Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 02:14 PM EST

PDB ID	:	1ARG
Title	:	Aspartate aminotransferase, phospho-5'-pyridoxyl aspartate complex
Authors	:	Malashkevich, V.N.; Jansonius, J.N.
Deposited on	:	1995-08-23
Resolution	:	2.20 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 (1)) were used in the production of this report:

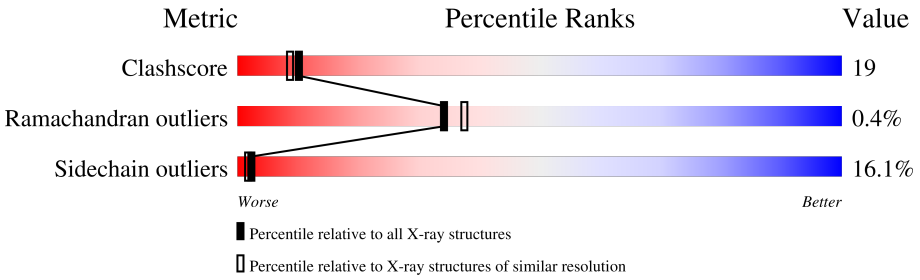
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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	59% 31% 10% •
1	B	396	58% 31% 11% •

2 Entry composition (i)

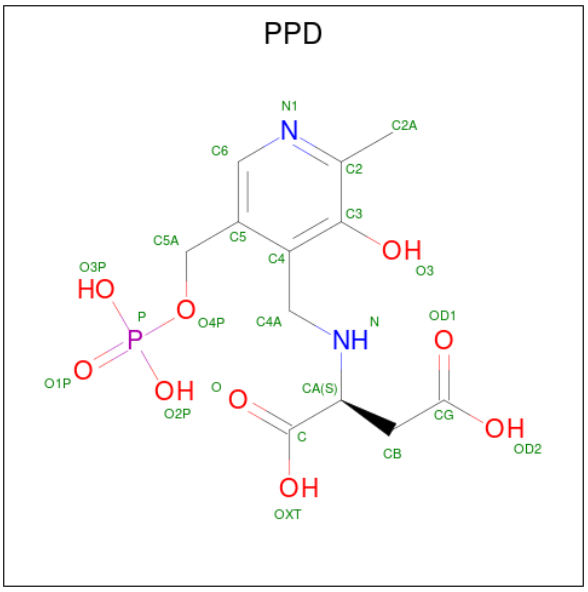
There are 3 unique types of molecules in this entry. The entry contains 6688 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	3069	1936	536	584	13	0	0	0
1	B	396	3069	1936	536	584	13	0	0	0

- Molecule 2 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYLENE)-AMINO]-SUCCINIC ACID (three-letter code: PPD) (formula: $C_{12}H_{17}N_2O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	24	12	2	9	1	0	0
2	B	1	24	12	2	9	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	255	255	255	0	0
			Total	O		
3	B	247	247	247	0	0

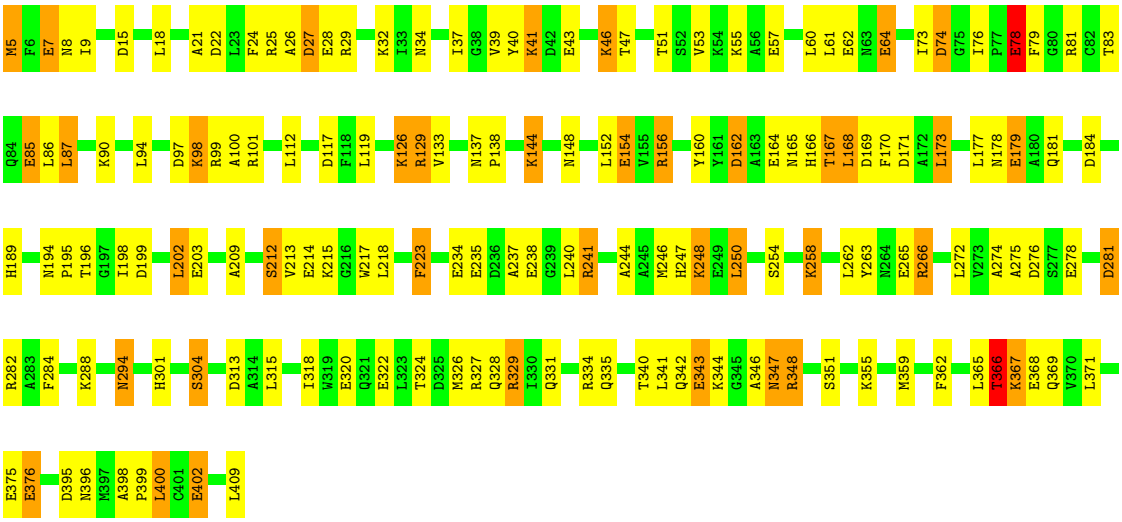
3 Residue-property plots (i)

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.

