Full wwPDB X-ray Structure Validation Report (i)

Feb 8, 2022 – 08:13 AM EST

PDB ID	:	1AHX
Title	:	ASPARTATE AMINOTRANSFERASE HEXAMUTANT
Authors	:	Malashkevich, V.N.; Jansonius, J.N.
Deposited on	:	1995-02-21
Resolution	:	2.00 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:

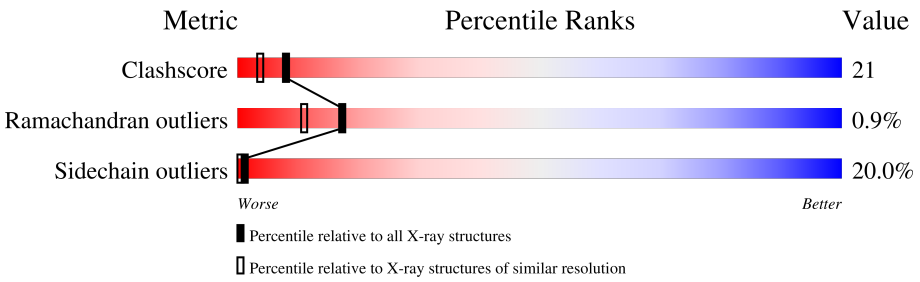
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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	57% 30% 12% •
1	B	396	55% 31% 11% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6723 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.

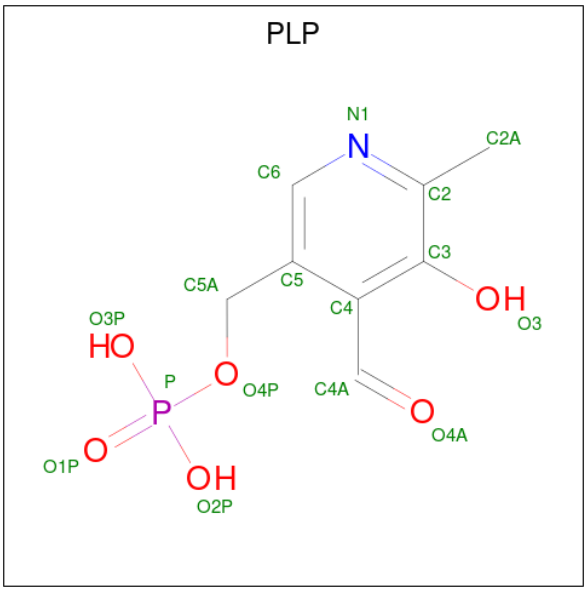
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

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:

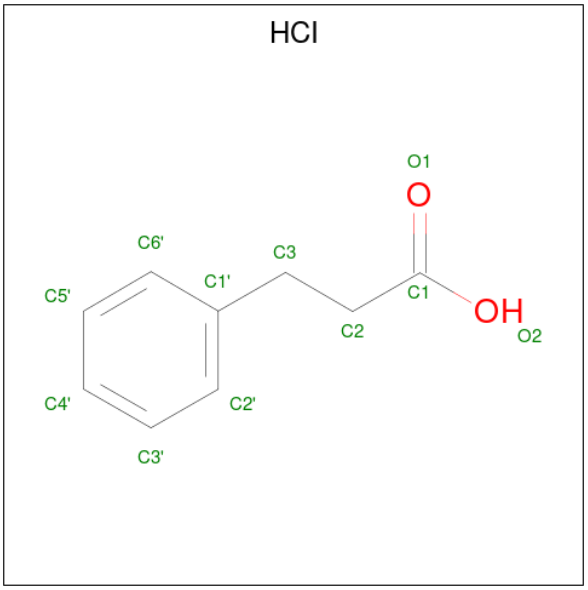
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LEU	VAL	conflict	UNP P00509
A	41	TYR	LYS	conflict	UNP P00509
A	47	ILE	THR	conflict	UNP P00509
A	69	LEU	ASN	conflict	UNP P00509
A	109	SER	THR	conflict	UNP P00509
A	297	SER	ASN	conflict	UNP P00509
B	39	LEU	VAL	conflict	UNP P00509
B	41	TYR	LYS	conflict	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 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
			Total	C	N	O	P		
2	B	1	15	8	1	5	1	0	0

- Molecule 3 is HYDROCINNAMIC ACID (three-letter code: HCI) (formula: $C_9H_{10}O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	O				
3	A	1	11	9	2			0	0
			Total	C	O				
3	B	1	11	9	2			0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	279	279	279	0	0
			Total	O		
4	B	250	250	250	0	0

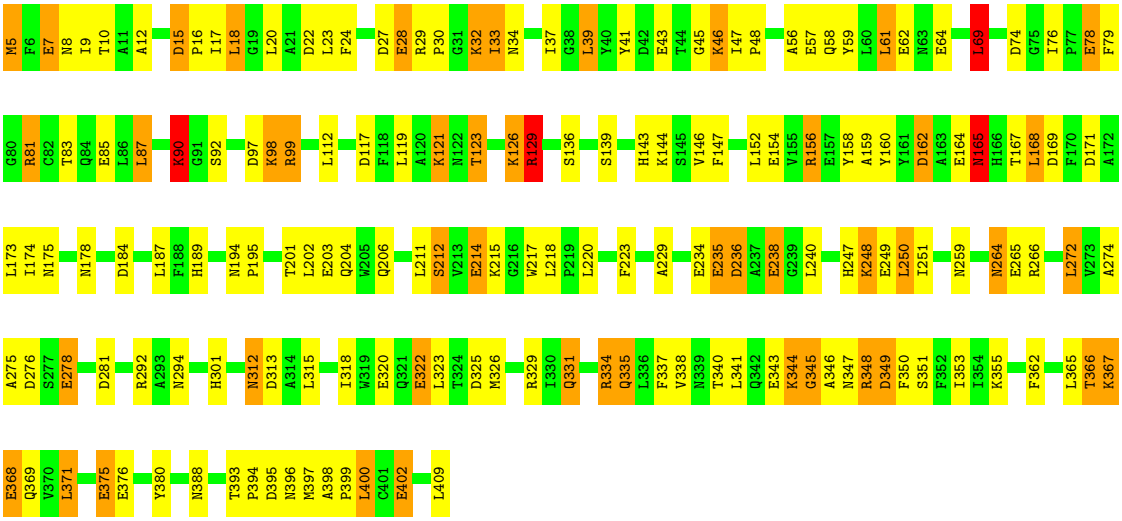
3 Residue-property plots (i)

