



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:31 am GMT

PDB ID : 1AHY
Title : ASPARTATE AMINOTRANSFERASE HEXAMUTANT
Authors : Malashkevich, V.N.; Jansonius, J.N.
Deposited on : 1995-02-21
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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

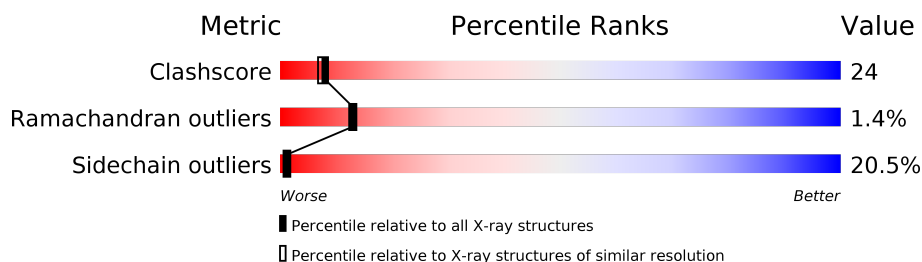
1 Overall quality at a glance

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	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (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	 53% 32% 14% .
1	B	396	 56% 30% 12% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6710 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:

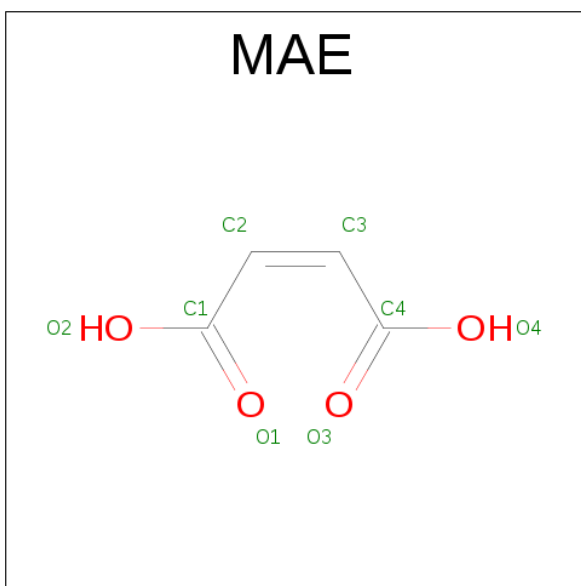
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LEU	VAL	CONFLICT	UNP P00509
A	41	TYR	LYS	CONFLICT	UNP P00509
A	47	ILE	THR	CONFLICT	UNP P00509
A	69	LEU	ASN	CONFLICT	UNP P00509
A	109	SER	THR	CONFLICT	UNP P00509
A	297	SER	ASN	CONFLICT	UNP P00509
B	39	LEU	VAL	CONFLICT	UNP P00509
B	41	TYR	LYS	CONFLICT	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 PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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

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



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

- Molecule 4 is water.

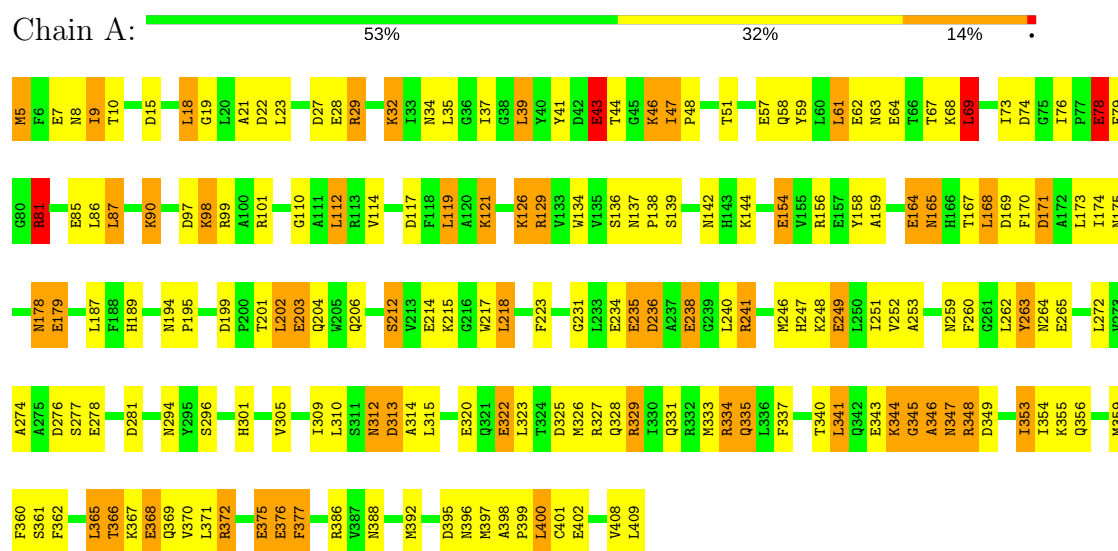
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	285	Total 285	O 285	0	0
4	B	237	Total 237	O 237	0	0

