



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 08:34 PM UTC

PDB ID : 3L3O / pdb_00003l3o
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)

This is a wwPDB X-ray Structure Validation Summary 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

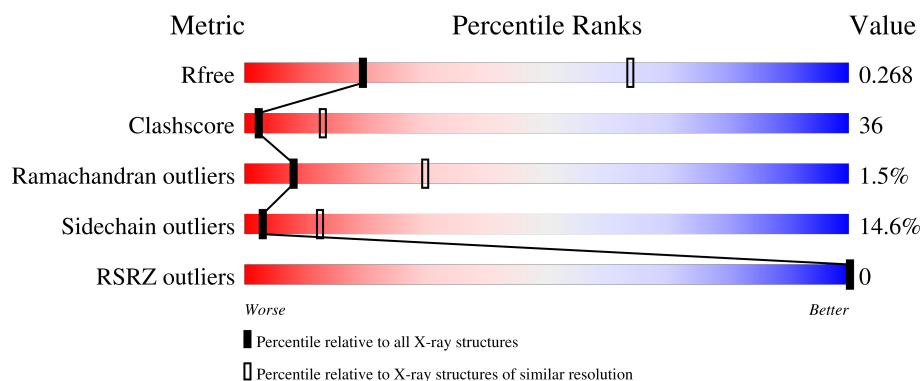
1 Overall quality at a glance

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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 $\leq 5\%$. 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	
1	D	645	
2	B	206	
2	E	206	
3	M	88	

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Mol	Chain	Length	Quality of chain
3	P	88	 39% 45% 11% 5%
4	C	343	 37% 38% 10% 14%
4	F	343	 38% 38% 10% 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			

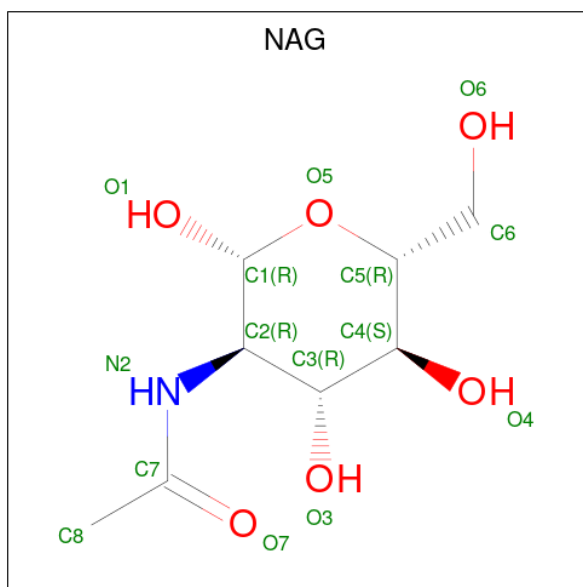
There are 6 discrepancies between the modelled and reference sequences:

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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

