



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 03:46 AM EDT

PDB ID : 1ECB / pdb\_00001ecb  
Title : ESCHERICHIA COLI GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE (PRPP) AMIDOTRANSFERASE COMPLEXED WITH 2 GMP, 1 MG PER SUBUNIT  
Authors : Krahn, J.M.; Smith, J.L.  
Deposited on : 1997-07-15  
Resolution : 2.70 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](mailto: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>.

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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)  
Xtrriage (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

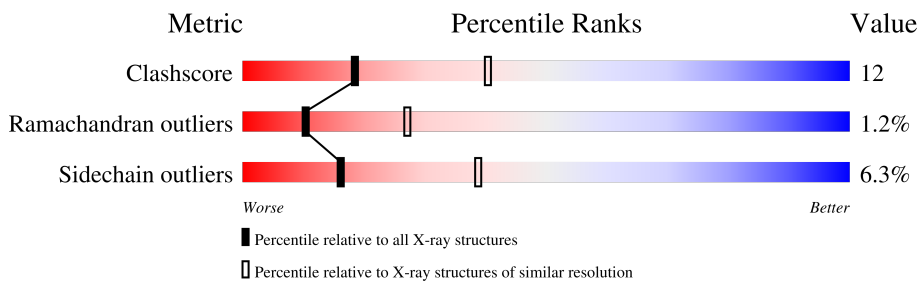
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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  $\geq 3$ , 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	504	
1	B	504	
1	C	504	
1	D	504	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15139 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.

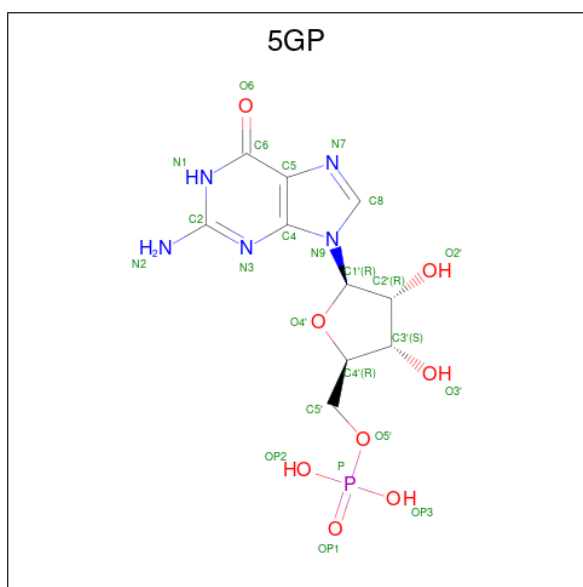
- Molecule 1 is a protein called GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	475	Total 3724	C 2345	N 657	O 705	S 17	0	0	0
1	B	470	Total 3685	C 2320	N 651	O 697	S 17	0	0	0
1	C	482	Total 3787	C 2381	N 675	O 714	S 17	0	0	0
1	D	473	Total 3708	C 2334	N 654	O 703	S 17	0	0	0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	D	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	D	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 4 is water.

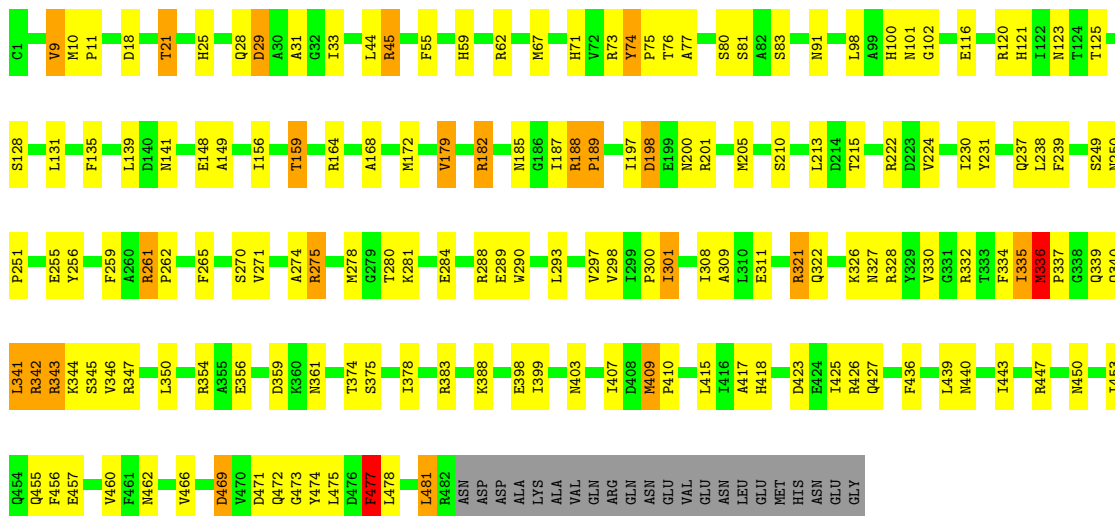
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	8	Total	O	0	0
			8	8		
4	C	13	Total	O	0	0
			13	13		
4	D	11	Total	O	0	0
			11	11		



VAL  
GLN  
ARG  
GLN  
MIO  
ASN  
GLU  
VAL  
GLU  
ASN  
LEU  
GLU  
MET  
HIS  
ASN  
GLU  
GLY

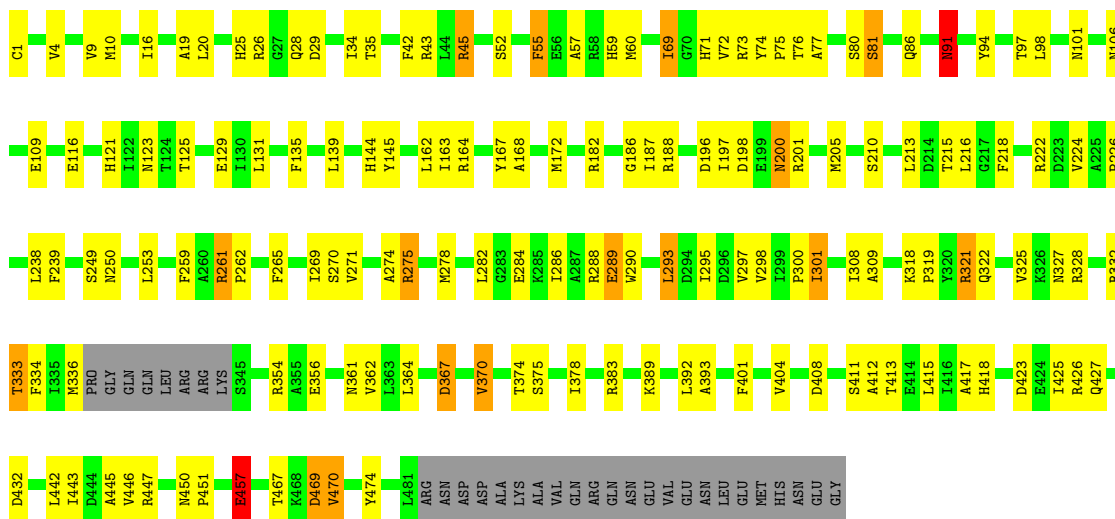
• Molecule 1: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE

Chain C:  64% 27%



• Molecule 1: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE

Chain D:  63% 27% 6%



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	95.80Å 113.20Å 199.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70	Depositor
% Data completeness (in resolution range)	97.7 (15.00-2.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.208 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	15139	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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: MG, 5GP

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	0.79	2/3791 (0.1%)	1.15	25/5133 (0.5%)
1	B	0.83	2/3751 (0.1%)	1.16	28/5078 (0.6%)
1	C	0.81	0/3855	1.14	24/5218 (0.5%)
1	D	0.79	0/3774	1.15	27/5110 (0.5%)
All	All	0.80	4/15171 (0.0%)	1.15	104/20539 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	301	ILE	CA-CB	-6.55	1.47	1.53
1	A	453	ILE	CA-CB	5.37	1.59	1.53
1	A	60	MET	SD-CE	-5.07	1.66	1.79
1	B	158	ALA	CA-CB	-5.06	1.45	1.53

