



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:41 AM UTC

PDB ID : 1XKB / pdb_00001xkb
Title : FACTOR XA COMPLEXED WITH A SYNTHETIC INHIBITOR FX-2212
A,(2S)-(3'-AMIDINO-3-BIPHENYLYL)-5-(4-PYRIDYLAMINO)PENTANO
IC ACID
Authors : Kamata, K.; Kim, S.H.
Deposited on : 1998-03-19
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

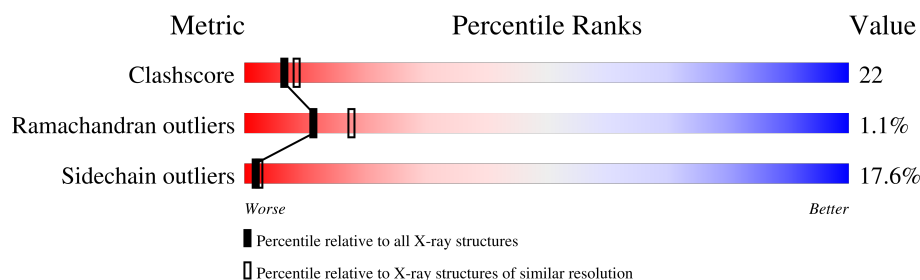
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

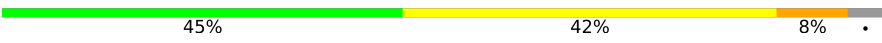
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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	95	
1	B	95	
2	C	235	
2	D	235	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5433 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 BLOOD COAGULATION FACTOR XA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	91	Total	C	N	O	S	0	0	0
			682	408	116	145	13			
1	B	90	Total	C	N	O	S	0	0	0
			676	405	117	141	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	BHD	ASP	modified residue	UNP P00742
B	63	BHD	ASP	modified residue	UNP P00742

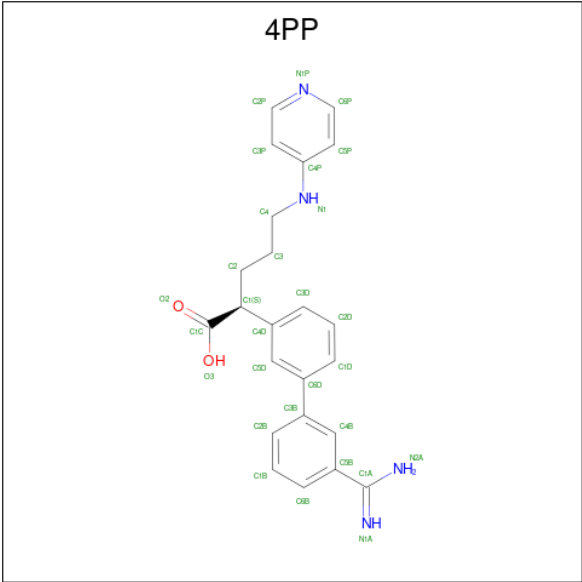
- Molecule 2 is a protein called BLOOD COAGULATION FACTOR XA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	235	Total	C	N	O	S	0	0	0
			1863	1172	327	350	14			
2	D	234	Total	C	N	O	S	0	0	0
			1852	1166	323	349	14			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is (2S)-(3'-AMIDINO-3-BIPHENYL)-5-(4-PYRIDYLAMINO)PENTANOIC ACID (CCD ID: 4PP) (formula: C₂₃H₂₄N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			29	23	4	2		
4	D	1	Total	C	N	O	0	0
			29	23	4	2		

- Molecule 5 is water.

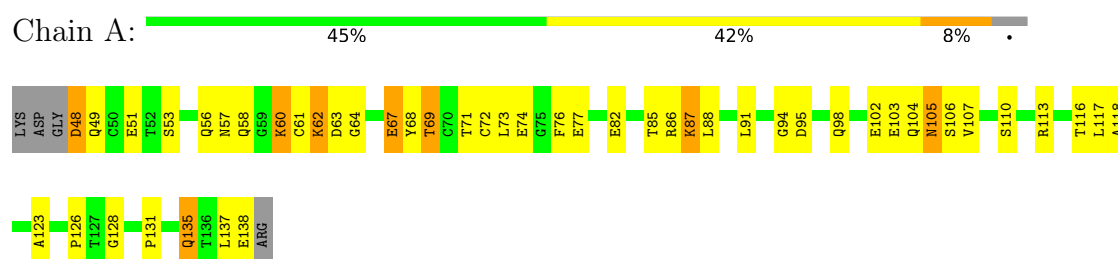
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total	O	0	0
			27	27		
5	C	123	Total	O	0	0
			123	123		
5	B	25	Total	O	0	0
			25	25		
5	D	124	Total	O	0	0
			124	124		

3 Residue-property plots [i](#)

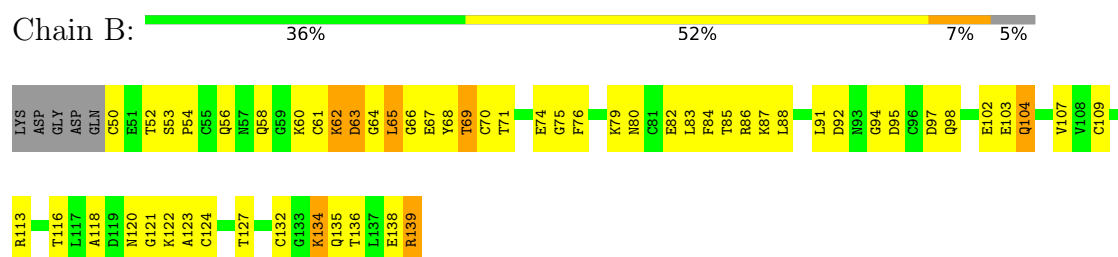
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

