



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:31 AM UTC

PDB ID : 1GPM / pdb_00001gpm
Title : ESCHERICHIA COLI GMP SYNTHETASE COMPLEXED WITH AMP
AND PYROPHOSPHATE
Authors : Tesmer, J.J.G.
Deposited on : 1995-04-04
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 ⓘ 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

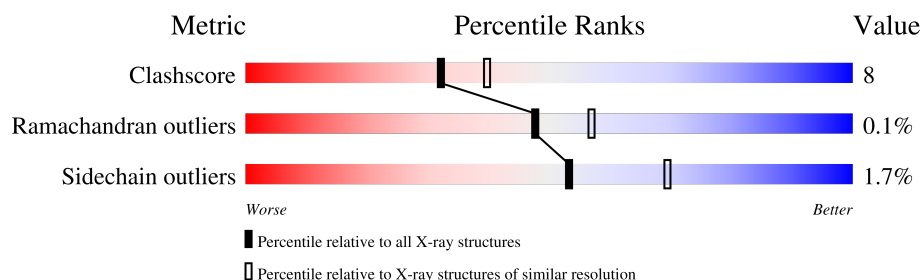
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	525	
1	B	525	
1	C	525	
1	D	525	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	528	-	X	-	-
2	PO4	B	528	-	X	-	-

2 Entry composition [i](#)

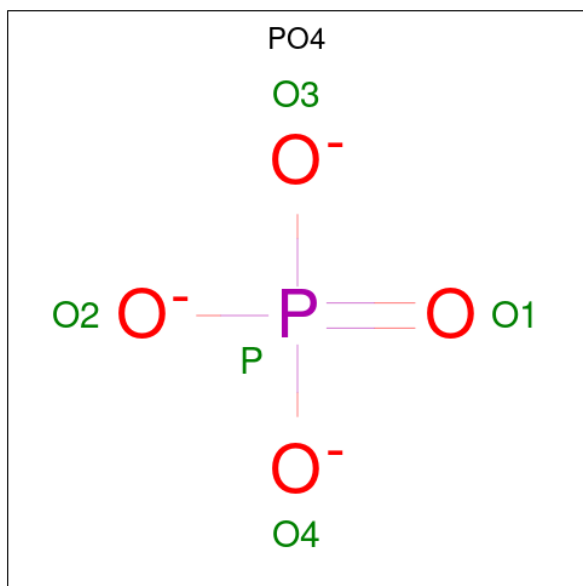
There are 7 unique types of molecules in this entry. The entry contains 16797 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GMP SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3955	2520	678	737	20			
1	B	499	Total	C	N	O	S	0	0	0
			3947	2516	676	734	21			
1	C	501	Total	C	N	O	S	0	0	0
			3955	2520	678	737	20			
1	D	499	Total	C	N	O	S	0	0	0
			3947	2516	676	734	21			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



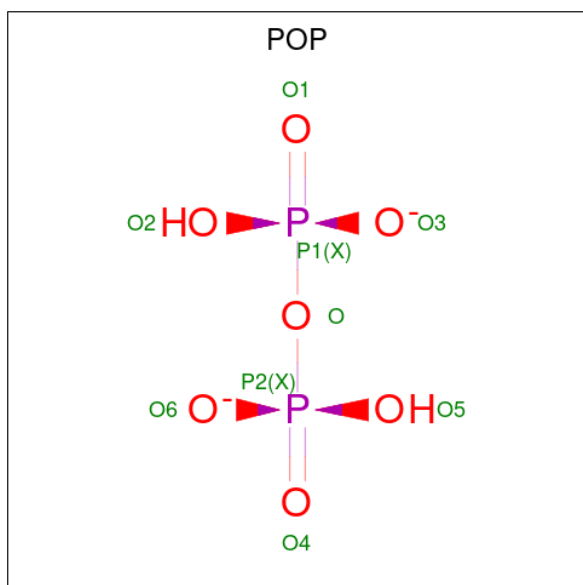
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

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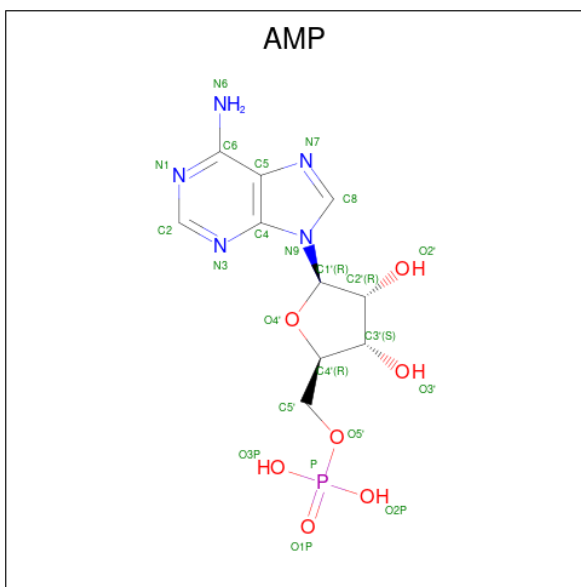
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



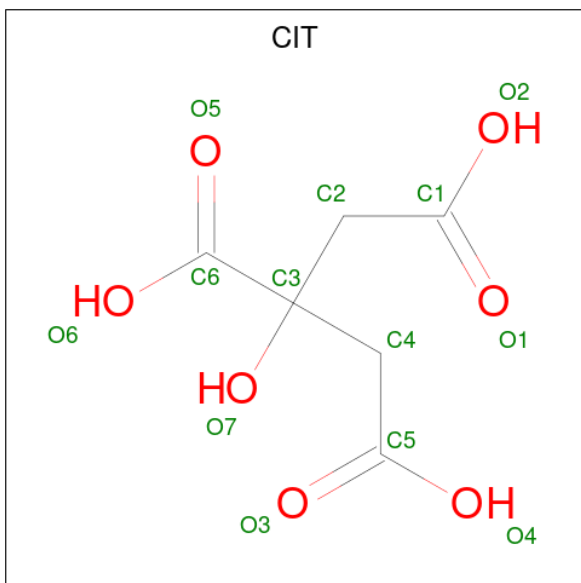
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			9	7	2		
3	B	1	Total	O	P	0	0
			9	7	2		
3	C	1	Total	O	P	0	0
			9	7	2		
3	D	1	Total	O	P	0	0
			9	7	2		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $\text{C}_{10}\text{H}_{14}\text{N}_5\text{O}_7\text{P}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 6 7	0	0
5	B	1	Total C O 13 6 7	0	0
5	C	1	Total C O 13 6 7	0	0
5	D	1	Total C O 13 6 7	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	242	Total O 242 242	0	0
7	B	174	Total O 174 174	0	0
7	C	219	Total O 219 219	0	0
7	D	155	Total O 155 155	0	0

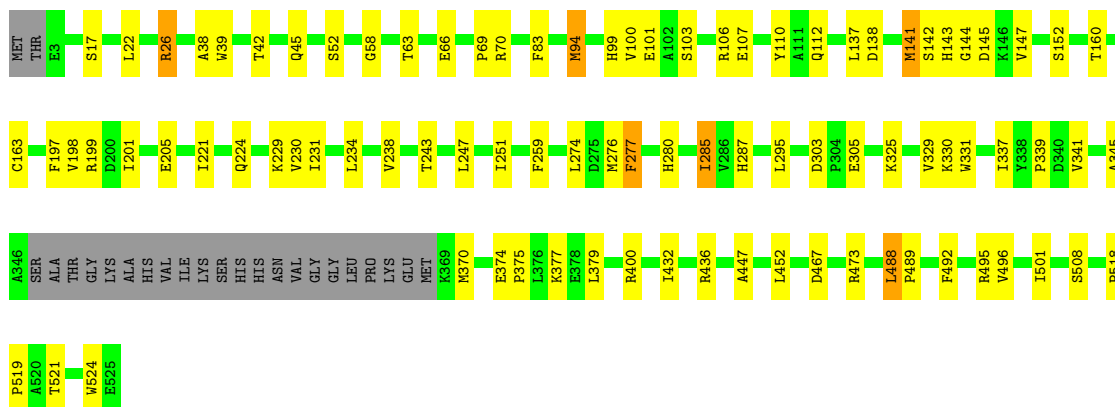
3 Residue-property plots [i](#)

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.

