



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:26 PM GMT

PDB ID : 1ARH  
Title : ASPARTATE AMINOTRANSFERASE, Y225R/R386A MUTANT  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

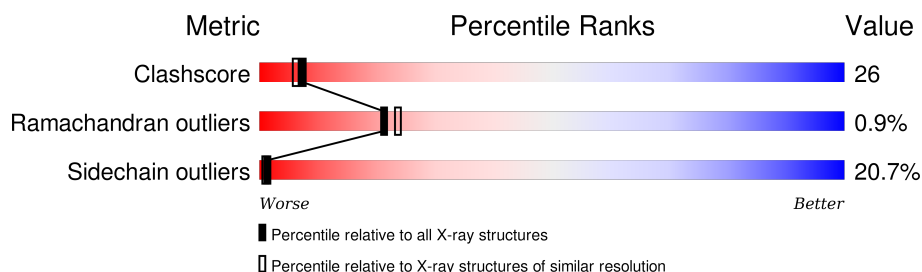
# 1 Overall quality at a glance ⓘ

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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	
1	B	396	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6543 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.

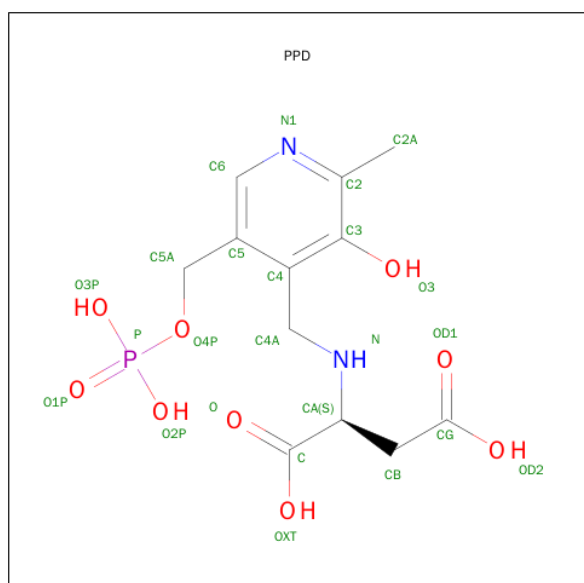
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3062	1930	536	583	13			
1	B	396	Total	C	N	O	S	0	0	0
			3062	1930	536	583	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	ARG	TYR	ENGINEERED	UNP P00509
A	386	ALA	ARG	ENGINEERED	UNP P00509
B	225	ARG	TYR	ENGINEERED	UNP P00509
B	386	ALA	ARG	ENGINEERED	UNP P00509

- Molecule 2 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDI N-4-YLMETHYLENE)-AMINO]-SUCCINIC ACID (three-letter code: PPD) (formula: C<sub>12</sub>H<sub>17</sub>N<sub>2</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	12	2	9	1		
2	B	1	Total	C	N	O	P	0	0
			24	12	2	9	1		

- Molecule 3 is water.

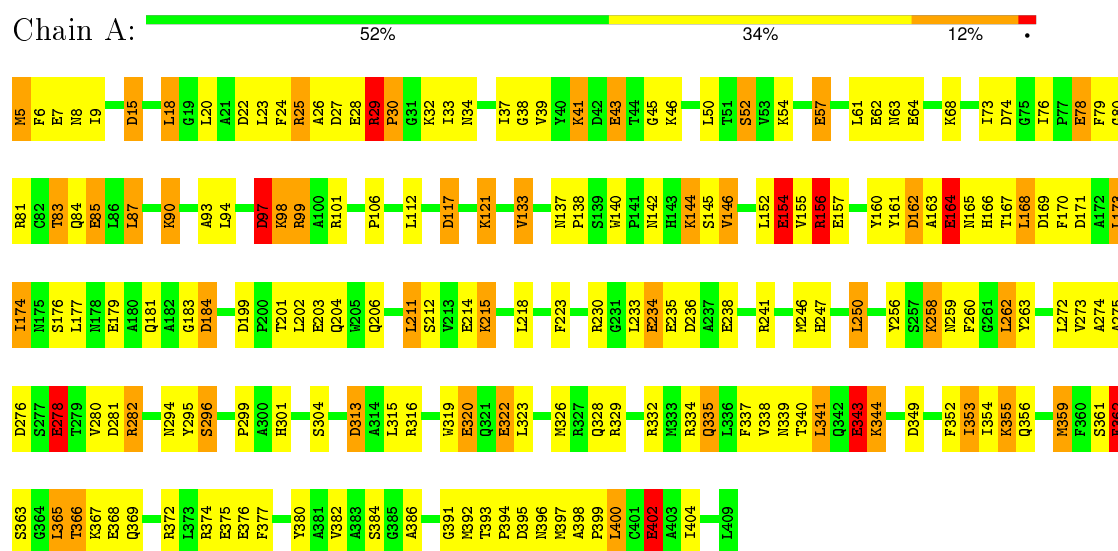
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	192	Total	O	0	0
			192	192		
3	B	179	Total	O	0	0
			179	179		

