Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2024 – 01:02 pm GMT

PDB ID	:	8OS5
Title	:	Crystal structure of the Factor XII heavy chain reveals an interlocking dimer with a FnII to kringle domain interaction
Authors	:	Li, C.; Saleem, M.; Kaira, B.G.; Brown, A.; Wilson, C.; Philippou, H.; Emsley, J.
Deposited on	:	2023-04-18
Resolution	:	3.40 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:

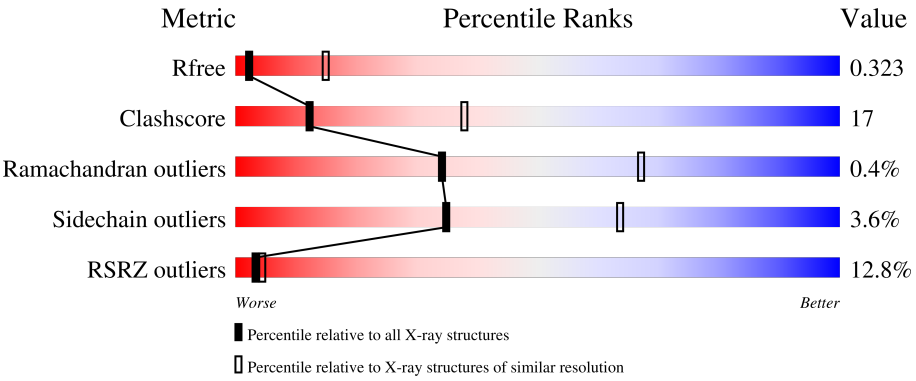
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 <=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.

Mol	Chain	Length	Quality of chain
1	A	295	9% 61% 24% · 12%
1	B	295	16% 51% 15% · 32%
1	C	295	6% 53% 30% · · 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5690 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 XII-Mie.

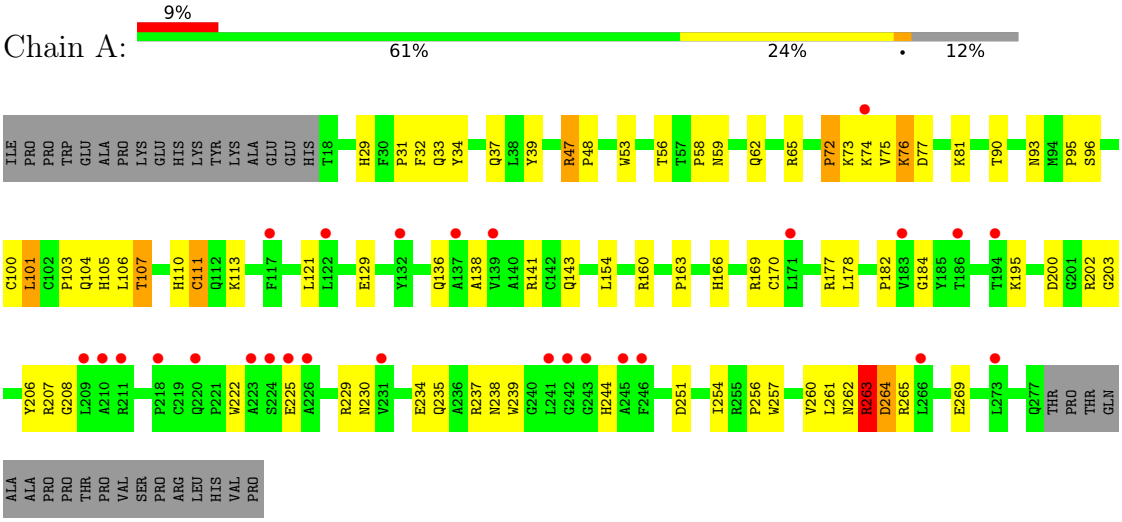
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	2	0	0
			2063	1278	393	365	27			
1	B	201	Total	C	N	O	S	1	0	0
			1573	963	304	283	23			
1	C	259	Total	C	N	O	S	3	0	0
			2054	1273	391	363	27			

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 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.

