



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:22 PM GMT

PDB ID : 1AHF
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

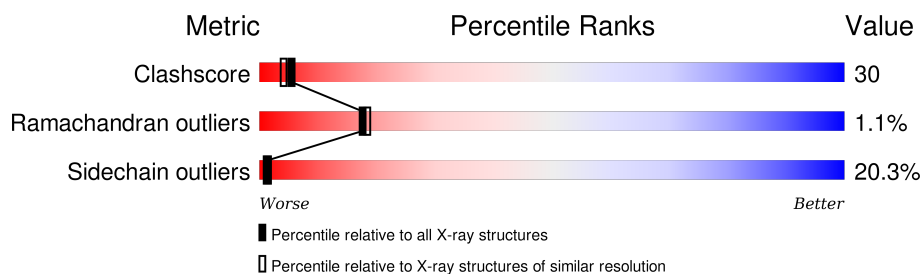
1 Overall quality at a glance

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 ≥ 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	

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
4	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:

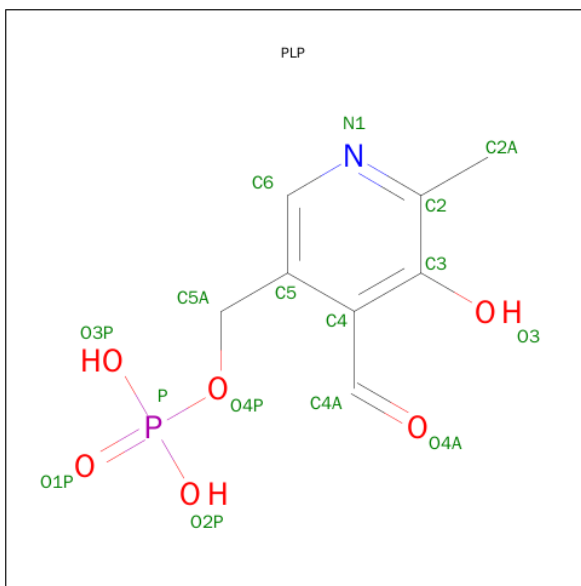
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LEU	VAL	CONFLICT	UNP P00509
A	41	TYR	LYS	CONFLICT	UNP P00509
A	47	ILE	THR	CONFLICT	UNP P00509
A	69	LEU	ASN	CONFLICT	UNP P00509
A	109	SER	THR	CONFLICT	UNP P00509
A	297	SER	ASN	CONFLICT	UNP P00509
B	39	LEU	VAL	CONFLICT	UNP P00509
B	41	TYR	LYS	CONFLICT	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 SULFATE ION (three-letter code: SO4) (formula: O₄S).



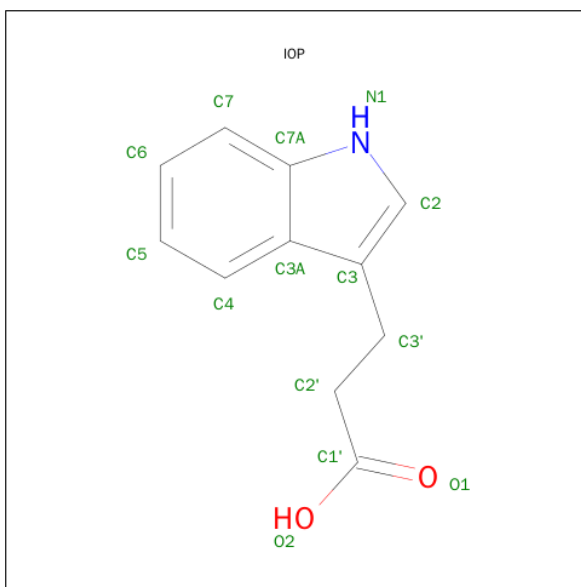
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 4 is INDOLYLPROPIONIC ACID (three-letter code: IOP) (formula: C₁₁H₁₁NO₂).



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

- Molecule 5 is water.