### 3 Residue-property plots

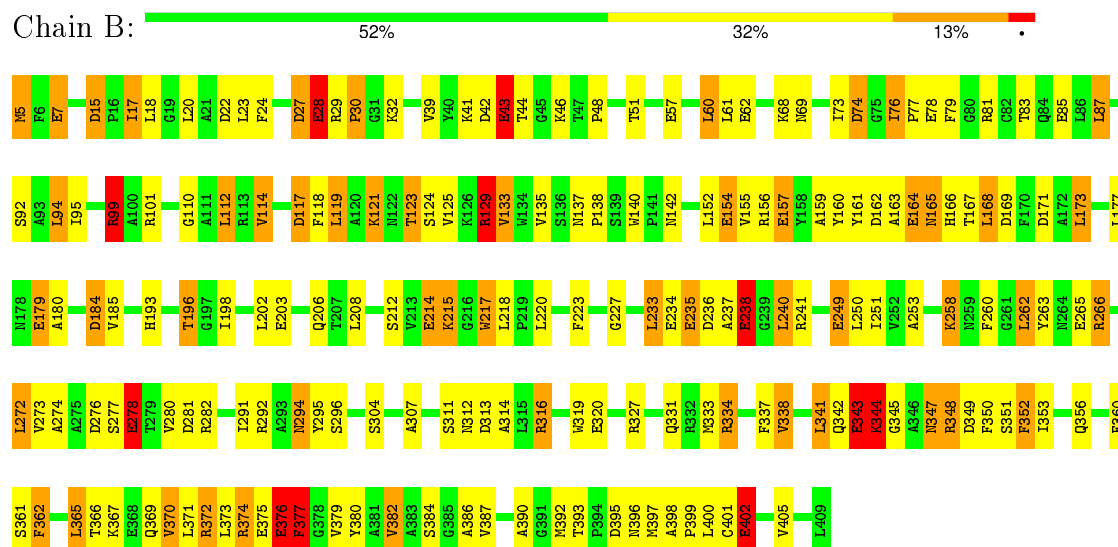
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

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 will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.12Å 79.61Å 89.85Å 90.00° 117.91° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	96.2 (8.00-2.30)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT V. 4-C	Depositor
R, $R_{free}$	0.219 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6543	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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: PPD

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	0.90	23/3122 (0.7%)	1.24	36/4229 (0.9%)
1	B	0.89	24/3122 (0.8%)	1.22	39/4229 (0.9%)
All	All	0.89	47/6244 (0.8%)	1.23	75/8458 (0.9%)

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	GLU	CD-OE1	6.90	1.33	1.25
1	A	179	GLU	CD-OE2	6.54	1.32	1.25
1	A	320	GLU	CD-OE2	6.34	1.32	1.25
1	B	320	GLU	CD-OE1	6.32	1.32	1.25
1	B	278	GLU	CD-OE2	6.30	1.32	1.25
1	A	43	GLU	CD-OE1	6.26	1.32	1.25
1	B	214	GLU	CD-OE2	6.22	1.32	1.25
1	B	62	GLU	CD-OE2	6.20	1.32	1.25
1	A	85	GLU	CD-OE1	6.11	1.32	1.25
1	A	164	GLU	CD-OE2	6.09	1.32	1.25
1	B	85	GLU	CD-OE1	6.06	1.32	1.25
1	B	234	GLU	CD-OE2	6.04	1.32	1.25
1	B	402	GLU	CD-OE2	6.04	1.32	1.25
1	A	62	GLU	CD-OE2	6.00	1.32	1.25
1	A	57	GLU	CD-OE1	5.99	1.32	1.25
1	B	265	GLU	CD-OE1	5.95	1.32	1.25
1	A	238	GLU	CD-OE2	5.94	1.32	1.25
1	B	43	GLU	CD-OE1	5.92	1.32	1.25
1	B	238	GLU	CD-OE2	5.91	1.32	1.25
1	A	343	GLU	CD-OE2	5.84	1.32	1.25
1	A	375	GLU	CD-OE2	5.83	1.32	1.25
1	A	7	GLU	CD-OE2	5.82	1.32	1.25
1	B	343	GLU	CD-OE2	5.79	1.32	1.25
1	A	402	GLU	CD-OE1	5.79	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	235	GLU	CD-OE1	5.73	1.31	1.25
1	A	214	GLU	CD-OE1	5.71	1.31	1.25
1	B	28	GLU	CD-OE1	5.68	1.31	1.25
1	A	322	GLU	CD-OE2	5.67	1.31	1.25
1	A	203	GLU	CD-OE1	5.63	1.31	1.25
1	B	376	GLU	CD-OE1	5.58	1.31	1.25
1	B	78	GLU	CD-OE1	5.58	1.31	1.25
1	B	157	GLU	CD-OE2	5.56	1.31	1.25
1	A	64	GLU	CD-OE2	5.56	1.31	1.25
1	B	7	GLU	CD-OE1	5.55	1.31	1.25
1	A	28	GLU	CD-OE2	5.49	1.31	1.25
1	A	78	GLU	CD-OE2	5.47	1.31	1.25
1	B	179	GLU	CD-OE2	5.47	1.31	1.25
1	B	375	GLU	CD-OE1	5.42	1.31	1.25
1	B	154	GLU	CD-OE1	5.42	1.31	1.25
1	A	234	GLU	CD-OE1	5.32	1.31	1.25
1	A	278	GLU	CD-OE1	5.27	1.31	1.25
1	A	376	GLU	CD-OE1	5.24	1.31	1.25
1	B	203	GLU	CD-OE1	5.24	1.31	1.25
1	B	249	GLU	CD-OE2	5.20	1.31	1.25
1	B	57	GLU	CD-OE2	5.09	1.31	1.25
1	B	164	GLU	CD-OE2	5.09	1.31	1.25
1	A	154	GLU	CD-OE2	5.06	1.31	1.25

