



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:15 PM UTC

PDB ID : 1ARI / pdb_00001ari
Title : Aspartate aminotransferase, W140H mutant, maleate complex
Authors : Malashkevich, V.N.; Jansonius, J.N.
Deposited on : 1995-08-23
Resolution : 2.30 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

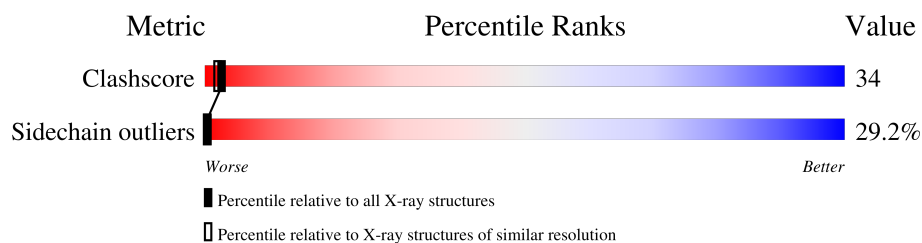
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

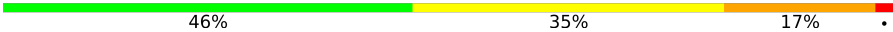
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	 46% 35% 17% •
1	B	396	 40% 41% 17% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6883 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.

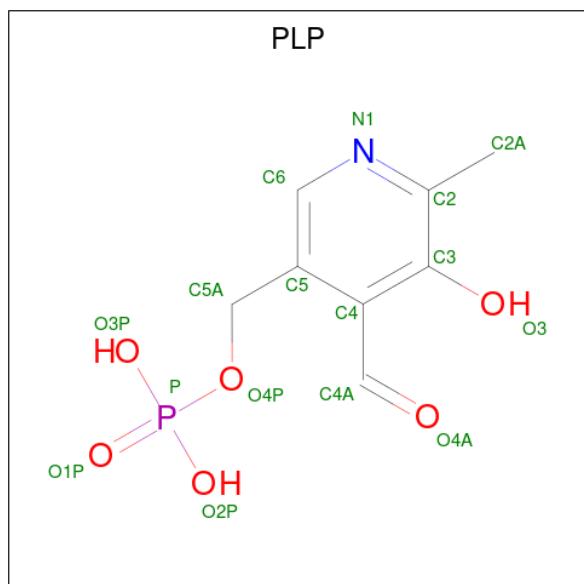
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3065	1931	537	584	13			
1	B	396	Total	C	N	O	S	0	0	0
			3065	1931	537	584	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	HIS	TRP	engineered mutation	UNP P00509
B	140	HIS	TRP	engineered mutation	UNP P00509

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



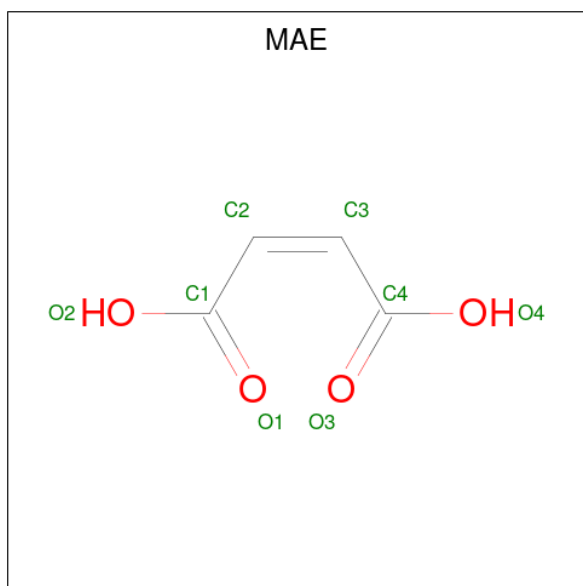
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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

- Molecule 3 is MALEIC ACID (CCD ID: MAE) (formula: $C_4H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		
3	B	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is water.

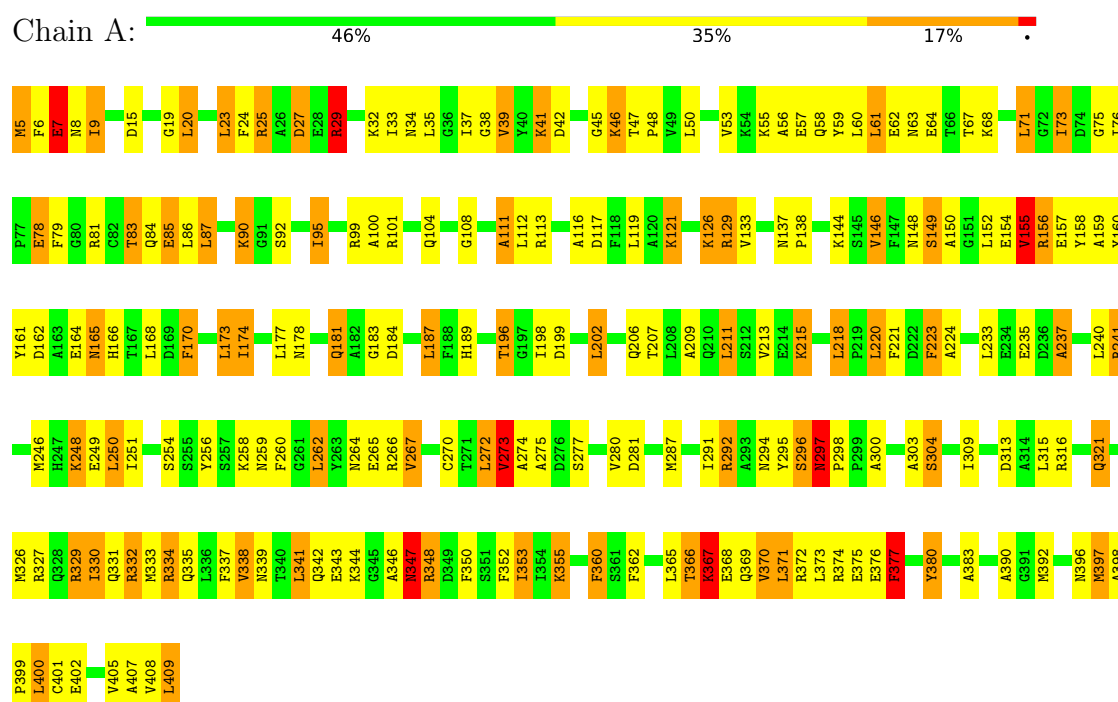
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	366	Total	O	0	0
			366	366		
4	B	341	Total	O	0	0
			341	341		