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.

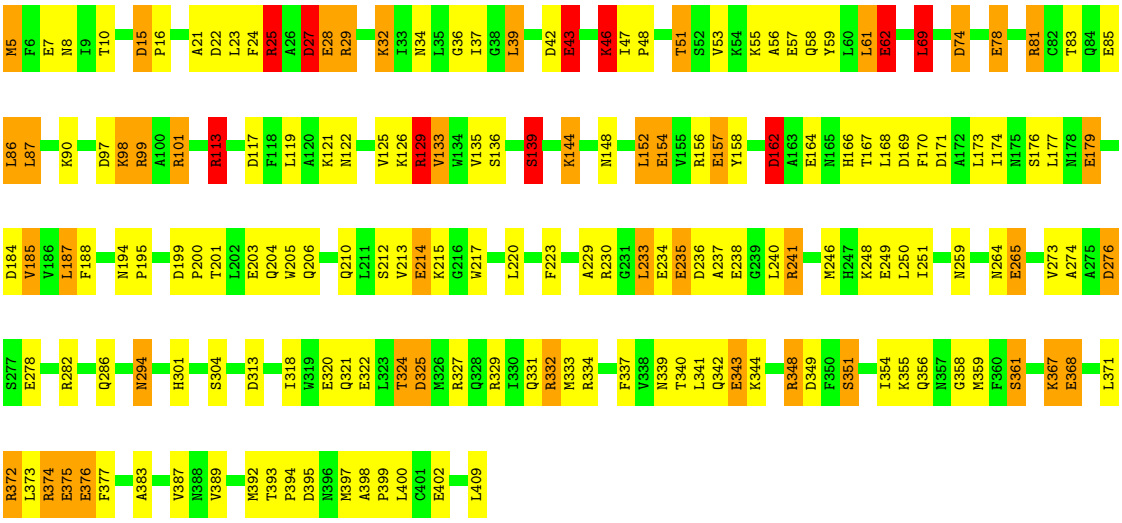
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain A: 57% 30% 12%



• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain B: 55% 31% 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	84.98Å 78.69Å 89.28Å 90.00° 118.32° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	93.5 (8.00-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.226 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6723	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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, HCI

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	1.05	24/3133 (0.8%)	1.29	35/4244 (0.8%)
1	B	1.03	24/3133 (0.8%)	1.34	35/4244 (0.8%)
All	All	1.04	48/6266 (0.8%)	1.32	70/8488 (0.8%)

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	0	1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	GLU	CD-OE1	9.08	1.35	1.25
1	B	320	GLU	CD-OE1	8.91	1.35	1.25
1	A	320	GLU	CD-OE1	8.19	1.34	1.25
1	B	265	GLU	CD-OE1	7.21	1.33	1.25
1	B	235	GLU	CD-OE2	7.18	1.33	1.25
1	A	376	GLU	CD-OE1	7.15	1.33	1.25
1	B	164	GLU	CD-OE2	7.12	1.33	1.25
1	B	375	GLU	CD-OE2	6.96	1.33	1.25
1	B	28	GLU	CD-OE1	6.96	1.33	1.25
1	B	376	GLU	CD-OE2	6.92	1.33	1.25
1	A	322	GLU	CD-OE1	6.89	1.33	1.25
1	A	238	GLU	CD-OE2	6.83	1.33	1.25
1	A	43	GLU	CD-OE2	6.81	1.33	1.25
1	A	234	GLU	CD-OE1	6.79	1.33	1.25
1	B	179	GLU	CD-OE2	6.74	1.33	1.25
1	B	214	GLU	CD-OE2	6.72	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	GLU	CD-OE2	6.71	1.33	1.25
1	B	249	GLU	CD-OE2	6.69	1.33	1.25
1	A	402	GLU	CD-OE2	6.62	1.32	1.25
1	A	375	GLU	CD-OE2	6.45	1.32	1.25
1	B	343	GLU	CD-OE2	6.29	1.32	1.25
1	B	203	GLU	CD-OE2	6.21	1.32	1.25
1	B	43	GLU	CD-OE2	6.17	1.32	1.25
1	A	278	GLU	CD-OE1	6.17	1.32	1.25
1	A	214	GLU	CD-OE1	6.09	1.32	1.25
1	A	164	GLU	CD-OE2	6.03	1.32	1.25
1	A	368	GLU	CD-OE1	6.02	1.32	1.25
1	A	85	GLU	CD-OE1	6.01	1.32	1.25
1	B	387	VAL	CB-CG1	-6.00	1.40	1.52
1	B	278	GLU	CD-OE2	5.96	1.32	1.25
1	A	203	GLU	CD-OE2	5.96	1.32	1.25
1	A	28	GLU	CD-OE1	5.93	1.32	1.25
1	A	343	GLU	CD-OE1	5.92	1.32	1.25
1	B	157	GLU	CD-OE2	5.88	1.32	1.25
1	B	238	GLU	CD-OE2	5.88	1.32	1.25
1	A	62	GLU	CD-OE2	5.68	1.31	1.25
1	A	7	GLU	CD-OE2	5.68	1.31	1.25
1	B	62	GLU	CD-OE2	5.67	1.31	1.25
1	B	78	GLU	CD-OE1	5.59	1.31	1.25
1	A	249	GLU	CD-OE2	5.52	1.31	1.25
1	B	85	GLU	CD-OE1	5.40	1.31	1.25
1	A	57	GLU	CD-OE2	5.38	1.31	1.25
1	B	234	GLU	CD-OE2	5.38	1.31	1.25
1	B	154	GLU	CD-OE1	5.29	1.31	1.25
1	B	368	GLU	CD-OE2	5.23	1.31	1.25
1	B	57	GLU	CD-OE1	-5.11	1.20	1.25
1	A	123	THR	C-N	-5.01	1.22	1.34
1	A	64	GLU	CD-OE2	5.01	1.31	1.25

