Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 03:46 PM EDT

PDB ID	:	1ARI
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 (i) symbol.

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

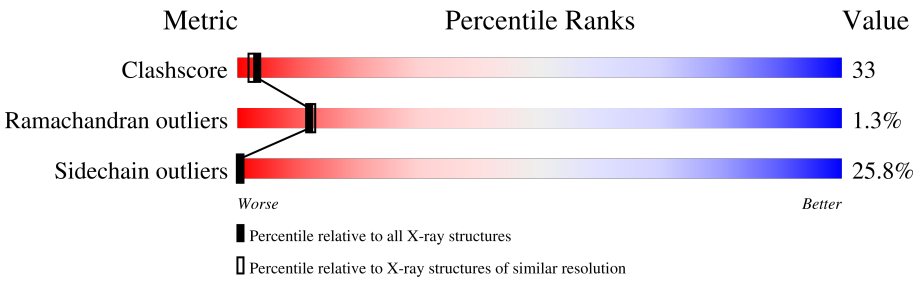
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	44% 38% 17% •
1	B	396	39% 43% 15% •

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.

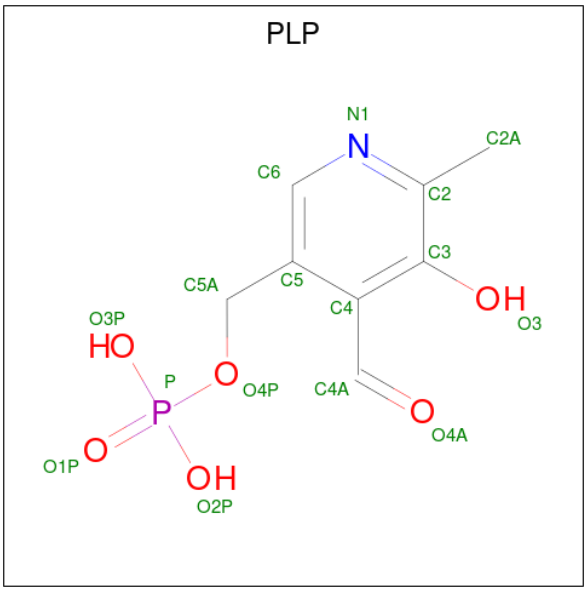
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

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

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 (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

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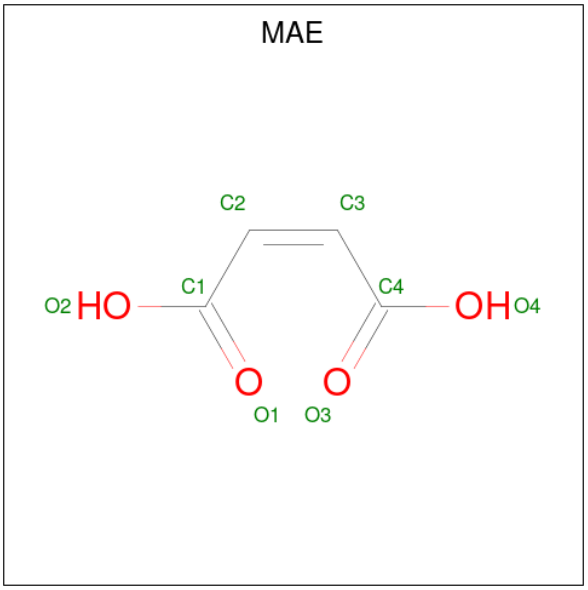
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	15	8	1	5	1	0	0

- Molecule 3 is MALEIC ACID (three-letter code: MAE) (formula: $C_4H_4O_4$).



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

- Molecule 4 is water.