3 Residue-property plots

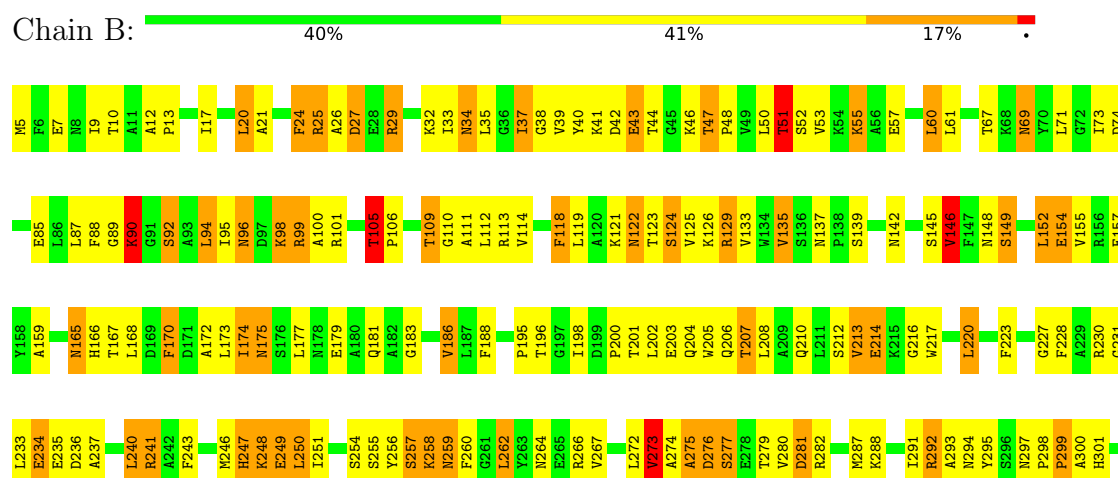
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

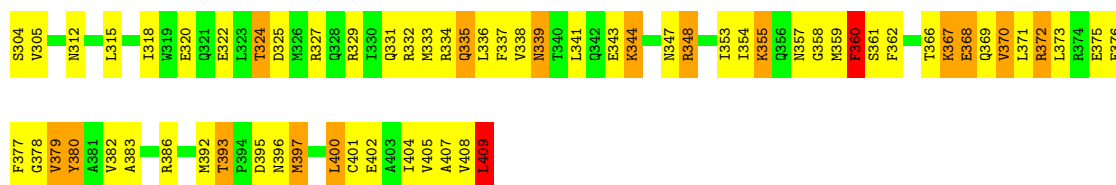
Note EDS was not executed.

• Molecule 1: ASPARTATE AMINOTRANSFERASE



• Molecule 1: ASPARTATE AMINOTRANSFERASE





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.40 Å 79.00 Å 90.80 Å 90.00° 118.80° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	92.0 (8.00-2.30)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 4C	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6883	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAE, 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	1.07	0/3125	1.64	42/4232 (1.0%)
1	B	1.10	0/3125	1.68	48/4232 (1.1%)
All	All	1.08	0/6250	1.66	90/8464 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0

There are no bond length outliers.

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	300	ALA	N-CA-C	9.94	121.70	111.07
1	B	106	PRO	N-CA-CB	8.89	108.70	102.65
1	A	300	ALA	N-CA-C	8.31	120.34	111.28
1	B	275	ALA	N-CA-C	7.88	119.88	111.28
1	B	273	VAL	N-CA-CB	7.74	123.24	110.86
1	A	155	VAL	N-CA-C	7.26	118.33	107.80
1	B	146	VAL	N-CA-CB	6.96	118.21	110.62
1	B	325	ASP	CA-CB-CG	6.79	119.39	112.60
1	B	258	LYS	CB-CA-C	6.78	121.64	109.29
1	A	258	LYS	CB-CA-C	6.61	123.39	111.03
1	A	42	ASP	CA-CB-CG	6.53	119.13	112.60
1	B	148	ASN	CA-CB-CG	6.38	118.98	112.60
1	B	51	THR	CB-CA-C	6.32	121.59	110.85
1	B	360	PHE	N-CA-C	6.31	120.14	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	GLY	N-CA-C	6.27	128.04	113.18
1	A	196	THR	N-CA-C	6.14	119.96	112.23
1	A	360	PHE	N-CA-C	6.06	119.53	110.14
1	B	90	LYS	N-CA-C	-6.06	103.04	111.52
1	A	199	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	67	THR	N-CA-C	6.03	118.35	109.24
1	A	84	GLN	N-CA-CB	6.02	119.57	110.30
1	A	215	LYS	N-CA-C	6.01	119.80	112.23
1	B	96	ASN	N-CA-C	5.97	119.66	112.38
1	A	71	LEU	N-CA-C	-5.90	102.20	110.35
1	B	237	ALA	N-CA-C	5.90	120.47	113.28
1	A	78	GLU	O-C-N	5.88	128.44	122.09
1	B	264	ASN	N-CA-C	5.86	120.15	112.89
1	A	367	LYS	CA-C-N	5.85	128.60	120.29
1	A	367	LYS	C-N-CA	5.85	128.60	120.29
1	A	396	ASN	CA-CB-CG	5.83	118.43	112.60
1	B	92	SER	CA-C-N	5.81	127.99	120.44
1	B	92	SER	C-N-CA	5.81	127.99	120.44
1	B	196	THR	N-CA-C	5.78	118.52	111.82
1	B	409	LEU	N-CA-CB	5.75	120.28	110.50
1	B	51	THR	N-CA-C	5.73	117.61	111.36
1	A	27	ASP	CA-CB-CG	5.72	118.32	112.60
1	B	92	SER	CA-C-O	5.72	128.69	120.51
1	A	313	ASP	N-CA-C	5.71	117.99	111.02
1	B	186	VAL	CB-CA-C	5.70	117.51	110.73
1	B	380	TYR	N-CA-C	5.69	118.00	108.96
1	A	407	ALA	CA-C-N	-5.67	115.02	122.16
1	A	407	ALA	C-N-CA	-5.67	115.02	122.16
1	A	250	LEU	N-CA-CB	-5.67	102.61	111.56
1	A	297	ASN	N-CA-CB	5.66	116.59	111.27
1	B	339	ASN	CA-CB-CG	-5.66	106.94	112.60
1	B	243	PHE	CA-CB-CG	5.65	119.45	113.80
1	A	292	ARG	N-CA-C	5.65	118.98	111.75
1	A	347	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	296	SER	N-CA-C	5.55	122.63	110.80
1	B	29	ARG	CA-C-N	5.54	126.76	119.84
1	B	29	ARG	C-N-CA	5.54	126.76	119.84
1	B	282	ARG	NE-CZ-NH2	5.47	124.13	119.20
1	B	172	ALA	N-CA-C	-5.47	104.85	112.45
1	A	298	PRO	N-CA-C	5.42	117.31	110.70
1	A	29	ARG	CA-C-N	5.42	126.61	119.84
1	A	29	ARG	C-N-CA	5.42	126.61	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	TYR	N-CA-C	5.37	117.50	108.96
1	B	335	GLN	N-CA-CB	5.36	118.19	110.20
1	B	298	PRO	N-CA-C	5.33	117.21	110.70
1	A	339	ASN	CA-CB-CG	-5.31	107.29	112.60
1	B	216	GLY	CA-C-N	-5.31	113.58	122.92
1	B	216	GLY	C-N-CA	-5.31	113.58	122.92
1	A	397	MET	N-CA-C	5.29	117.73	111.33
1	A	237	ALA	N-CA-C	5.27	119.43	112.89
1	B	71	LEU	N-CA-C	-5.27	103.93	110.41
1	A	334	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	A	184	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	75	GLY	CA-C-N	5.24	126.36	122.59
1	A	75	GLY	C-N-CA	5.24	126.36	122.59
1	B	188	PHE	CB-CA-C	-5.23	100.40	110.24
1	B	267	VAL	N-CA-C	5.20	115.53	107.78
1	B	165	ASN	CB-CA-C	5.20	118.75	109.29
1	A	298	PRO	CA-C-N	5.18	126.31	119.84
1	A	298	PRO	C-N-CA	5.18	126.31	119.84
1	A	7	GLU	N-CA-C	5.17	119.07	112.87
1	B	292	ARG	CA-C-N	-5.11	115.04	122.86
1	B	292	ARG	C-N-CA	-5.11	115.04	122.86
1	B	247	HIS	N-CA-C	5.10	117.44	110.55
1	B	24	PHE	CA-CB-CG	-5.09	108.71	113.80
1	A	273	VAL	N-CA-CB	5.08	123.81	111.81
1	B	105	THR	N-CA-C	5.08	113.98	108.14
1	B	118	PHE	CA-C-N	5.05	127.81	120.79
1	B	118	PHE	C-N-CA	5.05	127.81	120.79
1	B	105	THR	N-CA-CB	-5.04	104.95	111.35
1	B	170	PHE	N-CA-C	5.03	117.15	111.11
1	A	377	PHE	N-CA-C	5.03	120.25	113.72
1	B	299	PRO	CB-CA-C	-5.01	106.84	111.40
1	A	111	ALA	CA-C-N	5.01	127.75	120.79
1	A	111	ALA	C-N-CA	5.01	127.75	120.79
1	B	216	GLY	O-C-N	-5.01	116.19	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	409	LEU	CA