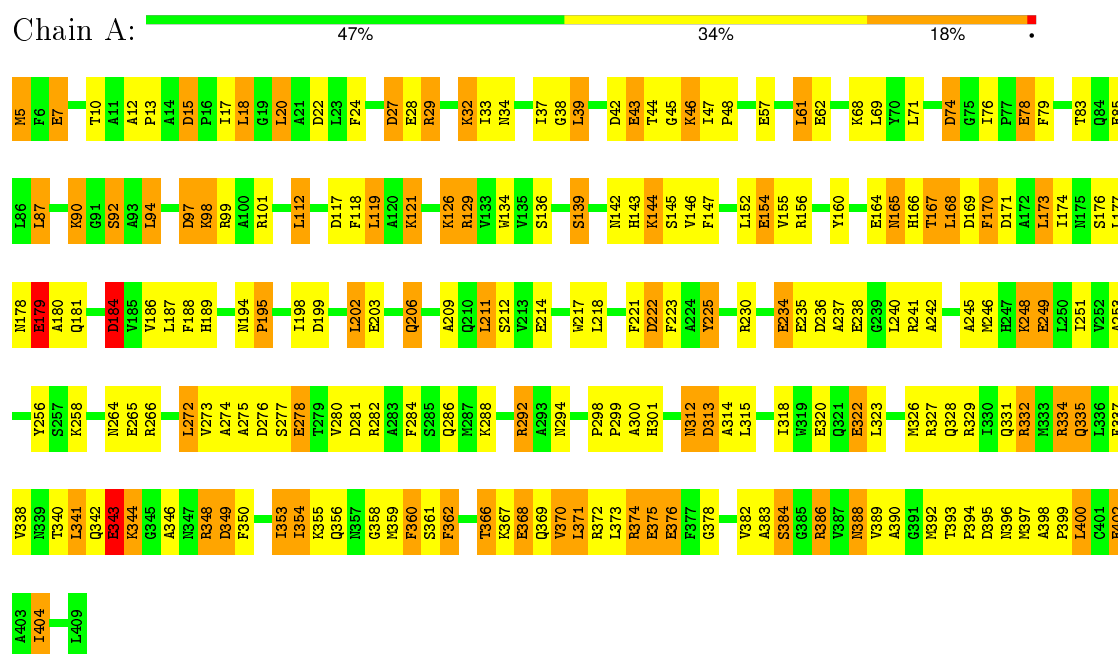
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total	O	0	0
			215	215		
5	B	187	Total	O	0	0
			187	187		

3 Residue-property plots

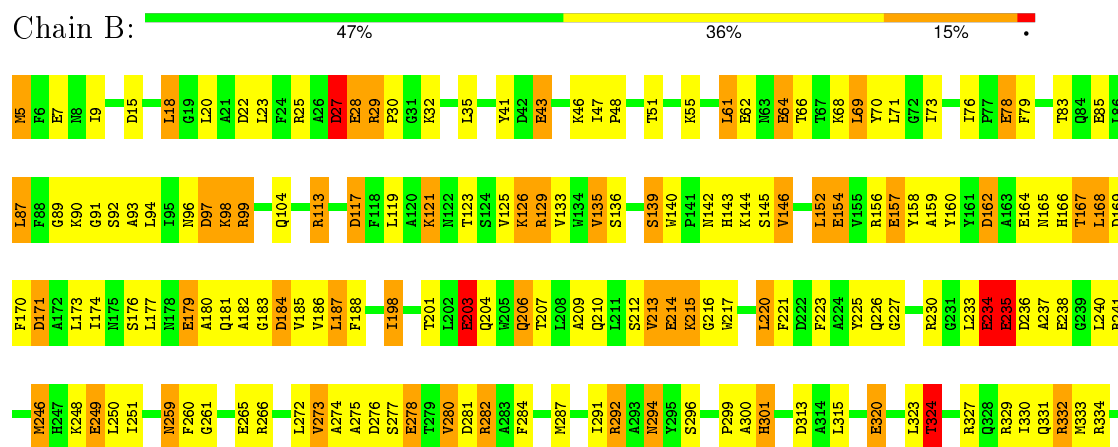
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, SO4, IOP