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

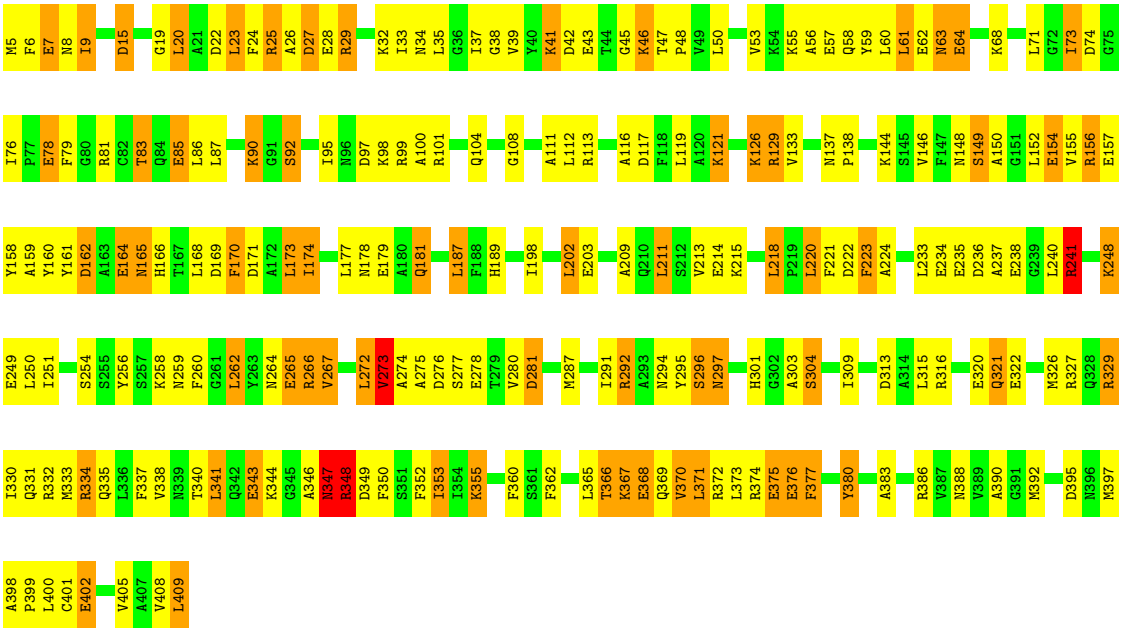
3 Residue-property plots (i)

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.

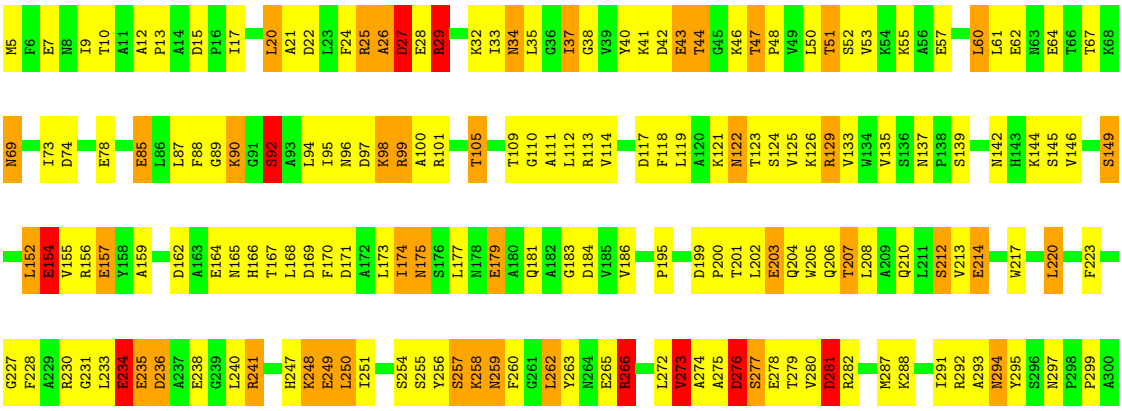
• Molecule 1: ASPARTATE AMINOTRANSFERASE

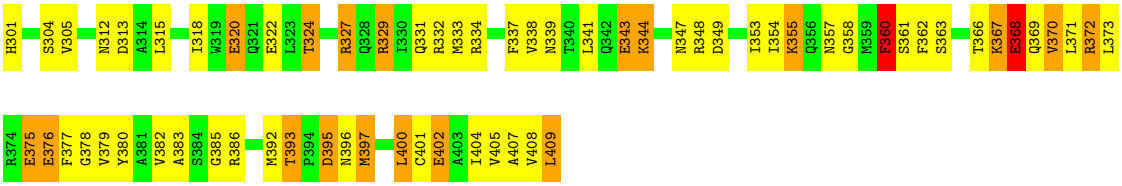
Chain A: 44% 38% 17%



• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain B: 39% 43% 15%




H301
S304
V305
N312
D313
A314
L315
I318
W319
E320
Q321
E322
L323
T324
R327
Q328
R329
I330
Q331
R332
M333
R334
F337
V338
N339
T340
L341
Q342
E343
K344
N347
R348
D349
I353
I354
K355
Q356
N357
G358
M359
F360
S361
F362
S363
T366
K367
E368
Q369
V370
L371
R372
L373
R374
E375
E376
F377
G378
V379
Y380
A381
V382
A383
S384
G385
R386
M392
T393
P394
D395
N396
M397
L400
C401
E402
A403
I404
V405
A407
V408
L409

