



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2016 – 04:34 AM EDT

PDB ID : 5I25
Title : human recombinant coagulation FXI in complex with a peptide derived from human high molecular weight kininogen (HKP)
Authors : Hall, G.A.F.; Wong, S.S.; Emsley, J.
Deposited on : 2016-02-08
Resolution : 2.85 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
<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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027674
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027674

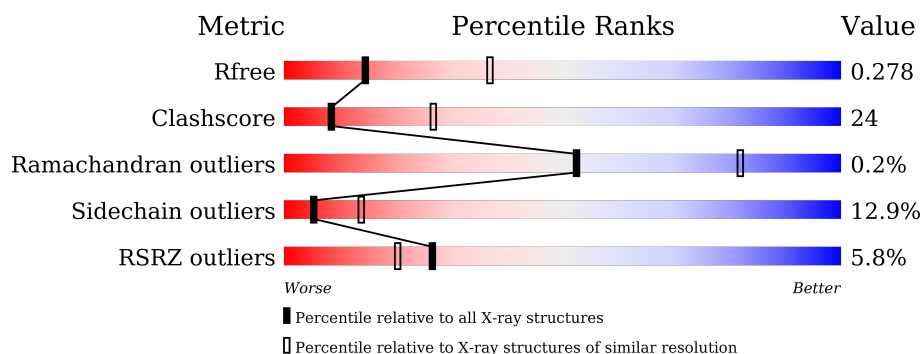
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	607	<div> <div>5%</div> <div>55%</div> <div>36%</div> <div>7%</div> <div>.</div> </div>
2	B	8	<div> <div>38%</div> <div>38%</div> <div>50%</div> <div>13%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4842 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.

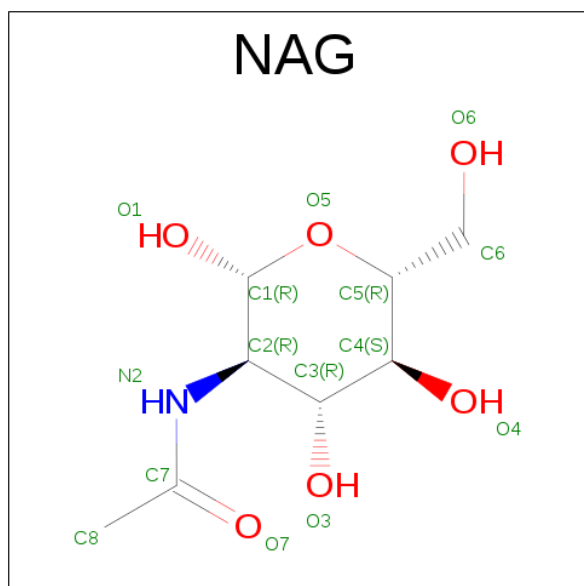
- Molecule 1 is a protein called Coagulation factor XI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4684	2950	815	878	41			

- Molecule 2 is a protein called ASN-PRO-ILE-SER-ASP-PHE-PRO-ASP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	0	0	0
			63	40	9	14			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