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	1.01	23/3133 (0.7%)	1.35	36/4244 (0.8%)
1	B	1.04	27/3133 (0.9%)	1.35	39/4244 (0.9%)
All	All	1.02	50/6266 (0.8%)	1.35	75/8488 (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 (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	91	GLY	C-N	-9.22	1.12	1.34
1	A	402	GLU	CD-OE2	7.48	1.33	1.25
1	A	85	GLU	CD-OE1	7.39	1.33	1.25
1	B	62	GLU	CD-OE2	7.20	1.33	1.25
1	A	320	GLU	CD-OE1	6.94	1.33	1.25
1	A	62	GLU	CD-OE2	6.92	1.33	1.25
1	B	238	GLU	CD-OE2	6.82	1.33	1.25
1	A	43	GLU	CD-OE1	6.55	1.32	1.25
1	A	249	GLU	CD-OE2	6.50	1.32	1.25
1	A	375	GLU	CD-OE1	6.46	1.32	1.25
1	A	164	GLU	CD-OE2	6.38	1.32	1.25
1	B	368	GLU	CD-OE2	6.38	1.32	1.25
1	A	203	GLU	CD-OE2	6.35	1.32	1.25
1	B	375	GLU	CD-OE2	6.33	1.32	1.25
1	B	320	GLU	CD-OE1	6.30	1.32	1.25
1	B	265	GLU	CD-OE1	6.28	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	GLU	CD-OE1	6.23	1.32	1.25
1	B	179	GLU	CD-OE2	6.22	1.32	1.25
1	B	402	GLU	CD-OE2	6.17	1.32	1.25
1	A	238	GLU	CD-OE2	6.15	1.32	1.25
1	A	28	GLU	CD-OE1	6.14	1.32	1.25
1	B	214	GLU	CD-OE2	6.13	1.32	1.25
1	B	234	GLU	CD-OE2	6.12	1.32	1.25
1	B	249	GLU	CD-OE2	6.11	1.32	1.25
1	B	235	GLU	CD-OE2	6.07	1.32	1.25
1	A	343	GLU	CD-OE1	6.07	1.32	1.25
1	B	164	GLU	CD-OE2	6.00	1.32	1.25
1	B	28	GLU	CD-OE1	5.96	1.32	1.25
1	B	43	GLU	CD-OE1	5.95	1.32	1.25
1	B	203	GLU	CD-OE1	5.93	1.32	1.25
1	B	343	GLU	CD-OE2	5.92	1.32	1.25
1	A	154	GLU	CD-OE2	5.88	1.32	1.25
1	A	78	GLU	CD-OE1	5.82	1.32	1.25
1	B	89	GLY	N-CA	5.80	1.54	1.46
1	A	368	GLU	CD-OE1	5.77	1.31	1.25
1	B	157	GLU	CD-OE2	5.75	1.31	1.25
1	A	214	GLU	CD-OE1	5.73	1.31	1.25
1	B	64	GLU	CD-OE2	5.70	1.31	1.25
1	A	278	GLU	CD-OE1	5.65	1.31	1.25
1	A	322	GLU	CD-OE1	5.63	1.31	1.25
1	B	278	GLU	CD-OE2	5.63	1.31	1.25
1	B	92	SER	N-CA	-5.59	1.35	1.46
1	A	234	GLU	CD-OE1	5.55	1.31	1.25
1	A	179	GLU	CD-OE2	5.40	1.31	1.25
1	A	235	GLU	CD-OE2	5.28	1.31	1.25
1	B	78	GLU	CD-OE1	5.22	1.31	1.25
1	B	376	GLU	CD-OE2	5.21	1.31	1.25
1	B	154	GLU	CD-OE1	5.18	1.31	1.25
1	A	265	GLU	CD-OE2	-5.11	1.20	1.25
1	A	7	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	225	TYR	CB-CG-CD1	-11.13	114.32	121.00
1	B	117	ASP	CB-CG-OD1	-8.41	110.73	118.30
1	B	169	ASP	CB-CG-OD2	-8.20	110.92	118.30
1	A	15	ASP	CB-CG-OD2	-8.09	111.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	TYR	CB-CG-CD2	8.09	125.85	121.00
1	B	225	TYR	CB-CG-CD2	7.98	125.79	121.00
1	A	171	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	B	225	TYR	CB-CG-CD1	-7.83	116.30	121.00
1	A	22	ASP	CB-CG-OD1	-7.68	111.39	118.30
1	B	22	ASP	CB-CG-OD1	-7.64	111.43	118.30
1	B	117	ASP	CB-CG-OD2	7.22	124.80	118.30
1	B	171	ASP	CB-CG-OD1	-7.17	111.85	118.30
1	A	276	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	A	74	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	A	313	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	97	ASP	CB-CG-OD1	-6.86	112.13	118.30
1	A	117	ASP	CB-CG-OD2	6.81	124.43	118.30
1	A	169	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	B	15	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	B	313	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	A	117	ASP	CB-CG-OD1	-6.62	112.35	118.30
1	A	27	ASP	CB-CG-OD2	-6.57	112.38	118.30
1	B	162	ASP	CB-CG-OD1	6.57	124.21	118.30
1	A	276	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	395	ASP	CB-CG-OD1	6.47	124.12	118.30
1	B	91	GLY	O-C-N	-6.44	112.39	122.70
1	A	15	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	27	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	184	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	A	395	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	A	74	ASP	CB-CG-OD1	6.21	123.89	118.30
1	B	409	LEU	CB-CA-C	6.21	122.00	110.20
1	B	184	ASP	CB-CG-OD1	-6.16	112.75	118.30
1	B	15	ASP	CB-CG-OD1	6.06	123.76	118.30
1	B	162	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	B	334	ARG	N-CA-CB	6.00	121.39	110.60
1	A	236	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	22	ASP	CB-CG-OD2	5.96	123.67	118.30
1	B	395	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	A	171	ASP	CB-CG-OD1	5.91	123.62	118.30
1	B	266	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	B	171	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	349	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	B	281	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	29	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	A	236	ASP	CB-CG-OD1	-5.79	113.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ASP	CB-CG-OD2	5.77	123.50	118.30
1	B	169	ASP	CB-CG-OD1	5.73	123.45	118.30
1	B	276	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	B	97	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	27	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	395	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	236	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	329	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	B	372	ARG	NE-CZ-NH2	5.61	123.10	120.30
1	B	374	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	B	27	ASP	CB-CA-C	5.53	121.46	110.40
1	A	118	PHE	CB-CG-CD1	5.52	124.66	120.80
1	B	324	THR	N-CA-CB	5.50	120.76	110.30
1	B	313	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	360	PHE	CB-CA-C	-5.50	99.40	110.40
1	A	222	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	199	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	332	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	B	97	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	B	282	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	B	349	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	B	276	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	230	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	374	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	A	195	PRO	CB-CA-C	-5.14	99.14	112.00
1	A	404	ILE	N-CA-CB	5.13	122.59	110.80
1	B	334	ARG	CB-CA-C	5.05	120.51	110.40
1	B	372	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	A	221	PHE	CB-CG-CD2	-5.01	117.29	120.80

