



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 04:12 PM EDT

PDB ID : 1IOE  
Title : Human coagulation factor Xa in complex with M55532  
Authors : Shiromizu, I.; Matsusue, T.  
Deposited on : unknown  
Resolution : 2.90 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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

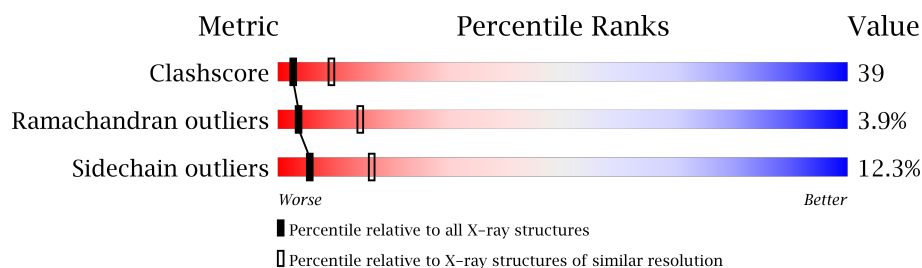
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)

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	235	
2	L	96	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2278 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 COAGULATION FACTOR XA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1864	1172	327	351	14			

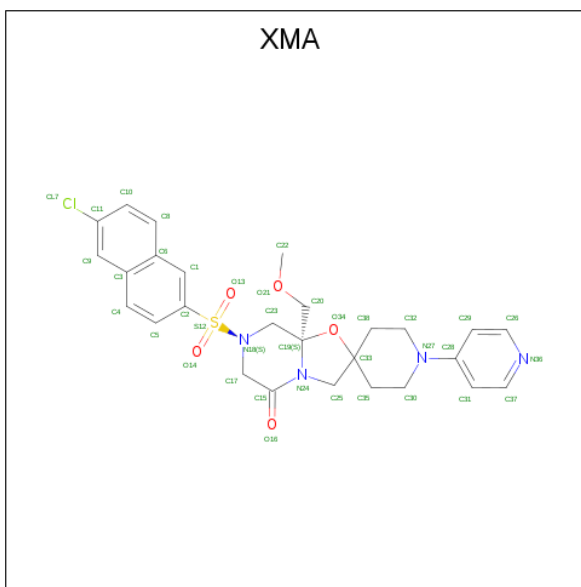
- Molecule 2 is a protein called COAGULATION FACTOR XA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	51	Total	C	N	O	S	0	0	0
			375	226	65	77	7			

- 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		

- Molecule 4 is (-)-7-[(6-CHLORO-2-NAPHTHALENYL)SULFONYL]TETRAHYDRO-8A-(METHOXYMETHYL)-1'-(4-PYRIDINYL)-SPIRO[5H-OXAZOLO[3,2-A]PYRAZINE-2(3H),4'-PIPERIDIN]-5-ONE (three-letter code: XMA) (formula: C<sub>27</sub>H<sub>29</sub>ClN<sub>4</sub>O<sub>5</sub>S).



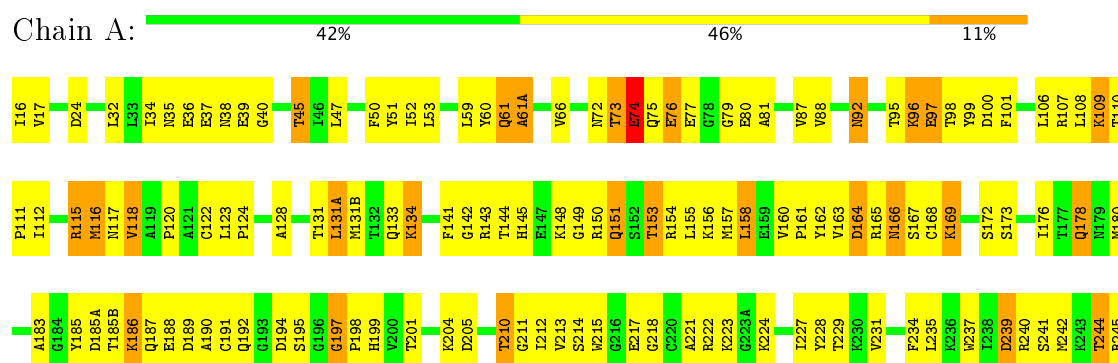
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			38	27	1	4	5	1		

