



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:29 PM UTC

PDB ID : 1AHF / pdb_00001ahf
Title : ASPARTATE AMINOTRANSFERASE HEXAMUTANT
Authors : Malashkevich, V.N.; Jansonius, J.N.
Deposited on : 1995-02-22
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

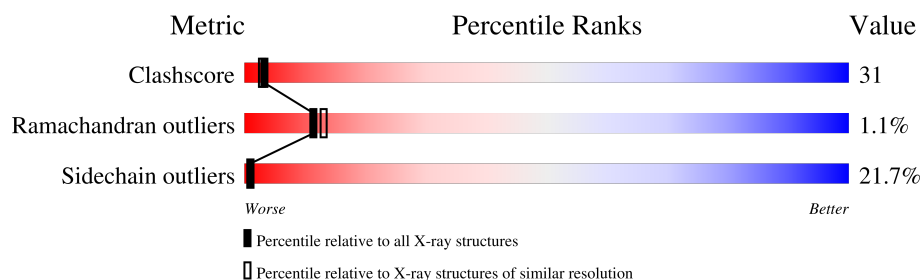
1 Overall quality at a glance

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)
Ramachandran outliers	187476	6854 (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	
1	B	396	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOP	A	411	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6593 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.

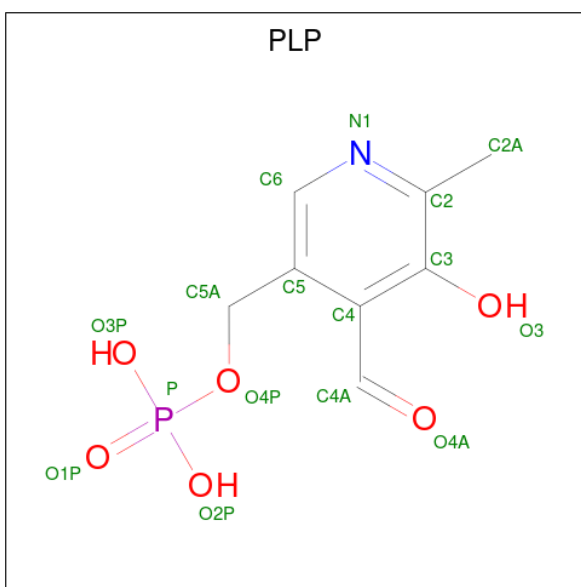
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3071	1942	533	583	13			
1	B	396	Total	C	N	O	S	0	0	0
			3071	1942	533	583	13			

There are 12 discrepancies between the modelled and reference sequences:

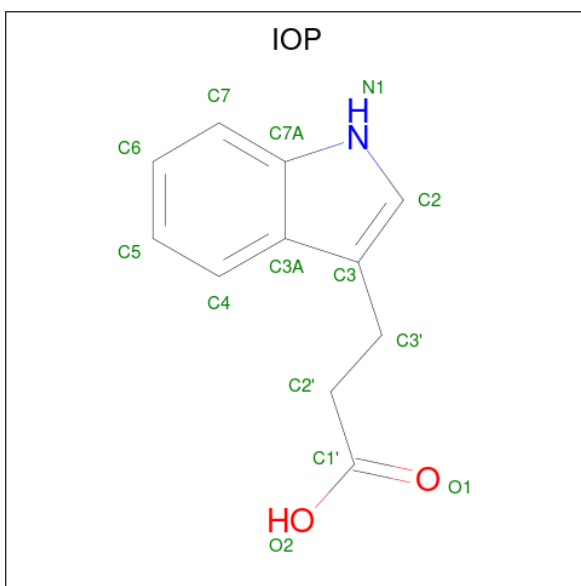
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LEU	VAL	conflict	UNP P00509
A	41	TYR	LYS	conflict	UNP P00509
A	47	ILE	THR	conflict	UNP P00509
A	69	LEU	ASN	conflict	UNP P00509
A	109	SER	THR	conflict	UNP P00509
A	297	SER	ASN	conflict	UNP P00509
B	39	LEU	VAL	conflict	UNP P00509
B	41	TYR	LYS	conflict	UNP P00509
B	47	ILE	THR	conflict	UNP P00509
B	69	LEU	ASN	conflict	UNP P00509
B	109	SER	THR	conflict	UNP P00509
B	297	SER	ASN	conflict	UNP P00509

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



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

- Molecule 3 is INDOLYLPROPIONIC ACID (CCD ID: IOP) (formula: $C_{11}H_{11}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	11	1	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 5 is water.

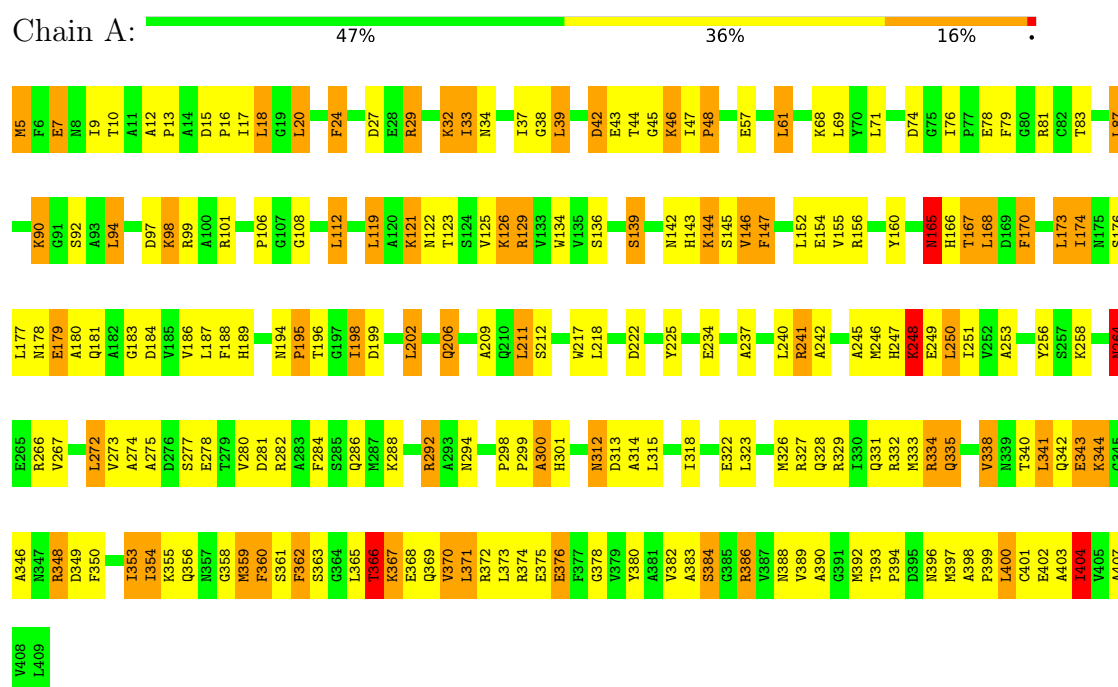
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total	O	0	0
			215	215		
5	B	187	Total	O	0	0
			187	187		