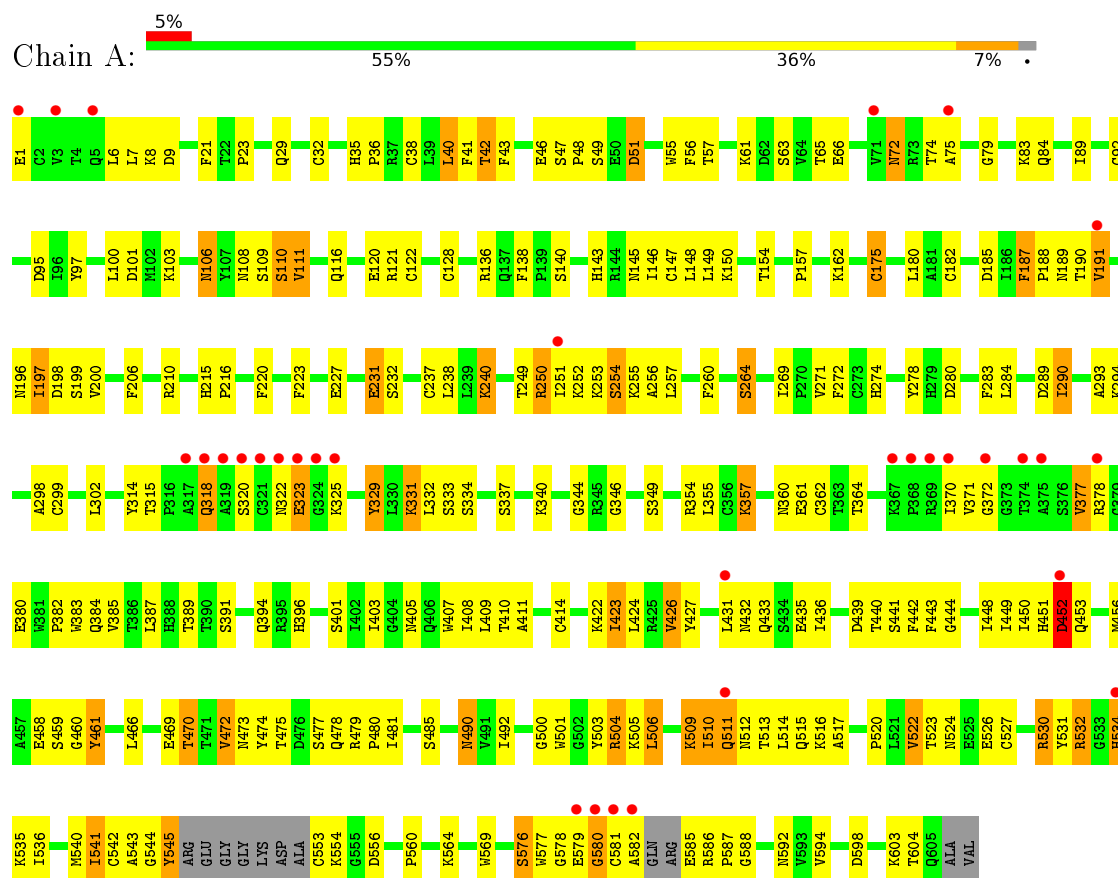
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	2	Total	O	0	0
			2	2		

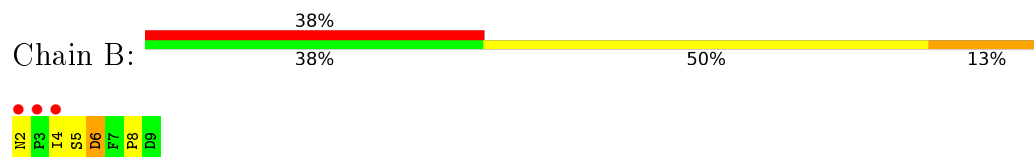
3 Residue-property plots

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.

• Molecule 1: Coagulation factor XI



• Molecule 2: ASN-PRO-ILE-SER-ASP-PHE-PRO-ASP



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.59 Å 80.59 Å 251.81 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.79 – 2.85 36.33 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.79-2.85) 99.7 (36.33-2.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.85 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.226 , 0.288 0.218 , 0.278	Depositor DCC
R_{free} test set	2057 reflections (11.34%)	DCC
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4842	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.56	1/4793 (0.0%)	0.71	2/6490 (0.0%)
2	B	0.52	0/65	0.60	0/89
All	All	0.56	1/4858 (0.0%)	0.71	2/6579 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	452	ASP	CB-CG	5.20	1.62	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	GLY	N-CA-C	-5.90	98.36	113.10
1	A	460	GLY	N-CA-C	5.42	126.64	113.10

There are no chirality outliers.

There are no planarity outliers.

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	4684	0	4571	226	0
2	B	63	0	52	7	0
3	A	42	0	39	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	51	0	0	2	0
4	B	2	0	0	2	0
All	All	4842	0	4662	227	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 24.

