



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:56 PM UTC

PDB ID : 1B4N / pdb_00001b4n
Title : FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE FROM PYRO-
COCCUS FURIOSUS, COMPLEXED WITH GLUTARATE
Authors : Hu, Y.L.; Faham, S.; Roy, R.; Adams, M.W.W.; Rees, D.C.
Deposited on : 1998-12-24
Resolution : 2.40 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

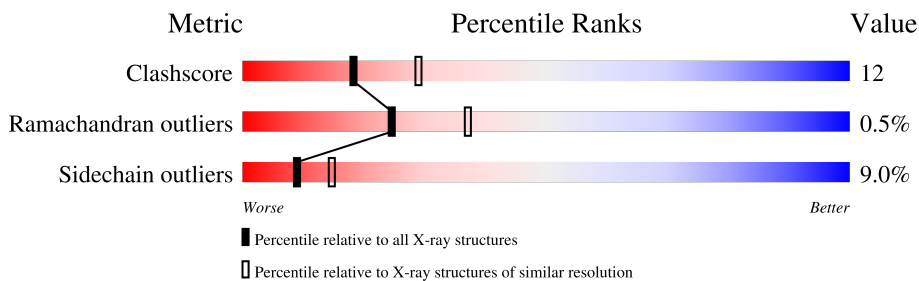
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	619	 66% 28% . .
1	B	619	 66% 28% . .
1	C	619	 64% 29% 5% .
1	D	619	 71% 24% . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19600 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.

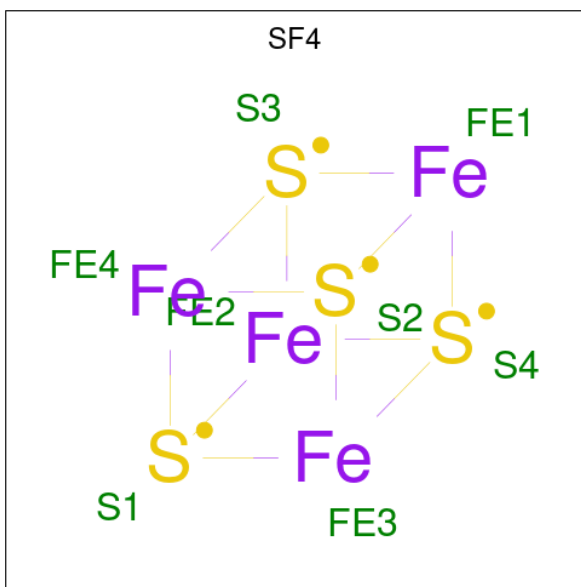
- Molecule 1 is a protein called FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4786	3067	809	888	22			
1	B	611	Total	C	N	O	S	0	0	0
			4786	3067	809	888	22			
1	C	611	Total	C	N	O	S	0	0	0
			4786	3067	809	888	22			
1	D	611	Total	C	N	O	S	0	0	0
			4786	3067	809	888	22			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

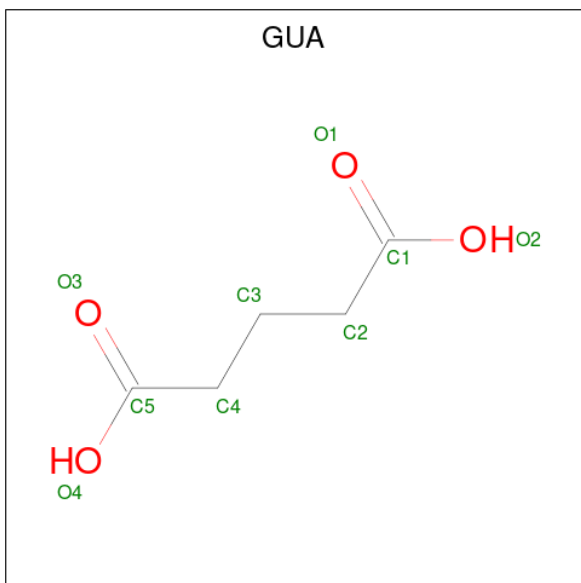
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



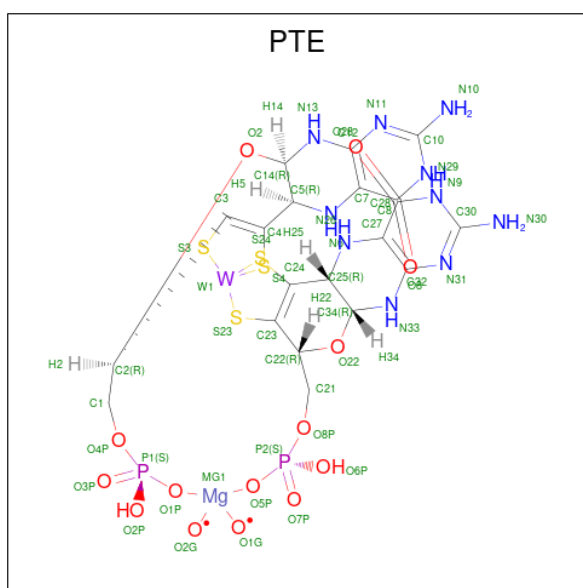
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is GLUTARIC ACID (CCD ID: GUA) (formula: C₅H₈O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 9 5 4	0	0
4	B	1	Total C O 9 5 4	0	0
4	C	1	Total C O 9 5 4	0	0
4	D	1	Total C O 9 5 4	0	0

- Molecule 5 is TUNGSTOPTERIN COFACTOR (CCD ID: PTE) (formula: $C_{20}H_{22}MgN_{10}O_{14}P_2S_4W$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C Mg N O P S W 50 20 1 10 12 2 4 1	0	0
5	B	1	Total C Mg N O P S W 50 20 1 10 12 2 4 1	0	0
5	C	1	Total C Mg N O P S W 50 20 1 10 12 2 4 1	0	0
5	D	1	Total C Mg N O P S W 50 20 1 10 12 2 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	38	Total O 38 38	0	0
6	B	46	Total O 46 46	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	49	Total	O	0	0
			49	49		
6	D	51	Total	O	0	0
			51	51		

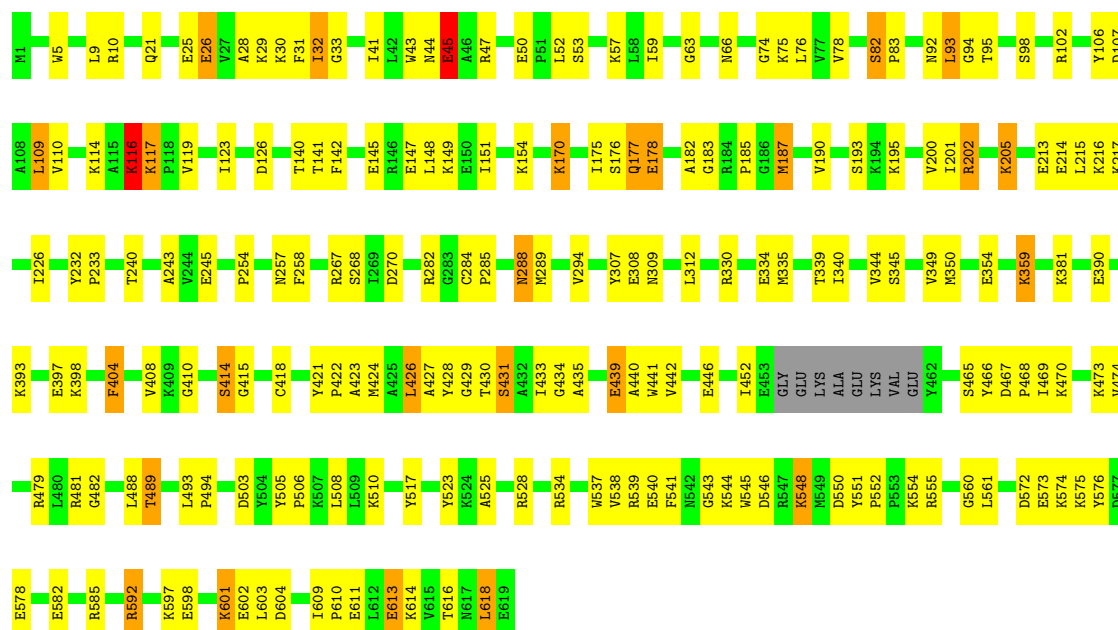
3 Residue-property plots

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.

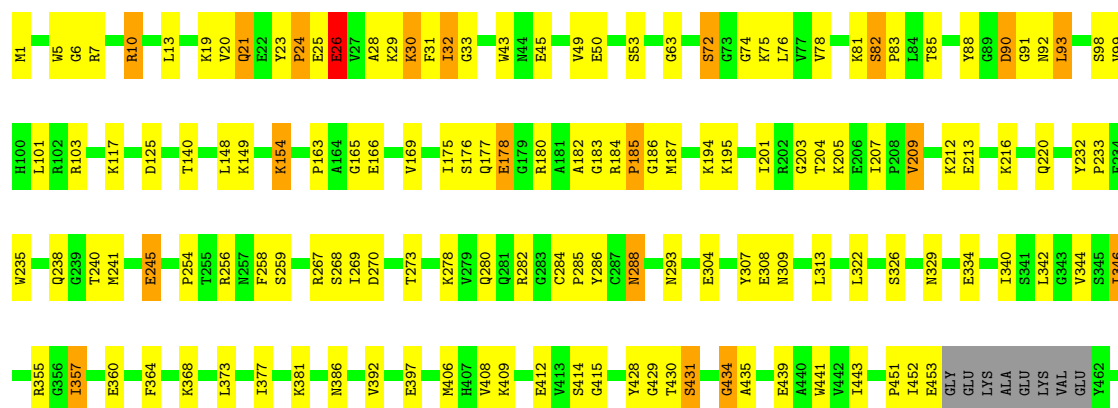
• Molecule 1: FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE

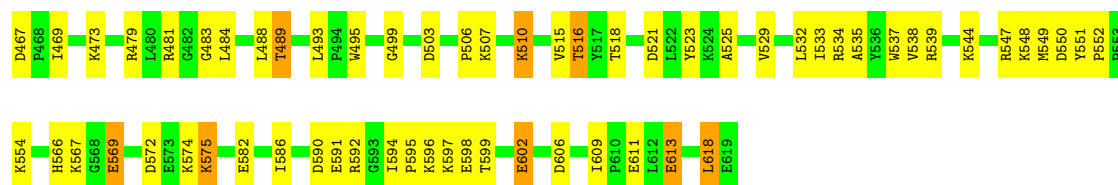
Chain A: 



