W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 28, 2023 – 06:47 AM EDT

PDB ID : 3L3O

Title : Staphylococcal Complement Inhibitor (SCIN) in complex with Human Complement Component C3c

Authors : Geisbrecht, B.V.; Garcia, B.G.

Deposited on : 2009-12-17

Resolution : 3.40 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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)	:	2.35

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 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.
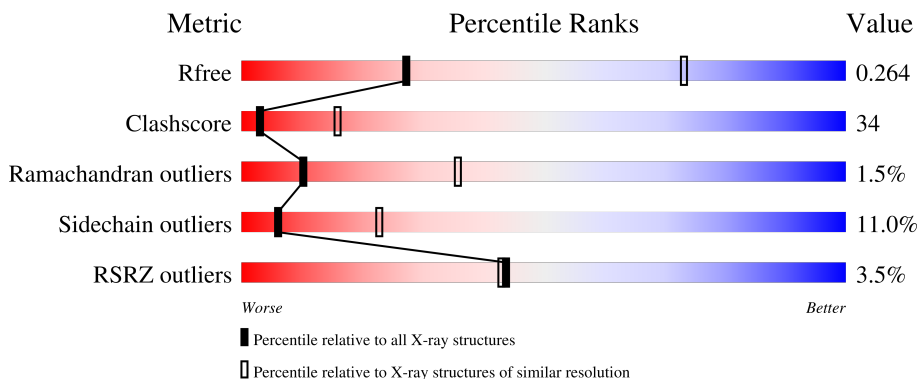
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	645	3% — 47% 48% ··
1	D	645	3% — 49% 46% ··
2	B	206	36% 43% 10% 11%
2	E	206	38% 41% 10% 11%
3	M	88	2% — 50% 35% 10% 5%

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Mol	Chain	Length	Quality of chain
3	P	88	2% ▮ 48% 36% 11% 5%
4	C	343	6% ▮ 39% 38% 9% 14%
4	F	343	6% ▮ 39% 38% 9% 14%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 19090 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	639	Total	C	N	O	S	0	0	0
			4979	3169	844	951	15			
1	D	639	Total	C	N	O	S	0	0	0
			4979	3169	844	951	15			

- Molecule 2 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	184	Total	C	N	O	S	0	0	0
			1488	956	250	277	5			
2	E	184	Total	C	N	O	S	0	0	0
			1488	956	250	277	5			

- Molecule 3 is a protein called Staphylococcal complement inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
3	P	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	GLY	-	expression tag	UNP Q931M7
M	-1	THR	-	expression tag	UNP Q931M7
M	0	SER	-	expression tag	UNP Q931M7
P	-2	GLY	-	expression tag	UNP Q931M7
P	-1	THR	-	expression tag	UNP Q931M7
P	0	SER	-	expression tag	UNP Q931M7

- Molecule 4 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	294	Total	C	N	O	S	0	0	0
			2382	1500	391	471	20			
4	C	294	Total	C	N	O	S	0	0	0
			2382	1500	391	471	20			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
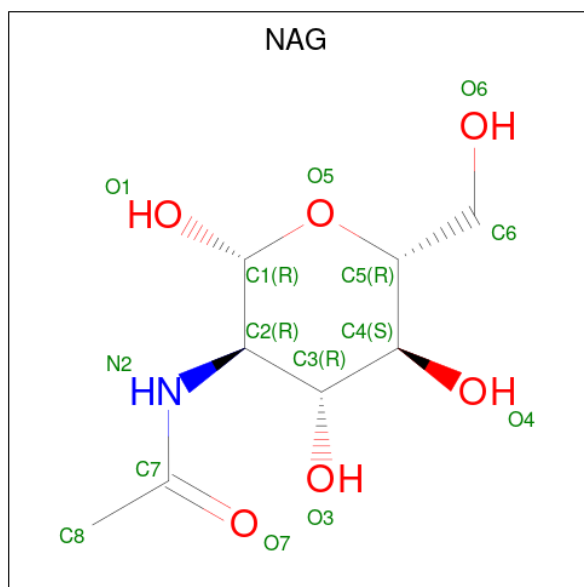
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots ⓘ

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: Complement C3

• Molecule 1: Complement C3

• Molecule 2: Complement C3

Chain B:

• Molecule 2: Complement C3

Chain E:

C794 V795 A796 V803 M804 Q805 D806 F807 F808 I809 D810 L811 R812 L813 V817 V818 R819 N820 I825 Y830 N831 Y832 R833 Q834 N835 Q836 E837 L838 K839 V840 R841 V842 E843 L844 L845 C851 S852 L853 A854 Q861 Q862 T863 V864 P868 K869 S870 S871 L872 S873 V877 I878 V879

K882 T883 E887 V888 E889 V890 K891 A892 A893 V894 Y895 H896 H897 F898 I899 G902 V903 L907 K908 V909 V910 E911 E912 GLY ILE ARG MET ASN LYS THR VAL ALA VAL ARG THR LEU ASP PRO GLU ARG LEU GLY ARG
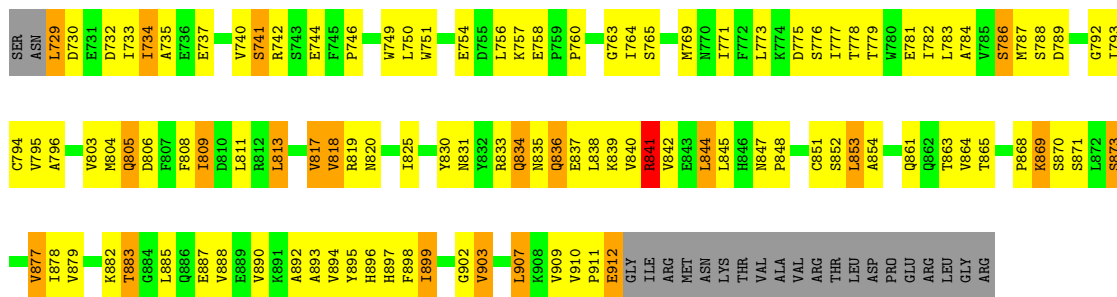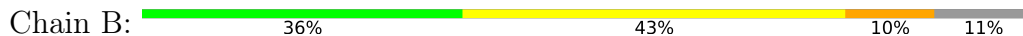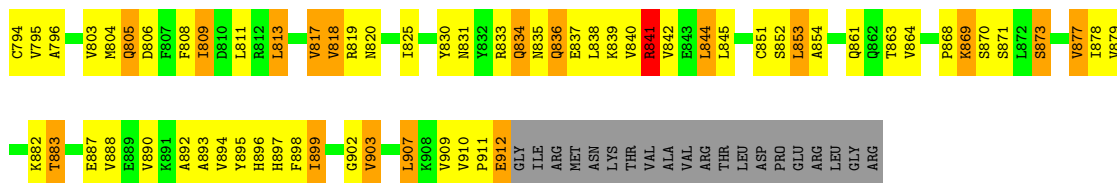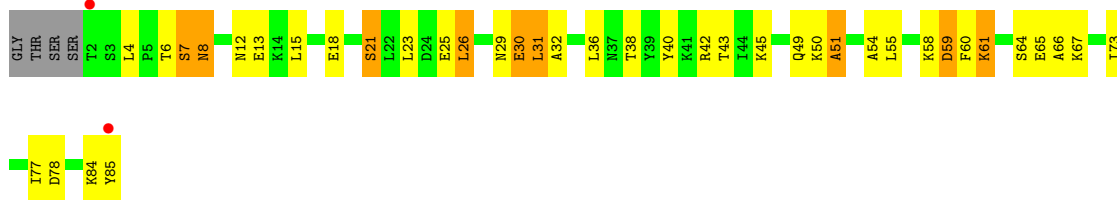
• Molecule 3: Staphylococcal complement inhibitor

Chain M:

2%
50% 35% 10% 5%

GLY THR SER SER T2 S3 L4 P5 T6 S7 N8 N12 E13 K14 L15 E18 S21 L22 L23 D24 E25 L26 N29 E30 L31 A32 L36 N37 T38 Y39 Y40 K41 R42 T43 I44 K45 Q49 K50 A51 A54 L55 K58 D59 F60 K61 S64 E65 A66 K67 I73

I77 D78 K84 Y85

• Molecule 3: Staphylococcal complement inhibitor

Chain P:

2%
48% 36% 11% 5%

GLY THR SER SER T2 S3 L4 P5 T6 S7 N8 Q11 N12 E13 K14 L15 E18 S21 L22 L23 D24 E25 L26 N29 E30 L31 A32 L36 N37 T38 Y39 Y40 K41 R42 T43 I44 K45 Q49 K50 A51 A54 L55 K58 D59 F60 K61 S64 E65 A66 K67