3 Residue-property plots

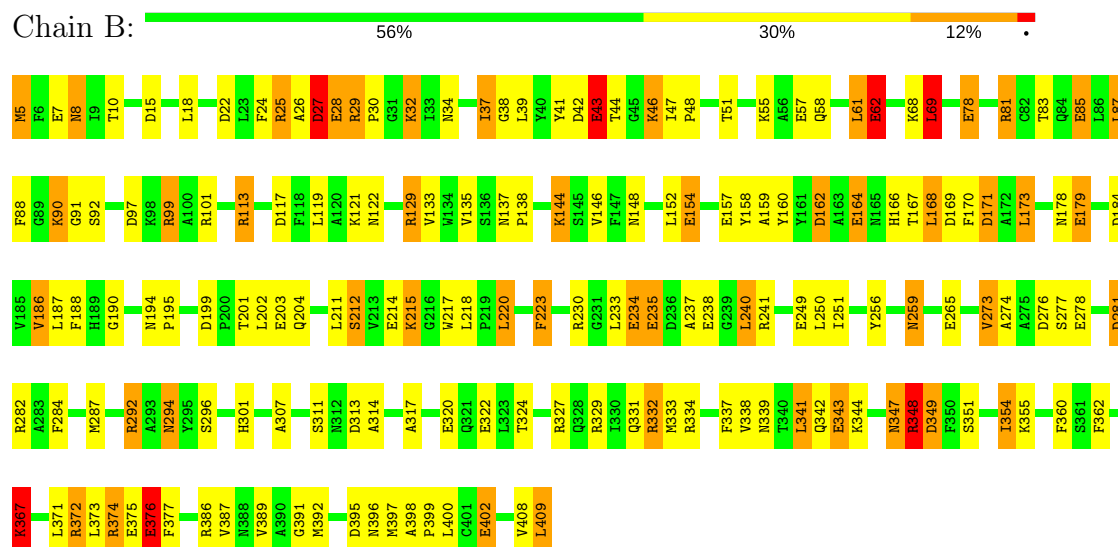
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.93Å 79.09Å 89.72Å 90.00° 118.70° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	90.5 (8.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.207 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6710	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.94	27/3133 (0.9%)	1.21	33/4244 (0.8%)
1	B	0.97	24/3133 (0.8%)	1.24	31/4244 (0.7%)
All	All	0.96	51/6266 (0.8%)	1.22	64/8488 (0.8%)

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	367	LYS	C-N	8.02	1.52	1.34
1	A	320	GLU	CD-OE1	7.50	1.33	1.25
1	B	320	GLU	CD-OE1	7.21	1.33	1.25
1	A	179	GLU	CD-OE2	7.21	1.33	1.25
1	A	322	GLU	CD-OE2	6.94	1.33	1.25
1	B	203	GLU	CD-OE2	6.84	1.33	1.25
1	A	43	GLU	CD-OE1	6.83	1.33	1.25
1	A	278	GLU	CD-OE1	6.71	1.33	1.25
1	B	214	GLU	CD-OE2	6.70	1.33	1.25
1	B	343	GLU	CD-OE2	6.63	1.32	1.25
1	A	235	GLU	CD-OE2	6.53	1.32	1.25
1	A	375	GLU	CD-OE1	6.46	1.32	1.25
1	A	78	GLU	CD-OE2	6.41	1.32	1.25
1	A	345	GLY	C-N	-6.39	1.19	1.34
1	B	28	GLU	CD-OE1	6.38	1.32	1.25
1	B	367	LYS	CA-C	-6.38	1.36	1.52
1	B	235	GLU	CD-OE2	6.37	1.32	1.25
1	A	62	GLU	CD-OE2	6.37	1.32	1.25
1	B	78	GLU	CD-OE1	6.31	1.32	1.25
1	B	375	GLU	CD-OE2	6.17	1.32	1.25
1	A	376	GLU	CD-OE2	6.16	1.32	1.25
1	B	43	GLU	CD-OE1	6.15	1.32	1.25
1	B	238	GLU	CD-OE2	6.12	1.32	1.25
1	A	154	GLU	CD-OE2	6.04	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	402	GLU	CD-OE2	6.02	1.32	1.25
1	B	164	GLU	CD-OE2	6.01	1.32	1.25
1	B	278	GLU	CD-OE2	6.01	1.32	1.25
1	B	234	GLU	CD-OE2	5.97	1.32	1.25
1	A	28	GLU	CD-OE1	5.96	1.32	1.25
1	A	214	GLU	CD-OE1	5.96	1.32	1.25
1	A	238	GLU	CD-OE2	5.90	1.32	1.25
1	B	62	GLU	CD-OE1	5.88	1.32	1.25
1	B	249	GLU	CD-OE2	5.85	1.32	1.25
1	A	402	GLU	CD-OE2	5.84	1.32	1.25
1	A	343	GLU	CD-OE2	5.83	1.32	1.25
1	A	85	GLU	CD-OE1	5.81	1.32	1.25
1	A	368	GLU	CD-OE1	5.79	1.32	1.25
1	B	179	GLU	CD-OE2	5.69	1.31	1.25
1	B	376	GLU	CD-OE2	5.61	1.31	1.25
1	A	164	GLU	CD-OE2	5.48	1.31	1.25
1	A	203	GLU	CD-OE2	5.48	1.31	1.25
1	A	249	GLU	CD-OE2	5.47	1.31	1.25
1	B	57	GLU	CD-OE2	5.45	1.31	1.25
1	A	64	GLU	CD-OE2	5.34	1.31	1.25
1	A	7	GLU	CD-OE2	5.26	1.31	1.25
1	A	265	GLU	CD-OE1	5.24	1.31	1.25
1	A	57	GLU	CD-OE2	5.21	1.31	1.25
1	B	154	GLU	CD-OE1	5.09	1.31	1.25
1	A	234	GLU	CD-OE1	5.08	1.31	1.25
1	B	322	GLU	CD-OE2	5.01	1.31	1.25
1	B	265	GLU	CD-OE1	5.01	1.31	1.25