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	276	ASP	CB-CG-OD2	-8.67	110.50	118.30
1	B	162	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	A	395	ASP	CB-CG-OD2	-7.65	111.41	118.30
1	A	169	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	B	27	ASP	N-CA-CB	7.33	123.80	110.60
1	B	171	ASP	CB-CG-OD2	-7.21	111.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	266	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	27	ASP	CB-CG-OD1	7.14	124.72	118.30
1	A	81	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	A	15	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	B	395	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	22	ASP	CB-CG-OD1	-6.94	112.05	118.30
1	B	27	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	A	117	ASP	CB-CG-OD2	6.78	124.40	118.30
1	B	162	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	184	ASP	CB-CG-OD1	-6.69	112.28	118.30
1	A	165	ASN	N-CA-CB	6.64	122.55	110.60
1	B	241	ARG	NE-CZ-NH2	6.61	123.61	120.30
1	B	276	ASP	CB-CG-OD1	6.48	124.13	118.30
1	B	97	ASP	CB-CG-OD1	-6.47	112.48	118.30
1	A	97	ASP	CB-CG-OD1	-6.46	112.49	118.30
1	B	169	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	A	171	ASP	CB-CG-OD2	-6.43	112.52	118.30
1	B	395	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	A	27	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	B	46	LYS	CB-CA-C	6.26	122.93	110.40
1	B	97	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	15	ASP	CB-CG-OD1	6.12	123.80	118.30
1	B	129	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	B	69	LEU	CB-CA-C	-6.02	98.75	110.20
1	A	395	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	329	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	276	ASP	CB-CG-OD1	5.84	123.55	118.30
1	A	184	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	169	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	345	GLY	O-C-N	-5.72	113.56	122.70
1	B	184	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	69	LEU	CB-CG-CD2	-5.70	101.30	111.00
1	A	349	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	B	184	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	B	199	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	250	LEU	N-CA-CB	-5.67	99.07	110.40
1	A	117	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	A	276	ASP	CB-CG-OD2	-5.63	113.24	118.30
1	A	313	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	281	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	25	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	A	236	ASP	CB-CG-OD2	5.52	123.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	162	ASP	CB-CA-C	5.51	121.42	110.40
1	B	15	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	B	250	LEU	N-CA-CB	5.49	121.37	110.40
1	B	129	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	B	325	ASP	CB-CG-OD2	5.45	123.21	118.30
1	B	22	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	A	99	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	A	74	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	313	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	B	241	ARG	CG-CD-NE	5.37	123.07	111.80
1	B	113	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	B	139	SER	N-CA-CB	5.27	118.40	110.50
1	B	376	GLU	N-CA-CB	-5.23	101.18	110.60
1	A	129	ARG	NE-CZ-NH1	-5.23	117.68	120.30
1	B	241	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	B	74	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	266	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	175	ASN	CB-CA-C	5.13	120.66	110.40
1	A	325	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	A	325	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	169	ASP	CB-CG-OD1	5.06	122.86	118.30
1	B	117	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	ARG	Sidechain

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	121	0
1	B	3071	0	3020	150	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	11	0	9	1	0
3	B	11	0	9	0	0
4	A	279	0	0	6	0
4	B	250	0	0	21	0
All	All	6723	0	6070	263	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 21.