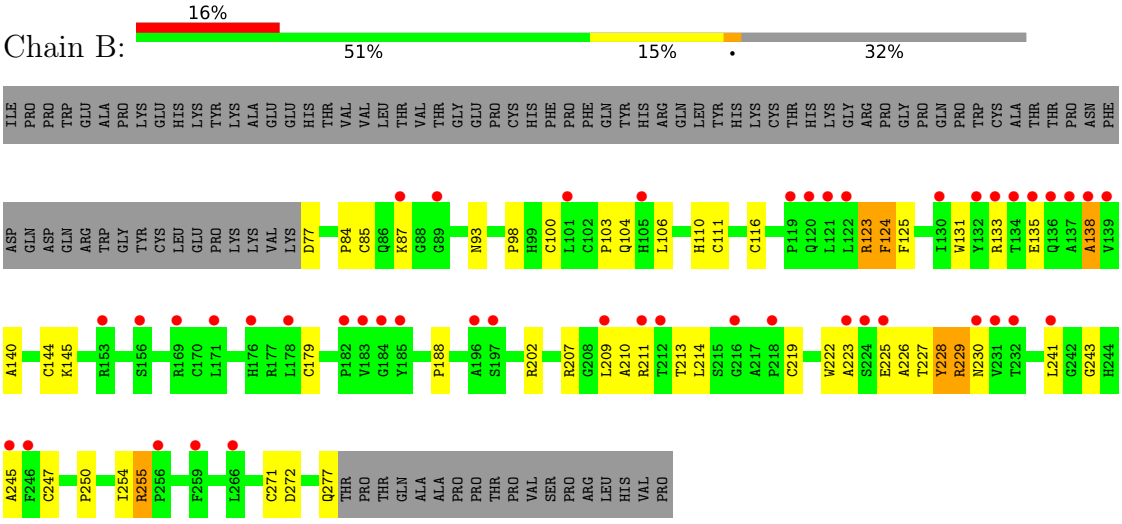
• Molecule 1: Coagulation factor XII-Mie

Chain A:



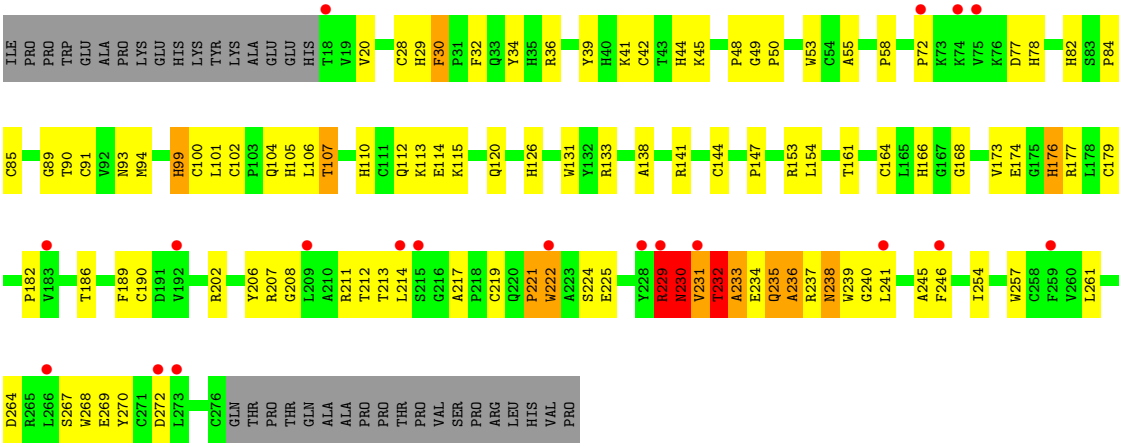
• Molecule 1: Coagulation factor XII-Mie

Chain B:



• Molecule 1: Coagulation factor XII-Mie

Chain C:


ILE PRO PRO TRP GLU ALA PRO LYS GLU HIS LYS TYR LYS ALA GLU GLU HIS T18 V19 V20 C28 H29 F30 P31 F32 Q33 Y34 H35 R36 Y39 H40 K41 C42 T43 H44 K45 P48 G49 P50 W53 C54 A55 P58 P72 K73 K74 V75 K76 D77 H78 H82 S83 P84
C85 G89 T90 C91 V92 N93 M94 H99 C100 L101 C102 P103 Q104 H105 L106 T107 H110 C111 Q112 K113 E114 K115 Q120 H126 W131 Y132 R133 A138 R141 C144 P147 R153 L154 T161 C164 L165 H166 G167 G168 V173 E174 G175 H176 R177 L178 C179
P182 V183 T186 F189 C190 D191 V192 R202 Y206 R207 G208 L209 A210 R211 T212 T213 L214 S215 G216 A217 P218 C219 Q220 P221 W222 A223 S224 E225 Y228 R229 N230 V231 T232 A233 E234 Q235 A236 R237 M238 W239 G240 L241 A245 F246 I254 W257 C258 F259 V260 L261
D264 R265 L266 S267 W268 E269 Y270 C271 D272 L273 C276 GLN THR PRO THR GLN ALA ALA PRO PRO PRO THR PRO VAL SER PRO ARG LEU HIS VAL PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	144.54Å 144.59Å 155.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.97 – 3.40 77.97 – 3.39	Depositor EDS
% Data completeness (in resolution range)	61.2 (77.97-3.40) 61.0 (77.97-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 3.41Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.255 , 0.319 0.271 , 0.323	Depositor DCC
R_{free} test set	1416 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å^2)	118.9	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.074 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	5690	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.62	0/2129	0.98	4/2891 (0.1%)
1	B	0.55	0/1618	0.95	6/2193 (0.3%)
1	C	0.67	0/2120	1.01	9/2879 (0.3%)
All	All	0.62	0/5867	0.98	19/7963 (0.2%)

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	A	0	4
1	B	0	4
1	C	0	3
All	All	0	11

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	31	PRO	N-CA-C	-6.97	93.98	112.10
1	C	236	ALA	CB-CA-C	6.74	120.21	110.10
1	C	230	ASN	N-CA-C	-6.60	93.19	111.00
1	A	138	ALA	N-CA-CB	6.17	118.74	110.10
1	C	238	ASN	N-CA-CB	5.95	121.31	110.60
1	B	138	ALA	N-CA-CB	5.88	118.33	110.10
1	C	176	HIS	CB-CA-C	-5.79	98.82	110.40
1	C	233	ALA	CB-CA-C	5.70	118.65	110.10
1	B	104	GLN	N-CA-CB	5.70	120.85	110.60
1	A	111	CYS	CA-CB-SG	5.48	123.86	114.00
1	B	124	PHE	N-CA-CB	-5.38	100.91	110.60
1	B	85	CYS	CB-CA-C	5.36	121.12	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	44	HIS	N-CA-C	-5.33	96.60	111.00
1	C	232	THR	N-CA-C	-5.23	96.89	111.00
1	A	121	LEU	CB-CG-CD2	5.21	119.86	111.00
1	C	229	ARG	N-CA-C	5.14	124.88	111.00
1	B	277	GLN	CB-CA-C	5.11	120.61	110.40
1	B	277	GLN	N-CA-C	-5.01	97.46	111.00
1	C	99	HIS	N-CA-CB	5.01	119.61	110.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	ARG	Sidechain
1	A	263	ARG	Sidechain
1	A	47	ARG	Sidechain
1	A	65	ARG	Sidechain
1	B	123	ARG	Sidechain
1	B	207	ARG	Sidechain
1	B	229	ARG	Sidechain
1	B	255	ARG	Sidechain
1	C	207	ARG	Sidechain
1	C	229	ARG	Sidechain
1	C	237	ARG	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	2063	0	1917	59	0
1	B	1573	0	1452	38	0
1	C	2054	0	1909	89	0
All	All	5690	0	5278	186	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 17.