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	B	184	ASP	CB-CG-OD1	-8.17	110.95	118.30
1	B	42	ASP	CB-CG-OD2	-7.84	111.24	118.30
1	A	376	GLU	CB-CA-C	-7.81	94.79	110.40
1	B	15	ASP	CB-CG-OD2	-7.65	111.42	118.30
1	A	169	ASP	CB-CG-OD1	7.64	125.18	118.30
1	A	169	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	A	377	PHE	CB-CG-CD2	-7.52	115.53	120.80
1	B	171	ASP	CB-CG-OD1	-7.29	111.74	118.30
1	B	169	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	B	15	ASP	CB-CG-OD1	7.07	124.66	118.30
1	A	236	ASP	CB-CG-OD1	-6.96	112.03	118.30
1	B	162	ASP	CB-CG-OD1	6.92	124.52	118.30
1	B	184	ASP	CB-CG-OD2	6.77	124.40	118.30
1	A	22	ASP	CB-CG-OD1	-6.77	112.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	B	22	ASP	CB-CG-OD1	6.58	124.23	118.30
1	B	42	ASP	CB-CG-OD1	6.43	124.08	118.30
1	A	117	ASP	CB-CG-OD1	-6.35	112.58	118.30
1	A	22	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	236	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	184	ASP	CB-CG-OD2	6.07	123.77	118.30
1	B	236	ASP	CB-CG-OD2	6.07	123.76	118.30
1	B	313	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	B	27	ASP	CB-CG-OD1	6.01	123.70	118.30
1	A	199	ASP	CB-CG-OD2	5.97	123.68	118.30
1	B	266	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	313	ASP	CB-CG-OD1	-5.93	112.96	118.30
1	B	162	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	A	15	ASP	CB-CG-OD1	5.93	123.63	118.30
1	A	276	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	282	ARG	NE-CZ-NH1	-5.89	117.36	120.30
1	A	97	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	74	ASP	CB-CG-OD2	5.84	123.55	118.30
1	B	281	ASP	CB-CG-OD1	-5.83	113.05	118.30
1	A	162	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	184	ASP	CB-CG-OD1	-5.83	113.06	118.30
1	A	162	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	B	377	PHE	CB-CA-C	-5.80	98.81	110.40
1	B	276	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	B	27	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	B	169	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	199	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	A	171	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	B	171	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	97	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	B	217	TRP	CA-CB-CG	5.66	124.46	113.70
1	A	362	PHE	CB-CG-CD1	5.63	124.75	120.80
1	A	117	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	377	PHE	N-CA-CB	5.59	120.66	110.60
1	A	395	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	B	276	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	236	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	276	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	281	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	74	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	A	395	ASP	CB-CG-OD2	5.36	123.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ASP	CB-CG-OD1	-5.35	113.49	118.30
1	B	349	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	B	74	ASP	CB-CG-OD2	5.34	123.10	118.30
1	B	313	ASP	CB-CG-OD1	5.33	123.10	118.30
1	B	395	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	395	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	B	154	GLU	N-CA-CB	5.30	120.13	110.60
1	A	156	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	A	281	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	B	352	PHE	CB-CG-CD1	5.15	124.41	120.80
1	B	349	ASP	CB-CG-OD1	5.15	122.93	118.30
1	B	99	ARG	N-CA-CB	-5.14	101.34	110.60
1	A	250	LEU	N-CA-CB	-5.10	100.20	110.40
1	A	15	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	B	129	ARG	CB-CA-C	-5.07	100.25	110.40
1	B	217	TRP	CB-CA-C	-5.04	100.31	110.40
1	A	281	ASP	CB-CG-OD2	5.02	122.81	118.30
1	B	117	ASP	CB-CG-OD2	5.01	122.81	118.30

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	3062	0	3014	160	0
1	B	3062	0	3014	163	0
2	A	24	0	12	0	0
2	B	24	0	12	1	0
3	A	192	0	0	10	0
3	B	179	0	0	7	0
All	All	6543	0	6052	314	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 26.