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	3071	0	3020	190	0
1	B	3071	0	3019	194	0
2	B	5	0	0	1	0
3	A	15	0	6	1	0
3	B	15	0	6	0	0
4	A	14	0	10	8	0
5	A	215	0	0	11	0
5	B	187	0	0	12	0
All	All	6593	0	6061	364	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 30.

All (364) 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:A:17:ILE:HG21	4:A:411:IOP:H2	1.43	1.00
1:A:37:ILE:HG13	4:A:411:IOP:H3'2	1.44	0.96
1:A:323:LEU:HA	1:A:326:MET:HE2	1.49	0.94
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: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:272:LEU:HD22	1:B:287:MET:HE1	1.63	0.80
1:B:272:LEU:HD22	1:B:287:MET:CE	2.11	0.80
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	4:A:411:IOP:H2	2.11	0.80
1:A:129:ARG:HD2	1:A:134:TRP:NE1	1.97	0.80
1:A:165:ASN:HD22	1:A:165:ASN:H	1.30	0.79
1:A:37:ILE:HG13	4: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:249:GLU:HA	1:B:273:VAL:O	1.87	0.75
1:A:198:ILE:HA	5:A:478:HOH:O	1.87	0.75
1:A:248:LYS:HG3	1:A:275:ALA:HB2	1.69	0.74
1:A:38:GLY:H	4: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:398:ALA:HB3	1:A:399:PRO:HD3	1.70	0.73
1:B:129:ARG:HE	1:B:154:GLU:HB3	1.54	0.72
1:A:71:LEU:HD11	1:A:300:ALA:HB2	1.72	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: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: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:B:250:LEU:HD12	1:B:273:VAL:HG13	1.76	0.68
1:B:96:ASN:N	1:B:96:ASN:HD22	1.90	0.68
1:A:136:SER:O	1:A:139:SER:HB2	1.94	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:366:THR:HG23	1:A:369:GLN:OE1	1.94	0.66
1:A:362:PHE:HE1	1:A:384:SER:HB2	1.60	0.66
1:A:278:GLU:HG2	1:A:282:ARG:NH1	2.11	0.66
1:A:386:ARG:HH22	4: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:B:397:MET:CE	1:B:400:LEU:HD22	2.26	0.65
1:A:249:GLU:OE1	1:B:5:MET:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:ARG:HD3	1:A:275:ALA:O	1.96	0.65
1:A:15:ASP:HB3	1:A:18:LEU:HB2	1.78	0.65
1:B:99:ARG:NH1	1:B:274:ALA:O	2.30	0.64
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:B:382:VAL:HG12	1:B:384:SER:H	1.65	0.61
1:B:327:ARG:O	1:B:331:GLN:HG3	2.00	0.61
1:A:170:PHE:CE2	1:A:174:ILE:HD11	2.34	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:B:237:ALA:O	1:B:241:ARG:HG3	2.01	0.60
1:A:144:LYS:CD	1:A:155:VAL:HG11	2.31	0.60
1:B:201:THR:OG1	1:B:204:GLN:HG3	2.02	0.60
1:B:212:SER:HB3	1:B:217:TRP:CE3	2.38	0.59
1:A:312:ASN:ND2	1:A:314:ALA:H	2.01	0.59
1:A:372:ARG:O	1:A:376:GLU:HB2	2.02	0.59
1:A:343:GLU:HG2	1:A:343:GLU:O	2.01	0.58
1:B:213:VAL:HG12	1:B:214:GLU:N	2.16	0.58
1:B:96:ASN:ND2	1:B:96:ASN:N	2.51	0.58
1:B:292:ARG:NH1	5:B:598:HOH:O	2.35	0.58
1:A:386:ARG:NH2	4:A:411:IOP:O2	2.31	0.58
1:B:372:ARG:O	1:B:376:GLU:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:237:ALA:HB1	1:A:241:ARG:HD3	1.85	0.57
1:A:160:TYR:O	1:A:168:LEU:HD23	2.05	0.57
1:A:57:GLU:OE2	1:A:301:HIS:HE1	1.87	0.57
1:B:272:LEU:HB2	1:B:287:MET:CE	2.35	0.56
1:B:274:ALA:HB3	1:B:280:VAL:HB	1.87	0.56