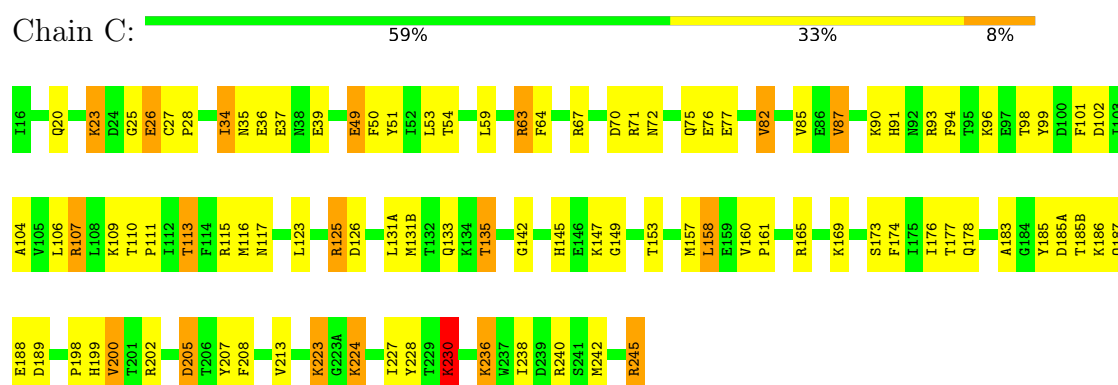
• Molecule 1: BLOOD COAGULATION FACTOR XA



• Molecule 1: BLOOD COAGULATION FACTOR XA

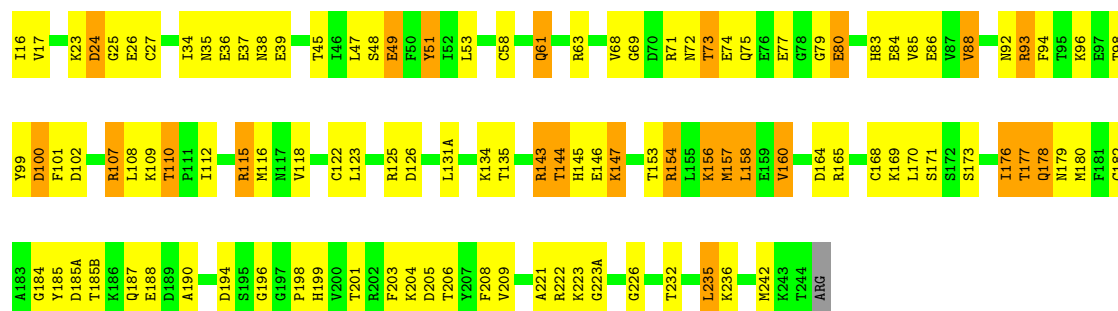


• Molecule 2: BLOOD COAGULATION FACTOR XA



• Molecule 2: BLOOD COAGULATION FACTOR XA





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	58.27Å 105.22Å 63.24Å 90.00° 103.40° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40	Depositor
% Data completeness (in resolution range)	86.3 (8.00-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.206 , 0.294	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5433	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: 4PP, BHD, 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	0.42	0/682	0.96	3/916 (0.3%)
1	B	0.47	0/676	0.86	0/907
2	C	0.47	0/1901	0.93	7/2560 (0.3%)
2	D	0.50	0/1890	0.97	11/2546 (0.4%)
All	All	0.48	0/5149	0.94	21/6929 (0.3%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	123	LEU	N-CA-C	-6.87	99.66	109.62
2	D	190	ALA	N-CA-C	-6.65	102.23	110.41
2	C	173	SER	N-CA-C	-6.58	104.88	113.17
2	D	179	ASN	N-CA-C	-6.57	105.58	112.93
2	D	51	TYR	N-CA-C	6.51	120.08	109.59
1	A	72	CYS	N-CA-C	6.45	118.63	110.24
1	A	128	GLY	CA-C-N	6.44	125.66	118.97
1	A	128	GLY	C-N-CA	6.44	125.66	118.97
2	D	73	THR	N-CA-C	6.30	120.44	112.87
2	D	196	GLY	N-CA-C	-6.17	106.23	114.25
2	C	205	ASP	N-CA-C	5.57	119.65	112.86
2	C	135	THR	N-CA-C	5.46	117.27	109.14
2	C	123	LEU	N-CA-C	-5.44	101.73	109.62
2	C	199	HIS	N-CA-C	-5.42	98.38	108.02
2	D	160	VAL	N-CA-C	5.37	113.74	107.89
2	D	27	CYS	CA-C-N	5.23	124.84	119.56
2	D	27	CYS	C-N-CA	5.23	124.84	119.56
2	D	100	ASP	N-CA-C	-5.16	102.64	110.28
2	D	199	HIS	N-CA-C	-5.13	98.92	107.80
2	C	96	LYS	N-CA-C	5.12	117.60	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	198	PRO	N-CA-C	5.05	120.11	111.68

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	682	0	614	33	0
1	B	676	0	614	45	0
2	C	1863	0	1821	81	0
2	D	1852	0	1808	69	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	C	29	0	22	1	0
4	D	29	0	22	1	0
5	A	27	0	0	0	0
5	B	25	0	0	0	0
5	C	123	0	0	6	0
5	D	124	0	0	8	0
All	All	5433	0	4901	218	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 22.

