



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 22, 2018 – 03:23 PM EST

PDB ID : 5O35  
Title : Structure of complement proteins complex  
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Deposited on : 2017-05-23  
Resolution : 4.20 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) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030736

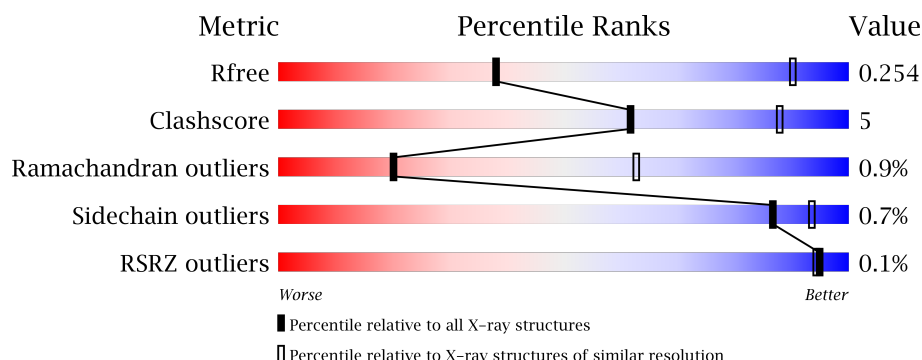
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*




The reported resolution of this entry is 4.20 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))
$R_{free}$	100719	1177 (4.80-3.60)
Clashscore	112137	1025 (4.72-3.66)
Ramachandran outliers	110173	1024 (4.76-3.62)
Sidechain outliers	110143	1008 (4.76-3.62)
RSRZ outliers	101464	1188 (4.80-3.60)

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.

Mol	Chain	Length	Quality of chain
1	A	645	 87% 13%
2	B	915	 84% 15%
3	C	383	 84% 10% . .

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15181 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 Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5007	3187	848	957	15			

- Molecule 2 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	912	Total	C	N	O	S	0	0	0
			7285	4613	1227	1407	38			

- Molecule 3 is a protein called Complement factor H, Complement factor H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	367	Total	C	N	O	S	0	0	0
			2861	1789	491	552	29			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1095	GLY	-	linker	UNP P08603
C	1096	GLY	-	linker	UNP P08603
C	1097	GLY	-	linker	UNP P08603
C	1098	GLY	-	linker	UNP P08603
C	1099	GLY	-	linker	UNP P08603
C	1100	GLY	-	linker	UNP P08603
C	1101	GLY	-	linker	UNP P08603
C	1102	GLY	-	linker	UNP P08603
C	1103	GLY	-	linker	UNP P08603
C	1104	GLY	-	linker	UNP P08603
C	1105	GLY	-	linker	UNP P08603
C	1106	GLY	-	linker	UNP P08603

