Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 04:36 PM EDT

PDB ID	:	1AHE
Title	:	ASPARTATE AMINOTRANSFERASE HEXAMUTANT
Authors	:	Malashkevich, V.N.; Jansonius, J.N.
Deposited on	:	1995-02-22
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

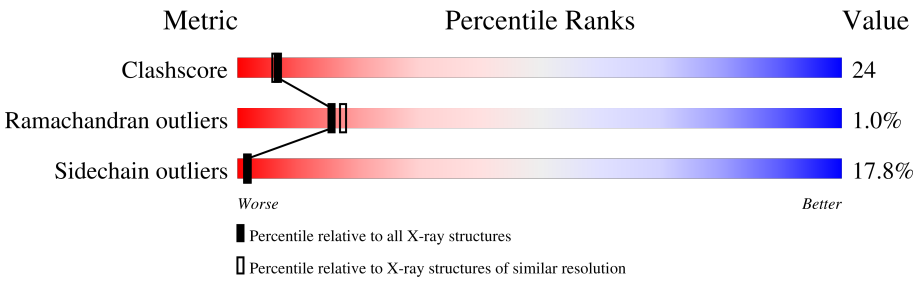
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	51% 36% 12% •
1	B	396	52% 35% 11% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PLP	B	412	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6582 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.

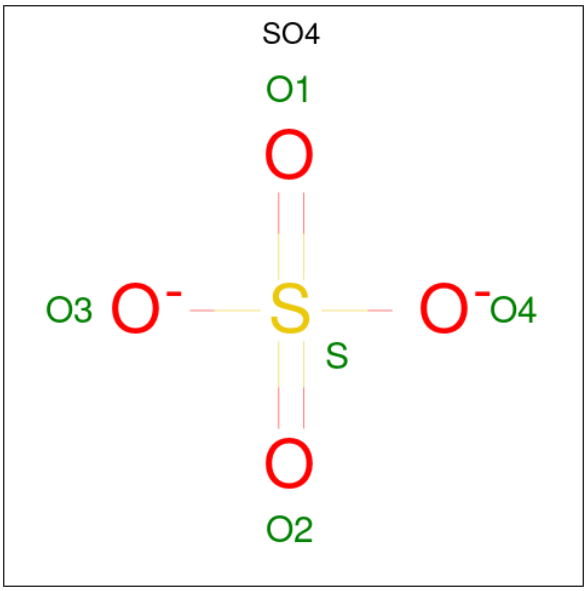
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

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

There are 12 discrepancies between the modelled and reference sequences:

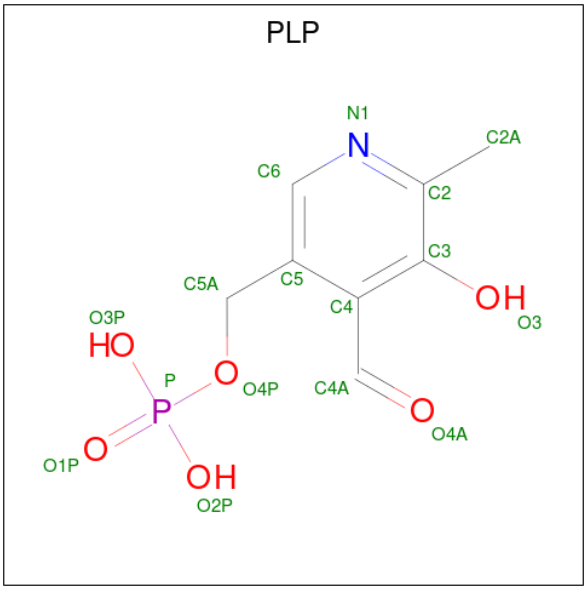
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LEU	VAL	conflict	UNP P00509
A	41	TYR	LYS	conflict	UNP P00509
A	47	ILE	THR	conflict	UNP P00509
A	69	LEU	ASN	conflict	UNP P00509
A	109	SER	THR	conflict	UNP P00509
A	297	SER	ASN	conflict	UNP P00509
B	39	LEU	VAL	conflict	UNP P00509
B	41	TYR	LYS	conflict	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: O_4S).



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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	209	209	209	0	0
			Total	O		
4	B	191	191	191	0	0

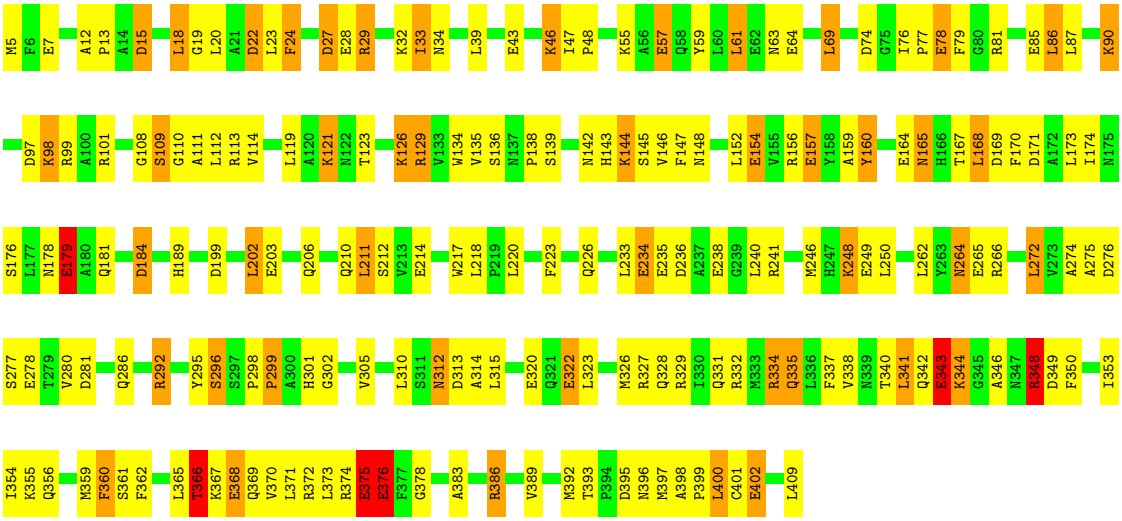
3 Residue-property plots (i)

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.