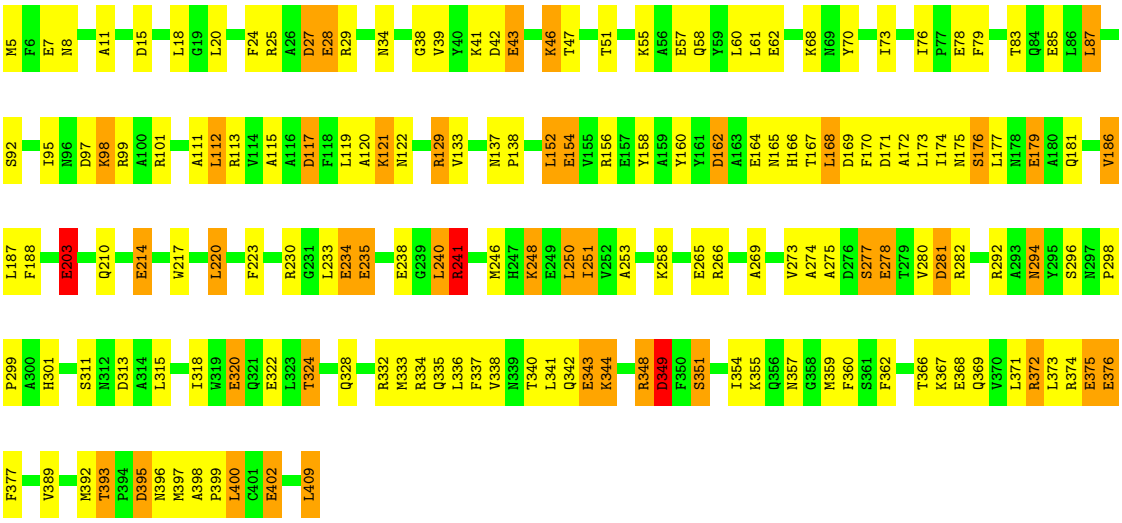
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain A: 59% 31% 10%



• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain B: 58% 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	85.39Å 78.95Å 89.29Å 90.00° 118.54° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	95.1 (8.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 4C	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6688	wwPDB-VP
Average B, all atoms (Å^2)	28.0	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: PPD

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	0.92	21/3130 (0.7%)	1.20	33/4240 (0.8%)
1	B	0.91	22/3130 (0.7%)	1.20	27/4240 (0.6%)
All	All	0.92	43/6260 (0.7%)	1.20	60/8480 (0.7%)

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	320	GLU	CD-OE1	7.48	1.33	1.25
1	A	320	GLU	CD-OE1	7.24	1.33	1.25
1	B	375	GLU	CD-OE2	6.82	1.33	1.25
1	B	43	GLU	CD-OE1	6.80	1.33	1.25
1	A	43	GLU	CD-OE1	6.54	1.32	1.25
1	B	203	GLU	CD-OE1	6.46	1.32	1.25
1	B	238	GLU	CD-OE2	6.46	1.32	1.25
1	A	7	GLU	CD-OE2	6.42	1.32	1.25
1	A	203	GLU	CD-OE1	6.41	1.32	1.25
1	B	164	GLU	CD-OE2	6.37	1.32	1.25
1	B	343	GLU	CD-OE2	6.36	1.32	1.25
1	A	235	GLU	CD-OE2	6.32	1.32	1.25
1	A	234	GLU	CD-OE1	6.29	1.32	1.25
1	A	85	GLU	CD-OE1	6.29	1.32	1.25
1	A	343	GLU	CD-OE1	6.22	1.32	1.25
1	A	179	GLU	CD-OE1	6.19	1.32	1.25
1	A	164	GLU	CD-OE2	6.17	1.32	1.25
1	A	214	GLU	CD-OE1	6.13	1.32	1.25
1	B	179	GLU	CD-OE1	6.09	1.32	1.25
1	A	265	GLU	CD-OE1	6.06	1.32	1.25
1	A	278	GLU	CD-OE1	6.03	1.32	1.25
1	B	28	GLU	CD-OE1	5.93	1.32	1.25
1	A	154	GLU	CD-OE2	5.89	1.32	1.25
1	B	78	GLU	CD-OE1	5.84	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	GLU	CD-OE2	5.80	1.32	1.25
1	A	402	GLU	CD-OE2	5.79	1.32	1.25
1	A	78	GLU	CD-OE2	5.79	1.32	1.25
1	A	28	GLU	CD-OE1	5.69	1.31	1.25
1	B	402	GLU	CD-OE2	5.68	1.31	1.25
1	A	376	GLU	CD-OE1	5.63	1.31	1.25
1	B	235	GLU	CD-OE2	5.53	1.31	1.25
1	B	85	GLU	CD-OE1	5.47	1.31	1.25
1	B	278	GLU	CD-OE2	5.40	1.31	1.25
1	A	62	GLU	CD-OE2	5.38	1.31	1.25
1	B	265	GLU	CD-OE1	5.31	1.31	1.25
1	B	154	GLU	CD-OE1	5.29	1.31	1.25
1	B	368	GLU	CD-OE2	-5.29	1.19	1.25
1	A	238	GLU	CD-OE2	5.25	1.31	1.25
1	A	64	GLU	CD-OE2	5.22	1.31	1.25
1	B	62	GLU	CD-OE2	5.22	1.31	1.25
1	B	234	GLU	CD-OE2	5.05	1.31	1.25
1	B	376	GLU	CD-OE2	5.05	1.31	1.25
1	B	57	GLU	CD-OE2	5.05	1.31	1.25

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	409	LEU	N-CA-CB	8.90	128.20	110.40
1	A	329	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	A	27	ASP	CB-CG-OD1	7.87	125.39	118.30
1	B	266	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	B	169	ASP	CB-CG-OD2	-7.44	111.60	118.30
1	A	266	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	B	395	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	A	313	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	B	27	ASP	CB-CG-OD1	-7.15	111.86	118.30
1	A	329	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	A	169	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	A	22	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	15	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	B	113	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	22	ASP	CB-CG-OD1	-6.68	112.29	118.30
1	B	281	ASP	CB-CG-OD2	6.67	124.31	118.30
1	B	171	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	B	313	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	A	27	ASP	CB-CG-OD2	-6.51	112.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	97	ASP	CB-CG-OD1	-6.33	112.60	118.30
1	A	74	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	395	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	A	276	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	B	46	LYS	N-CA-CB	6.05	121.49	110.60
1	B	162	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	A	117	ASP	CB-CG-OD1	-6.03	112.88	118.30
1	A	171	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	B	281	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	B	117	ASP	CB-CG-OD2	5.96	123.66	118.30
1	B	313	ASP	CB-CG-OD1	5.91	123.61	118.30
1	B	15	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	A	241	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	B	162	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	241	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	15	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	395	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	162	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	40	TYR	CB-CG-CD1	-5.68	117.59	121.00
1	A	184	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	A	97	ASP	CB-CG-OD2	5.61	123.34	118.30
1	A	366	THR	N-CA-CB	-5.61	99.65	110.30
1	B	117	ASP	CB-CG-OD1	-5.53	113.33	118.30
1	A	162	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	276	ASP	CB-CG-OD1	5.45	123.20	118.30
1	B	349	ASP	CB-CG-OD1	-5.44	113.41	118.30
1	B	156	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	250	LEU	N-CA-CB	-5.40	99.59	110.40
1	B	97	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	A	74	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	169	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	15	ASP	CB-CG-OD1	5.35	123.12	118.30
1	B	169	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	409	LEU	CB-CA-C	-5.28	100.16	110.20
1	A	281	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	199	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	171	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	349	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	334	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	395	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	313	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