All (186) 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:231:VAL:HA	1:C:235:GLN:HE22	1.20	1.01
1:C:231:VAL:HA	1:C:235:GLN:NE2	1.79	0.96
1:A:29:HIS:CE1	1:A:58:PRO:HG3	2.05	0.92
1:C:36:ARG:HH11	1:C:36:ARG:HG2	1.37	0.89
1:C:106:LEU:HA	1:C:113:LYS:O	1.75	0.86
1:B:87:LYS:O	1:B:87:LYS:HG3	1.77	0.84
1:B:228:TYR:O	1:B:229:ARG:HG3	1.78	0.83
1:C:211:ARG:HH21	1:C:245:ALA:HB3	1.44	0.83
1:C:261:LEU:HD11	1:C:264:ASP:HA	1.63	0.80
1:A:90:THR:HB	1:A:101:LEU:HD11	1.68	0.74
1:A:76:LYS:HB2	1:A:81:LYS:HE3	1.74	0.70
1:B:123:ARG:HE	1:B:125:PHE:HE1	1.38	0.70
1:C:232:THR:HG23	1:C:235:GLN:OE1	1.92	0.69
1:A:76:LYS:HZ3	1:A:76:LYS:H	1.40	0.69
1:C:36:ARG:HG2	1:C:36:ARG:NH1	2.03	0.69
1:A:105:HIS:O	1:A:106:LEU:HB2	1.93	0.69
1:A:163:PRO:HG3	1:A:177:ARG:HH21	1.57	0.68
1:B:214:LEU:HD11	1:B:255:ARG:HH11	1.58	0.68
1:C:231:VAL:HG23	1:C:235:GLN:HB2	1.76	0.67
1:C:212:THR:HG23	1:C:272:ASP:HB2	1.76	0.67
1:A:106:LEU:O	1:A:111:CYS:HA	1.95	0.66
1:A:32:PHE:HA	1:A:58:PRO:O	1.96	0.65
1:C:107:THR:HG21	1:C:126:HIS:CE1	2.32	0.65
1:C:231:VAL:CA	1:C:235:GLN:HE22	2.05	0.65
1:A:34:TYR:HB3	1:A:39:TYR:CE2	2.32	0.65
1:C:161:THR:HB	1:C:177:ARG:HH22	1.63	0.64
1:B:211:ARG:HG2	1:B:211:ARG:O	1.97	0.64
1:C:214:LEU:HD11	1:C:270:TYR:HB2	1.79	0.64
1:A:90:THR:O	1:A:101:LEU:HG	1.98	0.63
1:B:228:TYR:O	1:B:228:TYR:CD1	2.51	0.63
1:C:85:CYS:SG	1:C:91:CYS:HB2	2.39	0.63
1:A:107:THR:O	1:A:113:LYS:HB2	1.98	0.63
1:C:41:LYS:HG3	1:C:42:CYS:N	2.14	0.62
1:A:237:ARG:HG3	1:A:238:ASN:N	2.14	0.62
1:B:87:LYS:O	1:B:87:LYS:CG	2.47	0.62
1:B:211:ARG:HG2	1:B:211:ARG:HH11	1.64	0.62
1:A:72:PRO:HB2	1:A:74:LYS:NZ	2.15	0.61
1:A:184:GLY:HA3	1:A:195:LYS:HE3	1.81	0.61
1:C:138:ALA:HB3	1:C:153:ARG:HH11	1.66	0.60
1:A:251:ASP:OD2	1:A:257:TRP:CZ2	2.55	0.60
1:B:219:CYS:HB2	1:B:245:ALA:O	2.02	0.59
1:C:222:TRP:CG	1:C:241:LEU:HD22	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:TYR:HB3	1:C:39:TYR:CE2	2.38	0.58
1:C:232:THR:OG1	1:C:234:GLU:HG2	2.03	0.58
1:A:72:PRO:HB2	1:A:74:LYS:HZ1	1.68	0.58
1:B:227:THR:HG23	1:B:228:TYR:N	2.19	0.58
1:C:166:HIS:O	1:C:182:PRO:HG3	2.03	0.58
1:A:104:GLN:O	1:A:107:THR:HB	2.04	0.57