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

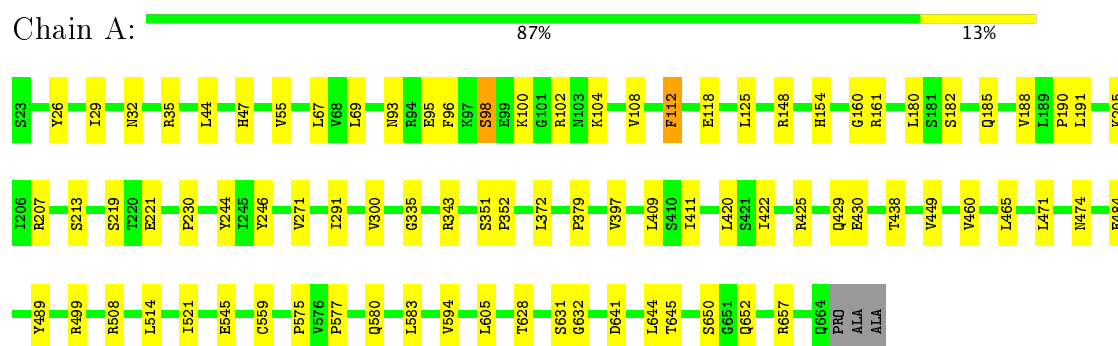


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

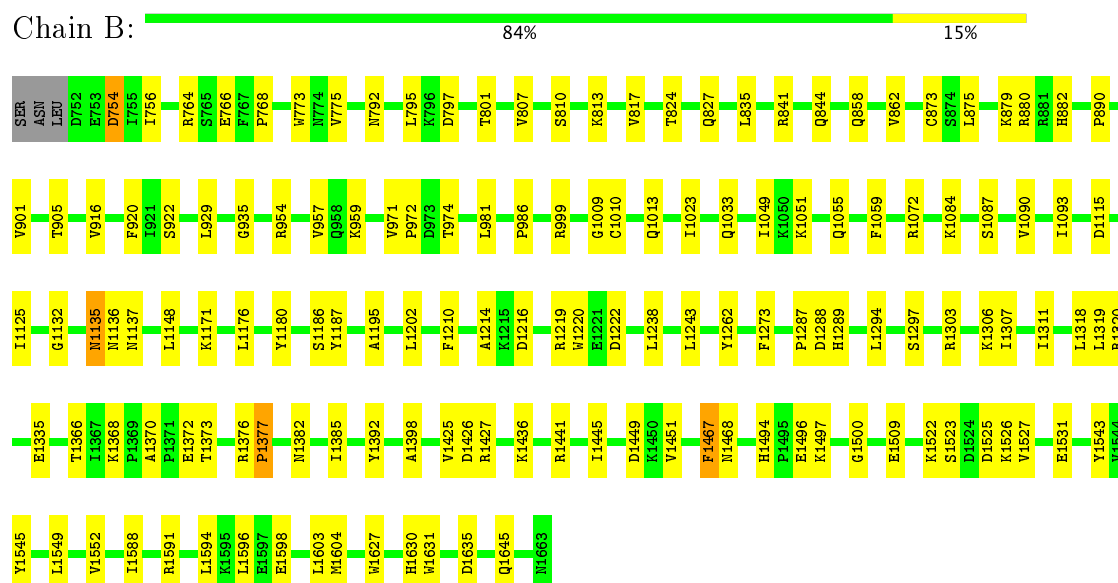
### 3 Residue-property plots

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.

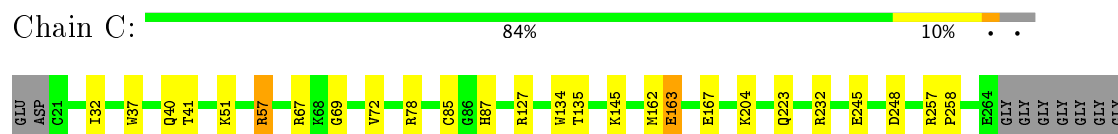
#### • Molecule 1: Complement C3

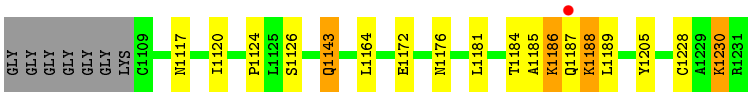


#### • Molecule 2: Complement C3



#### • Molecule 3: Complement factor H, Complement factor H





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.90Å 142.90Å 312.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.88 – 4.20 61.88 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (61.88-4.20) 99.9 (61.88-4.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 4.14Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.216 , 0.246 0.222 , 0.254	Depositor DCC
$R_{free}$ test set	1392 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	106.6	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 69.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.064 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	15181	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.28	0/5108	0.52	1/6940 (0.0%)
2	B	0.30	0/7431	0.54	0/10062
3	C	0.25	0/2935	0.47	1/3984 (0.0%)
All	All	0.28	0/15474	0.52	2/20986 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1186	LYS	C-N-CA	5.29	134.93	121.70
1	A	559	CYS	CA-CB-SG	5.01	123.02	114.00

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	5007	0	5065	55	0
2	B	7285	0	7208	85	0
3	C	2861	0	2680	27	0
4	B	28	0	25	0	0
All	All	15181	0	14978	153	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 5.