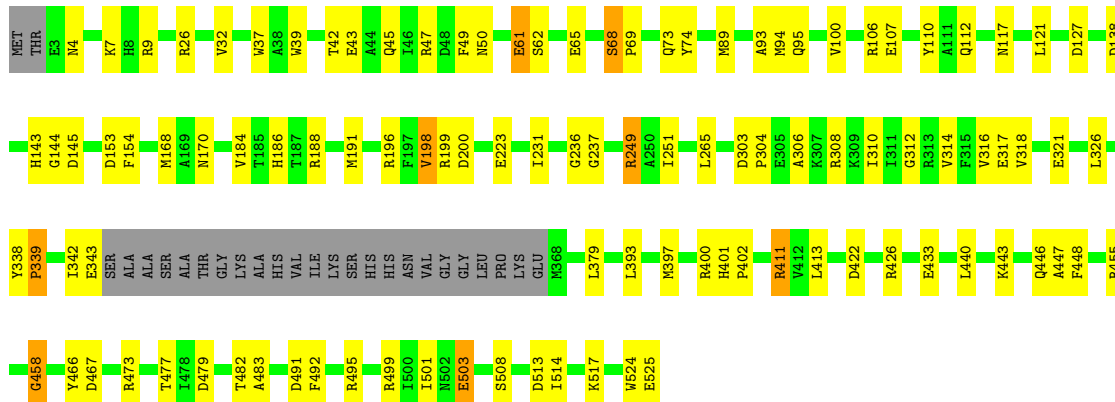
• Molecule 1: GMP SYNTHETASE

Chain A:  78% 16% • 5%



• Molecule 1: GMP SYNTHETASE

Chain B:  74% 19% • 5%

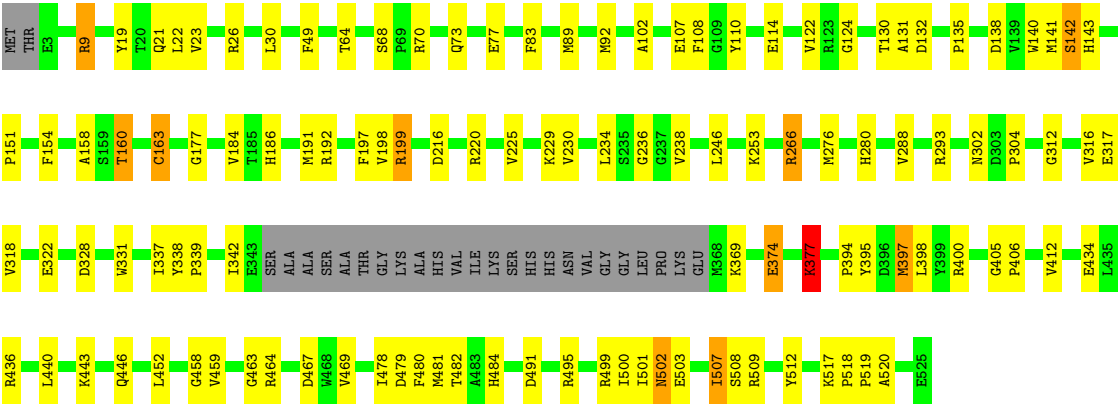


• Molecule 1: GMP SYNTHETASE

Chain C:  76% 18% • 5%



● Molecule 1: GMP SYNTHETASE



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	156.00Å 102.00Å 78.80Å 90.00° 96.70° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.20)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16797	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: AMP, POP, PO4, CIT, MG

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	0.56	1/4040 (0.0%)	0.96	16/5474 (0.3%)
1	B	0.49	0/4032	0.95	11/5462 (0.2%)
1	C	0.55	0/4040	0.96	12/5474 (0.2%)
1	D	0.50	0/4032	0.94	13/5462 (0.2%)
All	All	0.53	1/16144 (0.0%)	0.95	52/21872 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	MET	SD-CE	-6.74	1.62	1.79

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	238	VAL	N-CA-C	7.64	118.38	110.36
1	C	201	ILE	N-CA-C	7.40	117.48	110.53
1	C	238	VAL	N-CA-C	7.18	117.17	110.42
1	A	374	GLU	CA-C-N	7.13	126.83	119.56
1	A	374	GLU	C-N-CA	7.13	126.83	119.56
1	C	463	GLY	N-CA-C	-7.10	105.52	115.32
1	B	236	GLY	N-CA-C	-7.06	105.75	114.92
1	A	238	VAL	N-CA-C	6.95	117.06	110.53
1	A	66	GLU	N-CA-C	6.89	119.38	111.11
1	D	377	LYS	N-CA-C	6.87	120.54	111.75
1	C	458	GLY	N-CA-C	6.76	129.21	113.18
1	D	225	VAL	N-CA-C	6.64	117.52	111.81
1	B	68	SER	CA-C-N	6.51	126.54	119.90
1	B	68	SER	C-N-CA	6.51	126.54	119.90
1	D	160	THR	N-CA-C	-6.38	99.37	109.07
1	D	135	PRO	N-CA-C	6.30	120.74	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	458	GLY	N-CA-C	6.29	121.19	112.57
1	B	251	ILE	N-CA-C	6.20	118.14	112.43
1	D	374	GLU	CA-C-N	6.18	126.08	119.28
1	D	374	GLU	C-N-CA	6.18	126.08	119.28
1	C	466	TYR	N-CA-C	6.03	118.50	108.20
1	B	4	ASN	N-CA-C	-6.01	101.38	110.28
1	D	236	GLY	N-CA-C	-5.95	107.61	114.69
1	A	251	ILE	N-CA-C	5.93	118.59	112.90
1	A	277	PHE	N-CA-C	5.88	117.50	111.14
1	A	379	LEU	N-CA-C	5.80	119.51	110.17
1	B	411	ARG	N-CA-C	-5.76	106.09	113.23
1	A	201	ILE	N-CA-C	5.72	115.92	110.42
1	D	412	VAL	N-CA-C	-5.72	97.62	106.72
1	D	163	CYS	CA-C-N	5.69	125.54	119.28
1	D	163	CYS	C-N-CA	5.69	125.54	119.28
1	C	198	VAL	N-CA-C	5.65	115.84	110.53
1	B	379	LEU	N-CA-C	5.61	118.87	109.95
1	A	488	LEU	CA-C-N	5.56	125.88	119.93
1	A	488	LEU	C-N-CA	5.56	125.88	119.93
1	C	285	ILE	N-CA-C	5.55	115.86	107.75
1	A	152	SER	N-CA-C	5.42	117.19	111.28
1	C	239	ASP	N-CA-C	5.41	116.86	111.07
1	A	285	ILE	N-CA-C	5.38	115.64	108.11
1	A	198	VAL	N-CA-C	5.35	115.56	110.53
1	C	379	LEU	N-CA-C	5.31	118.72	110.17
1	A	205	GLU	N-CA-C	-5.30	103.39	110.55
1	A	52	SER	N-CA-C	-5.21	106.93	113.28
1	B	503	GLU	N-CA-C	5.20	118.78	112.23
1	C	485	TRP	N-CA-C	-5.17	102.21	109.96
1	C	377	LYS	N-CA-C	5.14	118.65	112.38
1	D	198	VAL	N-CA-C	5.08	115.30	110.42
1	D	122	VAL	N-CA-C	5.07	117.09	112.43
1	A	345	ALA	N-CA-C	-5.07	106.27	112.90
1	B	121	LEU	N-CA-C	5.07	116.80	111.28
1	B	198	VAL	N-CA-C	5.04	115.26	110.42
1	C	269	GLU	N-CA-C	5.02	116.44	110.97