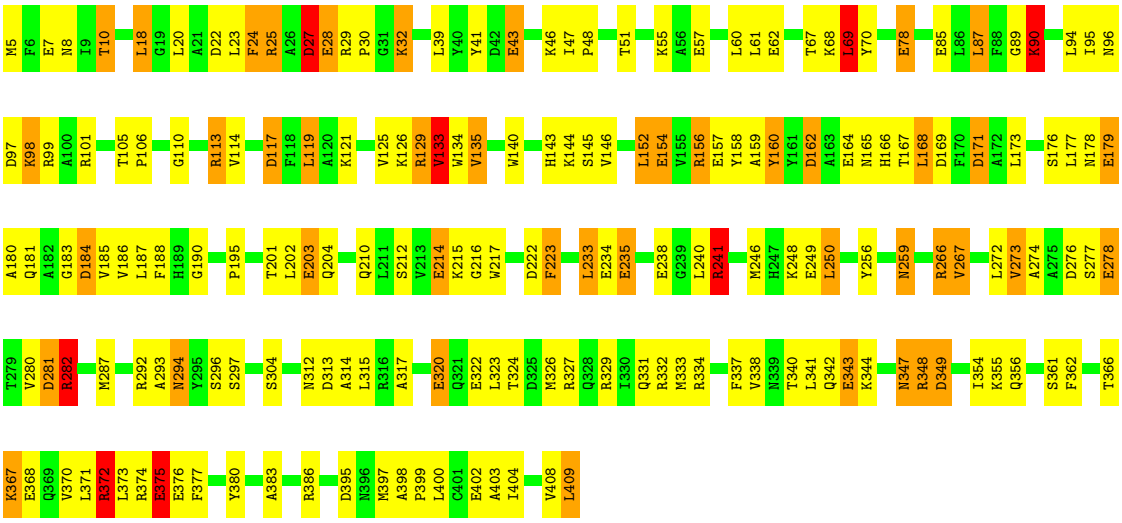
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain A: 51% 36% 12% •



• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain B: 52% 35% 11% •



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	85.07Å 77.98Å 88.86Å 90.00° 118.63° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	96.0 (8.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6582	wwPDB-VP
Average B, all atoms (Å^2)	42.0	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

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	1.02	25/3133 (0.8%)	1.29	35/4244 (0.8%)
1	B	1.01	22/3133 (0.7%)	1.33	39/4244 (0.9%)
All	All	1.02	47/6266 (0.8%)	1.31	74/8488 (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	A	1	0

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	THR	C-N	-8.61	1.14	1.34
1	A	85	GLU	CD-OE1	6.93	1.33	1.25
1	B	179	GLU	CD-OE1	6.92	1.33	1.25
1	A	203	GLU	CD-OE2	6.86	1.33	1.25
1	B	62	GLU	CD-OE2	6.85	1.33	1.25
1	A	43	GLU	CD-OE1	6.77	1.33	1.25
1	B	238	GLU	CD-OE2	6.46	1.32	1.25
1	A	320	GLU	CD-OE1	6.43	1.32	1.25
1	A	278	GLU	CD-OE1	6.39	1.32	1.25
1	A	164	GLU	CD-OE2	6.36	1.32	1.25
1	B	375	GLU	CD-OE2	6.29	1.32	1.25
1	A	238	GLU	CD-OE2	6.29	1.32	1.25
1	B	278	GLU	CD-OE2	6.27	1.32	1.25
1	B	28	GLU	CD-OE1	6.26	1.32	1.25
1	B	78	GLU	CD-OE1	6.23	1.32	1.25
1	A	28	GLU	CD-OE1	6.08	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	322	GLU	CD-OE2	6.04	1.32	1.25
1	A	402	GLU	CD-OE2	6.04	1.32	1.25
1	B	235	GLU	CD-OE2	5.93	1.32	1.25
1	B	214	GLU	CD-OE2	5.91	1.32	1.25
1	A	375	GLU	CD-OE1	5.89	1.32	1.25
1	B	320	GLU	CD-OE1	5.83	1.32	1.25
1	B	203	GLU	CD-OE1	5.82	1.32	1.25
1	A	376	GLU	CD-OE1	5.81	1.32	1.25
1	B	164	GLU	CD-OE2	5.81	1.32	1.25
1	B	43	GLU	CD-OE1	5.79	1.32	1.25
1	A	179	GLU	CD-OE2	5.71	1.31	1.25
1	A	235	GLU	CD-OE2	5.70	1.31	1.25
1	B	85	GLU	CD-OE1	5.67	1.31	1.25
1	A	157	GLU	CD-OE2	5.61	1.31	1.25
1	A	78	GLU	CD-OE2	5.59	1.31	1.25
1	B	90	LYS	C-N	-5.59	1.23	1.33
1	A	64	GLU	CD-OE2	5.57	1.31	1.25
1	A	265	GLU	CD-OE1	5.54	1.31	1.25
1	B	322	GLU	CD-OE2	5.51	1.31	1.25
1	A	343	GLU	CD-OE2	5.49	1.31	1.25
1	B	57	GLU	CD-OE2	5.44	1.31	1.25
1	B	154	GLU	CD-OE1	5.42	1.31	1.25
1	B	402	GLU	CD-OE2	5.37	1.31	1.25
1	B	343	GLU	CD-OE2	5.35	1.31	1.25
1	A	214	GLU	CD-OE1	5.31	1.31	1.25
1	A	154	GLU	CD-OE2	5.29	1.31	1.25
1	A	368	GLU	CD-OE1	5.17	1.31	1.25
1	A	234	GLU	CD-OE1	5.14	1.31	1.25
1	B	249	GLU	CD-OE2	5.08	1.31	1.25
1	B	368	GLU	CD-OE2	5.06	1.31	1.25
1	A	57	GLU	CD-OE2	5.04	1.31	1.25