### 3 Residue-property plots

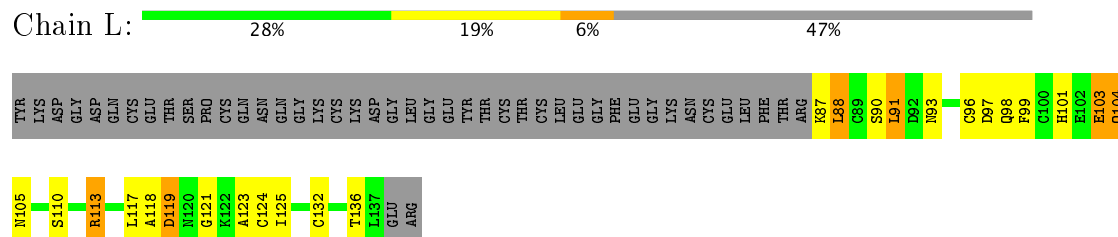
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: COAGULATION FACTOR XA



#### • Molecule 2: 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 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.70 Å 78.17 Å 56.04 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	81.9 (8.00-2.90)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNX 2000	Depositor
R, $R_{free}$	0.201 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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, XMA

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	0.40	0/1902	0.67	0/2560
2	L	0.39	0/381	0.67	0/515
All	All	0.40	0/2283	0.67	0/3075

There are no bond length outliers.

There are no bond angle outliers.

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	1864	0	1821	150	0
2	L	375	0	343	36	0
3	A	1	0	0	0	0
4	A	38	0	29	3	0
All	All	2278	0	2193	176	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 39.