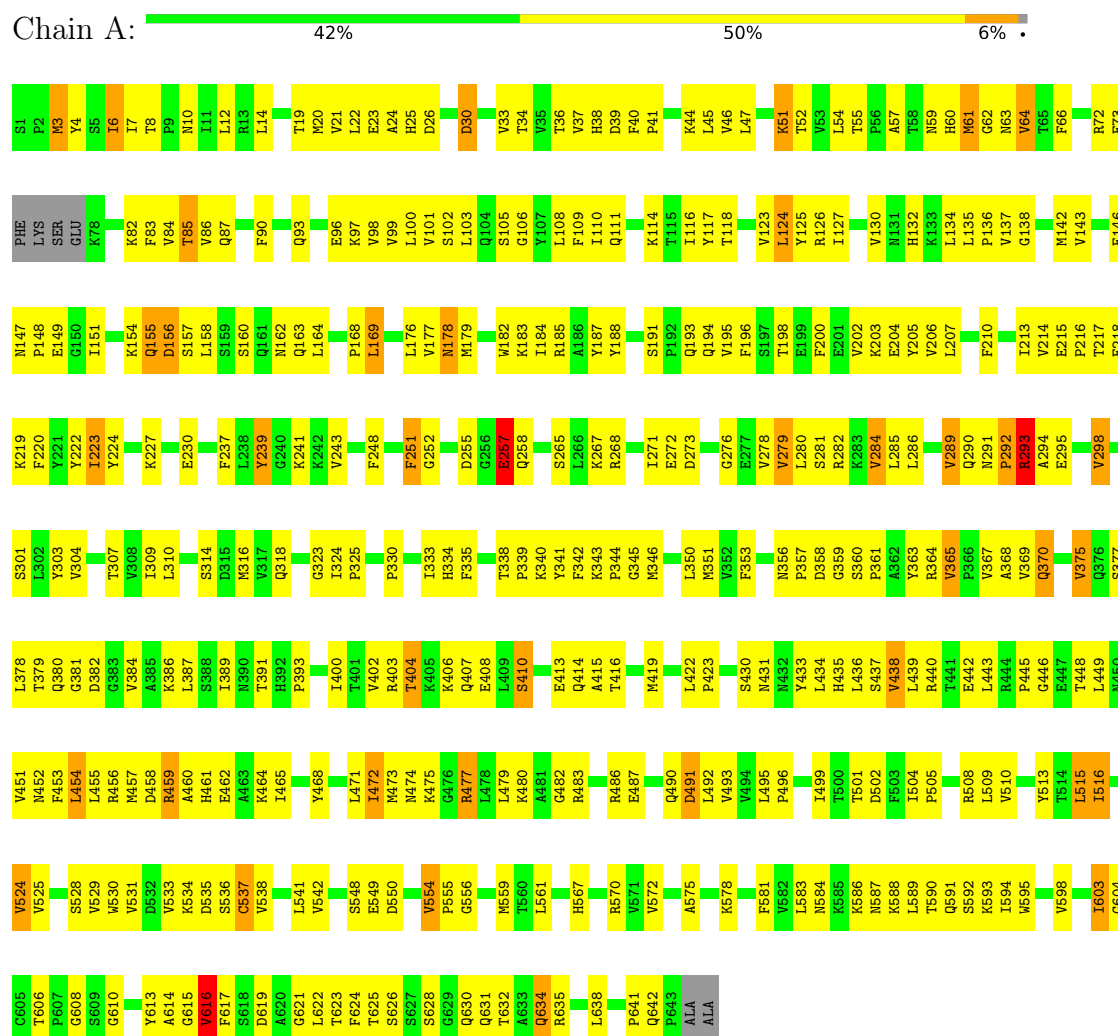


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

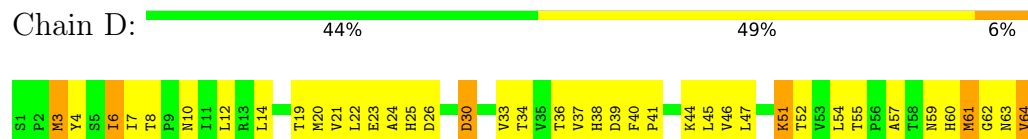
3 Residue-property plots

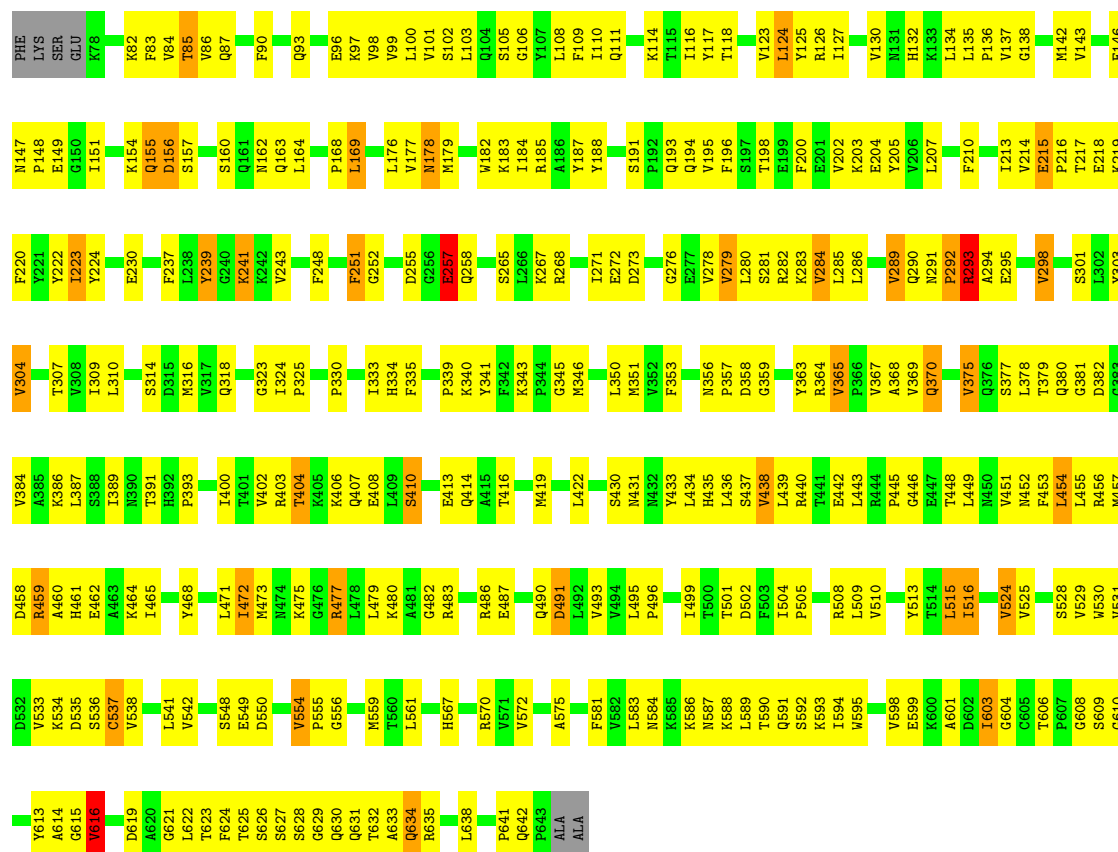
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



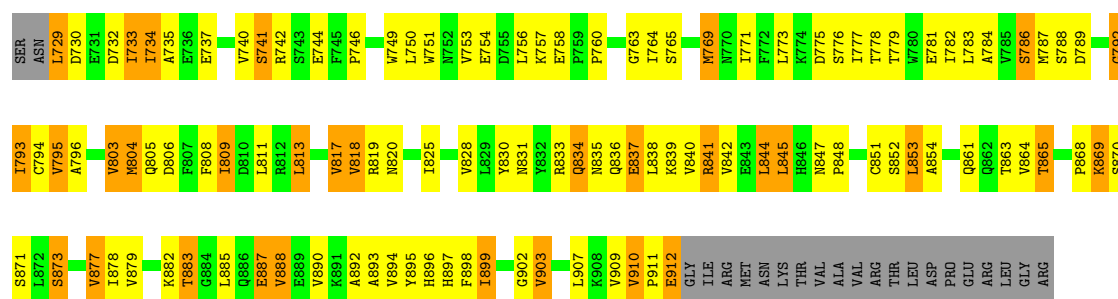
• Molecule 1: Complement C3