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	301	ILE	CA-C-N	10.10	130.18	119.78
1	B	301	ILE	C-N-CA	10.10	130.18	119.78
1	C	259	PHE	N-CA-C	9.21	122.30	111.71
1	A	187	ILE	N-CA-C	9.20	119.06	110.42
1	A	301	ILE	CA-C-N	9.11	129.18	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	ILE	C-N-CA	9.11	129.18	119.89
1	D	301	ILE	CA-C-N	8.72	128.79	119.89
1	D	301	ILE	C-N-CA	8.72	128.79	119.89
1	B	259	PHE	N-CA-C	8.59	121.73	111.33
1	A	469	ASP	N-CA-C	8.47	123.03	112.87
1	D	259	PHE	N-CA-C	8.13	122.16	111.75
1	C	168	ALA	N-CA-C	-7.87	95.46	108.76
1	B	188	ARG	CA-C-N	7.76	127.69	119.85
1	B	188	ARG	C-N-CA	7.76	127.69	119.85
1	D	457	GLU	N-CA-C	-7.45	97.92	109.76
1	B	301	ILE	N-CA-C	-7.40	99.69	107.60
1	A	110	LEU	N-CA-C	7.20	119.12	111.28
1	D	362	VAL	N-CA-C	7.11	120.46	108.86
1	C	255	GLU	N-CA-C	-7.09	103.48	111.07
1	D	367	ASP	N-CA-C	7.09	119.01	111.28
1	A	168	ALA	N-CA-C	-7.04	96.86	108.76
1	D	401	PHE	CA-C-N	6.88	127.12	119.90
1	D	401	PHE	C-N-CA	6.88	127.12	119.90
1	A	289	GLU	N-CA-C	6.84	121.21	113.01
1	B	74	TYR	N-CA-C	-6.82	101.05	109.65
1	B	407	ILE	N-CA-C	-6.81	97.92	107.80
1	B	147	LEU	N-CA-C	-6.76	101.60	110.53
1	D	470	VAL	N-CA-C	6.74	118.76	109.80
1	A	74	TYR	N-CA-C	-6.69	101.63	109.93
1	A	474	TYR	N-CA-C	-6.69	103.92	111.14
1	C	301	ILE	CA-C-N	6.63	126.65	119.89
1	C	301	ILE	C-N-CA	6.63	126.65	119.89
1	D	81	SER	N-CA-C	-6.56	102.56	111.55
1	D	10	MET	CA-C-N	6.49	127.95	119.84
1	D	10	MET	C-N-CA	6.49	127.95	119.84
1	B	82	ALA	N-CA-C	-6.35	103.15	113.19
1	C	159	THR	N-CA-C	-6.34	104.28	111.07
1	B	289	GLU	N-CA-C	6.30	120.83	113.20
1	D	450	ASN	CA-C-N	6.26	125.94	119.56
1	D	450	ASN	C-N-CA	6.26	125.94	119.56
1	A	129	GLU	N-CA-C	-6.25	104.35	112.23
1	A	224	VAL	N-CA-C	-6.24	99.60	108.58
1	C	330	VAL	N-CA-C	-6.22	98.72	108.86
1	A	361	ASN	N-CA-C	-6.22	99.10	109.24
1	D	224	VAL	N-CA-C	-6.19	100.67	108.84
1	C	361	ASN	N-CA-C	-6.13	99.28	109.46
1	B	462	ASN	N-CA-C	6.13	120.64	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	469	ASP	N-CA-C	6.11	118.01	111.36
1	B	362	VAL	N-CA-C	6.07	118.12	108.89
1	B	129	GLU	N-CA-C	-6.06	104.79	111.82
1	A	9	VAL	N-CA-C	-6.06	106.86	112.43
1	A	162	LEU	N-CA-C	6.05	118.78	111.40
1	A	255	GLU	N-CA-C	-6.04	104.78	111.36
1	C	334	PHE	N-CA-C	6.00	119.68	110.20
1	B	168	ALA	N-CA-C	-6.00	98.63	108.41
1	D	187	ILE	N-CA-C	5.99	116.05	110.42
1	D	168	ALA	N-CA-C	-5.98	98.54	108.34
1	B	283	GLY	N-CA-C	-5.94	105.61	112.50
1	B	224	VAL	N-CA-C	-5.81	100.21	108.58
1	D	289	GLU	N-CA-C	5.80	120.20	113.18
1	D	196	ASP	N-CA-C	5.80	118.86	110.28
1	A	259	PHE	N-CA-C	5.78	123.11	110.80
1	A	246	ASN	CA-C-N	5.73	125.67	119.76
1	A	246	ASN	C-N-CA	5.73	125.67	119.76
1	A	117	GLU	N-CA-C	5.70	117.58	111.36
1	C	224	VAL	N-CA-C	-5.70	101.31	108.84
1	C	189	PRO	N-CA-C	5.67	121.16	111.68
1	B	361	ASN	N-CA-C	-5.67	99.28	108.41
1	D	162	LEU	N-CA-C	5.62	117.21	111.14
1	B	306	CYS	N-CA-C	5.62	117.85	111.11
1	C	74	TYR	N-CA-C	-5.62	101.47	109.62
1	C	308	ILE	N-CA-C	-5.62	105.25	110.53
1	D	144	HIS	N-CA-C	5.61	117.78	110.43
1	B	246	ASN	CA-C-N	5.61	125.89	119.83
1	B	246	ASN	C-N-CA	5.61	125.89	119.83
1	A	170	VAL	N-CA-C	-5.59	100.25	108.85
1	B	80	SER	N-CA-C	5.58	122.69	110.80
1	D	55	PHE	N-CA-C	5.57	118.60	107.62
1	B	49	GLY	N-CA-C	5.57	118.53	111.85
1	C	116	GLU	N-CA-C	5.56	117.42	111.36
1	C	9	VAL	CB-CA-C	-5.51	104.93	111.65
1	D	129	GLU	N-CA-C	-5.50	105.30	112.23
1	D	333	THR	N-CA-C	-5.43	99.88	108.73
1	A	147	LEU	N-CA-C	-5.43	103.37	110.53
1	A	362	VAL	N-CA-C	5.40	117.17	108.85
1	D	91	ASN	N-CA-C	5.39	119.12	112.54
1	C	477	PHE	N-CA-C	-5.36	105.09	111.69
1	D	361	ASN	N-CA-C	-5.36	100.50	109.24
1	C	83	SER	N-CA-C	-5.34	103.64	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	PHE	N-CA-C	5.32	117.64	107.75
1	B	43	ARG	N-CA-C	-5.23	100.38	108.90
1	A	333	THR	N-CA-C	-5.22	98.75	107.99
1	B	170	VAL	N-CA-C	-5.20	100.75	108.45
1	C	450	ASN	CA-C-N	5.17	124.97	119.28
1	C	450	ASN	C-N-CA	5.17	124.97	119.28
1	C	29	ASP	N-CA-C	5.15	116.97	111.36
1	B	54	VAL	N-CA-C	5.12	115.34	110.53
1	C	281	LYS	N-CA-C	5.09	116.83	111.28
1	C	462	ASN	N-CA-C	5.08	119.55	112.90
1	B	134	ILE	N-CA-C	-5.07	105.55	110.42
1	A	100	HIS	N-CA-C	5.05	117.39	108.75
1	A	305	SER	N-CA-C	5.01	119.16	113.19
1	D	116	GLU	N-CA-C	5.01	116.83	111.36
1	C	128	SER	N-CA-C	-5.00	105.92	112.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	145	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3724	0	3687	95	0
1	B	3685	0	3645	86	0
1	C	3787	0	3757	99	0
1	D	3708	0	3667	89	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	48	0	22	6	0
3	B	48	0	22	2	0
3	C	48	0	21	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	48	0	22	3	0
4	A	7	0	0	0	0
4	B	8	0	0	0	0
4	C	13	0	0	1	0
4	D	11	0	0	0	0
All	All	15139	0	14843	359	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 (359) 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:C:336:MET:HB2	1:C:337:PRO:HD3	1.39	1.02
1:C:164:ARG:HD2	1:C:469:ASP:HB3	1.47	0.94
1:A:80:SER:HB2	1:A:83:SER:HB2	1.52	0.90
1:C:342:ARG:HA	1:C:342:ARG:NE	1.85	0.89
1:B:80:SER:HB2	1:B:83:SER:HB2	1.52	0.88
1:D:29:ASP:HB2	1:D:75:PRO:HD3	1.58	0.83
1:C:341:LEU:HD13	1:C:342:ARG:N	1.98	0.78
1:C:29:ASP:HB2	1:C:75:PRO:HD3	1.64	0.77
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.49	0.77
1:C:383:ARG:HG3	1:C:383:ARG:HH11	1.50	0.76
1:B:301:ILE:HD13	1:B:378:ILE:HD13	1.68	0.76
1:A:76:THR:HG23	1:A:79:SER:HB2	1.67	0.75
1:B:383:ARG:HG3	1:B:383:ARG:HH11	1.50	0.75
1:D:383:ARG:HG3	1:D:383:ARG:HH11	1.50	0.74
1:D:182:ARG:HD2	1:D:188:ARG:O	1.88	0.74
1:C:410:PRO:HD2	1:C:415:LEU:HD21	1.72	0.72
1:C:332:ARG:HH12	1:C:343:ARG:NH2	1.86	0.71
1:A:383:ARG:HG3	1:A:383:ARG:HH11	1.54	0.71
1:B:45:ARG:HG3	1:B:59:HIS:HB3	1.71	0.71
1:A:265:PHE:CE2	1:A:270:SER:HB2	2.27	0.70
1:D:301:ILE:HD13	1:D:378:ILE:HD13	1.75	0.69
1:D:404:VAL:HG21	1:D:470:VAL:HG21	1.75	0.69
1:D:417:ALA:HA	1:D:425:ILE:HD11	1.75	0.69
1:C:182:ARG:HD2	1:C:188:ARG:O	1.92	0.69
1:B:417:ALA:HA	1:B:425:ILE:HD11	1.74	0.68
1:C:341:LEU:HD13	1:C:342:ARG:H	1.58	0.67
1:D:34:ILE:HD11	1:D:42:PHE:HB3	1.78	0.66
1:B:293:LEU:HD22	1:B:295:ILE:HG23	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ILE:HD13	1:B:446:VAL:HG12	1.77	0.65
1:C:262:PRO:HA	1:C:271:VAL:HB	1.78	0.65
1:D:321:ARG:HG2	1:D:356:GLU:OE1	1.95	0.65
1:B:293:LEU:HD13	1:B:293:LEU:O	1.98	0.64
1:D:274:ALA:O	1:D:278:MET:HG3	1.97	0.63
1:B:76:THR:HG23	1:B:79:SER:HB2	1.79	0.63
1:B:119:ARG:HD2	1:D:94:TYR:CE1	2.34	0.63
1:B:321:ARG:HG2	1:B:321:ARG:HH11	1.63	0.62
1:A:58:ARG:HG2	1:A:58:ARG:NH1	2.13	0.62
1:A:321:ARG:HG2	1:A:356:GLU:OE1	1.99	0.62
1:C:301:ILE:HD13	1:C:378:ILE:HD13	1.79	0.62
1:C:321:ARG:HG2	1:C:356:GLU:OE1	2.00	0.62
1:A:86:GLN:HB3	1:A:87:PRO:HA	1.82	0.61
1:A:439:LEU:O	1:A:443:ILE:HG13	2.01	0.61
1:D:135:PHE:CZ	1:D:139:LEU:HD11	2.36	0.61
1:B:80:SER:CB	1:B:83:SER:HB2	2.27	0.61
1:B:58:ARG:HG2	1:B:58:ARG:HH11	1.66	0.60
1:C:336:MET:HB2	1:C:337:PRO:CD	2.23	0.60