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ASP	CB-CG-OD1	-8.20	110.92	118.30
1	A	360	PHE	CB-CA-C	-7.92	94.57	110.40
1	A	97	ASP	CB-CG-OD1	-7.75	111.32	118.30
1	B	15	ASP	CB-CG-OD1	-7.70	111.37	118.30
1	A	169	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	B	97	ASP	CB-CG-OD1	-7.40	111.64	118.30
1	A	15	ASP	CB-CG-OD2	-7.24	111.79	118.30
1	B	171	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	A	22	ASP	CB-CG-OD1	-7.00	112.00	118.30
1	B	69	LEU	CB-CA-C	-6.94	97.01	110.20
1	B	367	LYS	O-C-N	6.92	133.77	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	395	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	A	117	ASP	CB-CG-OD1	-6.68	112.29	118.30
1	B	22	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	A	74	ASP	CB-CG-OD1	6.48	124.14	118.30
1	B	349	ASP	CB-CG-OD1	-6.42	112.53	118.30
1	B	281	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	A	349	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	15	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	313	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	B	169	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	276	ASP	CB-CG-OD2	-6.21	112.72	118.30
1	B	162	ASP	CB-CG-OD2	-6.18	112.73	118.30
1	A	22	ASP	CB-CG-OD2	6.09	123.79	118.30
1	B	27	ASP	CB-CG-OD1	-6.06	112.85	118.30
1	B	313	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	B	276	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	313	ASP	CB-CG-OD1	5.95	123.66	118.30
1	A	74	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	A	97	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	169	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	97	ASP	CB-CG-OD2	5.85	123.56	118.30
1	B	276	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	117	ASP	CB-CG-OD2	5.83	123.54	118.30
1	B	15	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	360	PHE	N-CA-C	5.79	126.64	111.00
1	B	349	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	395	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	B	184	ASP	CB-CG-OD1	-5.71	113.17	118.30
1	A	334	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	B	91	GLY	O-C-N	5.68	131.78	122.70
1	B	292	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	B	395	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	117	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	B	162	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	241	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	313	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	81	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	B	281	ASP	CB-CG-OD1	5.25	123.02	118.30
1	B	27	ASP	N-CA-CB	5.24	120.04	110.60
1	A	199	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	A	236	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	171	ASP	CB-CG-OD2	5.18	122.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	46	LYS	N-CA-CB	5.18	119.92	110.60
1	A	276	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	199	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	A	27	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	27	ASP	CB-CG-OD1	5.09	122.89	118.30
1	A	325	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	236	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	B	22	ASP	CB-CG-OD1	5.04	122.83	118.30
1	A	359	MET	CG-SD-CE	5.03	108.25	100.20
1	B	129	ARG	NE-CZ-NH2	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3071	0	3019	162	0
1	B	3071	0	3020	142	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
3	A	8	0	2	0	0
3	B	8	0	2	0	0
4	A	285	0	0	20	0
4	B	237	0	0	18	0
All	All	6710	0	6055	290	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 (290) 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:366:THR:HG22	1:A:369:GLN:H	1.16	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HG13	1:B:69:LEU:HD21	1.38	1.03
1:B:29:ARG:HH11	1:B:29:ARG:HG3	1.23	1.03
1:A:347:ASN:HD21	1:A:409:LEU:HB3	1.28	0.97
1:A:165:ASN:H	1:A:165:ASN:HD22	0.96	0.95
1:B:187:LEU:HD12	1:B:188:PHE:N	1.87	0.90
1:B:347:ASN:HB2	1:B:409:LEU:HD12	1.55	0.89
1:A:165:ASN:H	1:A:165:ASN:ND2	1.74	0.85