All (153) 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:26:TYR:HB3	1:A:112:PHE:CE1	2.14	0.82
2:B:1216:ASP:OD2	2:B:1219:ARG:NH1	2.14	0.78
1:A:594:VAL:HG12	2:B:775:VAL:HG22	1.68	0.75
1:A:26:TYR:HB3	1:A:112:PHE:CD1	2.22	0.73
3:C:1120:ILE:HD11	3:C:1124:PRO:HG3	1.70	0.72
3:C:32:ILE:HG22	3:C:51:LYS:HB3	1.72	0.71
2:B:1288:ASP:OD2	2:B:1289:HIS:ND1	2.24	0.71
2:B:1135:ASN:O	2:B:1137:ASN:N	2.25	0.70
2:B:835:LEU:HG	2:B:929:LEU:HD23	1.73	0.70
2:B:1549:LEU:HD12	2:B:1598:GLU:HA	1.75	0.69
1:A:411:ILE:HD11	1:A:420:LEU:HD21	1.73	0.69
1:A:98:SER:HB3	1:A:104:LYS:HE2	1.73	0.69
2:B:1398:ALA:HB3	2:B:1451:VAL:HG22	1.75	0.68
1:A:474:ASN:HB3	1:A:514:LEU:HD11	1.76	0.68
1:A:650:SER:OG	1:A:652:GLN:OE1	2.12	0.68
1:A:460:VAL:HG13	1:A:471:LEU:HD11	1.78	0.65
2:B:1594:LEU:HB3	2:B:1596:LEU:HD13	1.79	0.63
2:B:862:VAL:HG22	2:B:916:VAL:HG12	1.80	0.63
3:C:232:ARG:NH2	3:C:248:ASP:OD2	2.32	0.63
2:B:764:ARG:HB3	2:B:797:ASP:HB3	1.81	0.62
3:C:1172:GLU:O	3:C:1176:ASN:ND2	2.33	0.61
2:B:1549:LEU:HD11	2:B:1552:VAL:HG23	1.83	0.60
2:B:972:PRO:HB2	2:B:1509:GLU:OE1	2.01	0.60
3:C:1205:TYR:HA	3:C:1230:LYS:HA	1.82	0.60
2:B:873:CYS:HB3	2:B:901:VAL:HB	1.85	0.59
3:C:223:GLN:HE22	3:C:1126:SER:HA	1.65	0.59
1:A:148:ARG:HG3	2:B:773:TRP:CZ2	2.38	0.59
1:A:55:VAL:HG22	1:A:112:PHE:HD2	1.68	0.58
1:A:35:ARG:HD3	1:A:154:HIS:CD2	2.38	0.58
2:B:1522:LYS:HD2	2:B:1526:LYS:HE2	1.84	0.58
2:B:1214:ALA:HB2	2:B:1220:TRP:CZ2	2.38	0.58
2:B:844:GLN:HA	2:B:901:VAL:HG22	1.85	0.58
2:B:1051:LYS:NZ	2:B:1055:GLN:OE1	2.33	0.57
2:B:1176:LEU:O	2:B:1180:TYR:HB2	2.04	0.57
2:B:954:ARG:HH12	2:B:959:LYS:HB2	1.67	0.56
2:B:999:ARG:HD2	2:B:1262:TYR:CE2	2.41	0.55
2:B:754:ASP:OD1	3:C:78:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:O	1:A:213:SER:HB3	2.07	0.55
1:A:429:GLN:O	1:A:430:GLU:HG2	2.07	0.55
2:B:1294:LEU:HB2	2:B:1311:ILE:HB	1.88	0.55
1:A:449:VAL:HB	1:A:545:GLU:HG3	1.89	0.54
2:B:1588:ILE:HG23	2:B:1591:ARG:NH1	2.22	0.54
2:B:810:SER:HB3	2:B:813:LYS:HB2	1.90	0.54
3:C:1186:LYS:HA	3:C:1187:GLN:HB2	1.90	0.54
2:B:1148:LEU:HD23	2:B:1195:ALA:HB1	1.88	0.54
2:B:1630:HIS:O	2:B:1645:GLN:NE2	2.40	0.54
3:C:67:ARG:HE	3:C:72:VAL:HG21	1.73	0.54
2:B:1186:SER:N	2:B:1222:ASP:OD2	2.41	0.54
1:A:44:LEU:HD13	1:A:55:VAL:HG11	1.90	0.53
2:B:1049:ILE:HG22	2:B:1093:ILE:HD13	1.90	0.53
1:A:67:LEU:HD21	3:C:257:ARG:HE	1.74	0.53
2:B:875:LEU:O	2:B:880:ARG:NH1	2.41	0.53