All (218) 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)
2:D:232:THR:HA	2:D:235:LEU:HD22	1.54	0.89
1:A:62:LYS:HG3	1:A:69:THR:HG22	1.54	0.89
1:B:138:GLU:HG3	1:B:139:ARG:CZ	2.05	0.87
1:A:48:ASP:HA	1:A:51:GLU:HB2	1.61	0.83
1:B:138:GLU:HG2	2:D:116:MET:SD	2.21	0.79
2:D:86:GLU:HB2	2:D:109:LYS:HG2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:34:ILE:HD11	2:C:82:VAL:HG13	1.66	0.78
2:C:70:ASP:HB3	5:C:584:HOH:O	1.86	0.75
1:B:94:GLY:O	1:B:95:ASP:HB2	1.86	0.75
2:C:165:ARG:HH21	2:C:178:GLN:HA	1.51	0.74
1:B:62:LYS:O	1:B:68:TYR:HA	1.87	0.74
2:C:147:LYS:HG2	2:D:145:HIS:HE1	1.54	0.73
1:B:50:CYS:SG	1:B:68:TYR:HB2	2.28	0.72
1:B:65:LEU:N	1:B:65:LEU:HD23	2.03	0.71
1:A:63:BHD:HA	1:A:68:TYR:HA	1.71	0.71
2:C:213:VAL:HG13	5:C:561:HOH:O	1.90	0.71
2:D:232:THR:HG23	5:D:765:HOH:O	1.92	0.70
1:B:98:GLN:HG3	1:B:124:CYS:SG	2.31	0.70
1:B:54:PRO:HB2	1:B:68:TYR:CE2	2.26	0.69
2:D:73:THR:HG23	2:D:153:THR:O	1.93	0.69
2:C:87:VAL:CG1	2:C:107:ARG:HB3	2.24	0.68
2:D:182:CYS:HB2	2:D:226:GLY:O	1.93	0.68
2:C:116:MET:O	2:C:117:ASN:HB2	1.93	0.67
2:D:17:VAL:O	2:D:188:GLU:HA	1.95	0.67
1:B:136:THR:O	2:D:116:MET:SD	2.53	0.66
1:A:103:GLU:O	1:A:104:GLN:HB2	1.95	0.66
1:B:135:GLN:HB3	2:D:25:GLY:O	1.95	0.66
2:C:87:VAL:HG13	2:C:107:ARG:HB3	1.78	0.65
2:D:49:GLU:CD	2:D:49:GLU:H	2.03	0.65
2:D:171:SER:HB2	2:D:223(A):GLY:O	1.96	0.65
1:B:56:GLN:HG2	1:B:80:ASN:HB3	1.79	0.65
1:B:65:LEU:N	1:B:65:LEU:CD2	2.60	0.64
2:D:157:MET:HE1	5:D:687:HOH:O	1.97	0.64
2:D:144:THR:HG22	2:D:156:LYS:NZ	2.12	0.64
2:D:158:LEU:HD13	2:D:160:VAL:HG13	1.80	0.63
2:C:50:PHE:CZ	2:C:111:PRO:HG3	2.34	0.63
2:D:185(B):THR:HB	2:D:223:LYS:HD3	1.80	0.63
2:D:24:ASP:HB3	2:D:116:MET:CE	2.29	0.62
2:C:64:PHE:CE1	2:C:85:VAL:HG21	2.35	0.62
2:C:238:ILE:O	2:C:242:MET:HG3	1.98	0.61
1:A:98:GLN:HG2	2:C:208:PHE:HZ	1.65	0.61
1:B:53:SER:N	1:B:54:PRO:HD3	2.15	0.61
1:A:87:LYS:HB2	1:A:91:LEU:HD23	1.82	0.61
2:C:49:GLU:HG3	2:C:111:PRO:HB3	1.81	0.61
2:C:165:ARG:NH1	2:C:169:LYS:HD2	2.13	0.61
2:D:48:SER:HB2	2:D:49:GLU:OE2	2.01	0.61
2:D:204:LYS:O	2:D:205:ASP:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LYS:HD3	1:A:95:ASP:OD2	2.02	0.60
2:C:236:LYS:HZ2	2:C:240:ARG:HG3	1.66	0.60
1:B:138:GLU:HG3	1:B:139:ARG:NH1	2.17	0.60
2:C:165:ARG:NH2	2:C:178:GLN:HA	2.16	0.60
2:C:145:HIS:HD2	2:C:147:LYS:H	1.50	0.60
2:D:100:ASP:CG	2:D:177:THR:HG21	2.27	0.59
2:C:71:ARG:HD3	5:C:582:HOH:O	2.00	0.59
2:D:92:ASN:ND2	2:D:93:ARG:HG2	2.18	0.59
2:C:236:LYS:NZ	2:C:240:ARG:HG3	2.18	0.59
1:B:61:CYS:HA	1:B:69:THR:O	2.03	0.59
1:A:60:LYS:HD2	1:A:62:LYS:NZ	2.18	0.59
2:C:34:ILE:HD13	2:C:67:ARG:HB2	1.85	0.57
1:B:63:BHD:OD1	1:B:63:BHD:N	2.35	0.57
1:A:105:ASN:HD22	1:A:105:ASN:N	2.03	0.57
2:C:23:LYS:O	2:C:26:GLU:HB2	2.04	0.57
2:D:35:ASN:OD1	2:D:39:GLU:HG2	2.05	0.57
2:D:24:ASP:HB3	2:D:116:MET:HE3	1.87	0.57
2:C:183:ALA:HB3	2:C:228:TYR:CE1	2.41	0.56
2:C:213:VAL:HG22	2:C:228:TYR:HE2	1.70	0.56
1:B:65:LEU:HD23	1:B:65:LEU:H	1.70	0.56
2:C:158:LEU:HD13	2:C:160:VAL:CG1	2.35	0.56
2:D:16:ILE:N	2:D:194:ASP:OD2	2.39	0.56
1:A:60:LYS:HD2	1:A:62:LYS:HZ1	1.71	0.55
2:C:185(B):THR:HB	2:C:223:LYS:HG3	1.87	0.55
2:C:113:THR:O	2:C:113:THR:HG22	2.06	0.55
1:A:82:GLU:N	1:A:82:GLU:OE1	2.39	0.55
2:C:165:ARG:HH22	2:C:177:THR:C	2.14	0.55
2:C:64:PHE:HE1	2:C:85:VAL:HG21	1.71	0.54