1:A:251:ILE:HG12	1:A:272:LEU:HD23	1.87	0.56
1:B:301:HIS:ND1	5:B:467:HOH:O	2.33	0.56
1:A:350:PHE:O	1:A:353:ILE:HB	2.05	0.56
1:B:46:LYS:HD2	1:B:47:ILE:N	2.18	0.56
1:A:248:LYS:HG3	1:A:275:ALA:CB	2.35	0.56
1:A:329:ARG:NH2	1:A:392:MET:O	2.39	0.56
1:B:332:ARG:HG2	1:B:333:MET:HE2	1.88	0.56
1:A:46:LYS:CD	1:A:47:ILE:H	2.11	0.56
1:B:98:LYS:HA	1:B:98:LYS:HZ3	1.70	0.56
1:A:362:PHE:CE1	1:A:384:SER:HB2	2.40	0.56
1:B:99:ARG:HG2	1:B:99:ARG:NH1	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:397:MET:HE1	1:B:400:LEU:HD22	1.89	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:144:LYS:HD2	1:A:155:VAL:HG11	1.87	0.55
1:A:12:ALA:HB1	1:A:13:PRO:HD2	1.88	0.55
1:B:158:TYR:CD1	1:B:173:LEU:HD12	2.41	0.55
1:B:272:LEU:HD22	1:B:287:MET:HE2	1.89	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:372:ARG:HG2	1:B:408:VAL:CG1	2.38	0.54
1:A:400:LEU:HD11	1:A:404:ILE:HD12	1.90	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:B:344:LYS:HD2	1:B:402:GLU:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:GLN:OE1	1:B:361:SER:HA	2.07	0.54
1:A:348:ARG:CG	1:A:348:ARG:HH11	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:376:GLU:HG2	1:B:377:PHE:CE2	2.42	0.53
1:B:126:LYS:HD2	5:B:417:HOH:O	2.08	0.53
1:B:129:ARG:HD3	1:B:154:GLU:HG2	1.90	0.53
1:A:337:PHE:HD1	1:A:397:MET:HE2	1.74	0.53
1:B:248:LYS:HE3	1:B:275:ALA:HB1	1.89	0.53
1:B:129:ARG:HD3	1:B:154:GLU:CG	2.39	0.53
1:A:99:ARG:HD2	1:A:274:ALA:O	2.09	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:A:234:GLU:CD	1:A:241:ARG:HH22	2.11	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:5:MET:HE2	1:B:125:VAL:HG23	1.91	0.52
1:A:222:ASP:OD2	3: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:A:5:MET:HE1	1:B:125:VAL:HG22	1.91	0.51
1:B:76:ILE:O	1:B:79:PHE:HB3	2.10	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:B:160:TYR:HD1	1:B:173:LEU:HD13	1.76	0.51
1:A:189:HIS:HD2	1:A:194:ASN:H	1.59	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:259:ASN:HD22	1:B:259:ASN:C	2.14	0.50
1:A:397:MET:HE1	1:A:400:LEU:CD2	2.41	0.50
1:B:119:LEU:HD21	1:B:185:VAL:HG21	1.94	0.50
1:A:142:ASN:O	1:A:146:VAL:HG13	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ARG:HD2	1:A:266:ARG:N	2.25	0.50
1:A:29:ARG:HH22	1:A:378:GLY:HA2	1.77	0.50
1:A:312:ASN:HD21	1:A:314:ALA:HB3	1.76	0.50
1:A:286:GLN:HG3	1:B:9:ILE:CG2	2.42	0.50
1:B:46:LYS:CG	1:B:47:ILE:H	2.25	0.50
1:A:371:LEU:HD23	5:A:481:HOH:O	2.10	0.50
1:B:187:LEU:C	1:B:187:LEU:HD12	2.30	0.49
1:B:76:ILE:HG22	1:B:79:PHE:H	1.76	0.49
1:A:186:VAL:HG12	1:A:188:PHE:CE2	2.47	0.49
1:B:201:THR:HG23	1:B:204:GLN:CD	2.32	0.49
1:B:227:GLY:HA3	1:B:323:LEU:HD21	1.94	0.49
1:A:249:GLU:HA	1:A:273:VAL:O	2.12	0.49
1:B:397:MET:HG3	1:B:397:MET:O	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:B:158:TYR:HD1	1:B:173:LEU:HD12	1.77	0.48
1:B:99:ARG:HG2	1:B:99:ARG:HH11	1.77	0.48
1:A:340:THR:O	1:A:344:LYS:HB2	2.12	0.48
1:A:277:SER:HA	1:A:280:VAL:HG12	1.95	0.48
1:A:42:ASP:O	1:A:45:GLY:N	2.30	0.48
1:B:259:ASN:ND2	1:B:259:ASN:N	2.61	0.48