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	3069	0	3018	119	0
1	B	3069	0	3018	120	0
2	A	24	0	12	2	0
2	B	24	0	12	1	0
3	A	255	0	0	13	0
3	B	247	0	0	16	0
All	All	6688	0	6060	231	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 19.

All (231) 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:NZ	1:A:47:THR:H	1.59	0.98
1:B:46:LYS:HD2	1:B:47:THR:H	1.37	0.88
1:A:46:LYS:HZ2	1:A:47:THR:H	1.18	0.88
1:B:98:LYS:HE2	1:B:98:LYS:HA	1.55	0.86
1:B:332:ARG:HD2	1:B:333:MET:CE	2.05	0.86
1:A:126:LYS:HE2	1:A:129:ARG:HB3	1.58	0.85
1:A:46:LYS:HG3	1:A:47:THR:N	1.93	0.84
1:B:120:ALA:HB2	1:B:152:LEU:HD21	1.59	0.84
1:A:248:LYS:HB2	1:A:248:LYS:NZ	1.94	0.80
1:B:99:ARG:HG2	1:B:274:ALA:O	1.83	0.79
1:A:126:LYS:HE2	1:A:129:ARG:HD3	1.64	0.78
1:B:46:LYS:CD	1:B:47:THR:H	1.97	0.78
1:B:324:THR:O	1:B:328:GLN:HG3	1.84	0.77
1:A:324:THR:O	1:A:328:GLN:HG3	1.85	0.75
1:A:85:GLU:OE2	1:A:90:LYS:HG3	1.88	0.73
1:A:154:GLU:OE2	1:A:156:ARG:HD3	1.89	0.73
1:A:348:ARG:CB	1:A:348:ARG:HH11	2.01	0.72
1:A:99:ARG:HD2	1:A:274:ALA:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:O	1:A:331:GLN:HG3	1.89	0.71
1:B:337:PHE:HB2	1:B:392:MET:HE3	1.74	0.68
1:B:187:LEU:HD23	3:B:637:HOH:O	1.93	0.67
1:A:41:LYS:HE3	3:A:585:HOH:O	1.93	0.67
1:A:340:THR:O	1:A:344:LYS:HB2	1.93	0.67
1:A:46:LYS:HZ3	1:A:47:THR:H	1.43	0.67
1:B:92:SER:HB3	1:B:95:ILE:HG13	1.74	0.67
1:A:398:ALA:O	1:A:402:GLU:HG3	1.94	0.66
1:B:348:ARG:HH11	1:B:348:ARG:HB2	1.60	0.66
1:B:398:ALA:HB3	1:B:399:PRO:HD3	1.76	0.66
1:B:269:ALA:N	3:B:808:HOH:O	2.29	0.66
1:A:27:ASP:OD2	1:A:29:ARG:NH1	2.29	0.66
1:A:41:LYS:NZ	3:A:483:HOH:O	2.28	0.66
1:A:398:ALA:HB3	1:A:399:PRO:HD3	1.76	0.66
1:B:240:LEU:O	1:B:240:LEU:HD22	1.97	0.65
1:B:46:LYS:CG	1:B:47:THR:H	2.10	0.65
1:A:98:LYS:HD2	3:A:563:HOH:O	1.97	0.65
1:B:5:MET:N	1:B:7:GLU:OE1	2.30	0.65
1:B:248:LYS:HG2	1:B:275:ALA:HB2	1.79	0.65
1:B:344:LYS:NZ	1:B:402:GLU:OE2	2.30	0.65
1:A:166:HIS:ND1	3:A:565:HOH:O	2.29	0.65
1:A:347:ASN:HD21	1:A:409:LEU:HB2	1.61	0.65
1:B:332:ARG:HD2	1:B:333:MET:HE3	1.79	0.65
1:A:215:LYS:HE2	3:A:635:HOH:O	1.95	0.65
1:B:250:LEU:HD13	1:B:273:VAL:HB	1.79	0.65
1:B:372:ARG:NH1	1:B:376:GLU:OE2	2.30	0.65
1:B:101:ARG:NH1	1:B:281:ASP:OD1	2.30	0.64
1:A:61:LEU:HD21	1:B:58:GLN:HG3	1.78	0.64
1:B:27:ASP:OD2	1:B:29:ARG:NH1	2.30	0.64
1:A:126:LYS:NZ	1:A:129:ARG:NE	2.45	0.63
1:A:209:ALA:O	1:A:213:VAL:HG23	1.98	0.63
1:A:366:THR:HG22	1:A:369:GLN:H	1.63	0.63
1:A:126:LYS:CE	1:A:129:ARG:HD3	2.28	0.63
1:B:98:LYS:HA	1:B:98:LYS:CE	2.26	0.63
1:B:186:VAL:HG12	1:B:217:TRP:HB3	1.80	0.63
1:A:24:PHE:CE1	1:A:34:ASN:HB2	2.33	0.63
1:B:170:PHE:CE2	1:B:174:ILE:HD11	2.34	0.62
1:B:210:GLN:HE21	1:B:214:GLU:HG3	1.63	0.62
1:A:81:ARG:HG3	1:A:81:ARG:HH11	1.63	0.61
1:B:99:ARG:HD2	1:B:275:ALA:O	2.01	0.61
1:A:348:ARG:HH11	1:A:348:ARG:HB2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD23	1:B:73:ILE:CG1	2.31	0.60
1:A:248:LYS:HB2	1:A:248:LYS:HZ3	1.64	0.60
1:A:126:LYS:HZ3	1:A:129:ARG:NE	1.99	0.60
1:A:101:ARG:NH1	1:A:281:ASP:OD1	2.30	0.60
1:B:389:VAL:HG13	1:B:392:MET:HE1	1.82	0.59
1:A:18:LEU:HD23	1:B:73:ILE:HD11	1.84	0.59
1:A:99:ARG:NH2	3:A:454:HOH:O	2.29	0.59
1:B:393:THR:HG22	1:B:396:ASN:H	1.68	0.59
1:A:7:GLU:O	1:B:282:ARG:NH2	2.37	0.58
1:B:376:GLU:HB3	1:B:377:PHE:CD1	2.39	0.58
1:B:332:ARG:HG2	3:B:829:HOH:O	2.04	0.57
1:A:18:LEU:HD23	1:B:73:ILE:HG13	1.85	0.56
1:B:43:GLU:CD	1:B:43:GLU:H	2.07	0.56
1:B:101:ARG:HD3	3:B:723:HOH:O	2.04	0.56
1:B:318:ILE:O	1:B:322:GLU:HG3	2.05	0.56
1:B:38:GLY:C	1:B:359:MET:HE1	2.26	0.56