2:C:131(A):LEU:O	2:C:133:GLN:HB2	2.07	0.54
1:B:50:CYS:HA	1:B:54:PRO:CG	2.36	0.54
1:A:104:GLN:C	1:A:105:ASN:HD22	2.15	0.54
2:C:145:HIS:CD2	2:C:147:LYS:H	2.26	0.54
2:C:99:TYR:O	2:C:102:ASP:HB2	2.08	0.53
2:C:185(B):THR:CB	2:C:223:LYS:HG3	2.39	0.53
2:D:69:GLY:HA3	2:D:79:GLY:O	2.07	0.53
1:B:75:GLY:O	1:B:85:THR:N	2.40	0.53
2:C:34:ILE:HD11	2:C:82:VAL:CG1	2.38	0.53
1:B:87:LYS:CD	1:B:92:ASP:HB2	2.39	0.53
1:B:87:LYS:HD3	1:B:91:LEU:O	2.09	0.53
1:B:95:ASP:HB3	1:B:122:LYS:HG2	1.91	0.53
2:D:58:CYS:HA	2:D:61:GLN:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:VAL:O	2:D:80:GLU:HA	2.09	0.52
1:B:60:LYS:O	1:B:70:CYS:HA	2.10	0.52
1:A:61:CYS:HA	1:A:69:THR:O	2.09	0.52
2:C:35:ASN:HD21	2:C:39:GLU:HB2	1.73	0.52
1:B:118:ALA:CB	1:B:123:ALA:HB3	2.40	0.52
1:B:50:CYS:HA	1:B:54:PRO:CD	2.40	0.52
2:C:147:LYS:HG2	2:D:145:HIS:CE1	2.41	0.52
2:C:98:THR:O	2:C:99:TYR:HB2	2.10	0.52
2:C:93:ARG:HB2	2:C:101:PHE:CD2	2.46	0.51
2:C:125:ARG:NH1	2:C:126:ASP:OD1	2.44	0.51
2:D:37:GLU:O	2:D:38:ASN:HB2	2.11	0.51
2:C:158:LEU:HD13	2:C:160:VAL:HG13	1.93	0.51
2:C:165:ARG:NH2	2:C:177:THR:C	2.68	0.51
1:B:50:CYS:C	1:B:52:THR:H	2.18	0.51
2:C:20:GLN:NE2	2:C:23:LYS:NZ	2.59	0.51
2:C:35:ASN:ND2	2:C:39:GLU:HB2	2.25	0.51
1:B:87:LYS:HD3	1:B:92:ASP:HB2	1.93	0.51
2:D:98:THR:O	2:D:99:TYR:HB2	2.10	0.51
1:A:94:GLY:O	1:A:95:ASP:HB2	2.11	0.50
2:C:59:LEU:CD1	2:C:90:LYS:HB2	2.41	0.50
1:A:77:GLU:CD	1:A:85:THR:HG22	2.36	0.50
2:D:72:ASN:OD1	2:D:72:ASN:C	2.54	0.50
1:A:126:PRO:CB	1:A:131:PRO:HG3	2.42	0.50
2:C:67:ARG:HD3	2:C:70:ASP:HB2	1.93	0.50
2:D:145:HIS:CD2	2:D:147:LYS:HD2	2.47	0.50
1:B:56:GLN:HG3	1:B:82:GLU:HB3	1.93	0.50
2:D:45:THR:OG1	2:D:198:PRO:HB3	2.12	0.49
1:A:73:LEU:HD23	1:A:74:GLU:N	2.27	0.49
1:A:104:GLN:O	1:A:105:ASN:HB2	2.13	0.49
2:C:200:VAL:CG1	2:C:207:TYR:HD2	2.26	0.49
1:A:117:LEU:HD12	1:A:123:ALA:O	2.12	0.49
2:C:165:ARG:HH11	2:C:169:LYS:NZ	2.11	0.48
2:D:80:GLU:O	2:D:80:GLU:HG2	2.10	0.48
2:C:185(A):ASP:O	5:C:565:HOH:O	2.20	0.48
2:D:83:HIS:ND1	2:D:110:THR:HG22	2.28	0.48
2:D:232:THR:HA	2:D:235:LEU:CD2	2.33	0.48
2:C:54:THR:HG22	2:C:104:ALA:HB3	1.96	0.48
2:D:156:LYS:HG3	5:D:694:HOH:O	2.13	0.48
1:A:77:GLU:OE2	1:A:85:THR:HG22	2.14	0.47
1:A:88:LEU:HA	1:A:107:VAL:CG2	2.44	0.47
2:C:230:LYS:NZ	5:C:542:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LYS:HD2	1:A:71:THR:OG1	2.14	0.47
1:B:134:LYS:HE2	2:D:206:THR:OG1	2.13	0.47
2:C:51:TYR:CZ	2:C:107:ARG:HG3	2.49	0.47
1:A:87:LYS:HE2	1:A:91:LEU:HG	1.97	0.47
2:D:51:TYR:CD2	2:D:242:MET:HG2	2.50	0.47
2:D:185:TYR:O	5:D:800:HOH:O	2.20	0.47
2:D:143:ARG:NH1	2:D:146:GLU:O	2.48	0.47
1:A:64:GLY:N	1:A:67:GLU:O	2.39	0.47
2:C:25:GLY:N	2:C:117:ASN:OD1	2.41	0.47
1:B:84:PHE:CD1	1:B:84:PHE:N	2.83	0.47
2:D:158:LEU:HD13	2:D:160:VAL:CG1	2.43	0.46
2:C:149:GLY:HA3	5:D:631:HOH:O	2.16	0.46
2:C:202:ARG:HB2	2:C:207:TYR:CE2	2.50	0.46
2:D:94:PHE:HA	2:D:101:PHE:HB2	1.96	0.46
1:B:103:GLU:O	1:B:104:GLN:HG2	2.15	0.46
2:D:184:GLY:HA3	5:D:645:HOH:O	2.14	0.46
2:C:213:VAL:HG22	2:C:228:TYR:CE2	2.50	0.46
1:A:135:GLN:NE2	2:C:26:GLU:O	2.49	0.46
2:C:107:ARG:CZ	2:C:245:ARG:O	2.64	0.46
1:B:103:GLU:O	1:B:104:GLN:C	2.58	0.45
1:B:82:GLU:HG2	1:B:83:LEU:CD1	2.47	0.45
2:C:93:ARG:HB2	2:C:101:PHE:CG	2.51	0.45
2:C:76:GLU:HA	2:C:76:GLU:OE1	2.17	0.45