3 Residue-property plots

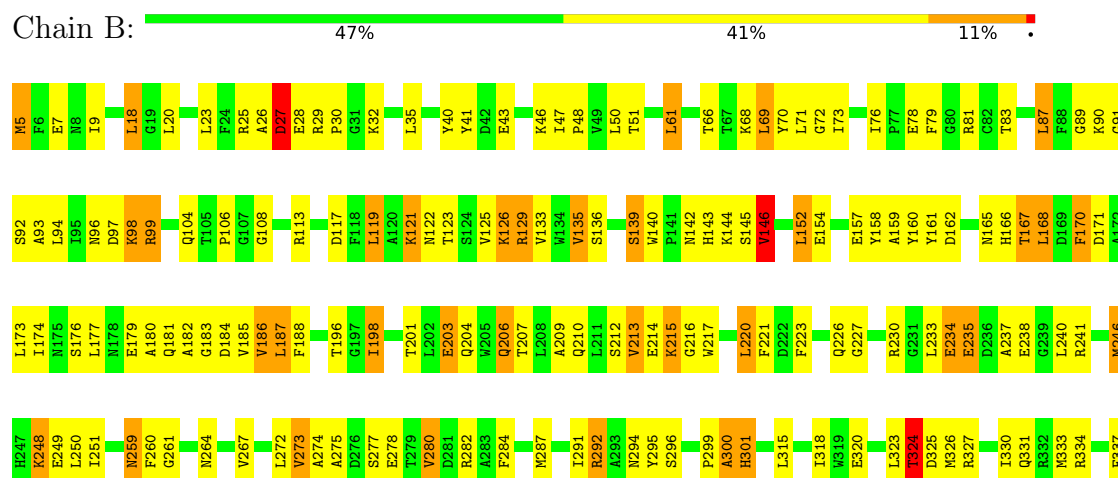
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

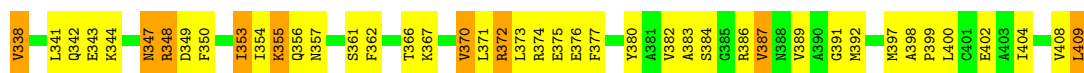
Note EDS was not executed.

• 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	85.92Å 79.39Å 88.80Å 90.00° 118.99° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	99.0 (8.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.232 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6593	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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: IOP, 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	1.17	1/3133 (0.0%)	1.61	32/4244 (0.8%)
1	B	1.24	3/3133 (0.1%)	1.64	31/4244 (0.7%)
All	All	1.20	4/6266 (0.1%)	1.63	63/8488 (0.7%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	91	GLY	C-N	-14.95	1.12	1.33
1	B	92	SER	N-CA	-8.32	1.35	1.46
1	B	89	GLY	N-CA	7.26	1.54	1.45
1	A	366	THR	CB-OG1	5.40	1.52	1.43

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	THR	N-CA-C	8.41	120.52	111.36
1	A	300	ALA	N-CA-C	8.12	119.91	111.14
1	A	248	LYS	N-CA-C	-8.06	103.39	113.55
1	B	91	GLY	O-C-N	-7.93	112.39	122.70
1	B	196	THR	N-CA-C	7.86	121.36	111.69
1	B	334	ARG	N-CA-CB	7.85	121.39	110.01
1	B	325	ASP	CA-CB-CG	7.28	119.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	VAL	N-CA-CB	7.26	118.56	110.51
1	B	91	GLY	CA-C-N	-7.23	111.08	121.42
1	B	91	GLY	C-N-CA	-7.23	111.08	121.42
1	B	161	TYR	N-CA-C	7.02	120.38	109.07
1	B	300	ALA	N-CA-C	6.94	120.22	111.69
1	B	324	THR	N-CA-CB	6.84	120.76	110.22
1	A	199	ASP	CA-CB-CG	6.75	119.35	112.60
1	B	27	ASP	CB-CA-C	6.73	121.46	110.22
1	A	125	VAL	N-CA-C	-6.71	100.08	109.21
1	B	106	PRO	N-CA-CB	6.60	107.14	102.65
1	A	404	ILE	N-CA-CB	6.59	122.59	110.40
1	A	147	PHE	CA-CB-CG	-6.57	107.23	113.80
1	A	106	PRO	N-CA-CB	6.41	107.00	102.65
1	A	359	MET	N-CA-C	6.29	119.12	111.82
1	B	409	LEU	CB-CA-C	6.26	122.00	110.10
1	A	24	PHE	CA-CB-CG	-6.21	107.59	113.80
1	B	334	ARG	CB-CA-C	6.13	120.51	110.88
1	A	122	ASN	CA-C-N	-6.11	111.73	121.44
1	A	122	ASN	C-N-CA	-6.11	111.73	121.44
1	A	247	HIS	CA-CB-CG	-5.90	107.90	113.80
1	B	248	LYS	N-CA-C	-5.86	104.30	112.45
1	B	146	VAL	N-CA-CB	5.79	117.33	110.55
1	A	7	GLU	CB-CA-C	-5.75	101.61	110.81
1	A	407	ALA	CA-C-N	-5.74	115.70	122.36
1	A	407	ALA	C-N-CA	-5.74	115.70	122.36
1	B	27	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	165	ASN	N-CA-CB	5.74	118.79	110.47
1	B	170	PHE	N-CA-C	5.66	117.93	111.02
1	B	122	ASN	CA-CB-CG	-5.66	106.94	112.60
1	B	264	ASN	N-CA-C	5.66	120.05	113.20
1	A	123	THR	CA-C-N	-5.61	114.94	124.31
1	A	123	THR	C-N-CA	-5.61	114.94	124.31
1	B	186	VAL	N-CA-CB	5.59	118.71	111.67
1	A	264	ASN	N-CA-C	5.58	119.95	113.20
1	A	108	GLY	N-CA-C	-5.56	105.65	112.77
1	A	48	PRO	N-CA-C	5.55	120.00	111.57
1	A	403	ALA	N-CA-C	-5.53	106.38	113.01
1	B	72	GLY	N-CA-C	-5.53	106.25	112.33
1	A	338	VAL	N-CA-CB	5.50	116.62	110.51
1	B	238	GLU	N-CA-C	5.41	117.88	111.33
1	B	68	LYS	CA-C-N	5.33	129.87	121.56
1	B	68	LYS	C-N-CA	5.33	129.87	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	PHE	CB-CA-C	-5.29	99.40	109.66
1	A	170	PHE	N-CA-CB	5.24	117.74	109.94
1	A	363	SER	N-CA-C	5.22	118.75	112.38
1	A	165	ASN	N-CA-C	5.20	119.25	113.02
1	A	146	VAL	N-CA-CB	5.17	116.26	110.62
1	B	409	LEU	N-CA-CB	5.16	119.26	110.50
1	B	68	LYS	CB-CA-C	5.15	119.36	111.02
1	A	195	PRO	CB-CA-C	-5.14	99.14	112.00
1	A	42	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	250	LEU	CB-CA-C	-5.07	101.19	110.62
1	B	108	GLY	N-CA-C	-5.05	108.05	114.16
1	B	186	VAL	CB-CA-C	5.03	118.18	111.19
1	B	26	ALA	CA-C-N	-5.00	115.55	122.30
1	B	26	ALA	C-N-CA	-5.00	115.55	122.30