1:A:77:ASP:HB3	1:A:93:ASN:CG	2.25	0.57
1:C:49:GLY:N	1:C:50:PRO:CD	2.67	0.57
1:A:264:ASP:N	1:A:264:ASP:OD1	2.38	0.56
1:C:206:TYR:CZ	1:C:208:GLY:HA3	2.40	0.56
1:C:179:CYS:SG	1:C:189:PHE:HA	2.45	0.56
1:B:145:LYS:O	1:B:145:LYS:HG3	2.05	0.56
1:C:120:GLN:OE1	1:C:133:ARG:HG3	2.06	0.56
1:B:222:TRP:CG	1:B:241:LEU:HD22	2.40	0.56
1:A:106:LEU:O	1:A:111:CYS:CA	2.55	0.55
1:B:227:THR:CG2	1:B:228:TYR:N	2.69	0.55
1:B:106:LEU:HD13	1:B:111:CYS:O	2.06	0.55
1:A:166:HIS:O	1:A:182:PRO:HG3	2.07	0.54
1:B:230:ASN:OD1	1:B:230:ASN:O	2.25	0.54
1:C:105:HIS:HA	1:C:115:LYS:HB2	1.89	0.54
1:C:20:VAL:HG21	1:C:41:LYS:NZ	2.23	0.54
1:C:202:ARG:HD2	1:C:254:ILE:HA	1.90	0.53
1:C:89:GLY:O	1:C:90:THR:HG23	2.09	0.53
1:C:114:GLU:OE1	1:C:147:PRO:HB3	2.09	0.53
1:C:138:ALA:HB3	1:C:153:ARG:NH1	2.24	0.53
1:C:173:VAL:HG12	1:C:174:GLU:N	2.23	0.53
1:B:225:GLU:HG2	1:B:226:ALA:N	2.24	0.53
1:A:47:ARG:HB2	1:A:48:PRO:HD3	1.91	0.52
1:A:48:PRO:O	1:A:53:TRP:CD1	2.63	0.52
1:C:29:HIS:O	1:C:32:PHE:HD2	1.92	0.52
1:A:90:THR:HG22	1:A:101:LEU:HD21	1.91	0.52
1:C:100:CYS:HB2	1:C:110:HIS:HA	1.92	0.52
1:B:211:ARG:HG2	1:B:211:ARG:NH1	2.25	0.51
1:A:262:ASN:HB2	1:A:265:ARG:HB3	1.92	0.51
1:C:41:LYS:HG3	1:C:42:CYS:H	1.75	0.51
1:C:232:THR:O	1:C:233:ALA:C	2.47	0.51
1:C:49:GLY:H	1:C:50:PRO:CD	2.24	0.51
1:A:77:ASP:HB3	1:A:93:ASN:OD1	2.10	0.50
1:C:222:TRP:HB3	1:C:241:LEU:HD22	1.93	0.50
1:C:222:TRP:CD1	1:C:246:PHE:O	2.64	0.50
1:C:229:ARG:HE	1:C:230:ASN:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:TRP:HH2	1:C:257:TRP:CZ2	2.30	0.50
1:A:34:TYR:HB3	1:A:39:TYR:HE2	1.76	0.50
1:A:239:TRP:CD1	1:A:239:TRP:N	2.79	0.50
1:A:235:GLN:HB3	1:A:239:TRP:CZ3	2.46	0.50
1:A:32:PHE:CZ	1:A:39:TYR:HB2	2.47	0.50
1:A:178:LEU:C	1:A:178:LEU:HD12	2.33	0.50
1:A:222:TRP:HD1	1:A:244:HIS:O	1.94	0.50
1:A:261:LEU:HG	1:A:263:ARG:O	2.11	0.50
1:C:29:HIS:O	1:C:32:PHE:HB3	2.12	0.50
1:A:141:ARG:HB2	1:A:154:LEU:HD11	1.94	0.49
1:C:36:ARG:NH1	1:C:36:ARG:CG	2.73	0.49
1:A:160:ARG:HH11	1:A:160:ARG:HG3	1.78	0.49
1:A:73:LYS:NZ	1:A:95:PRO:HA	2.28	0.49
1:A:48:PRO:HB2	1:A:53:TRP:CD1	2.48	0.49
1:A:234:GLU:O	1:A:237:ARG:HG2	2.13	0.49
1:C:49:GLY:H	1:C:50:PRO:HD3	1.76	0.49