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	3955	0	3911	52	0
1	B	3947	0	3905	72	0
1	C	3955	0	3911	64	0
1	D	3947	0	3905	75	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	A	9	0	0	0	0
3	B	9	0	0	1	0
3	C	9	0	0	0	0
3	D	9	0	0	0	0
4	A	23	0	12	1	0
4	B	23	0	12	0	0
4	C	23	0	12	0	0
4	D	23	0	12	0	0
5	A	13	0	5	0	0
5	B	13	0	5	0	0
5	C	13	0	5	0	0
5	D	13	0	5	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	242	0	0	3	0
7	B	174	0	0	5	0
7	C	219	0	0	3	0
7	D	155	0	0	4	0
All	All	16797	0	15700	255	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 8.

All (255) 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:459:VAL:HB	1:D:463:GLY:HA3	1.53	0.89
1:C:457:VAL:HG22	1:C:466:TYR:CE1	2.12	0.84
1:D:110:TYR:HE1	1:D:138:ASP:HB3	1.47	0.78
1:D:500:ILE:HG22	1:D:507:ILE:HG21	1.67	0.77
1:A:160:THR:HG22	1:A:163:CYS:HB3	1.66	0.76
1:D:184:VAL:HG12	1:D:186:HIS:H	1.51	0.76
1:B:43:GLU:O	1:B:47:ARG:HG2	1.88	0.74
1:C:276:MET:HE1	1:C:397:MET:HE1	1.71	0.72
1:D:160:THR:HG22	1:D:163:CYS:HB3	1.72	0.72
1:C:266:ARG:HD2	1:C:403:PHE:CZ	2.26	0.71
1:B:499:ARG:O	1:B:503:GLU:HG2	1.95	0.67
1:D:9:ARG:HG2	1:D:9:ARG:HH11	1.59	0.67
1:C:129:LEU:HD12	1:D:276:MET:HE2	1.78	0.66
1:B:93:ALA:HB2	1:B:168:MET:HE1	1.77	0.66
1:C:188:ARG:HB2	7:C:680:HOH:O	1.97	0.65
1:A:400:ARG:HG2	1:A:400:ARG:HH11	1.63	0.64
1:A:231:ILE:HD11	1:A:370:MET:HE1	1.80	0.63
1:B:94:MET:HE2	1:B:94:MET:HA	1.79	0.63
1:C:266:ARG:HD3	1:C:269:GLU:OE1	1.97	0.63
1:B:491:ASP:O	1:B:495:ARG:HG3	1.99	0.63
1:C:107:GLU:O	1:C:142:SER:HA	1.99	0.63
1:B:7:LYS:HG2	7:B:615:HOH:O	1.98	0.62
1:A:518:PRO:HB2	1:A:519:PRO:HA	1.80	0.62
1:B:26:ARG:HD2	1:B:191:MET:SD	2.40	0.62
1:A:141:MET:HE3	1:A:143:HIS:CD2	2.34	0.62
1:B:188:ARG:HG3	1:B:188:ARG:HH11	1.64	0.62
1:A:42:THR:H	1:A:45:GLN:HE21	1.47	0.62
1:C:518:PRO:HB2	1:C:519:PRO:HA	1.82	0.62
1:C:129:LEU:HD23	1:C:135:PRO:HA	1.82	0.61
1:D:130:THR:HG22	1:D:132:ASP:H	1.65	0.61
1:A:277:PHE:HB3	1:A:285:ILE:HD11	1.82	0.61
1:C:400:ARG:HG2	1:C:400:ARG:HH11	1.65	0.61
1:A:276:MET:O	1:A:280:HIS:HB3	2.01	0.60
1:D:9:ARG:HG2	1:D:9:ARG:NH1	2.15	0.60
1:D:151:PRO:HB2	1:D:154:PHE:CD1	2.36	0.60
1:D:110:TYR:CE1	1:D:138:ASP:HB3	2.34	0.59
1:B:411:ARG:HD2	7:B:602:HOH:O	2.01	0.59
1:A:39:TRP:CE2	1:A:69:PRO:HB3	2.38	0.59
1:B:393:LEU:HD13	1:B:397:MET:HE1	1.84	0.59
1:B:440:LEU:HA	1:B:443:LYS:HG2	1.85	0.59
1:C:229:LYS:HD2	1:C:328:ASP:HB2	1.84	0.59
1:C:457:VAL:HG22	1:C:466:TYR:HE1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ILE:HG22	1:B:343:GLU:HG3	1.86	0.58
1:C:266:ARG:NH2	1:C:400:ARG:HD2	2.18	0.58
1:D:9:ARG:HD3	1:D:49:PHE:CZ	2.38	0.58
1:B:73:GLN:NE2	1:B:95:GLN:HE21	2.02	0.58
1:D:107:GLU:HB3	1:D:143:HIS:HB3	1.85	0.58
1:A:94:MET:HE3	1:A:99:HIS:HA	1.85	0.57
1:B:184:VAL:HG12	1:B:186:HIS:H	1.68	0.57
1:B:401:HIS:HB3	1:B:446:GLN:OE1	2.04	0.57
1:C:188:ARG:NH1	1:D:395:TYR:CD1	2.73	0.57
1:D:338:TYR:CE2	1:D:342:ILE:HD11	2.40	0.56
1:D:374:GLU:O	1:D:377:LYS:HD2	2.05	0.56
1:A:101:GLU:O	1:A:145:ASP:HB3	2.05	0.56
1:A:230:VAL:HG22	1:A:331:TRP:HB2	1.88	0.56
1:C:396:ASP:O	1:C:400:ARG:HB2	2.06	0.56
1:B:37:TRP:HH2	1:B:49:PHE:HB2	1.71	0.55
1:C:114:GLU:OE2	1:C:134:LYS:HD2	2.06	0.55
1:D:479:ASP:HB3	1:D:482:THR:HB	1.88	0.55
1:D:337:ILE:HG13	1:D:339:PRO:HD2	1.89	0.55
1:D:230:VAL:HG22	1:D:331:TRP:HB2	1.89	0.55
1:C:280:HIS:HB2	7:D:574:HOH:O	2.06	0.55
1:D:400:ARG:HD2	7:D:542:HOH:O	2.07	0.55
1:D:467:ASP:HB2	1:D:508:SER:HB3	1.89	0.55
1:B:100:VAL:CG1	1:B:145:ASP:HB3	2.38	0.54
1:A:141:MET:HE3	1:A:143:HIS:HD2	1.72	0.54
1:B:482:THR:HA	1:B:517:LYS:O	2.08	0.53
1:A:341:VAL:HG22	1:A:377:LYS:HE2	1.88	0.53
1:D:491:ASP:O	1:D:495:ARG:HG3	2.08	0.53
1:B:479:ASP:HB3	1:B:482:THR:HB	1.91	0.53
1:D:64:THR:HG21	1:D:102:ALA:H	1.73	0.53
1:B:73:GLN:HE22	1:B:95:GLN:HE21	1.55	0.53
1:C:19:TYR:HE2	1:C:108:PHE:HZ	1.56	0.53
1:C:188:ARG:HG2	1:C:189:GLN:HE21	1.74	0.53
1:C:401:HIS:HB3	1:C:402:PRO:HD2	1.91	0.53
1:A:524:TRP:O	1:C:457:VAL:HG23	2.08	0.53
1:C:276:MET:O	1:C:280:HIS:HB3	2.07	0.52
1:D:229:LYS:HD2	1:D:328:ASP:HB2	1.92	0.52