All (227) 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:452:ASP:OD1	1:A:453:GLN:HG2	1.53	1.09
1:A:579:GLU:O	1:A:579:GLU:HG3	1.42	1.05
1:A:541:ILE:HD11	1:A:592:ASN:CG	1.78	1.03
1:A:9:ASP:OD1	1:A:74:THR:HA	1.60	1.01
1:A:189:ASN:HD22	1:A:254:SER:HA	1.37	0.90
1:A:377:VAL:HG22	1:A:378:ARG:H	1.45	0.81
1:A:189:ASN:ND2	1:A:254:SER:HA	1.97	0.80
1:A:407:TRP:CE2	1:A:604:THR:HG22	2.17	0.79
1:A:433:GLN:O	1:A:436:ILE:HG13	1.82	0.77
1:A:474:TYR:CZ	1:A:480:PRO:HG3	2.21	0.76
1:A:83:LYS:HB3	1:A:354:ARG:HD3	1.68	0.76
1:A:187:PHE:HD2	1:A:187:PHE:N	1.83	0.76
1:A:384:GLN:HE22	1:A:560:PRO:HD3	1.51	0.76
1:A:472:VAL:HG12	1:A:478:GLN:NE2	2.02	0.75
1:A:582:ALA:C	1:A:585:GLU:HA	2.07	0.75
1:A:187:PHE:CD2	1:A:187:PHE:N	2.50	0.75
1:A:405:ASN:O	1:A:472:VAL:HG23	1.86	0.75
1:A:511:GLN:HE21	1:A:512:ASN:H	1.36	0.74
1:A:354:ARG:NH2	4:A:1001:HOH:O	2.20	0.74
1:A:505:LYS:HD2	1:A:506:LEU:H	1.50	0.74
1:A:522:VAL:HG13	1:A:543:ALA:HA	1.70	0.74
1:A:283:PHE:O	1:A:331:LYS:HE3	1.87	0.73
1:A:461:TYR:N	1:A:461:TYR:CD1	2.52	0.72
1:A:72:ASN:ND2	3:A:901:NAG:O5	2.23	0.72
1:A:40:LEU:HD12	1:A:61:LYS:HB2	1.70	0.71
1:A:432:ASN:ND2	3:A:903:NAG:O5	2.24	0.71
1:A:92:CYS:SG	1:A:175:CYS:N	2.64	0.70
1:A:293:ALA:HB3	1:A:314:TYR:HE1	1.57	0.70
1:A:473:ASN:O	1:A:478:GLN:NE2	2.23	0.70
1:A:196:ASN:OD1	1:A:238:LEU:HD13	1.91	0.69
1:A:452:ASP:CG	1:A:453:GLN:HG2	2.12	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:GLN:HE21	1:A:384:GLN:HA	1.57	0.69
1:A:541:ILE:HD11	1:A:592:ASN:CB	2.22	0.68
1:A:371:VAL:O	1:A:371:VAL:HG23	1.93	0.68
1:A:384:GLN:NE2	1:A:560:PRO:HG3	2.09	0.68
1:A:227:GLU:O	1:A:255:LYS:HD3	1.93	0.67
1:A:387:LEU:HD13	1:A:426:VAL:HG13	1.76	0.67
1:A:511:GLN:HE21	1:A:512:ASN:N	1.91	0.67
1:A:389:THR:O	1:A:394:GLN:HA	1.93	0.67
1:A:580:GLY:O	1:A:581:CYS:C	2.32	0.67
1:A:469:GLU:HB2	1:A:470:THR:HG22	1.77	0.66
1:A:250:ARG:O	1:A:250:ARG:HG2	1.95	0.66
1:A:197:ILE:O	1:A:198:ASP:HB2	1.95	0.65
1:A:122:CYS:O	1:A:128:CYS:HB3	1.96	0.65
1:A:503:TYR:HE1	1:A:506:LEU:HA	1.61	0.65
1:A:51:ASP:N	1:A:51:ASP:OD2	2.20	0.64
1:A:322:ASN:OD1	1:A:323:GLU:HG3	1.98	0.64
1:A:510:ILE:HG23	1:A:511:GLN:N	2.12	0.64
1:A:370:ILE:HD12	1:A:371:VAL:H	1.62	0.64
1:A:360:ASN:ND2	1:A:362:CYS:SG	2.71	0.64
1:A:540:MET:C	1:A:541:ILE:HD13	2.18	0.63
1:A:401:SER:OG	1:A:560:PRO:HB3	1.99	0.63
1:A:531:TYR:OH	1:A:587:PRO:O	2.17	0.63
1:A:461:TYR:H	1:A:461:TYR:HD1	1.45	0.62
1:A:280:ASP:OD1	1:A:344:GLY:HA2	1.99	0.62
1:A:424:LEU:CD1	1:A:448:ILE:HD11	2.29	0.62
1:A:514:LEU:HD12	1:A:515:GLN:N	2.14	0.62
1:A:541:ILE:HD11	1:A:592:ASN:ND2	2.15	0.62
