.21	0.41
1:A:178:VAL:O	1:A:204:ASN:HB2	2.20	0.41
1:B:149:GLY:CA	3:B:1505:HOH:O	2.65	0.41
1:A:192:ILE:O	1:A:196:GLN:HG3	2.20	0.41
1:A:214:PHE:C	1:A:216:ASN:N	2.79	0.41
1:B:8:TYR:OH	1:B:69:TYR:HB3	2.20	0.41
1:A:39:PRO:O	1:A:348:ARG:NH1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:VAL:HG21	1:A:172:LEU:HD13	2.03	0.41
1:A:158:GLY:O	1:A:182:ILE:HA	2.20	0.41
1:A:472:GLU:HB3	3:A:1465:HOH:O	2.21	0.41
1:A:489:LYS:N	3:A:1423:HOH:O	2.53	0.41
1:B:307:ILE:HG23	1:B:308:LEU:N	2.35	0.41
1:B:370:LEU:HD12	1:B:370:LEU:HA	1.93	0.41
1:B:2:PRO:HA	1:B:6:GLN:OE1	2.21	0.41
1:B:22:GLU:HG3	1:B:138:PHE:CG	2.56	0.41
1:B:310:ARG:NH2	1:B:318:GLU:O	2.53	0.41
1:B:393:GLU:OE1	1:B:432:ARG:HD2	2.21	0.41
1:A:154:ILE:CG2	1:A:155:THR:N	2.84	0.40
1:B:25:ILE:CD1	1:B:245:ALA:HB2	2.42	0.40
1:B:162:GLY:O	1:B:193:GLN:HB3	2.21	0.40
1:B:214:PHE:C	1:B:216:ASN:N	2.79	0.40
1:A:2:PRO:HA	1:A:6:GLN:OE1	2.21	0.40
1:A:102:ASN:HD21	1:A:109:ASN:HD22	1.68	0.40
1:A:278:ASN:O	1:A:338:ASN:HB2	2.20	0.40
1:A:279:PHE:HB2	1:A:336:SER:OG	2.21	0.40
1:A:511:LYS:HB3	1:A:511:LYS:HE3	1.87	0.40
1:B:186:THR:C	1:B:188:ARG:N	2.80	0.40
1:B:191:PRO:O	1:B:195:GLU:HG3	2.22	0.40
1:B:267:SER:OG	1:B:269:LYS:HG3	2.21	0.40
1:B:509:LEU:HD12	1:B:511:LYS:HB2	2.03	0.40
1:B:346:LEU:HD23	1:B:346:LEU:HA	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	505/514 (98%)	456 (90%)	39 (8%)	10 (2%)	6 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	505/514 (98%)	452 (90%)	44 (9%)	9 (2%)	6	18
All	All	1010/1028 (98%)	908 (90%)	83 (8%)	19 (2%)	6	17

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	LYS
1	B	228	LYS
1	A	148	GLU
1	A	235	ASN
1	A	265	LYS
1	B	148	GLU
1	B	235	ASN
1	B	265	LYS
1	A	227	ASP
1	A	491	LYS
1	B	227	ASP
1	B	491	LYS
1	A	147	PRO
1	A	495	ARG
1	B	495	ARG
1	B	147	PRO
1	A	202	ASP
1	A	162	GLY
1	B	162	GLY

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	425/438 (97%)	396 (93%)	29 (7%)	14	35
1	B	425/438 (97%)	396 (93%)	29 (7%)	14	35
All	All	850/876 (97%)	792 (93%)	58 (7%)	14	35

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	43	GLN
1	A	59	GLN
1	A	67	ARG
1	A	99	LEU
1	A	123	PHE
1	A	139	LEU
1	A	140	GLN
1	A	141	ARG
1	A	183	LEU
1	A	206	GLN
1	A	218	GLN
1	A	225	PHE
1	A	230	PHE
1	A	234	HIS
1	A	269	LYS
1	A	270	VAL
1	A	293	LEU
1	A	304	GLU
1	A	321	ASP
1	A	391	THR
1	A	401	SER
1	A	415	LYS
1	A	420	ASP
1	A	447	LEU
1	A	478	GLU
1	A	485	THR
1	A	502	LYS
1	A	512	MSE
1	B	7	VAL
1	B	43	GLN
1	B	59	GLN
1	B	67	ARG
1	B	99	LEU
1	B	123	PHE
1	B	128	LEU
1	B	139	LEU
1	B	141	ARG
1	B	183	LEU
1	B	206	GLN
1	B	218	GLN
1	B	225	PHE
1	B	230	PHE