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	3065	0	3012	218	0
1	B	3065	0	3012	210	0
2	A	15	0	6	1	0
2	B	15	0	6	3	0
3	A	8	0	2	1	0
3	B	8	0	2	2	0
4	A	366	0	0	31	0
4	B	341	0	0	29	0
All	All	6883	0	6040	416	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 34.

All (416) 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:347:ASN:H	1:A:347:ASN:HD22	1.03	0.99
1:B:393:THR:HG22	1:B:396:ASN:H	1.29	0.94
1:A:260:PHE:HB3	1:A:262:LEU:HD22	1.54	0.89
1:A:344:LYS:HE2	1:A:402:GLU:HG2	1.54	0.89
1:B:332:ARG:HD2	1:B:333:MET:CE	2.02	0.89
1:B:400:LEU:HD23	1:B:404:ILE:HD12	1.56	0.88
1:A:294:ASN:HD21	1:B:294:ASN:HD21	1.21	0.88
1:B:129:ARG:HD3	1:B:154:GLU:HG2	1.56	0.85
1:B:348:ARG:NH1	1:B:409:LEU:HD22	1.94	0.83
1:A:126:LYS:HE2	1:A:129:ARG:HD3	1.61	0.82
1:A:347:ASN:H	1:A:347:ASN:ND2	1.76	0.82
1:A:32:LYS:C	1:A:33:ILE:HD13	2.05	0.82
1:B:99:ARG:HG2	1:B:274:ALA:O	1.82	0.80
1:A:20:LEU:HA	1:A:23:LEU:HD12	1.64	0.78
1:A:34:ASN:O	1:A:35:LEU:HD23	1.84	0.77
1:A:370:VAL:HG21	1:A:383:ALA:HA	1.65	0.77
1:A:165:ASN:H	1:A:165:ASN:HD22	1.30	0.77
1:B:37:ILE:HB	4:B:789:HOH:O	1.85	0.77
1:A:235:GLU:HG2	4:A:642:HOH:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LEU:HD13	1:A:177:LEU:HD12	1.66	0.77
1:B:53:VAL:HG13	1:B:305:VAL:HG11	1.67	0.76
1:A:350:PHE:O	1:A:353:ILE:HB	1.85	0.76
1:A:367:LYS:HD2	4:A:555:HOH:O	1.85	0.76
1:B:124:SER:HB2	4:B:690:HOH:O	1.85	0.76
1:B:393:THR:HG22	1:B:396:ASN:N	2.00	0.76
1:A:46:LYS:O	1:A:48:PRO:HD3	1.84	0.76
1:A:126:LYS:HE2	1:A:129:ARG:HB3	1.65	0.76
1:B:272:LEU:HD22	1:B:287:MET:CE	2.16	0.75
1:B:397:MET:CE	1:B:400:LEU:HD13	2.17	0.75
1:B:46:LYS:CD	1:B:47:THR:H	1.99	0.75
1:B:55:LYS:HE2	4:B:545:HOH:O	1.84	0.75
1:B:366:THR:OG1	1:B:369:GLN:HG3	1.86	0.75
1:A:272:LEU:HD12	1:A:287:MET:SD	2.27	0.74
1:B:260:PHE:HB3	1:B:262:LEU:HD22	1.68	0.73
1:B:376:GLU:HB3	1:B:377:PHE:CD2	2.22	0.73
1:A:398:ALA:O	1:A:402:GLU:HG3	1.89	0.73
1:B:123:THR:OG1	1:B:125:VAL:HG23	1.89	0.73
1:A:46:LYS:HE2	1:A:47:THR:H	1.54	0.72
1:A:397:MET:HE3	1:A:400:LEU:HD23	1.71	0.72
1:B:332:ARG:HD2	1:B:333:MET:HE2	1.70	0.72
1:A:397:MET:CE	1:A:400:LEU:HD23	2.20	0.72
1:A:39:VAL:HG21	1:B:69:ASN:HD21	1.55	0.72
1:B:397:MET:HE3	1:B:400:LEU:HD13	1.72	0.71
1:B:348:ARG:HG3	1:B:348:ARG:HH11	1.54	0.71
1:B:256:TYR:HA	1:B:259:ASN:HD21	1.55	0.71
1:A:126:LYS:CE	1:A:129:ARG:HD3	2.20	0.71
1:B:397:MET:HE3	1:B:397:MET:HA	1.73	0.71
1:A:327:ARG:O	1:A:331:GLN:HG3	1.89	0.70
1:B:42:ASP:HB2	1:B:43:GLU:OE2	1.90	0.70
1:B:201:THR:OG1	1:B:204:GLN:HG3	1.91	0.70
1:B:214:GLU:HB3	4:B:526:HOH:O	1.89	0.70
1:A:223:PHE:O	1:A:254:SER:HA	1.91	0.70
1:B:367:LYS:HZ1	1:B:367:LYS:N	1.89	0.70
1:B:367:LYS:HB2	1:B:367:LYS:HZ2	1.54	0.70
1:A:60:LEU:HD11	1:A:304:SER:HB3	1.72	0.70
1:A:92:SER:HB3	1:A:95:ILE:HG13	1.73	0.70
1:A:348:ARG:HD3	4:A:661:HOH:O	1.90	0.70
1:A:366:THR:HG22	1:A:369:GLN:H	1.58	0.69
1:B:21:ALA:O	1:B:25:ARG:HB2	1.92	0.69
1:A:209:ALA:O	1:A:213:VAL:HG23	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:MET:HA	1:A:5:MET:HE3	1.74	0.69
2:B:410:PLP:C4A	3:B:411:MAE:H2	2.23	0.69
1:A:333:MET:HA	1:A:333:MET:HE2	1.73	0.69
1:A:260:PHE:HB3	1:A:262:LEU:CD2	2.23	0.68
1:B:38:GLY:C	1:B:359:MET:HE1	2.18	0.68
1:B:393:THR:HG23	1:B:395:ASP:H	1.58	0.68
1:A:79:PHE:O	1:A:83:THR:HG23	1.93	0.68
1:B:43:GLU:CD	1:B:43:GLU:H	2.00	0.67
1:B:368:GLU:HB3	4:B:714:HOH:O	1.93	0.67
1:A:81:ARG:HD2	4:A:587:HOH:O	1.93	0.67
1:B:129:ARG:HD3	1:B:154:GLU:CG	2.24	0.67
1:A:85:GLU:OE1	1:A:90:LYS:HD2	1.94	0.66
1:B:372:ARG:HH21	1:B:408:VAL:HA	1.59	0.66
1:B:341:LEU:HD13	1:B:401:CYS:SG	2.35	0.66
1:B:344:LYS:HD3	1:B:402:GLU:HG3	1.77	0.66
1:B:46:LYS:HD2	1:B:47:THR:H	1.59	0.66
1:A:126:LYS:O	1:A:126:LYS:HG2	1.94	0.66
1:B:318:ILE:O	1:B:322:GLU:HG3	1.96	0.66
1:A:181:GLN:HG3	4:A:431:HOH:O	1.96	0.65
1:A:29:ARG:NH2	4:A:536:HOH:O	2.30	0.65
1:A:39:VAL:HG21	4:B:460:HOH:O	1.95	0.65
1:A:248:LYS:HE2	4:A:566:HOH:O	1.97	0.65
1:A:344:LYS:HE2	1:A:402:GLU:CG	2.26	0.65
1:A:374:ARG:NE	4:A:615:HOH:O	2.30	0.65
1:B:291:ILE:HG23	1:B:295:TYR:CZ	2.32	0.65
1:A:5:MET:N	1:A:7:GLU:OE1	2.29	0.65
1:A:347:ASN:ND2	1:A:409:LEU:HD12	2.10	0.65
1:B:137:ASN:ND2	4:B:734:HOH:O	2.29	0.65
1:A:99:ARG:NH1	1:A:274:ALA:O	2.30	0.65
1:A:329:ARG:NH2	1:A:392:MET:O	2.29	0.65
1:B:401:CYS:O	1:B:405:VAL:HG23	1.96	0.65
1:B:40:TYR:O	1:B:47:THR:HG23	1.95	0.65
1:B:320:GLU:O	1:B:324:THR:HG22	1.96	0.64
1:B:327:ARG:NE	4:B:722:HOH:O	2.29	0.64
1:A:129:ARG:HH22	1:A:181:GLN:NE2	1.96	0.64
1:B:366:THR:O	1:B:370:VAL:HG13	1.98	0.64
1:B:230:ARG:NH1	4:B:495:HOH:O	2.30	0.64
1:A:338:VAL:HG12	1:A:353:ILE:HG21	1.79	0.63
1:B:272:LEU:HB2	1:B:287:MET:HE1	1.79	0.63