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	3071	0	3020	194	0
1	B	3071	0	3020	198	0
2	A	15	0	6	1	0
2	B	15	0	6	0	0
3	A	14	0	10	8	0
4	B	5	0	0	1	0
5	A	215	0	0	11	0
5	B	187	0	0	12	0
All	All	6593	0	6062	374	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 31.

All (374) 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:B:117:ASP:O	1:B:121:LYS:HD2	1.57	1.03
1:B:272:LEU:HD22	1:B:287:MET:HE2	1.42	1.02
1:A:17:ILE:HG21	3:A:411:IOP:H2	1.43	1.00
1:A:37:ILE:HG13	3:A:411:IOP:H3'2	1.44	0.96
1:B:129:ARG:HG3	5:B:426:HOH:O	1.69	0.89
1:A:46:LYS:HD2	1:A:47:ILE:H	1.33	0.89
1:A:165:ASN:N	1:A:165:ASN:HD22	1.68	0.86
1:B:272:LEU:HB2	1:B:287:MET:HE1	1.58	0.85
1:A:129:ARG:HB2	1:A:154:GLU:HB3	1.58	0.85
1:A:121:LYS:NZ	1:A:121:LYS:HB3	1.94	0.83
1:B:98:LYS:NZ	1:B:98:LYS:HA	1.94	0.83
1:B:348:ARG:HG3	1:B:348:ARG:HH11	1.41	0.82
1:B:397:MET:HE3	1:B:397:MET:HA	1.60	0.81
1:A:292:ARG:CZ	1:B:18:LEU:HD22	2.12	0.80
1:B:46:LYS:HD2	1:B:47:ILE:H	1.46	0.80
1:A:17:ILE:CG2	3:A:411:IOP:H2	2.11	0.80
1:A:129:ARG:HD2	1:A:134:TRP:NE1	1.97	0.80
1:B:272:LEU:HD22	1:B:287:MET:CE	2.11	0.79
1:A:165:ASN:HD22	1:A:165:ASN:H	1.30	0.79
1:A:5:MET:HE2	1:B:125:VAL:HG23	1.64	0.79
1:A:37:ILE:HG13	3:A:411:IOP:C3'	2.11	0.78
1:A:248:LYS:CG	1:A:275:ALA:HB2	2.14	0.77
1:A:348:ARG:HG2	1:A:348:ARG:HH11	1.50	0.77
1:A:46:LYS:O	1:A:48:PRO:HD3	1.85	0.77
1:B:187:LEU:HD12	1:B:188:PHE:N	2.00	0.77
1:B:398:ALA:HB3	1:B:399:PRO:HD3	1.65	0.76
1:B:162:ASP:OD2	1:B:165:ASN:HB2	1.85	0.76
1:B:83:THR:HG22	1:B:87:LEU:HD22	1.65	0.75
1:A:198:ILE:HA	5:A:478:HOH:O	1.87	0.75
1:B:249:GLU:HA	1:B:273:VAL:O	1.87	0.75
1:A:248:LYS:HG3	1:A:275:ALA:HB2	1.69	0.74
1:A:38:GLY:H	3:A:411:IOP:H3'2	1.51	0.74
1:B:46:LYS:CD	1:B:47:ILE:H	2.00	0.74
1:A:323:LEU:HA	1:A:326:MET:CE	2.19	0.73
1:A:382:VAL:HG12	1:A:384:SER:H	1.51	0.73
1:A:129:ARG:HD2	1:A:134:TRP:HE1	1.53	0.73
1:A:323:LEU:HA	1:A:326:MET:HE2	1.71	0.73
1:A:398:ALA:HB3	1:A:399:PRO:HD3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LEU:HD11	1:A:300:ALA:HB2	1.72	0.72
1:B:129:ARG:HE	1:B:154:GLU:HB3	1.54	0.72
1:B:333:MET:HE2	1:B:333:MET:HA	1.70	0.72
1:A:24:PHE:CZ	1:A:34:ASN:HB2	2.26	0.70
1:A:388:ASN:HD21	1:A:390:ALA:HB3	1.54	0.70
1:B:170:PHE:CE2	1:B:174:ILE:HD11	2.26	0.70
1:B:27:ASP:OD1	1:B:29:ARG:HB2	1.92	0.70
1:B:98:LYS:HA	1:B:98:LYS:HZ3	1.53	0.70
1:B:129:ARG:NE	1:B:154:GLU:HB3	2.07	0.70
1:B:372:ARG:HG2	1:B:408:VAL:HG12	1.75	0.69
1:A:87:LEU:O	1:A:241:ARG:HD2	1.93	0.69
1:A:397:MET:HE3	1:A:400:LEU:HD23	1.72	0.69
1:A:328:GLN:O	1:A:332:ARG:HG3	1.93	0.68
1:A:46:LYS:HD2	1:A:47:ILE:N	2.08	0.68
1:B:46:LYS:O	1:B:48:PRO:HD3	1.93	0.68
1:B:160:TYR:CE1	1:B:168:LEU:HD21	2.27	0.68
1:B:98:LYS:HA	1:B:98:LYS:CE	2.24	0.68
1:A:206:GLN:O	1:A:209:ALA:HB3	1.94	0.68
1:A:136:SER:O	1:A:139:SER:HB2	1.94	0.68
1:B:96:ASN:HD22	1:B:96:ASN:N	1.90	0.68
1:B:250:LEU:HD12	1:B:273:VAL:HG13	1.76	0.68
1:A:24:PHE:CE1	1:A:34:ASN:HB2	2.28	0.67
1:A:15:ASP:OD2	1:B:292:ARG:HD2	1.94	0.67
1:B:212:SER:HB3	1:B:217:TRP:HE3	1.60	0.66
1:A:362:PHE:HE1	1:A:384:SER:HB2	1.60	0.66
1:A:366:THR:HG23	1:A:369:GLN:OE1	1.94	0.66
1:A:278:GLU:HG2	1:A:282:ARG:NH1	2.11	0.66
1:A:386:ARG:HH22	3:A:411:IOP:C1'	2.07	0.66
1:B:372:ARG:NH1	1:B:376:GLU:OE2	2.29	0.66
1:A:78:GLU:HB2	5:A:486:HOH:O	1.95	0.66
1:A:249:GLU:OE1	1:B:5:MET:N	2.29	0.65
1:B:397:MET:CE	1:B:400:LEU:HD22	2.26	0.65
