



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:31 PM GMT

PDB ID : 1XKB  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

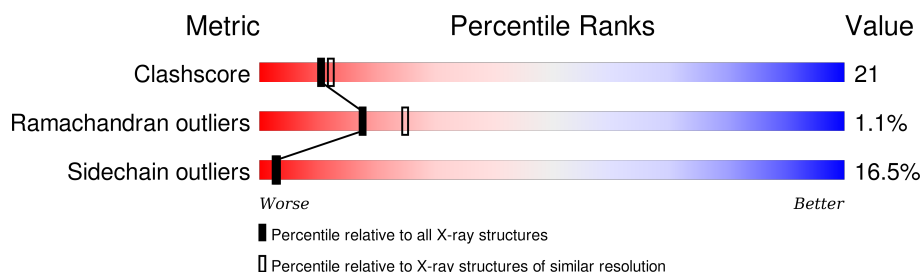
# 1 Overall quality at a glance

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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

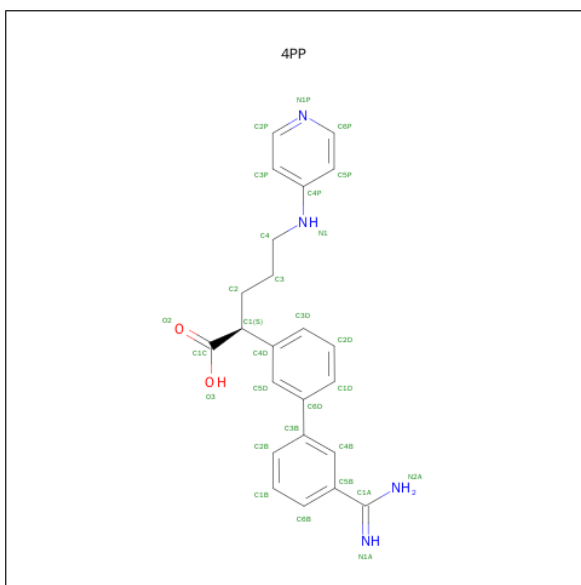
- Molecule 2 is a protein called BLOOD COAGULATION FACTOR XA.

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 (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is (2S)-(3'-AMIDINO-3-BIPHENYL)-5-(4-PYRIDYLAMINO)PENTANOIC ACID (three-letter code: 4PP) (formula: C<sub>23</sub>H<sub>24</sub>N<sub>4</sub>O<sub>2</sub>).



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

- Molecule 5 is water.

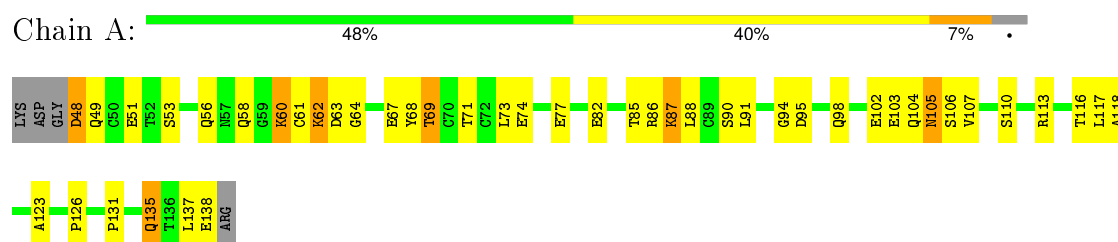
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	27	Total O 27 27	0	0
5	B	25	Total O 25 25	0	0
5	C	123	Total O 123 123	0	0
5	D	124	Total O 124 124	0	0

### 3 Residue-property plots

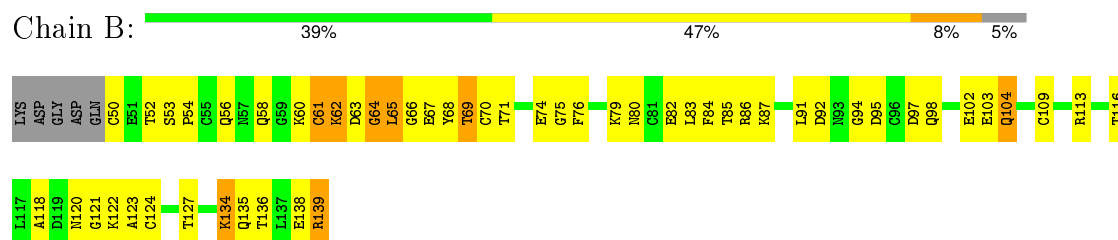
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