1:D:397:MET:HE3	1:D:398:LEU:HD23	1.91	0.52
1:C:521:THR:HB	2:C:528:PO4:O2	2.09	0.52
1:C:467:ASP:HB2	1:C:508:SER:HB3	1.90	0.52
1:C:263:GLY:O	1:C:425:ARG:NH2	2.43	0.52
1:B:422:ASP:O	1:B:426:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:VAL:HA	1:C:465:LYS:O	2.10	0.52
1:A:341:VAL:HG21	1:A:377:LYS:HG2	1.91	0.52
1:B:308:ARG:HH21	1:B:525:GLU:C	2.18	0.52
1:B:107:GLU:HB2	1:B:143:HIS:CE1	2.45	0.51
1:D:434:GLU:OE2	1:D:499:ARG:NH1	2.44	0.51
1:B:413:LEU:HD11	1:B:524:TRP:CE3	2.46	0.51
1:C:151:PRO:HB2	1:C:154:PHE:CD1	2.46	0.51
1:D:73:GLN:HG2	1:D:77:GLU:OE2	2.10	0.51
1:A:521:THR:HG23	1:C:458:GLY:HA2	1.92	0.51
1:D:394:PRO:HD2	1:D:397:MET:HG2	1.92	0.51
4:A:527:AMP:H5'1	4:A:527:AMP:H8	1.77	0.50
1:D:377:LYS:HD2	1:D:377:LYS:H	1.77	0.50
1:B:447:ALA:HA	1:B:473:ARG:O	2.12	0.50
1:A:160:THR:CG2	1:A:163:CYS:HB3	2.40	0.50
1:C:106:ARG:HA	1:C:144:GLY:HA2	1.94	0.50
1:C:189:GLN:OE1	1:C:192:ARG:NH1	2.40	0.50
1:D:130:THR:HG22	1:D:131:ALA:N	2.27	0.50
1:C:277:PHE:HB3	1:C:285:ILE:HD11	1.94	0.50
1:D:440:LEU:HA	1:D:443:LYS:HG2	1.94	0.50
1:B:306:ALA:O	1:B:310:ILE:HG13	2.13	0.49
1:B:249:ARG:NH1	7:B:676:HOH:O	2.44	0.49
1:A:432:ILE:O	1:A:436:ARG:HG3	2.11	0.49
1:B:231:ILE:HD12	1:B:326:LEU:HD12	1.94	0.49
1:B:61:GLU:HB2	7:B:629:HOH:O	2.11	0.49
1:D:440:LEU:HA	1:D:443:LYS:CG	2.43	0.49
1:C:114:GLU:CD	1:C:134:LYS:HD2	2.38	0.48
1:D:30:LEU:O	1:D:199:ARG:NH1	2.46	0.48
1:D:30:LEU:CD2	1:D:191:MET:HE3	2.43	0.48
1:B:154:PHE:CD1	1:B:154:PHE:N	2.81	0.48
1:D:107:GLU:O	1:D:142:SER:HA	2.13	0.48
1:C:26:ARG:HD2	1:C:191:MET:SD	2.53	0.48
1:D:400:ARG:NH2	7:D:666:HOH:O	2.42	0.48
1:B:112:GLN:HG2	1:B:138:ASP:OD1	2.14	0.48
1:D:140:TRP:HB2	1:D:186:HIS:HB2	1.96	0.48
1:D:436:ARG:HG3	1:D:436:ARG:HH11	1.78	0.48
1:A:38:ALA:HB1	7:A:660:HOH:O	2.14	0.47
1:B:501:ILE:HG21	1:D:519:PRO:HB2	1.95	0.47
1:C:102:ALA:HA	1:C:145:ASP:OD1	2.14	0.47
1:C:436:ARG:NH1	7:C:687:HOH:O	2.46	0.47
1:C:455:ARG:NH1	1:C:466:TYR:O	2.47	0.47
1:A:341:VAL:CG2	1:A:377:LYS:HE2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:TRP:CE2	1:B:69:PRO:HB3	2.49	0.47
1:B:196:ARG:O	1:B:200:ASP:HB2	2.14	0.47
1:B:42:THR:OG1	1:B:45:GLN:HG3	2.14	0.47
1:B:153:ASP:HB3	1:B:170:ASN:ND2	2.30	0.47
1:A:107:GLU:O	1:A:142:SER:HA	2.15	0.47
1:B:154:PHE:N	1:B:154:PHE:HD1	2.12	0.47
1:B:310:ILE:O	1:B:314:VAL:HG23	2.14	0.47
1:C:230:VAL:HG22	1:C:331:TRP:HB2	1.95	0.47
1:D:293:ARG:HH22	1:D:317:GLU:HB3	1.80	0.47
1:D:22:LEU:O	1:D:26:ARG:HG2	2.15	0.47
1:D:478:ILE:HG13	1:D:484:HIS:CE1	2.50	0.47
1:C:160:THR:HG22	1:C:163:CYS:HB3	1.98	0.46
1:C:436:ARG:NH2	7:C:728:HOH:O	2.45	0.46
1:B:446:GLN:HG3	1:B:448:PHE:CE1	2.50	0.46
1:B:127:ASP:OD1	1:B:188:ARG:HD2	2.15	0.46
1:C:266:ARG:HD2	1:C:403:PHE:CE1	2.50	0.46
1:B:65:GLU:HB2	1:B:68:SER:HB3	1.97	0.46
1:B:458:GLY:HA2	1:B:508:SER:HB3	1.96	0.46
1:D:293:ARG:HH11	1:D:318:VAL:HG22	1.81	0.46
1:D:458:GLY:HA3	1:D:464:ARG:O	2.15	0.46
1:B:237:GLY:HA3	3:B:526:POP:O1	2.16	0.46
1:A:106:ARG:HG2	1:A:144:GLY:HA2	1.98	0.46
1:C:330:LYS:C	1:C:370:MET:HB2	2.40	0.46
1:A:400:ARG:HH11	1:A:400:ARG:CG	2.29	0.46
1:D:405:GLY:N	1:D:406:PRO:CD	2.79	0.46
1:A:488:LEU:HA	1:A:489:PRO:HD3	1.84	0.45
1:C:338:TYR:HB3	1:C:339:PRO:HD3	1.98	0.45
1:B:492:PHE:HD1	1:B:495:ARG:HH21	1.63	0.45
1:D:83:PHE:HB2	1:D:197:PHE:CE1	2.51	0.45
1:D:160:THR:CG2	1:D:163:CYS:HB3	2.45	0.45
1:B:312:GLY:O	1:B:316:VAL:HG23	2.15	0.45
1:C:246:LEU:HD23	1:C:246:LEU:HA	1.74	0.45
1:D:266:ARG:HH11	1:D:266:ARG:HB2	1.81	0.45
1:A:42:THR:H	1:A:45:GLN:NE2	2.13	0.45
1:B:440:LEU:HD23	1:B:443:LYS:HG3	1.99	0.45
1:B:89:MET:HG2	1:B:168:MET:HE3	1.99	0.45
1:C:331:TRP:CE3	1:C:371:GLY:HA3	2.51	0.45
1:D:108:PHE:HA	1:D:141:MET:O	2.17	0.45
1:D:276:MET:O	1:D:280:HIS:HB3	2.17	0.45
1:B:110:TYR:CE2	1:B:138:ASP:HB3	2.52	0.44
1:B:477:THR:HA	1:B:483:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ARG:NH1	7:A:675:HOH:O	2.50	0.44
1:C:412:VAL:HA	1:C:451:PHE:HB3	1.99	0.44
1:A:22:LEU:O	1:A:26:ARG:HG2	2.18	0.44
1:A:199:ARG:HG3	1:A:199:ARG:HH11	1.82	0.44
1:A:229:LYS:HB2	1:A:329:VAL:HA	1.99	0.44