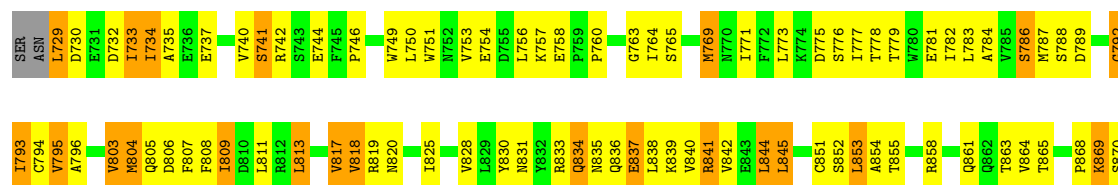
• Molecule 2: Complement C3

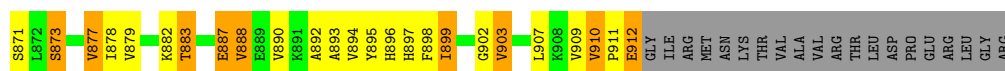
Chain B: 35% 39% 16% 11%



• Molecule 2: Complement C3

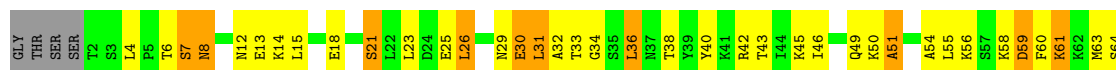
Chain E: 35% 39% 15% 11%





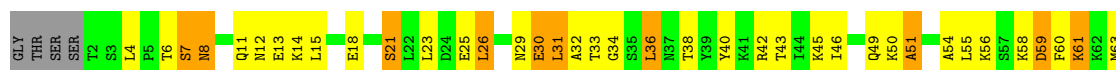
• Molecule 3: Staphylococcal complement inhibitor