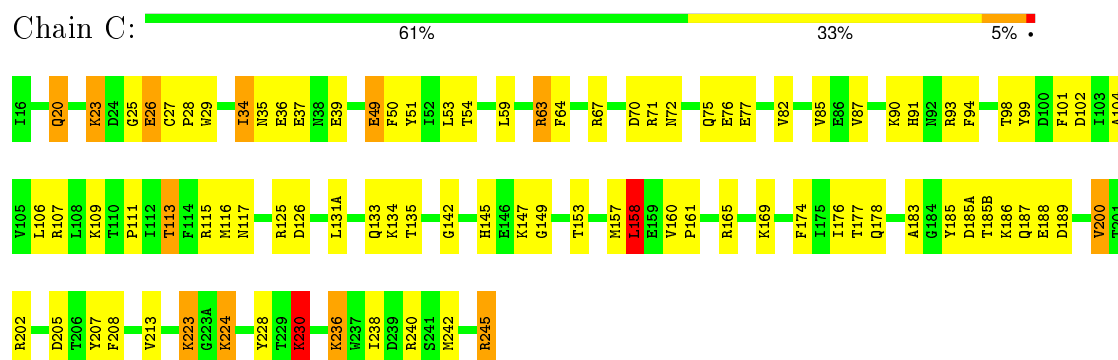
#### • Molecule 1: BLOOD COAGULATION FACTOR XA



#### • 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 will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.27 Å   105.22 Å   63.24 Å 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 <sup>2</sup> )	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: CA, BHD, 4PP

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	0.37	0/682	0.61	0/916
1	B	0.39	0/676	0.62	1/907 (0.1%)
2	C	0.38	0/1901	0.65	1/2560 (0.0%)
2	D	0.40	0/1890	0.66	1/2546 (0.0%)
All	All	0.39	0/5149	0.64	3/6929 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	158	LEU	CA-CB-CG	6.31	129.81	115.30
1	B	64	GLY	N-CA-C	-5.65	98.98	113.10
2	D	115	ARG	NE-CZ-NH2	-5.62	117.49	120.30

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	32	0
1	B	676	0	614	44	0
2	C	1863	0	1821	82	0
2	D	1852	0	1808	67	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	7	0
All	All	5433	0	4901	215	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 21.