• Molecule 1: FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE

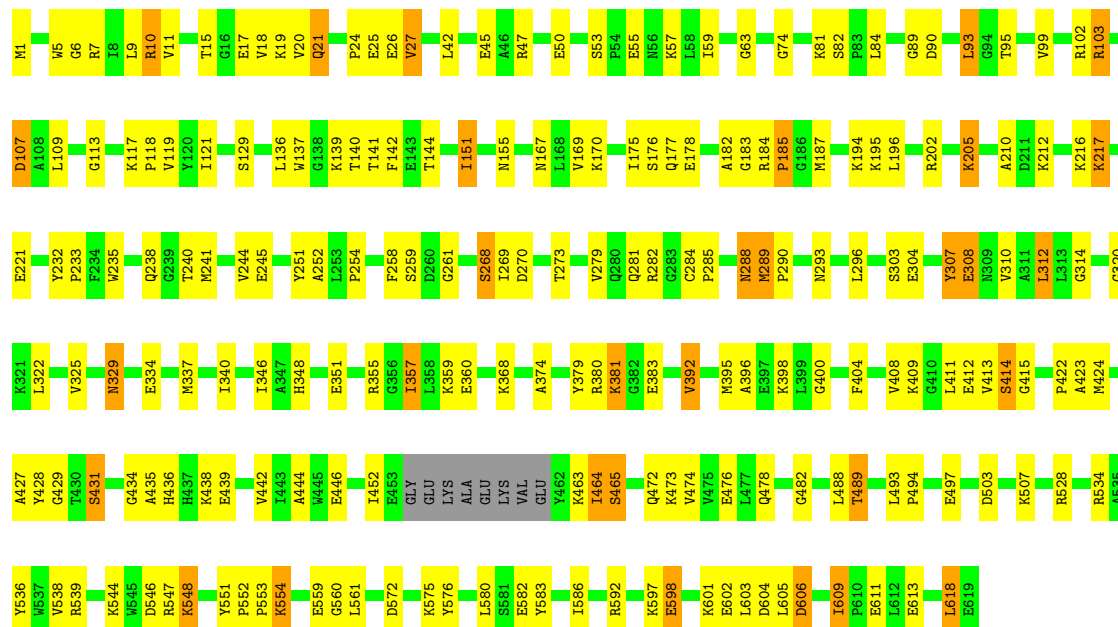
Chain B: 





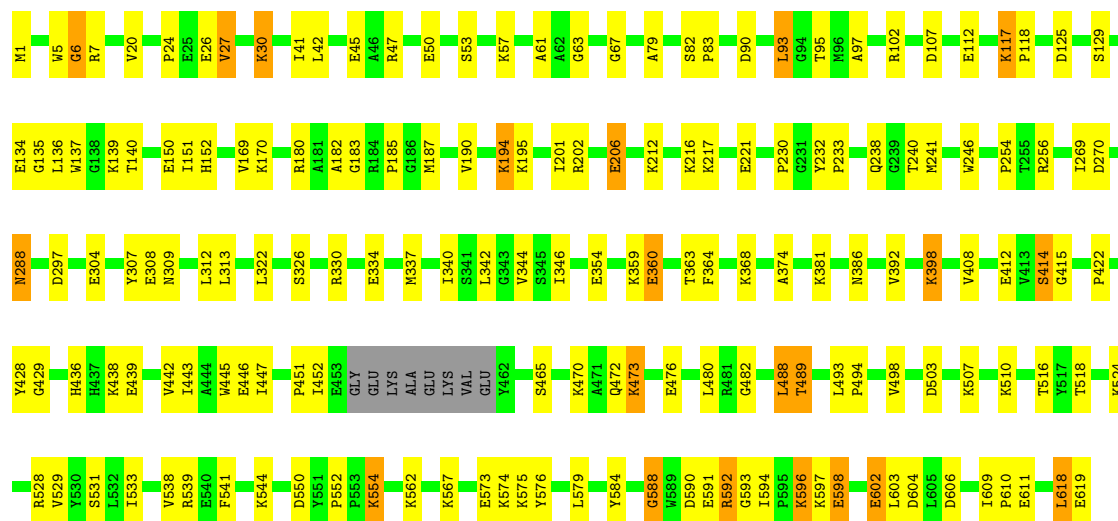
• Molecule 1: FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE

Chain C: 64% 29% 5% .



• Molecule 1: FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE

Chain D: 71% 24% . .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.40Å 170.50Å 180.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	77.0 (30.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.177 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19600	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: GUA, SF4, PTE, CA

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	0.48	0/4896	0.94	13/6619 (0.2%)
1	B	0.49	0/4896	0.97	16/6619 (0.2%)
1	C	0.50	0/4896	0.96	18/6619 (0.3%)
1	D	0.48	0/4896	0.96	18/6619 (0.3%)
All	All	0.49	0/19584	0.96	65/26476 (0.2%)

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	VAL	N-CA-C	-8.25	98.99	109.30
1	D	5	TRP	N-CA-C	-8.01	103.64	113.41
1	B	5	TRP	N-CA-C	-7.75	103.95	113.41
1	B	207	ILE	N-CA-C	7.60	115.16	108.63
1	B	82	SER	CA-C-N	7.13	126.76	119.56
1	B	82	SER	C-N-CA	7.13	126.76	119.56
1	B	82	SER	N-CA-C	6.99	119.78	109.50
1	A	439	GLU	N-CA-C	6.88	118.86	111.36
1	C	107	ASP	N-CA-C	-6.87	105.05	113.50
1	C	27	VAL	N-CA-C	-6.73	103.92	110.72
1	C	82	SER	CA-C-N	6.46	126.09	119.56
1	C	82	SER	C-N-CA	6.46	126.09	119.56
1	A	45	GLU	N-CA-C	6.32	120.72	112.89
1	C	497	GLU	N-CA-C	6.32	119.11	111.40
1	D	27	VAL	N-CA-C	-6.24	103.83	112.50
1	C	325	VAL	N-CA-C	-6.17	104.48	110.72
1	B	23	TYR	CA-C-N	6.13	127.50	119.84
1	B	23	TYR	C-N-CA	6.13	127.50	119.84
1	D	6	GLY	N-CA-C	-5.97	105.70	114.90
1	D	61	ALA	N-CA-C	5.91	118.88	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	TRP	N-CA-C	-5.91	104.24	112.45
1	A	190	VAL	N-CA-C	-5.89	105.11	110.82
1	D	152	HIS	N-CA-C	5.85	120.14	112.89
1	B	273	THR	N-CA-C	-5.79	104.88	111.14
1	C	289	MET	CA-C-N	5.75	125.75	119.89
1	C	289	MET	C-N-CA	5.75	125.75	119.89
1	B	6	GLY	N-CA-C	-5.70	107.09	115.30
1	C	81	LYS	N-CA-C	-5.68	101.43	109.96
1	C	45	GLU	N-CA-C	5.66	120.18	112.88
1	C	6	GLY	N-CA-C	-5.64	107.47	115.43
1	B	81	LYS	N-CA-C	-5.64	101.70	110.10
1	C	210	ALA	N-CA-C	5.61	117.07	111.07
1	B	45	GLU	N-CA-C	5.56	120.34	113.50
1	D	541	PHE	N-CA-C	-5.46	106.46	113.02
1	D	518	THR	N-CA-C	-5.46	103.49	110.53
1	A	82	SER	N-CA-C	5.43	117.49	109.50
1	D	79	ALA	N-CA-C	5.41	117.02	108.96
1	A	107	ASP	N-CA-C	-5.41	106.85	113.50
1	A	44	ASN	N-CA-C	5.40	117.02	111.03
1	D	194	LYS	N-CA-C	-5.36	106.33	112.92
1	A	289	MET	CA-C-N	5.34	125.35	119.90
1	A	289	MET	C-N-CA	5.34	125.35	119.90
1	D	125	ASP	CB-CA-C	-5.32	110.46	116.63
1	B	434	GLY	N-CA-C	-5.27	106.67	112.04
1	D	579	LEU	N-CA-C	-5.25	105.73	111.82
1	B	49	VAL	N-CA-C	5.25	116.14	110.21
1	D	169	VAL	N-CA-C	-5.22	101.95	108.84
1	D	170	LYS	N-CA-C	5.18	118.39	111.75
1	A	592	ARG	N-CA-C	-5.18	107.13	113.50
1	A	421	TYR	CA-C-N	5.13	124.58	119.24
1	A	421	TYR	C-N-CA	5.13	124.58	119.24
1	B	165	GLY	N-CA-C	-5.13	106.28	112.49
1	C	547	ARG	N-CA-C	5.13	116.87	111.28
1	D	45	GLU	N-CA-C	5.12	119.22	112.92
1	D	488	LEU	N-CA-C	5.12	116.67	111.14
1	C	307	TYR	N-CA-C	5.11	116.54	111.07
1	D	190	VAL	N-CA-C	-5.11	105.43	111.00
1	B	26	GLU	N-CA-C	-5.07	105.84	112.23
1	D	588	GLY	N-CA-C	-5.06	108.07	115.72
1	C	273	THR	N-CA-C	-5.05	105.86	111.36
1	C	592	ARG	N-CA-C	-5.05	107.11	114.12
1	C	169	VAL	N-CA-C	-5.04	103.00	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	LYS	N-CA-C	-5.04	106.65	112.89
1	C	59	ILE	N-CA-C	5.04	115.22	108.17
1	D	67	GLY	N-CA-C	-5.02	109.11	115.08

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	4786	0	4773	133	0
1	B	4786	0	4773	120	0
1	C	4786	0	4773	119	0
1	D	4786	0	4773	95	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	8	0	0	0	0
3	B	8	0	0	1	0
3	C	8	0	0	1	0
3	D	8	0	0	0	0
4	A	9	0	0	2	0
4	B	9	0	0	3	0
4	C	9	0	0	2	0
4	D	9	0	0	1	0
5	A	50	0	20	1	0
5	B	50	0	20	1	0
5	C	50	0	19	1	0
5	D	50	0	20	1	0
6	A	38	0	0	1	0
6	B	46	0	0	3	0
6	C	49	0	0	3	0
6	D	51	0	0	2	0
All	All	19600	0	19171	467	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 12.