1:A:121:LYS:HZ1	1:A:121:LYS:HB3	1.77	0.48
1:B:333:MET:CE	1:B:333:MET:HA	2.43	0.48
1:B:347:ASN:HD22	1:B:348:ARG:HH12	1.60	0.48
1:A:97:ASP:N	1:A:97:ASP:OD1	2.45	0.48
1:A:112:LEU:HD13	1:A:253:ALA:CB	2.44	0.48
1:B:181:GLN:HB2	5:B:427:HOH:O	2.13	0.48
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.56	0.48
1:B:46:LYS:C	1:B:48:PRO:HD3	2.35	0.48
1:A:156:ARG:HD2	5:A:474:HOH:O	2.14	0.48
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:98:LYS:HA	1:A:98:LYS:CE	2.38	0.47
1:B:210:GLN:O	1:B:214:GLU:HG3	2.14	0.47
1:A:318:ILE:O	1:A:322:GLU:HG3	2.15	0.47
1:B:170:PHE:HE2	1:B:207:THR:HG21	1.80	0.47
1:A:144:LYS:HD3	1:A:155:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LEU:HB2	1:B:287:MET:HE1	1.96	0.47
1:B:246:MET:HE3	1:B:246:MET:HB3	1.80	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:397:MET:HA	1:B:397:MET:CE	2.44	0.47
1:A:146:VAL:HG23	1:A:147:PHE:N	2.29	0.47
1:B:204:GLN:O	1:B:207:THR:HB	2.15	0.47
1:B:203:GLU:HG2	1:B:203:GLU:H	1.58	0.47
1:A:121:LYS:HZ2	1:A:121:LYS:HB3	1.77	0.47
1:B:159:ALA:O	1:B:173:LEU:HA	2.15	0.47
1:A:312:ASN:ND2	1:A:314:ALA:N	2.62	0.47
1:A:301:HIS:HD2	5:A:447:HOH:O	1.98	0.46
1:A:344:LYS:NZ	1:A:402:GLU:OE2	2.37	0.46
1:B:64:GLU:OE1	1:B:68:LYS:NZ	2.46	0.46
1:A:5:MET:HE1	1:B:125:VAL:CG2	2.46	0.46
1:B:250:LEU:CD1	1:B:273:VAL:HG13	2.45	0.46
1:B:315:LEU:HA	1:B:315:LEU:HD23	1.37	0.46
1:B:43:GLU:CD	1:B:43:GLU:H	2.19	0.46
1:B:168:LEU:HA	1:B:168:LEU:HD23	1.73	0.46
1:B:220:LEU:HD12	1:B:220:LEU:C	2.36	0.46
1:A:76:ILE:O	1:A:79:PHE:HB3	2.15	0.46
1:A:237:ALA:O	1:A:241:ARG:HD3	2.15	0.46
1:A:397:MET:HE1	1:A:400:LEU:HD23	1.96	0.46
1:A:400:LEU:CD1	1:A:404:ILE:HD12	2.44	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:177:LEU:O	1:B:180:ALA:HB3	2.15	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:B:277:SER:HA	1:B:280:VAL:HG12	1.97	0.46
1:B:248:LYS:HB3	1:B:275:ALA:HB2	1.98	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:117:ASP:O	1:B:121:LYS:CD	2.47	0.46
1:A:165:ASN:ND2	1:A:165:ASN:H	2.06	0.46
1:A:5:MET:CE	1:B:125:VAL:HG23	2.45	0.45
1:A:39:LEU:HD21	1:B:69:LEU:CD2	2.46	0.45
1:A:292:ARG:NH2	1:B:18:LEU:HD22	2.29	0.45
1:A:74:ASP:OD1	1:A:74:ASP:N	2.43	0.45
1:B:226:GLN:NE2	5:B:510:HOH:O	2.39	0.45
1:A:292:ARG:NE	1:B:18:LEU:HD22	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:HE3	1:A:90:LYS:HB3	1.67	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:382:VAL:CG1	1:A:383:ALA:N	2.80	0.45
1:A:92:SER:OG	1:A:94:LEU:N	2.50	0.45
1:B:46:LYS:CG	1:B:47:ILE:N	2.80	0.45
1:A:348:ARG:HH21	1:A:369:GLN:HE22	1.64	0.45
1:A:225:TYR:HE1	1:A:359:MET:HE3	1.81	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:HG2	1:B:235:GLU:H	1.56	0.44
1:B:272:LEU:HB2	1:B:287:MET:HE3	1.99	0.44
1:B:76:ILE:O	1:B:76:ILE:HG22	2.14	0.44
1:B:344:LYS:HD2	1:B:402:GLU:CG	2.46	0.44
1:A:266:ARG:HG2	1:B:299:PRO:HA	1.98	0.44
1:A:393:THR:HB	1:A:394:PRO:HD2	1.98	0.44
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:79:PHE:CD2	1:B:104:GLN:HB2	2.52	0.44
1:A:170:PHE:CE2	1:A:174:ILE:CD1	2.99	0.44