1:A:456:MET:O	1:A:459:SER:HB2	2.00	0.62
1:A:198:ASP:OD1	1:A:199:SER:N	2.32	0.61
1:A:443:PHE:CZ	1:A:472:VAL:HG13	2.35	0.61
1:A:384:GLN:NE2	1:A:560:PRO:HD3	2.15	0.61
1:A:385:VAL:HG21	1:A:408:ILE:HD12	1.81	0.61
1:A:564:LYS:HB2	1:A:569:TRP:CZ3	2.35	0.61
1:A:424:LEU:HD11	1:A:448:ILE:HD11	1.82	0.61
1:A:436:ILE:HG22	1:A:440:THR:HG21	1.83	0.60
1:A:384:GLN:NE2	1:A:384:GLN:HA	2.15	0.60
1:A:188:PRO:HA	1:A:257:LEU:HG	1.83	0.60
1:A:187:PHE:HD2	1:A:187:PHE:H	1.50	0.60
1:A:576:SER:OG	1:A:577:TRP:CD1	2.54	0.60
1:A:405:ASN:O	1:A:472:VAL:CG2	2.49	0.60
1:A:182:CYS:SG	1:A:264:SER:HB3	2.42	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:GLY:O	1:A:516:LYS:CE	2.50	0.59
1:A:299:CYS:SG	1:A:314:TYR:HB2	2.43	0.59
1:A:576:SER:OG	1:A:577:TRP:HD1	1.85	0.59
1:A:532:ARG:HH22	1:A:586:ARG:NH2	2.00	0.58
1:A:23:PRO:HB2	1:A:97:TYR:CE2	2.38	0.58
1:A:116:GLN:O	1:A:120:GLU:HG3	2.03	0.58
1:A:380:GLU:OE2	1:A:516:LYS:NZ	2.34	0.58
1:A:407:TRP:CD2	1:A:604:THR:HG22	2.38	0.58
1:A:377:VAL:HA	1:A:431:LEU:HD13	1.85	0.58
1:A:444:GLY:HA3	1:A:469:GLU:HG3	1.85	0.58
1:A:579:GLU:O	1:A:579:GLU:CG	2.30	0.58
1:A:206:PHE:O	1:A:210:ARG:HG3	2.05	0.57
1:A:492:ILE:HD12	1:A:492:ILE:N	2.19	0.57
1:A:196:ASN:OD1	1:A:240:LYS:HD2	2.04	0.57
1:A:564:LYS:HB2	1:A:569:TRP:CH2	2.40	0.57
1:A:511:GLN:NE2	1:A:512:ASN:H	2.00	0.57
1:A:461:TYR:N	1:A:461:TYR:HD1	1.97	0.56
1:A:522:VAL:HG22	1:A:542:CYS:HB2	1.86	0.56
1:A:318:GLN:NE2	1:A:318:GLN:HA	2.19	0.56
1:A:272:PHE:HB3	1:A:355:LEU:HB3	1.87	0.56
1:A:427:TYR:CE2	1:A:442:PHE:HB3	2.40	0.56
1:A:503:TYR:CE1	1:A:506:LEU:HA	2.40	0.55
1:A:511:GLN:CA	1:A:511:GLN:HE21	2.20	0.55
1:A:517:ALA:HB2	1:A:554:LYS:HE2	1.89	0.55
1:A:534:HIS:N	1:A:534:HIS:ND1	2.53	0.55
1:A:294:LYS:HE2	1:A:325:LYS:HE2	1.88	0.55
1:A:432:ASN:O	1:A:435:GLU:HB3	2.06	0.55
1:A:43:PHE:CE2	1:A:56:PHE:HA	2.42	0.55
1:A:293:ALA:HB3	1:A:314:TYR:CE1	2.41	0.54
1:A:40:LEU:CD1	1:A:61:LYS:HB2	2.37	0.54
1:A:535:LYS:HG3	1:A:536:ILE:N	2.22	0.53
1:A:531:TYR:HD2	1:A:536:ILE:HD11	1.72	0.53
1:A:108:ASN:HD21	3:A:902:NAG:C5	2.21	0.53
1:A:505:LYS:CD	1:A:506:LEU:H	2.20	0.53
1:A:540:MET:O	1:A:541:ILE:HD13	2.08	0.53
1:A:377:VAL:HG22	1:A:378:ARG:N	2.18	0.53
1:A:426:VAL:HG23	1:A:443:PHE:O	2.09	0.52
1:A:106:ASN:HB2	2:B:4:ILE:HB	1.90	0.52
1:A:148:LEU:HG	1:A:150:LYS:HE2	1.92	0.52
1:A:143:HIS:CD2	2:B:8:PRO:CD	2.93	0.52
1:A:396:HIS:HB3	1:A:510:ILE:HD11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLU:OE1	1:A:162:LYS:HE3	2.09	0.52
1:A:298:ALA:O	1:A:302:LEU:HD23	2.09	0.52
1:A:110:SER:HB2	1:A:121:ARG:NH1	2.24	0.52