1:B:24:PHE:CE1	1:B:34:ASN:HB2	2.13	0.84
1:A:397:MET:HE3	1:A:400:LEU:HD23	1.60	0.83
1:B:46:LYS:HG3	1:B:47:ILE:H	1.44	0.83
1:A:165:ASN:N	1:A:165:ASN:HD22	1.72	0.80
1:A:366:THR:HG22	1:A:369:GLN:N	1.97	0.79
1:B:337:PHE:HD1	1:B:397:MET:HE2	1.48	0.78
1:B:348:ARG:HH11	1:B:348:ARG:HG2	1.49	0.78
1:A:398:ALA:HB3	1:A:399:PRO:HD3	1.67	0.77
1:B:42:ASP:HB2	1:B:43:GLU:OE2	1.84	0.76
1:A:46:LYS:HB3	4:A:570:HOH:O	1.85	0.76
1:A:47:ILE:HG13	1:B:69:LEU:CD2	2.16	0.76
1:B:27:ASP:O	1:B:32:LYS:HE3	1.86	0.75
1:B:347:ASN:HB2	1:B:409:LEU:CD1	2.16	0.75
1:A:335:GLN:HA	1:A:354:ILE:HD11	1.70	0.74
1:A:154:GLU:OE2	1:A:156:ARG:HD2	1.88	0.74
1:A:8:ASN:HB3	4:A:688:HOH:O	1.88	0.72
1:A:366:THR:HG23	1:A:368:GLU:H	1.55	0.71
1:A:366:THR:HG21	4:A:590:HOH:O	1.89	0.71
1:A:46:LYS:O	1:A:48:PRO:HD3	1.90	0.71
1:A:129:ARG:HD2	1:A:134:TRP:NE1	2.06	0.70
1:A:90:LYS:HG2	4:A:540:HOH:O	1.90	0.70
1:B:327:ARG:O	1:B:331:GLN:HG3	1.92	0.69
1:A:327:ARG:HG2	1:A:331:GLN:HE21	1.58	0.69
1:A:335:GLN:HB3	4:A:639:HOH:O	1.95	0.67
1:A:347:ASN:OD1	1:A:348:ARG:HG2	1.94	0.66
1:A:329:ARG:NH2	1:A:392:MET:O	2.29	0.66
1:B:113:ARG:NH2	4:B:412:HOH:O	2.29	0.66
1:B:337:PHE:HB2	1:B:392:MET:HE3	1.77	0.66
1:B:397:MET:CE	1:B:400:LEU:HD22	2.25	0.66
1:B:218:LEU:HD13	4:B:512:HOH:O	1.95	0.66
1:A:347:ASN:ND2	1:A:409:LEU:HB3	2.07	0.66
1:A:129:ARG:HB3	1:A:129:ARG:CZ	2.27	0.65
1:B:87:LEU:O	1:B:241:ARG:NH1	2.29	0.65
1:A:101:ARG:NH1	1:A:281:ASP:OD1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ARG:NH1	1:B:376:GLU:OE2	2.30	0.65
1:A:121:LYS:NZ	1:A:121:LYS:O	2.30	0.65
1:A:99:ARG:NH2	4:A:546:HOH:O	2.30	0.65
1:A:328:GLN:NE2	4:A:636:HOH:O	2.29	0.65
1:B:348:ARG:HH11	1:B:348:ARG:CG	2.11	0.64
1:A:397:MET:HE3	1:A:400:LEU:CD2	2.27	0.63
1:B:29:ARG:NH2	1:B:374:ARG:O	2.31	0.63
1:A:129:ARG:HD2	1:A:134:TRP:HE1	1.61	0.63
1:A:59:TYR:O	1:A:63:ASN:ND2	2.30	0.63
1:B:332:ARG:HG2	1:B:333:MET:HE3	1.81	0.63
1:A:372:ARG:NE	1:A:376:GLU:OE2	2.29	0.63
1:B:29:ARG:NH1	1:B:29:ARG:HG3	2.03	0.62
1:B:398:ALA:N	1:B:399:PRO:HD2	2.14	0.62
1:B:46:LYS:CG	1:B:47:ILE:H	2.12	0.61
1:B:99:ARG:HG2	1:B:99:ARG:HH11	1.65	0.61
1:A:327:ARG:CG	1:A:331:GLN:HE21	2.13	0.61
1:B:190:GLY:HA3	1:B:223:PHE:CD1	2.36	0.61
1:A:78:GLU:HG2	4:A:474:HOH:O	2.00	0.61
1:B:43:GLU:CD	1:B:43:GLU:H	2.03	0.61
1:A:87:LEU:O	1:A:241:ARG:HD2	2.01	0.61
1:B:195:PRO:HB3	1:B:386:ARG:HD3	1.83	0.61
1:B:250:LEU:HD12	1:B:273:VAL:HG13	1.82	0.61
1:B:46:LYS:HG3	1:B:47:ILE:N	2.15	0.60
1:A:372:ARG:O	1:A:376:GLU:HB2	2.02	0.60
1:A:47:ILE:CG1	1:B:69:LEU:HD21	2.22	0.60
1:A:46:LYS:HG3	1:A:47:ILE:N	2.16	0.60
1:A:137:ASN:ND2	4:A:550:HOH:O	2.34	0.59
1:A:345:GLY:O	1:A:346:ALA:C	2.39	0.59
1:B:201:THR:OG1	1:B:204:GLN:HG3	2.02	0.59
1:B:99:ARG:HG2	1:B:274:ALA:O	2.03	0.59
1:A:366:THR:CG2	1:A:368:GLU:H	2.14	0.59
1:B:24:PHE:CZ	1:B:34:ASN:HB2	2.37	0.58
1:A:69:LEU:HD21	1:B:47:ILE:CD1	2.33	0.58
1:B:372:ARG:HD2	1:B:376:GLU:OE2	2.05	0.57
1:B:78:GLU:HA	1:B:78:GLU:OE1	2.05	0.57
1:A:212:SER:HB2	1:A:217:TRP:HE3	1.68	0.57
1:B:202:LEU:O	1:B:202:LEU:HD12	2.05	0.57
1:B:397:MET:HE1	1:B:400:LEU:HD22	1.86	0.56
1:A:398:ALA:HB3	1:A:399:PRO:CD	2.35	0.56
1:B:81:ARG:HG2	4:B:631:HOH:O	2.04	0.56
1:A:18:LEU:O	1:A:21:ALA:HB3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:SER:HB2	1:A:217:TRP:CE3	2.41	0.56
1:A:37:ILE:HB	4:A:605:HOH:O	2.05	0.56
1:A:337:PHE:HD1	1:A:397:MET:HE1	1.71	0.55
1:A:5:MET:HE3	4:B:458:HOH:O	2.06	0.55
1:A:312:ASN:HD21	1:A:314:ALA:HB3	1.70	0.55
1:B:5:MET:N	1:B:7:GLU:OE1	2.40	0.55
1:B:186:VAL:HG22	1:B:188:PHE:CE2	2.42	0.55
1:A:170:PHE:CE2	1:A:174:ILE:HD11	2.42	0.55
1:A:9:ILE:HD13	1:B:122:ASN:HB3	1.88	0.55
1:B:337:PHE:HD1	1:B:397:MET:CE	2.18	0.55
1:A:340:THR:O	1:A:344:LYS:HB2	2.06	0.54
1:A:69:LEU:HD21	1:B:47:ILE:HD12	1.89	0.54
1:B:28:GLU:OE1	1:B:28:GLU:HA	2.08	0.54
1:B:348:ARG:HG2	1:B:348:ARG:NH1	2.20	0.54
1:B:344:LYS:NZ	1:B:402:GLU:OE2	2.29	0.54
1:A:372:ARG:HG2	1:A:376:GLU:OE2	2.08	0.54
1:A:126:LYS:HE3	1:A:129:ARG:NH1	2.23	0.54
1:B:27:ASP:N	1:B:27:ASP:OD1	2.38	0.53
1:B:292:ARG:NH1	1:B:296:SER:OG	2.39	0.53
1:B:337:PHE:HB2	1:B:392:MET:CE	2.37	0.53
1:A:341:LEU:HD13	1:A:401:CYS:SG	2.48	0.53
1:B:27:ASP:OD2	1:B:29:ARG:NH1	2.41	0.53