1:B:76:ILE:O	1:B:79:PHE:HB3	2.06	0.56
1:B:374:ARG:NH2	3:B:617:HOH:O	2.39	0.56
1:B:129:ARG:HD3	1:B:154:GLU:CD	2.26	0.55
1:A:73:ILE:HD11	1:B:18:LEU:HD23	1.88	0.55
2:A:411:PPD:N	2:A:411:PPD:O3	2.40	0.55
1:A:189:HIS:CD2	1:A:194:ASN:H	2.25	0.55
1:A:18:LEU:HD23	1:B:73:ILE:CD1	2.37	0.55
1:A:94:LEU:HD11	1:A:244:ALA:HB1	1.88	0.55
1:A:46:LYS:HG3	1:A:47:THR:H	1.70	0.55
1:A:126:LYS:HE2	1:A:129:ARG:CD	2.36	0.55
1:B:46:LYS:HD2	1:B:47:THR:N	2.15	0.54
1:B:87:LEU:O	1:B:241:ARG:HD3	2.06	0.54
1:B:99:ARG:NH2	3:B:663:HOH:O	2.40	0.54
1:A:262:LEU:HD23	1:B:68:LYS:HD3	1.89	0.54
1:A:366:THR:HG23	1:A:368:GLU:OE1	2.07	0.54
1:B:210:GLN:HE21	1:B:214:GLU:CG	2.21	0.54
1:A:76:ILE:O	1:A:79:PHE:HB3	2.08	0.54
1:B:400:LEU:C	1:B:400:LEU:HD23	2.29	0.53
1:B:99:ARG:NH1	1:B:274:ALA:O	2.41	0.53
1:B:8:ASN:HB2	3:B:638:HOH:O	2.08	0.53
1:A:322:GLU:O	1:A:326:MET:HG3	2.09	0.53
1:A:237:ALA:O	1:A:241:ARG:HD3	2.09	0.52
1:A:156:ARG:HG3	3:A:645:HOH:O	2.07	0.52
1:B:162:ASP:OD2	1:B:165:ASN:HB3	2.09	0.52
1:B:220:LEU:HD22	1:B:251:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:SER:HB2	1:A:217:TRP:HE3	1.74	0.52
1:B:112:LEU:HD13	1:B:253:ALA:CB	2.39	0.52
1:B:42:ASP:HB2	1:B:43:GLU:OE2	2.09	0.52
1:A:46:LYS:HZ2	1:A:47:THR:N	1.97	0.52
1:A:162:ASP:O	1:A:166:HIS:N	2.43	0.52
1:A:83:THR:HG22	1:A:87:LEU:HD22	1.92	0.51
1:B:366:THR:OG1	1:B:369:GLN:HG3	2.10	0.51
1:A:99:ARG:HD3	1:A:275:ALA:O	2.11	0.51
1:B:277:SER:HA	1:B:280:VAL:HG12	1.93	0.51
1:A:60:LEU:O	1:A:64:GLU:HB2	2.11	0.51
1:A:25:ARG:HD2	3:A:507:HOH:O	2.10	0.51
1:B:162:ASP:O	1:B:166:HIS:N	2.39	0.51
1:A:53:VAL:O	1:A:57:GLU:HG3	2.11	0.50
1:B:117:ASP:O	1:B:121:LYS:HE2	2.11	0.50
1:A:294:ASN:C	1:A:294:ASN:HD22	2.13	0.50
1:B:165:ASN:OD1	1:B:165:ASN:O	2.30	0.50
1:A:282:ARG:HG3	1:B:11:ALA:HB2	1.94	0.50
1:B:115:ALA:HB2	1:B:251:ILE:HD11	1.94	0.50
1:A:24:PHE:CZ	1:A:32:LYS:HG3	2.47	0.50
1:A:396:ASN:O	1:A:400:LEU:HB3	2.12	0.50
1:A:258:LYS:HB3	1:A:359:MET:CE	2.42	0.50
1:A:24:PHE:CZ	1:A:34:ASN:HB2	2.47	0.49
1:B:398:ALA:N	1:B:399:PRO:HD2	2.28	0.49
1:A:25:ARG:O	1:A:27:ASP:N	2.45	0.49
1:B:230:ARG:NH2	1:B:235:GLU:HB2	2.27	0.49
1:A:5:MET:N	1:A:7:GLU:OE1	2.45	0.49
1:A:78:GLU:HA	1:A:78:GLU:OE1	2.13	0.49
1:B:335:GLN:HG3	3:B:758:HOH:O	2.11	0.49
1:A:51:THR:O	1:A:55:LYS:HG3	2.13	0.48
1:B:392:MET:HB3	1:B:392:MET:HE2	1.64	0.48
1:A:258:LYS:HE2	2:A:411:PPD:H4A2	1.94	0.48
1:A:318:ILE:O	1:A:322:GLU:HG3	2.12	0.48
1:A:162:ASP:HB3	1:A:167:THR:HG22	1.95	0.48
1:A:212:SER:HB2	1:A:217:TRP:CE3	2.48	0.48
1:B:186:VAL:HG22	1:B:188:PHE:CE1	2.49	0.48
1:A:100:ALA:O	1:A:101:ARG:HD2	2.14	0.48
1:A:126:LYS:NZ	1:A:129:ARG:HD3	2.28	0.48
1:B:294:ASN:C	1:B:294:ASN:HD22	2.16	0.48
1:B:28:GLU:OE1	1:B:28:GLU:HA	2.13	0.48
1:A:41:LYS:HD2	3:A:562:HOH:O	2.14	0.48
1:B:393:THR:CG2	1:B:395:ASP:H	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ARG:HH11	1:B:333:MET:HE1	1.78	0.47
1:B:311:SER:HB2	3:B:806:HOH:O	2.14	0.47
1:B:348:ARG:HH11	1:B:348:ARG:CB	2.27	0.47
1:A:189:HIS:HD2	1:A:194:ASN:H	1.61	0.47
1:B:298:PRO:HB2	1:B:299:PRO:HD2	1.97	0.47
1:B:349:ASP:OD2	1:B:351:SER:OG	2.33	0.47
1:A:223:PHE:O	1:A:254:SER:HA	2.14	0.47
1:B:336:LEU:HD23	1:B:397:MET:HE2	1.96	0.47
1:A:98:LYS:HD2	1:A:98:LYS:HA	1.64	0.47
1:A:398:ALA:N	1:A:399:PRO:HD2	2.28	0.47
1:B:172:ALA:O	1:B:176:SER:HB2	2.14	0.47
1:B:83:THR:HG22	1:B:87:LEU:HD22	1.97	0.46
1:A:9:ILE:HD13	1:B:122:ASN:HB3	1.95	0.46
1:A:21:ALA:O	1:A:25:ARG:HG3	2.14	0.46
1:A:196:THR:O	1:A:198:ILE:HD12	2.16	0.46
1:A:160:TYR:O	1:A:168:LEU:HD23	2.16	0.46