4 Data and refinement statistics (i)

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	86.40Å 79.00Å 90.80Å 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, MAE

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	0.93	23/3125 (0.7%)	1.33	35/4232 (0.8%)
1	B	0.95	23/3125 (0.7%)	1.37	39/4232 (0.9%)
All	All	0.94	46/6250 (0.7%)	1.35	74/8464 (0.9%)

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 (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	GLU	CD-OE2	6.48	1.32	1.25
1	B	320	GLU	CD-OE1	6.35	1.32	1.25
1	B	234	GLU	CD-OE2	6.32	1.32	1.25
1	A	85	GLU	CD-OE1	6.30	1.32	1.25
1	B	265	GLU	CD-OE1	6.20	1.32	1.25
1	A	179	GLU	CD-OE1	6.15	1.32	1.25
1	A	214	GLU	CD-OE1	6.14	1.32	1.25
1	B	78	GLU	CD-OE1	6.11	1.32	1.25
1	A	43	GLU	CD-OE1	6.05	1.32	1.25
1	A	62	GLU	CD-OE2	6.04	1.32	1.25
1	A	203	GLU	CD-OE1	6.02	1.32	1.25
1	B	62	GLU	CD-OE2	5.96	1.32	1.25
1	B	28	GLU	CD-OE1	5.94	1.32	1.25
1	B	375	GLU	CD-OE2	5.89	1.32	1.25
1	A	234	GLU	CD-OE1	5.89	1.32	1.25
1	A	78	GLU	CD-OE2	5.87	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	GLU	CD-OE2	5.84	1.32	1.25
1	B	238	GLU	CD-OE2	5.83	1.32	1.25
1	A	375	GLU	CD-OE1	5.78	1.32	1.25
1	B	278	GLU	CD-OE2	5.75	1.31	1.25
1	A	28	GLU	CD-OE1	5.65	1.31	1.25
1	A	320	GLU	CD-OE1	5.64	1.31	1.25
1	B	164	GLU	CD-OE2	5.55	1.31	1.25
1	B	154	GLU	CD-OE1	5.54	1.31	1.25
1	A	368	GLU	CD-OE1	5.54	1.31	1.25
1	B	43	GLU	CD-OE1	5.53	1.31	1.25
1	A	278	GLU	CD-OE1	5.52	1.31	1.25
1	B	402	GLU	CD-OE2	5.50	1.31	1.25
1	B	235	GLU	CD-OE2	5.49	1.31	1.25
1	A	265	GLU	CD-OE1	5.48	1.31	1.25
1	B	203	GLU	CD-OE1	5.48	1.31	1.25
1	B	343	GLU	CD-OE2	5.47	1.31	1.25
1	B	85	GLU	CD-OE1	5.47	1.31	1.25
1	B	376	GLU	CD-OE2	5.45	1.31	1.25
1	A	343	GLU	CD-OE2	5.39	1.31	1.25
1	B	179	GLU	CD-OE1	5.36	1.31	1.25
1	A	322	GLU	CD-OE2	5.35	1.31	1.25
1	B	157	GLU	CD-OE1	5.31	1.31	1.25
1	A	376	GLU	CD-OE2	5.27	1.31	1.25
1	A	402	GLU	CD-OE2	5.25	1.31	1.25
1	A	64	GLU	CD-OE2	5.16	1.31	1.25
1	B	368	GLU	CD-OE1	5.10	1.31	1.25
1	A	238	GLU	CD-OE2	5.08	1.31	1.25
1	A	157	GLU	CD-OE2	5.05	1.31	1.25
1	B	64	GLU	CD-OE2	5.05	1.31	1.25
1	A	164	GLU	CD-OE2	5.03	1.31	1.25