1:A:290:TRP:O	1:A:292:ASP:N	2.34	0.60
1:C:188:ARG:HG3	1:C:188:ARG:HH11	1.67	0.60
1:D:205:MET:HE2	1:D:213:LEU:HD12	1.82	0.59
1:D:370:VAL:HG13	3:D:505:5GP:OP3	2.02	0.59
1:B:321:ARG:HG2	1:B:356:GLU:OE1	2.02	0.59
1:A:371:ARG:HH11	1:A:371:ARG:HB3	1.66	0.59
1:C:417:ALA:HA	1:C:425:ILE:HD11	1.84	0.59
1:C:205:MET:HE2	1:C:213:LEU:HD12	1.83	0.59
1:B:166:ALA:CB	1:B:405:TYR:HB3	2.32	0.59
1:D:121:HIS:HE1	1:D:123:ASN:OD1	1.86	0.59
1:B:256:TYR:O	1:B:275:ARG:HD2	2.02	0.58
1:C:45:ARG:HG2	1:C:55:PHE:CD1	2.39	0.58
1:D:94:TYR:HE1	1:D:145:TYR:HD2	1.52	0.58
1:B:474:TYR:O	1:B:478:LEU:HG	2.03	0.57
1:A:45:ARG:HG3	1:A:59:HIS:HB3	1.85	0.57
1:B:383:ARG:HG3	1:B:383:ARG:NH1	2.20	0.57
1:C:164:ARG:CD	1:C:469:ASP:HB3	2.28	0.57
1:D:238:LEU:HD12	1:D:239:PHE:N	2.19	0.56
1:B:45:ARG:HB3	1:B:55:PHE:HE1	1.70	0.56
1:D:94:TYR:CE1	1:D:145:TYR:HD2	2.23	0.56
1:C:453:ILE:HG21	1:C:456:PHE:CE1	2.41	0.56
1:D:25:HIS:CE1	1:D:261:ARG:HG3	2.41	0.56
1:C:321:ARG:HG2	1:C:321:ARG:HH11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ARG:HD2	1:B:329:TYR:CE1	2.41	0.56
1:A:44:LEU:HG	1:A:45:ARG:N	2.21	0.55
1:D:200:ASN:N	1:D:200:ASN:ND2	2.54	0.55
1:D:262:PRO:HA	1:D:271:VAL:HB	1.88	0.55
1:D:289:GLU:O	1:D:290:TRP:HD1	1.90	0.55
1:B:179:VAL:HA	1:B:230:ILE:O	2.06	0.55
1:A:164:ARG:NH1	1:A:469:ASP:HB3	2.21	0.55
1:B:80:SER:C	1:B:82:ALA:H	2.14	0.55
1:C:284:GLU:O	1:C:288:ARG:HG3	2.06	0.55
1:A:471:ASP:O	1:A:474:TYR:HB3	2.06	0.55
1:C:250:ASN:OD1	1:C:466:VAL:HG21	2.07	0.55
1:C:261:ARG:NH2	1:D:327:ASN:OD1	2.40	0.55
1:D:442:LEU:O	1:D:445:ALA:HB3	2.07	0.54
1:A:371:ARG:HD3	3:A:505:5GP:OP3	2.06	0.54
1:B:371:ARG:O	1:B:416:ILE:HB	2.07	0.54
1:B:267:ASP:O	1:B:268:LYS:HB2	2.07	0.54
1:A:86:GLN:HG2	1:A:88:PHE:CE2	2.43	0.54
1:B:160:ASN:ND2	1:B:167:TYR:OH	2.41	0.54
1:B:321:ARG:HH11	1:B:321:ARG:CG	2.21	0.54
1:D:443:ILE:O	1:D:447:ARG:HB2	2.07	0.54
1:A:228:GLU:HG2	1:A:229:ALA:N	2.23	0.53
1:A:301:ILE:HD13	1:A:378:ILE:HD13	1.91	0.53
1:C:332:ARG:HH12	1:C:343:ARG:HH22	1.52	0.53
1:A:265:PHE:HA	1:A:269:ILE:O	2.08	0.53
1:B:80:SER:HB2	1:B:83:SER:CB	2.32	0.53
1:B:285:LYS:HG2	1:B:435:ILE:HD11	1.90	0.53
1:B:45:ARG:HB3	1:B:55:PHE:CE1	2.43	0.53
1:C:238:LEU:HD12	1:C:239:PHE:N	2.23	0.53
1:D:163:ILE:HD11	1:D:167:TYR:CZ	2.44	0.53
1:A:80:SER:CB	1:A:83:SER:HB2	2.34	0.53
1:C:383:ARG:HG3	1:C:383:ARG:NH1	2.21	0.53
1:D:45:ARG:HG2	1:D:55:PHE:CD1	2.43	0.53
1:D:238:LEU:HD12	1:D:239:PHE:H	1.73	0.53
1:C:443:ILE:O	1:C:447:ARG:HB2	2.08	0.53
1:A:443:ILE:O	1:A:447:ARG:HB2	2.09	0.53
1:B:477:PHE:HD1	1:B:477:PHE:O	1.91	0.53
1:D:164:ARG:HB3	1:D:469:ASP:OD2	2.08	0.53
1:B:86:GLN:HB3	1:B:87:PRO:HA	1.92	0.52
1:D:282:LEU:O	1:D:286:ILE:HG13	2.09	0.52
1:C:415:LEU:O	1:C:418:HIS:HB3	2.10	0.52
1:C:135:PHE:CZ	1:C:139:LEU:HD11	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:CYS:O	1:A:180:ALA:HA	2.10	0.52
1:C:33:ILE:HG13	1:C:55:PHE:CZ	2.44	0.52
1:A:346:VAL:HG23	1:A:377:GLN:OE1	2.10	0.52
1:C:73:ARG:NH1	1:C:81:SER:HA	2.25	0.52
1:B:297:VAL:CG1	1:B:362:VAL:HG12	2.40	0.51
1:C:475:LEU:HD23	1:C:478:LEU:HD12	1.91	0.51
1:B:290:TRP:O	1:B:293:LEU:HD12	2.10	0.51
1:A:285:LYS:HG2	1:A:435:ILE:HD11	1.93	0.51
1:B:439:LEU:O	1:B:443:ILE:HG13	2.11	0.51
1:C:328:ARG:HH22	3:D:506:5GP:H5'2	1.76	0.51
1:A:23:LEU:HD21	1:A:209:GLU:HB2	1.91	0.51
1:C:251:PRO:HG2	1:C:456:PHE:CD1	2.46	0.51
1:D:282:LEU:HD21	1:D:393:ALA:HB1	1.92	0.51
1:C:439:LEU:HG	1:C:443:ILE:HD11	1.93	0.51
1:B:471:ASP:O	1:B:475:LEU:HG	2.10	0.50
1:D:269:ILE:HD13	1:D:446:VAL:HG12	1.93	0.50
1:C:342:ARG:O	1:C:344:LYS:N	2.44	0.50
1:C:344:LYS:HD3	1:C:345:SER:H	1.77	0.50
1:B:195:ARG:NH1	1:B:203:GLU:OE1	2.44	0.50
1:C:478:LEU:HA	1:C:481:LEU:HD21	1.93	0.50
1:B:397:PRO:HG2	1:B:439:LEU:HA	1.93	0.50
1:C:18:ASP:HA	1:C:21:THR:OG1	2.12	0.50
1:C:256:TYR:O	1:C:275:ARG:HD2	2.12	0.50
1:C:188:ARG:HG3	1:C:189:PRO:HD2	1.93	0.50
1:B:28:GLN:HB3	1:B:50:LEU:HD23	1.93	0.50
1:B:94:TYR:O	1:D:121:HIS:HB2	2.12	0.50
1:C:471:ASP:C	1:C:473:GLY:H	2.20	0.50
1:C:399:ILE:HG21	1:C:409:MET:HE2	1.93	0.49
1:D:250:ASN:O	1:D:457:GLU:HB2	2.12	0.49
1:D:71:HIS:ND1	1:D:86:GLN:HB2	2.28	0.49
1:A:118:LYS:O	1:A:119:ARG:HB2	2.13	0.49
1:B:420:ARG:HG2	1:B:424:GLU:CD	2.37	0.49
1:D:253:LEU:HD21	1:D:442:LEU:HD23	1.94	0.49
1:A:251:PRO:HG2	1:A:456:PHE:CD1	2.48	0.49
1:D:389:LYS:HA	1:D:432:ASP:OD2	2.13	0.49
1:C:280:THR:N	1:C:311:GLU:HG2	2.28	0.49
1:B:166:ALA:HB2	1:B:405:TYR:HB3	1.95	0.48
1:C:73:ARG:HG2	1:C:74:TYR:N	2.27	0.48
1:B:265:PHE:CE2	1:B:270:SER:HB2	2.48	0.48
1:C:237:GLN:NE2	1:C:239:PHE:CZ	2.81	0.48
1:B:74:TYR:O	1:B:76:THR:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:HG3	1:B:272:TYR:HE2	1.79	0.48
1:B:24:GLN:O	1:B:24:GLN:HG3	2.14	0.48
1:B:280:THR:N	1:B:311:GLU:HG2	2.29	0.48
1:B:80:SER:C	1:B:82:ALA:N	2.72	0.48
1:C:45:ARG:HD2	1:C:59:HIS:CD2	2.48	0.48
1:C:73:ARG:HH12	1:C:81:SER:HA	1.78	0.48
1:C:289:GLU:O	1:C:290:TRP:HD1	1.97	0.48
1:D:426:ARG:HG2	1:D:426:ARG:HH11	1.77	0.48
1:C:403:ASN:HB2	1:C:460:VAL:CG1	2.43	0.48
1:D:321:ARG:HG2	1:D:321:ARG:HH11	1.79	0.48
1:A:160:ASN:ND2	1:A:167:TYR:OH	2.47	0.47
1:C:25:HIS:CE1	1:C:261:ARG:HG3	2.49	0.47
1:A:74:TYR:OH	3:A:505:5GP:O6	2.33	0.47
1:A:411:SER:OG	1:A:414:GLU:HG3	2.15	0.47
1:A:370:VAL:HB	3:A:505:5GP:OP3	2.15	0.47
1:B:118:LYS:O	1:B:119:ARG:HB2	2.14	0.47
1:B:293:LEU:CD2	1:B:295:ILE:HG23	2.44	0.47
1:D:197:ILE:HB	1:D:201:ARG:O	2.15	0.47
1:D:284:GLU:O	1:D:288:ARG:HG3	2.15	0.47
1:D:383:ARG:HG3	1:D:383:ARG:NH1	2.23	0.47
1:A:328:ARG:HH22	3:B:506:5GP:H5'2	1.79	0.47
1:D:297:VAL:HG21	1:D:321:ARG:HB2	1.97	0.47
1:B:1:CYS:O	1:B:26:ARG:HD3	2.15	0.47
1:B:71:HIS:HE1	1:B:73:ARG:HB2	1.79	0.47
1:B:336:MET:HE2	1:B:336:MET:HA	1.95	0.47
1:C:336:MET:CB	1:C:337:PRO:HD3	2.28	0.47
1:B:34:ILE:HA	1:B:43:ARG:O	2.14	0.46
1:D:34:ILE:HG23	1:D:172:MET:CE	2.45	0.46
1:A:204:TYR:HB2	1:A:232:ILE:HD13	1.96	0.46
1:A:345:SER:O	1:A:348:ARG:HB2	2.16	0.46
1:C:321:ARG:HH11	1:C:321:ARG:CG	2.28	0.46
1:C:481:LEU:H	1:C:481:LEU:HD23	1.80	0.46
1:A:359:ASP:C	1:A:388:LYS:HE2	2.41	0.46
1:D:19:ALA:HB2	1:D:216:LEU:HD11	1.97	0.46
1:A:321:ARG:HG2	1:A:321:ARG:HH11	1.79	0.46
1:A:200:ASN:OD1	1:A:200:ASN:N	2.48	0.46
1:A:417:ALA:HA	1:A:425:ILE:HD11	1.98	0.46
1:D:321:ARG:HH11	1:D:321:ARG:CG	2.29	0.46
1:C:426:ARG:HD3	4:C:515:HOH:O	2.16	0.46
3:C:506:5GP:N2	1:D:325:VAL:HG13	2.31	0.46
1:D:4:VAL:HG11	1:D:16:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:ARG:NH1	1:C:343:ARG:NH2	2.60	0.45
1:D:28:GLN:N	1:D:28:GLN:OE1	2.49	0.45
1:A:371:ARG:O	1:A:416:ILE:HB	2.16	0.45
1:D:45:ARG:HG2	1:D:55:PHE:CE1	2.50	0.45
1:A:12:VAL:O	1:A:16:ILE:HG13	2.17	0.45
1:C:148:GLU:O	1:C:149:ALA:C	2.60	0.45
1:A:86:GLN:HG2	1:A:88:PHE:CD2	2.51	0.45
1:A:140:ASP:O	1:A:143:ARG:NH2	2.49	0.45
1:B:326:LYS:HA	1:B:350:LEU:HD23	1.98	0.45
1:A:110:LEU:HD22	1:A:134:ILE:HD11	1.99	0.45
1:B:86:GLN:HG2	1:B:88:PHE:CD2	2.52	0.45
1:C:200:ASN:O	1:C:201:ARG:HG3	2.17	0.45
1:C:423:ASP:O	1:C:427:GLN:HG3	2.16	0.45
1:C:265:PHE:CE1	1:C:270:SER:HB2	2.52	0.45