1:C:112:GLN:HG2	1:C:113:LYS:N	2.27	0.49
1:A:237:ARG:HG3	1:A:238:ASN:H	1.77	0.49
1:C:28:CYS:HB2	1:C:30:PHE:CE1	2.47	0.49
1:C:231:VAL:CA	1:C:235:GLN:NE2	2.65	0.49
1:B:202:ARG:HD2	1:B:254:ILE:HA	1.95	0.48
1:A:206:TYR:CZ	1:A:208:GLY:HA3	2.48	0.48
1:B:211:ARG:O	1:B:211:ARG:CG	2.62	0.48
1:C:29:HIS:O	1:C:32:PHE:CD2	2.66	0.48
1:B:179:CYS:HB2	1:B:188:PRO:O	2.14	0.48
1:B:213:THR:HA	1:B:271:CYS:HA	1.96	0.48
1:C:267:SER:OG	1:C:268:TRP:N	2.46	0.48
1:B:209:LEU:O	1:B:210:ALA:C	2.49	0.48
1:B:131:TRP:HZ3	1:B:144:CYS:HB2	1.79	0.47
1:B:228:TYR:O	1:B:228:TYR:HD1	1.95	0.47
1:C:41:LYS:CG	1:C:42:CYS:N	2.77	0.47
1:C:176:HIS:N	1:C:176:HIS:ND1	2.62	0.47
1:B:214:LEU:HA	1:B:272:ASP:HB2	1.96	0.47
1:C:30:PHE:O	1:C:32:PHE:CD2	2.67	0.47
1:A:129:GLU:O	1:A:143:GLN:HA	2.15	0.47
1:B:84:PRO:HG3	1:B:98:PRO:HG2	1.97	0.47
1:B:116:CYS:O	1:B:124:PHE:HA	2.14	0.47
1:C:236:ALA:O	1:C:240:GLY:N	2.44	0.47
1:B:223:ALA:HB2	1:B:243:GLY:HA2	1.96	0.47
1:C:30:PHE:HA	1:C:32:PHE:CD2	2.50	0.47
1:C:94:MET:CE	1:C:99:HIS:CD2	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:CYS:HB3	1:C:106:LEU:O	2.15	0.47
1:B:210:ALA:O	1:B:247:CYS:SG	2.74	0.46
1:A:75:VAL:O	1:A:76:LYS:C	2.55	0.46
1:C:94:MET:HE2	1:C:99:HIS:CD2	2.51	0.45
1:A:203:GLY:HA3	1:A:256:PRO:HG3	1.99	0.45
1:A:163:PRO:HD2	1:A:170:CYS:SG	2.57	0.45
1:A:230:ASN:O	1:A:230:ASN:OD1	2.35	0.45
1:C:78:HIS:HB2	1:C:93:ASN:ND2	2.32	0.45
1:C:213:THR:HG21	1:C:217:ALA:HB3	1.98	0.45
1:A:90:THR:CG2	1:A:101:LEU:HD21	2.46	0.45
1:C:131:TRP:CZ3	1:C:144:CYS:HB2	2.52	0.45
1:C:229:ARG:CZ	1:C:229:ARG:HB2	2.46	0.45
1:C:235:GLN:HB3	1:C:239:TRP:CZ3	2.53	0.45
1:B:214:LEU:HD11	1:B:255:ARG:NH1	2.30	0.44
1:C:234:GLU:O	1:C:235:GLN:C	2.56	0.44
1:A:34:TYR:HB3	1:A:39:TYR:CD2	2.52	0.44
1:C:141:ARG:HD3	1:C:154:LEU:HD11	1.99	0.44
1:C:41:LYS:CG	1:C:42:CYS:H	2.30	0.44
1:C:224:SER:O	1:C:225:GLU:C	2.55	0.44
1:A:260:VAL:HG21	1:A:269:GLU:OE2	2.18	0.44
1:C:82:HIS:O	1:C:84:PRO:HD3	2.18	0.44
1:C:48:PRO:O	1:C:53:TRP:CD1	2.71	0.43
1:A:103:PRO:O	1:A:105:HIS:O	2.36	0.43
1:C:164:CYS:HB2	1:C:168:GLY:HA3	1.99	0.43
1:C:219:CYS:O	1:C:245:ALA:HB1	2.19	0.43