1:B:314:ALA:O	1:B:317:ALA:HB3	2.07	0.53
1:A:263:TYR:HB2	1:B:68:LYS:O	2.09	0.53
1:B:398:ALA:H	1:B:399:PRO:HD2	1.74	0.53
1:B:58:GLN:O	1:B:62:GLU:HG3	2.09	0.53
1:A:189:HIS:CD2	1:A:194:ASN:H	2.27	0.52
1:A:175:ASN:O	1:A:178:ASN:HB2	2.09	0.52
1:B:376:GLU:HB3	1:B:377:PHE:CD1	2.45	0.52
1:A:158:TYR:CE1	1:A:173:LEU:HD21	2.45	0.52
1:B:212:SER:HB2	1:B:217:TRP:HE3	1.75	0.52
1:A:101:ARG:HD3	4:A:425:HOH:O	2.08	0.51
1:B:159:ALA:O	1:B:173:LEU:HB2	2.09	0.51
1:B:187:LEU:C	1:B:187:LEU:HD12	2.30	0.51
1:A:356:GLN:OE1	1:A:361:SER:HA	2.10	0.51
1:B:46:LYS:O	1:B:48:PRO:HD3	2.10	0.51
1:A:61:LEU:HD12	1:B:61:LEU:HD12	1.91	0.51
1:A:187:LEU:C	1:A:187:LEU:HD23	2.31	0.51
1:A:142:ASN:ND2	4:A:650:HOH:O	2.30	0.51
1:A:235:GLU:O	1:A:238:GLU:HG3	2.10	0.51
1:A:43:GLU:HG3	4:A:536:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:TYR:HA	1:B:259:ASN:HD21	1.75	0.51
1:A:249:GLU:HB3	4:A:623:HOH:O	2.11	0.51
1:A:41:TYR:O	1:A:329:ARG:NH1	2.44	0.50
1:A:203:GLU:HB2	4:A:576:HOH:O	2.12	0.50
1:A:333:MET:CE	1:A:333:MET:HA	2.42	0.50
1:B:37:ILE:HG13	1:B:38:GLY:N	2.25	0.50
1:A:51:THR:N	1:A:322:GLU:OE2	2.35	0.50
1:A:78:GLU:OE1	1:A:78:GLU:HA	2.09	0.50
1:A:158:TYR:CD1	1:A:173:LEU:HD22	2.46	0.50
1:B:237:ALA:HB1	1:B:241:ARG:NH1	2.27	0.50
1:B:173:LEU:C	1:B:173:LEU:HD12	2.33	0.50
1:B:284:PHE:CE1	1:B:287:MET:HE2	2.47	0.50
1:B:5:MET:HG3	1:B:5:MET:O	2.12	0.50
1:A:73:ILE:HG13	1:B:18:LEU:HD23	1.94	0.49
1:B:344:LYS:HD3	1:B:402:GLU:HG3	1.95	0.49
1:B:374:ARG:NH2	4:B:612:HOH:O	2.45	0.49
1:B:81:ARG:HG3	4:B:521:HOH:O	2.13	0.49
1:B:173:LEU:O	1:B:173:LEU:HD12	2.12	0.49
1:A:312:ASN:ND2	1:A:314:ALA:H	2.11	0.49
1:B:372:ARG:HG2	1:B:408:VAL:HG12	1.93	0.49
1:A:165:ASN:N	1:A:165:ASN:ND2	2.41	0.49
1:A:126:LYS:HD3	1:A:129:ARG:NH2	2.28	0.48
1:B:240:LEU:O	1:B:240:LEU:HD22	2.13	0.48
1:B:85:GLU:OE1	1:B:90:LYS:HG2	2.12	0.48
1:A:347:ASN:OD1	1:A:409:LEU:HD13	2.14	0.48
1:B:351:SER:O	1:B:354:ILE:HG13	2.13	0.48
1:B:83:THR:HG22	1:B:87:LEU:HD22	1.94	0.48
1:B:29:ARG:HB3	1:B:30:PRO:HD2	1.94	0.48
1:A:61:LEU:HD11	1:B:58:GLN:HA	1.96	0.48
1:A:305:VAL:O	1:A:309:ILE:HG13	2.14	0.48
1:A:323:LEU:HD12	1:A:326:MET:HE3	1.94	0.48
1:B:294:ASN:HD22	1:B:294:ASN:C	2.16	0.48
1:B:332:ARG:HD2	4:B:587:HOH:O	2.13	0.48
1:A:76:ILE:O	1:A:79:PHE:HB3	2.14	0.48
1:A:294:ASN:HD21	1:B:294:ASN:HD21	1.60	0.48
1:A:348:ARG:HG2	1:A:348:ARG:H	1.51	0.47
1:B:41:TYR:CD1	1:B:391:GLY:HA2	2.49	0.47
1:A:158:TYR:HE1	1:A:173:LEU:HD21	1.79	0.47
1:B:24:PHE:C	1:B:26:ALA:H	2.18	0.47
1:A:195:PRO:HB3	1:A:386:ARG:HD3	1.96	0.47
1:A:99:ARG:HD2	1:A:274:ALA:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:LYS:HD3	4:B:527:HOH:O	2.13	0.47
1:A:409:LEU:HA	1:A:409:LEU:HD23	1.67	0.47
1:B:83:THR:O	1:B:87:LEU:HB2	2.14	0.47
1:A:34:ASN:O	1:A:35:LEU:HD23	2.15	0.47
1:B:162:ASP:O	1:B:166:HIS:N	2.48	0.47
1:B:397:MET:HE3	1:B:400:LEU:HD22	1.96	0.47
1:A:212:SER:HA	1:A:217:TRP:CE3	2.50	0.46
1:B:220:LEU:HD13	1:B:251:ILE:HB	1.97	0.46
1:A:397:MET:HA	1:A:397:MET:HE2	1.97	0.46
1:A:167:THR:OG1	1:A:168:LEU:N	2.48	0.46
1:A:137:ASN:HD22	1:A:138:PRO:HA	1.81	0.46
1:A:202:LEU:HD22	1:A:206:GLN:OE1	2.15	0.46
1:A:397:MET:HA	1:A:397:MET:CE	2.46	0.46
1:A:396:ASN:O	1:A:400:LEU:HB3	2.14	0.46
1:A:37:ILE:HG23	1:A:39:LEU:HD22	1.97	0.46
1:B:329:ARG:NH1	1:B:329:ARG:HG2	2.31	0.46
1:B:48:PRO:HG2	4:B:600:HOH:O	2.16	0.46
1:A:158:TYR:HD1	1:A:173:LEU:HD22	1.80	0.46
1:A:19:GLY:O	1:A:23:LEU:HD12	2.14	0.46
1:B:160:TYR:O	1:B:168:LEU:HD23	2.16	0.46
1:A:328:GLN:HG2	4:A:619:HOH:O	2.15	0.46
1:B:212:SER:HB2	1:B:217:TRP:CE3	2.51	0.46
1:A:312:ASN:ND2	1:A:315:LEU:H	2.13	0.46
1:B:389:VAL:HG13	1:B:392:MET:HE2	1.97	0.46
1:B:237:ALA:CB	1:B:241:ARG:NH1	2.79	0.45
1:B:99:ARG:HG2	1:B:99:ARG:NH1	2.29	0.45
1:A:29:ARG:O	1:A:32:LYS:HG2	2.16	0.45
1:A:73:ILE:CG1	1:B:18:LEU:HD23	2.46	0.45
1:B:284:PHE:CE1	1:B:287:MET:CE	2.99	0.45
1:B:284:PHE:HE1	1:B:287:MET:CE	2.28	0.45
1:A:126:LYS:CE	1:A:129:ARG:NH1	2.80	0.45
1:A:98:LYS:HE2	4:A:425:HOH:O	2.16	0.45
1:B:68:LYS:HB2	4:B:421:HOH:O	2.16	0.45
1:A:333:MET:HE2	1:A:333:MET:HA	1.98	0.45
1:A:126:LYS:CE	1:A:129:ARG:HH12	2.30	0.45
1:B:29:ARG:HB3	1:B:30:PRO:CD	2.46	0.45