1:D:9:ARG:HD3	1:D:49:PHE:CE2	2.53	0.44
1:A:221:ILE:HD13	1:A:247:LEU:HD23	2.00	0.44
1:A:325:LYS:NZ	7:A:561:HOH:O	2.47	0.44
1:A:492:PHE:O	1:A:496:VAL:HG23	2.18	0.44
1:C:163:CYS:HA	1:C:164:PRO:HD2	1.88	0.44
1:D:312:GLY:O	1:D:316:VAL:HG23	2.17	0.44
1:D:518:PRO:HB2	1:D:519:PRO:HA	1.98	0.44
1:C:457:VAL:HG12	1:C:458:GLY:N	2.32	0.44
1:B:106:ARG:HG2	1:B:144:GLY:HA2	2.00	0.44
1:B:188:ARG:HG3	1:B:188:ARG:NH1	2.31	0.44
1:B:400:ARG:HH11	1:B:400:ARG:HG2	1.81	0.44
1:B:514:ILE:HD13	1:D:512:TYR:HB2	2.00	0.44
1:A:110:TYR:HE1	1:A:138:ASP:HB3	1.83	0.44
1:A:243:THR:HG23	1:A:375:PRO:HG2	2.00	0.44
1:C:112:GLN:HG2	1:C:138:ASP:OD1	2.17	0.44
1:A:330:LYS:HD3	1:A:330:LYS:HA	1.91	0.43
1:B:440:LEU:HA	1:B:443:LYS:CG	2.47	0.43
1:C:440:LEU:HA	1:C:443:LYS:HD2	1.99	0.43
1:D:114:GLU:O	1:D:158:ALA:HA	2.19	0.43
1:D:30:LEU:HD21	1:D:191:MET:HE3	2.00	0.43
1:D:502:ASN:C	1:D:502:ASN:HD22	2.27	0.43
1:A:63:THR:O	1:A:70:ARG:NH2	2.48	0.43
1:A:337:ILE:HD12	1:A:339:PRO:HD2	2.00	0.43
1:B:32:VAL:HG21	1:B:198:VAL:CG1	2.48	0.43
1:B:338:TYR:HB3	1:B:339:PRO:HD3	1.99	0.43
1:C:420:TYR:N	1:C:420:TYR:CD1	2.82	0.43
1:B:43:GLU:HG3	1:B:74:TYR:CG	2.53	0.43
1:A:17:SER:HB2	1:A:58:GLY:C	2.42	0.43
1:C:221:ILE:HD11	1:C:375:PRO:HB3	1.99	0.43
1:C:401:HIS:CE1	1:C:444:VAL:HG23	2.53	0.43
1:C:415:GLU:OE1	1:C:417:LYS:NZ	2.51	0.43
1:D:517:LYS:HA	1:D:520:ALA:O	2.18	0.43
1:A:447:ALA:HA	1:A:473:ARG:O	2.19	0.43
1:C:17:SER:HB2	1:C:58:GLY:C	2.44	0.43
1:A:303:ASP:OD2	1:A:305:GLU:HB2	2.19	0.43
1:D:68:SER:HB2	1:D:70:ARG:HH12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:GLY:HA2	1:D:124:GLY:O	2.19	0.42
1:D:502:ASN:HD22	1:D:503:GLU:N	2.17	0.42
1:C:287:HIS:O	1:C:289:PRO:HD3	2.19	0.42
1:C:403:PHE:CD1	1:C:404:PRO:HD2	2.54	0.42
1:B:9:ARG:HH21	1:B:50:ASN:HB3	1.83	0.42
1:C:419:GLU:O	1:C:423:LEU:HG	2.19	0.42
1:B:62:SER:HB3	1:B:65:GLU:HG2	2.02	0.42
1:B:127:ASP:HB3	1:B:188:ARG:HE	1.84	0.42
1:C:489:PRO:HG2	1:C:492:PHE:HB3	2.01	0.42
1:B:37:TRP:CH2	1:B:49:PHE:HB2	2.51	0.42
1:B:433:GLU:CD	1:B:499:ARG:HH12	2.27	0.42
1:D:288:VAL:HG21	1:D:322:GLU:HG3	2.02	0.42
1:A:274:LEU:HD11	1:A:287:HIS:CE1	2.55	0.42
1:A:295:LEU:HD23	1:A:295:LEU:HA	1.87	0.42
1:D:501:ILE:HA	1:D:507:ILE:HG22	2.02	0.42
1:A:234:LEU:O	1:A:259:PHE:HD1	2.02	0.42
1:B:455:ARG:HA	1:B:467:ASP:O	2.20	0.42
1:D:130:THR:CG2	1:D:131:ALA:N	2.82	0.42
1:D:192:ARG:HD2	7:D:637:HOH:O	2.18	0.41
1:D:480:PHE:CD2	1:D:481:MET:SD	3.13	0.41
1:B:317:GLU:O	1:B:321:GLU:HG3	2.21	0.41
1:D:338:TYR:HB3	1:D:339:PRO:HD3	2.02	0.41
1:A:518:PRO:CB	1:A:519:PRO:HA	2.49	0.41
1:B:303:ASP:HA	1:B:304:PRO:HD2	1.87	0.41
1:A:501:ILE:HG23	1:A:508:SER:HA	2.02	0.41
1:D:89:MET:O	1:D:92:MET:HB3	2.19	0.41
1:A:100:VAL:HG22	1:A:147:VAL:HG22	2.02	0.41
1:B:314:VAL:O	1:B:318:VAL:HG23	2.20	0.41
1:B:402:PRO:HG2	1:B:446:GLN:NE2	2.35	0.41
1:C:3:GLU:O	1:C:3:GLU:HG3	2.21	0.41
1:D:89:MET:HG3	1:D:177:GLY:C	2.45	0.41
1:A:224:GLN:O	1:A:224:GLN:HG2	2.21	0.41
1:B:199:ARG:HD3	7:B:638:HOH:O	2.20	0.41
1:C:157:VAL:HB	1:C:167:ILE:HG22	2.03	0.41
1:D:452:LEU:HD12	1:D:469:VAL:HG12	2.02	0.41
1:A:112:GLN:HA	1:A:137:LEU:O	2.21	0.40
1:D:246:LEU:HD23	1:D:246:LEU:HA	1.91	0.40
1:C:54:ILE:O	1:C:82:VAL:HA	2.21	0.40
1:D:19:TYR:O	1:D:23:VAL:HG23	2.21	0.40
1:D:216:ASP:O	1:D:220:ARG:HG3	2.21	0.40
1:A:467:ASP:HB2	1:A:508:SER:OG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:TYR:CZ	1:D:304:PRO:HG2	2.57	0.40
1:C:303:ASP:HA	1:C:304:PRO:HD3	1.92	0.40
1:A:83:PHE:HB2	1:A:197:PHE:CE1	2.57	0.40
1:B:110:TYR:CD1	1:B:110:TYR:C	2.99	0.40
1:B:467:ASP:HB2	1:B:508:SER:HB3	2.03	0.40
1:C:132:ASP:OD2	1:C:134:LYS:HE3	2.21	0.40
1:A:103:SER:HB2	1:A:145:ASP:HA	2.03	0.40
1:B:513:ASP:OD2	1:D:509:ARG:HD3	2.21	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	472/525 (90%)	456 (97%)	16 (3%)	0	100	100
1	B	480/525 (91%)	458 (95%)	22 (5%)	0	100	100
1	C	497/525 (95%)	482 (97%)	14 (3%)	1 (0%)	43	51
1	D	495/525 (94%)	474 (96%)	20 (4%)	1 (0%)	43	51
All	All	1944/2100 (93%)	1870 (96%)	72 (4%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	459	VAL
1	D	253	LYS