2:C:72:ASN:HA	2:C:153:THR:O	2.17	0.45
2:C:245:ARG:CZ	2:C:245:ARG:HB2	2.43	0.45
2:C:20:GLN:HE21	2:C:23:LYS:HZ2	1.64	0.45
2:C:113:THR:O	2:C:115:ARG:HD3	2.17	0.44
2:C:242:MET:HE2	2:C:242:MET:HB3	1.81	0.44
1:B:50:CYS:C	1:B:52:THR:N	2.73	0.44
1:A:87:LYS:CB	1:A:91:LEU:HD23	2.46	0.44
2:C:131(B):MET:HE3	2:C:131(B):MET:HB3	1.80	0.44
2:D:115:ARG:HG2	2:D:118:VAL:HB	2.00	0.44
1:B:62:LYS:HD2	1:B:62:LYS:HA	1.47	0.44
2:C:188:GLU:O	2:C:189:ASP:HB2	2.18	0.44
2:C:183:ALA:HB3	2:C:228:TYR:HE1	1.83	0.44
2:C:185:TYR:CB	2:C:186:LYS:HB3	2.48	0.44
2:D:51:TYR:CG	2:D:242:MET:HG2	2.53	0.44
2:C:169:LYS:CG	2:C:176:ILE:HB	2.48	0.44
1:B:60:LYS:HB2	1:B:71:THR:OG1	2.17	0.44
2:D:34:ILE:O	2:D:34:ILE:HG13	2.18	0.44
2:D:47:LEU:HD11	2:D:53:LEU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131(A):LEU:HG	2:D:201:THR:HB	1.99	0.44
2:D:222:ARG:HD3	5:D:638:HOH:O	2.17	0.43
2:C:87:VAL:HG13	2:C:107:ARG:CB	2.45	0.43
1:B:116:THR:HG23	1:B:127:THR:CG2	2.48	0.43
2:C:72:ASN:OD1	2:C:153:THR:HG22	2.19	0.43
1:B:135:GLN:NE2	2:D:26:GLU:O	2.50	0.43
4:D:999:4PP:H5P	4:D:999:4PP:H42	1.83	0.43
2:C:147:LYS:NZ	2:D:187:GLN:OE1	2.51	0.43
2:D:145:HIS:NE2	2:D:147:LYS:HD2	2.34	0.43
2:D:49:GLU:HA	2:D:112:ILE:HB	2.01	0.43
2:D:156:LYS:HE2	2:D:156:LYS:HB3	1.78	0.43
2:C:91:HIS:CE1	2:C:101:PHE:CD2	3.07	0.42
2:D:168:CYS:SG	2:D:176:ILE:HD12	2.59	0.42
2:D:185(A):ASP:O	2:D:223(A):GLY:N	2.51	0.42
1:A:138:GLU:O	1:A:138:GLU:HG2	2.20	0.42
2:C:53:LEU:HD12	2:C:104:ALA:O	2.19	0.42
1:A:57:ASN:CG	1:A:76:PHE:CE1	2.97	0.42
2:C:27:CYS:N	2:C:28:PRO:CD	2.82	0.42
2:C:174:PHE:CG	4:C:998:4PP:H2P	2.55	0.42
1:A:62:LYS:O	1:A:63:BHD:C	2.68	0.42
1:B:82:GLU:OE1	1:B:82:GLU:N	2.43	0.42
1:B:109:CYS:HB2	1:B:121:GLY:O	2.19	0.42
2:D:187:GLN:HA	2:D:221:ALA:HB1	2.01	0.42
2:C:63:ARG:HE	2:C:63:ARG:HB2	1.39	0.42
2:C:135:THR:HG22	2:C:161:PRO:HA	2.01	0.42
2:D:185(A):ASP:OD1	2:D:185(A):ASP:C	2.62	0.42
2:D:85:VAL:HG11	2:D:88:VAL:HG12	2.01	0.42
1:B:84:PHE:N	1:B:84:PHE:HD1	2.17	0.42
2:D:134:LYS:HG2	2:D:135:THR:HG23	2.02	0.41
1:A:73:LEU:HD23	1:A:74:GLU:H	1.85	0.41
2:D:126:ASP:HB2	5:D:722:HOH:O	2.20	0.41
2:D:131(A):LEU:HD21	2:D:208:PHE:HB2	2.03	0.41
2:D:178:GLN:C	2:D:180:MET:H	2.27	0.41
1:A:105:ASN:N	1:A:105:ASN:ND2	2.68	0.41
1:A:126:PRO:HB3	1:A:131:PRO:HG3	2.02	0.41
2:C:109:LYS:HB2	2:C:109:LYS:HE3	1.76	0.41
1:B:118:ALA:HB3	1:B:120:ASN:OD1	2.20	0.41
2:D:71:ARG:O	2:D:154:ARG:HA	2.20	0.41
2:C:94:PHE:HA	2:C:101:PHE:HB2	2.03	0.41
2:C:224:LYS:O	5:C:565:HOH:O	2.22	0.41
1:A:118:ALA:CB	1:A:123:ALA:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ALA:HB2	1:B:123:ALA:HB3	2.03	0.41
1:B:138:GLU:HG3	1:B:139:ARG:NH2	2.33	0.41
2:D:99:TYR:O	2:D:102:ASP:HB2	2.20	0.41
2:C:236:LYS:HD3	2:C:236:LYS:O	2.20	0.41
2:D:203:PHE:CE2	2:D:204:LYS:HD2	2.56	0.40
2:D:51:TYR:CE1	2:D:107:ARG:HG3	2.56	0.40
1:B:132:CYS:C	2:D:122:CYS:SG	3.05	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	88/95 (93%)	79 (90%)	9 (10%)	0	100	100
1	B	87/95 (92%)	71 (82%)	13 (15%)	3 (3%)	3	2
2	C	233/235 (99%)	217 (93%)	13 (6%)	3 (1%)	9	14
2	D	232/235 (99%)	216 (93%)	15 (6%)	1 (0%)	30	43
All	All	640/660 (97%)	583 (91%)	50 (8%)	7 (1%)	11	18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	GLY
1	B	64	GLY
2	D	125	ARG
2	C	142	GLY
2	C	187	GLN
2	C	230	LYS
1	B	58	GLN