All (215) 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
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:HD23	1:B:65:LEU:N	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:24:ASP:HB3	2:D:116:MET:HE2	1.80	0.62
2:C:238:ILE:O	2:C:242:MET:HG3	1.98	0.61
1:B:53:SER:N	1:B:54:PRO:HD3	2.15	0.61
1:A:98:GLN:HG2	2:C:208:PHE:HZ	1.65	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
2:D:49:GLU:H	2:D:49:GLU:CD	2.03	0.60
1:B:138:GLU:HG3	1:B:139:ARG:NH1	2.17	0.60
1:A:87:LYS:HD3	1:A:95:ASP:OD2	2.02	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: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
1:B:61:CYS:HA	1:B:69:THR:O	2.03	0.59
2:C:236:LYS:NZ	2:C:240:ARG:HG3	2.18	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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:16:ILE:N	2:D:194:ASP:OD2	2.39	0.56
2:C:185(B):THR:HB	2:C:223:LYS:HG3	1.87	0.55
2:C:113:THR:HG22	2:C:113:THR:O	2.06	0.55
2:D:100:ASP:CG	2:D:177:THR:HG21	2.27	0.55
1:A:82:GLU:OE1	1:A:82:GLU:N	2.39	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
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
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
1:B:118:ALA:CB	1:B:123:ALA:HB3	2.40	0.52
2:C:35:ASN:HD21	2:C:39:GLU:HB2	1.73	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
1:A:60:LYS:HD2	1:A:62:LYS:HZ1	1.75	0.51
2:D:37:GLU:O	2:D:38:ASN:HB2	2.11	0.51
2:C:125:ARG:NH1	2:C:126:ASP:OD1	2.44	0.51
2:C:158:LEU:HD13	2:C:160:VAL:HG13	1.93	0.51
2:C:20:GLN:NE2	2:C:23:LYS:NZ	2.59	0.51
2:D:98:THR:O	2:D:99:TYR:HB2	2.10	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
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
2:C:67:ARG:HD3	2:C:70:ASP:HB2	1.93	0.50
2:C:165:ARG:HH22	2:C:177:THR:C	2.14	0.50
2:D:145:HIS:CD2	2:D:147:LYS:HD2	2.47	0.50
1:A:126:PRO:CB	1:A:131:PRO:HG3	2.42	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C	1:A:105:ASN:HD22	2.15	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:D:232:THR:HA	2:D:235:LEU:CD2	2.33	0.48
2:D:83:HIS:ND1	2:D:110:THR:HG22	2.28	0.48
2:C:185(A):ASP:O	5:C:565:HOH:O	2.20	0.48
2:D:156:LYS:HG3	5:D:694:HOH:O	2.13	0.48
2:C:54:THR:HG22	2:C:104:ALA:HB3	1.96	0.48
1:A:77:GLU:OE2	1:A:85:THR:HG22	2.14	0.47
2:C:230:LYS:NZ	5:C:542:HOH:O	2.47	0.47
1:A:88:LEU:HA	1:A:107:VAL:CG2	2.44	0.47
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:185:TYR:O	5:D:800:HOH:O	2.20	0.47
2:D:51:TYR:CD2	2:D:242:MET:HG2	2.50	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:N	1:B:84:PHE:CD1	2.83	0.47
2:C:165:ARG:HH11	2:C:169:LYS:HZ2	1.61	0.47
2:D:158:LEU:HD13	2:D:160:VAL:CG1	2.43	0.46
2:C:165:ARG:NH2	2:C:177:THR:C	2.68	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
2:C:149:GLY:HA3	5:D:631:HOH:O	2.16	0.46
1:B:50:CYS:C	1:B:52:THR:H	2.18	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
1:A:77:GLU:CD	1:A:85:THR:HG22	2.36	0.46
2:C:107:ARG:CZ	2:C:245:ARG:O	2.64	0.46
2:D:72:ASN:C	2:D:72:ASN:OD1	2.54	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE1	2:C:76:GLU:HA	2.17	0.45
2:C:245:ARG:HB2	2:C:245:ARG:CZ	2.43	0.45
2:C:72:ASN:HA	2:C:153:THR:O	2.17	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
1:A:87:LYS:CB	1:A:91:LEU:HD23	2.46	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:47:LEU:HD11	2:D:53:LEU:HB2	2.00	0.44
2:D:131(A):LEU:HG	2:D:201:THR:HB	1.99	0.44
2:D:34:ILE:HG13	2:D:34:ILE:O	2.18	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
2:C:236:LYS:HZ3	2:C:240:ARG:HG3	1.83	0.43
1:B:116:THR:HG23	1:B:127:THR:CG2	2.48	0.43
1:B:135:GLN:NE2	2:D:26:GLU:O	2.50	0.43
2:C:72:ASN:OD1	2:C:153:THR:HG22	2.19	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:156:LYS:HB3	2:D:156:LYS:HE2	1.78	0.43
2:D:49:GLU:HA	2:D:112:ILE:HB	2.01	0.43
2:D:185(A):ASP:O	2:D:223(A):GLY:N	2.51	0.42
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:C:53:LEU:HD12	2:C:104:ALA:O	2.19	0.42
1:A:138:GLU:HG2	1:A:138:GLU:O	2.20	0.42
2:C:174:PHE:CG	4:C:998:4PP:H2P	2.55	0.42
2:C:27:CYS:N	2:C:28:PRO:CD	2.82	0.42
1:A:62:LYS:O	1:A:63:BHD:C	2.68	0.42
2:D:187:GLN:HA	2:D:221:ALA:HB1	2.01	0.42
1:B:82:GLU:N	1:B:82:GLU:OE1	2.43	0.42
1:B:109:CYS:HB2	1:B:121:GLY:O	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:85:VAL:HG11	2:D:88:VAL:HG12	2.01	0.42
2:C:236:LYS:HZ2	2:C:240:ARG:HG3	1.83	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:131(A):LEU:HD21	2:D:208:PHE:HB2	2.03	0.41
2:D:126:ASP:HB2	5:D:722:HOH:O	2.20	0.41
1:A:105:ASN:ND2	1:A:105:ASN:N	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
1:B:50:CYS:C	1:B:52:THR:N	2.73	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
2:C:147:LYS:HZ1	2:D:145:HIS:CE1	2.39	0.41
1:B:118:ALA:HB2	1:B:123:ALA:HB3	2.03	0.41
1:A:118:ALA:CB	1:A:123:ALA:HB3	2.50	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
1:B:103:GLU:O	1:B:104:GLN:C	2.58	0.41
2:C:236:LYS:O	2:C:236:LYS:HD3	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
2:D:116:MET:O	2:D:117:ASN:HB2	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	88/95 (93%)	79 (90%)	9 (10%)	0	100	100
1	B	87/95 (92%)	71 (82%)	13 (15%)	3 (3%)	5	4
2	C	233/235 (99%)	217 (93%)	13 (6%)	3 (1%)	15	21
2	D	232/235 (99%)	216 (93%)	15 (6%)	1 (0%)	39	56
All	All	640/660 (97%)	583 (91%)	50 (8%)	7 (1%)	17	25