All (314) 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:344:LYS:HD2	1:B:402:GLU:HG3	1.24	1.16
1:B:260:PHE:HB3	1:B:262:LEU:HD22	1.40	1.02
1:A:201:THR:H	1:A:204:GLN:HE21	1.08	1.01
1:A:201:THR:H	1:A:204:GLN:NE2	1.69	0.89
1:B:344:LYS:CD	1:B:402:GLU:HG3	2.03	0.88
1:A:337:PHE:HD1	1:A:397:MET:HE1	1.37	0.88
1:B:24:PHE:CZ	1:B:32:LYS:HE3	2.10	0.87
1:A:352:PHE:HA	1:A:355:LYS:HD3	1.60	0.83
1:A:260:PHE:HB3	1:A:262:LEU:HD22	1.58	0.83
1:A:337:PHE:CD1	1:A:397:MET:HE1	2.15	0.81
1:B:29:ARG:HB3	1:B:30:PRO:HD2	1.62	0.81
1:B:337:PHE:HD1	1:B:397:MET:HE2	1.44	0.81
1:B:123:THR:CG2	1:B:125:VAL:H	1.94	0.79
1:A:156:ARG:NH1	1:A:156:ARG:HA	1.96	0.79
1:A:41:LYS:HD2	1:A:45:GLY:HA2	1.65	0.79
1:B:331:GLN:NE2	3:B:571:HOH:O	2.16	0.78
1:A:24:PHE:CE1	1:A:34:ASN:HB2	2.18	0.78
1:B:333:MET:HE2	1:B:393:THR:HA	1.65	0.78
1:A:41:LYS:HD2	1:A:45:GLY:C	2.04	0.77
1:B:333:MET:HE2	1:B:393:THR:CA	2.15	0.77
1:A:202:LEU:O	1:A:206:GLN:HG3	1.83	0.77
1:B:196:THR:CG2	1:B:198:ILE:H	1.97	0.77
1:A:174:ILE:HD13	1:A:211:LEU:CD2	2.17	0.75
1:B:344:LYS:O	1:B:344:LYS:HE2	1.87	0.74
1:A:398:ALA:HB3	1:A:399:PRO:HD3	1.70	0.74
1:A:174:ILE:HD13	1:A:211:LEU:HD23	1.70	0.74
1:A:398:ALA:O	1:A:402:GLU:HG2	1.88	0.73
1:A:162:ASP:OD1	1:A:164:GLU:HG2	1.88	0.72
1:A:41:LYS:HD2	1:A:45:GLY:CA	2.17	0.72
1:B:123:THR:HG22	1:B:125:VAL:H	1.54	0.72
1:B:344:LYS:HD2	1:B:402:GLU:CG	2.14	0.72
1:B:94:LEU:HD23	1:B:94:LEU:N	2.05	0.71
1:A:41:LYS:HB3	1:A:41:LYS:NZ	2.05	0.71
1:B:202:LEU:O	1:B:206:GLN:HG3	1.89	0.71
1:B:164:GLU:C	1:B:165:ASN:HD22	1.94	0.71
1:B:196:THR:HG22	1:B:198:ILE:H	1.54	0.71
1:B:185:VAL:HG22	1:B:218:LEU:HD23	1.72	0.70
1:B:196:THR:CG2	1:B:198:ILE:HB	2.21	0.70
1:B:334:ARG:HH12	1:B:361:SER:HG	1.35	0.70
1:B:165:ASN:N	1:B:165:ASN:HD22	1.89	0.69
1:A:328:GLN:O	1:A:332:ARG:HD3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLU:HG3	1:A:165:ASN:OD1	1.93	0.69
1:A:201:THR:N	1:A:204:GLN:HE21	1.86	0.69
1:A:41:LYS:HE3	1:A:391:GLY:HA2	1.74	0.69
1:A:23:LEU:HD12	1:A:380:TYR:HE2	1.58	0.69
1:B:161:TYR:CE2	1:B:163:ALA:HA	2.28	0.69
1:B:123:THR:CG2	1:B:125:VAL:HG23	2.22	0.69
1:A:98:LYS:HE3	1:A:101:ARG:HD3	1.73	0.68
1:A:294:ASN:HD21	1:B:294:ASN:HD21	1.39	0.68
1:B:161:TYR:HH	1:B:166:HIS:HD1	1.40	0.68
1:A:79:PHE:O	1:A:83:THR:HG23	1.94	0.68
1:B:99:ARG:HG2	1:B:99:ARG:HH11	1.56	0.68
1:A:98:LYS:CE	1:A:101:ARG:HD3	2.23	0.67
1:A:29:ARG:HD2	1:A:30:PRO:HD2	1.75	0.67
1:A:24:PHE:CE1	1:A:32:LYS:HD2	2.30	0.66
1:A:384:SER:HB3	3:A:440:HOH:O	1.96	0.66
1:A:211:LEU:CD1	1:A:215:LYS:HD3	2.26	0.66
1:B:382:VAL:HG23	1:B:386:ALA:O	1.95	0.65
1:B:99:ARG:HG2	1:B:99:ARG:NH1	2.11	0.65
1:A:8:ASN:ND2	3:A:599:HOH:O	2.30	0.65
1:A:137:ASN:ND2	1:A:157:GLU:OE1	2.29	0.65
1:A:29:ARG:O	1:A:32:LYS:HG2	1.96	0.65
1:B:312:ASN:O	1:B:316:ARG:HB2	1.96	0.65
1:B:154:GLU:OE2	1:B:156:ARG:NH1	2.30	0.65
1:A:24:PHE:CZ	1:A:34:ASN:HB2	2.32	0.64
1:A:183:GLY:HA2	1:B:5:MET:CE	2.28	0.64
1:A:211:LEU:HD12	1:A:215:LYS:HD3	1.78	0.64
1:A:117:ASP:O	1:A:121:LYS:HG2	1.98	0.64
1:A:382:VAL:HG23	1:A:386:ALA:O	1.98	0.64
1:B:99:ARG:NH1	1:B:274:ALA:O	2.30	0.64
1:A:258:LYS:HG2	1:A:359:MET:HE3	1.79	0.63
1:B:160:TYR:O	1:B:168:LEU:HD23	1.97	0.63
1:A:41:LYS:NZ	1:A:45:GLY:HA2	2.13	0.63
1:A:154:GLU:OE2	1:A:156:ARG:NH2	2.30	0.63
1:A:25:ARG:NH2	3:A:547:HOH:O	2.30	0.63
1:A:340:THR:O	1:A:344:LYS:HB2	1.99	0.62
1:B:237:ALA:O	1:B:241:ARG:HD3	1.99	0.62
1:A:366:THR:HG22	1:A:369:GLN:H	1.64	0.62
1:A:263:TYR:HB2	1:B:68:LYS:O	1.99	0.62
1:B:23:LEU:HD23	1:B:23:LEU:O	2.00	0.62
1:B:398:ALA:HB3	1:B:399:PRO:HD3	1.80	0.61
1:A:97:ASP:N	1:A:97:ASP:OD1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:CD	1:A:45:GLY:HA2	2.30	0.61
1:B:238:GLU:HA	1:B:238:GLU:OE1	2.00	0.60
1:A:183:GLY:HA2	1:B:5:MET:HE3	1.83	0.60
1:A:316:ARG:O	1:A:320:GLU:HG3	2.01	0.60
1:A:41:LYS:HE2	3:A:578:HOH:O	2.02	0.60
1:A:352:PHE:CA	1:A:355:LYS:HD3	2.32	0.60
1:B:123:THR:HG21	1:B:125:VAL:HG23	1.84	0.60
1:A:87:LEU:O	1:A:241:ARG:HD2	2.02	0.60
1:A:29:ARG:HH11	1:A:29:ARG:CG	2.15	0.60
1:A:98:LYS:NZ	1:A:101:ARG:HD3	2.17	0.59
1:A:78:GLU:HB3	3:A:543:HOH:O	2.02	0.59
1:B:123:THR:HG23	1:B:125:VAL:H	1.68	0.59
1:B:356:GLN:NE2	1:B:361:SER:OG	2.35	0.59
1:A:33:ILE:CD1	1:A:400:LEU:HB2	2.32	0.58
1:B:292:ARG:HA	1:B:296:SER:HA	1.85	0.58
1:B:372:ARG:HG3	1:B:376:GLU:HG2	1.85	0.58
1:B:24:PHE:HB2	1:B:380:TYR:CD2	2.39	0.58
1:B:334:ARG:NH1	1:B:361:SER:OG	2.31	0.57
1:B:341:LEU:HD13	1:B:401:CYS:HB3	1.85	0.57
1:B:212:SER:HA	1:B:217:TRP:CD1	2.40	0.57
1:B:129:ARG:HH11	1:B:129:ARG:CG	2.18	0.57
1:A:29:ARG:CG	1:A:30:PRO:HD2	2.34	0.57
1:B:334:ARG:HH11	1:B:334:ARG:HG2	1.69	0.57
1:A:278:GLU:OE1	1:A:282:ARG:NH1	2.30	0.57
1:A:29:ARG:HG3	1:A:30:PRO:HD2	1.87	0.57
1:B:401:CYS:O	1:B:405:VAL:HG23	2.04	0.57