1:A:367:LYS:HD3	1:A:368:GLU:OE2	2.16	0.45
1:B:230:ARG:NH1	3:B:647:HOH:O	2.50	0.45
1:B:170:PHE:CE2	1:B:174:ILE:CD1	3.00	0.45
1:A:212:SER:OG	1:A:247:HIS:NE2	2.48	0.45
1:B:160:TYR:O	1:B:168:LEU:HD23	2.17	0.45
1:A:87:LEU:O	1:A:241:ARG:HD2	2.16	0.45
1:A:126:LYS:HZ1	1:A:129:ARG:HD3	1.80	0.45
1:A:346:ALA:HB3	3:A:569:HOH:O	2.16	0.45
1:B:340:THR:O	1:B:344:LYS:HB2	2.16	0.45
1:B:186:VAL:CG1	1:B:217:TRP:HB3	2.46	0.45
1:B:46:LYS:CG	1:B:47:THR:N	2.79	0.44
1:B:137:ASN:ND2	3:B:823:HOH:O	2.49	0.44
1:B:332:ARG:HH11	1:B:333:MET:CE	2.29	0.44
1:B:115:ALA:CB	1:B:251:ILE:HD11	2.47	0.44
1:A:348:ARG:H	1:A:348:ARG:HG2	1.58	0.44
1:B:372:ARG:HH11	1:B:376:GLU:CD	2.20	0.44
1:A:126:LYS:NZ	1:A:129:ARG:CD	2.80	0.44
1:A:398:ALA:N	1:A:399:PRO:CD	2.80	0.44
1:B:111:ALA:HB2	3:B:808:HOH:O	2.17	0.44
1:A:347:ASN:HD21	1:A:409:LEU:CB	2.29	0.44
1:B:338:VAL:HG21	1:B:354:ILE:HG13	2.00	0.44
1:A:367:LYS:HB3	3:A:660:HOH:O	2.17	0.43
1:B:179:GLU:OE1	1:B:179:GLU:HA	2.18	0.43
1:B:360:PHE:HD2	3:B:790:HOH:O	2.01	0.43
1:A:367:LYS:HG2	1:A:368:GLU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASP:OD2	1:A:165:ASN:HB2	2.18	0.43
1:B:98:LYS:HE2	1:B:98:LYS:CA	2.37	0.43
1:B:292:ARG:HA	1:B:296:SER:HA	2.00	0.43
1:A:60:LEU:HD11	1:A:304:SER:HB3	2.01	0.43
1:B:320:GLU:O	1:B:324:THR:HG23	2.19	0.43
1:A:137:ASN:HA	1:A:138:PRO:HA	1.76	0.43
1:A:202:LEU:HD22	1:A:202:LEU:O	2.19	0.43
1:B:203:GLU:H	1:B:203:GLU:HG2	1.63	0.43
1:B:334:ARG:HB3	1:B:389:VAL:HG11	2.01	0.43
1:A:166:HIS:HD2	3:A:546:HOH:O	2.02	0.43
1:A:344:LYS:HE3	1:A:402:GLU:HG2	2.01	0.43
1:B:315:LEU:HA	1:B:315:LEU:HD23	1.57	0.43
1:B:158:TYR:CD1	1:B:173:LEU:HD13	2.54	0.42
1:A:74:ASP:OD1	1:A:74:ASP:N	2.44	0.42
1:A:266:ARG:HD2	1:A:266:ARG:N	2.34	0.42
1:B:278:GLU:OE2	1:B:282:ARG:HD3	2.20	0.42
1:A:39:VAL:O	1:A:39:VAL:HG12	2.19	0.42
1:A:194:ASN:HA	1:A:195:PRO:HA	1.75	0.42
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.74	0.42
1:A:170:PHE:O	1:A:173:LEU:HB3	2.19	0.42
1:B:175:ASN:ND2	3:B:735:HOH:O	2.53	0.42
1:B:177:LEU:HD23	1:B:177:LEU:HA	1.85	0.42
1:B:398:ALA:N	1:B:399:PRO:CD	2.83	0.42
1:B:396:ASN:O	1:B:400:LEU:HB3	2.20	0.41
2:B:411:PPD:H5A1	2:B:411:PPD:H4A1	1.93	0.41
1:A:167:THR:HG23	1:A:168:LEU:N	2.35	0.41
1:A:248:LYS:CG	1:A:275:ALA:HB2	2.50	0.41
1:B:374:ARG:O	1:B:374:ARG:HG2	2.16	0.41
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.97	0.41
1:A:348:ARG:HH11	1:A:348:ARG:HB3	1.84	0.41
1:B:70:TYR:HD1	3:B:809:HOH:O	2.03	0.41
1:B:374:ARG:NE	3:B:713:HOH:O	2.32	0.41
1:A:398:ALA:HB3	1:A:399:PRO:CD	2.49	0.41
1:B:24:PHE:CE1	1:B:34:ASN:HB2	2.56	0.41
1:B:87:LEU:HD12	1:B:87:LEU:HA	1.86	0.41
1:B:137:ASN:HA	1:B:138:PRO:HA	1.87	0.41
1:B:298:PRO:CB	1:B:299:PRO:HD2	2.51	0.41
1:A:284:PHE:CE2	1:A:288:LYS:HD2	2.56	0.40
1:B:5:MET:HE2	1:B:5:MET:HB2	1.78	0.40
1:A:258:LYS:HG3	1:A:263:TYR:HE1	1.86	0.40
1:B:168:LEU:HD23	1:B:168:LEU:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LYS:HD3	1:A:148:ASN:OD1	2.21	0.40
1:B:18:LEU:HD12	1:B:18:LEU:HA	1.86	0.40
1:A:25:ARG:C	1:A:27:ASP:H	2.25	0.40
1:A:101:ARG:HD3	3:A:514:HOH:O	2.22	0.40
1:B:393:THR:HG22	1:B:395:ASP:H	1.85	0.40
1:A:129:ARG:NH2	1:A:181:GLN:NE2	2.70	0.40
1:A:341:LEU:HD23	1:A:341:LEU:HA	1.85	0.40
1:B:341:LEU:HD23	1:B:341:LEU:HA	1.91	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%)	379 (96%)	13 (3%)	2 (0%)	29	31
1	B	394/396 (100%)	374 (95%)	19 (5%)	1 (0%)	41	46
All	All	788/792 (100%)	753 (96%)	32 (4%)	3 (0%)	34	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ALA
1	B	301	HIS
1	A	301	HIS