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	423/442 (96%)	420 (99%)	3 (1%)	76	87
1	B	423/442 (96%)	417 (99%)	6 (1%)	59	75
1	C	423/442 (96%)	417 (99%)	6 (1%)	59	75
1	D	423/442 (96%)	410 (97%)	13 (3%)	35	48
All	All	1692/1768 (96%)	1664 (98%)	28 (2%)	53	69

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	94	MET
1	A	452	LEU
1	B	61	GLU
1	B	117	ASN
1	B	223	GLU
1	B	249	ARG
1	B	265	LEU
1	B	339	PRO
1	C	126	GLU
1	C	210	PRO
1	C	266	ARG
1	C	343	GLU
1	C	390	GLU
1	C	459	VAL
1	D	9	ARG
1	D	21	GLN
1	D	142	SER
1	D	199	ARG
1	D	234	LEU
1	D	266	ARG
1	D	302	ASN
1	D	369	LYS
1	D	377	LYS
1	D	397	MET
1	D	446	GLN
1	D	502	ASN
1	D	507	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	45	GLN
1	A	50	ASN
1	A	73	GLN
1	A	179	GLN
1	A	284	ASN
1	A	505	ASN
1	B	45	GLN
1	B	50	ASN
1	B	73	GLN
1	B	280	HIS
1	B	302	ASN
1	B	498	ASN
1	C	45	GLN
1	C	50	ASN
1	C	179	GLN
1	C	186	HIS
1	C	287	HIS
1	D	248	HIS
1	D	268	ASN
1	D	272	GLN
1	D	284	ASN
1	D	487	HIS
1	D	502	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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
2	PO4	C	528	-	4,4,4	1.83	1 (25%)	6,6,6	2.14	2 (33%)
4	AMP	C	527	6	25,25,25	0.99	0	37,38,38	0.87	1 (2%)
4	AMP	B	527	6	25,25,25	0.96	1 (4%)	37,38,38	0.94	3 (8%)
3	POP	C	526	6	6,8,8	1.45	1 (16%)	12,13,13	1.36	1 (8%)
4	AMP	D	527	6	25,25,25	0.86	0	37,38,38	1.01	2 (5%)
4	AMP	A	527	-	25,25,25	0.92	1 (4%)	37,38,38	0.99	1 (2%)
2	PO4	D	528	-	4,4,4	2.04	2 (50%)	6,6,6	2.24	1 (16%)
5	CIT	A	529	-	12,12,12	1.52	2 (16%)	17,17,17	0.92	2 (11%)
5	CIT	C	529	-	12,12,12	1.18	0	17,17,17	1.22	3 (17%)
3	POP	A	526	-	6,8,8	1.45	0	12,13,13	1.41	2 (16%)
3	POP	D	526	6	6,8,8	1.34	1 (16%)	12,13,13	0.86	0
3	POP	B	526	6	6,8,8	1.15	0	12,13,13	1.34	1 (8%)
2	PO4	B	528	-	4,4,4	1.75	2 (50%)	6,6,6	2.01	3 (50%)
2	PO4	A	528	-	4,4,4	1.77	2 (50%)	6,6,6	2.17	2 (33%)
5	CIT	D	529	-	12,12,12	1.18	0	17,17,17	1.43	3 (17%)
5	CIT	B	529	-	12,12,12	1.41	2 (16%)	17,17,17	1.24	2 (11%)