1:B:334:ARG:NH2	1:B:360:PHE:O	2.38	0.56
1:B:112:LEU:HD13	1:B:253:ALA:CB	2.36	0.56
1:A:85:GLU:OE1	1:A:90:LYS:HD2	2.05	0.56
1:B:352:PHE:CE1	1:B:353:ILE:HD12	2.40	0.56
1:B:337:PHE:CD1	1:B:397:MET:HE2	2.33	0.56
1:B:196:THR:HG23	1:B:198:ILE:H	1.70	0.56
1:B:117:ASP:O	1:B:121:LYS:HD2	2.06	0.56
1:A:41:LYS:CE	1:A:45:GLY:HA2	2.36	0.56
1:B:94:LEU:HD23	1:B:94:LEU:H	1.68	0.56
1:B:344:LYS:HD2	1:B:402:GLU:HA	1.86	0.56
1:A:234:GLU:OE1	1:A:241:ARG:NH2	2.39	0.56
1:A:99:ARG:NH1	1:A:274:ALA:O	2.39	0.56
1:A:6:PHE:HB3	1:A:9:ILE:HD12	1.88	0.56
1:A:29:ARG:CD	1:A:30:PRO:HD2	2.36	0.55
1:A:73:ILE:HD11	1:B:18:LEU:HD23	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ARG:CG	1:B:99:ARG:HH11	2.19	0.55
1:B:196:THR:HG23	1:B:198:ILE:HB	1.87	0.55
1:B:28:GLU:OE1	1:B:28:GLU:HA	2.07	0.55
1:A:29:ARG:HH11	1:A:29:ARG:HG3	1.70	0.55
1:A:161:TYR:CZ	1:A:163:ALA:HA	2.41	0.55
1:B:240:LEU:O	1:B:240:LEU:HD22	2.06	0.55
1:A:156:ARG:CB	1:A:156:ARG:HH11	2.20	0.54
1:B:73:ILE:HD13	1:B:292:ARG:HB2	1.89	0.54
1:B:369:GLN:O	1:B:373:LEU:HB2	2.06	0.54
1:B:334:ARG:CG	1:B:334:ARG:HH11	2.21	0.54
1:B:5:MET:N	1:B:7:GLU:OE1	2.41	0.54
1:A:323:LEU:HA	1:A:326:MET:HE2	1.90	0.54
1:A:25:ARG:HG2	1:A:26:ALA:N	2.21	0.54
1:B:77:PRO:O	1:B:81:ARG:HD3	2.08	0.54
1:A:33:ILE:HG22	1:A:34:ASN:N	2.22	0.54
1:A:173:LEU:C	1:A:173:LEU:HD12	2.28	0.54
1:A:335:GLN:HA	1:A:354:ILE:HD11	1.90	0.54
1:B:278:GLU:CD	1:B:282:ARG:HH12	2.11	0.53
1:B:46:LYS:O	1:B:48:PRO:HD3	2.08	0.53
1:B:374:ARG:HB2	1:B:379:VAL:O	2.09	0.53
1:B:180:ALA:HB3	1:B:217:TRP:CZ3	2.44	0.53
1:B:291:ILE:HG23	1:B:295:TYR:CZ	2.44	0.53
1:A:258:LYS:HG2	1:A:359:MET:CE	2.39	0.52
1:A:32:LYS:HG3	1:A:32:LYS:O	2.09	0.52
1:B:196:THR:HG23	1:B:198:ILE:HD12	1.91	0.52
1:B:129:ARG:HG3	1:B:129:ARG:HH11	1.75	0.52
1:A:247:HIS:HD2	3:A:502:HOH:O	1.92	0.52
1:A:46:LYS:HD2	3:A:559:HOH:O	2.10	0.52
1:B:396:ASN:O	1:B:400:LEU:HB2	2.10	0.52
1:A:33:ILE:HD12	1:A:400:LEU:HB2	1.92	0.52
1:B:133:VAL:O	1:B:155:VAL:HA	2.09	0.52
1:B:249:GLU:HA	1:B:273:VAL:O	2.09	0.52
1:B:24:PHE:HD1	1:B:380:TYR:CD1	2.27	0.51
1:B:260:PHE:CB	1:B:262:LEU:HD22	2.29	0.51
1:B:352:PHE:CD1	1:B:353:ILE:HD12	2.44	0.51
1:A:5:MET:HE3	1:A:5:MET:HA	1.93	0.51
1:B:258:LYS:NZ	2:B:411:PPD:H4A2	2.26	0.51
1:B:344:LYS:CE	1:B:402:GLU:HG3	2.40	0.51
1:B:43:GLU:CD	1:B:43:GLU:H	2.14	0.51
1:B:382:VAL:HG12	3:B:435:HOH:O	2.10	0.51
1:A:106:PRO:HD3	1:A:295:TYR:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:THR:HG23	1:A:368:GLU:OE1	2.12	0.50
1:A:156:ARG:HA	1:A:156:ARG:HH11	1.73	0.50
1:A:68:LYS:HD3	1:B:262:LEU:HD12	1.94	0.50
1:A:352:PHE:HB2	1:A:355:LYS:HZ2	1.77	0.50
1:B:341:LEU:CD1	1:B:401:CYS:HB3	2.42	0.50
1:A:8:ASN:HB3	3:A:544:HOH:O	2.12	0.50
1:B:327:ARG:O	1:B:331:GLN:HG3	2.11	0.49
1:A:398:ALA:N	1:A:399:PRO:HD2	2.27	0.49
1:A:299:PRO:HA	1:B:266:ARG:HG2	1.93	0.49
1:B:165:ASN:N	1:B:165:ASN:ND2	2.59	0.49
1:A:362:PHE:HD1	1:A:386:ALA:HB2	1.77	0.49
1:B:398:ALA:N	1:B:399:PRO:HD2	2.26	0.49
1:A:201:THR:N	1:A:204:GLN:NE2	2.49	0.49
1:A:99:ARG:HG2	1:A:274:ALA:O	2.13	0.49
1:B:101:ARG:HD3	3:B:499:HOH:O	2.12	0.49
1:A:41:LYS:HZ3	1:A:45:GLY:HA2	1.77	0.49
1:A:362:PHE:CD1	1:A:386:ALA:HB2	2.48	0.49
1:B:333:MET:HB3	1:B:392:MET:HE2	1.95	0.49
1:A:398:ALA:HB3	1:A:399:PRO:CD	2.40	0.49
1:B:344:LYS:CD	1:B:402:GLU:HA	2.43	0.49
1:A:366:THR:HG23	1:A:368:GLU:H	1.78	0.49
1:B:377:PHE:CD1	1:B:377:PHE:N	2.79	0.48
1:A:57:GLU:OE2	1:A:301:HIS:NE2	2.35	0.48
1:B:334:ARG:O	1:B:338:VAL:HG13	2.14	0.48
1:B:161:TYR:OH	1:B:166:HIS:ND1	2.31	0.48
1:B:193:HIS:ND1	1:B:196:THR:HB	2.28	0.48
1:A:140:TRP:CZ2	1:A:142:ASN:HB3	2.48	0.48
1:A:352:PHE:HB2	1:A:355:LYS:NZ	2.28	0.48
1:B:294:ASN:HD22	1:B:294:ASN:C	2.16	0.48
1:B:398:ALA:HB3	1:B:399:PRO:CD	2.44	0.48
1:B:129:ARG:NH1	1:B:129:ARG:HG3	2.27	0.48
1:A:400:LEU:O	1:A:400:LEU:HD12	2.13	0.48
1:B:123:THR:HG23	1:B:124:SER:N	2.28	0.48
1:A:142:ASN:O	1:A:146:VAL:HG13	2.14	0.48
1:A:339:ASN:O	1:A:343:GLU:HG2	2.13	0.48
1:A:174:ILE:CD1	1:A:211:LEU:HD23	2.42	0.48
1:A:27:ASP:HB2	1:A:380:TYR:OH	2.14	0.48
1:A:76:ILE:O	1:A:79:PHE:HB3	2.14	0.48
1:A:99:ARG:HG2	1:A:99:ARG:HH11	1.78	0.48
1:B:110:GLY:O	1:B:114:VAL:HG13	2.13	0.48
1:B:362:PHE:CE1	1:B:384:SER:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:GLU:O	1:B:345:GLY:N	2.47	0.47
1:A:29:ARG:HG3	1:A:30:PRO:CD	2.44	0.47
1:B:304:SER:HB3	3:B:568:HOH:O	2.14	0.47
1:B:159:ALA:O	1:B:173:LEU:HB2	2.14	0.47
1:B:41:LYS:HB2	1:B:390:ALA:O	2.14	0.47
1:A:5:MET:HE3	1:A:5:MET:CA	2.44	0.47
1:A:41:LYS:HB3	1:A:41:LYS:HZ2	1.76	0.47
1:A:258:LYS:HB3	1:A:359:MET:HE1	1.97	0.47
1:A:367:LYS:NZ	1:A:368:GLU:OE2	2.40	0.47
1:B:118:PHE:HD1	1:B:119:LEU:HD13	1.78	0.47
1:B:24:PHE:CE1	1:B:32:LYS:HE3	2.49	0.47
1:A:52:SER:OG	1:A:322:GLU:OE1	2.31	0.47
1:A:161:TYR:CE2	1:A:163:ALA:HA	2.49	0.47