1:B:105:THR:HG21	1:B:111:ALA:HB2	1.79	0.63
1:B:46:LYS:O	1:B:48:PRO:HD3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASN:H	1:A:165:ASN:ND2	1.97	0.63
1:A:371:LEU:HD13	1:A:371:LEU:O	1.98	0.63
1:A:32:LYS:O	1:A:33:ILE:HD13	1.98	0.62
1:B:213:VAL:HG23	1:B:247:HIS:NE2	2.13	0.62
1:A:46:LYS:HG3	1:A:47:THR:N	2.14	0.62
1:B:301:HIS:O	1:B:305:VAL:HG23	2.00	0.62
1:A:162:ASP:OD2	1:A:165:ASN:ND2	2.33	0.61
1:B:200:PRO:HG2	1:B:205:TRP:CE2	2.34	0.61
1:A:7:GLU:HG2	4:A:750:HOH:O	2.00	0.61
1:A:99:ARG:HD2	1:A:274:ALA:O	2.00	0.61
1:B:207:THR:HG22	1:B:208:LEU:N	2.15	0.61
1:B:376:GLU:HG2	1:B:377:PHE:CE2	2.35	0.61
1:A:241:ARG:HG2	4:A:450:HOH:O	2.01	0.61
1:A:371:LEU:HD21	4:A:586:HOH:O	1.99	0.61
1:A:50:LEU:HD13	4:A:498:HOH:O	2.01	0.61
1:A:265:GLU:OE1	1:A:265:GLU:HA	2.02	0.60
1:A:347:ASN:HD22	1:A:347:ASN:N	1.85	0.60
1:B:348:ARG:NH1	1:B:348:ARG:HG3	2.16	0.60
1:B:170:PHE:CD1	1:B:173:LEU:HD23	2.37	0.60
1:B:272:LEU:HD22	1:B:287:MET:HE2	1.84	0.60
1:A:126:LYS:NZ	1:A:129:ARG:HD3	2.16	0.60
1:A:173:LEU:CD1	1:A:177:LEU:HD12	2.32	0.60
1:B:24:PHE:CE1	1:B:32:LYS:HG3	2.37	0.60
1:B:260:PHE:HB3	1:B:262:LEU:CD2	2.32	0.59
1:B:99:ARG:NH1	1:B:274:ALA:O	2.34	0.59
1:B:125:VAL:HA	4:B:523:HOH:O	2.02	0.59
1:B:248:LYS:HG2	1:B:275:ALA:HB2	1.83	0.59
1:A:126:LYS:HZ3	1:A:129:ARG:CZ	2.16	0.59
1:B:99:ARG:O	1:B:280:VAL:HG11	2.02	0.59
1:B:234:GLU:HG3	1:B:241:ARG:NH2	2.18	0.58
1:A:33:ILE:HD13	1:A:33:ILE:N	2.17	0.58
1:A:100:ALA:O	1:A:101:ARG:HD2	2.03	0.58
1:A:346:ALA:HB3	4:A:547:HOH:O	2.03	0.58
1:A:372:ARG:NH2	4:A:656:HOH:O	2.35	0.58
1:B:383:ALA:HB3	4:B:662:HOH:O	2.04	0.58
1:A:347:ASN:HD21	1:A:409:LEU:CB	2.17	0.58
1:A:326:MET:O	1:A:330:ILE:HG13	2.02	0.58
1:A:233:LEU:HG	4:A:711:HOH:O	2.03	0.58
1:A:60:LEU:O	1:A:64:GLU:HB2	2.03	0.58
1:A:76:ILE:O	1:A:79:PHE:HB3	2.03	0.58
1:A:347:ASN:OD1	1:A:409:LEU:HB3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PHE:HD1	1:A:380:TYR:CD1	2.22	0.57
1:A:248:LYS:HG3	1:A:275:ALA:HB2	1.85	0.57
1:A:397:MET:HE2	1:A:401:CYS:SG	2.44	0.57
1:B:35:LEU:N	1:B:380:TYR:O	2.34	0.57
1:A:71:LEU:HD13	1:A:76:ILE:HG13	1.86	0.57
1:B:400:LEU:CD2	1:B:404:ILE:HD12	2.31	0.57
1:A:198:ILE:HG12	4:A:640:HOH:O	2.04	0.57
1:B:118:PHE:O	1:B:122:ASN:ND2	2.30	0.57
1:B:48:PRO:HD2	4:B:630:HOH:O	2.05	0.57
1:A:256:TYR:HB2	1:A:267:VAL:HB	1.87	0.57
1:B:367:LYS:H	1:B:367:LYS:NZ	2.03	0.56
1:A:165:ASN:ND2	1:A:165:ASN:N	2.53	0.56
1:A:294:ASN:ND2	1:B:294:ASN:HD21	1.98	0.56
1:B:129:ARG:HD3	1:B:154:GLU:CD	2.31	0.56
1:A:34:ASN:C	1:A:35:LEU:HD23	2.31	0.56
1:A:372:ARG:HD3	1:A:408:VAL:CG1	2.36	0.56
1:A:371:LEU:HD23	4:A:591:HOH:O	2.06	0.56
1:B:250:LEU:HG	1:B:273:VAL:HG13	1.87	0.56
1:B:367:LYS:N	1:B:367:LYS:NZ	2.53	0.56
2:B:410:PLP:C4A	3:B:411:MAE:H3	2.36	0.56
1:A:159:ALA:O	1:A:173:LEU:HA	2.07	0.55
1:A:366:THR:CG2	1:A:368:GLU:HB2	2.36	0.55
1:A:398:ALA:HB3	1:A:399:PRO:HD3	1.88	0.55
1:A:39:VAL:HG21	1:B:69:ASN:ND2	2.20	0.55
1:A:273:VAL:HG23	1:A:274:ALA:N	2.20	0.55
1:A:309:ILE:O	1:A:316:ARG:HB2	2.07	0.55
1:B:110:GLY:O	1:B:114:VAL:HG13	2.06	0.55
1:B:33:ILE:HG22	1:B:35:LEU:HG	1.89	0.55
1:B:337:PHE:O	1:B:341:LEU:HB2	2.06	0.55
1:A:156:ARG:HD2	1:A:156:ARG:N	2.20	0.55
1:A:352:PHE:O	1:A:355:LYS:HG2	2.05	0.55
1:A:373:LEU:HA	1:A:377:PHE:HD1	1.71	0.55
1:B:34:ASN:C	1:B:34:ASN:HD22	2.13	0.55
1:A:202:LEU:HD22	1:A:202:LEU:O	2.07	0.55
1:B:212:SER:HA	1:B:217:TRP:CE3	2.42	0.55
1:A:146:VAL:HA	1:B:293:ALA:HB1	1.90	0.54
1:A:294:ASN:HD21	1:B:294:ASN:ND2	1.98	0.54
1:B:113:ARG:NH2	4:B:485:HOH:O	2.39	0.54
1:A:38:GLY:HA3	4:A:654:HOH:O	2.08	0.53
1:A:64:GLU:OE1	1:A:68:LYS:NZ	2.40	0.53
1:A:220:LEU:HD23	1:A:221:PHE:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:PHE:CZ	1:B:32:LYS:HG3	2.43	0.53
1:B:135:VAL:O	1:B:157:GLU:HA	2.07	0.53
1:A:126:LYS:N	4:A:474:HOH:O	2.30	0.53
1:B:126:LYS:N	4:B:523:HOH:O	2.30	0.53
1:A:73:ILE:HD13	1:A:292:ARG:HB2	1.91	0.53
1:A:46:LYS:HE2	1:A:46:LYS:HA	1.89	0.53
1:B:348:ARG:HH11	1:B:409:LEU:HD22	1.73	0.53
1:A:367:LYS:HB2	4:A:505:HOH:O	2.08	0.53
1:A:294:ASN:O	1:B:109:THR:HG22	2.08	0.52
1:A:129:ARG:HB2	1:A:154:GLU:O	2.09	0.52
1:B:234:GLU:HB2	4:B:675:HOH:O	2.09	0.52
1:B:9:ILE:HG22	1:B:10:THR:N	2.25	0.52
1:A:344:LYS:NZ	1:A:402:GLU:OE2	2.35	0.52
1:B:175:ASN:N	1:B:175:ASN:HD22	2.07	0.52
1:A:46:LYS:CE	1:A:47:THR:H	2.20	0.52
1:A:321:GLN:O	1:A:321:GLN:NE2	2.43	0.52
1:A:338:VAL:HG12	1:A:353:ILE:CG2	2.40	0.51
1:B:273:VAL:HG23	1:B:274:ALA:N	2.25	0.51
1:A:129:ARG:HH21	1:A:181:GLN:HB2	1.75	0.51
1:B:37:ILE:HG13	1:B:38:GLY:N	2.25	0.51
1:A:330:ILE:HD13	1:A:390:ALA:HB2	1.92	0.51
1:A:291:ILE:HG23	1:A:295:TYR:CZ	2.46	0.51
1:B:327:ARG:O	1:B:331:GLN:HG3	2.09	0.51