1:A:165:ASN:N	1:A:165:ASN:ND2	2.43	0.65
1:B:277:SER:N	5:B:555:HOH:O	2.29	0.65
1:B:28:GLU:OE1	1:B:28:GLU:HA	1.96	0.65
1:B:181:GLN:O	1:B:184:ASP:HB2	1.97	0.65
1:A:212:SER:HB3	1:A:217:TRP:CE3	2.31	0.65
1:A:334:ARG:NH1	1:A:358:GLY:O	2.29	0.65
1:A:15:ASP:HB3	1:A:18:LEU:HB2	1.78	0.65
1:A:99:ARG:HD3	1:A:275:ALA:O	1.96	0.65
1:B:99:ARG:NH1	1:B:274:ALA:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:GLU:O	1:B:179:GLU:HG3	1.97	0.64
1:A:372:ARG:NE	1:A:376:GLU:OE1	2.29	0.64
1:A:167:THR:OG1	1:A:168:LEU:N	2.30	0.64
1:B:87:LEU:O	1:B:241:ARG:NH1	2.31	0.63
1:A:129:ARG:HH22	1:A:181:GLN:HE21	1.46	0.63
1:B:348:ARG:HG3	1:B:348:ARG:NH1	2.11	0.63
1:A:61:LEU:HD12	1:B:61:LEU:HD12	1.81	0.62
1:A:126:LYS:NZ	1:A:154:GLU:OE1	2.30	0.62
1:A:237:ALA:O	1:A:241:ARG:HB2	1.99	0.62
1:A:5:MET:N	1:A:7:GLU:OE1	2.32	0.62
1:A:170:PHE:CE2	1:A:174:ILE:HD11	2.34	0.61
1:B:327:ARG:O	1:B:331:GLN:HG3	2.00	0.61
1:B:382:VAL:HG12	1:B:384:SER:H	1.65	0.61
1:B:83:THR:HG22	1:B:87:LEU:CD2	2.29	0.61
1:A:294:ASN:HD21	1:B:294:ASN:HD21	1.48	0.61
1:A:366:THR:O	1:A:370:VAL:HG13	2.01	0.61
1:A:312:ASN:ND2	1:A:315:LEU:H	1.99	0.60
1:B:230:ARG:HD3	5:B:451:HOH:O	2.00	0.60
1:A:29:ARG:O	1:A:32:LYS:HG2	2.01	0.60
1:A:189:HIS:CD2	1:A:194:ASN:H	2.19	0.60
1:A:5:MET:HE2	1:B:125:VAL:CG2	2.31	0.60
1:A:144:LYS:CD	1:A:155:VAL:HG11	2.31	0.60
1:B:237:ALA:O	1:B:241:ARG:HG3	2.01	0.60
1:B:201:THR:OG1	1:B:204:GLN:HG3	2.02	0.60
1:A:312:ASN:ND2	1:A:314:ALA:H	2.01	0.59
1:B:212:SER:HB3	1:B:217:TRP:CE3	2.38	0.59
1:A:372:ARG:O	1:A:376:GLU:HB2	2.02	0.59
1:A:121:LYS:HB3	1:A:121:LYS:HZ1	1.65	0.59
1:A:343:GLU:O	1:A:343:GLU:HG2	2.01	0.58
1:B:213:VAL:HG12	1:B:214:GLU:N	2.16	0.58
1:A:323:LEU:HD12	1:A:326:MET:HE3	1.86	0.58
1:B:96:ASN:N	1:B:96:ASN:ND2	2.51	0.58
1:B:292:ARG:NH1	5:B:598:HOH:O	2.35	0.58
1:A:386:ARG:NH2	3:A:411:IOP:O2	2.31	0.58
1:B:372:ARG:O	1:B:376:GLU:HB3	2.03	0.58
1:B:210:GLN:HE21	1:B:214:GLU:HG3	1.69	0.58
1:A:211:LEU:HD13	1:A:217:TRP:CH2	2.39	0.57
1:B:234:GLU:HG3	1:B:241:ARG:HH21	1.69	0.57
1:A:234:GLU:CD	1:A:241:ARG:HH22	2.11	0.57
1:A:160:TYR:O	1:A:168:LEU:HD23	2.05	0.57
1:A:237:ALA:HB1	1:A:241:ARG:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLU:OE2	1:A:301:HIS:HE1	1.87	0.57
1:A:251:ILE:HG12	1:A:272:LEU:HD23	1.87	0.56
1:A:350:PHE:O	1:A:353:ILE:HB	2.05	0.56
1:B:274:ALA:HB3	1:B:280:VAL:HB	1.87	0.56
1:B:301:HIS:ND1	5:B:467:HOH:O	2.33	0.56
1:A:248:LYS:HG3	1:A:275:ALA:CB	2.35	0.56
1:B:46:LYS:HD2	1:B:47:ILE:N	2.18	0.56
1:A:329:ARG:NH2	1:A:392:MET:O	2.39	0.56
1:A:46:LYS:CD	1:A:47:ILE:H	2.11	0.56
1:B:259:ASN:C	1:B:259:ASN:HD22	2.14	0.56
1:A:362:PHE:CE1	1:A:384:SER:HB2	2.40	0.56
1:B:99:ARG:NH1	1:B:99:ARG:HG2	2.20	0.56
1:B:398:ALA:HB3	1:B:399:PRO:CD	2.35	0.56
1:B:398:ALA:O	1:B:402:GLU:HG3	2.06	0.56
1:B:113:ARG:NH2	5:B:509:HOH:O	2.39	0.55
1:B:259:ASN:HD22	1:B:260:PHE:N	2.04	0.55
1:B:71:LEU:HD11	1:B:300:ALA:HB2	1.87	0.55
1:B:220:LEU:HD13	1:B:251:ILE:HB	1.86	0.55
1:A:12:ALA:HB1	1:A:13:PRO:HD2	1.88	0.55
1:A:144:LYS:HD2	1:A:155:VAL:HG11	1.87	0.55
1:B:158:TYR:CD1	1:B:173:LEU:HD12	2.41	0.55
1:A:29:ARG:NH2	1:A:378:GLY:HA2	2.22	0.55
1:B:183:GLY:N	1:B:216:GLY:O	2.31	0.55
1:B:186:VAL:HG12	1:B:217:TRP:HB3	1.87	0.55
1:A:397:MET:CE	1:A:400:LEU:HD23	2.37	0.55
1:A:398:ALA:HB3	1:A:399:PRO:CD	2.35	0.54
1:B:123:THR:HB	5:B:449:HOH:O	2.07	0.54