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	77/80 (96%)	58 (75%)	19 (25%)	1	1
1	B	76/80 (95%)	60 (79%)	16 (21%)	1	1
2	C	200/200 (100%)	174 (87%)	26 (13%)	4	5
2	D	199/200 (100%)	163 (82%)	36 (18%)	2	2
All	All	552/560 (99%)	455 (82%)	97 (18%)	2	2

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	49	GLN
1	A	53	SER
1	A	56	GLN
1	A	58	GLN
1	A	60	LYS
1	A	62	LYS
1	A	67	GLU
1	A	69	THR
1	A	86	ARG
1	A	87	LYS
1	A	102	GLU
1	A	105	ASN
1	A	106	SER
1	A	110	SER
1	A	113	ARG
1	A	116	THR
1	A	135	GLN
1	A	137	LEU
2	C	23	LYS
2	C	26	GLU
2	C	34	ILE
2	C	36	GLU
2	C	37	GLU

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Mol	Chain	Res	Type
2	C	49	GLU
2	C	63	ARG
2	C	75	GLN
2	C	77	GLU
2	C	82	VAL
2	C	87	VAL
2	C	106	LEU
2	C	107	ARG
2	C	110	THR
2	C	113	THR
2	C	125	ARG
2	C	157	MET
2	C	158	LEU
2	C	200	VAL
2	C	205	ASP
2	C	223	LYS
2	C	224	LYS
2	C	227	ILE
2	C	230	LYS
2	C	236	LYS
2	C	245	ARG
1	B	62	LYS
1	B	65	LEU
1	B	67	GLU
1	B	69	THR
1	B	74	GLU
1	B	76	PHE
1	B	79	LYS
1	B	86	ARG
1	B	88	LEU
1	B	97	ASP
1	B	102	GLU
1	B	104	GLN
1	B	107	VAL
1	B	113	ARG
1	B	134	LYS
1	B	139	ARG
2	D	23	LYS
2	D	24	ASP
2	D	36	GLU
2	D	49	GLU
2	D	61	GLN