Chain M: 40% 44% 11% 5%



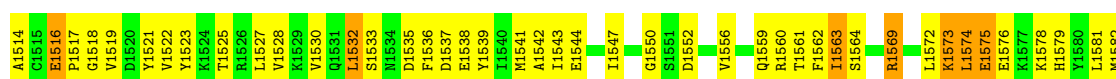
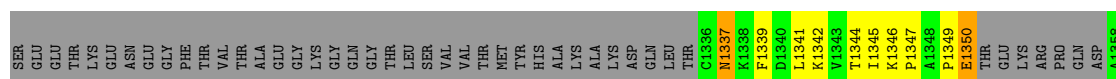
• Molecule 3: Staphylococcal complement inhibitor

Chain P: 39% 45% 11% 5%



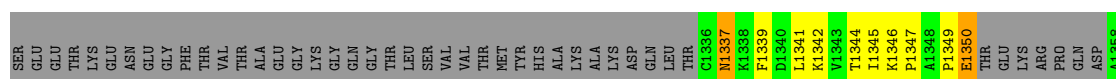
• Molecule 4: Complement C3

Chain F: 38% 38% 10% 14%



• Molecule 4: Complement C3

Chain C: 37% 38% 10% 14%



L1581	M1582	W1583	G1584	L1585	S1586		F1589	W1590		K1593		L1596	S1597	Y1598	I1599	T1600	G1601	K1602	D1603	T1604	W1605	V1606	E1607	H1608	V1609	P1610		Q1623		T1631	E1632	V1635	V1636		H1641																								
A1514	G1515	E1516	P1517	G1518	V1519	D1520	Y1521	V1522	Y1523	K1524	T1525	R1526	L1527	V1528	K1529	V1530	V1531	L1532	S1533	N1534	D1535	F1536	D1537	E1538	Y1539	T1540	M1541	A1542	I1543	E1544		T1547		G1550	S1551	D1552	E1553	V1554	Q1555	V1556		Q1559	R1560	T1561	F1562	I1563	S1564		R1569		L1572	K1573	L1574	E1575	E1576	K1577	K1578	H1579	Y1580
S1430	H1431	S1432	E1433		L1437	A1438		V1441	H1442	Q1443	Y1444	F1445	N1446	V1447		I1450	Q1451	P1452		Y1468	A1469	Y1461		E1465		T1468	R1469		H1472	P1473	E1474	K1475		G1478	K1479		C1484		E1487		E1493		I1498	GLN	LYS	SER	ASP	ASP	K1504	V1505	T1506	L1507	E1508	E1509	R1510	L1511	D1512	K1513	
K1359	N1360	T1361	M1362		E1365		R1369	Y1370	R1371		D1375	A1376	T1377	R1378	S1379	L1380	L1381		M1385	M1386	T1387	G1388	F1389	A1390	F1391	D1392	T1393	D1394	D1395	L1396	K1397	Q1398		V1403	D1404	R1405	Y1406	T1407	S1408	K1409	Y1410	E1411	L1412	D1413	K1414	A1415	F1416	S1417	D1418	R1419	R1420	T1421	L1422	I1423		L1426	D1427	K1428	V1429

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 34.52 – 3.40	Depositor EDS
% Data completeness (in resolution range)	91.0 (34.52-3.40) 91.1 (34.52-3.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.223 , 0.271 0.216 , 0.268	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)	0.26 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.429 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.52	0/5079	0.95	10/6902 (0.1%)
1	D	0.53	0/5079	0.95	10/6902 (0.1%)
2	B	0.63	0/1520	0.97	5/2066 (0.2%)
2	E	0.63	0/1520	0.97	5/2066 (0.2%)
3	M	0.51	0/690	0.85	1/923 (0.1%)
3	P	0.51	0/690	0.84	1/923 (0.1%)
4	C	0.45	0/2427	0.87	3/3271 (0.1%)
4	F	0.45	0/2427	0.87	3/3271 (0.1%)
All	All	0.52	0/19432	0.93	38/26324 (0.1%)