1:B:187:LEU:HD12	1:B:187:LEU:C	2.30	0.54
1:A:400:LEU:HD11	1:A:404:ILE:HD12	1.90	0.54
1:B:372:ARG:HG2	1:B:408:VAL:CG1	2.38	0.54
1:B:201:THR:HG23	1:B:204:GLN:CD	2.32	0.54
1:B:198:ILE:HA	5:B:498:HOH:O	2.08	0.54
1:A:181:GLN:O	1:A:184:ASP:HB2	2.07	0.54
1:A:344:LYS:NZ	1:A:402:GLU:OE2	2.37	0.54
1:B:344:LYS:HD2	1:B:402:GLU:HG2	1.90	0.54
1:B:356:GLN:OE1	1:B:361:SER:HA	2.07	0.54
1:A:348:ARG:HH11	1:A:348:ARG:CG	2.19	0.53
1:B:135:VAL:O	1:B:157:GLU:HA	2.08	0.53
1:B:344:LYS:CD	1:B:402:GLU:HG2	2.37	0.53
1:B:126:LYS:HD2	5:B:417:HOH:O	2.08	0.53
1:B:376:GLU:HG2	1:B:377:PHE:CE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:HD3	1:B:154:GLU:HG2	1.90	0.53
1:B:248:LYS:HE3	1:B:275:ALA:HB1	1.89	0.53
1:A:99:ARG:HD2	1:A:274:ALA:O	2.09	0.53
1:B:129:ARG:HD3	1:B:154:GLU:CG	2.39	0.53
1:A:212:SER:HB3	1:A:217:TRP:HE3	1.74	0.53
1:A:356:GLN:OE1	1:A:361:SER:HA	2.09	0.53
1:B:220:LEU:HD12	1:B:221:PHE:N	2.23	0.52
1:A:389:VAL:O	1:A:392:MET:HB2	2.10	0.52
1:B:46:LYS:C	1:B:48:PRO:HD3	2.35	0.52
1:B:78:GLU:HB2	5:B:505:HOH:O	2.09	0.52
1:A:39:LEU:HD21	1:B:69:LEU:HD21	1.92	0.52
1:B:366:THR:O	1:B:370:VAL:HG13	2.10	0.52
1:A:129:ARG:HH22	1:A:181:GLN:NE2	2.08	0.52
1:A:327:ARG:NH2	5:A:453:HOH:O	2.39	0.52
1:A:222:ASP:OD2	2:A:410:PLP:N1	2.43	0.52
1:A:129:ARG:NH2	1:A:181:GLN:HE21	2.08	0.51
1:A:284:PHE:CE2	1:A:288:LYS:HD2	2.45	0.51
1:B:76:ILE:O	1:B:79:PHE:HB3	2.10	0.51
1:A:333:MET:HA	1:A:333:MET:HE2	1.93	0.51
1:B:206:GLN:O	1:B:209:ALA:HB3	2.11	0.51
1:A:97:ASP:HB2	1:A:99:ARG:HG3	1.92	0.51
1:A:189:HIS:HD2	1:A:194:ASN:H	1.59	0.51
1:B:160:TYR:HD1	1:B:173:LEU:HD13	1.76	0.51
1:B:220:LEU:HD12	1:B:220:LEU:C	2.36	0.51
1:B:35:LEU:HD11	1:B:400:LEU:HD11	1.92	0.51
1:B:182:ALA:HB2	1:B:215:LYS:O	2.11	0.51
1:A:5:MET:N	1:B:249:GLU:OE1	2.44	0.50
1:B:43:GLU:CD	1:B:43:GLU:H	2.19	0.50
1:A:142:ASN:O	1:A:146:VAL:HG13	2.12	0.50
1:B:119:LEU:HD21	1:B:185:VAL:HG21	1.94	0.50
1:A:266:ARG:HD2	1:A:266:ARG:N	2.25	0.50
1:A:348:ARG:NH2	5:A:510:HOH:O	2.30	0.50
1:B:99:ARG:CG	1:B:99:ARG:HH11	2.24	0.50
1:B:320:GLU:O	1:B:324:THR:HG23	2.12	0.50
1:A:29:ARG:HH22	1:A:378:GLY:HA2	1.77	0.50
1:A:286:GLN:HG3	1:B:9:ILE:CG2	2.42	0.50
1:A:312:ASN:HD21	1:A:314:ALA:HB3	1.76	0.50
1:A:371:LEU:HD23	5:A:481:HOH:O	2.10	0.50
1:B:46:LYS:CG	1:B:47:ILE:H	2.25	0.50
1:A:186:VAL:HG12	1:A:188:PHE:CE2	2.47	0.49
1:A:397:MET:HE2	1:A:401:CYS:SG	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ILE:HG22	1:B:79:PHE:H	1.76	0.49
1:B:227:GLY:HA3	1:B:323:LEU:HD21	1.94	0.49
1:A:183:GLY:HA2	1:B:5:MET:HE1	1.94	0.49
1:A:249:GLU:HA	1:A:273:VAL:O	2.12	0.49
1:B:397:MET:O	1:B:397:MET:HG3	2.12	0.49
1:B:404:ILE:O	1:B:408:VAL:HG22	2.12	0.49
1:A:18:LEU:HD23	1:B:292:ARG:HD3	1.94	0.49
1:B:167:THR:HG22	1:B:355:LYS:HE2	1.95	0.49
1:A:143:HIS:O	1:A:146:VAL:HG22	2.13	0.49
1:B:167:THR:CG2	1:B:355:LYS:HE2	2.43	0.49
1:B:27:ASP:O	1:B:32:LYS:NZ	2.29	0.49
1:A:277:SER:HA	1:A:280:VAL:HG12	1.95	0.48
1:A:340:THR:O	1:A:344:LYS:HB2	2.12	0.48
1:B:99:ARG:HG2	1:B:99:ARG:HH11	1.77	0.48
1:B:158:TYR:HD1	1:B:173:LEU:HD12	1.77	0.48
1:A:42:ASP:O	1:A:45:GLY:N	2.30	0.48
1:B:272:LEU:HB2	1:B:287:MET:CE	2.35	0.48
1:B:259:ASN:N	1:B:259:ASN:ND2	2.61	0.48
1:A:97:ASP:OD1	1:A:97:ASP:N	2.45	0.48
1:A:112:LEU:HD13	1:A:253:ALA:CB	2.44	0.48
1:B:347:ASN:HD22	1:B:348:ARG:HH12	1.60	0.48
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.56	0.48