All (467) 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:D:93:LEU:HB3	1:D:182:ALA:HB2	1.34	1.05
1:A:93:LEU:HB3	1:A:182:ALA:HB2	1.39	1.02
1:C:93:LEU:HB3	1:C:182:ALA:HB2	1.39	1.02
1:C:572:ASP:OD2	1:C:575:LYS:HG3	1.65	0.97
1:B:93:LEU:HB3	1:B:182:ALA:HB2	1.47	0.94
1:A:426:LEU:HD23	1:A:474:VAL:HG21	1.51	0.93
1:B:288:ASN:H	1:B:288:ASN:HD22	1.15	0.91
1:B:308:GLU:HG2	1:B:340:ILE:HD11	1.50	0.91
1:C:74:GLY:HA3	1:C:285:PRO:HG2	1.53	0.89
1:A:439:GLU:HG2	1:A:482:GLY:HA3	1.54	0.86
1:A:232:TYR:HB3	1:A:233:PRO:HD3	1.58	0.85
1:A:534:ARG:O	1:A:538:VAL:HG23	1.78	0.84
1:B:510:LYS:HZ2	1:B:510:LYS:HB2	1.43	0.84
1:B:26:GLU:O	1:B:30:LYS:HB2	1.80	0.82
1:C:103:ARG:O	1:C:205:LYS:HB2	1.80	0.81
1:C:268:SER:HB2	1:C:320:GLY:O	1.80	0.80
1:A:187:MET:N	1:A:187:MET:HE2	1.98	0.78
1:B:24:PRO:HB3	1:B:26:GLU:OE2	1.84	0.78
1:C:50:GLU:HB2	1:C:53:SER:HB3	1.67	0.77
1:C:9:LEU:HD23	1:C:109:LEU:HD13	1.68	0.76
1:B:572:ASP:OD2	1:B:575:LYS:HG3	1.86	0.76
1:D:308:GLU:HG2	1:D:340:ILE:HD11	1.69	0.75
1:C:444:ALA:HB3	6:C:639:HOH:O	1.86	0.74
1:A:572:ASP:OD2	1:A:575:LYS:HG3	1.88	0.73
1:A:214:GLU:OE1	1:A:217:LYS:HD3	1.88	0.72
1:D:340:ILE:O	1:D:344:VAL:HG23	1.90	0.72
1:A:345:SER:O	1:A:349:VAL:HG23	1.89	0.71
1:B:149:LYS:HD3	1:B:154:LYS:HA	1.71	0.71
1:D:297:ASP:HB3	1:D:326:SER:HB3	1.74	0.70
1:A:330:ARG:O	1:A:334:GLU:HG2	1.92	0.70
1:A:414:SER:HB2	1:A:428:TYR:OH	1.91	0.70
1:C:11:VAL:HG22	1:C:18:VAL:HG22	1.74	0.70
1:A:50:GLU:HB2	1:A:53:SER:HB3	1.72	0.69
1:B:7:ARG:NH1	1:B:20:VAL:HG11	2.07	0.69
1:C:284:CYS:HB3	1:C:285:PRO:HD2	1.75	0.68
1:C:308:GLU:HG2	1:C:340:ILE:HD11	1.76	0.66
1:D:136:LEU:O	1:D:139:LYS:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ARG:HG2	1:B:364:PHE:CG	2.30	0.66
1:B:481:ARG:HH22	4:B:622:GUA:C1	2.09	0.66
1:A:187:MET:HE2	1:A:187:MET:H	1.59	0.66
1:B:93:LEU:HA	5:B:623:PTE:O5P	1.96	0.65
1:C:474:VAL:O	1:C:478:GLN:HG3	1.97	0.65
1:A:74:GLY:HA3	1:A:285:PRO:HG2	1.79	0.65
1:A:598:GLU:O	1:A:602:GLU:HB2	1.96	0.65
1:C:140:THR:HB	1:C:334:GLU:HB2	1.77	0.65
1:B:83:PRO:HD2	1:B:185:PRO:O	1.97	0.65
1:C:24:PRO:HD2	1:C:27:VAL:HG21	1.79	0.65
1:D:238:GLN:O	1:D:241:MET:HB2	1.96	0.64
1:C:381:LYS:NZ	1:C:381:LYS:HB3	2.13	0.64
1:B:50:GLU:HB2	1:B:53:SER:HB3	1.79	0.64
1:C:288:ASN:HD22	1:C:288:ASN:H	1.44	0.64
1:C:503:ASP:O	1:C:507:LYS:HG3	1.97	0.64
1:A:597:LYS:HZ3	1:A:618:LEU:HB3	1.63	0.64
1:B:238:GLN:O	1:B:241:MET:HB2	1.98	0.64
1:C:238:GLN:O	1:C:241:MET:HB2	1.98	0.63
1:D:588:GLY:O	1:D:596:LYS:HG3	1.98	0.63
1:D:50:GLU:HB2	1:D:53:SER:HB3	1.80	0.63
1:B:288:ASN:HD22	1:B:288:ASN:N	1.90	0.62
1:C:183:GLY:HA3	1:C:187:MET:HB2	1.80	0.62
1:C:431:SER:HB3	1:C:434:GLY:O	1.99	0.62
1:D:232:TYR:HB3	1:D:233:PRO:HD3	1.79	0.62
1:A:288:ASN:HD22	1:A:288:ASN:H	1.47	0.62
1:C:424:MET:O	1:C:427:ALA:HB3	2.00	0.62
1:B:7:ARG:HH11	1:B:20:VAL:HG11	1.65	0.62
1:A:427:ALA:HB1	1:A:440:ALA:HB3	1.82	0.62
1:D:414:SER:HB3	1:D:428:TYR:OH	2.00	0.62
1:D:118:PRO:HB3	1:D:137:TRP:CE3	2.35	0.62
1:C:439:GLU:HG2	1:C:482:GLY:HA3	1.82	0.62
1:A:43:TRP:O	1:A:539:ARG:NH2	2.31	0.61
1:A:431:SER:HB3	1:A:434:GLY:O	2.00	0.61
1:D:7:ARG:NH1	1:D:20:VAL:HG11	2.16	0.61
1:A:63:GLY:HA3	1:A:488:LEU:O	2.02	0.60
1:B:148:LEU:HD23	1:C:151:ILE:HD12	1.82	0.60
1:B:13:LEU:HD12	1:B:194:LYS:HB3	1.83	0.60
1:B:308:GLU:OE2	1:B:415:GLY:N	2.28	0.60
1:C:99:VAL:O	1:C:103:ARG:HG3	2.01	0.59
1:C:281:GLN:NE2	1:C:293:ASN:OD1	2.35	0.59
1:D:381:LYS:NZ	1:D:381:LYS:HB3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:HIS:O	1:B:569:GLU:HB2	2.02	0.59
1:B:503:ASP:O	1:B:506:PRO:HD2	2.03	0.59
1:D:342:LEU:O	1:D:346:ILE:HG13	2.01	0.59
1:C:355:ARG:HB2	1:C:357:ILE:HD12	1.85	0.59
1:D:254:PRO:HG2	1:D:415:GLY:HA2	1.84	0.58
1:C:308:GLU:OE2	1:C:415:GLY:N	2.33	0.58
1:C:47:ARG:NH1	1:C:611:GLU:OE2	2.36	0.58
1:A:151:ILE:HG13	1:D:151:ILE:HG13	1.84	0.58
1:B:381:LYS:NZ	1:B:381:LYS:HB3	2.19	0.58
1:B:429:GLY:O	1:B:550:ASP:HA	2.02	0.58
1:C:217:LYS:O	1:C:221:GLU:HG3	2.03	0.58
1:A:393:LYS:HD2	1:A:410:GLY:HA2	1.84	0.58
1:B:99:VAL:O	1:B:103:ARG:HG2	2.04	0.58
1:B:342:LEU:O	1:B:346:ILE:HG13	2.03	0.58
1:C:355:ARG:CB	1:C:357:ILE:HD12	2.34	0.58
1:A:543:GLY:HA3	1:A:616:THR:HG23	1.84	0.57
1:B:431:SER:HB3	1:B:434:GLY:O	2.04	0.57
1:D:26:GLU:CD	1:D:26:GLU:H	2.12	0.57
1:A:441:TRP:HB2	1:A:481:ARG:NH2	2.20	0.57
1:D:337:MET:HE1	1:D:374:ALA:O	2.02	0.57
1:A:610:PRO:O	1:A:614:LYS:HG3	2.04	0.57
1:C:167:ASN:ND2	1:C:379:TYR:HA	2.20	0.57
1:A:308:GLU:CG	1:A:340:ILE:HD11	2.34	0.57
1:B:532:LEU:O	1:B:535:ALA:HB3	2.05	0.57
1:B:240:THR:O	1:B:307:TYR:HB2	2.04	0.57
1:C:392:VAL:CG2	1:C:412:GLU:HG3	2.35	0.57
1:B:185:PRO:HD3	6:B:629:HOH:O	2.05	0.56
1:D:354:GLU:OE2	1:D:363:THR:HB	2.05	0.56
1:A:63:GLY:N	1:A:66:ASN:OD1	2.39	0.56
1:A:429:GLY:O	1:A:550:ASP:HA	2.05	0.56
1:C:175:ILE:HG22	1:C:176:SER:N	2.19	0.56
1:C:212:LYS:O	1:C:216:LYS:HG3	2.05	0.56
1:A:45:GLU:HB3	1:A:57:LYS:HE2	1.87	0.56
1:A:93:LEU:HA	5:A:623:PTE:O5P	2.05	0.56
1:D:117:LYS:HB2	6:D:664:HOH:O	2.06	0.56
1:C:142:PHE:CE1	1:C:178:GLU:HA	2.41	0.55
1:D:308:GLU:CG	1:D:340:ILE:HD11	2.36	0.55
1:D:524:LYS:HE3	1:D:528:ARG:NH2	2.21	0.55
1:A:539:ARG:HD2	1:A:540:GLU:OE2	2.05	0.55
1:A:147:GLU:HB3	1:D:151:ILE:HD11	1.87	0.55
1:A:597:LYS:NZ	1:A:618:LEU:HB3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:ARG:O	1:D:334:GLU:HG2	2.06	0.55
1:D:446:GLU:HG3	1:D:470:LYS:HE2	1.87	0.55
1:D:185:PRO:HD2	1:D:187:MET:CE	2.36	0.55
1:D:309:ASN:O	1:D:313:LEU:HB2	2.07	0.55
1:C:93:LEU:HA	5:C:623:PTE:O5P	2.07	0.55
1:A:308:GLU:HG2	1:A:340:ILE:HD11	1.88	0.54
1:D:598:GLU:O	1:D:602:GLU:HB2	2.07	0.54
1:A:503:ASP:O	1:A:506:PRO:HD2	2.06	0.54
1:D:1:MET:HE1	1:D:6:GLY:HA3	1.88	0.54
1:D:312:LEU:HG	1:D:340:ILE:HG23	1.89	0.54
1:A:52:LEU:HD22	1:A:193:SER:HB3	1.89	0.54
1:D:240:THR:O	1:D:307:TYR:HB2	2.07	0.54
1:B:103:ARG:HB2	1:B:203:GLY:HA3	1.89	0.54
1:A:404:PHE:HB3	1:A:555:ARG:NH2	2.23	0.54
1:A:534:ARG:NH1	1:A:545:TRP:HE1	2.06	0.54
1:B:309:ASN:O	1:B:313:LEU:HB2	2.08	0.54
1:B:91:GLY:HA3	1:B:183:GLY:H	1.73	0.53
1:C:534:ARG:O	1:C:538:VAL:HG23	2.08	0.53
1:B:103:ARG:O	1:B:205:LYS:HB2	2.08	0.53
1:D:206:GLU:HG2	1:D:206:GLU:O	2.08	0.53
1:A:76:LEU:HB2	1:A:98:SER:HB2	1.90	0.53
1:C:117:LYS:O	1:C:119:VAL:HG13	2.08	0.53
1:A:140:THR:HB	1:A:334:GLU:HB2	1.91	0.53
1:B:288:ASN:H	1:B:288:ASN:ND2	1.95	0.53
1:B:232:TYR:HB3	1:B:233:PRO:HD3	1.89	0.53
1:D:445:TRP:CD1	1:D:473:LYS:HE2	2.44	0.53
1:B:259:SER:HB2	6:B:656:HOH:O	2.09	0.52
1:B:183:GLY:HA3	1:B:187:MET:HB2	1.90	0.52
1:D:93:LEU:HA	5:D:623:PTE:O5P	2.09	0.52
1:A:404:PHE:N	1:A:404:PHE:CD1	2.78	0.52
1:A:468:PRO:HB2	1:A:582:GLU:HG2	1.90	0.52
1:A:226:ILE:HD11	1:A:494:PRO:HB3	1.91	0.52
1:C:55:GLU:O	1:C:57:LYS:NZ	2.41	0.52
1:C:251:TYR:HA	1:C:261:GLY:O	2.09	0.52
1:B:31:PHE:O	1:B:33:GLY:N	2.39	0.52
1:B:63:GLY:HA3	1:B:488:LEU:O	2.10	0.52
1:D:288:ASN:H	1:D:288:ASN:HD22	1.58	0.52
1:A:232:TYR:HB3	1:A:233:PRO:CD	2.36	0.52