1:B:92:SER:HB3	1:B:95:ILE:HD12	1.96	0.47
1:A:341:LEU:HA	1:A:341:LEU:HD12	1.83	0.46
1:A:161:TYR:HE1	1:A:166:HIS:HA	1.80	0.46
1:A:365:LEU:HD12	1:A:365:LEU:HA	1.72	0.46
1:A:99:ARG:HG2	1:A:99:ARG:NH1	2.29	0.46
1:A:329:ARG:NH2	1:A:392:MET:O	2.44	0.46
1:B:135:VAL:O	1:B:157:GLU:HA	2.15	0.45
1:B:333:MET:HB3	1:B:392:MET:CE	2.45	0.45
1:B:129:ARG:CB	1:B:129:ARG:HH11	2.28	0.45
1:A:234:GLU:CD	1:A:241:ARG:HH22	2.20	0.45
1:A:218:LEU:HD13	3:A:506:HOH:O	2.14	0.45
1:B:180:ALA:O	1:B:217:TRP:HZ3	1.99	0.45
1:B:365:LEU:HA	1:B:365:LEU:HD12	1.77	0.45
1:B:83:THR:HG22	1:B:87:LEU:HD22	1.99	0.45
1:B:251:ILE:HG12	1:B:272:LEU:HD23	1.98	0.45
1:B:382:VAL:HG13	3:B:513:HOH:O	2.16	0.45
1:A:93:ALA:O	1:A:97:ASP:OD1	2.35	0.45
1:A:164:GLU:CG	1:A:165:ASN:N	2.80	0.45
1:A:173:LEU:HD12	1:A:173:LEU:O	2.17	0.45
1:B:347:ASN:HD22	1:B:348:ARG:H	1.64	0.45
1:B:123:THR:CG2	1:B:124:SER:N	2.80	0.45
1:A:18:LEU:HD22	1:B:292:ARG:CZ	2.47	0.45
1:B:352:PHE:CE1	1:B:353:ILE:CD1	3.00	0.44
1:B:15:ASP:OD1	1:B:17:ILE:N	2.45	0.44
1:A:138:PRO:HG3	1:A:362:PHE:CE2	2.52	0.44
1:A:397:MET:CE	1:A:400:LEU:HD23	2.47	0.44
1:A:355:LYS:HB2	1:A:355:LYS:HE2	1.45	0.44
1:B:258:LYS:N	1:B:258:LYS:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ARG:HB2	1:B:350:PHE:CE1	2.52	0.44
1:B:376:GLU:OE1	1:B:376:GLU:HA	2.16	0.44
1:A:338:VAL:HG11	1:A:354:ILE:HG12	2.00	0.44
1:A:5:MET:HB3	1:A:5:MET:HE2	1.77	0.44
1:B:220:LEU:HD13	1:B:251:ILE:HB	1.99	0.44
1:A:356:GLN:OE1	1:A:361:SER:OG	2.29	0.44
1:B:343:GLU:HG2	1:B:344:LYS:N	2.33	0.43
1:A:15:ASP:HB3	1:A:18:LEU:HB2	1.99	0.43
1:B:77:PRO:HB2	1:B:81:ARG:NH1	2.33	0.43
1:B:39:VAL:HG22	1:B:263:TYR:CE1	2.53	0.43
1:A:144:LYS:HB2	1:A:144:LYS:HE3	1.50	0.43
1:A:80:GLY:O	1:A:84:GLN:HG3	2.18	0.43
1:A:161:TYR:OH	1:A:166:HIS:HD2	2.02	0.43
1:A:41:LYS:HD2	1:A:45:GLY:O	2.17	0.43
1:B:214:GLU:HG3	1:B:215:LYS:HD3	2.01	0.43
1:A:164:GLU:HG3	1:A:165:ASN:N	2.33	0.43
1:A:366:THR:HB	1:A:369:GLN:OE1	2.18	0.43
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.72	0.43
1:A:393:THR:HB	1:A:394:PRO:HD2	2.00	0.43
1:A:397:MET:HE3	1:A:400:LEU:HD23	2.01	0.42
1:B:129:ARG:HH11	1:B:129:ARG:HB2	1.84	0.42
1:A:211:LEU:HD11	1:A:215:LYS:HD3	1.98	0.42
1:B:294:ASN:ND2	3:B:519:HOH:O	2.52	0.42
1:A:315:LEU:HA	1:A:315:LEU:HD23	1.81	0.42
1:B:233:LEU:HD21	1:B:319:TRP:CH2	2.54	0.42
1:A:260:PHE:CE1	1:A:319:TRP:CZ2	3.07	0.42
1:A:63:ASN:ND2	3:A:562:HOH:O	2.47	0.42
1:B:123:THR:HG23	1:B:125:VAL:HG23	1.99	0.42
1:A:99:ARG:HD2	1:A:275:ALA:O	2.19	0.42
1:A:397:MET:HE3	1:A:400:LEU:CD2	2.49	0.42
1:B:382:VAL:HG12	3:B:459:HOH:O	2.18	0.42
1:A:396:ASN:O	1:A:400:LEU:HB3	2.18	0.42
1:B:196:THR:HG23	1:B:198:ILE:CB	2.48	0.42
1:B:215:LYS:HA	1:B:215:LYS:HD2	1.77	0.42
1:A:20:LEU:HA	1:A:20:LEU:HD23	1.70	0.42
1:B:129:ARG:NH1	1:B:184:ASP:OD1	2.52	0.42
1:B:312:ASN:OD1	1:B:314:ALA:HB3	2.19	0.42
1:B:208:LEU:HA	1:B:208:LEU:HD23	1.82	0.42
1:B:177:LEU:HA	1:B:177:LEU:HD23	1.64	0.42
1:A:161:TYR:CD1	1:A:162:ASP:N	2.88	0.41
1:B:307:ALA:O	1:B:311:SER:OG	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:TRP:CH2	1:B:142:ASN:HB3	2.56	0.41
1:B:366:THR:O	1:B:370:VAL:HG13	2.21	0.41
1:B:397:MET:CE	1:B:400:LEU:HD13	2.51	0.41
1:B:334:ARG:HG2	1:B:353:ILE:CG2	2.51	0.41
1:B:227:GLY:O	1:B:327:ARG:HD3	2.20	0.41
1:A:83:THR:HG22	1:A:256:TYR:OH	2.20	0.41
1:B:123:THR:HG21	1:B:125:VAL:CG2	2.48	0.41
1:B:347:ASN:HD22	1:B:348:ARG:N	2.19	0.41
1:A:29:ARG:NH1	1:A:29:ARG:CG	2.79	0.41
1:B:76:ILE:O	1:B:79:PHE:HB3	2.21	0.41
1:A:156:ARG:HB3	1:A:156:ARG:HH11	1.85	0.40
1:B:235:GLU:O	1:B:238:GLU:HB2	2.21	0.40
1:B:137:ASN:HA	1:B:138:PRO:HA	1.75	0.40
1:B:196:THR:HG21	1:B:198:ILE:HB	1.97	0.40
1:A:165:ASN:O	1:A:167:THR:HG23	2.21	0.40
1:B:23:LEU:HD23	1:B:23:LEU:C	2.40	0.40
1:B:118:PHE:CD1	1:B:119:LEU:HD13	2.55	0.40
1:A:352:PHE:CE1	1:A:353:ILE:HG13	2.57	0.40
1:A:133:VAL:O	1:A:155:VAL:HA	2.21	0.40
1:A:181:GLN:O	1:A:184:ASP:HB2	2.22	0.40
1:B:74:ASP:N	1:B:74:ASP:OD1	2.47	0.40
1:B:250:LEU:HD12	1:B:250:LEU:C	2.41	0.40
1:A:160:TYR:CE1	1:A:168:LEU:HD21	2.55	0.40
1:A:29:ARG:HG3	1:A:30:PRO:N	2.37	0.40
1:A:316:ARG:HG2	1:A:316:ARG:O	2.22	0.40
1:A:18:LEU:CD2	1:B:292:ARG:CZ	3.00	0.40
1:B:60:LEU:HD12	1:B:60:LEU:HA	1.79	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	394/396 (100%)	367 (93%)	22 (6%)	5 (1%)	15	15
1	B	394/396 (100%)	368 (93%)	24 (6%)	2 (0%)	34	41
All	All	788/792 (100%)	735 (93%)	46 (6%)	7 (1%)	21	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	30	PRO
1	A	30	PRO
1	B	344	LYS
1	A	296	SER
1	A	43	GLU
1	A	38	GLY
1	A	37	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	319/319 (100%)	250 (78%)	69 (22%)	1	1
1	B	319/319 (100%)	256 (80%)	63 (20%)	1	1
All	All	638/638 (100%)	506 (79%)	132 (21%)	1	1