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	267	VAL	CG1-CB-CG2	-10.42	94.22	110.90
1	A	123	THR	O-C-N	-10.15	106.47	122.70
1	B	282	ARG	NE-CZ-NH1	-8.21	116.19	120.30
1	A	171	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	A	27	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	169	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	B	162	ASP	CB-CG-OD2	-7.29	111.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	22	ASP	CB-CG-OD1	-7.25	111.77	118.30
1	A	74	ASP	CB-CG-OD1	7.23	124.81	118.30
1	B	276	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	B	90	LYS	O-C-N	-7.03	111.25	123.20
1	A	15	ASP	CB-CG-OD1	-7.00	112.00	118.30
1	B	281	ASP	CB-CG-OD2	-6.86	112.12	118.30
1	B	395	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	B	349	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	B	282	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	B	162	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	313	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	334	ARG	NE-CZ-NH1	-6.61	116.99	120.30
1	A	27	ASP	CB-CG-OD1	6.60	124.24	118.30
1	B	169	ASP	CB-CG-OD2	-6.59	112.36	118.30
1	B	313	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	B	22	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	B	171	ASP	CB-CG-OD2	-6.52	112.44	118.30
1	A	266	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	A	74	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	A	276	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	250	LEU	CB-CA-C	-6.37	98.09	110.20
1	A	360	PHE	CB-CA-C	-6.32	97.77	110.40
1	B	241	ARG	CG-CD-NE	6.29	125.02	111.80
1	B	276	ASP	CB-CG-OD1	6.24	123.92	118.30
1	B	24	PHE	CB-CG-CD1	-6.15	116.50	120.80
1	A	349	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	B	97	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	B	27	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	236	ASP	CB-CG-OD1	-6.03	112.87	118.30
1	A	276	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	395	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	313	ASP	CB-CG-OD1	-5.88	113.01	118.30
1	A	199	ASP	CB-CG-OD2	5.86	123.58	118.30
1	B	24	PHE	CB-CG-CD2	5.79	124.85	120.80
1	B	27	ASP	CB-CG-OD1	-5.75	113.13	118.30
1	B	409	LEU	CB-CA-C	5.68	121.00	110.20
1	B	184	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	295	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	B	266	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	B	22	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	184	ASP	CB-CG-OD1	-5.55	113.30	118.30
1	B	334	ARG	N-CA-CB	5.54	120.58	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	184	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	B	372	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	A	366	THR	N-CA-CB	-5.50	99.86	110.30
1	A	22	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	117	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	A	395	ASP	CB-CG-OD1	5.43	123.19	118.30
1	B	69	LEU	CB-CA-C	-5.42	99.89	110.20
1	A	199	ASP	CB-CG-OD1	-5.41	113.44	118.30
1	A	97	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	348	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	B	70	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	A	169	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	97	ASP	CB-CG-OD2	5.32	123.08	118.30
1	B	90	LYS	N-CA-C	-5.31	96.67	111.00
1	B	169	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	281	ASP	CB-CG-OD1	-5.29	113.53	118.30
1	B	281	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	171	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	97	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	A	24	PHE	CB-CG-CD1	-5.24	117.13	120.80
1	B	133	VAL	N-CA-CB	5.21	122.97	111.50
1	B	27	ASP	CB-CA-C	5.18	120.76	110.40
1	A	281	ASP	CB-CG-OD2	5.08	122.88	118.30
1	A	77	PRO	N-CA-CB	5.05	109.36	103.30
1	B	297	SER	N-CA-CB	5.04	118.06	110.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	165	ASN	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	3019	156	0
1	B	3071	0	3020	147	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	15	0	6	1	0
3	B	15	0	6	0	0
4	A	209	0	0	12	0
4	B	191	0	0	6	0
All	All	6582	0	6051	288	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 24.