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	535	ASP	CB-CA-C	-7.24	98.42	110.29
1	D	535	ASP	CB-CA-C	-7.23	98.44	110.29
4	F	1606	VAL	N-CA-C	6.95	118.12	108.12
4	C	1606	VAL	N-CA-C	6.95	118.12	108.12
1	D	151	ILE	N-CA-C	6.65	114.14	107.55

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	349	0
1	D	4979	0	5041	345	0
2	B	1488	0	1512	123	0
2	E	1488	0	1512	124	0
3	M	682	0	697	57	0
3	P	682	0	697	56	0
4	C	2382	0	2288	204	0
4	F	2382	0	2288	205	0
5	A	14	0	13	4	0
5	D	14	0	13	4	0
All	All	19090	0	19102	1360	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 36.

The worst 5 of 1360 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
2:E:912:GLU:H	2:E:912:GLU:CD	1.52	1.12
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

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	635/645 (98%)	554 (87%)	71 (11%)	10 (2%)	7	29
1	D	635/645 (98%)	554 (87%)	71 (11%)	10 (2%)	7	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	182/206 (88%)	162 (89%)	18 (10%)	2 (1%)	11	38
2	E	182/206 (88%)	162 (89%)	18 (10%)	2 (1%)	11	38
3	M	82/88 (93%)	60 (73%)	19 (23%)	3 (4%)	2	16
3	P	82/88 (93%)	60 (73%)	19 (23%)	3 (4%)	2	16
4	C	288/343 (84%)	245 (85%)	40 (14%)	3 (1%)	12	40
4	F	288/343 (84%)	245 (85%)	40 (14%)	3 (1%)	12	40
All	All	2374/2564 (93%)	2042 (86%)	296 (12%)	36 (2%)	8	30

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%)	503 (89%)	60 (11%)	6	23
1	D	563/567 (99%)	502 (89%)	61 (11%)	6	22
2	B	172/191 (90%)	135 (78%)	37 (22%)	1	3
2	E	172/191 (90%)	135 (78%)	37 (22%)	1	3
3	M	76/79 (96%)	65 (86%)	11 (14%)	3	13
3	P	76/79 (96%)	65 (86%)	11 (14%)	3	13
4	C	266/309 (86%)	217 (82%)	49 (18%)	1	7
4	F	266/309 (86%)	217 (82%)	49 (18%)	1	7
All	All	2154/2292 (94%)	1839 (85%)	315 (15%)	3	12

5 of 315 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	1344	THR
2	E	776	SER
4	C	1393	THR
4	C	1504	LYS
2	E	861	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	155	GLN
4	C	1531	GLN
1	D	392	HIS
3	P	8	ASN
1	D	144	ASN

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 oligosaccharides 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
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(°)	Ideal(°)
5	D	646	NAG	C1-O5-C5	4.92	118.78	112.19
5	A	646	NAG	C1-O5-C5	4.91	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 [i](#)

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, 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%)	-1.58	0 100 100	20, 103, 160, 191	0
1	D	639/645 (99%)	-1.57	0 100 100	20, 103, 160, 191	0
2	B	184/206 (89%)	-1.61	0 100 100	52, 77, 109, 129	0
2	E	184/206 (89%)	-1.63	0 100 100	52, 77, 109, 129	0
3	M	84/88 (95%)	-1.63	0 100 100	68, 87, 139, 187	0
3	P	84/88 (95%)	-1.62	0 100 100	68, 87, 139, 187	0
4	C	294/343 (85%)	-1.43	0 100 100	20, 134, 208, 240	0
4	F	294/343 (85%)	-1.42	0 100 100	20, 134, 208, 240	0
All	All	2402/2564 (93%)	-1.55	0 100 100	20, 97, 182, 240	0

There are no RSRZ outliers to report.

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 oligosaccharides 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. 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($\text{\AA}^2$)	Q<0.9
5	NAG	A	646	14/15	0.98	0.04	90,126,144,147	0
5	NAG	D	646	14/15	0.98	0.03	90,126,144,147	0

6.5 Other polymers [i](#)

There are no such residues in this entry.