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	18	LEU
1	A	25	ARG
1	A	29	ARG
1	A	39	VAL
1	A	41	LYS
1	A	50	LEU
1	A	52	SER
1	A	54	LYS

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Mol	Chain	Res	Type
1	A	61	LEU
1	A	81	ARG
1	A	83	THR
1	A	87	LEU
1	A	90	LYS
1	A	94	LEU
1	A	97	ASP
1	A	98	LYS
1	A	99	ARG
1	A	112	LEU
1	A	121	LYS
1	A	133	VAL
1	A	144	LYS
1	A	145	SER
1	A	146	VAL
1	A	152	LEU
1	A	154	GLU
1	A	156	ARG
1	A	164	GLU
1	A	168	LEU
1	A	170	PHE
1	A	173	LEU
1	A	174	ILE
1	A	176	SER
1	A	211	LEU
1	A	212	SER
1	A	215	LYS
1	A	223	PHE
1	A	230	ARG
1	A	233	LEU
1	A	246	MET
1	A	250	LEU
1	A	258	LYS
1	A	259	ASN
1	A	262	LEU
1	A	272	LEU
1	A	273	VAL
1	A	278	GLU
1	A	280	VAL
1	A	296	SER
1	A	304	SER
1	A	313	ASP

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Mol	Chain	Res	Type
1	A	334	ARG
1	A	335	GLN
1	A	341	LEU
1	A	343	GLU
1	A	344	LYS
1	A	349	ASP
1	A	353	ILE
1	A	355	LYS
1	A	359	MET
1	A	362	PHE
1	A	363	SER
1	A	365	LEU
1	A	366	THR
1	A	372	ARG
1	A	374	ARG
1	A	400	LEU
1	A	402	GLU
1	A	404	ILE
1	B	5	MET
1	B	17	ILE
1	B	20	LEU
1	B	27	ASP
1	B	28	GLU
1	B	43	GLU
1	B	44	THR
1	B	51	THR
1	B	60	LEU
1	B	61	LEU
1	B	69	ASN
1	B	76	ILE
1	B	87	LEU
1	B	94	LEU
1	B	99	ARG
1	B	112	LEU
1	B	114	VAL
1	B	119	LEU
1	B	121	LYS
1	B	123	THR
1	B	129	ARG
1	B	133	VAL
1	B	152	LEU
1	B	165	ASN