1:B:78:VAL:HG12	1:B:187:MET:HG3	1.92	0.52
1:C:337:MET:HE1	1:C:374:ALA:O	2.09	0.52
1:C:436:HIS:CE1	1:C:438:LYS:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:LEU:O	1:A:604:ASP:HB2	2.08	0.52
1:B:78:VAL:HG12	1:B:187:MET:CG	2.39	0.51
1:B:414:SER:HB2	1:B:428:TYR:CE1	2.44	0.51
1:C:113:GLY:O	1:C:194:LYS:HG2	2.11	0.51
1:D:488:LEU:N	1:D:489:THR:HA	2.26	0.51
1:A:202:ARG:NH1	1:A:202:ARG:HG3	2.25	0.51
1:B:180:ARG:HD2	1:B:180:ARG:N	2.26	0.51
1:D:494:PRO:O	1:D:498:VAL:HG22	2.11	0.51
1:A:340:ILE:O	1:A:344:VAL:HG23	2.10	0.51
1:B:1:MET:SD	1:B:25:GLU:HG3	2.49	0.51
1:B:245:GLU:OE1	1:B:270:ASP:OD2	2.29	0.51
1:B:598:GLU:O	1:B:602:GLU:HB2	2.11	0.51
1:C:142:PHE:CD1	1:C:178:GLU:HG2	2.46	0.51
1:D:230:PRO:O	1:D:233:PRO:HD2	2.10	0.51
1:D:452:ILE:HG13	1:D:452:ILE:O	2.11	0.51
1:A:466:TYR:O	1:A:467:ASP:C	2.51	0.51
1:D:584:TYR:CE1	1:D:593:GLY:HA2	2.46	0.51
1:D:603:LEU:O	1:D:604:ASP:HB2	2.09	0.51
1:D:270:ASP:OD1	1:D:270:ASP:C	2.53	0.51
1:B:609:ILE:O	1:B:613:GLU:HB2	2.11	0.50
1:C:580:LEU:O	1:C:583:TYR:HB3	2.11	0.50
1:D:439:GLU:HG2	1:D:482:GLY:HA3	1.93	0.50
1:B:409:LYS:HG2	1:B:549:MET:HE3	1.94	0.50
1:C:121:ILE:HG13	1:C:196:LEU:HD11	1.93	0.50
1:C:348:HIS:CG	1:C:392:VAL:HG12	2.46	0.50
1:D:562:LYS:O	1:D:567:LYS:HD2	2.12	0.50
1:A:28:ALA:O	1:A:32:ILE:N	2.41	0.50
1:A:47:ARG:NH1	1:A:611:GLU:OE2	2.44	0.50
1:C:442:VAL:HG22	1:C:442:VAL:O	2.11	0.50
1:D:140:THR:HB	1:D:334:GLU:HB2	1.92	0.50
1:D:180:ARG:N	1:D:180:ARG:HD2	2.25	0.50
1:B:308:GLU:OE1	4:B:622:GUA:O3	2.29	0.50
1:C:185:PRO:HD2	1:C:187:MET:CE	2.41	0.50
1:C:598:GLU:OE1	1:C:598:GLU:HA	2.12	0.50
1:D:256:ARG:HG2	1:D:364:PHE:CG	2.47	0.50
1:D:359:LYS:C	1:D:360:GLU:HG2	2.36	0.50
1:D:381:LYS:HB3	1:D:381:LYS:HZ2	1.76	0.50
1:D:392:VAL:HG22	1:D:412:GLU:HG3	1.93	0.50
1:B:596:LYS:O	1:B:599:THR:HB	2.12	0.50
1:C:414:SER:HB2	1:C:428:TYR:CE1	2.46	0.50
1:C:528:ARG:HG3	1:C:605:LEU:HD21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASP:OD1	1:A:270:ASP:C	2.55	0.49
1:A:546:ASP:C	1:A:546:ASP:OD1	2.54	0.49
1:B:50:GLU:HB2	1:B:53:SER:CB	2.43	0.49
1:A:243:ALA:HB2	6:A:631:HOH:O	2.11	0.49
1:B:479:ARG:HD3	1:B:523:TYR:HB3	1.94	0.49
1:C:1:MET:HE2	1:C:25:GLU:HB2	1.94	0.49
1:D:308:GLU:OE2	1:D:415:GLY:N	2.36	0.49
1:C:118:PRO:HB3	1:C:137:TRP:CE3	2.48	0.49
1:A:308:GLU:OE2	1:A:415:GLY:N	2.35	0.49
1:A:26:GLU:O	1:A:30:LYS:HB2	2.12	0.49
1:A:47:ARG:HG3	1:A:539:ARG:CZ	2.43	0.49
1:A:308:GLU:OE2	1:A:414:SER:HB3	2.13	0.49
1:C:554:LYS:O	1:C:554:LYS:HG2	2.12	0.49
1:D:97:ALA:HB1	1:D:201:ILE:HD12	1.95	0.49
1:B:88:TYR:HB3	1:B:533:ILE:HG23	1.95	0.49
1:A:145:GLU:O	1:A:149:LYS:HG3	2.12	0.49
1:B:74:GLY:HA3	1:B:285:PRO:HG2	1.95	0.49
1:D:288:ASN:HD22	1:D:288:ASN:N	2.10	0.49
1:B:90:ASP:OD1	1:B:90:ASP:C	2.56	0.48
1:C:408:VAL:O	1:C:409:LYS:HB2	2.13	0.48
1:C:348:HIS:CD2	1:C:395:MET:HE3	2.48	0.48
1:A:31:PHE:O	1:A:33:GLY:N	2.42	0.48
1:A:334:GLU:C	1:A:335:MET:HE2	2.38	0.48
1:C:597:LYS:O	1:C:601:LYS:HG3	2.13	0.48
4:D:622:GUA:C4	4:D:622:GUA:O1	2.66	0.48
1:B:344:VAL:HG12	1:B:392:VAL:HG11	1.95	0.48
1:C:184:ARG:HB2	1:C:185:PRO:HD3	1.95	0.48
1:A:488:LEU:N	1:A:489:THR:HA	2.28	0.48
1:B:254:PRO:HG2	1:B:415:GLY:HA2	1.95	0.48
1:C:232:TYR:HB3	1:C:233:PRO:HD3	1.95	0.48
1:C:488:LEU:N	1:C:489:THR:HA	2.29	0.48
1:A:183:GLY:HA3	1:A:187:MET:HB2	1.96	0.48
1:C:452:ILE:HG13	1:C:452:ILE:O	2.13	0.48
4:C:622:GUA:O1	4:C:622:GUA:C4	2.66	0.48
1:B:28:ALA:O	1:B:32:ILE:N	2.46	0.48
1:C:136:LEU:O	1:C:139:LYS:HG3	2.14	0.48
1:B:72:SER:HB3	3:B:621:SF4:S3	2.53	0.47
1:B:85:THR:HB	1:B:537:TRP:HH2	1.79	0.47
1:C:270:ASP:HB2	6:C:644:HOH:O	2.14	0.47
1:C:546:ASP:OD1	1:C:546:ASP:C	2.57	0.47
1:D:524:LYS:HE3	1:D:528:ARG:HH22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ILE:HG22	1:A:176:SER:N	2.28	0.47
1:A:423:ALA:HB2	1:A:470:LYS:HD3	1.96	0.47
1:B:26:GLU:CD	1:B:26:GLU:H	2.22	0.47
1:B:439:GLU:O	1:B:481:ARG:HB2	2.15	0.47
1:B:525:ALA:O	1:B:529:VAL:HG23	2.15	0.47
1:C:288:ASN:HD22	1:C:288:ASN:N	2.10	0.47
1:D:552:PRO:HD3	1:D:576:TYR:CZ	2.49	0.47
4:A:622:GUA:C4	4:A:622:GUA:O1	2.68	0.47
1:D:135:GLY:O	1:D:139:LYS:HE3	2.15	0.47
1:B:269:ILE:HA	1:B:322:LEU:HB2	1.96	0.47
1:C:408:VAL:HG11	1:C:429:GLY:HA2	1.96	0.47
1:C:603:LEU:O	1:C:604:ASP:HB2	2.14	0.47
1:B:510:LYS:HA	1:B:515:VAL:O	2.15	0.47
1:C:7:ARG:NH1	1:C:20:VAL:HG11	2.29	0.47
1:C:289:MET:N	1:C:290:PRO:CD	2.77	0.47
1:C:312:LEU:HG	1:C:340:ILE:HG23	1.96	0.47
1:B:140:THR:HB	1:B:334:GLU:HB2	1.95	0.47
1:B:408:VAL:HB	1:B:435:ALA:HB2	1.96	0.47
1:C:63:GLY:HA3	1:C:488:LEU:O	2.15	0.47
1:D:429:GLY:O	1:D:550:ASP:HA	2.14	0.47
1:A:202:ARG:HG3	1:A:202:ARG:HH11	1.80	0.47
1:A:215:LEU:HD12	1:A:508:LEU:CD2	2.45	0.47
1:B:414:SER:HB2	1:B:428:TYR:OH	2.15	0.47
1:B:510:LYS:HZ2	1:B:510:LYS:CB	2.21	0.47
1:B:582:GLU:O	1:B:586:ILE:HG13	2.15	0.47
1:C:310:VAL:O	1:C:314:GLY:N	2.47	0.47
1:A:408:VAL:HB	1:A:435:ALA:HB2	1.96	0.47
1:D:90:ASP:OD1	1:D:90:ASP:C	2.58	0.47
1:B:538:VAL:HG21	1:B:594:ILE:HG12	1.97	0.47
1:C:235:TRP:NE1	1:C:289:MET:HE3	2.30	0.47
1:B:209:VAL:HG11	1:B:212:LYS:HA	1.97	0.46
1:B:258:PHE:CD2	1:B:406:MET:HG3	2.49	0.46
1:B:467:ASP:CG	1:B:469:ILE:HG22	2.40	0.46
1:D:590:ASP:C	1:D:592:ARG:H	2.23	0.46
4:B:622:GUA:O1	4:B:622:GUA:C4	2.67	0.46
1:B:441:TRP:HB2	1:B:481:ARG:NH2	2.30	0.46
1:C:183:GLY:O	1:C:184:ARG:C	2.57	0.46
1:C:582:GLU:O	1:C:586:ILE:HG13	2.15	0.46
1:D:597:LYS:HG2	1:D:618:LEU:HD23	1.97	0.46
1:A:439:GLU:HG2	1:A:482:GLY:CA	2.37	0.46
1:A:452:ILE:O	1:A:452:ILE:HG13	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ARG:HD3	1:A:523:TYR:HB3	1.98	0.46
1:C:10:ARG:HD3	1:C:21:GLN:OE1	2.15	0.46
1:C:175:ILE:CG2	1:C:176:SER:N	2.78	0.46
1:C:472:GLN:O	1:C:476:GLU:HG3	2.15	0.46
1:A:116:LYS:H	1:A:116:LYS:HG2	1.44	0.46
1:A:240:THR:O	1:A:307:TYR:HB2	2.15	0.46
1:C:439:GLU:HG2	1:C:482:GLY:CA	2.45	0.46
1:C:244:VAL:HB	6:C:644:HOH:O	2.15	0.46
1:C:308:GLU:HG2	1:C:340:ILE:CD1	2.45	0.46
1:B:590:ASP:C	1:B:592:ARG:H	2.24	0.46
1:A:170:LYS:HD2	1:A:170:LYS:HA	1.68	0.46
1:B:10:ARG:HD3	1:B:21:GLN:OE1	2.15	0.46
1:B:101:LEU:HA	1:B:201:ILE:HG21	1.98	0.46
1:B:355:ARG:HB2	1:B:357:ILE:HD12	1.98	0.46
1:B:452:ILE:O	1:B:452:ILE:HG13	2.16	0.46
1:D:117:LYS:HB3	1:D:117:LYS:HZ2	1.81	0.46
1:B:235:TRP:CH2	1:B:493:LEU:HD13	2.51	0.45
1:C:74:GLY:CA	1:C:285:PRO:HG2	2.36	0.45
1:A:359:LYS:HA	1:A:359:LYS:HD3	1.52	0.45
1:A:534:ARG:HH11	1:A:545:TRP:HE1	1.64	0.45
1:C:411:LEU:O	1:C:435:ALA:HB3	2.16	0.45
1:C:606:ASP:O	1:C:609:ILE:HG13	2.16	0.45
1:D:472:GLN:O	1:D:476:GLU:HG3	2.16	0.45
1:B:184:ARG:HB2	6:B:629:HOH:O	2.17	0.45
1:A:82:SER:HA	1:A:83:PRO:HD3	1.78	0.45
1:A:422:PRO:HD2	1:A:446:GLU:OE2	2.16	0.45
1:A:148:LEU:HD13	1:A:200:VAL:CG2	2.47	0.45
1:B:43:TRP:O	1:B:539:ARG:NH2	2.46	0.45
1:B:175:ILE:HG22	1:B:176:SER:N	2.30	0.45
1:D:269:ILE:HA	1:D:322:LEU:HB2	1.98	0.45
1:D:538:VAL:HG21	1:D:594:ILE:HG23	1.98	0.45
1:C:15:THR:OG1	1:C:17:GLU:HB2	2.17	0.45
1:D:609:ILE:HB	1:D:610:PRO:CD	2.47	0.45