1:C:186:THR:O	1:C:190:CYS:HA	2.18	0.43
1:B:228:TYR:CD1	1:B:228:TYR:C	2.91	0.43
1:C:20:VAL:HG21	1:C:41:LYS:HZ1	1.84	0.43
1:A:73:LYS:HZ1	1:A:95:PRO:CA	2.32	0.43
1:C:104:GLN:O	1:C:105:HIS:O	2.37	0.43
1:A:106:LEU:O	1:A:111:CYS:CB	2.67	0.43
1:B:100:CYS:SG	1:B:110:HIS:HA	2.59	0.43
1:B:133:ARG:HB3	1:B:140:ALA:HB3	2.01	0.43
1:A:33:GLN:HB3	1:A:59:ASN:OD1	2.18	0.42
1:C:173:VAL:CG1	1:C:174:GLU:N	2.82	0.42
1:C:77:ASP:HB2	1:C:93:ASN:CG	2.40	0.42
1:B:135:GLU:HB2	1:B:138:ALA:O	2.19	0.42
1:C:30:PHE:HA	1:C:32:PHE:HD2	1.85	0.42
1:C:222:TRP:CB	1:C:241:LEU:HD22	2.48	0.42
1:B:77:ASP:HB2	1:B:93:ASN:ND2	2.35	0.42
1:A:100:CYS:HB2	1:A:110:HIS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:HH11	1:A:254:ILE:HA	1.84	0.42
1:B:131:TRP:CZ3	1:B:144:CYS:HB2	2.55	0.42
1:B:228:TYR:O	1:B:229:ARG:CG	2.60	0.42
1:C:131:TRP:CH2	1:C:144:CYS:HB2	2.55	0.42
1:A:103:PRO:O	1:A:104:GLN:C	2.58	0.42
1:C:257:TRP:HB3	1:C:270:TYR:HD1	1.85	0.41
1:C:32:PHE:HB2	1:C:55:ALA:HB3	2.02	0.41
1:C:213:THR:HG23	1:C:269:GLU:HB2	2.02	0.41
1:A:62:GLN:H	1:A:62:GLN:CD	2.23	0.41
1:A:251:ASP:OD2	1:A:257:TRP:HZ2	2.02	0.41
1:C:115:LYS:HE2	1:C:126:HIS:NE2	2.35	0.41
1:A:136:GLN:HG2	1:A:169:ARG:NH1	2.36	0.41
1:C:32:PHE:HA	1:C:58:PRO:O	2.21	0.41
1:C:221:PRO:O	1:C:224:SER:HB3	2.21	0.41
1:A:225:GLU:O	1:A:229:ARG:HB2	2.21	0.41
1:C:107:THR:HG23	1:C:113:LYS:NZ	2.36	0.41
1:C:213:THR:HG22	1:C:214:LEU:N	2.36	0.40
1:B:222:TRP:CZ3	1:B:250:PRO:HG3	2.56	0.40
1:C:84:PRO:O	1:C:110:HIS:HB2	2.21	0.40
1:C:213:THR:CB	1:C:217:ALA:HB3	2.51	0.40
1:C:257:TRP:HB3	1:C:270:TYR:CD1	2.57	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	258/295 (88%)	239 (93%)	18 (7%)	1 (0%)	34	67
1	B	199/295 (68%)	182 (92%)	16 (8%)	1 (0%)	29	61
1	C	257/295 (87%)	233 (91%)	23 (9%)	1 (0%)	34	67
All	All	714/885 (81%)	654 (92%)	57 (8%)	3 (0%)	34	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	72	PRO
1	A	72	PRO
1	B	103	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	223/254 (88%)	214 (96%)	9 (4%)	31	60
1	B	169/254 (66%)	168 (99%)	1 (1%)	86	94
1	C	222/254 (87%)	210 (95%)	12 (5%)	22	52
All	All	614/762 (81%)	592 (96%)	22 (4%)	35	63