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Mol	Chain	Res	Type
1	B	167	THR
1	B	168	LEU
1	B	173	LEU
1	B	179	GLU
1	B	196	THR
1	B	215	LYS
1	B	223	PHE
1	B	233	LEU
1	B	238	GLU
1	B	240	LEU
1	B	258	LYS
1	B	262	LEU
1	B	272	LEU
1	B	277	SER
1	B	278	GLU
1	B	280	VAL
1	B	294	ASN
1	B	316	ARG
1	B	334	ARG
1	B	338	VAL
1	B	341	LEU
1	B	342	GLN
1	B	343	GLU
1	B	344	LYS
1	B	347	ASN
1	B	348	ARG
1	B	351	SER
1	B	362	PHE
1	B	365	LEU
1	B	367	LYS
1	B	370	VAL
1	B	371	LEU
1	B	372	ARG
1	B	374	ARG
1	B	376	GLU
1	B	377	PHE
1	B	382	VAL
1	B	387	VAL
1	B	402	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	166	HIS
1	A	204	GLN
1	A	259	ASN
1	A	328	GLN
1	A	342	GLN
1	B	69	ASN
1	B	148	ASN
1	B	165	ASN
1	B	178	ASN
1	B	226	GLN
1	B	247	HIS
1	B	286	GLN
1	B	294	ASN
1	B	328	GLN
1	B	347	ASN
1	B	356	GLN

### 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 carbohydrates 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	PPD	A	411	-	18,24,24	1.67	1 (5%)	23,34,34	2.00	6 (26%)
2	PPD	B	411	-	18,24,24	2.08	2 (11%)	23,34,34	1.92	8 (34%)

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	PPD	A	411	-	-	0/13/19/19	0/1/1/1
2	PPD	B	411	-	-	0/13/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	411	PPD	C4A-C4	-7.48	1.43	1.51
2	A	411	PPD	C4A-C4	-5.86	1.45	1.51
2	B	411	PPD	C3-C2	2.17	1.42	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	PPD	C5-C6-N1	-3.03	118.61	123.86
2	B	411	PPD	C3-C2-N1	-2.52	117.14	120.61
2	A	411	PPD	C3-C2-N1	-2.43	117.25	120.61
2	B	411	PPD	C5-C6-N1	-2.35	119.78	123.86
2	B	411	PPD	C6-N1-C2	2.11	123.59	119.28
2	B	411	PPD	C2A-C2-C3	2.18	123.67	121.04
2	A	411	PPD	C6-N1-C2	2.48	124.34	119.28
2	B	411	PPD	C4A-C4-C5	2.54	121.97	119.71
2	B	411	PPD	O3P-P-O1P	2.76	119.47	110.58
2	A	411	PPD	C2A-C2-C3	2.77	124.37	121.04
2	B	411	PPD	C4A-N-CA	3.97	119.87	113.81
2	B	411	PPD	C6-C5-C4	4.04	121.10	118.09
2	A	411	PPD	C6-C5-C4	4.56	121.49	118.09
2	A	411	PPD	C4A-N-CA	5.12	121.63	113.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	411	PPD	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.