1:A:377:PHE:CD1	1:A:377:PHE:N	2.85	0.45
1:B:230:ARG:HD3	4:B:442:HOH:O	2.17	0.45
1:B:367:LYS:N	1:B:367:LYS:HE3	2.32	0.45
1:A:23:LEU:HD12	1:A:23:LEU:H	1.82	0.44
1:B:178:ASN:ND2	4:B:480:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ARG:CG	1:B:29:ARG:HH11	2.10	0.44
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.73	0.44
1:A:365:LEU:HA	1:A:365:LEU:HD12	1.84	0.44
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.70	0.44
1:B:101:ARG:NH1	1:B:281:ASP:OD1	2.50	0.44
1:B:398:ALA:N	1:B:399:PRO:CD	2.79	0.44
1:A:312:ASN:HD22	1:A:312:ASN:C	2.21	0.44
1:A:369:GLN:HG2	1:A:408:VAL:HG23	1.99	0.44
1:B:158:TYR:CD1	1:B:173:LEU:HD13	2.53	0.44
1:B:307:ALA:O	1:B:311:SER:HB2	2.17	0.44
1:A:260:PHE:HB3	1:A:262:LEU:HD12	1.99	0.44
1:A:170:PHE:CE2	1:A:174:ILE:CD1	3.00	0.44
1:B:211:LEU:HD11	1:B:215:LYS:HD3	2.00	0.44
1:B:348:ARG:NH1	1:B:409:LEU:CD1	2.81	0.44
1:A:398:ALA:N	1:A:399:PRO:HD2	2.32	0.43
1:B:334:ARG:HB3	1:B:389:VAL:HG11	2.00	0.43
1:A:194:ASN:HA	1:A:195:PRO:HA	1.75	0.43
1:A:159:ALA:O	1:A:173:LEU:HA	2.18	0.43
1:A:189:HIS:HD2	1:A:194:ASN:H	1.65	0.43
1:A:366:THR:CG2	1:A:368:GLU:N	2.80	0.43
1:A:158:TYR:CE1	1:A:173:LEU:CD2	3.01	0.43
1:A:218:LEU:HD21	4:A:623:HOH:O	2.17	0.43
1:A:353:ILE:HD13	1:A:361:SER:HB2	2.00	0.43
1:B:144:LYS:HD2	1:B:148:ASN:OD1	2.18	0.43
1:A:251:ILE:HG22	1:A:252:VAL:N	2.33	0.43
1:B:372:ARG:HG2	1:B:408:VAL:CG1	2.49	0.43
1:A:366:THR:CG2	1:A:368:GLU:HB2	2.49	0.43
1:A:170:PHE:CD2	1:A:174:ILE:HD12	2.54	0.43
1:A:347:ASN:HD21	1:A:409:LEU:CB	2.15	0.43
1:A:68:LYS:HB2	4:A:417:HOH:O	2.18	0.43
1:B:8:ASN:HB2	4:B:572:HOH:O	2.18	0.43
1:A:126:LYS:HE2	1:A:129:ARG:HH12	1.83	0.42
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.92	0.42
1:A:121:LYS:NZ	1:A:121:LYS:HB3	2.23	0.42
1:A:46:LYS:CG	1:A:47:ILE:N	2.83	0.42
1:A:18:LEU:HD22	1:B:292:ARG:CZ	2.50	0.42
1:B:78:GLU:HB2	4:B:477:HOH:O	2.19	0.42
1:A:67:THR:HG23	1:A:69:LEU:HB2	2.01	0.42
1:A:98:LYS:HD2	4:A:541:HOH:O	2.20	0.42
1:B:81:ARG:HD3	1:B:81:ARG:HH11	1.71	0.42
1:A:334:ARG:HH11	1:A:334:ARG:HD2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:HD13	1:A:361:SER:CB	2.49	0.42
1:A:37:ILE:HG21	1:A:37:ILE:HD13	1.75	0.42
1:A:9:ILE:O	1:B:282:ARG:NH1	2.45	0.42
1:B:194:ASN:HA	1:B:195:PRO:HA	1.74	0.42
1:B:256:TYR:HA	1:B:259:ASN:ND2	2.35	0.42
1:A:400:LEU:HD12	1:A:400:LEU:O	2.20	0.41
1:A:5:MET:HB2	4:B:512:HOH:O	2.19	0.41
1:B:135:VAL:O	1:B:157:GLU:HA	2.20	0.41
1:B:170:PHE:CE1	1:B:204:GLN:HB3	2.54	0.41
1:B:341:LEU:HA	1:B:341:LEU:HD12	1.95	0.41
1:B:284:PHE:HE1	1:B:287:MET:HE2	1.85	0.41
1:B:396:ASN:O	1:B:400:LEU:HB2	2.19	0.41
1:A:112:LEU:HD13	1:A:253:ALA:CB	2.50	0.41
1:A:78:GLU:CD	1:A:81:ARG:HH21	2.22	0.41
1:B:241:ARG:HH11	1:B:241:ARG:CG	2.33	0.41
1:A:201:THR:OG1	1:A:204:GLN:HG3	2.21	0.41
1:B:137:ASN:HA	1:B:138:PRO:HA	1.86	0.41
1:A:110:GLY:O	1:A:114:VAL:HG23	2.21	0.41
1:B:360:PHE:HD2	4:B:585:HOH:O	2.02	0.41
1:B:46:LYS:HA	1:B:46:LYS:HD2	1.96	0.41
1:A:170:PHE:CE1	1:A:204:GLN:HB3	2.56	0.41
1:A:158:TYR:CD1	1:A:173:LEU:CD2	3.03	0.41
1:A:335:GLN:HG2	1:A:335:GLN:H	1.41	0.41
1:B:372:ARG:O	1:B:376:GLU:HB2	2.21	0.41
1:A:121:LYS:HE3	1:A:121:LYS:HB3	1.53	0.41
1:A:327:ARG:O	1:A:331:GLN:HG3	2.20	0.41
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.82	0.41
1:B:329:ARG:HH11	1:B:329:ARG:CG	2.34	0.41
1:B:338:VAL:HG22	1:B:339:ASN:N	2.35	0.41
1:B:81:ARG:HD2	4:B:520:HOH:O	2.20	0.41
1:A:136:SER:O	1:A:139:SER:HB2	2.21	0.41
1:A:129:ARG:HG3	1:A:156:ARG:HG3	2.03	0.41
1:B:332:ARG:CG	1:B:333:MET:CE	2.99	0.40
1:B:367:LYS:HE2	4:B:527:HOH:O	2.20	0.40
1:B:337:PHE:CD1	1:B:397:MET:CE	3.03	0.40
1:B:344:LYS:CD	1:B:402:GLU:HG3	2.51	0.40
1:A:121:LYS:NZ	1:A:121:LYS:CB	2.82	0.40
1:A:126:LYS:HG2	1:A:126:LYS:O	2.19	0.40
1:A:212:SER:OG	1:A:247:HIS:NE2	2.51	0.40
1:A:231:GLY:O	1:A:236:ASP:HB2	2.21	0.40
1:B:88:PHE:O	1:B:241:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LEU:HA	1:A:341:LEU:HD12	1.79	0.40
1:B:348:ARG:CG	1:B:348:ARG:NH1	2.79	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%)	361 (92%)	27 (7%)	6 (2%)	12	11
1	B	394/396 (100%)	369 (94%)	20 (5%)	5 (1%)	14	14
All	All	788/792 (100%)	730 (93%)	47 (6%)	11 (1%)	13	13