1:A:68:LYS:HB2	1:B:261:GLY:O	2.17	0.44
1:B:7:GLU:N	1:B:7:GLU:OE1	2.35	0.44
1:A:12:ALA:HB1	1:A:13:PRO:CD	2.47	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:210:GLN:HE21	1:B:214:GLU:CG	2.31	0.43
1:B:140:TRP:CH2	1:B:142:ASN:HB3	2.53	0.43
1:B:140:TRP:HE3	1:B:143:HIS:CD2	2.35	0.43
1:A:176:SER:O	1:A:179:GLU:HG3	2.18	0.43
1:B:348:ARG:HD2	1:B:409:LEU:HD22	2.00	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:A:71:LEU:HD11	1:A:300:ALA:CB	2.46	0.43
1:A:388:ASN:HD22	1:A:388:ASN:C	2.22	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: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:A:202:LEU:HD23	1:A:202:LEU:HA	1.85	0.43
1:B:212:SER:CB	1:B:217:TRP:HE3	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LEU:HA	1:A:341:LEU:HD12	1.69	0.43
1:B:129:ARG:HD3	1:B:154:GLU:CD	2.39	0.42
1:B:212:SER:CB	1:B:217:TRP:CE3	3.02	0.42
1:B:158:TYR:CD1	1:B:173:LEU:CD1	3.02	0.42
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.87	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:101:ARG:HD3	1:A:281:ASP:OD1	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:A:342:GLN:C	1:A:344:LYS:H	2.23	0.42
1:B:386:ARG:NH2	2:B:411:SO4:O4	2.51	0.42
1:A:386:ARG:NH2	4:A:411:IOP:C1'	2.80	0.42
1:A:397:MET:HE3	1:A:400:LEU:HD23	2.01	0.42
1:A:79:PHE:CZ	1:A:256:TYR:HE2	2.37	0.42
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:HA	1:B:152:LEU:HD12	1.70	0.42
1:B:129:ARG:NE	1:B:154:GLU:CB	2.78	0.42
1:B:259:ASN:HD22	1:B:259:ASN:N	2.16	0.42
1:A:98:LYS:HD2	1:A:98:LYS:HA	1.46	0.42
1:A:20:LEU:HD23	1:A:20:LEU:HA	1.67	0.42
1:A:46:LYS:NZ	1:B:66:THR:O	2.51	0.41
1:B:113:ARG:HA	1:B:113:ARG:HD3	1.94	0.41
1:A:242:ALA:O	1:A:245:ALA:HB3	2.19	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:348:ARG:NH1	1:A:348:ARG:CG	2.80	0.41
1:A:87:LEU:HD12	1:A:87:LEU:HA	1.86	0.41
1:A:278:GLU:HG2	1:A:282:ARG:HH12	1.81	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:B:5:MET:N	1:B:7:GLU:OE1	2.53	0.41
1:A:160:TYR:HD1	1:A:173:LEU:HD23	1.85	0.41
1:A:33:ILE:HD13	1:A:396:ASN:HB2	2.03	0.41
1:B:83:THR:O	1:B:87:LEU:HD22	2.21	0.41
1:A:312:ASN:HD22	1:A:314:ALA:N	2.19	0.41
1:A:248:LYS:HG2	1:A:275:ALA:HB2	2.00	0.41
1:A:168:LEU:HD12	5:A:540:HOH:O	2.21	0.41
1:A:68:LYS:HB2	5:A:616:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:HD12	1:B:94:LEU:N	2.35	0.41
1:B:18:LEU:HA	1:B:18:LEU:HD12	1.78	0.41
1:B:162:ASP:O	1:B:166:HIS:N	2.44	0.41
1:A:27:ASP:OD1	1:A:29:ARG:HB2	2.21	0.41
1:A:367:LYS:HG3	1:A:368:GLU:N	2.37	0.40
1:A:5:MET:CE	1:B:125:VAL:CG2	3.00	0.40
1:A:373:LEU:HA	1:A:373:LEU:HD23	1.94	0.40
1:B:347:ASN:HB2	1:B:409:LEU:HD13	2.03	0.40
1:B:186:VAL:HG22	1:B:188:PHE:CE1	2.57	0.40
1:A:18:LEU:HA	1:A:18:LEU:HD12	1.82	0.40
1:A:78:GLU:OE1	1:A:78:GLU:HA	2.22	0.40
1:B:69:LEU:HD22	1:B:70:TYR:N	2.36	0.40
1:A:258:LYS:HB2	5:A:425:HOH:O	2.20	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%)	15	15
1	B	394/396 (100%)	370 (94%)	20 (5%)	4 (1%)	19	21
All	All	788/792 (100%)	728 (92%)	51 (6%)	9 (1%)	17	18