I73 I77 D78 K82 S83 K84 Y85

• Molecule 4: Complement C3

Chain F:

6%
39% 38% 9% 14%

SER GLU GLU THR LYS GLU ASN GLU GLY PHE THR VAL THR ALA GLU GLY LYS GLY GLN GLY THR LEU SER VAL VAL THR MET TYR HIS ALA LYS ALA ASP GLN LEU THR C1336 N1337 K1338 F1339 D1340 L1341 K1342 V1343 T1344 I1345 K1346 P1347 A1348 P1349 E1350 THR GLU LYS ARG PRO GLN ASP A1358

K1359 N1360 T1361 M1362 E1365 R1369 Y1370 R1371 A1376 T1377 M1378 S1379 I1380 L1381 M1385 M1386 T1387 G1388 F1389 A1390 P1391 D1392 D1393 D1394 D1395 K1396 K1397 Q1398 V1403 D1404 R1405 Y1406 I1407 S1408 K1409 Y1410 E1411 L1412 D1413 K1414 A1415 F1416 S1417 D1418 R1419 N1420 T1421 L1422 I1423 L1426 D1427 K1428 V1429 S1430

H1431 S1432 E1433 L1437 A1438 V1441 H1442 Q1443 Y1444 F1445 N1446 V1447 I1450 Q1451 P1452 Y1458 A1459 Y1460 Y1461 T1468 R1469 H1472 P1473 E1474 K1475 K1479 C1484 E1487 E1493 I1498 GLN LYS SER ASP ASP K1504 V1505 T1506 L1507 E1508 E1509 R1510 L1511 D1512 K1513 A1514 C1515 E1516 P1517

G1518 V1519 D1520 Y1521 V1522 Y1523 K1524 T1525 R1526 L1527 V1528 K1529 V1530 Q1531 L1532 S1533 N1534 D1535 F1536 E1538 Y1539 I1540 M1541 A1542 I1543 E1544 Q1545 T1546 I1547 G1550 S1551 D1552 Q1559 R1560 T1561 F1562 I1563 S1564 R1569 L1572 K1573 L1574 E1575 E1576 K1577 K1578 H1579 Y1580 L1581 M1582 W1583 G1584 L1585 S1586

F1589 W1590 K1593 L1596 S1597 Y1598 I1599 I1600 G1601 K1602 D1603 T1604 W1605 V1606 E1607 H1608 W1609 P1610 Q1623 T1631 E1632 S1633 M1634 V1635 V1636 N1641

• Molecule 4: Complement C3

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.11Å 217.03Å 115.65Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	34.52 – 3.40 49.97 – 3.40	Depositor EDS
% Data completeness (in resolution range)	91.0 (34.52-3.40) 91.0 (49.97-3.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.223 , 0.271 0.215 , 0.264	Depositor DCC
R_{free} test set	1988 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å^2)	57.2	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 45.1	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.429 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	19090	wwPDB-VP
Average B, all atoms (Å^2)	108.0	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.*

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[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 (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	0.41	0/5079	0.62	1/6902 (0.0%)
1	D	0.41	0/5079	0.62	2/6902 (0.0%)
2	B	0.51	0/1520	0.70	1/2066 (0.0%)
2	E	0.51	0/1520	0.70	1/2066 (0.0%)
3	M	0.39	0/690	0.59	0/923
3	P	0.39	0/690	0.59	0/923
4	C	0.36	0/2427	0.57	0/3271
4	F	0.36	0/2427	0.57	0/3271
All	All	0.42	0/19432	0.62	5/26324 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	535	ASP	CB-CA-C	-5.99	98.42	110.40
1	D	535	ASP	CB-CA-C	-5.98	98.44	110.40
1	D	291	ASN	C-N-CD	-5.26	109.02	120.60
2	E	841	ARG	NE-CZ-NH1	5.09	122.85	120.30
2	B	841	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	4979	0	5041	333	0
1	D	4979	0	5041	326	0
2	B	1488	0	1512	122	0
2	E	1488	0	1512	120	0
3	M	682	0	697	51	0
3	P	682	0	697	50	0
4	C	2382	0	2288	197	0
4	F	2382	0	2288	198	0
5	A	14	0	13	4	0
5	D	14	0	13	4	0
All	All	19090	0	19102	1298	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 34.