1:C:240:THR:O	1:C:307:TYR:HB2	2.16	0.45
1:A:418:CYS:SG	1:A:424:MET:HB3	2.57	0.45
1:B:373:LEU:O	1:B:377:ILE:HG13	2.16	0.45
1:B:518:THR:O	1:B:521:ASP:HB2	2.17	0.45
1:C:609:ILE:HG23	1:C:618:LEU:HD23	1.99	0.45
1:A:117:LYS:O	1:A:119:VAL:HG13	2.16	0.44
1:A:546:ASP:OD1	1:A:548:LYS:HB2	2.17	0.44
1:B:451:PRO:C	1:B:453:GLU:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ARG:NH1	1:C:107:ASP:OD1	2.50	0.44
1:A:350:MET:O	1:A:354:GLU:HG3	2.17	0.44
1:A:423:ALA:HB1	1:A:442:VAL:HG21	2.00	0.44
1:B:163:PRO:HA	1:B:166:GLU:HB2	1.99	0.44
1:B:548:LYS:HD2	1:B:548:LYS:HA	1.75	0.44
1:C:396:ALA:O	1:C:400:GLY:N	2.49	0.44
1:A:534:ARG:HH22	1:A:550:ASP:CG	2.26	0.44
1:A:548:LYS:HD2	1:A:548:LYS:HA	1.53	0.44
1:C:548:LYS:O	1:C:551:TYR:HB2	2.18	0.44
1:B:488:LEU:N	1:B:489:THR:HA	2.32	0.44
1:B:597:LYS:HG3	1:B:618:LEU:HB3	2.00	0.44
1:C:351:GLU:HG2	1:C:404:PHE:CE2	2.53	0.44
1:D:503:ASP:O	1:D:507:LYS:HG3	2.18	0.44
1:B:430:THR:O	1:B:431:SER:C	2.59	0.44
1:C:548:LYS:HE2	1:C:551:TYR:CE2	2.53	0.44
1:D:183:GLY:HA3	1:D:187:MET:HB2	2.00	0.44
1:A:41:ILE:HG23	1:A:45:GLU:HG3	2.00	0.44
1:A:76:LEU:O	1:A:92:ASN:HA	2.18	0.44
1:B:125:ASP:OD2	1:B:204:THR:OG1	2.36	0.44
1:B:551:TYR:HA	1:B:552:PRO:HD3	1.85	0.44
1:C:141:THR:OG1	1:C:334:GLU:HA	2.18	0.44
1:D:246:TRP:CD2	1:D:451:PRO:HG3	2.52	0.44
1:A:423:ALA:HB3	1:A:446:GLU:OE1	2.18	0.44
1:A:560:GLY:O	1:A:561:LEU:C	2.60	0.44
1:B:534:ARG:HG3	1:B:595:PRO:HD3	1.99	0.44
1:A:170:LYS:HG2	1:A:390:GLU:HA	2.00	0.44
1:B:547:ARG:NH1	1:B:591:GLU:OE1	2.48	0.44
1:A:254:PRO:HB3	1:A:258:PHE:CD1	2.53	0.43
1:B:278:LYS:HE2	1:B:293:ASN:OD1	2.18	0.43
1:C:359:LYS:HD3	1:C:359:LYS:HA	1.78	0.43
1:C:493:LEU:O	1:C:494:PRO:C	2.61	0.43
1:A:148:LEU:HD13	1:A:200:VAL:HG22	2.00	0.43
1:A:534:ARG:HA	1:A:534:ARG:HD3	1.78	0.43
1:B:484:LEU:O	1:B:488:LEU:HG	2.17	0.43
1:D:398:LYS:HZ3	1:D:398:LYS:HG3	1.74	0.43
1:D:24:PRO:HB3	1:D:26:GLU:OE2	2.18	0.43
1:D:246:TRP:CE3	1:D:451:PRO:HG3	2.54	0.43
1:A:142:PHE:N	1:A:142:PHE:CD1	2.86	0.43
1:C:89:GLY:O	1:C:90:ASP:HB3	2.18	0.43
1:D:529:VAL:O	1:D:533:ILE:HD12	2.18	0.43
1:A:312:LEU:N	1:A:312:LEU:HD22	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:ARG:NH1	1:D:611:GLU:OE2	2.50	0.43
1:D:422:PRO:HD2	1:D:446:GLU:OE2	2.19	0.43
1:D:554:LYS:O	1:D:554:LYS:HG2	2.18	0.43
1:A:78:VAL:HG12	1:A:187:MET:HG3	2.00	0.43
1:A:493:LEU:N	1:A:494:PRO:CD	2.82	0.43
1:B:185:PRO:HD2	1:B:187:MET:CE	2.48	0.43
1:A:141:THR:OG1	1:A:334:GLU:HA	2.17	0.43
1:B:284:CYS:HB3	1:B:285:PRO:HD2	2.00	0.43
1:D:26:GLU:O	1:D:30:LYS:HB2	2.19	0.43
1:A:50:GLU:CB	1:A:53:SER:HB3	2.46	0.43
1:B:177:GLN:O	1:B:178:GLU:C	2.61	0.43
1:B:414:SER:HB2	1:B:428:TYR:HE1	1.84	0.43
1:A:25:GLU:HG2	1:A:29:LYS:HE3	2.00	0.43
1:A:102:ARG:HA	1:A:106:TYR:O	2.18	0.43
1:C:329:ASN:C	1:C:329:ASN:HD22	2.26	0.43
1:A:75:LYS:HD2	1:A:92:ASN:OD1	2.19	0.43
1:B:76:LEU:HB2	1:B:98:SER:HB2	2.00	0.43
1:D:493:LEU:O	1:D:494:PRO:C	2.60	0.43
1:A:66:ASN:HB2	1:A:102:ARG:HG3	2.00	0.42
1:A:312:LEU:HD13	1:A:312:LEU:HA	1.77	0.42
1:B:408:VAL:HG11	1:B:429:GLY:HA2	2.01	0.42
1:D:42:LEU:HD23	1:D:42:LEU:HA	1.88	0.42
1:A:202:ARG:NH2	1:D:134:GLU:OE2	2.52	0.42
1:B:178:GLU:O	1:B:282:ARG:NH1	2.52	0.42
1:C:24:PRO:HD2	1:C:27:VAL:CG2	2.47	0.42
1:D:82:SER:HA	1:D:83:PRO:HD3	1.78	0.42
1:D:117:LYS:HB3	1:D:117:LYS:NZ	2.33	0.42
1:A:29:LYS:HA	1:A:517:TYR:OH	2.19	0.42
1:D:93:LEU:HB3	1:D:182:ALA:CB	2.25	0.42
1:D:436:HIS:CE1	1:D:438:LYS:HB2	2.54	0.42
1:A:59:ILE:HG23	1:A:110:VAL:HG22	2.02	0.42
1:D:408:VAL:HG11	1:D:429:GLY:HA2	2.01	0.42
1:A:177:GLN:O	1:A:178:GLU:C	2.62	0.42
1:A:284:CYS:HB3	1:A:285:PRO:HD2	2.02	0.42
1:C:5:TRP:HB3	1:C:7:ARG:HG3	2.00	0.42
1:C:177:GLN:O	1:C:178:GLU:C	2.63	0.42
1:A:548:LYS:O	1:A:551:TYR:HB2	2.20	0.42
1:C:42:LEU:O	1:C:536:TYR:HE2	2.02	0.42
1:C:552:PRO:HD3	1:C:576:TYR:CZ	2.55	0.42
1:A:466:TYR:N	1:A:466:TYR:CD1	2.87	0.42
1:A:609:ILE:O	1:A:613:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:LYS:HD2	1:B:92:ASN:OD1	2.19	0.42
1:C:269:ILE:HA	1:C:322:LEU:HB2	2.02	0.42
1:D:597:LYS:N	1:D:619:GLU:O	2.38	0.42
1:B:483:GLY:O	1:B:484:LEU:C	2.63	0.42
1:C:355:ARG:HB3	1:C:357:ILE:HD12	2.01	0.42
1:C:90:ASP:OD1	1:C:90:ASP:C	2.63	0.41
1:C:422:PRO:HG2	1:C:465:SER:O	2.20	0.41
1:D:185:PRO:HD2	1:D:187:MET:HE2	2.02	0.41
1:D:112:GLU:HA	1:D:194:LYS:HE3	2.01	0.41
1:A:185:PRO:HD2	1:A:187:MET:HE3	2.02	0.41
1:A:308:GLU:OE1	4:A:622:GUA:O3	2.38	0.41
1:B:392:VAL:HG22	1:B:412:GLU:HG3	2.01	0.41
1:B:495:TRP:O	1:B:499:GLY:HA2	2.21	0.41
1:C:423:ALA:HB3	1:C:446:GLU:CD	2.45	0.41
1:D:139:LYS:HA	6:D:660:HOH:O	2.19	0.41
1:C:251:TYR:O	1:C:261:GLY:HA3	2.21	0.41
1:C:413:VAL:HG21	1:C:553:PRO:HG2	2.02	0.41
1:B:479:ARG:HD3	1:B:523:TYR:CB	2.50	0.41
1:A:257:ASN:ND2	1:A:404:PHE:HB2	2.35	0.41
1:A:335:MET:HE2	1:A:335:MET:N	2.35	0.41
1:A:505:TYR:HB2	1:A:506:PRO:HD3	2.02	0.41
1:A:525:ALA:O	1:A:528:ARG:HB3	2.20	0.41
1:D:442:VAL:O	1:D:442:VAL:HG22	2.20	0.41
1:D:529:VAL:HG12	1:D:533:ILE:HD12	2.02	0.41
1:A:552:PRO:HD3	1:A:576:TYR:CZ	2.55	0.41
1:D:63:GLY:HA3	1:D:488:LEU:O	2.20	0.41
1:A:282:ARG:CZ	1:A:294:VAL:HG21	2.51	0.41
1:A:597:LYS:O	1:A:601:LYS:HG3	2.20	0.41
1:B:82:SER:HB3	1:B:85:THR:OG1	2.20	0.41
1:A:9:LEU:HD23	1:A:109:LEU:HD13	2.02	0.41
1:A:10:ARG:HD3	1:A:21:GLN:OE1	2.19	0.41
1:A:94:GLY:HA3	1:A:284:CYS:SG	2.61	0.41
1:A:126:ASP:OD2	1:A:205:LYS:NZ	2.54	0.41
1:A:585:ARG:NH1	1:A:585:ARG:HG2	2.36	0.41
1:B:72:SER:N	1:B:286:TYR:O	2.49	0.41
1:B:451:PRO:C	1:B:453:GLU:N	2.79	0.41
1:C:252:ALA:O	1:C:254:PRO:HD3	2.21	0.41
1:C:279:VAL:HG11	1:C:296:LEU:HG	2.03	0.41
1:A:430:THR:O	1:A:431:SER:C	2.62	0.41
1:B:285:PRO:O	1:B:286:TYR:HB2	2.21	0.41
1:C:84:LEU:HD13	1:C:170:LYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:PRO:HG2	1:C:415:GLY:HA2	2.03	0.41
1:B:184:ARG:C	1:B:186:GLY:H	2.29	0.40
1:C:136:LEU:HD22	1:C:144:THR:HG23	2.02	0.40
1:D:510:LYS:NZ	1:D:516:THR:OG1	2.49	0.40
1:A:123:ILE:O	1:A:201:ILE:HA	2.20	0.40
1:C:308:GLU:OE1	4:C:622:GUA:O3	2.39	0.40
1:C:560:GLY:O	1:C:561:LEU:C	2.64	0.40
1:A:288:ASN:HD22	1:A:288:ASN:N	2.14	0.40
1:A:309:ASN:CG	1:A:339:THR:HG21	2.46	0.40
1:A:582:GLU:OE1	1:A:582:GLU:HA	2.21	0.40
1:B:82:SER:HA	1:B:83:PRO:HD3	1.68	0.40
1:B:326:SER:O	1:B:329:ASN:HB3	2.22	0.40
1:B:516:THR:O	1:B:516:THR:HG22	2.20	0.40
1:C:379:TYR:O	1:C:380:ARG:C	2.64	0.40
1:D:443:ILE:O	1:D:447:ILE:HG13	2.21	0.40
1:A:537:TRP:O	1:A:541:PHE:HB2	2.21	0.40
1:C:290:PRO:HA	3:C:621:SF4:S2	2.62	0.40
1:D:217:LYS:O	1:D:221:GLU:HG3	2.21	0.40
1:B:184:ARG:HB2	1:B:185:PRO:HD3	2.02	0.40
1:D:102:ARG:NH1	1:D:107:ASP:OD1	2.55	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	607/619 (98%)	570 (94%)	34 (6%)	3 (0%)	24	37
1	B	607/619 (98%)	572 (94%)	31 (5%)	4 (1%)	18	28
1	C	607/619 (98%)	569 (94%)	35 (6%)	3 (0%)	24	37
1	D	607/619 (98%)	572 (94%)	34 (6%)	1 (0%)	43	58
All	All	2428/2476 (98%)	2283 (94%)	134 (6%)	11 (0%)	24	37