All (176) 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:A:72:ASN:ND2	1:A:154:ARG:HE	1.54	1.04
1:A:72:ASN:HD22	1:A:154:ARG:NE	1.64	0.95
2:L:113:ARG:HD3	2:L:113:ARG:H	1.34	0.93
1:A:240:ARG:HD3	1:A:245:ARG:HD3	1.48	0.93
2:L:103:GLU:HG2	2:L:104:GLN:HE22	1.33	0.91
1:A:211:GLY:HA2	1:A:231:VAL:HG23	1.52	0.90
1:A:72:ASN:HD22	1:A:154:ARG:HE	0.83	0.82
1:A:60:TYR:HE1	1:A:96:LYS:HD2	1.47	0.78
1:A:50:PHE:CZ	1:A:111:PRO:HG3	2.20	0.77
1:A:96:LYS:N	1:A:96:LYS:HD3	2.00	0.77
1:A:96:LYS:H	1:A:96:LYS:HD3	1.47	0.76
1:A:123:LEU:HD23	2:L:113:ARG:NH2	1.99	0.76
2:L:103:GLU:HG2	2:L:104:GLN:NE2	1.99	0.76
1:A:32:LEU:HD13	1:A:141:PHE:HD2	1.52	0.74
1:A:218:GLY:HA3	1:A:222:ARG:NE	2.04	0.73
1:A:116:MET:HG3	1:A:117:ASN:OD1	1.89	0.72
1:A:178:GLN:NE2	1:A:178:GLN:H	1.88	0.72
2:L:103:GLU:CG	2:L:104:GLN:HE22	2.03	0.71
1:A:35:ASN:HD21	1:A:37:GLU:HB2	1.55	0.71
1:A:195:SER:HA	1:A:213:VAL:HG12	1.73	0.71
1:A:217:GLU:HB2	1:A:224:LYS:HE2	1.72	0.71
1:A:16:ILE:HG13	1:A:156:LYS:HB2	1.73	0.70
1:A:165:ARG:O	1:A:168:CYS:HB3	1.91	0.69
1:A:52:ILE:HB	1:A:106:LEU:HB2	1.75	0.69
1:A:199:HIS:HB3	1:A:211:GLY:O	1.92	0.69
1:A:143:ARG:CD	1:A:192:GLN:HB3	2.22	0.68
1:A:240:ARG:CD	1:A:245:ARG:HD3	2.23	0.68
1:A:74:GLU:OE2	1:A:75:GLN:HG3	1.94	0.68
1:A:165:ARG:HG2	1:A:169:LYS:HE3	1.76	0.68
1:A:242:MET:C	1:A:244:THR:H	1.95	0.68
1:A:143:ARG:HD2	1:A:192:GLN:HB3	1.75	0.68
1:A:45:THR:HG23	1:A:198:PRO:HB3	1.74	0.68
2:L:113:ARG:HD3	2:L:113:ARG:N	2.09	0.67
1:A:183:ALA:HB3	1:A:228:TYR:CE1	2.30	0.67
1:A:96:LYS:H	1:A:96:LYS:CD	2.04	0.66
1:A:240:ARG:NH1	1:A:240:ARG:HB2	2.12	0.65
1:A:61:GLN:O	1:A:61(A):ALA:HB2	1.99	0.63
1:A:178:GLN:HE21	1:A:178:GLN:H	1.43	0.62
1:A:123:LEU:H	2:L:113:ARG:NH1	1.97	0.62
1:A:108:LEU:HD12	1:A:112:ILE:HG13	1.81	0.62
1:A:47:LEU:HD11	1:A:53:LEU:HB2	1.80	0.62
1:A:76:GLU:HG3	1:A:76:GLU:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:TRP:CZ2	1:A:227:ILE:HG21	2.35	0.61
1:A:158:LEU:HD13	1:A:160:VAL:CG1	2.31	0.60
2:L:98:GLN:HG3	2:L:124:CYS:SG	2.42	0.60
1:A:163:VAL:HG23	1:A:183:ALA:HA	1.83	0.60
1:A:50:PHE:CE2	1:A:111:PRO:HG3	2.36	0.60
1:A:242:MET:C	1:A:244:THR:N	2.56	0.59
1:A:95:THR:HB	1:A:97:GLU:OE1	2.02	0.59
1:A:189:ASP:OD1	4:A:401:XMA:H10	2.03	0.59
2:L:103:GLU:O	2:L:105:ASN:N	2.35	0.59
1:A:231:VAL:O	1:A:235:LEU:HD13	2.03	0.59
1:A:185(A):ASP:O	1:A:223:LYS:HA	2.03	0.58
1:A:47:LEU:HD22	1:A:123:LEU:HD21	1.84	0.58
1:A:195:SER:HA	1:A:213:VAL:CG1	2.34	0.58
1:A:87:VAL:HG22	1:A:107:ARG:HB3	1.84	0.58
1:A:36:GLU:C	1:A:38:ASN:H	2.07	0.58
1:A:143:ARG:HD2	1:A:192:GLN:OE1	2.04	0.58
1:A:240:ARG:HB2	1:A:240:ARG:HH11	1.68	0.57