The worst 5 of 1298 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)
4:C:1569:ARG:HG3	4:C:1569:ARG:HH11	0.99	1.15
4:C:1505:VAL:HG11	4:C:1510:ARG:HH21	1.06	1.14
4:F:1349:PRO:O	4:F:1350:GLU:HB2	1.47	1.12
4:F:1569:ARG:HG3	4:F:1569:ARG:HH11	0.99	1.11
4:C:1349:PRO:O	4:C:1350:GLU:HB2	1.47	1.10

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	635/645 (98%)	554 (87%)	71 (11%)	10 (2%)	9	34
1	D	635/645 (98%)	554 (87%)	71 (11%)	10 (2%)	9	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	182/206 (88%)	162 (89%)	18 (10%)	2 (1%)	14	44
2	E	182/206 (88%)	162 (89%)	18 (10%)	2 (1%)	14	44
3	M	82/88 (93%)	60 (73%)	19 (23%)	3 (4%)	3	20
3	P	82/88 (93%)	60 (73%)	19 (23%)	3 (4%)	3	20
4	C	288/343 (84%)	245 (85%)	40 (14%)	3 (1%)	15	46
4	F	288/343 (84%)	245 (85%)	40 (14%)	3 (1%)	15	46
All	All	2374/2564 (93%)	2042 (86%)	296 (12%)	36 (2%)	10	36

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	PRO
1	D	292	PRO
1	A	289	VAL
1	A	293	ARG
1	A	537	CYS

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	563/567 (99%)	530 (94%)	33 (6%)	19	49
1	D	563/567 (99%)	530 (94%)	33 (6%)	19	49
2	B	172/191 (90%)	142 (83%)	30 (17%)	2	7
2	E	172/191 (90%)	142 (83%)	30 (17%)	2	7
3	M	76/79 (96%)	67 (88%)	9 (12%)	5	19
3	P	76/79 (96%)	66 (87%)	10 (13%)	4	15
4	C	266/309 (86%)	220 (83%)	46 (17%)	2	7
4	F	266/309 (86%)	220 (83%)	46 (17%)	2	7
All	All	2154/2292 (94%)	1917 (89%)	237 (11%)	6	23

5 of 237 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	1535	ASP
2	E	836	GLN
1	D	251	PHE
2	E	818	VAL
2	E	912	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
4	F	1579	HIS
1	D	132	HIS
4	C	1579	HIS
1	D	392	HIS
3	P	8	ASN

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 ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

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
5	NAG	A	646	-	14,14,15	0.44	0	17,19,21	1.45	1 (5%)
5	NAG	D	646	-	14,14,15	0.44	0	17,19,21	1.45	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	646	-	-	4/6/23/26	0/1/1/1
5	NAG	D	646	-	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	646	NAG	C1-O5-C5	4.86	118.78	112.19
5	A	646	NAG	C1-O5-C5	4.85	118.76	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	646	NAG	O5-C5-C6-O6
5	A	646	NAG	O5-C5-C6-O6
5	A	646	NAG	C8-C7-N2-C2
5	A	646	NAG	O7-C7-N2-C2
5	D	646	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	646	NAG	4	0
5	D	646	NAG	4	0

5.7 Other polymers ⓘ

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	639/645 (99%)	0.09	21 (3%)	46	45	20, 103, 160, 191	0
1	D	639/645 (99%)	0.06	17 (2%)	54	53	20, 103, 160, 191	0
2	B	184/206 (89%)	-0.17	0	100	100	52, 77, 109, 129	0
2	E	184/206 (89%)	-0.22	0	100	100	52, 77, 109, 129	0
3	M	84/88 (95%)	-0.08	2 (2%)	59	57	68, 87, 139, 187	0
3	P	84/88 (95%)	-0.15	2 (2%)	59	57	68, 87, 139, 187	0
4	C	294/343 (85%)	0.31	21 (7%)	16	18	20, 134, 208, 240	0
4	F	294/343 (85%)	0.32	22 (7%)	14	16	20, 134, 208, 240	0
All	All	2402/2564 (93%)	0.08	85 (3%)	44	43	20, 97, 182, 240	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	421	ALA	5.2
4	C	1607	GLU	4.5
4	F	1607	GLU	4.4
3	M	85	TYR	4.3
1	A	347	PRO	4.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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. 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	B-factors(Å^2)	Q<0.9
5	NAG	D	646	14/15	0.82	0.20	90,126,144,147	0
5	NAG	A	646	14/15	0.84	0.22	90,126,144,147	0

6.5 Other polymers (i)

There are no such residues in this entry.