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	92	SER
1	A	301	HIS
1	A	346	ALA
1	B	301	HIS
1	B	347	ASN
1	B	25	ARG
1	A	69	LEU
1	A	263	TYR
1	B	348	ARG
1	A	90	LYS
1	A	164	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%)	256 (80%)	64 (20%)	1	1
1	B	320/320 (100%)	253 (79%)	67 (21%)	1	1
All	All	640/640 (100%)	509 (80%)	131 (20%)	1	1

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	9	ILE
1	A	10	THR
1	A	18	LEU
1	A	29	ARG
1	A	32	LYS
1	A	39	LEU
1	A	43	GLU
1	A	44	THR
1	A	46	LYS
1	A	47	ILE
1	A	58	GLN
1	A	61	LEU
1	A	69	LEU
1	A	78	GLU
1	A	81	ARG
1	A	86	LEU
1	A	87	LEU
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	165	ASN
1	A	168	LEU

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Mol	Chain	Res	Type
1	A	171	ASP
1	A	178	ASN
1	A	179	GLU
1	A	202	LEU
1	A	212	SER
1	A	215	LYS
1	A	218	LEU
1	A	223	PHE
1	A	240	LEU
1	A	246	MET
1	A	248	LYS
1	A	259	ASN
1	A	264	ASN
1	A	272	LEU
1	A	277	SER
1	A	296	SER
1	A	312	ASN
1	A	313	ASP
1	A	329	ARG
1	A	335	GLN
1	A	341	LEU
1	A	344	LYS
1	A	347	ASN
1	A	348	ARG
1	A	353	ILE
1	A	355	LYS
1	A	362	PHE
1	A	365	LEU
1	A	366	THR
1	A	367	LYS
1	A	370	VAL
1	A	371	LEU
1	A	372	ARG
1	A	375	GLU
1	A	377	PHE
1	A	388	ASN
1	A	400	LEU
1	B	5	MET
1	B	8	ASN
1	B	10	THR
1	B	25	ARG
1	B	27	ASP