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Mol	Chain	Res	Type
2	D	63	ARG
2	D	74	GLU
2	D	75	GLN
2	D	77	GLU
2	D	80	GLU
2	D	84	GLU
2	D	88	VAL
2	D	93	ARG
2	D	96	LYS
2	D	107	ARG
2	D	108	LEU
2	D	110	THR
2	D	115	ARG
2	D	143	ARG
2	D	144	THR
2	D	147	LYS
2	D	154	ARG
2	D	156	LYS
2	D	157	MET
2	D	158	LEU
2	D	164	ASP
2	D	165	ARG
2	D	169	LYS
2	D	170	LEU
2	D	173	SER
2	D	176	ILE
2	D	177	THR
2	D	178	GLN
2	D	209	VAL
2	D	235	LEU
2	D	236	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	56	GLN
1	A	105	ASN
1	A	135	GLN
2	C	20	GLN
2	C	30	GLN
2	C	145	HIS

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Mol	Chain	Res	Type
2	C	178	GLN
1	B	57	ASN
1	B	104	GLN
2	D	38	ASN
2	D	133	GLN
2	D	145	HIS
2	D	178	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	BHD	A	63	1,3	6,8,9	1.11	0	8,10,12	0.85	0
1	BHD	B	63	1	6,8,9	1.02	0	8,10,12	1.58	2 (25%)

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
1	BHD	A	63	1,3	-	4/9/10/12	-
1	BHD	B	63	1	-	5/9/10/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	BHD	OB-CB-CA	2.88	113.80	107.49
1	B	63	BHD	OD2-CG-CB	2.37	119.89	113.31

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63	BHD	OB-CB-CG-OD1
1	A	63	BHD	OB-CB-CG-OD2
1	B	63	BHD	CA-CB-CG-OD1
1	B	63	BHD	CA-CB-CG-OD2
1	A	63	BHD	CA-CB-CG-OD1
1	A	63	BHD	CA-CB-CG-OD2
1	B	63	BHD	OB-CB-CG-OD1
1	B	63	BHD	OB-CB-CG-OD2
1	B	63	BHD	N-CA-CB-OB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	63	BHD	2	0
1	B	63	BHD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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
4	4PP	C	998	-	31,31,31	2.14	15 (48%)	38,41,41	1.30	5 (13%)
4	4PP	D	999	-	31,31,31	2.25	18 (58%)	38,41,41	1.17	2 (5%)

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	4PP	C	998	-	-	2/23/23/23	0/3/3/3
4	4PP	D	999	-	-	6/23/23/23	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	998	4PP	C4P-N1	4.23	1.50	1.38
4	D	999	4PP	C4P-N1	4.18	1.50	1.38
4	C	998	4PP	C5B-C1A	3.78	1.54	1.47
4	D	999	4PP	C5B-C1A	3.56	1.54	1.47
4	D	999	4PP	C5D-C4D	3.47	1.44	1.39
4	C	998	4PP	C5D-C4D	3.24	1.43	1.39
4	D	999	4PP	C2D-C3D	3.13	1.44	1.38
4	C	998	4PP	C2P-N1P	2.95	1.42	1.33
4	D	999	4PP	C6P-N1P	2.94	1.42	1.33
4	C	998	4PP	C6P-N1P	2.86	1.41	1.33
4	C	998	4PP	C5P-C4P	2.83	1.44	1.39
4	D	999	4PP	C4D-C1	2.80	1.56	1.52
4	D	999	4PP	C2P-N1P	2.74	1.41	1.33
4	D	999	4PP	C3D-C4D	2.67	1.43	1.39
4	D	999	4PP	C1B-C2B	2.56	1.43	1.38
4	D	999	4PP	C6B-C5B	2.56	1.43	1.39
4	D	999	4PP	C5P-C4P	2.50	1.43	1.39
4	D	999	4PP	C2D-C1D	2.47	1.43	1.38
4	D	999	4PP	C1B-C6B	2.39	1.43	1.38
4	D	999	4PP	C4-N1	2.35	1.50	1.45
4	C	998	4PP	C1B-C2B	2.26	1.42	1.38
4	C	998	4PP	C3B-C6D	2.25	1.54	1.49
4	C	998	4PP	C2D-C1D	2.22	1.42	1.38
4	D	999	4PP	C3P-C2P	2.22	1.42	1.38
4	C	998	4PP	C5D-C6D	2.17	1.43	1.39
4	C	998	4PP	C2D-C3D	2.17	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	999	4PP	C5D-C6D	2.16	1.43	1.39
4	C	998	4PP	C1B-C6B	2.14	1.42	1.38
4	C	998	4PP	C4B-C5B	2.13	1.42	1.39
4	C	998	4PP	C3D-C4D	2.10	1.42	1.39
4	D	999	4PP	C2B-C3B	2.08	1.43	1.39
4	C	998	4PP	C6B-C5B	2.05	1.42	1.39
4	D	999	4PP	C4B-C5B	2.02	1.42	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	998	4PP	C4-N1-C4P	-4.68	112.58	122.92
4	D	999	4PP	C4-N1-C4P	-4.22	113.58	122.92
4	C	998	4PP	C3-C2-C1	-2.54	108.68	114.06
4	C	998	4PP	C5P-C6P-N1P	-2.26	119.75	123.60
4	C	998	4PP	O3-C1C-O2	-2.25	118.96	124.08
4	C	998	4PP	C3P-C2P-N1P	-2.25	119.75	123.60
4	D	999	4PP	C3P-C2P-N1P	-2.15	119.94	123.60