1:C:398:GLU:HG3	1:C:436:PHE:CE2	2.51	0.45
1:B:121:HIS:HB3	1:D:91:ASN:O	2.17	0.45
1:B:171:ALA:HB3	1:B:179:VAL:HG22	1.99	0.45
1:A:163:ILE:HD11	1:A:167:TYR:CZ	2.52	0.45
1:C:74:TYR:OH	3:C:505:5GP:O6	2.34	0.45
1:C:346:VAL:HG21	1:C:374:THR:HA	1.99	0.45
1:A:45:ARG:NH1	1:A:54:VAL:O	2.50	0.45
1:A:222:ARG:NH2	1:A:228:GLU:OE2	2.50	0.45
1:B:45:ARG:NH1	1:B:54:VAL:O	2.48	0.45
1:B:286:ILE:O	1:B:290:TRP:HB2	2.17	0.45
1:C:121:HIS:HE1	1:C:123:ASN:OD1	1.99	0.45
1:C:197:ILE:O	1:C:198:ASP:HB3	2.17	0.45
1:D:74:TYR:HE2	1:D:408:ASP:HB3	1.82	0.45
1:A:34:ILE:O	1:A:34:ILE:HG23	2.17	0.44
1:B:274:ALA:O	1:B:277:ASN:HB2	2.18	0.44
1:B:301:ILE:HD13	1:B:378:ILE:CD1	2.44	0.44
1:C:327:ASN:OD1	1:D:261:ARG:NH2	2.49	0.44
1:C:332:ARG:HH21	1:D:57:ALA:HB2	1.82	0.44
1:D:1:CYS:O	1:D:26:ARG:HD3	2.17	0.44
1:D:293:LEU:HD13	1:D:295:ILE:HG23	1.98	0.44
1:D:374:THR:HG22	1:D:378:ILE:CD1	2.47	0.44
1:D:467:THR:C	1:D:469:ASP:N	2.75	0.44
1:A:211:VAL:HG13	1:A:264:SER:OG	2.18	0.44
1:A:302:PRO:HA	1:A:303:GLU:HA	1.70	0.44
1:D:364:LEU:O	1:D:392:LEU:HD12	2.18	0.44
1:A:13:ASN:O	1:A:60:MET:HE1	2.17	0.44
1:A:43:ARG:NH1	1:A:62:ARG:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:HH11	1:A:321:ARG:CG	2.31	0.44
1:B:232:ILE:HG12	1:B:238:LEU:HD13	1.98	0.44
1:A:110:LEU:HD22	1:A:134:ILE:CD1	2.47	0.44
1:A:121:HIS:HB3	1:C:91:ASN:O	2.16	0.44
1:C:250:ASN:HA	1:C:455:GLN:O	2.18	0.44
1:D:328:ARG:O	1:D:328:ARG:HG2	2.17	0.44
1:A:371:ARG:NH1	1:A:414:GLU:HB3	2.33	0.44
1:D:60:MET:HE3	1:D:60:MET:HB3	1.86	0.44
1:D:200:ASN:H	1:D:200:ASN:HD22	1.65	0.44
1:D:45:ARG:HD2	1:D:59:HIS:CG	2.52	0.44
1:D:265:PHE:CE1	1:D:270:SER:HB2	2.53	0.44
1:D:297:VAL:HG23	1:D:319:PRO:O	2.17	0.44
1:A:267:ASP:O	1:A:268:LYS:HB2	2.18	0.43
1:D:367:ASP:OD1	3:D:505:5GP:O3'	2.37	0.43
1:B:140:ASP:O	1:B:143:ARG:NH2	2.50	0.43
1:C:359:ASP:C	1:C:388:LYS:HE2	2.43	0.43
1:A:1:CYS:HA	1:A:72:VAL:O	2.18	0.43
1:C:474:TYR:HA	1:C:477:PHE:HB3	1.99	0.43
1:D:69:ILE:HD11	1:D:97:THR:HG23	2.01	0.43
3:A:506:5GP:H5'2	1:B:328:ARG:HH22	1.83	0.43
1:B:10:MET:HB2	1:B:11:PRO:HD2	2.01	0.43
1:C:59:HIS:O	1:C:62:ARG:HG2	2.18	0.43
1:C:156:ILE:O	1:C:159:THR:HB	2.18	0.43
1:C:475:LEU:HD23	1:C:475:LEU:HA	1.87	0.43
1:C:28:GLN:N	1:C:28:GLN:OE1	2.52	0.43
1:C:342:ARG:HA	1:C:342:ARG:HE	1.79	0.43
1:D:73:ARG:NH1	1:D:81:SER:HA	2.34	0.43
1:A:24:GLN:O	1:A:24:GLN:HG3	2.19	0.43
1:A:250:ASN:HA	1:A:455:GLN:O	2.19	0.43
1:B:29:ASP:HB2	1:B:75:PRO:HD3	2.00	0.43
1:C:300:PRO:HB3	1:C:309:ALA:HB3	2.00	0.43
1:B:211:VAL:HG13	1:B:264:SER:OG	2.19	0.43
1:C:335:ILE:HG22	1:C:340:GLN:H	1.83	0.43
1:D:411:SER:O	1:D:412:ALA:C	2.59	0.43
1:D:467:THR:C	1:D:469:ASP:H	2.27	0.43
1:A:34:ILE:HA	1:A:43:ARG:O	2.19	0.43
1:C:403:ASN:HB2	1:C:460:VAL:HG13	2.00	0.43
1:D:20:LEU:HD22	1:D:72:VAL:HG13	2.00	0.43
1:B:285:LYS:HE3	1:B:289:GLU:OE1	2.18	0.43
1:A:353:ASN:C	1:A:353:ASN:HD22	2.27	0.42
1:A:383:ARG:HG3	1:A:383:ARG:NH1	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:SER:HB2	1:A:465:TYR:CE2	2.53	0.42
1:B:477:PHE:CD1	1:B:477:PHE:C	2.97	0.42
1:D:94:TYR:CE1	1:D:145:TYR:CD2	3.05	0.42
1:D:205:MET:HG2	1:D:218:PHE:CD2	2.55	0.42
1:D:447:ARG:NH1	1:D:451:PRO:O	2.52	0.42
1:A:92:SER:HA	1:A:93:PRO:C	2.44	0.42
1:B:265:PHE:HA	1:B:269:ILE:O	2.19	0.42
1:C:179:VAL:HA	1:C:230:ILE:O	2.20	0.42
1:C:359:ASP:O	1:C:388:LYS:HE2	2.20	0.42
1:B:421:GLU:O	1:B:422:VAL:C	2.63	0.42
1:D:163:ILE:O	1:D:163:ILE:HG13	2.19	0.42
1:D:197:ILE:HG21	1:D:201:ARG:HE	1.85	0.42
1:A:24:GLN:HG2	1:B:329:TYR:CD2	2.54	0.42
1:A:286:ILE:O	1:A:290:TRP:HB2	2.20	0.42
1:B:415:LEU:O	1:B:418:HIS:HB3	2.20	0.42
1:A:301:ILE:HD12	1:A:366:ASP:HB2	2.01	0.42
1:B:34:ILE:HG23	1:B:34:ILE:O	2.18	0.42
1:B:92:SER:HA	1:B:93:PRO:C	2.45	0.42
1:B:166:ALA:HB3	1:B:405:TYR:HB3	2.01	0.42
1:C:44:LEU:HG	1:C:45:ARG:N	2.34	0.42
1:C:439:LEU:HG	1:C:443:ILE:CD1	2.49	0.42
1:A:80:SER:C	1:A:82:ALA:H	2.27	0.42
1:C:102:GLY:HA2	1:C:188:ARG:HD2	2.02	0.42
1:A:93:PRO:HB2	1:A:94:TYR:CD2	2.55	0.42
1:A:94:TYR:OH	1:A:147:LEU:HD21	2.20	0.42
1:A:127:ASP:HA	1:A:130:ILE:HG13	2.00	0.42
1:D:186:GLY:HA3	1:D:226:PRO:HG3	2.01	0.42
1:A:290:TRP:CG	1:A:293:LEU:HD12	2.55	0.42
1:A:359:ASP:O	1:A:388:LYS:HE2	2.20	0.42
1:C:297:VAL:HG22	1:C:298:VAL:N	2.34	0.42
1:C:326:LYS:HA	1:C:350:LEU:HD23	2.02	0.42
1:C:383:ARG:NH1	1:C:383:ARG:CG	2.82	0.42
1:A:465:TYR:CG	1:A:470:VAL:HG11	2.54	0.41
3:A:506:5GP:O4'	1:B:328:ARG:NH2	2.52	0.41
1:B:477:PHE:HD1	1:B:477:PHE:C	2.28	0.41
1:C:31:ALA:HA	1:C:71:HIS:O	2.20	0.41
1:C:250:ASN:O	1:C:457:GLU:HB2	2.20	0.41
1:B:230:ILE:HG23	1:B:238:LEU:HD11	2.02	0.41
1:A:331:GLY:H	1:A:348:ARG:HH12	1.67	0.41
1:B:375:SER:O	1:B:379:ILE:HD12	2.20	0.41
1:D:415:LEU:HB2	1:D:418:HIS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:ARG:O	1:D:308:ILE:HG12	2.21	0.41
1:C:185:ASN:HB2	1:C:187:ILE:HG13	2.02	0.41
1:A:383:ARG:NH1	1:A:383:ARG:CG	2.83	0.41
1:B:258:TYR:CE1	3:B:505:5GP:H2'	2.55	0.41
1:C:29:ASP:OD2	1:C:81:SER:HB3	2.20	0.41
1:C:478:LEU:HA	1:C:481:LEU:CD2	2.50	0.41
1:D:336:MET:HE2	1:D:336:MET:HA	2.01	0.41
1:D:383:ARG:NH1	1:D:383:ARG:CG	2.83	0.41
1:A:179:VAL:HA	1:A:230:ILE:O	2.21	0.41
1:A:221:LEU:O	1:A:222:ARG:HB3	2.20	0.41
1:D:198:ASP:OD1	1:D:200:ASN:ND2	2.53	0.41
1:D:297:VAL:HG22	1:D:298:VAL:N	2.35	0.41
1:D:300:PRO:HB3	1:D:309:ALA:CB	2.50	0.41
1:C:335:ILE:HD12	1:C:335:ILE:H	1.85	0.41
1:D:106:ASN:HB2	1:D:109:GLU:HG2	2.02	0.41
1:A:43:ARG:HH11	1:A:62:ARG:HG2	1.84	0.41
1:A:92:SER:HB3	1:C:120:ARG:HA	2.02	0.41
1:A:126:SER:C	1:A:128:SER:H	2.28	0.41
1:A:142:PHE:CD2	1:A:151:ASN:HB3	2.56	0.41
1:D:332:ARG:HG3	1:D:334:PHE:CZ	2.56	0.41
1:D:470:VAL:HG13	1:D:474:TYR:HD2	1.85	0.41
1:A:26:ARG:NH2	1:A:255:GLU:OE1	2.54	0.41
1:A:144:HIS:O	1:A:144:HIS:ND1	2.54	0.41
1:A:178:MET:HE2	1:A:232:ILE:HD12	2.02	0.41
1:A:290:TRP:CD2	1:A:293:LEU:HD12	2.56	0.41
1:B:86:GLN:HG2	1:B:88:PHE:CE2	2.56	0.41
1:B:230:ILE:CG2	1:B:238:LEU:HD11	2.51	0.41
1:D:318:LYS:HD3	1:D:318:LYS:HA	1.92	0.41
1:A:74:TYR:O	1:A:76:THR:N	2.53	0.40
1:A:438:ASP:HB3	1:A:440:ASN:OD1	2.21	0.40
1:B:474:TYR:O	1:B:477:PHE:HB3	2.21	0.40
1:A:328:ARG:HD2	1:A:329:TYR:CE1	2.56	0.40
1:B:321:ARG:CG	1:B:321:ARG:NH1	2.80	0.40
1:C:10:MET:HB2	1:C:11:PRO:HD2	2.03	0.40
1:D:423:ASP:O	1:D:427:GLN:HG3	2.21	0.40
1:A:156:ILE:O	1:A:159:THR:HB	2.22	0.40
1:A:258:TYR:CE1	3:A:505:5GP:H2'	2.57	0.40
1:C:67:MET:HG2	1:C:172:MET:SD	2.62	0.40
1:C:274:ALA:O	1:C:278:MET:HG3	2.21	0.40
1:A:5:GLY:HA3	1:A:170:VAL:HG21	2.04	0.40
1:D:35:THR:OG1	1:D:43:ARG:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLY:HA2	1:A:74:TYR:HA	2.03	0.40
1:B:191:VAL:O	1:B:206:VAL:HA	2.21	0.40
1:C:179:VAL:HG12	1:C:231:TYR:HD1	1.86	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	471/504 (94%)	427 (91%)	38 (8%)	6 (1%)	9	25
1	B	466/504 (92%)	427 (92%)	36 (8%)	3 (1%)	21	44
1	C	480/504 (95%)	431 (90%)	39 (8%)	10 (2%)	5	15
1	D	469/504 (93%)	431 (92%)	35 (8%)	3 (1%)	21	44
All	All	1886/2016 (94%)	1716 (91%)	148 (8%)	22 (1%)	10	27

