



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:24 am GMT

PDB ID : 2A73
Title : Human Complement Component C3
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Deposited on : 2005-07-04
Resolution : 3.30 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

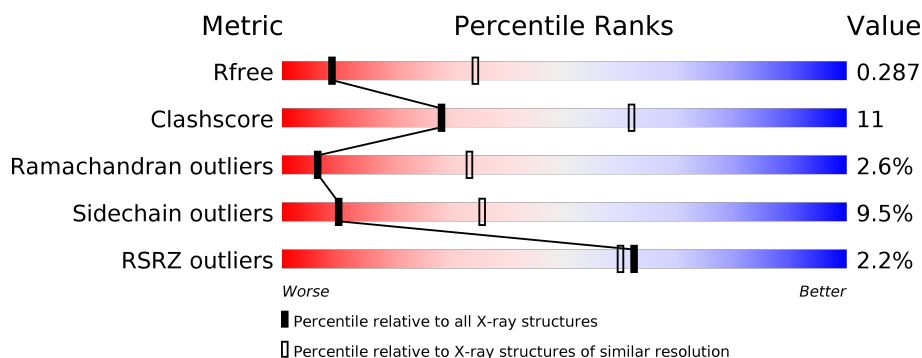
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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	643	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>••</div> </div> </div>
2	B	991	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>29%</div> <div>7%</div> <div>••</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	B	3	X	-	-	-
3	MAN	B	5	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12860 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	635	Total	C	N	O	S	0	0	0
			4950	3153	837	945	15			

- Molecule 2 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	976	Total	C	N	O	S	0	0	0
			7821	4943	1331	1501	46			

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

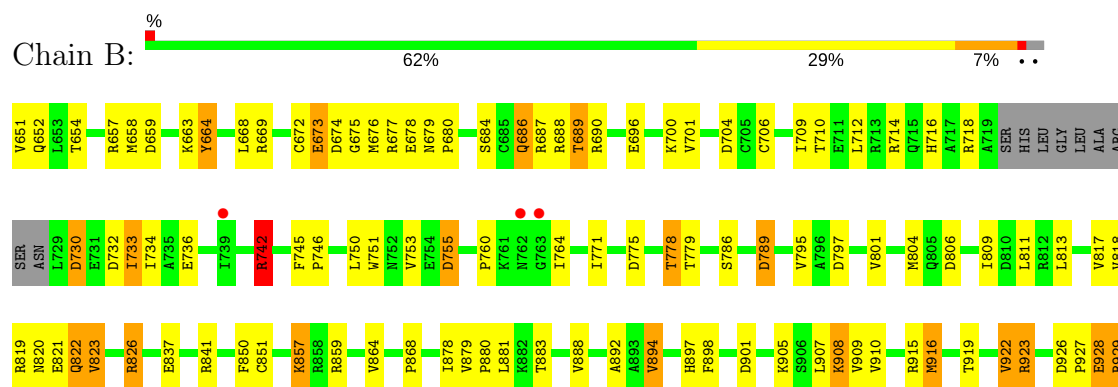
3 Residue-property plots [i](#)

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



L930	D1007	A1120	Q1255	E1350	A1438	L1532
Q931	E1008	L1121	A1256	T1351	F1439	E1544
R932	K1014	V1125	K1262	R1354	K1440	D1552
E933	L1126	L1126	D1263	P1355	Y1444	Q1555
G934	E1018	Q1130	D1266	Q1356	E1448	Q1558
K937	L1024	A1131	H1267	D1357	L1449	I1566
E938	K1029	A1132	Q1268	T1361	I1450	C1568
D939	K1029	K1133	E1269	R1371	Q1451	K1577
I940	Q1033	D1134	L1270	R1372	V1457	W1583
D944	P1040	E1137	D1273	D1373	Y1460	D1588
D947	S1041	L1143	L1276	Q1374	Y1461	G1591
Q948	S1042	P1144	L1277	D1375	W1462	E1592
V949	A1043	I1147	Q1278	A1376	L1463	K1593
P950	F1044	D1152	K1284	T1377	E1464	P1594
D951	P1052	N1157	I1285	M1378	R1469	H1595
T952	T1057	I1169	W1291	S1379	P1473	L1596
E953	S1065	L1180	E1292	I1380	E1474	I1599
S954	D1074	R1197	W1291	L1381	K1475	G1602
E955	Q1076	D1200	S1293	D1382	K1476	D1603
T956	C1079	Q1204	A1294	M1385	E1477	T1604
Q961	K1083	Y1206	S1295	M1386	D1477	W1605
G962	K1091	V1208	R1298	T1387	Q1478	D1613
P963	P1092	L1215	T1302	A1390	K1479	D1617
V965	D1093	L1221	T1302	P1391	L1480	E1618
A966	V1095	D1225	V1310	T1393	N1481	E1619
E970	F1096	F1226	G1314	D1394	K1482	D1626
D971	A1100	P1227	K1315	D1395	L1483	E1632
D974	I1103	P1228	G1315	D1404	C1484	S1633
H980	H1104	P1229	L1320	S1408	R1485	M1634
L981	Q1105	Q1237	S1321	K1409	C1489	N1641
I982	E1106	R1238	V1322	Y1410	C1496	
V983	ILE	Y1239	V1323	E1411	F1497	
T984	GLY		T1324	L1412	I1498	
P985	LEU		M1325	D1413	Q1499	
C988	ARG		Y1326	K1414	K1500	
G989	N1113		H1327	A1415	S1501	
E990	N1114		A1330	F1416	D1502	
Q991	N1115		D1332	S1417	D1503	
I994	E1116		C1336	D1418	E1509	
G995	K1117		M1337	R1419	D1512	
M996	M1118		K1338	N1420	E1516	
T997	L1119		F1339	I1423	P1517	
P998			D1340	I1424	G1518	
T999			L1341	D1427	V1519	
V1000			I1345	K1428	D1520	
N1001			P1347	E1433	K1524	
A1002				D1434	L1527	
Y1005				D1435		
L1006						