1:A:191:VAL:HG22	1:A:251:ILE:HB	1.92	0.51
1:A:426:VAL:HG23	1:A:443:PHE:HB2	1.92	0.51
1:A:223:PHE:O	1:A:256:ALA:HA	2.10	0.51
1:A:42:THR:O	1:A:42:THR:HG22	2.09	0.51
1:A:6:LEU:C	1:A:7:LEU:HD23	2.30	0.51
1:A:252:LYS:O	1:A:253:LYS:HG2	2.10	0.51
1:A:501:TRP:O	1:A:511:GLN:HB2	2.10	0.51
1:A:514:LEU:HD12	1:A:515:GLN:H	1.74	0.51
1:A:106:ASN:ND2	4:B:101:HOH:O	2.41	0.51
1:A:21:PHE:O	1:A:157:PRO:HD2	2.11	0.51
1:A:532:ARG:NH2	1:A:586:ARG:NH2	2.58	0.51
1:A:541:ILE:HD11	1:A:592:ASN:HB2	1.93	0.51
1:A:490:ASN:N	1:A:490:ASN:OD1	2.43	0.50
1:A:284:LEU:HD12	1:A:340:LYS:HB3	1.93	0.50
1:A:382:PRO:HB2	1:A:479:ARG:H	1.77	0.50
1:A:504:ARG:CG	1:A:504:ARG:HH11	2.25	0.50
1:A:46:GLU:HG3	1:A:55:TRP:CZ3	2.47	0.50
1:A:46:GLU:HA	1:A:55:TRP:CD1	2.47	0.49
1:A:29:GLN:HG3	1:A:41:PHE:CE2	2.47	0.49
1:A:382:PRO:HB2	1:A:479:ARG:N	2.27	0.49
1:A:101:ASP:OD1	1:A:103:LYS:HE2	2.13	0.49
1:A:143:HIS:NE2	2:B:8:PRO:HD3	2.28	0.49
1:A:372:GLY:O	1:A:516:LYS:NZ	2.46	0.49
1:A:577:TRP:CD2	1:A:577:TRP:O	2.66	0.49
2:B:6:ASP:OD2	4:B:101:HOH:O	2.20	0.48
1:A:200:VAL:HG22	1:A:237:CYS:HB3	1.95	0.48
1:A:449:ILE:HG21	1:A:603:LYS:HD2	1.94	0.48
1:A:451:HIS:HD2	1:A:453:GLN:H	1.60	0.48
1:A:35:HIS:CG	1:A:36:PRO:HD2	2.48	0.48
1:A:384:GLN:NE2	1:A:560:PRO:CD	2.76	0.48
1:A:47:SER:HB2	1:A:48:PRO:HD2	1.96	0.48
1:A:432:ASN:OD1	1:A:513:THR:HA	2.14	0.48
1:A:451:HIS:CD2	1:A:453:GLN:H	2.32	0.47
1:A:423:ILE:HG13	1:A:423:ILE:O	2.13	0.47
1:A:475:THR:O	1:A:478:GLN:N	2.47	0.47
1:A:136:ARG:O	1:A:138:PHE:N	2.47	0.47
1:A:384:GLN:NE2	1:A:560:PRO:CG	2.77	0.47
1:A:143:HIS:CD2	2:B:8:PRO:HD3	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ILE:HB	1:A:466:LEU:HB2	1.96	0.47
1:A:410:THR:OG1	1:A:411:ALA:N	2.48	0.47
1:A:530:ARG:NE	1:A:545:TYR:OH	2.48	0.47
1:A:106:ASN:OD1	1:A:106:ASN:N	2.48	0.46
1:A:149:LEU:C	1:A:150:LYS:HG2	2.36	0.46
1:A:9:ASP:OD1	1:A:74:THR:CA	2.49	0.46
1:A:269:ILE:HG13	1:A:271:VAL:HG23	1.96	0.46
1:A:148:LEU:HD23	1:A:148:LEU:H	1.78	0.46
1:A:357:LYS:HA	1:A:357:LYS:HD3	1.38	0.46
1:A:154:THR:O	1:A:216:PRO:HG2	2.16	0.46
1:A:387:LEU:CD1	1:A:426:VAL:HG13	2.42	0.46
1:A:136:ARG:C	1:A:138:PHE:N	2.69	0.46
1:A:109:SER:HB2	2:B:4:ILE:CG2	2.45	0.46
1:A:46:GLU:HA	1:A:55:TRP:CG	2.51	0.46
1:A:29:GLN:HG3	1:A:41:PHE:HE2	1.81	0.45
1:A:200:VAL:CG2	1:A:237:CYS:HB3	2.45	0.45
1:A:1:GLU:HA	1:A:1:GLU:OE2	2.16	0.45
1:A:377:VAL:HA	1:A:431:LEU:CD1	2.46	0.45
1:A:210:ARG:NH2	4:A:1003:HOH:O	2.49	0.45
1:A:289:ASP:OD1	1:A:290:ILE:N	2.50	0.45
1:A:41:PHE:CE2	1:A:79:GLY:HA3	2.51	0.45
1:A:110:SER:O	1:A:146:ILE:HA	2.17	0.44