1:A:168:CYS:SG	1:A:176:ILE:HG21	2.45	0.57
1:A:81:ALA:HB2	1:A:115:ARG:HH22	1.69	0.56
1:A:134:LYS:HE3	1:A:134:LYS:HA	1.86	0.56
2:L:93:ASN:ND2	2:L:96:CYS:HB2	2.20	0.56
2:L:113:ARG:CD	2:L:113:ARG:H	2.08	0.56
1:A:131(B):MET:HA	1:A:162:TYR:CZ	2.40	0.56
1:A:158:LEU:HD13	1:A:160:VAL:HG12	1.87	0.56
1:A:73:THR:C	1:A:74:GLU:HG3	2.26	0.55
1:A:97:GLU:O	4:A:401:XMA:H26	2.07	0.55
1:A:98:THR:O	1:A:99:TYR:HB2	2.08	0.54
1:A:51:TYR:OH	1:A:107:ARG:HD2	2.07	0.54
1:A:59:LEU:O	1:A:60:TYR:HD2	1.90	0.54
1:A:35:ASN:ND2	1:A:37:GLU:HB2	2.23	0.54
1:A:160:VAL:HG23	1:A:160:VAL:O	2.08	0.54
2:L:87:LYS:HD2	2:L:105:ASN:O	2.08	0.53
1:A:185(B):THR:HA	1:A:223:LYS:HG2	1.91	0.53
1:A:215:TRP:CE2	1:A:227:ILE:HG21	2.42	0.53
1:A:195:SER:C	1:A:197:GLY:H	2.12	0.53
1:A:150:ARG:HH21	1:A:150:ARG:HG3	1.74	0.52
1:A:240:ARG:CB	1:A:240:ARG:HH11	2.22	0.52
1:A:212:ILE:HB	1:A:229:THR:HB	1.91	0.52
1:A:36:GLU:CD	1:A:36:GLU:H	2.14	0.52
1:A:72:ASN:ND2	1:A:75:GLN:NE2	2.58	0.52
1:A:234:PHE:O	1:A:237:TRP:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:118:ALA:HB2	2:L:125:ILE:HD11	1.93	0.51
2:L:88:LEU:HD23	2:L:91:LEU:HD23	1.93	0.50
1:A:211:GLY:CA	1:A:231:VAL:HG23	2.34	0.50
2:L:88:LEU:C	2:L:90:SER:H	2.13	0.50
2:L:97:ASP:CG	2:L:123:ALA:HA	2.32	0.50
1:A:124:PRO:HA	2:L:99:PHE:CE1	2.46	0.49
1:A:35:ASN:HD21	1:A:37:GLU:CB	2.22	0.49
1:A:186:LYS:HE2	1:A:188:GLU:OE2	2.12	0.49
1:A:88:VAL:HG13	1:A:88:VAL:O	2.12	0.49
1:A:164:ASP:OD2	1:A:167:SER:N	2.39	0.49
1:A:172:SER:OG	1:A:173:SER:N	2.46	0.49
1:A:155:LEU:HD12	1:A:156:LYS:H	1.78	0.48
1:A:79:GLY:O	1:A:115:ARG:NH2	2.46	0.48
2:L:103:GLU:C	2:L:105:ASN:H	2.17	0.48
1:A:128:ALA:O	1:A:131(A):LEU:HB2	2.14	0.48
2:L:103:GLU:C	2:L:104:GLN:CD	2.72	0.48
1:A:16:ILE:HB	1:A:156:LYS:HD3	1.96	0.48
1:A:201:THR:OG1	1:A:210:THR:HG21	2.13	0.48
1:A:61:GLN:O	1:A:61(A):ALA:CB	2.62	0.48
1:A:217:GLU:CB	1:A:224:LYS:HE2	2.43	0.48
1:A:240:ARG:CG	1:A:245:ARG:HD3	2.44	0.47
1:A:155:LEU:HD12	1:A:156:LYS:N	2.30	0.47
1:A:97:GLU:CD	1:A:97:GLU:H	2.18	0.47
1:A:81:ALA:CB	1:A:115:ARG:HH22	2.28	0.47
1:A:239:ASP:C	1:A:241:SER:N	2.69	0.46
1:A:80:GLU:N	1:A:80:GLU:OE2	2.46	0.46
1:A:122:CYS:SG	2:L:132:CYS:C	2.94	0.46
2:L:119:ASP:C	2:L:121:GLY:H	2.18	0.46
1:A:92:ASN:OD1	1:A:92:ASN:N	2.43	0.46
1:A:239:ASP:C	1:A:241:SER:H	2.20	0.46
1:A:109:LYS:O	1:A:109:LYS:HD2	2.16	0.46
1:A:141:PHE:CE1	1:A:155:LEU:HB2	2.51	0.45
1:A:34:ILE:HA	1:A:39:GLU:O	2.15	0.45
1:A:16:ILE:HD13	1:A:194:ASP:OD1	2.16	0.45
1:A:189:ASP:OD1	1:A:190:ALA:N	2.44	0.45
2:L:87:LYS:HG2	2:L:88:LEU:N	2.31	0.45
2:L:117:LEU:HD12	2:L:123:ALA:O	2.17	0.45