All (263) 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:46:LYS:HD2	1:A:47:ILE:H	1.23	1.04
1:A:366:THR:HG22	1:A:369:GLN:H	1.25	0.99
1:B:389:VAL:HG13	1:B:392:MET:HE2	1.46	0.96
1:B:29:ARG:HH11	1:B:29:ARG:HG3	1.29	0.95
1:A:18:LEU:HD12	1:A:37:ILE:HD12	1.49	0.94
1:B:359:MET:HE1	4:B:456:HOH:O	1.73	0.87
1:B:98:LYS:HE2	1:B:98:LYS:HA	1.57	0.87
1:B:389:VAL:HG13	1:B:392:MET:CE	2.08	0.84
1:A:248:LYS:CG	1:A:275:ALA:HB2	2.10	0.81
1:A:126:LYS:HE2	1:A:129:ARG:NH1	1.96	0.81
1:A:366:THR:HG22	1:A:369:GLN:N	1.97	0.79
1:A:366:THR:HG21	4:A:583:HOH:O	1.82	0.79
1:A:165:ASN:N	1:A:165:ASN:HD22	1.79	0.79
1:A:312:ASN:ND2	1:A:315:LEU:H	1.81	0.78
1:A:165:ASN:HD22	1:A:165:ASN:H	1.31	0.78
1:A:121:LYS:NZ	1:A:121:LYS:HB3	1.96	0.77
1:A:45:GLY:HA3	4:A:672:HOH:O	1.86	0.76
1:A:397:MET:HE3	1:A:400:LEU:HD21	1.67	0.75
1:B:348:ARG:HG2	1:B:348:ARG:HH11	1.51	0.74
1:B:201:THR:HG23	1:B:204:GLN:OE1	1.88	0.74
1:A:90:LYS:HG2	4:A:463:HOH:O	1.87	0.73
1:A:159:ALA:O	1:A:173:LEU:HD23	1.89	0.73
1:B:398:ALA:O	1:B:402:GLU:HG3	1.89	0.73
1:B:46:LYS:HD2	1:B:47:ILE:H	1.54	0.72
1:B:42:ASP:HB2	1:B:43:GLU:OE1	1.90	0.72
1:B:98:LYS:HA	1:B:98:LYS:CE	2.20	0.72
1:A:294:ASN:HD21	1:B:294:ASN:HD21	1.39	0.71
1:A:312:ASN:HD22	1:A:315:LEU:H	1.37	0.71
1:A:393:THR:HB	1:A:394:PRO:HD2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:SER:O	1:B:139:SER:HB2	1.91	0.70
1:A:41:TYR:CE2	1:A:47:ILE:HD11	2.26	0.69
1:A:235:GLU:O	1:A:238:GLU:HG3	1.92	0.69
1:B:200:PRO:HG2	1:B:205:TRP:CE2	2.28	0.68
1:A:366:THR:CG2	1:A:369:GLN:H	2.03	0.68
1:A:46:LYS:HD2	1:A:47:ILE:N	2.04	0.67
1:B:133:VAL:HB	1:B:185:VAL:HG23	1.76	0.67
1:B:201:THR:HG23	1:B:204:GLN:CD	2.15	0.67
1:B:389:VAL:CG1	1:B:392:MET:HE2	2.22	0.66
1:A:248:LYS:HG3	1:A:275:ALA:HB2	1.78	0.66
1:B:87:LEU:O	1:B:241:ARG:NH1	2.29	0.66
1:B:24:PHE:CZ	1:B:32:LYS:HG3	2.31	0.66
1:A:46:LYS:CD	1:A:47:ILE:H	2.06	0.65
1:A:251:ILE:HD13	1:A:272:LEU:HD23	1.78	0.65
1:B:99:ARG:NH2	4:B:481:HOH:O	2.29	0.65
1:B:29:ARG:NH2	1:B:374:ARG:O	2.29	0.65
1:A:78:GLU:OE1	1:A:81:ARG:NH2	2.29	0.65
1:B:187:LEU:HD12	1:B:188:PHE:N	2.12	0.65
1:B:321:GLN:NE2	1:B:325:ASP:OD1	2.30	0.65
1:A:18:LEU:CD1	1:A:37:ILE:HD12	2.27	0.65
1:A:162:ASP:OD2	1:A:165:ASN:ND2	2.30	0.65
1:B:21:ALA:O	1:B:25:ARG:HD2	1.97	0.65
1:A:99:ARG:NH2	4:A:476:HOH:O	2.30	0.64
1:A:29:ARG:HG3	4:A:571:HOH:O	1.98	0.64
1:B:27:ASP:OD2	1:B:29:ARG:NH1	2.29	0.64
1:B:81:ARG:NH1	4:B:641:HOH:O	2.31	0.63
1:A:398:ALA:HB3	1:A:399:PRO:HD3	1.79	0.63
1:A:37:ILE:HG23	1:A:39:LEU:HD22	1.79	0.63
1:A:126:LYS:HE2	1:A:129:ARG:HH12	1.63	0.63
1:B:46:LYS:O	1:B:48:PRO:HD3	1.97	0.63
1:B:43:GLU:CD	1:B:43:GLU:H	2.01	0.63
1:B:332:ARG:HD2	4:B:547:HOH:O	1.98	0.62
1:B:29:ARG:HG3	1:B:29:ARG:NH1	2.08	0.62
1:B:344:LYS:NZ	1:B:402:GLU:OE2	2.30	0.62
1:B:393:THR:HB	1:B:394:PRO:HD2	1.79	0.62
1:A:136:SER:O	1:A:139:SER:HB3	1.99	0.62
1:B:99:ARG:HG2	1:B:274:ALA:O	1.99	0.62
1:B:201:THR:HG21	4:B:510:HOH:O	1.99	0.61