1:A:100:LEU:HD12	1:A:100:LEU:HA	1.80	0.44
1:A:290:ILE:HD13	1:A:329:TYR:CE1	2.53	0.44
1:A:383:TRP:CE2	1:A:481:ILE:HD12	2.52	0.44
1:A:422:LYS:HA	1:A:422:LYS:HD3	1.79	0.44
1:A:396:HIS:HB3	1:A:510:ILE:CD1	2.48	0.43
1:A:403:ILE:HD13	1:A:409:LEU:HB2	1.99	0.43
1:A:111:VAL:HA	1:A:145:ASN:O	2.18	0.43
1:A:278:TYR:N	1:A:349:SER:O	2.48	0.43
1:A:577:TRP:N	1:A:577:TRP:CD1	2.86	0.43
1:A:361:GLU:O	1:A:364:THR:HG23	2.19	0.43
1:A:475:THR:C	1:A:477:SER:N	2.71	0.43
1:A:577:TRP:O	1:A:577:TRP:CG	2.70	0.43
1:A:6:LEU:HD23	1:A:6:LEU:N	2.33	0.43
1:A:215:HIS:HA	1:A:216:PRO:HD3	1.84	0.43
1:A:32:CYS:O	1:A:38:CYS:HB3	2.18	0.43
1:A:436:ILE:HD12	1:A:436:ILE:O	2.19	0.43
1:A:504:ARG:NH1	1:A:504:ARG:CG	2.82	0.43
1:A:505:LYS:HD2	1:A:506:LEU:N	2.26	0.42
1:A:520:PRO:HD2	1:A:544:GLY:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:PHE:N	1:A:206:PHE:CD1	2.86	0.42
1:A:332:LEU:C	1:A:332:LEU:HD12	2.39	0.42
1:A:46:GLU:HG3	1:A:55:TRP:CE3	2.54	0.42
1:A:74:THR:O	1:A:75:ALA:HB3	2.19	0.42
1:A:500:GLY:H	1:A:514:LEU:HD11	1.84	0.42
1:A:109:SER:HB2	2:B:4:ILE:HG23	2.01	0.42
1:A:475:THR:O	1:A:477:SER:N	2.52	0.42
1:A:424:LEU:HD12	1:A:448:ILE:HD11	2.01	0.42
1:A:544:GLY:O	1:A:545:TYR:HB2	2.20	0.42
1:A:21:PHE:HA	1:A:56:PHE:O	2.19	0.42
1:A:65:THR:C	1:A:66:GLU:HG3	2.40	0.42
1:A:444:GLY:O	1:A:469:GLU:HG2	2.20	0.42
1:A:511:GLN:CA	1:A:511:GLN:NE2	2.83	0.41
1:A:56:PHE:CZ	1:A:100:LEU:HD11	2.54	0.41
1:A:280:ASP:CG	1:A:344:GLY:HA2	2.41	0.41
1:A:578:GLY:HA3	1:A:588:GLY:HA2	2.01	0.41
1:A:191:VAL:CG1	1:A:253:LYS:HB2	2.50	0.41
1:A:220:PHE:HA	1:A:260:PHE:HA	2.02	0.41
1:A:280:ASP:OD2	1:A:346:GLY:HA2	2.21	0.41
1:A:231:GLU:OE2	1:A:232:SER:HA	2.20	0.41
1:A:377:VAL:CG2	1:A:378:ARG:H	2.23	0.41
1:A:411:ALA:HB3	1:A:414:CYS:SG	2.61	0.41
1:A:458:GLU:HG3	1:A:577:TRP:CD2	2.56	0.41
1:A:8:LYS:O	1:A:9:ASP:C	2.59	0.41
1:A:524:ASN:O	1:A:527:CYS:N	2.54	0.41
1:A:517:ALA:HB2	1:A:554:LYS:CE	2.49	0.41
1:A:371:VAL:O	1:A:371:VAL:CG2	2.65	0.40
1:A:185:ASP:O	1:A:187:PHE:HE2	2.04	0.40
1:A:72:ASN:OD1	1:A:72:ASN:N	2.49	0.40
1:A:210:ARG:HD2	1:A:274:HIS:CE1	2.56	0.40
1:A:333:SER:OG	1:A:334:SER:N	2.53	0.40
1:A:509:LYS:HE2	1:A:509:LYS:HB2	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	590/607 (97%)	567 (96%)	22 (4%)	1 (0%)	52	82
2	B	6/8 (75%)	6 (100%)	0	0	100	100
All	All	596/615 (97%)	573 (96%)	22 (4%)	1 (0%)	52	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	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	528/535 (99%)	462 (88%)	66 (12%)	6	15
2	B	8/8 (100%)	5 (62%)	3 (38%)	0	0
All	All	536/543 (99%)	467 (87%)	69 (13%)	5	14