All (288) 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:144:LYS:HZ3	1:A:148:ASN:HD21	1.11	0.98
1:A:366:THR:HG22	1:A:369:GLN:H	1.31	0.95
1:A:46:LYS:HD2	1:A:47:ILE:H	1.32	0.95
1:A:165:ASN:H	1:A:165:ASN:HD22	1.03	0.93
1:A:165:ASN:HD22	1:A:165:ASN:N	1.54	0.91
1:B:94:LEU:HD11	1:B:99:ARG:HH21	1.36	0.90
1:B:348:ARG:HG3	1:B:348:ARG:HH11	1.37	0.89
1:B:398:ALA:HB3	1:B:399:PRO:HD3	1.57	0.86
1:B:272:LEU:HD22	1:B:287:MET:CE	2.08	0.84
1:A:144:LYS:NZ	1:A:148:ASN:HD21	1.73	0.84
1:A:292:ARG:CZ	1:B:18:LEU:HD22	2.11	0.81
1:A:165:ASN:N	1:A:165:ASN:ND2	2.30	0.80
1:B:272:LEU:HD22	1:B:287:MET:HE2	1.65	0.79
1:B:187:LEU:HD12	1:B:188:PHE:N	1.98	0.79
1:A:121:LYS:NZ	1:A:121:LYS:HB3	1.96	0.78
1:B:94:LEU:HD11	1:B:99:ARG:NH2	1.98	0.78
1:B:397:MET:HE1	1:B:400:LEU:HD13	1.66	0.78
1:A:337:PHE:HD1	1:A:397:MET:HE1	1.49	0.77
1:A:398:ALA:HB3	1:A:399:PRO:HD3	1.66	0.77
1:A:99:ARG:HD2	1:A:274:ALA:O	1.86	0.76
1:B:46:LYS:O	1:B:48:PRO:HD3	1.85	0.76
1:A:24:PHE:O	1:A:32:LYS:NZ	2.19	0.75
1:B:327:ARG:O	1:B:331:GLN:HG3	1.88	0.72
1:A:129:ARG:HD2	1:A:134:TRP:NE1	2.05	0.72
1:A:90:LYS:HB2	4:A:597:HOH:O	1.88	0.71
1:B:46:LYS:HD2	1:B:47:ILE:H	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:SER:O	1:A:139:SER:HB2	1.90	0.71
1:B:27:ASP:OD1	1:B:29:ARG:HB2	1.90	0.71
1:B:162:ASP:OD2	1:B:165:ASN:HB2	1.91	0.70
1:B:24:PHE:O	1:B:32:LYS:HE3	1.92	0.70
1:B:98:LYS:HA	1:B:98:LYS:CE	2.22	0.70
1:B:28:GLU:OE1	1:B:28:GLU:HA	1.93	0.69
1:B:320:GLU:O	1:B:324:THR:HG23	1.92	0.69
1:A:323:LEU:HD12	1:A:326:MET:HE3	1.74	0.69
1:A:248:LYS:HG2	1:A:275:ALA:HB2	1.75	0.68
1:A:337:PHE:CD1	1:A:397:MET:HE1	2.29	0.68
1:A:24:PHE:CZ	1:A:34:ASN:HB2	2.28	0.68
1:A:337:PHE:HD1	1:A:397:MET:CE	2.07	0.68
1:A:248:LYS:CG	1:A:275:ALA:HB2	2.25	0.67
1:A:144:LYS:NZ	1:A:148:ASN:ND2	2.42	0.66
1:B:46:LYS:CD	1:B:47:ILE:H	2.07	0.66
1:B:94:LEU:CD1	1:B:99:ARG:HH21	2.08	0.66
1:B:372:ARG:O	1:B:376:GLU:HB3	1.95	0.66
1:B:374:ARG:HD3	1:B:380:TYR:CE2	2.30	0.66
1:A:99:ARG:HD3	1:A:275:ALA:O	1.96	0.66
1:B:90:LYS:HZ3	1:B:90:LYS:HB2	1.61	0.65
1:A:5:MET:N	1:A:7:GLU:OE1	2.30	0.65
1:B:337:PHE:HD1	1:B:397:MET:HE2	1.62	0.65
1:B:372:ARG:NH1	1:B:376:GLU:OE2	2.29	0.65
1:A:46:LYS:CD	1:A:47:ILE:H	2.08	0.64
1:B:25:ARG:NH1	4:B:415:HOH:O	2.31	0.64
1:B:250:LEU:HD12	1:B:273:VAL:HG13	1.80	0.64
1:B:348:ARG:HD2	1:B:409:LEU:HD22	1.78	0.64
1:A:167:THR:OG1	1:A:168:LEU:N	2.31	0.64
1:B:8:ASN:HB2	4:B:569:HOH:O	1.97	0.63
1:A:87:LEU:O	1:A:241:ARG:HD2	1.97	0.63
1:A:126:LYS:NZ	1:A:154:GLU:OE1	2.30	0.63
1:A:344:LYS:HE2	1:A:402:GLU:CG	2.28	0.63
1:B:241:ARG:HG3	1:B:241:ARG:HH11	1.64	0.63
1:B:179:GLU:O	1:B:179:GLU:HG3	1.99	0.63
1:B:348:ARG:HG3	1:B:348:ARG:NH1	2.09	0.63
1:A:27:ASP:OD1	1:A:29:ARG:HB2	1.99	0.63
1:A:129:ARG:HD2	1:A:134:TRP:HE1	1.63	0.63
1:B:201:THR:OG1	1:B:204:GLN:HG3	1.98	0.62
1:A:110:GLY:O	1:A:114:VAL:HG23	1.99	0.62
1:B:87:LEU:O	1:B:241:ARG:NH1	2.32	0.62
1:A:15:ASP:HB3	1:A:18:LEU:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PHE:CE1	1:A:34:ASN:HB2	2.36	0.61
1:B:278:GLU:OE2	1:B:282:ARG:NH1	2.32	0.61
1:A:211:LEU:HD13	1:A:217:TRP:CH2	2.35	0.61
1:B:89:GLY:O	1:B:90:LYS:O	2.19	0.61
1:A:312:ASN:ND2	1:A:315:LEU:H	2.00	0.60
1:A:46:LYS:HD2	1:A:47:ILE:N	2.12	0.60
1:B:398:ALA:HB3	1:B:399:PRO:CD	2.32	0.60
1:A:366:THR:HG23	1:A:368:GLU:H	1.67	0.59
1:A:206:GLN:O	1:A:210:GLN:HG3	2.03	0.59
1:B:210:GLN:HE21	1:B:214:GLU:HG3	1.68	0.59
1:B:96:ASN:HD22	1:B:96:ASN:N	2.00	0.59
1:A:33:ILE:CD1	1:A:396:ASN:HB2	2.33	0.59
1:A:81:ARG:NH2	4:A:587:HOH:O	2.34	0.59
1:A:249:GLU:OE1	1:B:5:MET:N	2.35	0.59
1:A:212:SER:HB3	1:A:217:TRP:CE3	2.38	0.58
1:A:343:GLU:O	1:A:343:GLU:HG2	2.02	0.58
1:B:367:LYS:HE3	1:B:383:ALA:O	2.03	0.58
1:B:98:LYS:HA	1:B:98:LYS:HE2	1.85	0.58
1:B:347:ASN:HB2	1:B:409:LEU:HD13	1.85	0.58
1:B:241:ARG:HH11	1:B:241:ARG:CG	2.17	0.58
1:A:327:ARG:O	1:A:331:GLN:HG3	2.04	0.57
1:A:57:GLU:OE2	1:A:301:HIS:HE1	1.87	0.57
1:B:98:LYS:HA	1:B:98:LYS:NZ	2.19	0.57
1:A:18:LEU:HD22	1:B:292:ARG:CZ	2.34	0.57
1:A:372:ARG:NE	1:A:376:GLU:OE1	2.35	0.57
1:B:210:GLN:HE21	1:B:214:GLU:CG	2.18	0.57
1:A:348:ARG:HG2	1:A:348:ARG:HH11	1.69	0.57
1:B:186:VAL:HG12	1:B:217:TRP:HB3	1.86	0.57
1:A:46:LYS:O	1:A:48:PRO:HD3	2.04	0.57
4:A:438:HOH:O	1:B:7:GLU:HG3	2.05	0.56
1:B:366:THR:O	1:B:370:VAL:HG13	2.05	0.56