1:A:189:HIS:HB2	4:A:688:HOH:O	2.09	0.51
1:B:288:LYS:HA	1:B:291:ILE:HD12	1.91	0.51
1:A:401:CYS:O	1:A:405:VAL:HG23	2.11	0.51
1:B:142:ASN:O	1:B:146:VAL:HG13	2.11	0.51
1:A:155:VAL:C	1:A:156:ARG:HD2	2.36	0.51
1:A:35:LEU:HB2	1:A:380:TYR:O	2.11	0.51
1:A:327:ARG:HG2	1:A:331:GLN:HE21	1.76	0.51
1:B:125:VAL:C	1:B:126:LYS:HG3	2.36	0.51
1:B:291:ILE:HG21	4:B:568:HOH:O	2.11	0.51
1:A:373:LEU:HA	1:A:377:PHE:CD1	2.47	0.50
1:B:90:LYS:HG2	4:B:705:HOH:O	2.10	0.50
1:B:379:VAL:HG12	1:B:379:VAL:O	2.11	0.50
1:A:165:ASN:HD22	1:A:165:ASN:N	2.00	0.50
1:B:125:VAL:O	1:B:126:LYS:HG3	2.11	0.50
1:B:372:ARG:NH2	1:B:408:VAL:HA	2.25	0.50
1:A:126:LYS:HZ3	1:A:129:ARG:NE	2.10	0.50
1:B:27:ASP:HB2	4:B:718:HOH:O	2.11	0.50
1:B:34:ASN:HA	1:B:380:TYR:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ALA:HB3	1:B:280:VAL:HB	1.93	0.50
1:A:50:LEU:HB2	4:A:498:HOH:O	2.12	0.50
1:B:44:THR:HG21	4:B:679:HOH:O	2.11	0.50
1:A:341:LEU:HD13	1:A:401:CYS:SG	2.52	0.50
1:B:145:SER:O	1:B:149:SER:OG	2.30	0.50
1:B:380:TYR:CD1	1:B:380:TYR:N	2.79	0.50
1:B:329:ARG:NH1	1:B:329:ARG:HG2	2.26	0.50
1:B:183:GLY:N	4:B:601:HOH:O	2.45	0.49
1:A:183:GLY:HA2	1:B:5:MET:HE1	1.93	0.49
1:A:211:LEU:HD22	1:A:215:LYS:HG3	1.95	0.49
1:A:59:TYR:O	1:A:63:ASN:ND2	2.46	0.49
1:A:87:LEU:O	1:A:241:ARG:NH1	2.45	0.49
1:A:101:ARG:HD3	4:A:421:HOH:O	2.11	0.49
1:B:277:SER:O	1:B:281:ASP:HB2	2.13	0.49
1:A:59:TYR:CD2	1:A:63:ASN:ND2	2.81	0.49
1:A:280:VAL:HG13	1:A:281:ASP:N	2.28	0.49
1:A:398:ALA:HB3	1:A:399:PRO:CD	2.43	0.49
1:B:37:ILE:HG21	4:B:474:HOH:O	2.12	0.49
1:B:266:ARG:HH22	2:B:410:PLP:P	2.35	0.49
1:B:367:LYS:HB2	4:B:719:HOH:O	2.12	0.49
1:A:237:ALA:HB1	1:A:241:ARG:HD2	1.95	0.49
1:B:42:ASP:OD1	1:B:44:THR:OG1	2.30	0.49
1:B:339:ASN:HD22	1:B:339:ASN:HA	1.35	0.49
1:A:397:MET:HE1	1:A:400:LEU:HD23	1.94	0.48
1:B:195:PRO:HB3	1:B:386:ARG:HD3	1.94	0.48
1:A:117:ASP:O	1:A:121:LYS:HB2	2.14	0.48
1:B:360:PHE:HB2	4:B:477:HOH:O	2.13	0.48
1:A:99:ARG:NH2	4:A:552:HOH:O	2.46	0.48
1:B:347:ASN:HD22	1:B:409:LEU:HD13	1.78	0.48
1:A:24:PHE:CE1	1:A:34:ASN:HB2	2.49	0.48
1:A:334:ARG:NH2	1:A:360:PHE:O	2.47	0.48
1:B:173:LEU:HD12	1:B:173:LEU:O	2.14	0.48
1:B:51:THR:HG22	4:B:535:HOH:O	2.14	0.47
1:B:170:PHE:O	1:B:173:LEU:HB3	2.14	0.47
1:B:312:ASN:HB3	1:B:315:LEU:HB2	1.96	0.47
1:A:78:GLU:HA	1:A:78:GLU:OE1	2.12	0.47
1:A:237:ALA:CB	1:A:241:ARG:HH11	2.27	0.47
1:A:332:ARG:HD3	4:A:581:HOH:O	2.13	0.47
1:B:210:GLN:HE21	1:B:214:GLU:HG2	1.78	0.47
1:B:234:GLU:N	4:B:675:HOH:O	2.29	0.47
1:A:248:LYS:HB2	1:A:248:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PHE:CE1	1:A:341:LEU:HD22	2.49	0.47
1:A:337:PHE:O	1:A:341:LEU:HB2	2.14	0.47
1:B:234:GLU:HG3	1:B:241:ARG:HH22	1.78	0.47
1:B:344:LYS:NZ	1:B:402:GLU:OE2	2.40	0.47
1:B:358:GLY:N	4:B:515:HOH:O	2.30	0.47
1:A:20:LEU:HA	1:A:23:LEU:CD1	2.38	0.47
1:A:41:LYS:HE2	4:A:619:HOH:O	2.14	0.47
1:A:59:TYR:CG	1:A:63:ASN:ND2	2.83	0.47
1:A:113:ARG:NH1	1:A:149:SER:HB3	2.29	0.47
1:B:400:LEU:HD23	1:B:400:LEU:C	2.40	0.47
1:A:211:LEU:HD22	1:A:215:LYS:CG	2.45	0.46
1:B:159:ALA:O	1:B:173:LEU:HA	2.15	0.46
1:B:170:PHE:HZ	1:B:208:LEU:HG	1.80	0.46
1:A:113:ARG:HG2	1:B:294:ASN:HD22	1.80	0.46
1:B:177:LEU:C	1:B:179:GLU:H	2.23	0.46
1:B:129:ARG:CD	1:B:154:GLU:HG2	2.38	0.46
1:B:380:TYR:N	1:B:380:TYR:HD1	2.13	0.46
1:B:372:ARG:NH1	1:B:376:GLU:OE2	2.48	0.46
1:A:280:VAL:CG1	1:A:281:ASP:N	2.79	0.46
1:A:341:LEU:HD12	1:A:341:LEU:HA	1.47	0.46
1:A:116:ALA:HB1	1:A:150:ALA:CB	2.46	0.45
1:A:126:LYS:HZ1	1:A:129:ARG:HD3	1.79	0.45
1:B:88:PHE:CD1	1:B:94:LEU:HD22	2.51	0.45
1:B:100:ALA:C	1:B:101:ARG:HG2	2.41	0.45
1:B:220:LEU:HD12	1:B:220:LEU:C	2.41	0.45
1:B:332:ARG:HD2	1:B:333:MET:HE1	1.94	0.45
1:B:367:LYS:NZ	1:B:367:LYS:CB	2.80	0.45
1:A:347:ASN:ND2	1:A:409:LEU:CD1	2.80	0.45
1:B:255:SER:OG	1:B:257:SER:HB2	2.16	0.45
1:A:108:GLY:O	1:A:111:ALA:HB3	2.17	0.45
1:A:237:ALA:HB1	1:A:241:ARG:HH11	1.82	0.45
1:B:165:ASN:OD1	1:B:165:ASN:O	2.34	0.45
1:B:367:LYS:HB2	1:B:367:LYS:NZ	2.25	0.45
1:B:37:ILE:HG13	1:B:38:GLY:H	1.82	0.45
1:B:276:ASP:O	1:B:279:THR:N	2.49	0.45
1:A:126:LYS:NZ	1:A:129:ARG:CD	2.80	0.45
1:A:333:MET:HE2	1:A:333:MET:CA	2.44	0.45
1:B:166:HIS:O	1:B:355:LYS:HE2	2.17	0.45
1:B:272:LEU:HD22	1:B:287:MET:HE1	1.97	0.45
1:A:397:MET:HE3	1:A:397:MET:O	2.17	0.45
1:A:85:GLU:OE2	1:A:90:LYS:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LYS:CG	1:B:47:THR:N	2.80	0.44
1:A:6:PHE:O	1:A:9:ILE:HG13	2.17	0.44
1:A:24:PHE:CD1	1:A:380:TYR:CD1	3.02	0.44
1:A:25:ARG:O	1:A:27:ASP:N	2.50	0.44
3:A:411:MAE:C1	1:B:292:ARG:HH12	2.31	0.44
1:A:113:ARG:O	1:A:113:ARG:HG3	2.17	0.44
1:A:347:ASN:ND2	1:A:347:ASN:N	2.52	0.44
1:B:9:ILE:CG2	1:B:10:THR:N	2.80	0.44