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	GLU
1	C	80	SER
1	C	339	GLN
1	C	343	ARG
1	D	80	SER
1	A	199	GLU
1	C	336	MET
1	D	77	ALA
1	D	354	ARG
1	B	80	SER
1	C	198	ASP
1	C	354	ARG

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Mol	Chain	Res	Type
1	A	200	ASN
1	A	354	ARG
1	C	341	LEU
1	B	75	PRO
1	B	354	ARG
1	C	141	ASN
1	C	472	GLN
1	C	77	ALA
1	A	75	PRO
1	A	11	PRO

### 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	397/422 (94%)	374 (94%)	23 (6%)	18 42
1	B	392/422 (93%)	372 (95%)	20 (5%)	21 48
1	C	403/422 (96%)	372 (92%)	31 (8%)	12 30
1	D	395/422 (94%)	369 (93%)	26 (7%)	15 36
All	All	1587/1688 (94%)	1487 (94%)	100 (6%)	16 39

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	45	ARG
1	A	131	LEU
1	A	144	HIS
1	A	150	ASP
1	A	179	VAL
1	A	188	ARG
1	A	200	ASN
1	A	215	THR
1	A	222	ARG
1	A	235	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	275	ARG
1	A	292	ASP
1	A	321	ARG
1	A	322	GLN
1	A	347	ARG
1	A	353	ASN
1	A	371	ARG
1	A	375	SER
1	A	409	MET
1	A	458	CYS
1	A	466	VAL
1	A	471	ASP
1	B	45	ARG
1	B	100	HIS
1	B	105	THR
1	B	131	LEU
1	B	144	HIS
1	B	179	VAL
1	B	188	ARG
1	B	199	GLU
1	B	275	ARG
1	B	292	ASP
1	B	293	LEU
1	B	305	SER
1	B	321	ARG
1	B	322	GLN
1	B	332	ARG
1	B	353	ASN
1	B	375	SER
1	B	413	THR
1	B	440	ASN
1	B	477	PHE
1	C	9	VAL
1	C	21	THR
1	C	45	ARG
1	C	76	THR
1	C	98	LEU
1	C	100	HIS
1	C	101	ASN
1	C	125	THR
1	C	131	LEU
1	C	179	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	182	ARG
1	C	188	ARG
1	C	210	SER
1	C	215	THR
1	C	222	ARG
1	C	249	SER
1	C	261	ARG
1	C	275	ARG
1	C	293	LEU
1	C	321	ARG
1	C	322	GLN
1	C	335	ILE
1	C	336	MET
1	C	342	ARG
1	C	347	ARG
1	C	375	SER
1	C	407	ILE
1	C	409	MET
1	C	440	ASN
1	C	477	PHE
1	C	481	LEU
1	D	9	VAL
1	D	45	ARG
1	D	52	SER
1	D	69	ILE
1	D	76	THR
1	D	91	ASN
1	D	98	LEU
1	D	101	ASN
1	D	125	THR
1	D	131	LEU
1	D	200	ASN
1	D	210	SER
1	D	215	THR
1	D	222	ARG
1	D	249	SER
1	D	261	ARG
1	D	275	ARG
1	D	293	LEU
1	D	321	ARG
1	D	322	GLN
1	D	333	THR

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Mol	Chain	Res	Type
1	D	370	VAL
1	D	375	SER
1	D	413	THR
1	D	457	GLU
1	D	469	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	160	ASN
1	A	250	ASN
1	A	322	GLN
1	A	353	ASN
1	A	454	GLN
1	B	71	HIS
1	B	101	ASN
1	B	141	ASN
1	B	160	ASN
1	B	185	ASN
1	B	250	ASN
1	B	322	GLN
1	B	353	ASN
1	B	437	GLN
1	B	454	GLN
1	C	91	ASN
1	C	101	ASN
1	C	121	HIS
1	C	237	GLN
1	C	322	GLN
1	C	339	GLN
1	C	340	GLN
1	D	61	GLN
1	D	121	HIS
1	D	185	ASN
1	D	200	ASN
1	D	237	GLN
1	D	250	ASN
1	D	322	GLN
1	D	437	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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$
3	5GP	B	505	2	26,26,26	1.24	2 (7%)	39,40,40	1.25	6 (15%)
3	5GP	C	505	2	26,26,26	1.20	3 (11%)	39,40,40	1.26	4 (10%)
3	5GP	D	506	-	26,26,26	1.23	2 (7%)	39,40,40	1.35	4 (10%)
3	5GP	C	506	-	26,26,26	1.45	3 (11%)	39,40,40	1.69	11 (28%)
3	5GP	A	505	2	26,26,26	1.51	6 (23%)	39,40,40	1.35	5 (12%)
3	5GP	B	506	-	26,26,26	1.40	4 (15%)	39,40,40	1.58	9 (23%)
3	5GP	D	505	2	26,26,26	1.09	1 (3%)	39,40,40	1.23	4 (10%)
3	5GP	A	506	-	26,26,26	1.32	1 (3%)	39,40,40	1.52	9 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5GP	B	505	2	-	0/10/26/26	0/3/3/3
3	5GP	C	505	2	-	0/10/26/26	0/3/3/3
3	5GP	D	506	-	-	6/10/26/26	0/3/3/3
3	5GP	C	506	-	-	6/10/26/26	0/3/3/3
3	5GP	A	505	2	-	0/10/26/26	0/3/3/3
3	5GP	B	506	-	-	6/10/26/26	0/3/3/3
3	5GP	D	505	2	-	0/10/26/26	0/3/3/3
3	5GP	A	506	-	-	5/10/26/26	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	505	5GP	C4-N3	3.78	1.42	1.34
3	C	506	5GP	C8-N9	-3.38	1.29	1.37
3	B	506	5GP	O4'-C4'	-3.32	1.37	1.45
3	D	506	5GP	O4'-C4'	-3.17	1.37	1.45
3	A	505	5GP	C6-N1	3.06	1.44	1.38
3	D	505	5GP	C6-N1	2.83	1.44	1.38
3	C	506	5GP	C5-N7	-2.82	1.33	1.39
3	B	505	5GP	C4-N3	2.79	1.40	1.34
3	C	505	5GP	C6-N1	2.75	1.44	1.38
3	C	505	5GP	C4-N3	2.71	1.40	1.34
3	B	506	5GP	C5'-C4'	-2.70	1.43	1.51
3	C	506	5GP	O2'-C2'	-2.54	1.36	1.43
3	B	505	5GP	C6-N1	2.50	1.43	1.38
3	A	506	5GP	O4'-C4'	-2.46	1.39	1.45
3	C	505	5GP	O4'-C1'	2.32	1.47	1.42
3	A	505	5GP	C5-N7	2.29	1.43	1.39
3	A	505	5GP	C4-N9	2.22	1.43	1.38
3	A	505	5GP	P-O5'	2.22	1.67	1.60
3	B	506	5GP	O2'-C2'	-2.21	1.37	1.43
3	D	506	5GP	C5'-C4'	-2.08	1.45	1.51
3	A	505	5GP	C5'-C4'	2.04	1.57	1.51
3	B	506	5GP	O4'-C1'	2.01	1.46	1.42