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
4	AMP	C	527	6	-	5/10/26/26	0/3/3/3
4	AMP	B	527	6	-	2/10/26/26	0/3/3/3
3	POP	C	526	6	-	1/6/6/6	-
4	AMP	D	527	6	-	1/10/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CIT	A	529	-	-	0/16/16/16	-
5	CIT	C	529	-	-	0/16/16/16	-
3	POP	A	526	-	-	3/6/6/6	-
3	POP	D	526	6	-	1/6/6/6	-
3	POP	B	526	6	-	0/6/6/6	-
4	AMP	A	527	-	-	0/10/26/26	0/3/3/3
5	CIT	D	529	-	-	0/16/16/16	-
5	CIT	B	529	-	-	0/16/16/16	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	528	PO4	P-O2	-2.94	1.46	1.54
5	B	529	CIT	O6-C6	-2.85	1.20	1.30
2	C	528	PO4	P-O2	-2.60	1.47	1.54
5	A	529	CIT	O6-C6	-2.55	1.21	1.30
3	D	526	POP	P1-O3	-2.49	1.45	1.54
5	B	529	CIT	C3-C6	2.22	1.55	1.53
4	B	527	AMP	O3'-C3'	2.18	1.48	1.43
2	A	528	PO4	P-O2	-2.18	1.48	1.54
3	C	526	POP	P1-O3	-2.14	1.46	1.54
4	A	527	AMP	O4'-C1'	2.12	1.46	1.42
2	D	528	PO4	P-O3	-2.07	1.48	1.54
2	B	528	PO4	P-O2	-2.06	1.48	1.54
5	A	529	CIT	O1-C1	2.04	1.28	1.22
2	B	528	PO4	P-O4	-2.04	1.48	1.54
2	A	528	PO4	P-O3	-2.02	1.48	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	528	PO4	O2-P-O1	-4.44	95.26	110.95
2	C	528	PO4	O3-P-O1	-4.06	96.58	110.95
2	A	528	PO4	O4-P-O1	-3.86	97.30	110.95
5	D	529	CIT	C3-C4-C5	3.56	123.66	113.92
5	B	529	CIT	C3-C4-C5	3.39	123.18	113.92
3	C	526	POP	O6-P2-O5	3.06	119.26	107.80
2	B	528	PO4	O3-P-O1	-3.05	100.16	110.95
2	A	528	PO4	O4-P-O2	3.05	117.41	107.91
4	C	527	AMP	O5'-P-O1P	-2.73	99.05	106.44
5	C	529	CIT	C3-C2-C1	2.65	121.16	113.92
3	A	526	POP	O5-P2-O4	-2.63	100.59	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	527	AMP	O5'-C5'-C4'	2.55	117.68	108.99
5	C	529	CIT	C3-C4-C5	2.53	120.85	113.92
5	A	529	CIT	C3-C4-C5	2.53	120.84	113.92
4	A	527	AMP	O5'-P-O1P	-2.46	99.78	106.44
3	A	526	POP	O6-P2-O4	2.44	120.35	110.83
5	D	529	CIT	C3-C2-C1	2.42	120.54	113.92
3	B	526	POP	O6-P2-O5	2.40	116.80	107.80
4	B	527	AMP	O2P-P-O5'	-2.34	100.56	106.67
2	B	528	PO4	O3-P-O2	2.33	115.15	107.91
2	B	528	PO4	O4-P-O2	2.21	114.79	107.91
2	C	528	PO4	O3-P-O2	2.18	114.69	107.91
5	D	529	CIT	O6-C6-C3	2.18	117.31	113.14
5	B	529	CIT	C3-C2-C1	2.11	119.68	113.92
5	C	529	CIT	O6-C6-C3	2.09	117.15	113.14
4	B	527	AMP	O5'-C5'-C4'	2.05	115.99	108.99
5	A	529	CIT	O6-C6-C3	2.03	117.04	113.14
4	B	527	AMP	O2P-P-O1P	2.03	118.74	110.83
4	D	527	AMP	O3P-P-O2P	2.02	115.39	107.80

There are no chirality outliers.

All (13) torsion outliers are listed below:

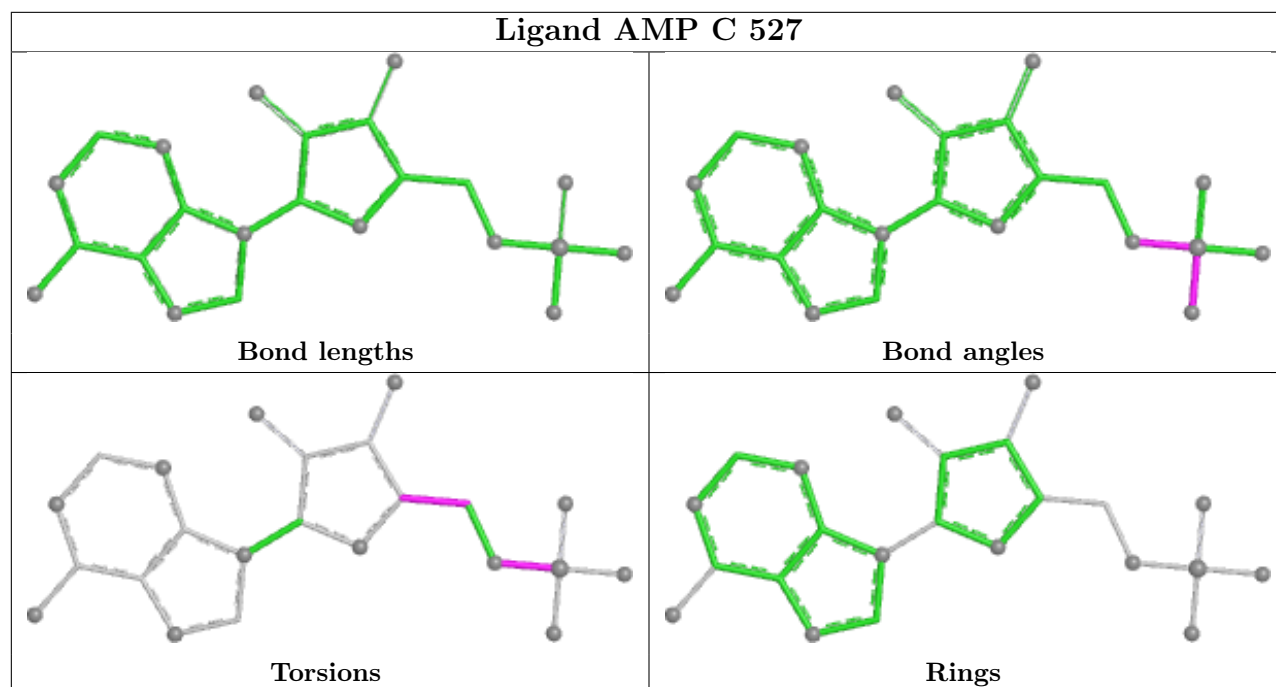
Mol	Chain	Res	Type	Atoms
3	A	526	POP	P1-O-P2-O5
3	A	526	POP	P1-O-P2-O6
4	B	527	AMP	C5'-O5'-P-O2P
4	B	527	AMP	C5'-O5'-P-O3P
4	C	527	AMP	C5'-O5'-P-O2P
4	C	527	AMP	C5'-O5'-P-O3P
4	C	527	AMP	C3'-C4'-C5'-O5'
4	C	527	AMP	O4'-C4'-C5'-O5'
4	C	527	AMP	C5'-O5'-P-O1P
3	C	526	POP	P1-O-P2-O4
4	D	527	AMP	O4'-C4'-C5'-O5'
3	D	526	POP	P1-O-P2-O4
3	A	526	POP	P1-O-P2-O4