1:A:126:LYS:NZ	1:A:129:ARG:CZ	2.80	0.44
1:B:240:LEU:C	1:B:240:LEU:HD22	2.42	0.44
1:B:372:ARG:NH2	1:B:407:ALA:O	2.50	0.44
1:A:237:ALA:CB	1:A:241:ARG:NH1	2.80	0.44
1:B:57:GLU:OE2	1:B:301:HIS:NE2	2.42	0.44
1:B:367:LYS:HG2	4:B:553:HOH:O	2.17	0.44
1:A:126:LYS:HE2	1:A:129:ARG:CD	2.40	0.44
1:A:160:TYR:HD1	1:A:173:LEU:HD23	1.82	0.44
1:B:85:GLU:OE2	1:B:90:LYS:HA	2.17	0.44
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.85	0.44
1:B:5:MET:HE2	1:B:5:MET:HB2	1.84	0.44
1:B:25:ARG:O	1:B:26:ALA:HB2	2.18	0.44
1:B:52:SER:O	1:B:55:LYS:HB2	2.18	0.44
1:B:98:LYS:NZ	1:B:98:LYS:HA	2.32	0.44
1:A:315:LEU:HA	1:A:315:LEU:HD23	1.60	0.44
1:B:338:VAL:HG21	1:B:354:ILE:HD11	1.99	0.44
1:B:392:MET:HG2	1:B:400:LEU:HD11	2.00	0.44
1:A:113:ARG:HG2	1:B:294:ASN:ND2	2.33	0.43
1:B:17:ILE:CG2	1:B:37:ILE:HD12	2.48	0.43
1:A:264:ASN:O	1:B:299:PRO:HA	2.19	0.43
1:A:372:ARG:HD3	1:A:408:VAL:HG12	1.99	0.43
1:A:397:MET:HE3	1:A:397:MET:HA	2.00	0.43
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.62	0.43
1:B:20:LEU:HD12	1:B:20:LEU:HA	1.80	0.43
1:B:272:LEU:O	1:B:280:VAL:HG21	2.18	0.43
1:B:368:GLU:CD	1:B:368:GLU:H	2.26	0.43
1:A:53:VAL:O	1:A:57:GLU:HG3	2.19	0.43
1:A:342:GLN:C	1:A:344:LYS:H	2.25	0.43
1:B:21:ALA:HB1	1:B:25:ARG:CZ	2.48	0.43
1:B:29:ARG:NH1	1:B:378:GLY:CA	2.82	0.43
1:B:98:LYS:HA	1:B:98:LYS:HZ3	1.84	0.43
1:B:152:LEU:HD13	1:B:152:LEU:N	2.34	0.43
1:A:380:TYR:CD1	1:A:380:TYR:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:GLY:O	1:B:236:ASP:HB2	2.19	0.43
1:A:161:TYR:CZ	1:A:166:HIS:HA	2.54	0.43
1:A:327:ARG:NH2	4:A:657:HOH:O	2.51	0.43
1:B:357:ASN:HB2	4:B:515:HOH:O	2.18	0.43
1:A:23:LEU:H	1:A:23:LEU:HG	1.69	0.43
1:A:246:MET:HE2	1:A:246:MET:HB3	1.74	0.43
1:A:347:ASN:HD21	1:A:409:LEU:HB3	1.82	0.43
1:B:38:GLY:O	1:B:359:MET:HE1	2.18	0.43
1:B:202:LEU:HD12	1:B:202:LEU:O	2.19	0.43
1:A:156:ARG:NH2	4:A:613:HOH:O	2.51	0.43
1:B:210:GLN:NE2	1:B:214:GLU:OE2	2.52	0.43
1:A:5:MET:HB3	1:B:249:GLU:OE1	2.19	0.42
1:B:249:GLU:C	1:B:250:LEU:HD23	2.43	0.42
1:B:341:LEU:HD12	1:B:341:LEU:HA	1.74	0.42
1:A:129:ARG:NH2	1:A:181:GLN:NE2	2.67	0.42
1:A:170:PHE:CE2	1:A:174:ILE:CD1	3.02	0.42
1:B:29:ARG:NH1	1:B:378:GLY:HA3	2.34	0.42
1:A:237:ALA:HB3	1:A:241:ARG:NH1	2.34	0.42
1:A:374:ARG:HB2	4:A:615:HOH:O	2.19	0.42
1:B:35:LEU:HB2	1:B:380:TYR:O	2.19	0.42
1:B:227:GLY:O	1:B:327:ARG:NH1	2.51	0.42
1:B:382:VAL:CG1	1:B:383:ALA:N	2.83	0.42
1:B:129:ARG:HA	1:B:154:GLU:O	2.20	0.42
1:A:366:THR:HG22	1:A:369:GLN:N	2.30	0.42
1:A:56:ALA:O	1:A:59:TYR:HB3	2.20	0.42
1:A:347:ASN:ND2	1:A:409:LEU:HB3	2.35	0.42
1:B:74:ASP:N	1:B:74:ASP:OD1	2.43	0.42
1:B:329:ARG:CG	1:B:329:ARG:HH11	2.33	0.42
1:A:81:ARG:HG3	1:A:81:ARG:HH11	1.85	0.42
1:B:177:LEU:HD23	1:B:177:LEU:HA	1.78	0.42
1:A:137:ASN:HA	1:A:138:PRO:HA	1.94	0.42
1:A:249:GLU:OE1	1:B:5:MET:HB3	2.19	0.42
1:B:5:MET:N	1:B:7:GLU:OE1	2.52	0.42
1:B:170:PHE:HE1	1:B:208:LEU:HD11	1.84	0.42
1:A:126:LYS:NZ	1:A:129:ARG:NE	2.68	0.41
1:B:173:LEU:HD12	1:B:173:LEU:C	2.44	0.41
1:A:187:LEU:HA	1:A:220:LEU:O	2.20	0.41
1:B:174:ILE:HG22	1:B:175:ASN:N	2.35	0.41
1:A:90:LYS:HB3	1:A:90:LYS:HE3	1.75	0.41
1:A:148:ASN:N	1:A:148:ASN:HD22	2.18	0.41
1:A:367:LYS:HG2	1:A:368:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ARG:HD3	1:A:408:VAL:HG11	2.01	0.41
1:B:329:ARG:O	1:B:332:ARG:HB3	2.19	0.41
1:B:402:GLU:HB3	4:B:684:HOH:O	2.20	0.41
1:A:46:LYS:CG	1:A:47:THR:N	2.83	0.41
1:A:371:LEU:HD22	1:A:371:LEU:HA	1.84	0.41
1:B:96:ASN:HD22	1:B:96:ASN:HA	1.50	0.41
1:A:34:ASN:HA	1:A:380:TYR:HB2	2.03	0.41
1:A:35:LEU:N	1:A:380:TYR:O	2.49	0.41
1:A:59:TYR:CD1	1:A:59:TYR:C	2.99	0.41
1:A:266:ARG:HH22	2:A:410:PLP:P	2.44	0.41
1:B:12:ALA:HA	1:B:13:PRO:HD3	1.93	0.41
1:B:60:LEU:HD12	1:B:60:LEU:HA	1.67	0.41
1:B:210:GLN:O	1:B:213:VAL:HB	2.21	0.41
1:A:270:CYS:SG	1:A:287:MET:HE1	2.60	0.41
1:A:158:TYR:HD2	1:A:173:LEU:HD22	1.86	0.40
1:A:297:ASN:O	1:B:266:ARG:HD2	2.21	0.40
1:B:73:ILE:O	1:B:73:ILE:HG22	2.21	0.40
1:A:41:LYS:HG3	1:A:45:GLY:HA2	2.03	0.40
1:B:46:LYS:CG	1:B:47:THR:H	2.34	0.40
1:A:25:ARG:C	1:A:27:ASP:H	2.30	0.40
1:A:224:ALA:HB2	4:A:430:HOH:O	2.21	0.40
1:B:123:THR:OG1	1:B:124:SER:N	2.51	0.40
1:A:15:ASP:O	1:A:19:GLY:HA3	2.21	0.40
1:A:71:LEU:HB2	4:A:523:HOH:O	2.21	0.40
1:A:104:GLN:NE2	1:A:303:ALA:HB2	2.36	0.40
1:B:177:LEU:C	1:B:179:GLU:N	2.80	0.40
1:B:228:PHE:HZ	1:B:258:LYS:O	2.05	0.40
1:B:392:MET:HG2	1:B:400:LEU:CD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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	320/320 (100%)	230 (72%)	90 (28%)	0	0
1	B	320/320 (100%)	223 (70%)	97 (30%)	0	0
All	All	640/640 (100%)	453 (71%)	187 (29%)	0	0