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	169	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	A	334	ARG	NE-CZ-NH1	-8.13	116.23	120.30
1	A	27	ASP	CB-CG-OD1	7.82	125.33	118.30
1	B	276	ASP	CB-CG-OD2	7.74	125.27	118.30
1	A	313	ASP	CB-CG-OD1	-7.67	111.40	118.30
1	B	282	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	B	276	ASP	CB-CG-OD1	-7.55	111.50	118.30
1	B	117	ASP	CB-CG-OD1	-7.50	111.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	27	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	B	15	ASP	CB-CG-OD1	-7.23	111.79	118.30
1	B	236	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	A	27	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	B	29	ARG	C-N-CD	-6.86	105.52	120.60
1	A	15	ASP	CB-CG-OD1	-6.71	112.27	118.30
1	A	15	ASP	CB-CG-OD2	6.68	124.31	118.30
1	B	395	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	A	349	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	A	222	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	258	LYS	CB-CA-C	6.49	123.39	110.40
1	B	360	PHE	CB-CG-CD2	-6.49	116.26	120.80
1	B	97	ASP	CB-CG-OD1	-6.47	112.47	118.30
1	B	199	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	A	169	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	B	313	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	171	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	B	327	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	B	92	SER	CA-C-N	-6.15	103.66	117.20
1	A	97	ASP	CB-CG-OD2	6.12	123.81	118.30
1	B	349	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	A	222	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	B	236	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	162	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	15	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	395	ASP	CB-CG-OD1	-6.04	112.86	118.30
1	A	97	ASP	CB-CG-OD1	-6.03	112.87	118.30
1	A	395	ASP	CB-CG-OD2	6.03	123.73	118.30
1	B	162	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	B	89	GLY	N-CA-C	5.97	128.04	113.10
1	A	241	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	A	349	ASP	CB-CG-OD1	5.94	123.64	118.30
1	A	22	ASP	CB-CG-OD1	-5.93	112.96	118.30
1	B	162	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	236	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	169	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	236	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	B	44	THR	CA-CB-CG2	-5.84	104.23	112.40
1	B	27	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	386	ARG	NE-CZ-NH2	5.77	123.18	120.30
1	B	117	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	276	ASP	CB-CG-OD2	-5.69	113.18	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	171	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	A	380	TYR	CB-CG-CD1	-5.64	117.62	121.00
1	B	281	ASP	CB-CG-OD1	-5.64	113.23	118.30
1	B	184	ASP	CB-CG-OD1	-5.63	113.23	118.30
1	B	258	LYS	CB-CA-C	5.62	121.64	110.40
1	A	273	VAL	N-CA-CB	5.59	123.81	111.50
1	A	340	THR	CA-CB-CG2	-5.55	104.62	112.40
1	B	22	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	B	22	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	273	VAL	N-CA-CB	5.34	123.24	111.50
1	B	395	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	22	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	327	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	281	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	B	171	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	74	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	281	ASP	CB-CG-OD2	5.16	122.95	118.30
1	B	329	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	A	292	ARG	NE-CZ-NH2	5.11	122.85	120.30
1	B	97	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	313	ASP	CB-CG-OD1	5.09	122.89	118.30
1	A	313	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	276	ASP	CB-CG-OD1	5.02	122.82	118.30
1	B	169	ASP	CB-CG-OD1	5.01	122.81	118.30

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3065	0	3012	212	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3065	0	3012	203	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	30	0
All	All	6883	0	6040	404	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 33.