1:A:388:ASN:HD22	1:A:388:ASN:C	2.22	0.48
1:B:181:GLN:HB2	5:B:427:HOH:O	2.13	0.48
1:A:156:ARG:HD2	5:A:474:HOH:O	2.14	0.48
1:A:98:LYS:CE	1:A:98:LYS:HA	2.38	0.47
1:B:173:LEU:O	1:B:176:SER:HB2	2.14	0.47
1:B:248:LYS:HE3	1:B:275:ALA:CB	2.44	0.47
1:A:318:ILE:O	1:A:322:GLU:HG3	2.15	0.47
1:A:323:LEU:HA	1:A:326:MET:HE3	1.96	0.47
1:A:342:GLN:C	1:A:344:LYS:H	2.23	0.47
1:B:210:GLN:O	1:B:214:GLU:HG3	2.14	0.47
1:A:144:LYS:HD3	1:A:155:VAL:HG11	1.96	0.47
1:B:129:ARG:HD3	1:B:154:GLU:CD	2.39	0.47
1:B:170:PHE:HE2	1:B:207:THR:HG21	1.80	0.47
1:B:333:MET:HE2	1:B:333:MET:CA	2.42	0.47
1:A:146:VAL:HG23	1:A:147:PHE:N	2.29	0.47
1:B:73:ILE:HG23	1:B:291:ILE:CG2	2.45	0.47
1:B:73:ILE:HG23	1:B:291:ILE:HG21	1.97	0.47
1:B:203:GLU:H	1:B:203:GLU:HG2	1.58	0.47
1:B:204:GLN:O	1:B:207:THR:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ASN:ND2	1:A:314:ALA:N	2.62	0.47
1:B:159:ALA:O	1:B:173:LEU:HA	2.15	0.47
1:A:225:TYR:HE1	1:A:359:MET:HE3	1.79	0.47
1:A:301:HIS:HD2	5:A:447:HOH:O	1.98	0.46
1:B:250:LEU:CD1	1:B:273:VAL:HG13	2.45	0.46
1:B:315:LEU:HD23	1:B:315:LEU:HA	1.37	0.46
1:A:76:ILE:O	1:A:79:PHE:HB3	2.15	0.46
1:B:168:LEU:HD23	1:B:168:LEU:HA	1.73	0.46
1:A:237:ALA:O	1:A:241:ARG:HD3	2.15	0.46
1:A:400:LEU:CD1	1:A:404:ILE:HD12	2.44	0.46
1:B:177:LEU:O	1:B:180:ALA:HB3	2.15	0.46
1:B:278:GLU:OE1	1:B:282:ARG:NH1	2.49	0.46
1:B:330:ILE:HG23	1:B:389:VAL:HG12	1.98	0.46
1:B:324:THR:HB	1:B:327:ARG:NH2	2.31	0.46
1:A:234:GLU:OE1	1:A:241:ARG:NH2	2.47	0.46
1:A:298:PRO:HB2	1:A:299:PRO:HD2	1.98	0.46
1:B:93:ALA:O	1:B:97:ASP:N	2.33	0.46
1:B:248:LYS:HB3	1:B:275:ALA:HB2	1.98	0.46
1:B:277:SER:HA	1:B:280:VAL:HG12	1.97	0.46
1:A:165:ASN:H	1:A:165:ASN:ND2	2.06	0.46
1:B:117:ASP:O	1:B:121:LYS:CD	2.47	0.46
1:A:39:LEU:HD21	1:B:69:LEU:CD2	2.46	0.45
1:A:74:ASP:OD1	1:A:74:ASP:N	2.43	0.45
1:A:292:ARG:NH2	1:B:18:LEU:HD22	2.29	0.45
1:B:226:GLN:NE2	5:B:510:HOH:O	2.39	0.45
1:A:90:LYS:HE3	1:A:90:LYS:HB3	1.67	0.45
1:A:292:ARG:NE	1:B:18:LEU:HD22	2.32	0.45
1:A:144:LYS:HD2	1:A:155:VAL:CG1	2.46	0.45
1:A:212:SER:CB	1:A:217:TRP:CE3	2.99	0.45
1:A:92:SER:OG	1:A:94:LEU:N	2.50	0.45
1:A:382:VAL:CG1	1:A:383:ALA:N	2.80	0.45
1:A:348:ARG:HH21	1:A:369:GLN:HE22	1.64	0.45
1:B:46:LYS:CG	1:B:47:ILE:N	2.80	0.45
1:A:312:ASN:C	1:A:312:ASN:HD22	2.25	0.45
1:A:92:SER:OG	1:A:94:LEU:HB2	2.17	0.45
1:B:41:TYR:CD1	1:B:391:GLY:HA2	2.52	0.44
1:B:235:GLU:H	1:B:235:GLU:HG2	1.56	0.44
1:B:76:ILE:O	1:B:76:ILE:HG22	2.14	0.44
1:A:266:ARG:HG2	1:B:299:PRO:HA	1.98	0.44
1:B:344:LYS:HD2	1:B:402:GLU:CG	2.46	0.44
1:A:393:THR:HB	1:A:394:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:SER:O	1:B:139:SER:HB2	2.18	0.44
1:A:335:GLN:HA	1:A:354:ILE:CD1	2.47	0.44
1:B:397:MET:HE2	1:B:400:LEU:HD22	1.99	0.44
1:B:79:PHE:CD2	1:B:104:GLN:HB2	2.52	0.44
1:A:68:LYS:HB2	1:B:261:GLY:O	2.17	0.44
1:A:170:PHE:CE2	1:A:174:ILE:CD1	2.99	0.44
1:A:12:ALA:HB1	1:A:13:PRO:CD	2.47	0.44
1:B:7:GLU:OE1	1:B:7:GLU:N	2.35	0.44
1:B:23:LEU:HD23	1:B:23:LEU:HA	1.74	0.44
1:B:170:PHE:CE2	1:B:174:ILE:CD1	3.00	0.43
1:B:140:TRP:HE3	1:B:143:HIS:CD2	2.35	0.43
1:B:140:TRP:CH2	1:B:142:ASN:HB3	2.53	0.43
1:B:210:GLN:HE21	1:B:214:GLU:CG	2.31	0.43
1:A:176:SER:O	1:A:179:GLU:HG3	2.18	0.43
1:A:15:ASP:CG	1:A:16:PRO:HD2	2.44	0.43
1:A:348:ARG:NH2	1:A:369:GLN:HE22	2.16	0.43
1:A:367:LYS:NZ	1:A:368:GLU:OE2	2.34	0.43
1:B:337:PHE:HE2	1:B:353:ILE:CD1	2.32	0.43