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	7	GLU
1	A	8	ASN
1	A	9	ILE
1	A	20	LEU
1	A	23	LEU
1	A	25	ARG
1	A	29	ARG
1	A	37	ILE
1	A	39	VAL
1	A	41	LYS
1	A	46	LYS
1	A	55	LYS
1	A	58	GLN
1	A	61	LEU
1	A	62	GLU
1	A	73	ILE
1	A	83	THR
1	A	85	GLU
1	A	86	LEU
1	A	87	LEU
1	A	90	LYS
1	A	95	ILE
1	A	112	LEU
1	A	119	LEU
1	A	121	LYS
1	A	126	LYS
1	A	129	ARG
1	A	133	VAL
1	A	144	LYS
1	A	146	VAL

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Mol	Chain	Res	Type
1	A	149	SER
1	A	152	LEU
1	A	155	VAL
1	A	156	ARG
1	A	157	GLU
1	A	164	GLU
1	A	165	ASN
1	A	168	LEU
1	A	170	PHE
1	A	173	LEU
1	A	174	ILE
1	A	178	ASN
1	A	181	GLN
1	A	187	LEU
1	A	196	THR
1	A	202	LEU
1	A	206	GLN
1	A	207	THR
1	A	211	LEU
1	A	218	LEU
1	A	220	LEU
1	A	223	PHE
1	A	240	LEU
1	A	241	ARG
1	A	248	LYS
1	A	250	LEU
1	A	251	ILE
1	A	259	ASN
1	A	262	LEU
1	A	267	VAL
1	A	272	LEU
1	A	273	VAL
1	A	277	SER
1	A	296	SER
1	A	297	ASN
1	A	304	SER
1	A	321	GLN
1	A	329	ARG
1	A	330	ILE
1	A	332	ARG
1	A	335	GLN
1	A	338	VAL