All (404) 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: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:32:LYS:C	1:A:33:ILE:HD13	2.05	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LYS:HE2	1:A:129:ARG:HB3	1.65	0.76
1:B:367:LYS:HB2	1:B:367:LYS:HZ2	1.50	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:B:332:ARG:HD2	1:B:333:MET:HE2	1.68	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:CE	1:A:400:LEU:HD23	2.20	0.72
1:B:397:MET:HE3	1:B:400:LEU:HD13	1.70	0.72
1:A:39:VAL:HG21	1:B:69:ASN:HD21	1.55	0.72
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: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: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
2:B:410:PLP:C4A	3:B:411:MAE:H2	2.23	0.69
1:A:260:PHE:HB3	1:A:262:LEU:CD2	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:397:MET:HE3	1:A:400:LEU:HD23	1.79	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:144:LYS:NZ	4:B:783:HOH:O	2.30	0.63
1:B:43:GLU:CD	1:B:43:GLU:H	2.00	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
1:B:367:LYS:HZ1	1:B:367:LYS:N	1.95	0.63
1:B:272:LEU:HB2	1:B:287:MET:HE1	1.79	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:126:LYS:HZ1	1:A:129:ARG:HD3	1.66	0.60
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:272:LEU:HD22	1:B:287:MET:HE2	1.83	0.60
1:B:170:PHE:CD1	1:B:173:LEU:HD23	2.37	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: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
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: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:A:397:MET:HE1	1:A:400:LEU:HD23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:202:LEU:HD22	1:A:202:LEU:O	2.07	0.55
1:A:397:MET:HE2	1:A:401:CYS:SG	2.47	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
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:397:MET:HE3	1:A:397:MET:O	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:129:ARG:HD3	1:B:154:GLU:CD	2.31	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:34:ASN:C	1:A:35:LEU:HD23	2.31	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: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: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:34:ASN:C	1:B:34:ASN:HD22	2.13	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:126:LYS:HZ1	1:A:129:ARG:CD	2.25	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: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:B:367:LYS:HZ2	1:B:367:LYS:CB	2.24	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
1:A:337:PHE:CE1	1:A:341:LEU:HD22	2.49	0.47
1:A:397:MET:HE1	1:A:400:LEU:CD2	2.45	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:A:211:LEU:HD22	1:A:215:LYS:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:155:VAL:C	1:A:156:ARG:HD2	2.36	0.46
1:A:113:ARG:HG2	1:B:294:ASN:HD22	1.80	0.46
1:B:125:VAL:C	1:B:126:LYS:HG3	2.36	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:B:88:PHE:CD1	1:B:94:LEU:HD22	2.51	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:A:126:LYS:NZ	1:A:129:ARG:CZ	2.80	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:B:166:HIS:O	1:B:355:LYS:HE2	2.17	0.45
1:A:85:GLU:OE2	1:A:90:LYS:HA	2.17	0.44
1:B:46:LYS:CG	1:B:47:THR:N	2.80	0.44
1:B:272:LEU:HD22	1:B:287:MET:HE1	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:SER:OG	1:B:385:GLY:O	2.32	0.44
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.85	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:A:126:LYS:HZ3	1:A:129:ARG:CZ	2.30	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: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:A:53:VAL:O	1:A:57:GLU:HG3	2.19	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
1:B:231:GLY:O	1:B:236:ASP:HB2	2.19	0.43
1:A:5:MET:HA	1:A:5:MET:CE	2.48	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:347:ASN:HD21	1:A:409:LEU:HB3	1.82	0.43
1:A:397:MET:HE3	1:A:397:MET:HA	2.01	0.43
1:B:202:LEU:HD12	1:B:202:LEU:O	2.19	0.43
1:B:397:MET:CE	1:B:397:MET:HA	2.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:400:LEU:HD23	1:B:400:LEU:C	2.40	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: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
1:A:372:ARG:HD3	1:A:408:VAL:HG11	2.01	0.41
1:B:177:LEU:C	1:B:179:GLU:H	2.23	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:333:MET:HA	1:A:333:MET:CE	2.50	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: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:B:220:LEU:C	1:B:220:LEU:HD12	2.41	0.41
1:B:100:ALA:C	1:B:101:ARG:HG2	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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)

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%)	351 (89%)	37 (9%)	6 (2%)	10	10
1	B	394/396 (100%)	351 (89%)	39 (10%)	4 (1%)	15	17
All	All	788/792 (100%)	702 (89%)	76 (10%)	10 (1%)	12	12

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ALA
1	A	348	ARG
1	B	26	ALA
1	B	266	ARG
1	B	92	SER
1	B	263	TYR
1	A	92	SER
1	A	296	SER
1	A	301	HIS

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Mol	Chain	Res	Type
1	A	347	ASN

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%)	241 (75%)	79 (25%)	0 0
1	B	320/320 (100%)	234 (73%)	86 (27%)	0 0
All	All	640/640 (100%)	475 (74%)	165 (26%)	0 0