1:B:90:LYS:HB2	1:B:90:LYS:NZ	2.18	0.56
1:A:98:LYS:HA	1:A:98:LYS:CE	2.33	0.56
1:A:292:ARG:NH2	1:B:18:LEU:HD22	2.19	0.56
1:A:372:ARG:O	1:A:376:GLU:HB2	2.05	0.56
1:B:133:VAL:HB	1:B:185:VAL:HB	1.88	0.56
1:B:143:HIS:NE2	1:B:222:ASP:OD2	2.29	0.55
1:A:121:LYS:HB3	1:A:121:LYS:HZ2	1.70	0.55
1:B:272:LEU:HD22	1:B:287:MET:HE1	1.88	0.55
1:B:125:VAL:HG11	1:B:185:VAL:CG2	2.36	0.55
1:B:210:GLN:O	1:B:214:GLU:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:GLU:HG2	1:B:377:PHE:CE2	2.42	0.54
1:B:135:VAL:O	1:B:157:GLU:HA	2.08	0.54
1:A:356:GLN:OE1	1:A:361:SER:HA	2.08	0.54
1:A:135:VAL:O	1:A:157:GLU:HA	2.07	0.54
1:B:43:GLU:CD	1:B:43:GLU:H	2.12	0.54
1:A:129:ARG:HH22	1:A:181:GLN:NE2	2.06	0.53
1:B:347:ASN:HD22	1:B:348:ARG:HH12	1.55	0.53
1:B:187:LEU:HD12	1:B:187:LEU:C	2.28	0.53
1:A:337:PHE:HA	1:A:397:MET:HE2	1.89	0.53
1:A:176:SER:O	1:A:179:GLU:HG3	2.08	0.53
1:B:94:LEU:HD12	1:B:99:ARG:HE	1.74	0.53
1:A:398:ALA:HB3	1:A:399:PRO:CD	2.35	0.53
1:A:234:GLU:OE1	1:A:241:ARG:NH2	2.40	0.52
1:B:397:MET:CE	1:B:400:LEU:HD13	2.38	0.52
1:A:329:ARG:NH2	1:A:393:THR:HG22	2.24	0.52
1:B:46:LYS:CG	1:B:47:ILE:H	2.21	0.52
1:B:202:LEU:HD12	1:B:202:LEU:O	2.10	0.52
1:A:341:LEU:HD13	1:A:401:CYS:SG	2.50	0.52
1:B:99:ARG:HG2	1:B:274:ALA:O	2.10	0.52
1:A:144:LYS:HZ3	1:A:148:ASN:ND2	1.92	0.51
1:A:286:GLN:HE21	1:B:10:THR:HG22	1.73	0.51
1:A:98:LYS:HE2	4:A:601:HOH:O	2.09	0.51
1:A:396:ASN:O	1:A:399:PRO:HD2	2.11	0.51
1:B:46:LYS:HD2	1:B:47:ILE:N	2.24	0.50
1:A:366:THR:HG22	1:A:369:GLN:N	2.13	0.50
1:B:5:MET:N	1:B:7:GLU:OE1	2.44	0.50
1:A:76:ILE:O	1:A:79:PHE:HB3	2.11	0.50
1:A:359:MET:O	1:A:389:VAL:N	2.45	0.50
1:B:158:TYR:CD2	1:B:177:LEU:HD21	2.46	0.50
1:B:113:ARG:NH2	4:B:508:HOH:O	2.44	0.50
1:A:340:THR:O	1:A:344:LYS:HB2	2.12	0.50
1:B:314:ALA:O	1:B:317:ALA:HB3	2.11	0.50
1:A:329:ARG:HH22	1:A:393:THR:HG22	1.77	0.49
1:A:146:VAL:HG23	1:A:147:PHE:N	2.28	0.49
1:A:160:TYR:HD1	1:A:173:LEU:CD2	2.24	0.49
1:A:248:LYS:HG3	1:A:275:ALA:HA	1.95	0.49
1:A:302:GLY:O	1:A:305:VAL:HB	2.12	0.49
1:B:140:TRP:HE3	1:B:143:HIS:CD2	2.30	0.49
1:A:323:LEU:HA	1:A:326:MET:HE2	1.94	0.49
1:B:181:GLN:O	1:B:184:ASP:HB2	2.13	0.49
1:B:160:TYR:O	1:B:168:LEU:HD23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ASN:C	1:B:294:ASN:HD22	2.14	0.48
1:B:158:TYR:CE1	1:B:173:LEU:HD11	2.48	0.48
1:B:400:LEU:C	1:B:400:LEU:HD23	2.34	0.48
1:A:59:TYR:CE1	1:A:63:ASN:ND2	2.81	0.48
1:A:360:PHE:CD1	1:A:386:ARG:HD3	2.47	0.48
1:A:129:ARG:HH22	1:A:181:GLN:HE21	1.61	0.48
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.63	0.48
1:B:101:ARG:NH1	1:B:281:ASP:OD1	2.47	0.48
1:A:342:GLN:C	1:A:344:LYS:H	2.17	0.48
1:B:159:ALA:O	1:B:173:LEU:HD12	2.13	0.48
1:B:162:ASP:O	1:B:166:HIS:N	2.45	0.47
1:A:386:ARG:NH2	2:A:411:SO4:O2	2.47	0.47
1:A:329:ARG:NH2	1:A:392:MET:O	2.46	0.47
1:A:373:LEU:O	1:A:378:GLY:N	2.47	0.47
1:B:312:ASN:OD1	1:B:314:ALA:HB3	2.15	0.47
1:A:109:SER:HB2	3:A:412:PLP:O2P	2.15	0.47
1:B:256:TYR:HA	1:B:259:ASN:HD21	1.80	0.47
1:B:400:LEU:HD23	1:B:404:ILE:HD12	1.96	0.47
1:A:328:GLN:O	1:A:332:ARG:HG3	2.15	0.47
1:B:95:ILE:O	1:B:98:LYS:HE2	2.14	0.47
1:A:156:ARG:HD2	4:A:477:HOH:O	2.14	0.47
1:B:212:SER:HB2	1:B:217:TRP:HB2	1.97	0.46
1:A:159:ALA:O	1:A:173:LEU:HD22	2.16	0.46
1:A:366:THR:O	1:A:370:VAL:HG13	2.16	0.46
1:B:277:SER:HA	1:B:280:VAL:HG12	1.97	0.46
1:A:212:SER:CB	1:A:217:TRP:CE3	2.99	0.46
1:B:201:THR:HG23	1:B:204:GLN:OE1	2.16	0.46
1:B:96:ASN:N	1:B:96:ASN:ND2	2.64	0.46
1:B:10:THR:HG22	1:B:10:THR:O	2.16	0.46
1:B:158:TYR:CD1	1:B:173:LEU:HD12	2.50	0.46
1:A:170:PHE:CE2	1:A:174:ILE:CD1	2.99	0.46
1:B:78:GLU:O	1:B:78:GLU:HG3	2.15	0.46
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.81	0.45
1:B:212:SER:CB	1:B:217:TRP:CE3	2.99	0.45
1:A:78:GLU:HG3	4:A:587:HOH:O	2.17	0.45
1:B:5:MET:O	1:B:5:MET:HG3	2.15	0.45
1:B:356:GLN:OE1	1:B:361:SER:HA	2.16	0.45
1:A:312:ASN:HD21	1:A:314:ALA:HB3	1.82	0.45
1:B:46:LYS:CG	1:B:47:ILE:N	2.80	0.45
1:B:177:LEU:O	1:B:180:ALA:HB3	2.16	0.45
1:A:18:LEU:HD22	1:B:292:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLY:O	1:A:22:ASP:N	2.47	0.45
1:A:396:ASN:C	1:A:399:PRO:HD2	2.37	0.45
1:A:46:LYS:CG	1:A:47:ILE:N	2.80	0.45
1:A:98:LYS:CA	1:A:98:LYS:HE3	2.47	0.45
1:B:89:GLY:O	1:B:90:LYS:HB3	2.16	0.45
1:B:129:ARG:HD3	1:B:154:GLU:HG2	1.98	0.45
1:A:338:VAL:HG13	1:A:354:ILE:HD11	1.97	0.45