1:B:46:LYS:HD2	1:B:47:ILE:HG13	1.82	0.61
1:B:241:ARG:CG	1:B:241:ARG:HH11	2.13	0.61
1:A:366:THR:HG22	1:A:369:GLN:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ARG:HH11	1:B:241:ARG:HG3	1.65	0.61
1:B:348:ARG:HG2	1:B:348:ARG:NH1	2.14	0.61
1:A:340:THR:O	1:A:344:LYS:HB2	2.01	0.60
1:B:348:ARG:HH11	1:B:348:ARG:CG	2.13	0.60
1:B:389:VAL:O	1:B:392:MET:HG3	2.02	0.60
1:B:372:ARG:O	1:B:376:GLU:HB3	2.01	0.60
1:B:29:ARG:HH11	1:B:29:ARG:CG	2.08	0.59
1:A:121:LYS:HB3	1:A:121:LYS:HZ2	1.68	0.59
1:B:376:GLU:HG2	1:B:377:PHE:CE1	2.37	0.59
1:A:129:ARG:CD	1:A:156:ARG:HG3	2.33	0.58
1:A:398:ALA:O	1:A:402:GLU:HG3	2.03	0.58
1:B:5:MET:N	1:B:7:GLU:OE1	2.36	0.58
1:B:229:ALA:HB3	1:B:236:ASP:OD1	2.04	0.58
1:B:337:PHE:HD1	1:B:397:MET:HE2	1.68	0.58
1:A:318:ILE:O	1:A:322:GLU:HG3	2.04	0.58
1:B:58:GLN:O	1:B:62:GLU:HG3	2.04	0.58
1:A:397:MET:HA	1:A:397:MET:CE	2.34	0.58
1:B:101:ARG:HG3	1:B:101:ARG:HH11	1.67	0.58
1:B:265:GLU:HB3	4:B:601:HOH:O	2.03	0.57
1:A:154:GLU:OE2	1:A:156:ARG:HD2	2.05	0.57
1:A:201:THR:OG1	1:A:204:GLN:HG3	2.05	0.57
1:A:46:LYS:O	1:A:48:PRO:HD3	2.05	0.57
1:A:366:THR:HB	1:A:369:GLN:OE1	2.05	0.56
1:B:46:LYS:HD2	1:B:47:ILE:N	2.19	0.56
1:A:248:LYS:HD2	1:A:275:ALA:CB	2.36	0.56
1:B:101:ARG:HG3	1:B:101:ARG:NH1	2.21	0.56
1:A:211:LEU:O	1:A:214:GLU:N	2.40	0.55
1:B:173:LEU:O	1:B:176:SER:HB2	2.07	0.55
1:B:237:ALA:HB1	1:B:241:ARG:NH1	2.21	0.55
1:A:397:MET:HE3	1:A:400:LEU:CD2	2.35	0.55
1:B:170:PHE:CE2	1:B:174:ILE:HD11	2.42	0.55
1:A:123:THR:HB	4:B:412:HOH:O	2.06	0.55
1:B:24:PHE:CZ	1:B:34:ASN:HB2	2.42	0.55
1:B:359:MET:CE	4:B:456:HOH:O	2.44	0.55
1:A:220:LEU:HG	1:A:251:ILE:HB	1.89	0.54
1:B:327:ARG:O	1:B:331:GLN:HG3	2.07	0.54
1:A:126:LYS:NZ	1:A:154:GLU:OE1	2.35	0.54
1:A:248:LYS:CD	1:A:275:ALA:HB2	2.38	0.54
1:B:389:VAL:HG22	1:B:392:MET:CE	2.38	0.53
1:A:165:ASN:N	1:A:165:ASN:ND2	2.53	0.53
1:B:324:THR:HG21	4:B:529:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ALA:N	1:A:399:PRO:HD2	2.23	0.52
1:B:230:ARG:NH2	1:B:235:GLU:HB2	2.24	0.52
1:B:397:MET:CE	1:B:400:LEU:HD22	2.39	0.52
1:B:144:LYS:HD2	1:B:148:ASN:OD1	2.10	0.52
1:B:129:ARG:HD3	1:B:154:GLU:OE2	2.10	0.52
1:B:179:GLU:O	1:B:179:GLU:HG3	2.08	0.52
1:A:248:LYS:HD2	1:A:275:ALA:HB2	1.92	0.52
1:B:28:GLU:OE1	1:B:28:GLU:HA	2.09	0.52
1:A:61:LEU:HD12	1:B:61:LEU:HD12	1.92	0.51
1:B:332:ARG:NH2	4:B:606:HOH:O	2.30	0.51
1:B:210:GLN:HA	1:B:246:MET:CE	2.40	0.51
1:B:212:SER:HB2	1:B:217:TRP:HE3	1.75	0.51
1:B:389:VAL:HG22	1:B:392:MET:HE2	1.92	0.51
1:A:126:LYS:HE2	1:A:129:ARG:CZ	2.40	0.51
1:A:76:ILE:O	1:A:79:PHE:HB3	2.09	0.51
1:A:33:ILE:CD1	1:A:396:ASN:HB2	2.41	0.50
1:A:278:GLU:O	1:A:278:GLU:HG2	2.11	0.50
1:B:53:VAL:O	1:B:56:ALA:HB3	2.11	0.50
1:B:133:VAL:HB	1:B:185:VAL:CG2	2.41	0.50
1:B:170:PHE:O	1:B:173:LEU:HB3	2.12	0.50
1:B:321:GLN:HB2	4:B:625:HOH:O	2.10	0.50
1:B:37:ILE:HG23	1:B:39:LEU:HD22	1.94	0.50
1:B:367:LYS:HE3	1:B:383:ALA:O	2.12	0.49