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	42	THR
1	A	49	SER
1	A	51	ASP
1	A	57	THR
1	A	63	SER
1	A	72	ASN
1	A	84	GLN
1	A	89	ILE
1	A	95	ASP
1	A	106	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	110	SER
1	A	111	VAL
1	A	140	SER
1	A	147	CYS
1	A	175	CYS
1	A	180	LEU
1	A	187	PHE
1	A	190	THR
1	A	191	VAL
1	A	197	ILE
1	A	231	GLU
1	A	240	LYS
1	A	249	THR
1	A	250	ARG
1	A	254	SER
1	A	264	SER
1	A	290	ILE
1	A	315	THR
1	A	318	GLN
1	A	320	SER
1	A	323	GLU
1	A	329	TYR
1	A	331	LYS
1	A	337	SER
1	A	357	LYS
1	A	391	SER
1	A	423	ILE
1	A	426	VAL
1	A	439	ASP
1	A	441	SER
1	A	450	ILE
1	A	452	ASP
1	A	461	TYR
1	A	470	THR
1	A	472	VAL
1	A	485	SER
1	A	490	ASN
1	A	504	ARG
1	A	506	LEU
1	A	509	LYS
1	A	510	ILE
1	A	511	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	522	VAL
1	A	523	THR
1	A	526	GLU
1	A	530	ARG
1	A	532	ARG
1	A	534	HIS
1	A	541	ILE
1	A	545	TYR
1	A	553	CYS
1	A	556	ASP
1	A	576	SER
1	A	594	VAL
1	A	598	ASP
2	B	2	ASN
2	B	5	SER
2	B	6	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	A	189	ASN
1	A	318	GLN
1	A	384	GLN
1	A	451	HIS
1	A	511	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