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%)	61 (80%)	15 (20%)	1	2
2	C	200/200 (100%)	177 (88%)	23 (12%)	7	9
2	D	199/200 (100%)	165 (83%)	34 (17%)	2	3
All	All	552/560 (99%)	461 (84%)	91 (16%)	3	3

All (91) 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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	58	GLN
1	A	60	LYS
1	A	62	LYS
1	A	69	THR
1	A	86	ARG
1	A	87	LYS
1	A	90	SER
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	20	GLN
2	C	23	LYS
2	C	26	GLU
2	C	29	TRP
2	C	34	ILE
2	C	36	GLU
2	C	37	GLU
2	C	49	GLU
2	C	63	ARG
2	C	75	GLN
2	C	77	GLU
2	C	106	LEU
2	C	113	THR
2	C	134	LYS
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	230	LYS
2	C	236	LYS
2	C	245	ARG
1	B	61	CYS
1	B	62	LYS
1	B	65	LEU
1	B	67	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	69	THR
1	B	74	GLU
1	B	76	PHE
1	B	79	LYS
1	B	86	ARG
1	B	97	ASP
1	B	102	GLU
1	B	104	GLN
1	B	113	ARG
1	B	134	LYS
1	B	139	ARG
2	D	20	GLN
2	D	23	LYS
2	D	24	ASP
2	D	29	TRP
2	D	36	GLU
2	D	61	GLN
2	D	71	ARG
2	D	74	GLU
2	D	77	GLU
2	D	80	GLU
2	D	84	GLU
2	D	93	ARG
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	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	185(B)	THR
2	D	209	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	235	LEU
2	D	236	LYS
2	D	239	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) 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	145	HIS
2	C	178	GLN
1	B	57	ASN
1	B	104	GLN
2	D	75	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	4,8,9	1.13	0	4,10,12	1.06	0
1	BHD	B	63	1	4,8,9	2.15	1 (25%)	4,10,12	1.79	1 (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	-	0/4/10/12	0/0/0/0
1	BHD	B	63	1	-	0/4/10/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	BHD	CA-CB	4.23	1.62	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	BHD	OB-CB-CA	2.86	113.80	107.44

There are no chirality outliers.

There are no torsion outliers.

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 carbohydrates 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	-	28,31,31	2.10	10 (35%)	34,41,41	1.25	3 (8%)
4	4PP	D	999	-	28,31,31	2.16	14 (50%)	34,41,41	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	-	-	0/19/23/23	0/3/3/3
4	4PP	D	999	-	-	0/19/23/23	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	999	4PP	C2D-C1D	2.06	1.43	1.38
4	D	999	4PP	C5D-C6D	2.06	1.43	1.39
4	C	998	4PP	C5D-C6D	2.06	1.43	1.39
4	C	998	4PP	C3B-C6D	2.07	1.54	1.49
4	D	999	4PP	C3P-C2P	2.07	1.42	1.38
4	D	999	4PP	C4B-C5B	2.09	1.42	1.39
4	C	998	4PP	C3D-C4D	2.09	1.42	1.39
4	D	999	4PP	C1B-C2B	2.13	1.43	1.38
4	C	998	4PP	C4B-C5B	2.21	1.42	1.39
4	D	999	4PP	C6B-C5B	2.34	1.43	1.39
4	D	999	4PP	C5P-C4P	2.59	1.43	1.39
4	D	999	4PP	C2P-N1P	2.59	1.41	1.33
4	D	999	4PP	C2D-C3D	2.60	1.44	1.38
4	D	999	4PP	C3D-C4D	2.63	1.43	1.39
4	C	998	4PP	C6P-N1P	2.71	1.41	1.33
4	D	999	4PP	C6P-N1P	2.78	1.42	1.33
4	C	998	4PP	C2P-N1P	2.79	1.42	1.33
4	C	998	4PP	C5D-C4D	2.92	1.43	1.39
4	C	998	4PP	C5P-C4P	2.94	1.44	1.39
4	D	999	4PP	C5D-C4D	3.12	1.44	1.39
4	D	999	4PP	C5B-C1A	3.93	1.54	1.47
4	D	999	4PP	C4P-N1	4.03	1.50	1.38
4	C	998	4PP	C4P-N1	4.07	1.50	1.38
4	C	998	4PP	C5B-C1A	4.17	1.54	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	998	4PP	C4-N1-C4P	-4.91	112.58	122.95
4	D	999	4PP	C4-N1-C4P	-4.44	113.58	122.95
4	C	998	4PP	C5P-C6P-N1P	-2.24	119.75	123.64
4	C	998	4PP	C3P-C2P-N1P	-2.23	119.75	123.64
4	D	999	4PP	C3P-C2P-N1P	-2.13	119.94	123.64

There are no chirality outliers.

There are no torsion outliers.

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

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.