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

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Mol	Chain	Res	Type
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%)	252 (79%)	68 (21%)	1	1
1	B	320/320 (100%)	258 (81%)	62 (19%)	2	1
All	All	640/640 (100%)	510 (80%)	130 (20%)	1	1

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	10	THR
1	A	18	LEU
1	A	20	LEU
1	A	29	ARG
1	A	32	LYS
1	A	39	LEU
1	A	44	THR
1	A	46	LYS
1	A	61	LEU
1	A	69	LEU
1	A	87	LEU
1	A	90	LYS
1	A	92	SER
1	A	94	LEU
1	A	98	LYS
1	A	112	LEU
1	A	119	LEU
1	A	121	LYS

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Mol	Chain	Res	Type
1	A	126	LYS
1	A	129	ARG
1	A	139	SER
1	A	144	LYS
1	A	145	SER
1	A	152	LEU
1	A	165	ASN
1	A	167	THR
1	A	168	LEU
1	A	170	PHE
1	A	178	ASN
1	A	179	GLU
1	A	184	ASP
1	A	187	LEU
1	A	195	PRO
1	A	202	LEU
1	A	206	GLN
1	A	211	LEU
1	A	218	LEU
1	A	223	PHE
1	A	240	LEU
1	A	246	MET
1	A	248	LYS
1	A	264	ASN
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	366	THR
1	A	370	VAL

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Mol	Chain	Res	Type
1	A	371	LEU
1	A	375	GLU
1	A	376	GLU
1	A	384	SER
1	A	386	ARG
1	A	388	ASN
1	A	400	LEU
1	B	5	MET
1	B	18	LEU
1	B	25	ARG
1	B	27	ASP
1	B	51	THR
1	B	55	LYS
1	B	61	LEU
1	B	69	LEU
1	B	87	LEU
1	B	90	LYS
1	B	98	LYS
1	B	99	ARG
1	B	113	ARG
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	156	ARG
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

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Mol	Chain	Res	Type
1	B	233	LEU
1	B	234	GLU
1	B	235	GLU
1	B	240	LEU
1	B	246	MET
1	B	259	ASN
1	B	273	VAL
1	B	280	VAL
1	B	292	ARG
1	B	294	ASN
1	B	324	THR
1	B	332	ARG
1	B	338	VAL
1	B	341	LEU
1	B	343	GLU
1	B	349	ASP
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	374	ARG
1	B	375	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	142	ASN
1	A	165	ASN
1	A	181	GLN
1	A	189	HIS
1	A	206	GLN
1	A	226	GLN
1	A	264	ASN
1	A	301	HIS
1	A	312	ASN
1	A	328	GLN

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Mol	Chain	Res	Type
1	A	357	ASN
1	A	388	ASN
1	B	63	ASN
1	B	84	GLN
1	B	96	ASN
1	B	122	ASN
1	B	165	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

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](#)

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	PLP	A	410	1	15,15,16	1.12	1 (6%)	21,22,23	2.07	7 (33%)
4	IOP	A	411	-	11,15,15	0.84	0	9,20,20	1.69	2 (22%)
2	SO4	B	411	-	4,4,4	0.18	0	6,6,6	0.61	0
3	PLP	B	412	1	15,15,16	1.31	3 (20%)	21,22,23	2.00	7 (33%)

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	PLP	A	410	1	-	0/6/6/8	0/1/1/1
4	IOP	A	411	-	-	0/3/5/5	0/2/2/2
2	SO4	B	411	-	-	0/0/0/0	0/0/0/0
3	PLP	B	412	1	-	0/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	412	PLP	C4A-C4	-2.41	1.46	1.51
3	B	412	PLP	P-O3P	-2.12	1.47	1.54
3	A	410	PLP	C5-C4	2.54	1.43	1.40
3	B	412	PLP	C5-C4	2.75	1.43	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	411	IOP	C3'-C2'-C1'	-4.18	105.09	112.75
3	A	410	PLP	C3-C4-C5	-3.24	115.24	118.78
3	B	412	PLP	C3-C2-N1	-2.40	117.29	120.61
3	B	412	PLP	C3-C4-C5	-2.39	116.17	118.78
4	A	411	IOP	C2'-C3'-C3	-2.32	108.51	112.32
3	A	410	PLP	C3-C2-N1	-2.30	117.43	120.61
3	B	412	PLP	C5A-C5-C6	-2.14	115.24	119.28
3	A	410	PLP	C5-C6-N1	-2.08	120.25	123.86
3	B	412	PLP	C5A-C5-C4	2.00	124.30	121.65
3	B	412	PLP	C6-C5-C4	2.51	120.28	118.15
3	B	412	PLP	O4P-C5A-C5	2.73	113.50	108.99
3	A	410	PLP	O4P-C5A-C5	3.07	114.07	108.99
3	A	410	PLP	O3P-P-O1P	3.33	121.29	110.58
3	A	410	PLP	C6-C5-C4	3.41	121.04	118.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	410	PLP	C4A-C4-C5	4.23	125.29	120.88
3	B	412	PLP	C4A-C4-C5	5.24	126.35	120.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

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

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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