3 ligands 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	$\# Z > 2$
3	NAG	A	901	-	14,14,15	0.54	0	15,19,21	0.85	0
3	NAG	A	902	-	14,14,15	0.77	0	15,19,21	1.75	4 (26%)
3	NAG	A	903	-	14,14,15	0.49	0	15,19,21	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	901	-	-	0/6/23/26	0/1/1/1
3	NAG	A	902	-	-	0/6/23/26	0/1/1/1
3	NAG	A	903	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	NAG	O7-C7-C8	-2.23	117.97	122.07
3	A	902	NAG	O3-C3-C2	2.20	114.09	109.37
3	A	902	NAG	C1-O5-C5	2.92	116.44	112.14
3	A	902	NAG	C2-N2-C7	3.21	127.28	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	NAG	1	0
3	A	902	NAG	1	0
3	A	903	NAG	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

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, 95th 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	596/607 (98%)	0.24	32 (5%) 29 23	38, 70, 112, 145	0
2	B	8/8 (100%)	1.66	3 (37%) 0 0	89, 100, 119, 127	0
All	All	604/615 (98%)	0.26	35 (5%) 26 20	38, 70, 112, 145	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	320	SER	6.7
2	B	2	ASN	6.2
1	A	321	CYS	5.8
1	A	319	ALA	5.3
1	A	369	ARG	4.9
1	A	318	GLN	4.6
1	A	1	GLU	4.4
1	A	324	GLY	4.4
1	A	317	ALA	4.3
1	A	372	GLY	4.3
1	A	374	THR	4.3
1	A	322	ASN	4.2
1	A	375	ALA	3.8
1	A	370	ILE	3.6
1	A	581	CYS	3.2
1	A	75	ALA	3.2
2	B	3	PRO	3.2
1	A	251	ILE	3.0
1	A	325	LYS	3.0
1	A	3	VAL	3.0
1	A	534	HIS	3.0
1	A	580	GLY	2.8
1	A	582	ALA	2.5
1	A	323	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	4	ILE	2.4
1	A	579	GLU	2.4
1	A	511	GLN	2.3
1	A	452	ASP	2.3
1	A	367	LYS	2.3
1	A	368	PRO	2.2
1	A	378	ARG	2.2
1	A	431	LEU	2.1
1	A	5	GLN	2.1
1	A	191	VAL	2.1
1	A	71	VAL	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	903	14/15	0.64	0.30	-	105,124,127,128	0
3	NAG	A	901	14/15	0.79	0.27	-	103,119,128,128	0
3	NAG	A	902	14/15	0.75	0.18	-	55,76,84,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.