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	GLU
1	B	24	PRO
1	B	178	GLU
1	D	591	GLU
1	C	258	PHE
1	A	32	ILE
1	A	414	SER
1	B	32	ILE
1	B	185	PRO
1	C	464	ILE
1	C	185	PRO

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	493/499 (99%)	449 (91%)	44 (9%)	9	15
1	B	493/499 (99%)	447 (91%)	46 (9%)	8	14
1	C	493/499 (99%)	443 (90%)	50 (10%)	7	11
1	D	493/499 (99%)	455 (92%)	38 (8%)	12	20
All	All	1972/1996 (99%)	1794 (91%)	178 (9%)	9	15

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	45	GLU
1	A	93	LEU
1	A	95	THR
1	A	109	LEU
1	A	114	LYS
1	A	116	LYS
1	A	117	LYS
1	A	154	LYS

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Mol	Chain	Res	Type
1	A	170	LYS
1	A	177	GLN
1	A	187	MET
1	A	195	LYS
1	A	202	ARG
1	A	205	LYS
1	A	213	GLU
1	A	216	LYS
1	A	245	GLU
1	A	267	ARG
1	A	268	SER
1	A	288	ASN
1	A	359	LYS
1	A	381	LYS
1	A	397	GLU
1	A	398	LYS
1	A	404	PHE
1	A	426	LEU
1	A	431	SER
1	A	433	ILE
1	A	465	SER
1	A	469	ILE
1	A	473	LYS
1	A	489	THR
1	A	510	LYS
1	A	544	LYS
1	A	548	LYS
1	A	554	LYS
1	A	573	GLU
1	A	574	LYS
1	A	578	GLU
1	A	592	ARG
1	A	601	LYS
1	A	613	GLU
1	A	618	LEU
1	B	10	ARG
1	B	19	LYS
1	B	21	GLN
1	B	26	GLU
1	B	29	LYS
1	B	30	LYS
1	B	72	SER

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Mol	Chain	Res	Type
1	B	90	ASP
1	B	93	LEU
1	B	117	LYS
1	B	154	LYS
1	B	195	LYS
1	B	209	VAL
1	B	213	GLU
1	B	216	LYS
1	B	220	GLN
1	B	245	GLU
1	B	267	ARG
1	B	268	SER
1	B	280	GLN
1	B	288	ASN
1	B	304	GLU
1	B	346	ILE
1	B	357	ILE
1	B	360	GLU
1	B	368	LYS
1	B	386	ASN
1	B	397	GLU
1	B	431	SER
1	B	443	ILE
1	B	473	LYS
1	B	489	THR
1	B	507	LYS
1	B	510	LYS
1	B	516	THR
1	B	544	LYS
1	B	554	LYS
1	B	567	LYS
1	B	569	GLU
1	B	574	LYS
1	B	575	LYS
1	B	602	GLU
1	B	606	ASP
1	B	611	GLU
1	B	613	GLU
1	B	618	LEU
1	C	10	ARG
1	C	19	LYS
1	C	21	GLN

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Mol	Chain	Res	Type
1	C	26	GLU
1	C	93	LEU
1	C	95	THR
1	C	103	ARG
1	C	129	SER
1	C	151	ILE
1	C	155	ASN
1	C	195	LYS
1	C	202	ARG
1	C	205	LYS
1	C	217	LYS
1	C	245	GLU
1	C	259	SER
1	C	268	SER
1	C	282	ARG
1	C	288	ASN
1	C	303	SER
1	C	304	GLU
1	C	308	GLU
1	C	312	LEU
1	C	329	ASN
1	C	346	ILE
1	C	357	ILE
1	C	360	GLU
1	C	368	LYS
1	C	381	LYS
1	C	383	GLU
1	C	392	VAL
1	C	398	LYS
1	C	414	SER
1	C	431	SER
1	C	463	LYS
1	C	464	ILE
1	C	465	SER
1	C	473	LYS
1	C	489	THR
1	C	539	ARG
1	C	544	LYS
1	C	548	LYS
1	C	554	LYS
1	C	559	GLU
1	C	598	GLU

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Mol	Chain	Res	Type
1	C	602	GLU
1	C	606	ASP
1	C	609	ILE
1	C	613	GLU
1	C	618	LEU
1	D	27	VAL
1	D	30	LYS
1	D	41	ILE
1	D	57	LYS
1	D	93	LEU
1	D	95	THR
1	D	117	LYS
1	D	129	SER
1	D	150	GLU
1	D	195	LYS
1	D	202	ARG
1	D	206	GLU
1	D	212	LYS
1	D	216	LYS
1	D	288	ASN
1	D	304	GLU
1	D	360	GLU
1	D	368	LYS
1	D	386	ASN
1	D	398	LYS
1	D	414	SER
1	D	465	SER
1	D	473	LYS
1	D	480	LEU
1	D	489	THR
1	D	531	SER
1	D	539	ARG
1	D	544	LYS
1	D	554	LYS
1	D	573	GLU
1	D	574	LYS
1	D	575	LYS
1	D	592	ARG
1	D	596	LYS
1	D	598	GLU
1	D	602	GLU
1	D	606	ASP

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Mol	Chain	Res	Type
1	D	618	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	GLN
1	A	288	ASN
1	A	301	GLN
1	B	281	GLN
1	B	288	ASN
1	B	293	ASN
1	C	288	ASN
1	D	288	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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
5	PTE	B	623	1,6,4,2	46,58,60	3.01	10 (21%)	42,93,98	4.31	22 (52%)
4	GUA	A	622	5	8,8,8	1.01	0	9,9,9	1.03	0
3	SF4	D	621	1	0,12,12	-	-	-	-	-
5	PTE	C	623	1,6,4,2	46,58,60	2.95	12 (26%)	42,93,98	5.10	18 (42%)
3	SF4	A	621	1	0,12,12	-	-	-	-	-
3	SF4	B	621	1	0,12,12	-	-	-	-	-
3	SF4	C	621	1	0,12,12	-	-	-	-	-
5	PTE	A	623	1,6,4,2	46,58,60	2.79	12 (26%)	42,93,98	6.75	21 (50%)
4	GUA	D	622	5	8,8,8	1.05	0	9,9,9	0.97	0
4	GUA	B	622	5	8,8,8	1.08	0	9,9,9	0.95	0
4	GUA	C	622	5	8,8,8	0.99	0	9,9,9	1.05	0
5	PTE	D	623	1,6,4,2	46,58,60	2.83	10 (21%)	42,93,98	3.50	26 (61%)

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
5	PTE	B	623	1,6,4,2	-	1/12/96/100	-
4	GUA	A	622	5	-	3/6/6/6	-
5	PTE	C	623	1,6,4,2	-	1/12/96/100	-
3	SF4	D	621	1	-	-	0/6/5/5
3	SF4	A	621	1	-	-	0/6/5/5
3	SF4	B	621	1	-	-	0/6/5/5
3	SF4	C	621	1	-	-	0/6/5/5
5	PTE	A	623	1,6,4,2	-	1/12/96/100	-
4	GUA	D	622	5	-	2/6/6/6	-
4	GUA	B	622	5	-	2/6/6/6	-
4	GUA	C	622	5	-	4/6/6/6	-
5	PTE	D	623	1,6,4,2	-	1/12/96/100	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	623	PTE	O28-C28	9.94	1.42	1.23
5	C	623	PTE	O8-C8	9.24	1.41	1.23
5	B	623	PTE	O8-C8	9.13	1.40	1.23
5	C	623	PTE	O28-C28	8.81	1.40	1.23
5	D	623	PTE	O28-C28	8.58	1.39	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	623	PTE	O8-C8	8.53	1.39	1.23
5	A	623	PTE	O28-C28	8.10	1.38	1.23
5	A	623	PTE	P1-O1P	7.49	1.62	1.50
5	A	623	PTE	O8-C8	7.31	1.37	1.23
5	B	623	PTE	P2-O5P	7.00	1.61	1.50
5	C	623	PTE	P2-O5P	6.92	1.61	1.50
5	B	623	PTE	C14-C5	6.53	1.58	1.53
5	B	623	PTE	P1-O1P	6.51	1.60	1.50
5	D	623	PTE	P2-O5P	6.26	1.60	1.50
5	A	623	PTE	C14-C5	6.09	1.58	1.53
5	D	623	PTE	P1-O1P	5.94	1.60	1.50
5	A	623	PTE	P2-O5P	5.79	1.59	1.50
5	C	623	PTE	C14-C5	5.71	1.58	1.53
5	D	623	PTE	C34-C25	5.68	1.58	1.53
5	C	623	PTE	P1-O1P	5.60	1.59	1.50
5	C	623	PTE	C27-C32	5.27	1.47	1.38
5	D	623	PTE	C14-C5	4.98	1.57	1.53
5	A	623	PTE	C27-C32	4.82	1.46	1.38
5	B	623	PTE	C27-C32	4.80	1.46	1.38
5	D	623	PTE	C7-C12	4.80	1.46	1.38
5	B	623	PTE	C7-C12	4.67	1.46	1.38
5	D	623	PTE	C27-C32	4.49	1.46	1.38
5	C	623	PTE	C7-C12	4.29	1.46	1.38
5	A	623	PTE	C7-C12	4.24	1.45	1.38
5	B	623	PTE	C34-C25	3.56	1.56	1.53
5	C	623	PTE	C34-C25	3.50	1.56	1.53
5	D	623	PTE	C25-N26	3.37	1.50	1.46
5	C	623	PTE	O2-C14	-3.09	1.39	1.43
5	A	623	PTE	C5-N6	3.06	1.49	1.46
5	A	623	PTE	C34-N33	3.02	1.50	1.45
5	C	623	PTE	C25-N26	2.73	1.49	1.46
5	A	623	PTE	C32-N33	2.64	1.38	1.35
5	C	623	PTE	C5-N6	2.62	1.49	1.46
5	C	623	PTE	C12-N13	2.45	1.38	1.35
5	B	623	PTE	C25-N26	2.43	1.49	1.46
5	A	623	PTE	C34-C25	2.35	1.55	1.53
5	D	623	PTE	C5-N6	2.29	1.49	1.46
5	B	623	PTE	O2-C14	-2.25	1.40	1.43
5	A	623	PTE	O2-C14	-2.16	1.40	1.43