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	998	4PP	C1C-C1-C2-C3
4	D	999	4PP	C4D-C1-C1C-O2
4	D	999	4PP	C2-C1-C1C-O3
4	D	999	4PP	C4D-C1-C1C-O3
4	C	998	4PP	C4D-C1-C2-C3
4	D	999	4PP	C2-C3-C4-N1
4	D	999	4PP	C2-C1-C1C-O2
4	D	999	4PP	C3-C4-N1-C4P

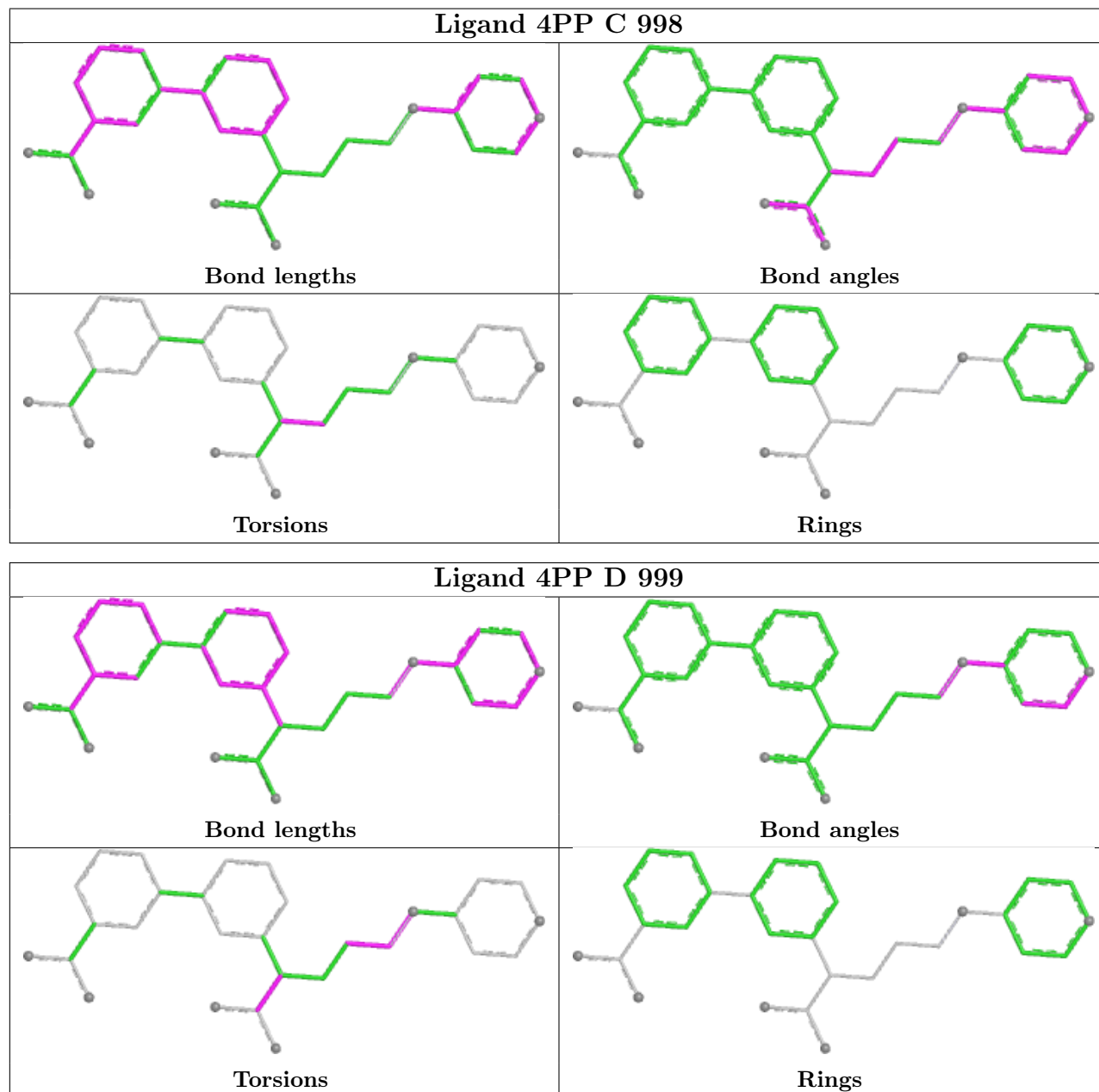
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	998	4PP	1	0
4	D	999	4PP	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.