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	506	5GP	N2-C2-N3	-4.74	110.43	119.67
3	C	506	5GP	O4'-C1'-C2'	-3.68	98.74	106.62
3	A	506	5GP	O4'-C4'-C5'	-3.60	97.80	109.33
3	C	506	5GP	O6-C6-N1	3.56	126.81	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	506	5GP	C6-C5-C4	3.56	124.19	118.83
3	D	505	5GP	C2'-C3'-C4'	3.51	109.39	102.61
3	C	505	5GP	C2'-C3'-C4'	3.17	108.74	102.61
3	A	506	5GP	C2-N3-C4	-3.10	106.95	112.30
3	A	505	5GP	OP2-P-OP3	2.93	118.80	107.80
3	C	506	5GP	O2'-C2'-C1'	-2.93	100.03	110.10
3	D	506	5GP	O2'-C2'-C1'	-2.90	100.12	110.10
3	D	506	5GP	O6-C6-N1	2.89	125.55	120.11
3	D	506	5GP	O4'-C4'-C5'	-2.83	100.27	109.33
3	B	506	5GP	O2'-C2'-C1'	-2.80	100.45	110.10
3	B	506	5GP	O4'-C4'-C5'	-2.80	100.37	109.33
3	A	506	5GP	N1-C2-N3	2.78	128.41	123.32
3	B	505	5GP	OP2-P-OP3	2.77	118.21	107.80
3	D	505	5GP	O3'-C3'-C4'	-2.77	103.13	111.08
3	C	505	5GP	OP2-P-OP3	2.70	117.92	107.80
3	C	506	5GP	C6-C5-N7	-2.68	125.40	130.29
3	B	506	5GP	O4'-C1'-C2'	-2.66	100.92	106.62
3	A	506	5GP	O2'-C2'-C1'	-2.65	100.99	110.10
3	C	506	5GP	C3'-C2'-C1'	2.58	106.35	101.46
3	A	505	5GP	C2-N3-C4	2.52	116.64	112.30
3	B	506	5GP	N2-C2-N1	2.51	122.06	116.76
3	C	505	5GP	C2-N3-C4	2.50	116.61	112.30
3	C	506	5GP	O4'-C4'-C5'	-2.48	101.38	109.33
3	A	506	5GP	O5'-P-OP1	-2.44	99.84	106.44
3	C	506	5GP	N9-C8-N7	2.44	117.92	113.40
3	D	505	5GP	OP2-P-OP3	2.42	116.88	107.80
3	A	505	5GP	C3'-C2'-C1'	2.40	106.00	101.46
3	C	506	5GP	OP2-P-O5'	-2.38	100.45	106.67
3	D	505	5GP	OP2-P-O5'	-2.36	100.52	106.67
3	B	506	5GP	N1-C2-N3	2.29	127.51	123.32
3	B	506	5GP	C6-C5-C4	2.27	122.24	118.83
3	A	506	5GP	C6-C5-C4	2.27	122.24	118.83
3	A	506	5GP	O5'-C5'-C4'	-2.27	101.27	108.99
3	B	506	5GP	C2-N3-C4	-2.27	108.39	112.30
3	B	505	5GP	N2-C2-N1	2.26	121.54	116.76
3	B	505	5GP	C2'-C3'-C4'	2.26	106.97	102.61
3	B	506	5GP	O6-C6-N1	2.24	124.33	120.11
3	B	505	5GP	C4'-O4'-C1'	2.21	114.34	109.47
3	A	505	5GP	N2-C2-N1	2.19	121.38	116.76
3	C	505	5GP	N2-C2-N1	2.18	121.36	116.76
3	A	506	5GP	C5'-C4'-C3'	2.17	123.04	115.21
3	B	505	5GP	OP2-P-O5'	-2.13	101.12	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	506	5GP	OP2-P-OP1	2.12	119.10	110.83
3	C	506	5GP	C5'-C6'-N1	-2.08	107.95	113.25
3	C	506	5GP	O5'-P-OP1	-2.07	100.84	106.44
3	D	506	5GP	C6'-C5'-C4	2.04	121.90	118.83
3	A	505	5GP	C4'-O4'-C1'	2.01	113.91	109.47
3	B	505	5GP	O3'-C3'-C2'	-2.00	105.40	111.82

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	506	5GP	C5'-O5'-P-OP1
3	A	506	5GP	C5'-O5'-P-OP3
3	A	506	5GP	C5'-O5'-P-OP2
3	B	506	5GP	C5'-O5'-P-OP1
3	B	506	5GP	C5'-O5'-P-OP3
3	B	506	5GP	C5'-O5'-P-OP2
3	C	506	5GP	C5'-O5'-P-OP1
3	C	506	5GP	C5'-O5'-P-OP3
3	C	506	5GP	C5'-O5'-P-OP2
3	D	506	5GP	C5'-O5'-P-OP1
3	D	506	5GP	C5'-O5'-P-OP3
3	D	506	5GP	C5'-O5'-P-OP2
3	D	506	5GP	O4'-C4'-C5'-O5'
3	B	506	5GP	C3'-C4'-C5'-O5'
3	D	506	5GP	C3'-C4'-C5'-O5'
3	B	506	5GP	O4'-C4'-C5'-O5'
3	C	506	5GP	C4'-C5'-O5'-P
3	A	506	5GP	O4'-C4'-C5'-O5'
3	C	506	5GP	C3'-C4'-C5'-O5'
3	D	506	5GP	C4'-C5'-O5'-P
3	C	506	5GP	O4'-C4'-C5'-O5'
3	B	506	5GP	C4'-C5'-O5'-P
3	A	506	5GP	C3'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 13 short contacts:

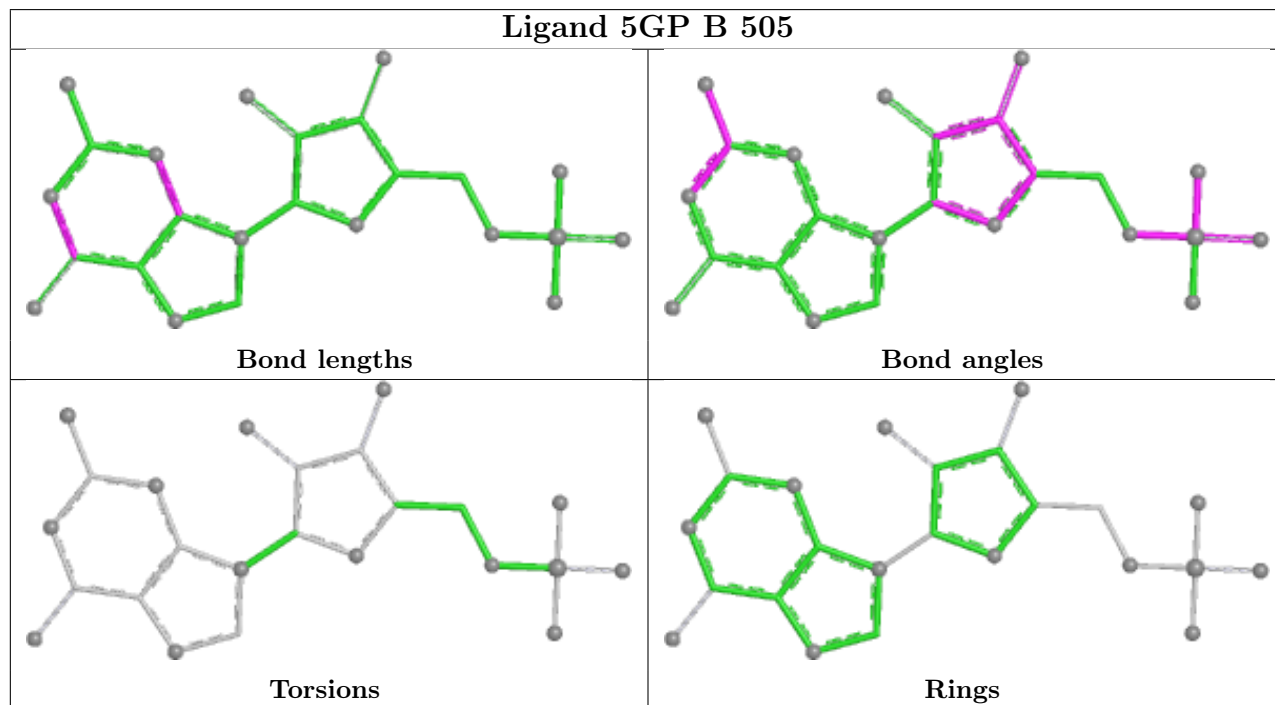
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	505	5GP	1	0
3	C	505	5GP	1	0