1:B:348:ARG:HD2	1:B:409:LEU:HD22	2.00	0.43
1:A:71:LEU:HD11	1:A:300:ALA:CB	2.46	0.43
1:B:73:ILE:CD1	1:B:292:ARG:HE	2.31	0.43
1:B:142:ASN:O	1:B:146:VAL:HG13	2.18	0.43
1:B:294:ASN:C	1:B:294:ASN:HD22	2.25	0.43
1:B:280:VAL:O	1:B:284:PHE:HB2	2.19	0.43
1:A:331:GLN:NE2	5:A:457:HOH:O	2.51	0.43
1:B:323:LEU:HA	1:B:326:MET:HE3	2.01	0.43
1:A:202:LEU:HD23	1:A:202:LEU:HA	1.85	0.43
1:A:341:LEU:HD12	1:A:341:LEU:HA	1.69	0.43
1:B:212:SER:CB	1:B:217:TRP:HE3	2.30	0.43
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.87	0.42
1:B:158:TYR:CD1	1:B:173:LEU:CD1	3.02	0.42
1:B:212:SER:CB	1:B:217:TRP:CE3	3.02	0.42
1:A:101:ARG:HD3	1:A:281:ASP:OD1	2.19	0.42
1:B:20:LEU:O	1:B:23:LEU:HB2	2.19	0.42
1:B:350:PHE:O	1:B:353:ILE:HB	2.19	0.42
1:A:388:ASN:ND2	1:A:390:ALA:H	2.16	0.42
1:B:210:GLN:O	1:B:213:VAL:HB	2.19	0.42
1:B:386:ARG:NH2	4:B:411:SO4:O4	2.51	0.42
1:A:27:ASP:OD2	1:A:380:TYR:OH	2.30	0.42
1:A:386:ARG:NH2	3:A:411:IOP:C1'	2.80	0.42
1:A:79:PHE:CZ	1:A:256:TYR:HE2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:GLU:OE2	1:B:282:ARG:NH1	2.51	0.42
1:A:165:ASN:O	1:A:166:HIS:HB2	2.20	0.42
1:B:152:LEU:HD12	1:B:152:LEU:HA	1.70	0.42
1:B:129:ARG:NE	1:B:154:GLU:CB	2.78	0.42
1:A:20:LEU:HD23	1:A:20:LEU:HA	1.67	0.42
1:A:98:LYS:HA	1:A:98:LYS:HD2	1.46	0.42
1:B:259:ASN:HD22	1:B:259:ASN:N	2.16	0.42
1:B:389:VAL:C	1:B:391:GLY:H	2.28	0.42
1:A:46:LYS:NZ	1:B:66:THR:O	2.51	0.41
1:A:242:ALA:O	1:A:245:ALA:HB3	2.19	0.41
1:B:113:ARG:HA	1:B:113:ARG:HD3	1.94	0.41
1:B:246:MET:HE3	1:B:246:MET:HB3	1.57	0.41
1:A:83:THR:HG22	1:A:87:LEU:HD22	2.00	0.41
1:A:112:LEU:HD12	1:A:112:LEU:HA	1.91	0.41
1:A:177:LEU:O	1:A:180:ALA:HB3	2.19	0.41
1:A:87:LEU:HA	1:A:87:LEU:HD12	1.86	0.41
1:A:278:GLU:HG2	1:A:282:ARG:HH12	1.81	0.41
1:A:348:ARG:CG	1:A:348:ARG:NH1	2.80	0.41
1:B:370:VAL:HG21	1:B:383:ALA:HA	2.02	0.41
1:B:374:ARG:HD3	1:B:380:TYR:CE2	2.55	0.41
1:A:33:ILE:HD13	1:A:396:ASN:HB2	2.03	0.41
1:A:160:TYR:HD1	1:A:173:LEU:HD23	1.85	0.41
1:B:5:MET:N	1:B:7:GLU:OE1	2.53	0.41
1:B:83:THR:O	1:B:87:LEU:HD22	2.21	0.41
1:B:387:VAL:CG1	1:B:392:MET:HE3	2.51	0.41
1:A:312:ASN:HD22	1:A:314:ALA:N	2.19	0.41
1:A:397:MET:CE	1:A:400:LEU:CD2	2.99	0.41
1:A:68:LYS:HB2	5:A:616:HOH:O	2.20	0.41
1:A:168:LEU:HD12	5:A:540:HOH:O	2.21	0.41
1:A:248:LYS:HG2	1:A:275:ALA:HB2	2.00	0.41
1:B:40:TYR:CD2	1:B:40:TYR:C	2.99	0.41
1:B:94:LEU:N	1:B:94:LEU:HD12	2.35	0.41
1:A:27:ASP:OD1	1:A:29:ARG:HB2	2.21	0.41
1:A:264:ASN:C	1:A:264:ASN:HD22	2.27	0.41
1:B:18:LEU:HD12	1:B:18:LEU:HA	1.78	0.41
1:B:162:ASP:O	1:B:166:HIS:N	2.44	0.41
1:A:367:LYS:HG3	1:A:368:GLU:N	2.37	0.40
1:A:373:LEU:HD23	1:A:373:LEU:HA	1.94	0.40
1:B:278:GLU:CD	1:B:282:ARG:NH1	2.79	0.40
1:B:284:PHE:CD1	1:B:287:MET:HE3	2.56	0.40
1:B:400:LEU:C	1:B:400:LEU:HD23	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD12	1:A:18:LEU:HA	1.82	0.40
1:A:78:GLU:OE1	1:A:78:GLU:HA	2.22	0.40
1:A:312:ASN:ND2	1:A:312:ASN:C	2.79	0.40
1:B:186:VAL:HG22	1:B:188:PHE:CE1	2.57	0.40
1:B:295:TYR:C	1:B:295:TYR:CD1	3.00	0.40
1:B:347:ASN:HB2	1:B:409:LEU:HD13	2.03	0.40
1:A:258:LYS:HB2	5:A:425:HOH:O	2.20	0.40
1:B:69:LEU:HD22	1:B:70:TYR:N	2.36	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	394/396 (100%)	358 (91%)	31 (8%)	5 (1%)	9	10
1	B	394/396 (100%)	370 (94%)	20 (5%)	4 (1%)	12	15
All	All	788/792 (100%)	728 (92%)	51 (6%)	9 (1%)	11	13