1:A:264:ASN:C	1:A:264:ASN:HD22	2.14	0.48
1:B:389:VAL:HA	1:B:392:MET:HE2	1.95	0.48
1:B:398:ALA:N	1:B:399:PRO:HD2	2.28	0.48
1:A:350:PHE:HB3	1:A:353:ILE:HD12	1.95	0.48
1:B:331:GLN:NE2	4:B:548:HOH:O	2.43	0.48
1:A:12:ALA:HB2	1:B:286:GLN:NE2	2.29	0.48
1:B:349:ASP:OD1	1:B:351:SER:OG	2.31	0.48
1:B:83:THR:HG22	1:B:87:LEU:HD22	1.95	0.47
1:A:366:THR:HG22	1:A:369:GLN:CB	2.44	0.47
1:B:113:ARG:HA	1:B:113:ARG:HD3	1.75	0.47
1:B:56:ALA:O	1:B:59:TYR:HB3	2.14	0.47
1:B:201:THR:HG23	1:B:204:GLN:CG	2.45	0.47
1:A:5:MET:N	1:A:7:GLU:OE1	2.48	0.47
1:B:51:THR:HG21	4:B:589:HOH:O	2.14	0.47
1:B:237:ALA:CB	1:B:241:ARG:NH1	2.78	0.47
1:B:37:ILE:N	4:B:563:HOH:O	2.29	0.47
1:B:318:ILE:O	1:B:322:GLU:HG3	2.14	0.47
1:B:101:ARG:HD2	1:B:101:ARG:HA	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ALA:HB3	1:A:236:ASP:OD1	2.15	0.46
1:B:389:VAL:HA	1:B:392:MET:HG3	1.98	0.46
1:A:146:VAL:HG23	1:A:147:PHE:N	2.31	0.46
1:B:74:ASP:N	1:B:74:ASP:OD1	2.42	0.46
1:B:212:SER:CB	1:B:217:TRP:HE3	2.29	0.46
1:B:332:ARG:HB2	4:B:586:HOH:O	2.15	0.46
1:A:29:ARG:O	1:A:32:LYS:HG2	2.16	0.46
1:B:101:ARG:HH11	1:B:101:ARG:CG	2.29	0.45
1:B:332:ARG:NE	4:B:586:HOH:O	2.46	0.45
1:A:398:ALA:HB3	1:A:399:PRO:CD	2.45	0.45
1:B:83:THR:O	1:B:87:LEU:HB2	2.17	0.45
1:B:158:TYR:CD1	1:B:173:LEU:CD1	3.00	0.45
1:B:389:VAL:CB	1:B:392:MET:HE2	2.46	0.45
1:A:24:PHE:HD1	1:A:380:TYR:CG	2.34	0.45
1:A:212:SER:OG	1:A:247:HIS:NE2	2.49	0.45
1:B:135:VAL:O	1:B:157:GLU:HA	2.17	0.45
1:B:162:ASP:O	1:B:166:HIS:N	2.50	0.45
1:A:337:PHE:HD1	1:A:397:MET:HE1	1.82	0.45
1:B:220:LEU:HD13	1:B:251:ILE:CG2	2.46	0.45
1:A:158:TYR:CD1	1:A:173:LEU:HD21	2.52	0.45
1:A:396:ASN:O	1:A:399:PRO:HD2	2.16	0.45
1:B:348:ARG:HD3	4:B:617:HOH:O	2.15	0.45
1:A:126:LYS:O	1:A:126:LYS:HG2	2.17	0.44
1:A:187:LEU:C	1:A:187:LEU:HD23	2.38	0.44
1:B:170:PHE:CE2	1:B:174:ILE:CD1	3.00	0.44
1:A:18:LEU:HD13	3:A:411:HCI:C5'	2.47	0.44
1:A:47:ILE:HG13	1:B:69:LEU:HD21	1.99	0.44
1:B:200:PRO:HG2	1:B:205:TRP:CZ2	2.53	0.44
1:A:121:LYS:HB3	1:A:121:LYS:HZ3	1.78	0.44
1:A:212:SER:HB2	1:A:217:TRP:HE3	1.82	0.44
1:B:47:ILE:HA	1:B:48:PRO:HD2	1.82	0.44
1:A:8:ASN:N	1:A:8:ASN:OD1	2.36	0.44
1:A:158:TYR:CD1	1:A:173:LEU:CD2	3.01	0.44
1:A:366:THR:HG23	1:A:368:GLU:H	1.82	0.44
1:A:69:LEU:O	1:B:264:ASN:HB3	2.18	0.44
1:B:329:ARG:NH1	1:B:329:ARG:HG2	2.32	0.44
1:A:9:ILE:HD13	1:B:122:ASN:HB3	1.99	0.43
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.47	0.43
1:A:41:TYR:CZ	1:A:47:ILE:HD11	2.53	0.43
1:A:194:ASN:HA	1:A:195:PRO:HA	1.81	0.43
1:B:158:TYR:CD1	1:B:173:LEU:HD13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LYS:CD	1:B:402:GLU:HG2	2.48	0.43
1:A:335:GLN:H	1:A:335:GLN:HG2	1.56	0.43
1:A:367:LYS:H	1:A:367:LYS:HG2	1.58	0.43
1:A:398:ALA:N	1:A:399:PRO:CD	2.81	0.43
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.61	0.43
1:A:349:ASP:CG	1:A:351:SER:HG	2.22	0.43
1:B:27:ASP:OD1	1:B:27:ASP:N	2.48	0.43