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%)	270 (84%)	50 (16%)	2 2
1	B	320/320 (100%)	267 (83%)	53 (17%)	2 1
All	All	640/640 (100%)	537 (84%)	103 (16%)	2 2

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	8	ASN
1	A	37	ILE
1	A	41	LYS
1	A	46	LYS
1	A	78	GLU
1	A	86	LEU
1	A	87	LEU
1	A	98	LYS
1	A	112	LEU
1	A	119	LEU
1	A	126	LYS
1	A	129	ARG
1	A	133	VAL
1	A	144	LYS
1	A	152	LEU
1	A	156	ARG
1	A	167	THR
1	A	168	LEU
1	A	173	LEU
1	A	178	ASN
1	A	179	GLU
1	A	202	LEU
1	A	212	SER
1	A	218	LEU
1	A	223	PHE
1	A	240	LEU
1	A	246	MET
1	A	248	LYS
1	A	250	LEU
1	A	258	LYS
1	A	272	LEU
1	A	294	ASN

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Mol	Chain	Res	Type
1	A	304	SER
1	A	329	ARG
1	A	335	GLN
1	A	342	GLN
1	A	343	GLU
1	A	347	ASN
1	A	348	ARG
1	A	351	SER
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	400	LEU
1	B	20	LEU
1	B	25	ARG
1	B	39	VAL
1	B	41	LYS
1	B	51	THR
1	B	55	LYS
1	B	60	LEU
1	B	61	LEU
1	B	87	LEU
1	B	98	LYS
1	B	112	LEU
1	B	119	LEU
1	B	121	LYS
1	B	129	ARG
1	B	133	VAL
1	B	152	LEU
1	B	167	THR
1	B	168	LEU
1	B	176	SER
1	B	181	GLN
1	B	186	VAL
1	B	203	GLU
1	B	220	LEU
1	B	223	PHE
1	B	233	LEU