2:B:1202:LEU:HD23	2:B:1243:LEU:HD11	1.91	0.53
1:A:148:ARG:CZ	1:A:594:VAL:HB	2.39	0.53
1:A:47:HIS:ND1	1:A:489:TYR:OH	2.30	0.52
1:A:230:PRO:HD3	1:A:605:LEU:HD11	1.90	0.52
3:C:1181:LEU:HD13	3:C:1189:LEU:HD12	1.91	0.52
1:A:575:PRO:HB3	2:B:795:LEU:HD11	1.91	0.52
3:C:1186:LYS:HB3	3:C:1188:LYS:N	2.25	0.52
1:A:93:ASN:HB3	1:A:95:GLU:HG2	1.93	0.51
1:A:205:LYS:HG3	1:A:221:GLU:HG2	1.93	0.51
1:A:397:VAL:HG12	1:A:409:LEU:HD22	1.92	0.51
2:B:1543:TYR:HB2	2:B:1545:TYR:CZ	2.45	0.51
1:A:244:TYR:CE2	1:A:246:TYR:HB2	2.46	0.51
2:B:1588:ILE:HG23	2:B:1591:ARG:HH12	1.76	0.51
1:A:32:ASN:HB3	1:A:657:ARG:HH11	1.76	0.50
2:B:1084:LYS:HG2	2:B:1273:PHE:HE2	1.77	0.50
1:A:102:ARG:NH1	2:B:1033:GLN:HG2	2.27	0.50
2:B:766:GLU:HG3	3:C:87:HIS:CD2	2.47	0.49
1:A:55:VAL:HG13	1:A:112:PHE:CD2	2.47	0.49
1:A:98:SER:HB3	1:A:104:LYS:CE	2.41	0.49
3:C:40:GLN:HG3	3:C:41:THR:HG23	1.94	0.49
2:B:1297:SER:HB2	2:B:1306:LYS:HD2	1.94	0.49
2:B:1549:LEU:HD11	2:B:1552:VAL:CG2	2.44	0.48
2:B:954:ARG:NH1	2:B:959:LYS:HB2	2.28	0.48
2:B:957:VAL:HG12	2:B:1335:GLU:HB3	1.96	0.48
1:A:352:PRO:O	1:A:379:PRO:HD3	2.14	0.48
2:B:1376:ARG:N	2:B:1377:PRO:HD3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:756:ILE:HD12	2:B:922:SER:HB3	1.95	0.48
2:B:1604:MET:HA	2:B:1627:TRP:O	2.15	0.47
1:A:108:VAL:O	1:A:118:GLU:HA	2.13	0.47
2:B:920:PHE:CZ	3:C:57:ARG:HD3	2.49	0.47
2:B:1087:SER:O	2:B:1090:VAL:HG22	2.15	0.47
1:A:484:GLU:O	1:A:508:ARG:NH1	2.38	0.46
2:B:1392:TYR:CD1	2:B:1398:ALA:HB2	2.50	0.46
1:A:465:LEU:HD21	1:A:521:ILE:HG13	1.97	0.46
2:B:1303:ARG:NH1	2:B:1307:ILE:HD11	2.30	0.46
2:B:981:LEU:HB3	2:B:1319:LEU:HD11	1.97	0.46
3:C:162:MET:HG2	3:C:163:GLU:H	1.79	0.46
2:B:807:VAL:HG22	2:B:817:VAL:HG22	1.98	0.46
2:B:1426:ASP:HB3	2:B:1449:ASP:HB2	1.97	0.46
2:B:1214:ALA:HB2	2:B:1220:TRP:CE2	2.51	0.46
2:B:1525:ASP:OD1	2:B:1525:ASP:N	2.45	0.46
1:A:577:PRO:HD2	2:B:827:GLN:HG3	1.98	0.46
3:C:223:GLN:NE2	3:C:1126:SER:HA	2.30	0.46
3:C:1143:GLN:O	3:C:1164:LEU:N	2.40	0.46
2:B:1370:ALA:HB2	2:B:1385:ILE:HG13	1.97	0.45
2:B:1171:LYS:NZ	3:C:1117:ASN:OD1	2.36	0.45
2:B:1180:TYR:OH	2:B:1210:PHE:HB2	2.17	0.45
2:B:858:GLN:C	2:B:890:PRO:HG3	2.37	0.45
3:C:1186:LYS:CA	3:C:1187:GLN:HB2	2.46	0.45
3:C:85:CYS:HB3	3:C:134:TRP:NE1	2.31	0.45
2:B:1010:CYS:HA	2:B:1059:PHE:CZ	2.52	0.45
1:A:185:GLN:HB3	1:A:188:VAL:O	2.17	0.44
1:A:335:GLY:HA3	2:B:1445:ILE:HD11	1.99	0.44