1:B:110:GLY:O	1:B:114:VAL:HG23	2.16	0.45
1:A:344:LYS:HE2	1:A:402:GLU:HG3	1.99	0.44
1:A:46:LYS:CD	1:A:47:ILE:N	2.78	0.44
1:A:226:GLN:HG2	1:A:233:LEU:HD23	1.99	0.44
1:A:370:VAL:HG21	1:A:383:ALA:HA	1.99	0.44
1:B:152:LEU:HD12	1:B:152:LEU:HA	1.84	0.44
1:A:108:GLY:O	1:A:111:ALA:HB3	2.18	0.44
1:A:312:ASN:HD22	1:A:315:LEU:H	1.62	0.44
1:A:189:HIS:HD2	4:A:425:HOH:O	2.01	0.44
1:A:46:LYS:HE2	1:B:67:THR:HB	2.00	0.44
1:A:202:LEU:HD22	1:A:202:LEU:O	2.17	0.43
1:A:98:LYS:HA	1:A:98:LYS:HE3	2.00	0.43
1:A:142:ASN:HD21	1:B:292:ARG:HG3	1.83	0.43
1:A:113:ARG:NH1	1:B:293:ALA:O	2.52	0.43
1:B:134:TRP:HA	1:B:156:ARG:O	2.18	0.43
1:B:20:LEU:HD12	1:B:20:LEU:HA	1.74	0.43
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.69	0.43
1:A:350:PHE:O	1:A:353:ILE:HB	2.17	0.43
1:B:69:LEU:HD23	1:B:69:LEU:HA	1.70	0.43
1:B:315:LEU:HA	1:B:315:LEU:HD23	1.77	0.43
1:A:335:GLN:H	1:A:335:GLN:HG2	1.54	0.43
1:B:18:LEU:HD12	1:B:18:LEU:HA	1.49	0.43
1:A:12:ALA:HB1	1:A:13:PRO:HD2	2.01	0.43
1:A:18:LEU:HA	1:A:18:LEU:HD12	1.45	0.43
1:A:5:MET:HE2	1:B:125:VAL:HG23	2.01	0.43
1:B:41:TYR:HE1	4:B:544:HOH:O	2.01	0.43
1:B:90:LYS:CG	4:B:579:HOH:O	2.66	0.43
1:A:156:ARG:NH2	4:A:602:HOH:O	2.51	0.42
1:A:274:ALA:HB3	1:A:280:VAL:HB	2.01	0.42
1:B:117:ASP:O	1:B:121:LYS:HD2	2.18	0.42
1:B:195:PRO:HB3	1:B:386:ARG:HD3	2.01	0.42
1:B:60:LEU:HD11	1:B:304:SER:HB2	2.01	0.42
1:A:129:ARG:HB2	1:A:154:GLU:HB3	2.01	0.42
1:A:264:ASN:C	1:A:264:ASN:HD22	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HD23	1:B:68:LYS:HD2	2.01	0.42
1:A:366:THR:CG2	1:A:368:GLU:H	2.32	0.42
1:B:158:TYR:CD1	1:B:173:LEU:CD1	3.02	0.42
1:B:177:LEU:HB3	1:B:217:TRP:CH2	2.54	0.42
1:A:272:LEU:HD23	1:A:272:LEU:HA	1.82	0.42
1:A:286:GLN:NE2	1:B:10:THR:HG22	2.35	0.42
1:B:348:ARG:NH1	1:B:348:ARG:CG	2.80	0.42
1:A:18:LEU:CD2	1:B:292:ARG:CZ	2.98	0.42
1:A:98:LYS:HA	1:A:98:LYS:HD2	1.60	0.42
1:A:341:LEU:HD12	1:A:341:LEU:HA	1.79	0.42
1:B:332:ARG:HG2	1:B:333:MET:HE3	2.02	0.42
1:A:69:LEU:HD23	1:B:39:LEU:HD22	2.02	0.42
1:A:143:HIS:O	1:A:146:VAL:HG22	2.19	0.42
1:B:29:ARG:NH1	1:B:375:GLU:O	2.53	0.41
1:B:94:LEU:HD12	1:B:94:LEU:HA	1.81	0.41
1:A:5:MET:HE3	4:B:499:HOH:O	2.19	0.41
1:A:160:TYR:HD1	1:A:173:LEU:HD21	1.84	0.41
1:A:298:PRO:HA	1:A:299:PRO:HD3	1.91	0.41
1:A:144:LYS:HZ2	1:A:148:ASN:ND2	2.17	0.41
1:A:292:ARG:NH1	1:A:296:SER:OG	2.53	0.41
1:A:301:HIS:HD2	4:A:451:HOH:O	2.03	0.41
1:A:338:VAL:CG1	1:A:354:ILE:HD11	2.50	0.41
1:B:23:LEU:HD23	1:B:23:LEU:HA	1.70	0.41
1:A:386:ARG:HD2	4:A:436:HOH:O	2.20	0.41
1:B:190:GLY:HA3	1:B:223:PHE:CD1	2.55	0.41
1:B:340:THR:O	1:B:344:LYS:HG3	2.21	0.41
1:B:397:MET:HE3	1:B:397:MET:HA	2.02	0.41
1:A:61:LEU:HA	1:A:61:LEU:HD23	1.79	0.41
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.85	0.41
1:B:158:TYR:HD1	1:B:173:LEU:HD12	1.86	0.41
1:B:272:LEU:HD13	1:B:287:MET:HE1	2.02	0.41
1:A:98:LYS:CE	1:A:98:LYS:CA	2.99	0.41
1:A:138:PRO:HB3	4:A:441:HOH:O	2.21	0.41
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.90	0.41
1:A:374:ARG:NH1	1:A:375:GLU:OE1	2.54	0.41
1:B:183:GLY:N	1:B:216:GLY:O	2.34	0.41
1:A:212:SER:HB2	1:A:217:TRP:HB2	2.03	0.41
1:A:220:LEU:C	1:A:220:LEU:HD23	2.41	0.41
1:A:312:ASN:HD22	1:A:312:ASN:C	2.24	0.41
1:A:348:ARG:CZ	1:A:409:LEU:HD22	2.51	0.41
1:B:119:LEU:HD12	1:B:119:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:SER:CB	1:B:217:TRP:HE3	2.34	0.41
1:A:86:LEU:HD12	1:A:86:LEU:HA	1.75	0.40
1:B:403:ALA:O	1:B:408:VAL:HG13	2.22	0.40
1:A:248:LYS:NZ	4:A:539:HOH:O	2.41	0.40
1:A:322:GLU:O	1:A:326:MET:HG3	2.21	0.40
1:B:125:VAL:HG11	1:B:185:VAL:HG23	2.02	0.40
1:B:129:ARG:HD3	1:B:154:GLU:CG	2.51	0.40
1:B:323:LEU:HD12	1:B:326:MET:HE3	2.03	0.40
1:B:329:ARG:O	1:B:329:ARG:HG2	2.21	0.40
1:A:299:PRO:HA	1:B:266:ARG:HG2	2.04	0.40
1:B:113:ARG:HA	1:B:113:ARG:HD3	1.95	0.40
1:B:274:ALA:HB3	1:B:280:VAL:HB	2.02	0.40
1:A:400:LEU:HD12	1:A:400:LEU:O	2.20	0.40
1:B:105:THR:HB	1:B:106:PRO:HD2	2.02	0.40
1:A:170:PHE:CE2	1:A:174:ILE:HD11	2.56	0.40
1:B:248:LYS:HD3	1:B:248:LYS:HA	1.87	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%)	368 (93%)	22 (6%)	4 (1%)	15 17
1	B	394/396 (100%)	369 (94%)	21 (5%)	4 (1%)	15 17
All	All	788/792 (100%)	737 (94%)	43 (6%)	8 (1%)	15 17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	346	ALA
1	A	343	GLU