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	41	LYS
1	A	42	ASP
1	A	46	LYS
1	A	55	LYS
1	A	58	GLN
1	A	61	LEU
1	A	63	ASN
1	A	73	ILE
1	A	83	THR
1	A	86	LEU
1	A	90	LYS
1	A	98	LYS
1	A	112	LEU
1	A	119	LEU

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Mol	Chain	Res	Type
1	A	121	LYS
1	A	126	LYS
1	A	129	ARG
1	A	133	VAL
1	A	144	LYS
1	A	149	SER
1	A	152	LEU
1	A	156	ARG
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	202	LEU
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	266	ARG
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	335	GLN
1	A	341	LEU
1	A	343	GLU

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Mol	Chain	Res	Type
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	388	ASN
1	A	409	LEU
1	B	20	LEU
1	B	25	ARG
1	B	27	ASP
1	B	29	ARG
1	B	34	ASN
1	B	37	ILE
1	B	41	LYS
1	B	47	THR
1	B	50	LEU
1	B	51	THR
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	95	ILE
1	B	98	LYS
1	B	99	ARG
1	B	105	THR
1	B	112	LEU
1	B	119	LEU
1	B	121	LYS
1	B	122	ASN
1	B	129	ARG
1	B	133	VAL

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Mol	Chain	Res	Type
1	B	139	SER
1	B	149	SER
1	B	152	LEU
1	B	154	GLU
1	B	155	VAL
1	B	156	ARG
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	203	GLU
1	B	206	GLN
1	B	207	THR
1	B	212	SER
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	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
1	B	266	ARG
1	B	273	VAL
1	B	276	ASP
1	B	277	SER
1	B	281	ASP
1	B	294	ASN
1	B	297	ASN
1	B	304	SER
1	B	324	THR
1	B	334	ARG
1	B	343	GLU

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Mol	Chain	Res	Type
1	B	344	LYS
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	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 (29) 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	181	GLN
1	A	226	GLN
1	A	259	ASN
1	A	321	GLN
1	A	331	GLN
1	A	339	ASN
1	A	347	ASN
1	B	34	ASN
1	B	63	ASN
1	B	69	ASN
1	B	84	GLN
1	B	96	ASN
1	B	137	ASN
1	B	165	ASN
1	B	175	ASN

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Mol	Chain	Res	Type
1	B	210	GLN
1	B	226	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 (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 monosaccharides 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	$\#\|Z\| > 2$
3	MAE	A	411	-	1,7,7	0.42	0	2,8,8	3.78	2 (100%)
2	PLP	B	410	1	15,15,16	1.61	2 (13%)	20,22,23	1.75	5 (25%)
2	PLP	A	410	1	15,15,16	1.29	1 (6%)	20,22,23	1.97	5 (25%)
3	MAE	B	411	-	1,7,7	0.72	0	2,8,8	5.61	2 (100%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	410	PLP	C4A-C4	-4.55	1.42	1.51
2	A	410	PLP	C4A-C4	-3.22	1.45	1.51
2	B	410	PLP	P-O3P	-2.68	1.44	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	411	MAE	C1-C2-C3	6.55	137.69	123.69
2	A	410	PLP	C6-C5-C4	5.65	122.61	118.16
3	B	411	MAE	C4-C3-C2	4.48	133.25	123.69
3	A	411	MAE	C4-C3-C2	3.95	132.13	123.69
3	A	411	MAE	C1-C2-C3	3.59	131.37	123.69
2	B	410	PLP	C6-C5-C4	3.47	120.89	118.16
2	B	410	PLP	C3-C2-N1	-3.29	116.52	120.77
2	B	410	PLP	C2A-C2-C3	3.26	124.92	120.89
2	A	410	PLP	C5-C6-N1	-3.20	118.49	123.82
2	B	410	PLP	C5-C6-N1	-2.78	119.18	123.82
2	B	410	PLP	C6-N1-C2	2.77	124.30	119.17
2	A	410	PLP	C3-C2-N1	-2.57	117.45	120.77
2	A	410	PLP	C6-N1-C2	2.30	123.42	119.17
2	A	410	PLP	O3P-P-O1P	2.14	119.06	110.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	411	MAE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	410	PLP	3	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.