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	623	PTE	O2-C14-N13	33.05	138.60	108.61
5	C	623	PTE	O2-C14-N13	26.99	133.10	108.61
5	A	623	PTE	O22-C34-N33	21.38	128.01	108.61
5	B	623	PTE	O22-C34-N33	17.75	124.71	108.61
5	C	623	PTE	O2-C14-C5	-9.26	102.78	108.96
5	B	623	PTE	C34-C25-N26	-9.21	98.82	107.87
5	B	623	PTE	O2-C14-N13	-9.04	100.40	108.61
5	A	623	PTE	O2-C14-C5	-7.91	103.69	108.96
5	A	623	PTE	C14-C5-N6	-7.83	100.17	107.87
5	B	623	PTE	O22-C34-C25	7.31	113.84	108.96
5	C	623	PTE	O22-C34-N33	7.19	115.13	108.61
5	D	623	PTE	O2-C14-C5	-7.07	104.25	108.96
5	D	623	PTE	C34-C25-N26	-6.94	101.05	107.87
5	D	623	PTE	O2-C14-N13	6.89	114.86	108.61
5	A	623	PTE	O22-C34-C25	-6.54	104.60	108.96
5	B	623	PTE	O22-C22-C23	6.49	118.26	109.09
5	D	623	PTE	O28-C28-C27	-5.93	112.96	127.26
5	D	623	PTE	O22-C34-N33	5.72	113.80	108.61
5	C	623	PTE	C14-C5-N6	-5.52	102.45	107.87
5	D	623	PTE	O6P-P2-O5P	5.10	123.75	108.12
5	D	623	PTE	N30-C30-N29	5.05	127.42	116.76
5	D	623	PTE	O8-C8-C7	-4.91	115.43	127.26
5	C	623	PTE	C10-N11-C12	4.77	121.77	113.36
5	A	623	PTE	C10-N11-C12	4.53	121.36	113.36
5	D	623	PTE	O22-C34-C25	-4.50	105.96	108.96
5	D	623	PTE	C10-N11-C12	4.49	121.28	113.36
5	C	623	PTE	C34-C25-N26	-4.46	103.48	107.87
5	C	623	PTE	C28-C27-N26	4.38	128.21	116.27
5	C	623	PTE	C8-C7-N6	4.26	127.89	116.27
5	D	623	PTE	O28-C28-N29	4.26	128.12	120.11
5	B	623	PTE	C10-N11-C12	4.23	120.82	113.36
5	B	623	PTE	C28-C27-N26	4.15	127.60	116.27
5	A	623	PTE	O8-C8-C7	-4.13	117.31	127.26
5	D	623	PTE	C30-N31-C32	4.06	120.53	113.36
5	A	623	PTE	C8-C7-N6	4.06	127.34	116.27
5	B	623	PTE	O2P-P1-O1P	4.02	120.43	108.12
5	A	623	PTE	C34-C25-N26	-3.97	103.96	107.87
5	C	623	PTE	C30-N31-C32	3.97	120.36	113.36
5	D	623	PTE	C8-C7-N6	3.92	126.96	116.27
5	B	623	PTE	O2-C2-C3	3.87	114.55	109.09
5	D	623	PTE	N10-C10-N9	3.87	124.92	116.76
5	C	623	PTE	N9-C10-N11	-3.73	116.50	123.32
5	D	623	PTE	C14-C5-N6	-3.68	104.25	107.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	623	PTE	O8-C8-C7	-3.65	118.46	127.26
5	D	623	PTE	C28-C27-N26	3.58	126.04	116.27
5	A	623	PTE	C30-N31-C32	3.55	119.62	113.36
5	B	623	PTE	O6P-P2-O5P	3.51	118.88	108.12
5	B	623	PTE	C30-N31-C32	3.41	119.38	113.36
5	D	623	PTE	C3-C4-S4	3.38	124.54	119.62
5	A	623	PTE	N29-C30-N31	-3.36	117.18	123.32
5	D	623	PTE	O8-C8-N9	3.34	126.39	120.11
5	B	623	PTE	C8-C7-N6	3.29	125.23	116.27
5	C	623	PTE	O28-C28-C27	-3.24	119.46	127.26
5	A	623	PTE	C28-C27-N26	3.21	125.03	116.27
5	B	623	PTE	O2-C14-C5	3.21	111.10	108.96
5	A	623	PTE	N10-C10-N9	3.18	123.47	116.76
5	C	623	PTE	C23-C24-S24	-3.17	115.02	119.62
5	A	623	PTE	O4P-C1-C2	3.15	116.36	108.58
5	D	623	PTE	N29-C30-N31	-3.10	117.64	123.32
5	D	623	PTE	N9-C10-N11	-3.02	117.80	123.32
5	C	623	PTE	N10-C10-N9	2.98	123.06	116.76
5	A	623	PTE	C7-C8-N9	2.92	120.16	112.13
5	B	623	PTE	N10-C10-N9	2.92	122.92	116.76
5	B	623	PTE	N29-C30-N31	-2.86	118.08	123.32
5	A	623	PTE	O28-C28-C27	-2.82	120.46	127.26
5	D	623	PTE	O6P-P2-O8P	-2.78	94.97	107.57
5	C	623	PTE	O8-C8-C7	-2.71	120.72	127.26
5	B	623	PTE	C4-C3-S3	-2.68	115.73	119.62
5	C	623	PTE	C27-C28-N29	2.67	119.46	112.13
5	D	623	PTE	C24-C23-S23	-2.61	115.84	119.62
5	A	623	PTE	O2P-P1-O1P	2.60	116.09	108.12
5	B	623	PTE	O28-C28-C27	-2.60	121.00	127.26
5	D	623	PTE	N30-C30-N31	-2.52	114.76	119.67
5	A	623	PTE	N9-C10-N11	-2.46	118.83	123.32
5	D	623	PTE	C27-C28-N29	2.45	118.86	112.13
5	B	623	PTE	C3-C4-S4	2.40	123.12	119.62
5	A	623	PTE	C27-C28-N29	2.40	118.73	112.13
5	D	623	PTE	C4-C3-S3	-2.38	116.17	119.62
5	A	623	PTE	N30-C30-N31	2.34	124.23	119.67
5	C	623	PTE	O6P-P2-O5P	2.28	115.11	108.12
5	B	623	PTE	O2P-P1-O4P	-2.27	97.29	107.57
5	C	623	PTE	O8P-C21-C22	-2.21	103.13	108.58
5	B	623	PTE	N9-C10-N11	-2.18	119.33	123.32
5	D	623	PTE	C7-C8-N9	2.17	118.09	112.13
5	B	623	PTE	C7-C8-N9	2.13	117.98	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	623	PTE	O4P-P1-O3P	2.05	117.05	108.94
5	C	623	PTE	C3-C4-S4	2.01	122.55	119.62

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	623	PTE	O4P-C1-C2-O2
5	D	623	PTE	C1-O4P-P1-O3P
5	A	623	PTE	O4P-C1-C2-O2
5	B	623	PTE	O4P-C1-C2-O2
4	A	622	GUA	C3-C4-C5-O3
4	B	622	GUA	C3-C4-C5-O3
4	D	622	GUA	C3-C4-C5-O3
4	C	622	GUA	C3-C4-C5-O3
4	A	622	GUA	C3-C4-C5-O4
4	B	622	GUA	C3-C4-C5-O4
4	D	622	GUA	C3-C4-C5-O4
4	C	622	GUA	C3-C4-C5-O4
4	C	622	GUA	O2-C1-C2-C3
4	A	622	GUA	O2-C1-C2-C3
4	C	622	GUA	O1-C1-C2-C3

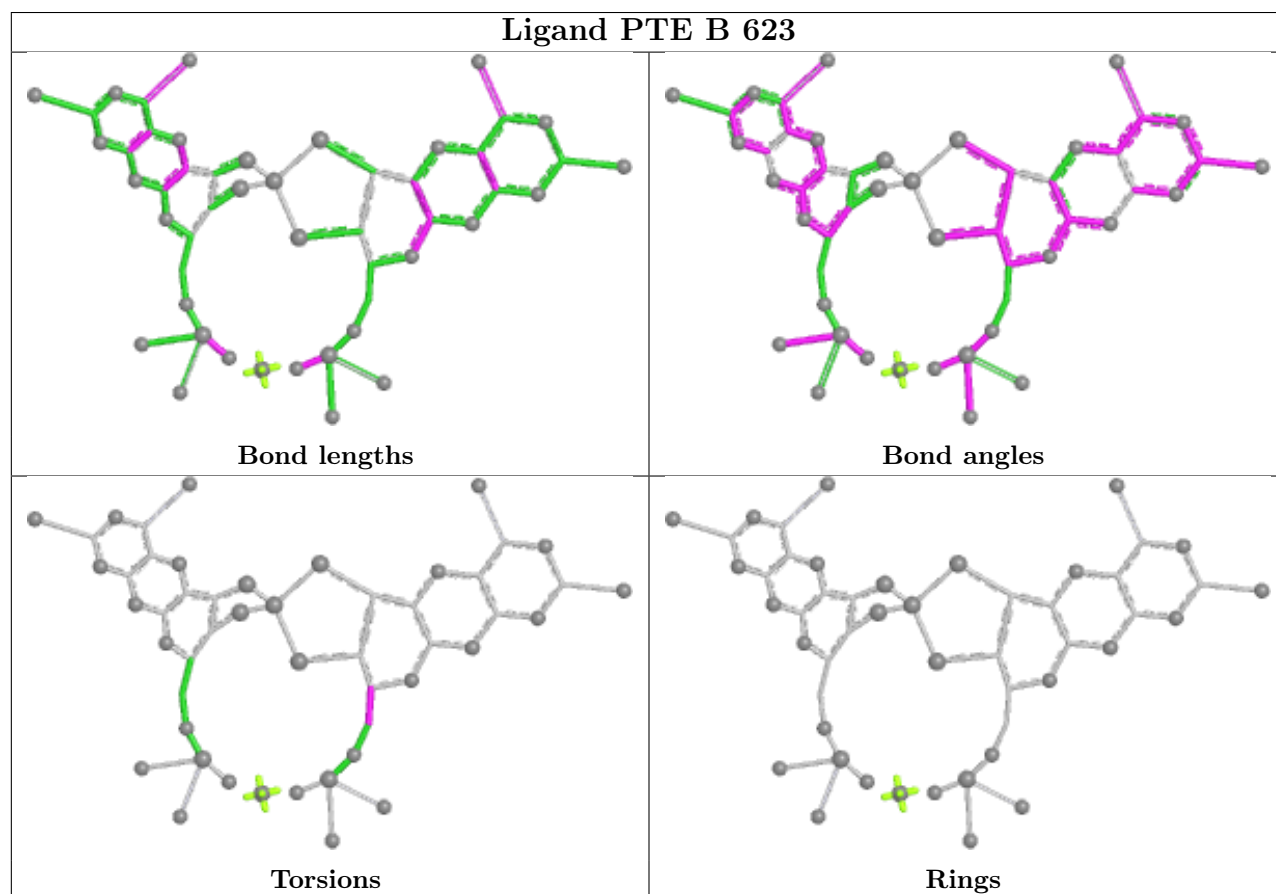
There are no ring outliers.