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Mol	Chain	Res	Type
1	B	347	ASN
1	A	20	LEU
1	B	30	PRO
1	B	90	LYS
1	B	160	TYR
1	A	160	TYR

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%)	264 (82%)	56 (18%)	2 2
1	B	320/320 (100%)	262 (82%)	58 (18%)	1 1
All	All	640/640 (100%)	526 (82%)	114 (18%)	2 1

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	23	LEU
1	A	29	ARG
1	A	33	ILE
1	A	39	LEU
1	A	46	LYS
1	A	55	LYS
1	A	61	LEU
1	A	69	LEU
1	A	86	LEU
1	A	90	LYS
1	A	98	LYS
1	A	101	ARG
1	A	109	SER
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	144	LYS
1	A	145	SER
1	A	152	LEU
1	A	165	ASN
1	A	168	LEU
1	A	178	ASN
1	A	179	GLU
1	A	184	ASP
1	A	202	LEU
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	277	SER
1	A	292	ARG
1	A	296	SER
1	A	299	PRO
1	A	312	ASN
1	A	334	ARG
1	A	335	GLN
1	A	341	LEU
1	A	344	LYS
1	A	348	ARG
1	A	355	LYS
1	A	362	PHE
1	A	365	LEU
1	A	366	THR
1	A	367	LYS
1	A	371	LEU
1	A	375	GLU
1	A	376	GLU
1	A	386	ARG
1	A	400	LEU
1	B	10	THR
1	B	18	LEU
1	B	25	ARG