1:A:228:TYR:N	1:A:228:TYR:CD1	2.85	0.45
1:A:51:TYR:HA	1:A:106:LEU:O	2.18	0.44
1:A:60:TYR:CE1	1:A:96:LYS:HD2	2.38	0.44
1:A:32:LEU:HD22	1:A:141:PHE:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:99:PHE:HB2	2:L:110:SER:OG	2.17	0.44
1:A:166:ASN:O	1:A:167:SER:C	2.55	0.44
1:A:117:ASN:O	1:A:118:VAL:CG2	2.66	0.44
1:A:73:THR:OG1	1:A:153:THR:HA	2.18	0.44
1:A:123:LEU:H	2:L:113:ARG:CZ	2.31	0.44
1:A:169:LYS:HD2	1:A:169:LYS:H	1.82	0.44
1:A:217:GLU:O	1:A:222:ARG:HD2	2.18	0.44
1:A:134:LYS:HE3	1:A:134:LYS:CA	2.47	0.44
1:A:150:ARG:NH2	1:A:150:ARG:HG3	2.31	0.44
2:L:119:ASP:C	2:L:121:GLY:N	2.72	0.43
2:L:87:LYS:O	2:L:88:LEU:CB	2.67	0.43
1:A:191:CYS:SG	1:A:192:GLN:N	2.91	0.43
1:A:187:GLN:NE2	1:A:221:ALA:O	2.52	0.43
1:A:36:GLU:C	1:A:38:ASN:N	2.70	0.43
1:A:16:ILE:CG1	1:A:156:LYS:HB2	2.45	0.42
1:A:240:ARG:HG2	1:A:245:ARG:HB3	2.01	0.42
1:A:40:GLY:O	1:A:151:GLN:NE2	2.52	0.42
1:A:120:PRO:O	2:L:132:CYS:HA	2.19	0.42
1:A:35:ASN:HD21	1:A:37:GLU:CD	2.22	0.42
1:A:116:MET:O	1:A:117:ASN:HB2	2.20	0.42
1:A:122:CYS:SG	2:L:132:CYS:O	2.78	0.42
1:A:72:ASN:ND2	1:A:75:GLN:CD	2.73	0.42
1:A:241:SER:O	1:A:244:THR:HA	2.20	0.42
1:A:123:LEU:H	2:L:113:ARG:HH12	1.65	0.42
1:A:142:GLY:N	1:A:194:ASP:OD2	2.51	0.42
1:A:35:ASN:HD21	1:A:37:GLU:CG	2.33	0.42
2:L:103:GLU:CG	2:L:104:GLN:NE2	2.74	0.41
1:A:161:PRO:HG2	1:A:185:TYR:CE1	2.55	0.41
1:A:66:VAL:HG11	1:A:108:LEU:CD2	2.50	0.41
1:A:204:LYS:O	1:A:205:ASP:HB2	2.20	0.41
1:A:35:ASN:O	1:A:38:ASN:N	2.50	0.41
1:A:116:MET:SD	2:L:136:THR:O	2.77	0.41
1:A:32:LEU:HD22	1:A:141:PHE:CE2	2.56	0.41
2:L:103:GLU:CD	2:L:104:GLN:HE22	2.24	0.41
1:A:24:ASP:OD2	1:A:117:ASN:OD1	2.38	0.41
1:A:115:ARG:HD3	1:A:118:VAL:HB	2.01	0.41
1:A:145:HIS:CE1	1:A:148:LYS:C	2.94	0.41
1:A:122:CYS:CA	2:L:113:ARG:HH12	2.34	0.41
1:A:100:ASP:O	1:A:101:PHE:HB2	2.21	0.41
1:A:150:ARG:O	1:A:151:GLN:C	2.59	0.41
1:A:214:SER:O	4:A:401:XMA:H4	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:103:GLU:O	2:L:105:ASN:OD1	2.38	0.41
1:A:53:LEU:HD11	1:A:212:ILE:HD11	2.03	0.40
2:L:88:LEU:C	2:L:90:SER:N	2.75	0.40
1:A:143:ARG:HG3	1:A:143:ARG:H	1.72	0.40
1:A:145:HIS:CE1	1:A:149:GLY:N	2.89	0.40
1:A:110:THR:HA	1:A:111:PRO:HD3	1.87	0.40
1:A:17:VAL:O	1:A:188:GLU:HA	2.19	0.40
1:A:231:VAL:HG12	1:A:235:LEU:CD1	2.51	0.40
1:A:240:ARG:O	1:A:245:ARG:HB3	2.21	0.40
1:A:73:THR:O	1:A:74:GLU:HG3	2.22	0.40
1:A:16:ILE:N	1:A:194:ASP:OD1	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	233/235 (99%)	183 (78%)	41 (18%)	9 (4%)	3	14
2	L	49/96 (51%)	38 (78%)	9 (18%)	2 (4%)	3	13
All	All	282/331 (85%)	221 (78%)	50 (18%)	11 (4%)	3	14