3:C:145:LYS:HB3	3:C:167:GLU:HG2	1.98	0.44
2:B:1425:VAL:HG11	2:B:1427:ARG:NH1	2.32	0.44
2:B:766:GLU:C	2:B:768:PRO:HD3	2.38	0.44
1:A:291:ILE:HD13	1:A:300:VAL:HB	1.98	0.44
2:B:1635:ASP:OD1	2:B:1635:ASP:N	2.49	0.44
2:B:841:ARG:HE	2:B:905:THR:HG23	1.81	0.44
1:A:148:ARG:HG3	2:B:773:TRP:HZ2	1.80	0.44
1:A:271:VAL:HG21	1:A:300:VAL:HG11	2.00	0.44
2:B:1603:LEU:HB2	2:B:1631:TRP:CE3	2.53	0.44
3:C:1205:TYR:HB3	3:C:1228:CYS:HB3	1.99	0.44
3:C:257:ARG:HA	3:C:258:PRO:HA	1.91	0.44
2:B:1467:PHE:HD1	2:B:1468:ASN:H	1.67	0.43
1:A:29:ILE:HG22	1:A:644:LEU:HD22	1.99	0.43
2:B:1522:LYS:HG3	2:B:1523:SER:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1436:LYS:NZ	2:B:1441:ARG:HG3	2.33	0.43
1:A:32:ASN:HA	1:A:645:THR:HG23	2.00	0.43
2:B:1072:ARG:NH1	2:B:1125:ILE:HD11	2.34	0.43
1:A:628:THR:OG1	1:A:641:ASP:HB3	2.18	0.42
2:B:1494:HIS:HB3	2:B:1497:LYS:HB2	2.00	0.42
2:B:1132:GLY:HA3	2:B:1187:TYR:CZ	2.55	0.42
2:B:935:GLY:HA3	2:B:971:VAL:HG21	2.02	0.42
2:B:1023:ILE:HD13	2:B:1273:PHE:CE1	2.55	0.42
1:A:335:GLY:CA	2:B:1445:ILE:HD11	2.50	0.42
2:B:801:THR:HA	2:B:824:THR:HA	2.01	0.42
1:A:351:SER:HA	1:A:352:PRO:HD3	1.93	0.42
1:A:180:LEU:HD22	1:A:191:LEU:HD21	2.02	0.42
1:A:161:ARG:N	1:A:182:SER:OG	2.45	0.42
1:A:207:ARG:HD3	1:A:219:SER:OG	2.20	0.41
1:A:631:SER:OG	1:A:632:GLY:N	2.52	0.41
1:A:425:ARG:HG2	1:A:438:THR:HB	2.01	0.41
2:B:1392:TYR:CG	2:B:1398:ALA:HB2	2.55	0.41
1:A:160:GLY:HA2	1:A:182:SER:HG	1.85	0.41
2:B:1238:LEU:HA	2:B:1238:LEU:HD23	1.83	0.41
1:A:160:GLY:HA2	1:A:182:SER:OG	2.21	0.41
2:B:971:VAL:O	2:B:974:THR:OG1	2.30	0.41
2:B:1318:LEU:HD23	2:B:1320:ARG:NH1	2.35	0.41
1:A:69:LEU:HD11	1:A:96:PHE:CZ	2.56	0.41
1:A:580:GLN:OE1	2:B:792:ASN:ND2	2.54	0.41
1:A:26:TYR:CB	1:A:112:PHE:CD1	2.97	0.41
2:B:1366:THR:HG21	2:B:1368:LYS:HE3	2.03	0.41
2:B:1009:GLY:HA3	2:B:1013:GLN:HB3	2.03	0.40
2:B:1549:LEU:HD12	2:B:1598:GLU:CA	2.49	0.40
1:A:583:LEU:HD12	1:A:583:LEU:HA	1.85	0.40
3:C:204:LYS:HB3	3:C:204:LYS:HE3	1.80	0.40
3:C:1185:ALA:O	3:C:1186:LYS:HB2	2.20	0.40
3:C:127:ARG:HG2	3:C:135:THR:O	2.22	0.40
1:A:372:LEU:HD21	1:A:422:ILE:HG21	2.03	0.40
2:B:1527:VAL:HA	2:B:1531:GLU:OE1	2.22	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	640/645 (99%)	613 (96%)	25 (4%)	2 (0%)	44	81
2	B	910/915 (100%)	861 (95%)	39 (4%)	10 (1%)	17	59
3	C	363/383 (95%)	332 (92%)	25 (7%)	6 (2%)	11	51
All	All	1913/1943 (98%)	1806 (94%)	89 (5%)	18 (1%)	20	63