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	346	ALA
1	A	343	GLU
1	A	374	ARG
1	B	30	PRO
1	B	301	HIS
1	A	173	LEU
1	B	347	ASN
1	B	296	SER
1	A	43	GLU

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	320/320 (100%)	246 (77%)	74 (23%)	1	1
1	B	320/320 (100%)	255 (80%)	65 (20%)	1	1
All	All	640/640 (100%)	501 (78%)	139 (22%)	1	1

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	9	ILE
1	A	10	THR
1	A	18	LEU
1	A	20	LEU
1	A	29	ARG
1	A	32	LYS
1	A	33	ILE
1	A	39	LEU
1	A	44	THR
1	A	46	LYS
1	A	61	LEU
1	A	69	LEU
1	A	81	ARG
1	A	87	LEU
1	A	90	LYS
1	A	94	LEU
1	A	98	LYS
1	A	112	LEU
1	A	119	LEU
1	A	121	LYS
1	A	126	LYS
1	A	129	ARG
1	A	139	SER
1	A	144	LYS
1	A	145	SER
1	A	152	LEU

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Mol	Chain	Res	Type
1	A	165	ASN
1	A	167	THR
1	A	168	LEU
1	A	174	ILE
1	A	178	ASN
1	A	179	GLU
1	A	187	LEU
1	A	195	PRO
1	A	198	ILE
1	A	202	LEU
1	A	206	GLN
1	A	211	LEU
1	A	218	LEU
1	A	240	LEU
1	A	241	ARG
1	A	246	MET
1	A	248	LYS
1	A	250	LEU
1	A	264	ASN
1	A	267	VAL
1	A	272	LEU
1	A	292	ARG
1	A	312	ASN
1	A	313	ASP
1	A	334	ARG
1	A	335	GLN
1	A	338	VAL
1	A	341	LEU
1	A	344	LYS
1	A	348	ARG
1	A	349	ASP
1	A	353	ILE
1	A	354	ILE
1	A	355	LYS
1	A	360	PHE
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

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Mol	Chain	Res	Type
1	A	376	GLU
1	A	384	SER
1	A	386	ARG
1	A	400	LEU
1	A	404	ILE
1	B	5	MET
1	B	18	LEU
1	B	25	ARG
1	B	27	ASP
1	B	50	LEU
1	B	51	THR
1	B	61	LEU
1	B	69	LEU
1	B	81	ARG
1	B	87	LEU
1	B	90	LYS
1	B	98	LYS
1	B	99	ARG
1	B	119	LEU
1	B	121	LYS
1	B	126	LYS
1	B	129	ARG
1	B	133	VAL
1	B	135	VAL
1	B	139	SER
1	B	144	LYS
1	B	145	SER
1	B	146	VAL
1	B	152	LEU
1	B	167	THR
1	B	168	LEU
1	B	171	ASP
1	B	187	LEU
1	B	198	ILE
1	B	203	GLU
1	B	206	GLN
1	B	213	VAL
1	B	215	LYS
1	B	220	LEU
1	B	223	PHE
1	B	233	LEU
1	B	234	GLU

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Mol	Chain	Res	Type
1	B	235	GLU
1	B	240	LEU
1	B	246	MET
1	B	259	ASN
1	B	267	VAL
1	B	273	VAL
1	B	280	VAL
1	B	292	ARG
1	B	318	ILE
1	B	324	THR
1	B	338	VAL
1	B	341	LEU
1	B	342	GLN
1	B	343	GLU
1	B	348	ARG
1	B	349	ASP
1	B	353	ILE
1	B	354	ILE
1	B	355	LYS
1	B	357	ASN
1	B	362	PHE
1	B	367	LYS
1	B	370	VAL
1	B	371	LEU
1	B	372	ARG
1	B	373	LEU
1	B	375	GLU
1	B	387	VAL

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	84	GLN
1	A	142	ASN
1	A	165	ASN
1	A	166	HIS
1	A	175	ASN
1	A	181	GLN
1	A	189	HIS
1	A	206	GLN
1	A	226	GLN
1	A	264	ASN

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Mol	Chain	Res	Type
1	A	301	HIS
1	A	312	ASN
1	A	328	GLN
1	A	335	GLN
1	A	339	ASN
1	A	342	GLN
1	A	357	ASN
1	A	388	ASN
1	B	8	ASN
1	B	63	ASN
1	B	84	GLN
1	B	96	ASN
1	B	175	ASN
1	B	206	GLN
1	B	210	GLN
1	B	226	GLN
1	B	247	HIS
1	B	259	ASN
1	B	294	ASN
1	B	328	GLN
1	B	339	ASN
1	B	347	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](#)

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	412	1	15,15,16	1.34	3 (20%)	21,22,23	2.03	8 (38%)
4	SO4	B	411	-	4,4,4	0.29	0	6,6,6	0.46	0
2	PLP	A	410	1	15,15,16	1.12	1 (6%)	21,22,23	2.05	10 (47%)
3	IOP	A	411	-	15,15,15	0.65	0	20,20,20	1.45	4 (20%)

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	412	1	-	2/6/6/8	0/1/1/1
2	PLP	A	410	1	-	2/6/6/8	0/1/1/1
3	IOP	A	411	-	-	2/5/5/5	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	412	PLP	C5-C4	2.82	1.43	1.40
2	A	410	PLP	C5-C4	2.60	1.43	1.40
2	B	412	PLP	C4A-C4	-2.43	1.46	1.51
2	B	412	PLP	P-O3P	-2.08	1.47	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	412	PLP	C4A-C4-C5	5.24	126.35	120.94
2	A	410	PLP	C4A-C4-C5	4.22	125.29	120.94
2	A	410	PLP	C6-C5-C4	3.59	121.04	118.10
3	A	411	IOP	C3'-C2'-C1'	-3.23	105.09	113.67
3	A	411	IOP	O1-C1'-C2'	-3.01	113.54	123.09
2	B	412	PLP	C3-C2-N1	-2.91	117.29	120.96
2	A	410	PLP	C3-C2-N1	-2.80	117.43	120.96
2	A	410	PLP	C3-C4-C5	-2.79	115.24	118.59
2	A	410	PLP	O3P-P-O1P	2.68	121.29	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	412	PLP	C6-C5-C4	2.66	120.28	118.10
3	A	411	IOP	O2-C1'-C2'	2.62	122.28	114.00
2	B	412	PLP	C5A-C5-C6	-2.53	115.24	119.36
2	A	410	PLP	O4P-C5A-C5	2.52	114.07	109.36
2	B	412	PLP	C6-N1-C2	2.26	123.30	119.20
2	B	412	PLP	O4P-C5A-C5	2.21	113.50	109.36
2	A	410	PLP	C5-C6-N1	-2.21	120.25	123.83
2	A	410	PLP	C5A-C5-C6	-2.19	115.79	119.36
2	A	410	PLP	C4-C3-C2	2.15	123.10	119.89
3	A	411	IOP	C2'-C3'-C3	-2.11	108.51	113.98
2	B	412	PLP	C5-C6-N1	-2.08	120.45	123.83
2	A	410	PLP	C6-N1-C2	2.06	122.93	119.20
2	B	412	PLP	C3-C4-C5	-2.02	116.17	118.59

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	410	PLP	C4-C5-C5A-O4P
2	A	410	PLP	C6-C5-C5A-O4P
2	B	412	PLP	C4-C5-C5A-O4P
2	B	412	PLP	C6-C5-C5A-O4P
3	A	411	IOP	O1-C1'-C2'-C3'
3	A	411	IOP	O2-C1'-C2'-C3'

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	411	SO4	1	0
2	A	410	PLP	1	0
3	A	411	IOP	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	91:GLY	C	92:SER	N	1.12

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.