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	116.98Å 156.26Å 271.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 39.12 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-3.30) 99.8 (39.12-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.230 , 0.289 0.228 , 0.287	Depositor DCC
R_{free} test set	1882 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	83.5	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 73.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12860	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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

5.1 Standard geometry

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

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	0.21	0/5048	0.56	27/6859 (0.4%)
2	B	0.21	0/7973	0.59	54/10779 (0.5%)
All	All	0.21	0/13021	0.58	81/17638 (0.5%)

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
3	B	2	0

There are no bond length outliers.

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	602	ASP	CB-CG-OD2	5.59	123.33	118.30
2	B	674	ASP	CB-CG-OD2	5.58	123.32	118.30
2	B	730	ASP	CB-CG-OD2	5.51	123.26	118.30
2	B	1512	ASP	CB-CG-OD2	5.51	123.26	118.30
2	B	1413	ASP	CB-CG-OD2	5.49	123.25	118.30
1	A	39	ASP	CB-CG-OD2	5.48	123.23	118.30
2	B	1382	ASP	CB-CG-OD2	5.46	123.22	118.30
2	B	1418	ASP	CB-CG-OD2	5.45	123.21	118.30
2	B	1394	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	535	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	255	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	550	ASP	CB-CG-OD2	5.37	123.14	118.30
2	B	1427	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	349	ASP	CB-CG-OD2	5.33	123.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1332	ASP	CB-CG-OD2	5.32	123.09	118.30
2	B	1273	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	382	ASP	CB-CG-OD2	5.29	123.07	118.30
2	B	1434	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	577	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	491	ASP	CB-CG-OD2	5.28	123.05	118.30
2	B	1392	ASP	CB-CG-OD2	5.26	123.03	118.30
2	B	901	ASP	CB-CG-OD2	5.25	123.03	118.30
2	B	1486	ASP	CB-CG-OD2	5.25	123.03	118.30
2	B	1099	ASP	CB-CG-OD2	5.25	123.03	118.30
2	B	789	ASP	CB-CG-OD2	5.25	123.02	118.30
2	B	806	ASP	CB-CG-OD2	5.24	123.02	118.30
2	B	1395	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	315	ASP	CB-CG-OD2	5.22	123.00	118.30
2	B	1617	ASP	CB-CG-OD2	5.21	122.99	118.30
2	B	1503	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	566	ASP	CB-CG-OD2	5.21	122.98	118.30
2	B	1357	ASP	CB-CG-OD2	5.20	122.98	118.30
2	B	1152	ASP	CB-CG-OD2	5.20	122.98	118.30
2	B	704	ASP	CB-CG-OD2	5.20	122.98	118.30
2	B	1373	ASP	CB-CG-OD2	5.20	122.98	118.30
2	B	1375	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	596	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	30	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	527	ASP	CB-CG-OD2	5.19	122.97	118.30
2	B	944	ASP	CB-CG-OD2	5.18	122.97	118.30
2	B	1074	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	612	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	26	ASP	CB-CG-OD2	5.17	122.95	118.30
2	B	1435	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	502	ASP	CB-CG-OD2	5.16	122.94	118.30
2	B	1520	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	358	ASP	CB-CG-OD2	5.16	122.94	118.30
2	B	1007	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	532	ASP	CB-CG-OD2	5.15	122.93	118.30
2	B	775	ASP	CB-CG-OD2	5.15	122.93	118.30
2	B	755	ASP	CB-CG-OD2	5.14	122.93	118.30
2	B	1266	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	458	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	113	ASP	CB-CG-OD2	5.13	122.92	118.30
2	B	797	ASP	CB-CG-OD2	5.13	122.92	118.30
2	B	1200	ASP	CB-CG-OD2	5.13	122.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1588	ASP	CB-CG-OD2	5.12	122.91	118.30
2	B	926	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	296	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	273	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	619	ASP	CB-CG-OD2	5.10	122.89	118.30
2	B	951	ASP	CB-CG-OD2	5.10	122.89	118.30
2	B	1263	ASP	CB-CG-OD2	5.10	122.89	118.30
2	B	1477	ASP	CB-CG-OD2	5.09	122.88	118.30
2	B	939	ASP	CB-CG-OD2	5.08	122.88	118.30
2	B	947	ASP	CB-CG-OD2	5.08	122.88	118.30
2	B	1613	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	172	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	156	ASP	CB-CG-OD2	5.05	122.85	118.30
2	B	1502	ASP	CB-CG-OD2	5.05	122.85	118.30
2	B	732	ASP	CB-CG-OD2	5.05	122.84	118.30
2	B	1603	ASP	CB-CG-OD2	5.04	122.84	118.30
2	B	971	ASP	CB-CG-OD2	5.03	122.83	118.30
2	B	1093	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	287	ASP	CB-CG-OD2	5.03	122.83	118.30
2	B	659	ASP	CB-CG-OD2	5.03	122.82	118.30
2	B	1552	ASP	CB-CG-OD2	5.03	122.82	118.30
2	B	974	ASP	CB-CG-OD2	5.02	122.82	118.30
2	B	1134	ASP	CB-CG-OD2	5.01	122.81	118.30
2	B	1118	ASP	CB-CG-OD2	5.01	122.81	118.30
2	B	1225	ASP	CB-CG-OD2	5.00	122.80	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	3	MAN	C1
3	B	5	MAN	C1