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Mol	Chain	Res	Type
1	B	234	GLU
1	B	240	LEU
1	B	241	ARG
1	B	246	MET
1	B	248	LYS
1	B	250	LEU
1	B	251	ILE
1	B	258	LYS
1	B	277	SER
1	B	294	ASN
1	B	324	THR
1	B	342	GLN
1	B	343	GLU
1	B	344	LYS
1	B	348	ARG
1	B	349	ASP
1	B	351	SER
1	B	355	LYS
1	B	357	ASN
1	B	362	PHE
1	B	367	LYS
1	B	371	LEU
1	B	372	ARG
1	B	373	LEU
1	B	375	GLU
1	B	393	THR
1	B	400	LEU
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	137	ASN
1	A	166	HIS
1	A	175	ASN
1	A	181	GLN
1	A	189	HIS
1	A	206	GLN
1	A	294	ASN
1	A	331	GLN
1	A	335	GLN
1	A	339	ASN

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Mol	Chain	Res	Type
1	A	357	ASN
1	A	388	ASN
1	B	84	GLN
1	B	96	ASN
1	B	137	ASN
1	B	165	ASN
1	B	175	ASN
1	B	206	GLN
1	B	210	GLN
1	B	294	ASN
1	B	331	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)

2 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	PPD	A	411	-	24,24,24	1.98	4 (16%)	30,34,34	1.81	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PPD	B	411	-	24,24,24	1.66	1 (4%)	30,34,34	1.96	8 (26%)

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	PPD	A	411	-	-	6/19/19/19	0/1/1/1
2	PPD	B	411	-	-	7/19/19/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	411	PPD	C4A-C4	-7.75	1.42	1.51
2	B	411	PPD	C4A-C4	-6.74	1.43	1.51
2	A	411	PPD	CA-C	-2.22	1.46	1.52
2	A	411	PPD	C3-C4	-2.15	1.36	1.40
2	A	411	PPD	P-O3P	-2.13	1.46	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	411	PPD	C6-C5-C4	4.62	121.39	118.12
2	B	411	PPD	C6-C5-C4	4.40	121.23	118.12
2	B	411	PPD	C4A-N-CA	4.06	121.61	113.92
2	A	411	PPD	C5-C6-N1	-3.72	117.61	123.82
2	B	411	PPD	C5-C6-N1	-3.48	118.02	123.82
2	B	411	PPD	C6-N1-C2	3.46	125.57	119.17
2	B	411	PPD	C2A-C2-C3	3.46	125.16	120.89
2	A	411	PPD	C4A-N-CA	3.28	120.14	113.92
2	B	411	PPD	C3-C2-N1	-3.23	116.59	120.77
2	A	411	PPD	C3-C2-N1	-3.17	116.67	120.77
2	A	411	PPD	C6-N1-C2	3.01	124.73	119.17
2	A	411	PPD	OD2-CG-CB	2.48	122.02	114.07
2	A	411	PPD	C2A-C2-C3	2.47	123.94	120.89
2	B	411	PPD	C4A-C4-C3	2.42	122.63	120.04
2	B	411	PPD	OD2-CG-CB	2.28	121.39	114.07

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	411	PPD	C5A-O4P-P-O2P
2	B	411	PPD	C5A-O4P-P-O3P
2	A	411	PPD	C5-C4-C4A-N
2	B	411	PPD	C5-C4-C4A-N
2	B	411	PPD	C5A-O4P-P-O1P
2	A	411	PPD	C-CA-N-C4A
2	B	411	PPD	C-CA-N-C4A
2	A	411	PPD	C3-C4-C4A-N
2	B	411	PPD	C3-C4-C4A-N
2	A	411	PPD	CB-CA-N-C4A
2	B	411	PPD	CB-CA-N-C4A
2	A	411	PPD	C5A-O4P-P-O3P
2	A	411	PPD	C4-C5-C5A-O4P

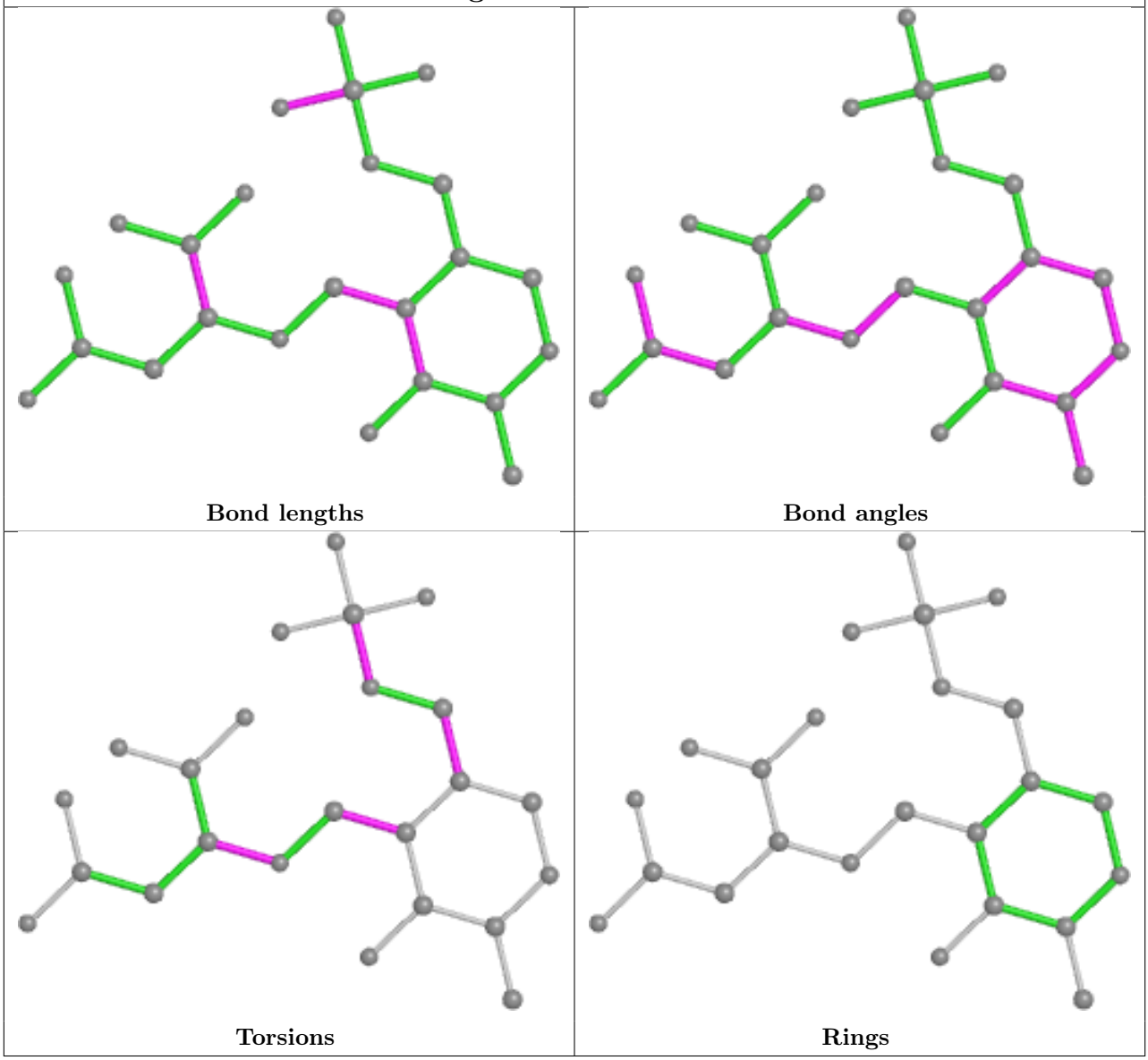
There are no ring outliers.