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Mol	Chain	Res	Type
1	B	234	HIS
1	B	269	LYS
1	B	270	VAL
1	B	293	LEU
1	B	304	GLU
1	B	321	ASP
1	B	391	THR
1	B	401	SER
1	B	415	LYS
1	B	420	ASP
1	B	447	LEU
1	B	478	GLU
1	B	485	THR
1	B	502	LYS
1	B	512	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	51	ASN
1	A	59	GLN
1	A	109	ASN
1	A	117	HIS
1	A	129	GLN
1	A	133	ASN
1	A	193	GLN
1	A	196	GLN
1	A	240	ASN
1	A	250	GLN
1	A	364	ASN
1	A	438	ASN
1	A	460	ASN
1	A	503	ASN
1	B	43	GLN
1	B	51	ASN
1	B	59	GLN
1	B	109	ASN
1	B	117	HIS
1	B	129	GLN
1	B	133	ASN
1	B	193	GLN

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Mol	Chain	Res	Type
1	B	196	GLN
1	B	218	GLN
1	B	240	ASN
1	B	250	GLN
1	B	260	GLN
1	B	364	ASN
1	B	438	ASN
1	B	460	ASN
1	B	503	ASN

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](#)

2 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	B	1400	1	15,15,16	3.86	7 (46%)	21,22,23	2.54	9 (42%)
2	PLP	A	1400	1	15,15,16	3.48	7 (46%)	21,22,23	2.62	10 (47%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	B	1400	1	-	2/6/6/8	0/1/1/1
2	PLP	A	1400	1	-	1/6/6/8	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1400	PLP	C5-C4	11.60	1.53	1.40
2	A	1400	PLP	C5-C4	10.17	1.52	1.40
2	B	1400	PLP	C3-C2	5.43	1.46	1.41
2	A	1400	PLP	C3-C2	4.40	1.45	1.41
2	B	1400	PLP	C4A-C4	-4.03	1.43	1.51
2	A	1400	PLP	C4A-C4	-3.92	1.43	1.51
2	B	1400	PLP	C2-N1	3.70	1.40	1.33
2	B	1400	PLP	C5A-C5	3.48	1.60	1.50
2	A	1400	PLP	P-O4P	3.28	1.70	1.60
2	A	1400	PLP	C5A-C5	3.11	1.59	1.50
2	A	1400	PLP	C2-N1	3.02	1.39	1.33
2	B	1400	PLP	C6-N1	2.17	1.38	1.34
2	B	1400	PLP	P-O4P	2.10	1.67	1.60
2	A	1400	PLP	P-O3P	-2.09	1.47	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1400	PLP	C2A-C2-C3	5.66	127.42	120.80
2	B	1400	PLP	C2A-C2-C3	5.46	127.19	120.80
2	A	1400	PLP	O4P-C5A-C5	4.69	118.15	109.36
2	B	1400	PLP	O4P-C5A-C5	4.20	117.22	109.36
2	A	1400	PLP	C6-N1-C2	4.07	126.59	119.20
2	B	1400	PLP	C6-N1-C2	3.91	126.28	119.20
2	B	1400	PLP	C4A-C4-C5	3.69	124.75	120.94
2	B	1400	PLP	O3-C3-C4	3.44	127.08	118.10
2	A	1400	PLP	C4A-C4-C5	3.41	124.45	120.94
2	B	1400	PLP	C3-C2-N1	-3.38	116.70	120.96
2	A	1400	PLP	O3-C3-C4	3.35	126.84	118.10
2	A	1400	PLP	C3-C2-N1	-3.32	116.77	120.96
2	A	1400	PLP	C5-C6-N1	-3.00	118.95	123.83
2	B	1400	PLP	C5-C6-N1	-2.90	119.11	123.83
2	A	1400	PLP	C4A-C4-C3	-2.75	115.94	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1400	PLP	C4A-C4-C3	-2.63	116.14	120.52
2	B	1400	PLP	O3-C3-C2	-2.31	112.79	117.58
2	A	1400	PLP	O3P-P-O2P	2.19	116.00	107.80
2	A	1400	PLP	O3-C3-C2	-2.03	113.37	117.58

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1400	PLP	C6-C5-C5A-O4P
2	B	1400	PLP	C6-C5-C5A-O4P
2	B	1400	PLP	C5A-O4P-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

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	503/514 (97%)	-0.04	5 (0%) 79 78	21, 44, 99, 100	0
1	B	503/514 (97%)	-0.23	5 (0%) 79 78	16, 38, 84, 100	0
All	All	1006/1028 (97%)	-0.13	10 (0%) 79 78	16, 42, 90, 100	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	VAL	2.9
1	A	148	GLU	2.6
1	A	374	GLY	2.4
1	B	215	ASP	2.3
1	A	225	PHE	2.3
1	A	496	ALA	2.2
1	B	227	ASP	2.1
1	B	150	GLU	2.1
1	B	230	PHE	2.0
1	B	508	GLU	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
2	PLP	A	1400	15/16	0.95	0.08	35,37,39,39	0
2	PLP	B	1400	15/16	0.97	0.07	39,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.