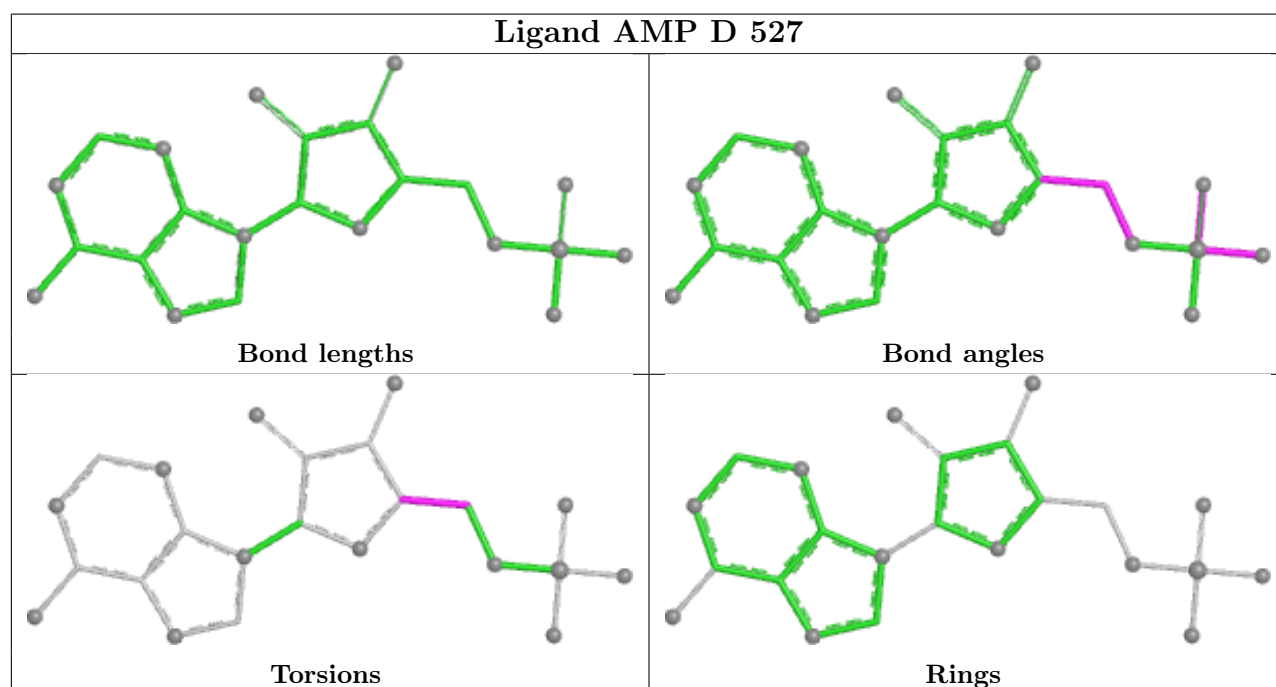
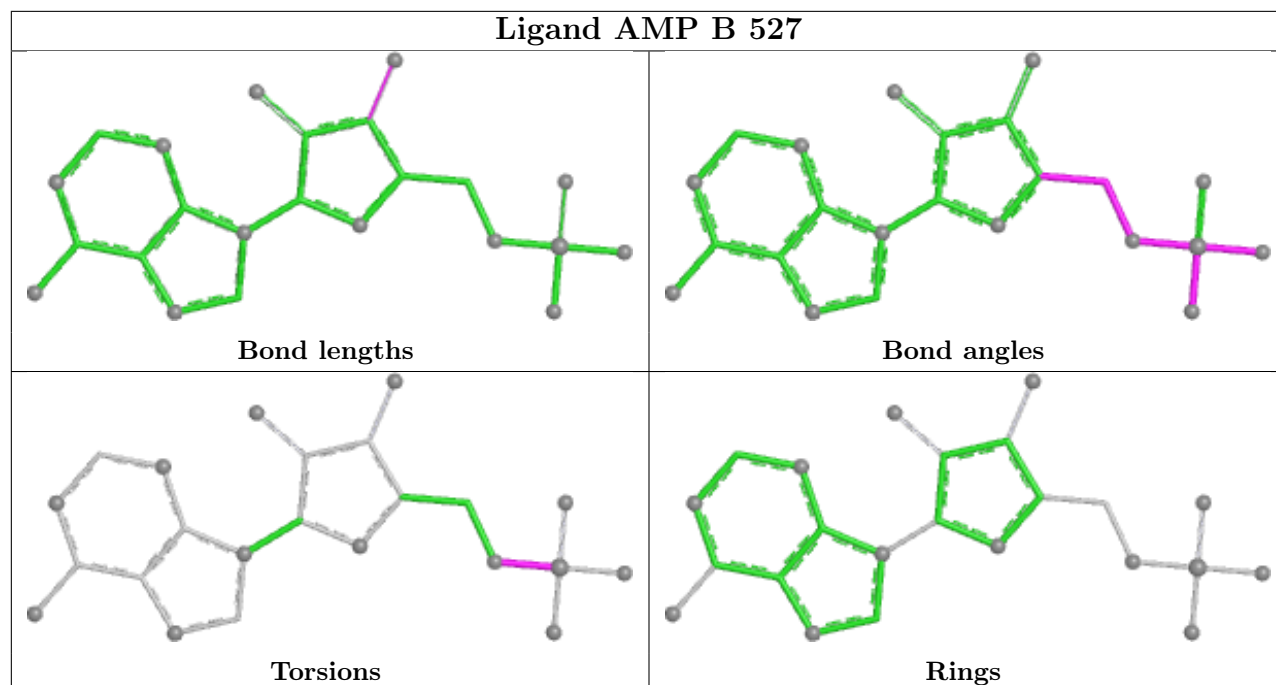
There are no ring outliers.

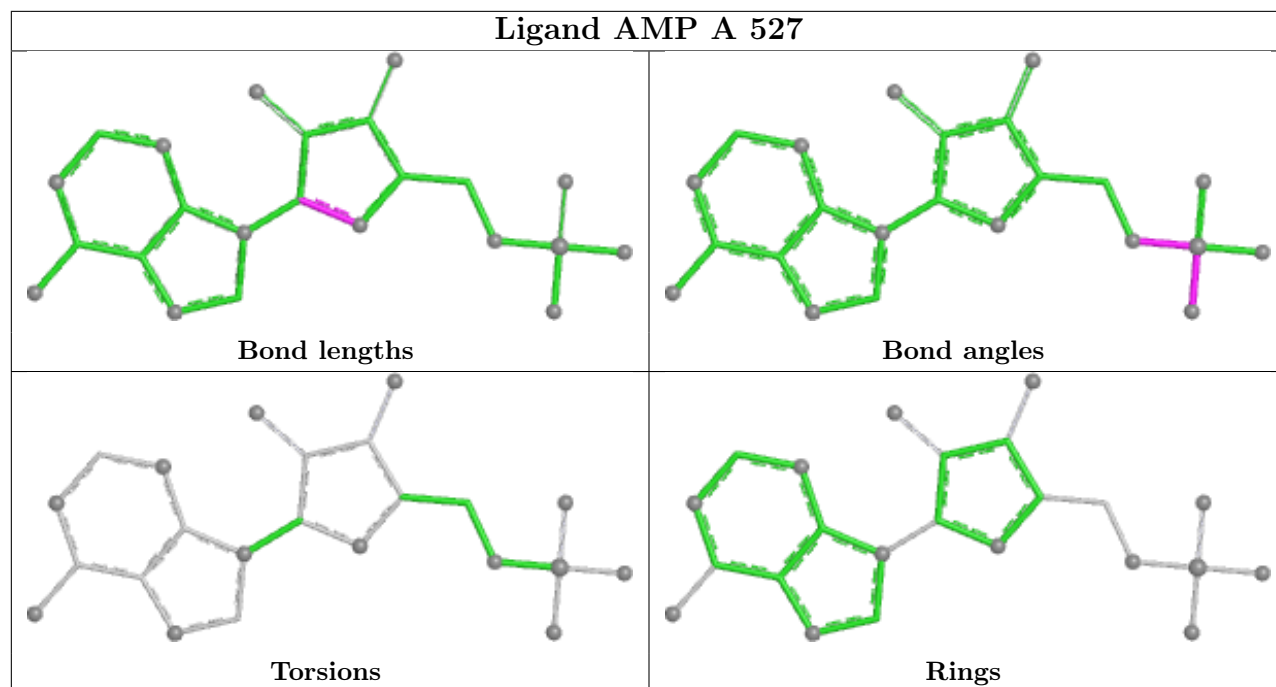
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	528	PO4	1	0
4	A	527	AMP	1	0
3	B	526	POP	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.







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.