1:B:332:ARG:HG2	1:B:333:MET:CE	2.49	0.43
1:B:398:ALA:N	1:B:399:PRO:CD	2.82	0.43
1:A:56:ALA:O	1:A:59:TYR:HB3	2.19	0.43
1:B:201:THR:HG22	4:B:618:HOH:O	2.18	0.43
1:A:24:PHE:CZ	1:A:34:ASN:HB2	2.54	0.43
1:B:86:LEU:HA	1:B:86:LEU:HD23	1.75	0.43
1:B:129:ARG:HD3	1:B:154:GLU:CD	2.38	0.43
1:B:210:GLN:NE2	1:B:214:GLU:OE2	2.52	0.43
1:B:324:THR:HG22	4:B:479:HOH:O	2.19	0.43
1:A:397:MET:HE2	1:A:397:MET:O	2.19	0.43
1:B:294:ASN:C	1:B:294:ASN:HD22	2.23	0.43
1:A:20:LEU:HD23	1:A:20:LEU:HA	1.82	0.42
1:A:7:GLU:O	1:B:282:ARG:NH2	2.52	0.42
1:A:167:THR:OG1	1:A:168:LEU:N	2.52	0.42
1:A:212:SER:HB2	1:A:217:TRP:CE3	2.54	0.42
1:B:133:VAL:HA	1:B:185:VAL:HG23	2.00	0.42
1:A:323:LEU:HD12	1:A:326:MET:HE3	2.00	0.42
1:A:15:ASP:HA	1:A:16:PRO:HD3	1.92	0.42
1:A:189:HIS:CD2	1:A:194:ASN:H	2.37	0.42
1:B:340:THR:O	1:B:344:LYS:HG3	2.20	0.42
1:B:46:LYS:C	1:B:48:PRO:HD3	2.40	0.42
1:A:17:ILE:O	1:A:20:LEU:HB2	2.19	0.42
1:B:348:ARG:H	1:B:348:ARG:HG3	1.48	0.42
1:B:356:GLN:OE1	1:B:361:SER:HA	2.19	0.42
1:B:144:LYS:HD2	4:B:629:HOH:O	2.19	0.42
1:B:177:LEU:HD23	1:B:177:LEU:HA	1.85	0.42
1:A:143:HIS:O	1:A:147:PHE:HD2	2.03	0.41
1:A:348:ARG:H	1:A:348:ARG:HG2	1.60	0.41
1:B:78:GLU:O	1:B:78:GLU:HG3	2.20	0.41
1:B:210:GLN:HA	1:B:246:MET:HE2	2.02	0.41
1:B:15:ASP:HA	1:B:16:PRO:HD3	1.88	0.41
1:B:98:LYS:HE2	1:B:98:LYS:CA	2.36	0.41
1:B:374:ARG:NH1	4:B:649:HOH:O	2.52	0.41
1:B:397:MET:HE3	1:B:400:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LYS:HD3	1:B:402:GLU:HG2	2.03	0.41
1:A:331:GLN:O	1:A:335:GLN:HG2	2.20	0.41
1:A:348:ARG:CZ	1:A:409:LEU:HD22	2.50	0.41
1:A:371:LEU:HD12	1:A:371:LEU:O	2.21	0.41
1:A:29:ARG:HA	1:A:30:PRO:HD2	1.82	0.41
1:A:98:LYS:HD2	4:A:464:HOH:O	2.19	0.41
1:B:359:MET:HB2	1:B:359:MET:HE2	1.96	0.41
1:A:46:LYS:CG	1:A:47:ILE:N	2.84	0.41
1:B:187:LEU:HD12	1:B:187:LEU:C	2.40	0.41
1:B:210:GLN:HG3	1:B:214:GLU:OE2	2.21	0.41
1:B:334:ARG:NH2	1:B:358:GLY:O	2.54	0.41
1:A:345:GLY:O	1:A:346:ALA:C	2.58	0.41
1:B:212:SER:CB	1:B:217:TRP:CE3	3.04	0.41
1:B:334:ARG:HB3	1:B:389:VAL:HG11	2.03	0.41
1:B:393:THR:HA	1:B:394:PRO:HD3	1.85	0.41
1:A:78:GLU:CD	1:A:81:ARG:HH21	2.24	0.41
1:A:160:TYR:O	1:A:168:LEU:HD23	2.21	0.41
1:A:81:ARG:HH11	1:A:81:ARG:HD3	1.72	0.40
1:B:170:PHE:CE1	1:B:204:GLN:HB3	2.55	0.40
1:A:9:ILE:CG2	1:B:286:GLN:HG3	2.51	0.40
1:B:125:VAL:CG1	1:B:185:VAL:HG22	2.52	0.40
1:A:393:THR:HB	1:A:394:PRO:CD	2.49	0.40
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.82	0.40
1:B:152:LEU:HA	1:B:152:LEU:HD12	1.65	0.40
1:B:339:ASN:HD22	1:B:339:ASN:HA	1.60	0.40
1:B:213:VAL:HG21	1:B:246:MET:HB3	2.02	0.40
1:A:83:THR:O	1:A:87:LEU:HB2	2.21	0.40
1:A:99:ARG:HD2	1:A:274:ALA:O	2.21	0.40
1:B:194:ASN:HA	1:B:195:PRO:HA	1.83	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%)	369 (94%)	22 (6%)	3 (1%)	19 13
1	B	394/396 (100%)	369 (94%)	21 (5%)	4 (1%)	15 9
All	All	788/792 (100%)	738 (94%)	43 (6%)	7 (1%)	17 11