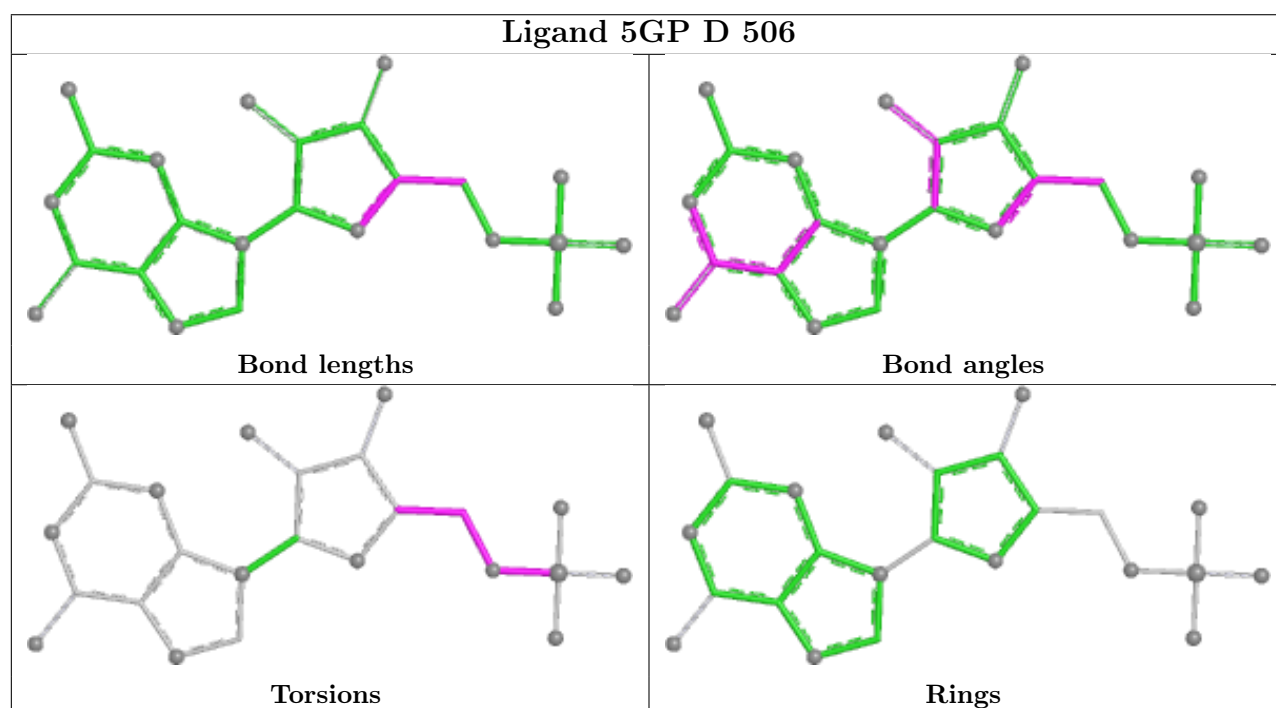
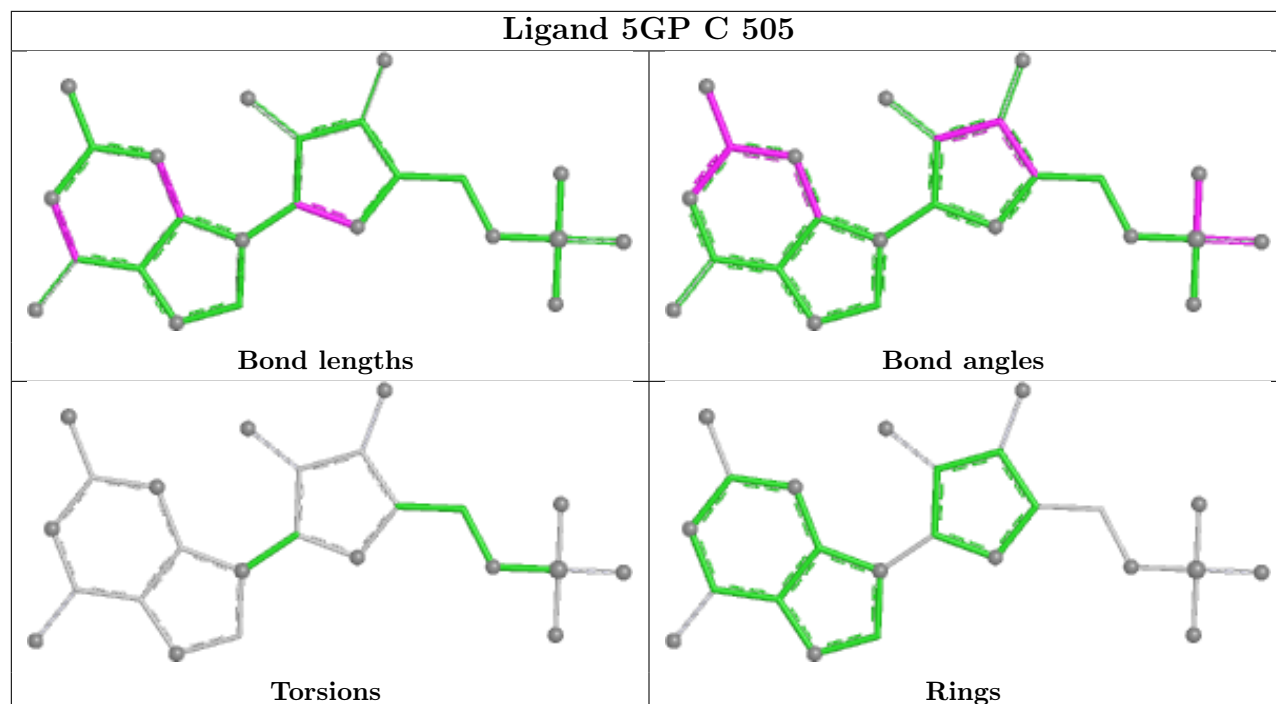
*Continued on next page...*

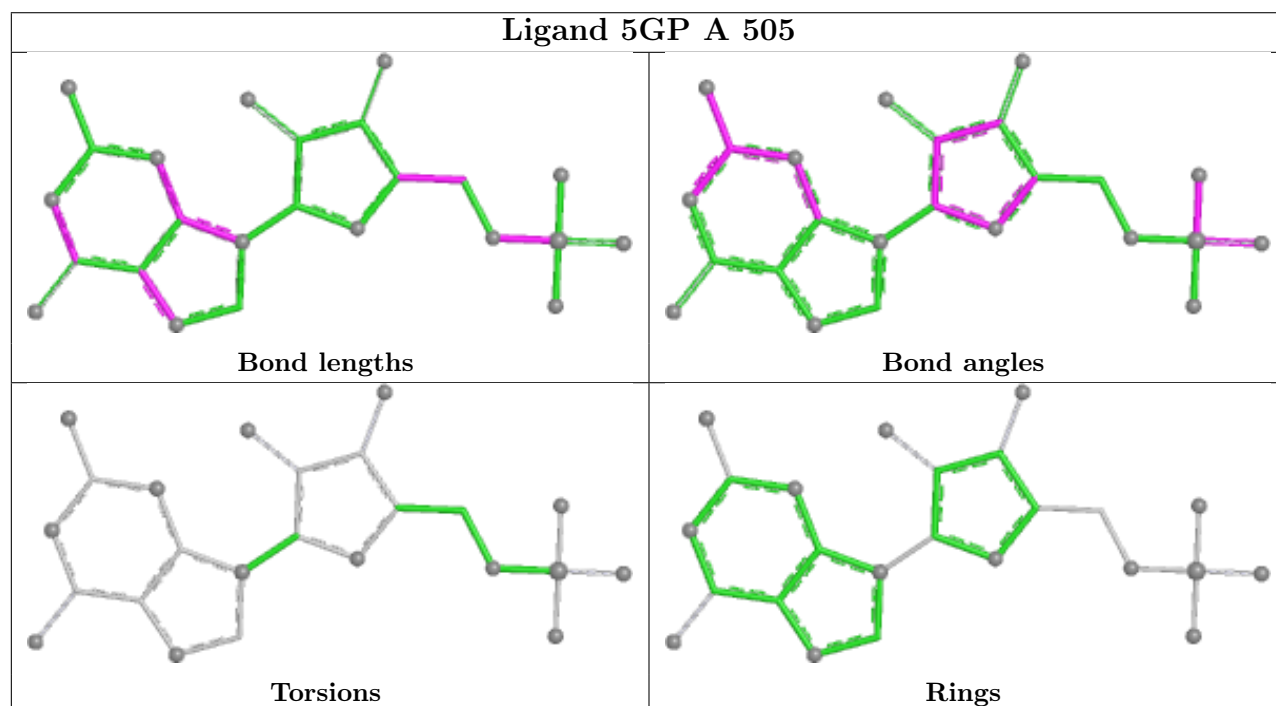
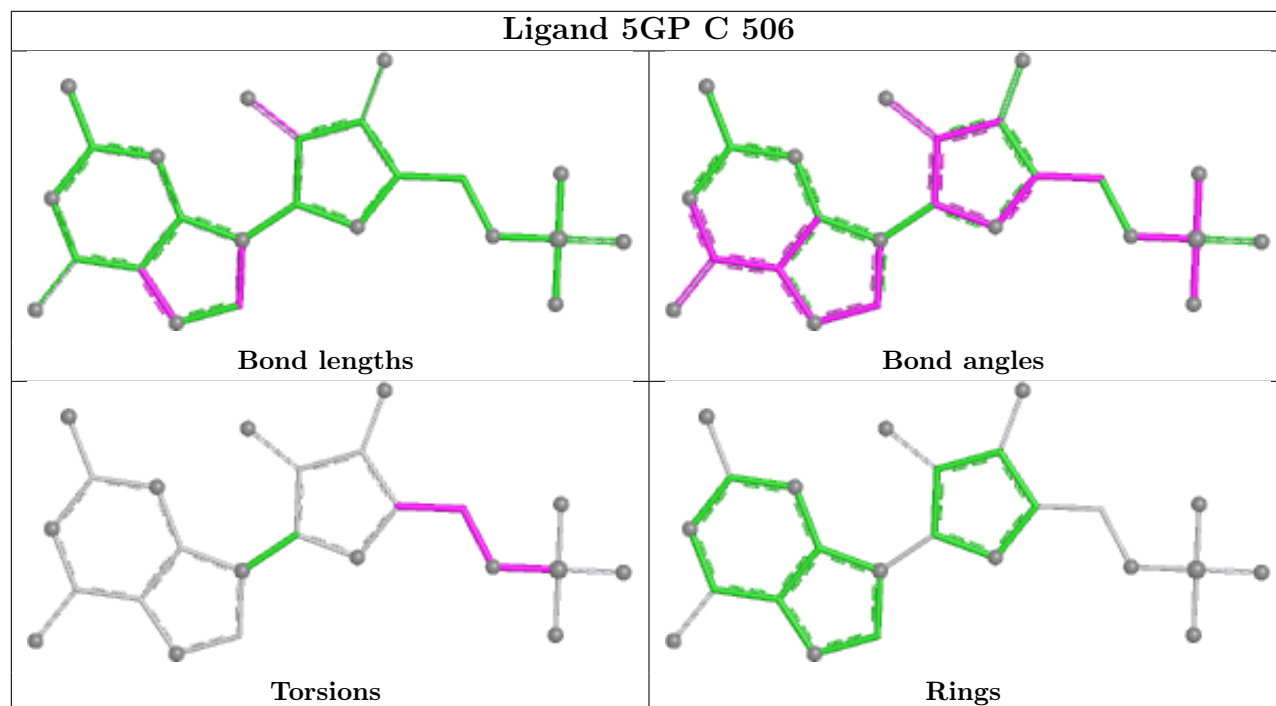
Continued from previous page...