2 monomers are involved in 3 short contacts:

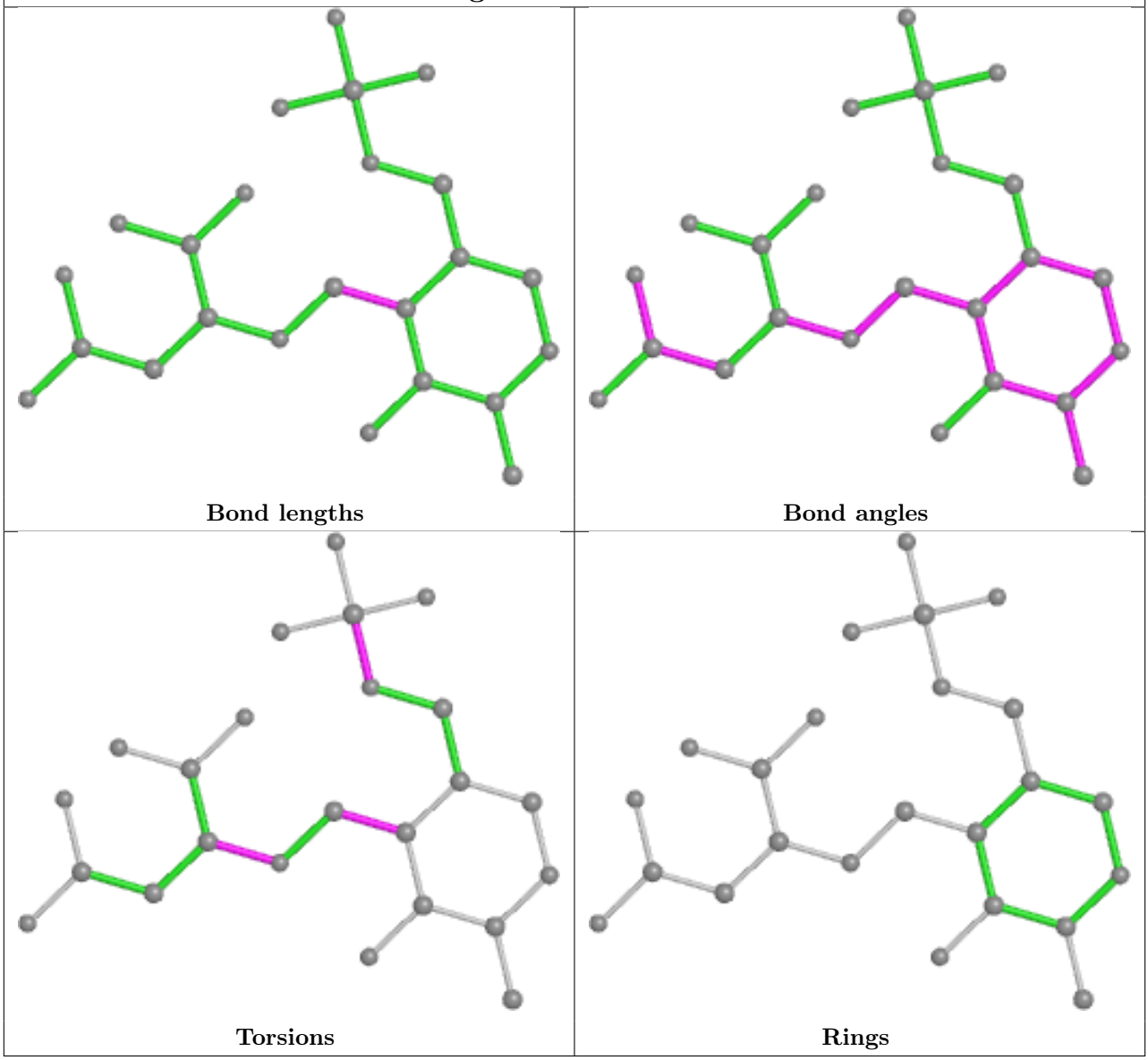
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	411	PPD	2	0
2	B	411	PPD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PPD A 411



Ligand PPD B 411



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.