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	56	THR
1	A	76	LYS
1	A	96	SER
1	A	101	LEU
1	A	107	THR
1	A	200	ASP
1	A	263	ARG
1	A	264	ASP
1	B	228	TYR
1	C	30	PHE
1	C	45	LYS
1	C	101	LEU
1	C	107	THR
1	C	221	PRO
1	C	222	TRP
1	C	229	ARG
1	C	230	ASN

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Mol	Chain	Res	Type
1	C	231	VAL
1	C	232	THR
1	C	235	GLN
1	C	238	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	HIS
1	C	99	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	260/295 (88%)	0.71	27 (10%) 6 8	76, 108, 146, 168	2 (0%)
1	B	201/295 (68%)	1.10	46 (22%) 0 1	105, 133, 158, 167	0
1	C	259/295 (87%)	0.55	19 (7%) 15 17	81, 110, 142, 162	1 (0%)
All	All	720/885 (81%)	0.76	92 (12%) 3 4	76, 116, 153, 168	3 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	74	LYS	9.8
1	B	138	ALA	9.3
1	B	223	ALA	8.0
1	B	225	GLU	7.5
1	B	137	ALA	5.8
1	B	136	GLN	5.4
1	A	241	LEU	5.2
1	C	209	LEU	4.9
1	B	139	VAL	4.9
1	A	74	LYS	4.7
1	B	134	THR	4.7
1	B	224	SER	4.6
1	A	223	ALA	4.6
1	A	242	GLY	4.6
1	A	194	THR	4.5
1	B	121	LEU	4.4
1	A	225	GLU	4.4
1	B	132	TYR	4.3
1	C	246	PHE	4.0
1	B	183	VAL	4.0
1	C	222	TRP	3.9
1	B	266	LEU	3.9
1	A	209	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	220	GLN	3.8
1	C	214	LEU	3.8
1	C	231	VAL	3.7
1	B	241	LEU	3.6
1	A	226	ALA	3.6
1	B	122	LEU	3.5
1	A	183	VAL	3.5
1	A	122	LEU	3.5
1	B	156	SER	3.4
1	C	75	VAL	3.4
1	B	130	ILE	3.3
1	B	216	GLY	3.3
1	B	211	ARG	3.3
1	B	133	ARG	3.0
1	A	224	SER	3.0
1	B	184	GLY	3.0
1	B	153	ARG	2.9
1	C	18	THR	2.8
1	A	246	PHE	2.8
1	A	273	LEU	2.8
1	B	231	VAL	2.8
1	B	196	ALA	2.8
1	B	87	LYS	2.8
1	C	241	LEU	2.7
1	B	169	ARG	2.7
1	A	266	LEU	2.7
1	B	212	THR	2.6
1	B	176	HIS	2.6
1	A	210	ALA	2.6
1	B	246	PHE	2.6
1	C	183	VAL	2.6
1	B	135	GLU	2.6
1	B	182	PRO	2.6
1	A	117	PHE	2.5
1	B	232	THR	2.5
1	B	218	PRO	2.5
1	B	209	LEU	2.5
1	A	231	VAL	2.4
1	C	192	VAL	2.4
1	B	105	HIS	2.4
1	A	243	GLY	2.4
1	C	229	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	245	ALA	2.4
1	C	215	SER	2.4
1	C	273	LEU	2.3
1	B	259	PHE	2.3
1	C	228	TYR	2.3
1	B	171	LEU	2.3
1	C	266	LEU	2.3
1	C	259	PHE	2.3
1	B	119	PRO	2.3
1	C	72	PRO	2.3
1	B	101	LEU	2.2
1	A	139	VAL	2.2
1	A	132	TYR	2.2
1	B	256	PRO	2.2
1	B	120	GLN	2.2
1	A	137	ALA	2.1
1	A	245	ALA	2.1
1	A	171	LEU	2.1
1	A	211	ARG	2.1
1	B	185	TYR	2.1
1	B	89	GLY	2.1
1	B	178	LEU	2.1
1	A	186	THR	2.0
1	B	230	ASN	2.0
1	B	197	SER	2.0
1	C	272	ASP	2.0
1	A	218	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.