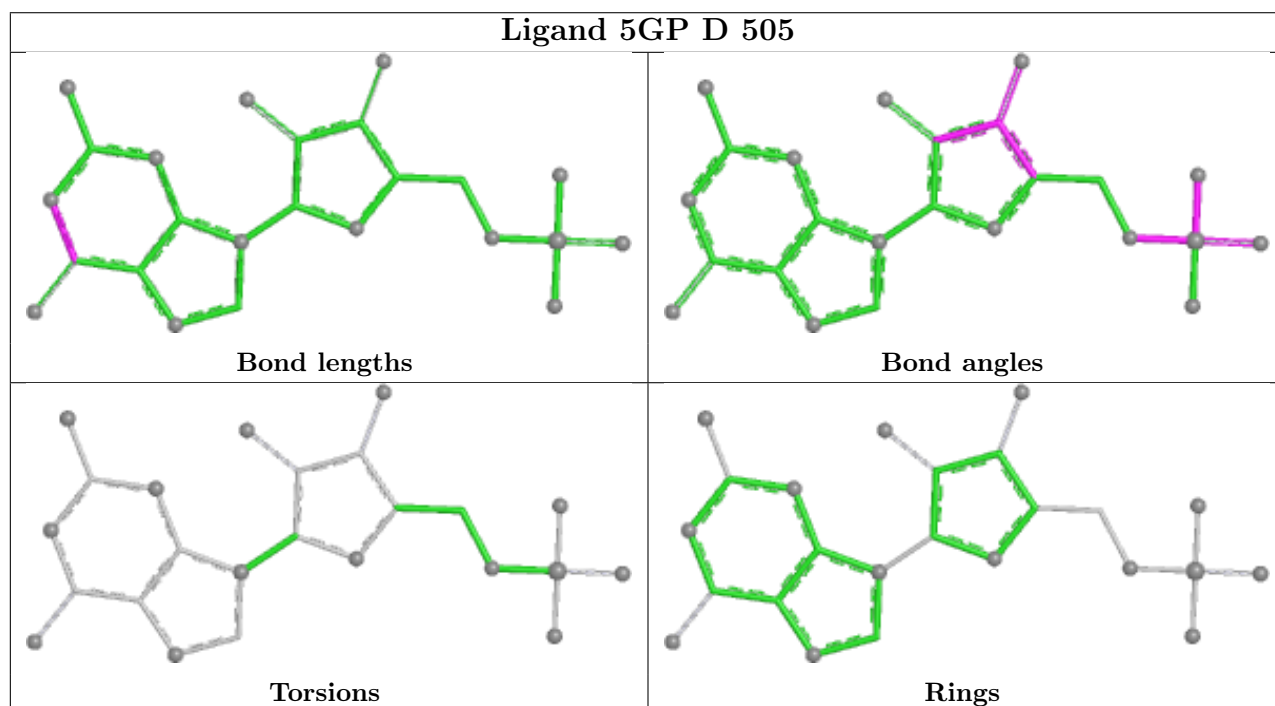
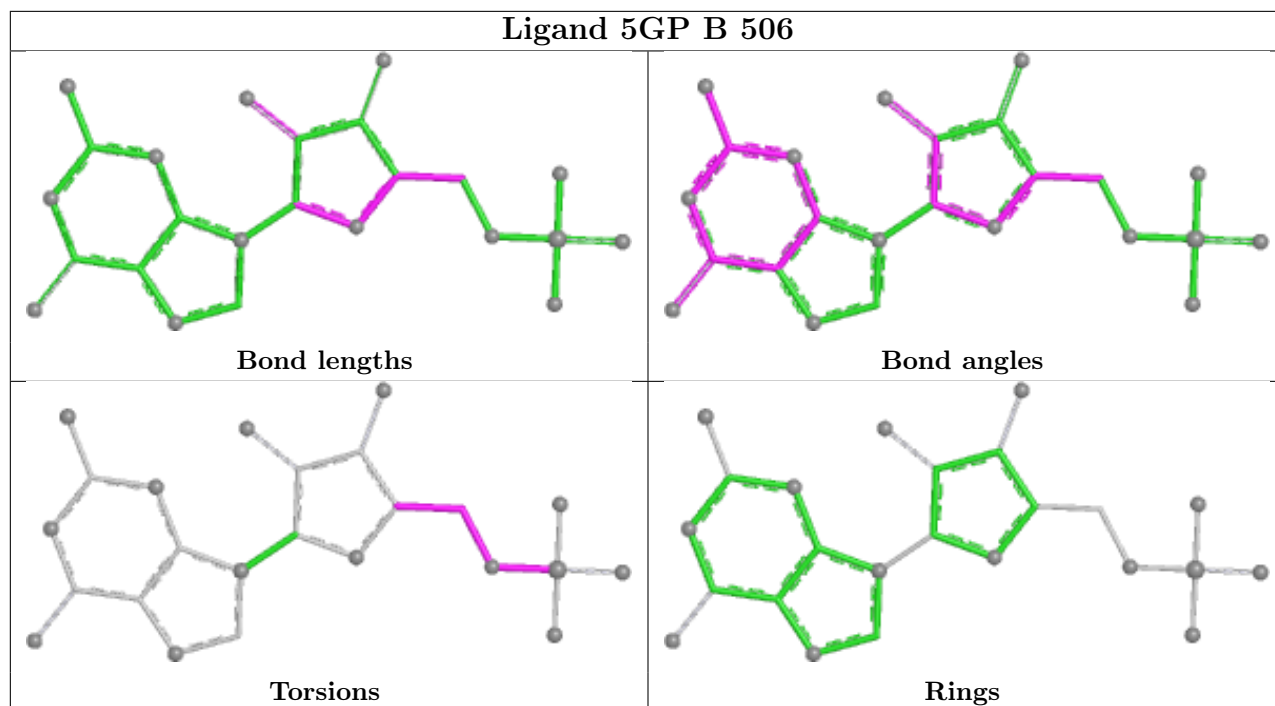
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	506	5GP	1	0
3	C	506	5GP	1	0
3	A	505	5GP	4	0
3	B	506	5GP	1	0
3	D	505	5GP	2	0
3	A	506	5GP	2	0

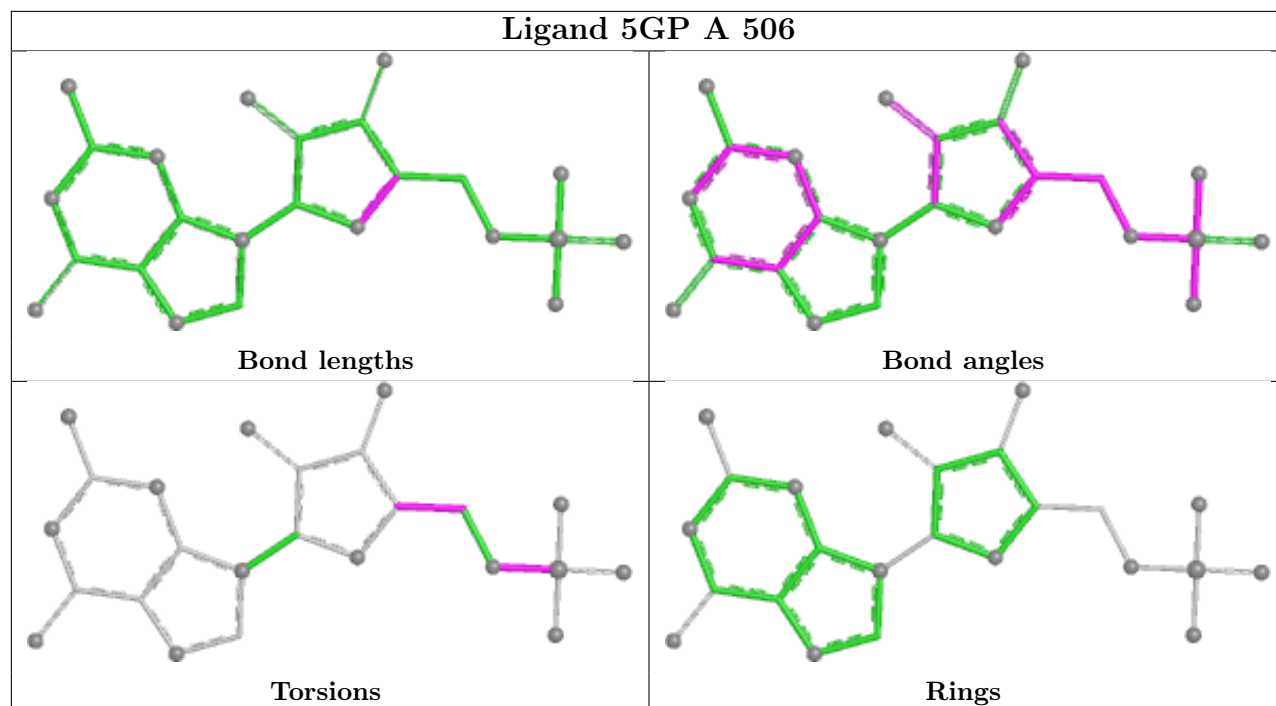
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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.