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	GLU
2	L	104	GLN
1	A	61	GLN
1	A	61(A)	ALA
1	A	76	GLU
1	A	244	THR
1	A	73	THR

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Mol	Chain	Res	Type
1	A	186	LYS
1	A	197	GLY
2	L	88	LEU
1	A	118	VAL

### 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	200/200 (100%)	175 (88%)	25 (12%)	5	16
2	L	43/82 (52%)	38 (88%)	5 (12%)	6	19
All	All	243/282 (86%)	213 (88%)	30 (12%)	5	16

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	74	GLU
1	A	77	GLU
1	A	92	ASN
1	A	96	LYS
1	A	97	GLU
1	A	109	LYS
1	A	115	ARG
1	A	116	MET
1	A	131	THR
1	A	131(A)	LEU
1	A	133	GLN
1	A	134	LYS
1	A	144	THR
1	A	151	GLN
1	A	153	THR
1	A	157	MET
1	A	158	LEU
1	A	164	ASP

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Mol	Chain	Res	Type
1	A	166	ASN
1	A	169	LYS
1	A	178	GLN
1	A	180	MET
1	A	210	THR
1	A	239	ASP
2	L	91	LEU
2	L	101	HIS
2	L	103	GLU
2	L	113	ARG
2	L	119	ASP

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

Mol	Chain	Res	Type
1	A	30	GLN
1	A	72	ASN
1	A	75	GLN
1	A	117	ASN
1	A	133	GLN
1	A	178	GLN
1	A	187	GLN
2	L	104	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	XMA	A	401	-	41,43,43	4.16	23 (56%)	54,66,66	1.91	12 (22%)

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	XMA	A	401	-	-	0/20/62/62	0/5/6/6

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	XMA	C29-C26	2.28	1.43	1.38
4	A	401	XMA	C31-C37	2.52	1.43	1.38
4	A	401	XMA	C8-C6	2.64	1.48	1.41
4	A	401	XMA	C4-C3	2.67	1.48	1.41
4	A	401	XMA	C17-C15	3.25	1.57	1.51
4	A	401	XMA	C8-C10	3.31	1.43	1.36
4	A	401	XMA	S12-N18	3.79	1.69	1.63
4	A	401	XMA	C4-C5	4.04	1.45	1.36
4	A	401	XMA	C28-N27	4.25	1.50	1.38
4	A	401	XMA	C38-C33	4.51	1.58	1.52
4	A	401	XMA	C29-C28	4.52	1.48	1.39
4	A	401	XMA	C31-C28	4.62	1.48	1.39
4	A	401	XMA	C9-C11	4.99	1.46	1.36
4	A	401	XMA	C1-C2	5.07	1.45	1.36
4	A	401	XMA	C10-C11	5.21	1.48	1.38
4	A	401	XMA	C35-C33	5.66	1.59	1.52
4	A	401	XMA	C30-N27	5.72	1.55	1.46
4	A	401	XMA	C32-N27	6.01	1.55	1.46
4	A	401	XMA	C6-C3	6.70	1.57	1.42
4	A	401	XMA	C15-N24	6.92	1.44	1.35
4	A	401	XMA	C5-C2	8.07	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	XMA	O14-S12	8.86	1.54	1.43
4	A	401	XMA	O13-S12	10.17	1.56	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	XMA	O14-S12-O13	-4.65	111.65	119.46
4	A	401	XMA	C38-C33-C35	-3.78	106.50	111.38
4	A	401	XMA	C23-N18-S12	-2.84	111.44	117.48
4	A	401	XMA	C22-O21-C20	2.14	116.72	112.27
4	A	401	XMA	C17-N18-C23	2.19	115.86	113.42
4	A	401	XMA	O14-S12-C2	2.30	111.00	108.00
4	A	401	XMA	C5-C2-S12	2.52	122.52	119.78
4	A	401	XMA	C32-N27-C30	2.72	117.34	111.57
4	A	401	XMA	O34-C33-C35	3.13	110.99	108.28
4	A	401	XMA	O14-S12-N18	4.02	110.49	106.69
4	A	401	XMA	C17-N18-S12	5.03	126.38	116.90
4	A	401	XMA	O34-C19-N24	5.79	105.80	102.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	XMA	3	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

### 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.