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Mol	Chain	Res	Type
1	B	27	ASP
1	B	32	LYS
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	113	ARG
1	B	119	LEU
1	B	126	LYS
1	B	129	ARG
1	B	133	VAL
1	B	135	VAL
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	176	SER
1	B	178	ASN
1	B	203	GLU
1	B	215	LYS
1	B	223	PHE
1	B	233	LEU
1	B	234	GLU
1	B	235	GLU
1	B	240	LEU
1	B	241	ARG
1	B	246	MET
1	B	250	LEU
1	B	259	ASN
1	B	267	VAL
1	B	273	VAL
1	B	282	ARG
1	B	294	ASN
1	B	296	SER
1	B	338	VAL

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Mol	Chain	Res	Type
1	B	341	LEU
1	B	342	GLN
1	B	343	GLU
1	B	348	ARG
1	B	349	ASP
1	B	354	ILE
1	B	355	LYS
1	B	362	PHE
1	B	367	LYS
1	B	371	LEU
1	B	372	ARG
1	B	373	LEU
1	B	375	GLU

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	63	ASN
1	A	84	GLN
1	A	137	ASN
1	A	142	ASN
1	A	148	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
1	A	335	GLN
1	A	339	ASN
1	A	357	ASN
1	A	388	ASN
1	B	84	GLN
1	B	96	ASN
1	B	166	HIS
1	B	206	GLN
1	B	210	GLN
1	B	226	GLN
1	B	259	ASN

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Mol	Chain	Res	Type
1	B	294	ASN
1	B	328	GLN
1	B	339	ASN
1	B	347	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	PLP	B	412	1	15,15,16	1.77	4 (26%)	20,22,23	1.85	10 (50%)
2	SO4	A	411	-	4,4,4	0.29	0	6,6,6	0.61	0
3	PLP	A	412	1	15,15,16	1.89	2 (13%)	20,22,23	2.56	8 (40%)
2	SO4	B	411	-	4,4,4	0.17	0	6,6,6	0.46	0

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	B	412	1	-	4/6/6/8	0/1/1/1
3	PLP	A	412	1	-	5/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	412	PLP	C5-C4	5.64	1.46	1.40
3	B	412	PLP	C5-C4	4.72	1.45	1.40
3	B	412	PLP	C5A-C5	2.60	1.58	1.50
3	A	412	PLP	P-O3P	-2.59	1.44	1.54
3	B	412	PLP	C4A-C4	-2.54	1.46	1.51
3	B	412	PLP	P-O3P	-2.30	1.46	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	412	PLP	C4A-C4-C5	6.00	127.11	120.94
3	A	412	PLP	C6-C5-C4	4.81	121.95	118.16
3	A	412	PLP	C3-C4-C5	-4.45	113.93	118.74
3	A	412	PLP	C5A-C5-C6	-3.04	114.37	119.37
3	B	412	PLP	C4A-C4-C5	3.00	124.02	120.94
3	B	412	PLP	C6-N1-C2	2.71	124.20	119.17
3	B	412	PLP	C6-C5-C4	2.49	120.12	118.16
3	B	412	PLP	C5A-C5-C6	-2.49	115.28	119.37
3	B	412	PLP	C3-C4-C5	-2.41	116.14	118.74
3	A	412	PLP	C5-C6-N1	-2.41	119.80	123.82
3	A	412	PLP	O3P-P-O1P	2.41	120.11	110.68
3	B	412	PLP	O4P-C5A-C5	2.41	113.94	109.35
3	A	412	PLP	O3P-P-O4P	-2.40	100.35	106.73
3	B	412	PLP	C5-C6-N1	-2.38	119.86	123.82
3	B	412	PLP	C3-C2-N1	-2.25	117.86	120.77
3	A	412	PLP	C2A-C2-C3	2.18	123.58	120.89
3	B	412	PLP	C2A-C2-C3	2.02	123.39	120.89
3	B	412	PLP	O3-C3-C4	2.00	123.37	118.10

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	412	PLP	C4-C5-C5A-O4P
3	A	412	PLP	C6-C5-C5A-O4P
3	A	412	PLP	C5A-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
3	A	412	PLP	C5A-O4P-P-O2P
3	A	412	PLP	C5A-O4P-P-O3P
3	B	412	PLP	C4-C5-C5A-O4P
3	B	412	PLP	C6-C5-C5A-O4P
3	B	412	PLP	C5A-O4P-P-O2P
3	B	412	PLP	C5A-O4P-P-O3P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	411	SO4	1	0
3	A	412	PLP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	123:THR	C	124:SER	N	1.14

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.