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Mol	Chain	Res	Type
1	B	29	ARG
1	B	32	LYS
1	B	37	ILE
1	B	39	LEU
1	B	43	GLU
1	B	44	THR
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	85	GLU
1	B	87	LEU
1	B	90	LYS
1	B	99	ARG
1	B	113	ARG
1	B	119	LEU
1	B	121	LYS
1	B	129	ARG
1	B	133	VAL
1	B	144	LYS
1	B	146	VAL
1	B	152	LEU
1	B	154	GLU
1	B	164	GLU
1	B	167	THR
1	B	168	LEU
1	B	171	ASP
1	B	173	LEU
1	B	179	GLU
1	B	186	VAL
1	B	212	SER
1	B	215	LYS
1	B	220	LEU
1	B	223	PHE
1	B	233	LEU
1	B	234	GLU
1	B	235	GLU
1	B	240	LEU
1	B	259	ASN
1	B	273	VAL

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Mol	Chain	Res	Type
1	B	277	SER
1	B	294	ASN
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	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	374	ARG
1	B	376	GLU
1	B	387	VAL
1	B	409	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	137	ASN
1	A	142	ASN
1	A	165	ASN
1	A	189	HIS
1	A	226	GLN
1	A	259	ASN
1	A	264	ASN
1	A	312	ASN
1	A	328	GLN
1	A	331	GLN
1	A	335	GLN
1	A	357	ASN
1	A	388	ASN
1	B	84	GLN
1	B	96	ASN
1	B	166	HIS
1	B	175	ASN

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Mol	Chain	Res	Type
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	331	GLN
1	B	339	ASN
1	B	342	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	PLP	A	410	1	15,15,16	1.71	3 (20%)	20,22,23	2.29	11 (55%)
3	MAE	A	411	-	1,7,7	0.46	0	0,8,8	0.00	-
2	PLP	B	410	1	15,15,16	1.61	4 (26%)	20,22,23	1.90	7 (35%)
3	MAE	B	411	-	1,7,7	0.54	0	0,8,8	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	410	1	-	0/6/6/8	0/1/1/1
3	MAE	A	411	-	-	0/0/5/5	0/0/0/0
2	PLP	B	410	1	-	0/6/6/8	0/1/1/1
3	MAE	B	411	-	-	0/0/5/5	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	410	PLP	C4A-C4	-2.77	1.46	1.51
2	B	410	PLP	C4A-C4	-2.32	1.46	1.51
2	B	410	PLP	P-O3P	-2.02	1.46	1.54
2	B	410	PLP	C5-C4	3.36	1.44	1.40
2	A	410	PLP	C5-C4	3.40	1.44	1.40
2	B	410	PLP	C3-C2	3.50	1.43	1.40
2	A	410	PLP	C3-C2	3.53	1.43	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	410	PLP	O3P-P-O4P	-3.05	98.61	106.73
2	A	410	PLP	C5A-C5-C6	-2.82	114.48	119.33
2	B	410	PLP	C3-C2-N1	-2.76	117.12	120.75
2	A	410	PLP	C3-C4-C5	-2.66	115.61	118.63
2	A	410	PLP	C3-C2-N1	-2.52	117.44	120.75
2	B	410	PLP	C3-C4-C5	-2.38	115.94	118.63
2	B	410	PLP	C5-C6-N1	-2.37	119.85	123.87
2	A	410	PLP	C5-C6-N1	-2.24	120.07	123.87
2	A	410	PLP	C6-N1-C2	2.21	123.51	119.26
2	B	410	PLP	C6-N1-C2	2.61	124.29	119.26
2	A	410	PLP	O3P-P-O1P	2.84	121.60	110.50
2	A	410	PLP	O2P-P-O4P	3.11	115.02	106.73
2	A	410	PLP	C2A-C2-C3	3.13	124.70	120.96
2	B	410	PLP	C4A-C4-C5	3.17	124.06	120.86
2	B	410	PLP	C6-C5-C4	3.24	120.89	118.18
2	A	410	PLP	C6-C5-C4	3.60	121.18	118.18
2	B	410	PLP	C2A-C2-C3	3.65	125.31	120.96
2	A	410	PLP	C4A-C4-C5	4.35	125.25	120.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.