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1136	ASN
2	B	1377	PRO
2	B	1382	ASN
2	B	1135	ASN
2	B	1496	GLU
2	B	1500	GLY
1	A	100	LYS
2	B	1372	GLU
1	A	98	SER
2	B	1115	ASP
2	B	1373	THR
3	C	163	GLU
3	C	245	GLU
3	C	1184	THR
3	C	1230	LYS
3	C	1188	LYS
3	C	69	GLY
2	B	1287	PRO

### 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	566/567 (100%)	562 (99%)	4 (1%)	87	93
2	B	807/810 (100%)	802 (99%)	5 (1%)	89	94
3	C	313/328 (95%)	310 (99%)	3 (1%)	80	90
All	All	1686/1705 (99%)	1674 (99%)	12 (1%)	87	93

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	PHE
1	A	190	PRO
1	A	343	ARG
1	A	499	ARG
2	B	754	ASP
2	B	879	LYS
2	B	882	HIS
2	B	986	PRO
2	B	1467	PHE
3	C	37	TRP
3	C	57	ARG
3	C	1143	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	223	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

2 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	$\# Z  > 2$
4	NAG	B	1701	2,4	14,14,15	0.96	1 (7%)	15,19,21	0.67	0
4	NAG	B	1702	4	14,14,15	0.95	2 (14%)	15,19,21	1.02	1 (6%)

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	NAG	B	1701	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1702	4	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1702	NAG	O5-C1	2.18	1.47	1.43
4	B	1702	NAG	C1-C2	2.61	1.56	1.52
4	B	1701	NAG	C1-C2	3.32	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1702	NAG	C1-O5-C5	3.48	116.96	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	642/645 (99%)	-0.14	0 <a href="#">100</a> <a href="#">100</a>	105, 143, 171, 206	0
2	B	912/915 (99%)	-0.21	0 <a href="#">100</a> <a href="#">100</a>	79, 129, 188, 252	0
3	C	367/383 (95%)	-0.12	1 (0%) <a href="#">93</a> <a href="#">91</a>	107, 168, 210, 247	0
All	All	1921/1943 (98%)	-0.17	1 (0%) <a href="#">95</a> <a href="#">94</a>	79, 141, 198, 252	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1187	GLN	2.1

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	B	1702	14/15	0.81	0.27	-	178,195,200,202	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	1701	14/15	0.88	0.20	-	169,192,199,207	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.