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Mol	Chain	Res	Type
1	A	341	LEU
1	A	343	GLU
1	A	347	ASN
1	A	348	ARG
1	A	353	ILE
1	A	355	LYS
1	A	362	PHE
1	A	365	LEU
1	A	366	THR
1	A	367	LYS
1	A	370	VAL
1	A	371	LEU
1	A	375	GLU
1	A	376	GLU
1	A	377	PHE
1	A	400	LEU
1	A	409	LEU
1	B	20	LEU
1	B	25	ARG
1	B	27	ASP
1	B	34	ASN
1	B	37	ILE
1	B	39	VAL
1	B	41	LYS
1	B	43	GLU
1	B	47	THR
1	B	50	LEU
1	B	51	THR
1	B	55	LYS
1	B	60	LEU
1	B	61	LEU
1	B	67	THR
1	B	69	ASN
1	B	87	LEU
1	B	90	LYS
1	B	92	SER
1	B	94	LEU
1	B	95	ILE
1	B	98	LYS
1	B	99	ARG
1	B	105	THR
1	B	109	THR

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Mol	Chain	Res	Type
1	B	112	LEU
1	B	119	LEU
1	B	121	LYS
1	B	122	ASN
1	B	124	SER
1	B	129	ARG
1	B	133	VAL
1	B	135	VAL
1	B	139	SER
1	B	146	VAL
1	B	149	SER
1	B	152	LEU
1	B	154	GLU
1	B	155	VAL
1	B	167	THR
1	B	168	LEU
1	B	174	ILE
1	B	175	ASN
1	B	181	GLN
1	B	186	VAL
1	B	198	ILE
1	B	203	GLU
1	B	206	GLN
1	B	207	THR
1	B	213	VAL
1	B	214	GLU
1	B	220	LEU
1	B	223	PHE
1	B	233	LEU
1	B	234	GLU
1	B	235	GLU
1	B	240	LEU
1	B	241	ARG
1	B	246	MET
1	B	248	LYS
1	B	249	GLU
1	B	250	LEU
1	B	251	ILE
1	B	254	SER
1	B	257	SER
1	B	259	ASN
1	B	262	LEU

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Mol	Chain	Res	Type
1	B	273	VAL
1	B	276	ASP
1	B	277	SER
1	B	281	ASP
1	B	297	ASN
1	B	304	SER
1	B	324	THR
1	B	334	ARG
1	B	335	GLN
1	B	336	LEU
1	B	343	GLU
1	B	344	LYS
1	B	348	ARG
1	B	353	ILE
1	B	355	LYS
1	B	360	PHE
1	B	361	SER
1	B	362	PHE
1	B	367	LYS
1	B	368	GLU
1	B	370	VAL
1	B	371	LEU
1	B	372	ARG
1	B	373	LEU
1	B	375	GLU
1	B	379	VAL
1	B	393	THR
1	B	397	MET
1	B	400	LEU
1	B	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	63	ASN
1	A	84	GLN
1	A	148	ASN
1	A	165	ASN
1	A	166	HIS
1	A	178	ASN
1	A	181	GLN

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Mol	Chain	Res	Type
1	A	189	HIS
1	A	226	GLN
1	A	259	ASN
1	A	286	GLN
1	A	297	ASN
1	A	321	GLN
1	A	328	GLN
1	A	331	GLN
1	A	339	ASN
1	A	342	GLN
1	A	347	ASN
1	A	388	ASN
1	B	34	ASN
1	B	63	ASN
1	B	69	ASN
1	B	96	ASN
1	B	137	ASN
1	B	165	ASN
1	B	175	ASN
1	B	178	ASN
1	B	206	GLN
1	B	210	GLN
1	B	259	ASN
1	B	294	ASN
1	B	328	GLN
1	B	339	ASN
1	B	342	GLN
1	B	347	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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	410	1	15,15,16	1.66	3 (20%)	21,22,23	1.79	5 (23%)
3	MAE	A	411	-	7,7,7	1.13	0	8,8,8	0.91	0
2	PLP	A	410	1	15,15,16	1.34	1 (6%)	21,22,23	2.02	7 (33%)
3	MAE	B	411	-	7,7,7	1.30	0	8,8,8	1.04	1 (12%)

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	410	1	-	0/6/6/8	0/1/1/1
3	MAE	A	411	-	-	4/5/5/5	-
2	PLP	A	410	1	-	0/6/6/8	0/1/1/1
3	MAE	B	411	-	-	2/5/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	410	PLP	C4A-C4	-4.73	1.42	1.51
2	A	410	PLP	C4A-C4	-3.34	1.45	1.51
2	B	410	PLP	P-O3P	-2.77	1.44	1.54
2	B	410	PLP	C5A-C5	2.04	1.56	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	410	PLP	C6-C5-C4	5.50	122.61	118.10
2	B	410	PLP	C2A-C2-C3	3.52	124.92	120.80
2	B	410	PLP	C3-C2-N1	-3.52	116.52	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	410	PLP	C6-C5-C4	3.41	120.89	118.10
2	A	410	PLP	C5-C6-N1	-3.28	118.49	123.83
2	B	410	PLP	C5-C6-N1	-2.86	119.18	123.83
2	B	410	PLP	C6-N1-C2	2.81	124.30	119.20
2	A	410	PLP	C5A-C5-C4	-2.80	117.11	122.64
2	A	410	PLP	C3-C2-N1	-2.79	117.45	120.96
2	A	410	PLP	C6-N1-C2	2.33	123.42	119.20
2	A	410	PLP	C2A-C2-C3	2.15	123.32	120.80
2	A	410	PLP	O3P-P-O1P	2.11	119.06	110.83
3	B	411	MAE	C3-C2-C1	2.09	137.69	127.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	411	MAE	O2-C1-C2-C3
3	A	411	MAE	O1-C1-C2-C3
3	A	411	MAE	C2-C3-C4-O3
3	A	411	MAE	C2-C3-C4-O4
3	B	411	MAE	C2-C3-C4-O3
3	B	411	MAE	C2-C3-C4-O4

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	410	PLP	3	0
3	A	411	MAE	1	0
2	A	410	PLP	1	0
3	B	411	MAE	2	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.