10 monomers are involved in 14 short contacts:

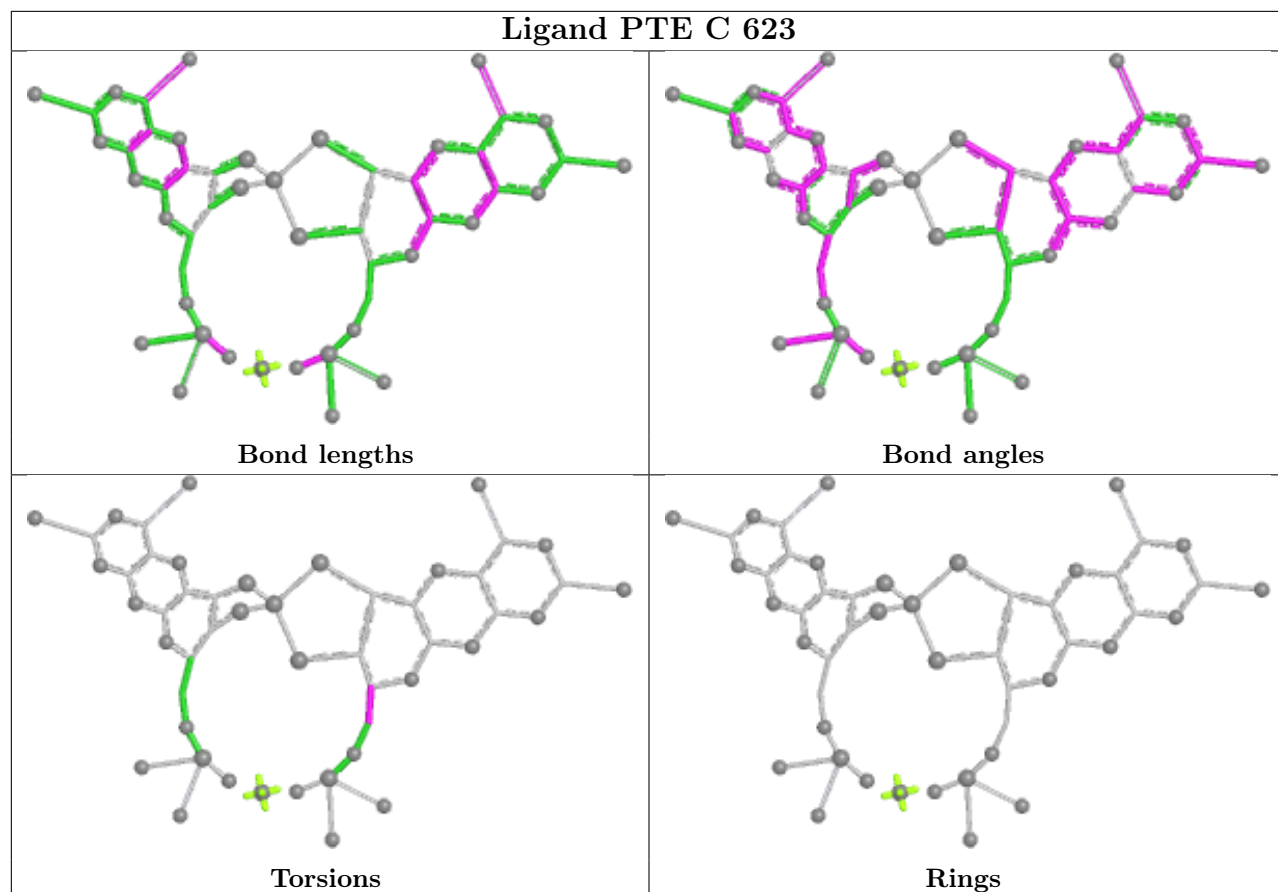
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	623	PTE	1	0
4	A	622	GUA	2	0
5	C	623	PTE	1	0
3	B	621	SF4	1	0
3	C	621	SF4	1	0
5	A	623	PTE	1	0
4	D	622	GUA	1	0
4	B	622	GUA	3	0
4	C	622	GUA	2	0
5	D	623	PTE	1	0

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

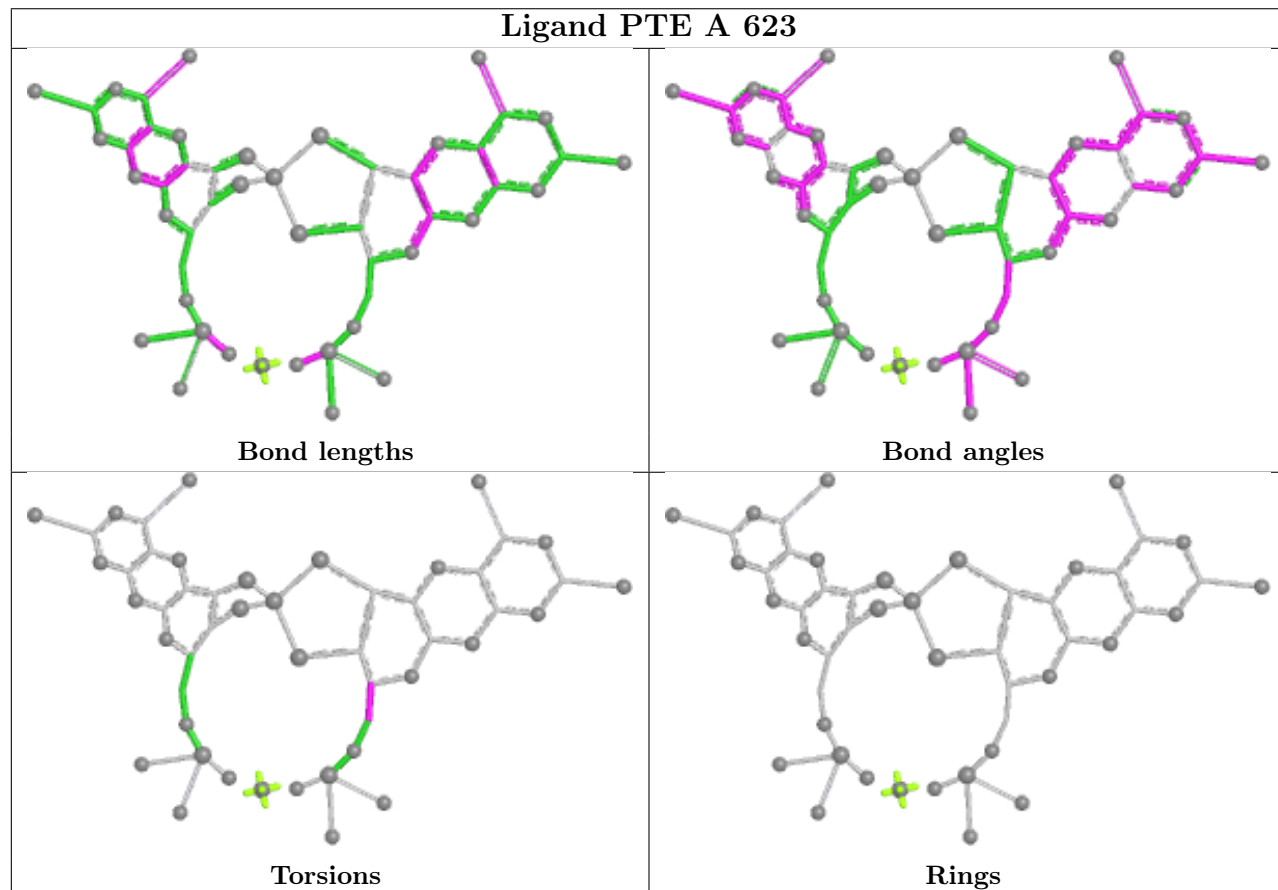
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

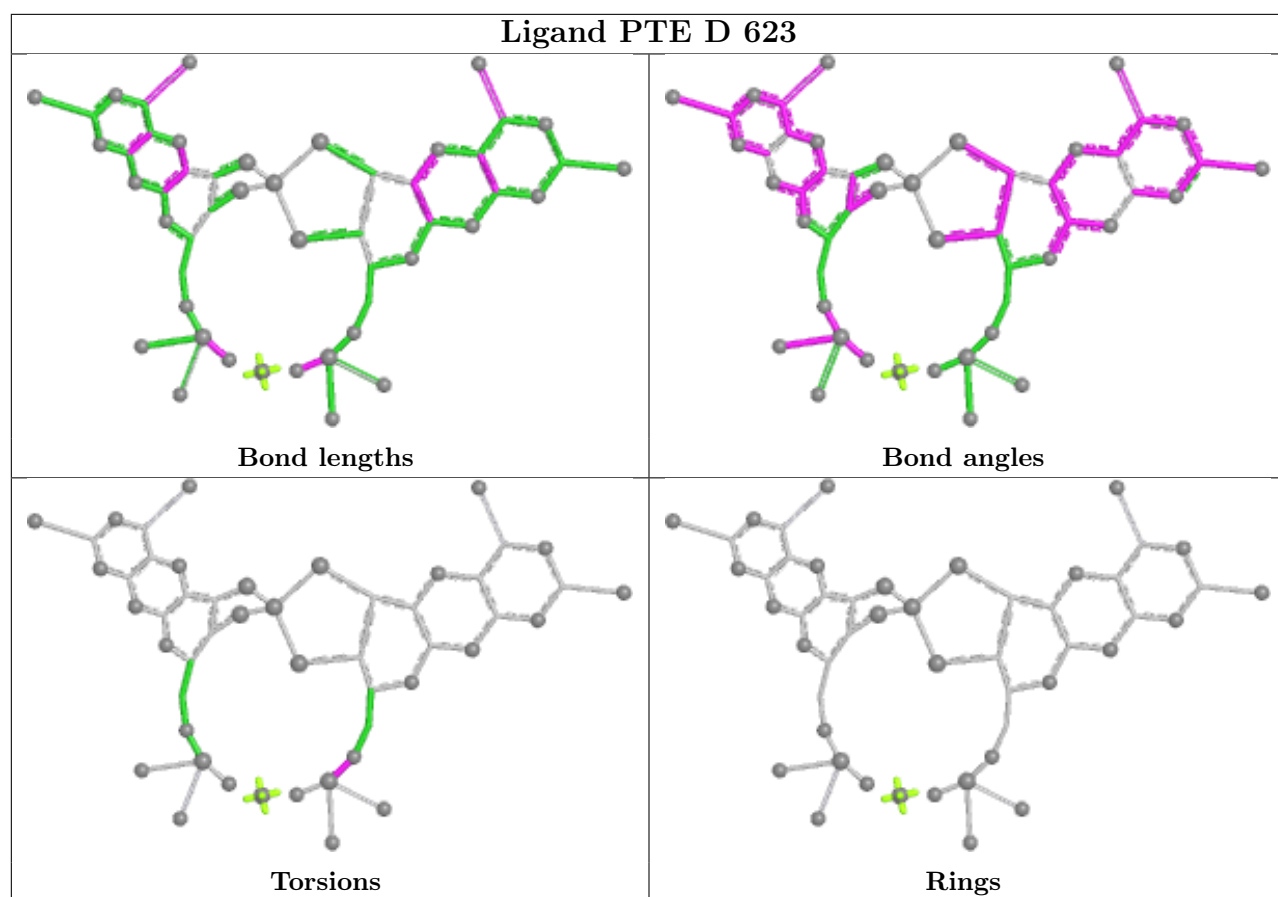


Ligand PTE C 623



Ligand PTE A 623





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.