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	69	LEU
1	B	233	LEU
1	A	90	LYS
1	B	301	HIS
1	A	69	LEU
1	A	301	HIS
1	B	36	GLY

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%)	259 (81%)	61 (19%)	1 0
1	B	320/320 (100%)	253 (79%)	67 (21%)	1 0
All	All	640/640 (100%)	512 (80%)	128 (20%)	1 0

All (128) 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	23	LEU
1	A	28	GLU
1	A	32	LYS
1	A	33	ILE
1	A	39	LEU
1	A	46	LYS

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Mol	Chain	Res	Type
1	A	58	GLN
1	A	61	LEU
1	A	69	LEU
1	A	78	GLU
1	A	87	LEU
1	A	90	LYS
1	A	92	SER
1	A	98	LYS
1	A	112	LEU
1	A	119	LEU
1	A	121	LYS
1	A	126	LYS
1	A	129	ARG
1	A	144	LYS
1	A	152	LEU
1	A	156	ARG
1	A	162	ASP
1	A	165	ASN
1	A	168	LEU
1	A	174	ILE
1	A	178	ASN
1	A	202	LEU
1	A	206	GLN
1	A	212	SER
1	A	215	LYS
1	A	218	LEU
1	A	223	PHE
1	A	240	LEU
1	A	248	LYS
1	A	250	LEU
1	A	259	ASN
1	A	264	ASN
1	A	272	LEU
1	A	292	ARG
1	A	312	ASN
1	A	331	GLN
1	A	334	ARG
1	A	335	GLN
1	A	338	VAL
1	A	341	LEU
1	A	344	LYS
1	A	347	ASN

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Mol	Chain	Res	Type
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	388	ASN
1	A	400	LEU
1	B	5	MET
1	B	8	ASN
1	B	10	THR
1	B	23	LEU
1	B	25	ARG
1	B	27	ASP
1	B	29	ARG
1	B	32	LYS
1	B	39	LEU
1	B	43	GLU
1	B	46	LYS
1	B	51	THR
1	B	55	LYS
1	B	61	LEU
1	B	62	GLU
1	B	69	LEU
1	B	81	ARG
1	B	86	LEU
1	B	87	LEU
1	B	90	LYS
1	B	98	LYS
1	B	99	ARG
1	B	101	ARG
1	B	113	ARG
1	B	119	LEU
1	B	121	LYS
1	B	126	LYS
1	B	129	ARG
1	B	133	VAL
1	B	139	SER
1	B	144	LYS
1	B	152	LEU

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Mol	Chain	Res	Type
1	B	156	ARG
1	B	162	ASP
1	B	167	THR
1	B	168	LEU
1	B	185	VAL
1	B	187	LEU
1	B	206	GLN
1	B	215	LYS
1	B	223	PHE
1	B	233	LEU
1	B	240	LEU
1	B	248	LYS
1	B	259	ASN
1	B	273	VAL
1	B	276	ASP
1	B	294	ASN
1	B	304	SER
1	B	324	THR
1	B	332	ARG
1	B	341	LEU
1	B	342	GLN
1	B	343	GLU
1	B	348	ARG
1	B	351	SER
1	B	354	ILE
1	B	355	LYS
1	B	361	SER
1	B	367	LYS
1	B	368	GLU
1	B	371	LEU
1	B	372	ARG
1	B	373	LEU
1	B	374	ARG
1	B	375	GLU
1	B	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	142	ASN
1	A	165	ASN

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Mol	Chain	Res	Type
1	A	189	HIS
1	A	206	GLN
1	A	226	GLN
1	A	259	ASN
1	A	264	ASN
1	A	312	ASN
1	A	328	GLN
1	A	357	ASN
1	A	388	ASN
1	B	63	ASN
1	B	84	GLN
1	B	96	ASN
1	B	206	GLN
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

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	HCI	B	411	-	8,11,11	0.59	0	10,13,13	1.21	1 (10%)
3	HCI	A	411	-	8,11,11	0.66	0	10,13,13	0.72	0
2	PLP	A	410	1	15,15,16	1.35	3 (20%)	20,22,23	2.07	8 (40%)
2	PLP	B	410	1	15,15,16	1.66	3 (20%)	20,22,23	1.81	7 (35%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	410	PLP	C5-C4	4.57	1.45	1.40
2	A	410	PLP	C5-C4	2.98	1.43	1.40
2	B	410	PLP	C3-C2	2.60	1.43	1.40
2	A	410	PLP	C3-C2	2.55	1.43	1.40
2	A	410	PLP	C4A-C4	-2.48	1.46	1.51
2	B	410	PLP	C5A-C5	2.06	1.56	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	410	PLP	C6-C5-C4	4.97	122.07	118.16
2	B	410	PLP	C3-C4-C5	-3.11	115.38	118.74
2	A	410	PLP	C3-C4-C5	-3.02	115.48	118.74
2	A	410	PLP	C2A-C2-C3	2.86	124.42	120.89
2	A	410	PLP	C5-C6-N1	-2.84	119.09	123.82
2	B	410	PLP	C3-C2-N1	-2.82	117.13	120.77
2	B	410	PLP	C6-N1-C2	2.59	123.96	119.17
2	A	410	PLP	C6-N1-C2	2.59	123.96	119.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	410	PLP	C6-C5-C4	2.57	120.18	118.16
2	B	410	PLP	C5-C6-N1	-2.39	119.83	123.82
2	B	410	PLP	C2A-C2-C3	2.36	123.80	120.89
3	B	411	HCI	C5'-C6'-C1'	2.32	124.19	120.63
2	A	410	PLP	O3P-P-O1P	2.27	119.55	110.68
2	B	410	PLP	C4A-C4-C5	2.19	123.19	120.94
2	A	410	PLP	C3-C2-N1	-2.11	118.04	120.77
2	A	410	PLP	O4P-C5A-C5	2.07	113.30	109.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	410	PLP	C4-C5-C5A-O4P
2	A	410	PLP	C6-C5-C5A-O4P
2	B	410	PLP	C6-C5-C5A-O4P
2	B	410	PLP	C5A-O4P-P-O1P
2	B	410	PLP	C5A-O4P-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section 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.