There are no planarity outliers.

5.2 Too-close contacts

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	4950	0	5012	83	0
2	B	7821	0	7743	211	0
3	B	61	0	52	4	0
4	A	28	0	25	0	0
All	All	12860	0	12832	286	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 11.

All (286) 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:584:ASN:HB3	1:A:585:LYS:CA	1.85	1.07
1:A:584:ASN:CB	1:A:585:LYS:HA	1.84	1.06
2:B:908:LYS:HE3	2:B:1417:SER:HA	1.38	1.05
2:B:1484:CYS:HA	2:B:1489:CYS:HB2	1.37	1.04
1:A:584:ASN:HB3	1:A:585:LYS:HA	0.99	0.98
1:A:203:LYS:O	1:A:204:GLU:HB3	1.65	0.96
1:A:554:VAL:HG22	1:A:555:PRO:HD2	1.50	0.91
2:B:1593:LYS:HB2	2:B:1594:PRO:HA	1.51	0.90
2:B:1228:PRO:HB2	2:B:1229:PRO:HD3	1.62	0.82
2:B:1484:CYS:HA	2:B:1489:CYS:CB	2.11	0.81
2:B:927:PRO:O	2:B:928:GLU:HB2	1.80	0.81
2:B:1404:ASP:N	2:B:1404:ASP:OD1	2.16	0.77
2:B:961:GLN:HG2	2:B:966:ALA:HB3	1.67	0.76
2:B:929:ARG:O	2:B:931:GLY:N	2.16	0.74
2:B:1325:MET:CE	3:B:1:NAG:H5	2.18	0.74
2:B:1524:LYS:HD3	2:B:1544:GLU:HB2	1.70	0.72
1:A:203:LYS:O	1:A:204:GLU:CB	2.38	0.72
2:B:822:GLN:HG3	2:B:879:VAL:HG22	1.73	0.71
2:B:1593:LYS:CB	2:B:1594:PRO:HA	2.21	0.69
2:B:686:GLN:H	2:B:686:GLN:CD	1.95	0.69
2:B:1249:ALA:O	2:B:1253:VAL:HG23	1.92	0.69
2:B:997:THR:HB	2:B:998:PRO:HD3	1.75	0.69
1:A:426:THR:HG21	1:A:432:ASN:H	1.58	0.69
2:B:811:LEU:HB3	2:B:905:LYS:HD2	1.74	0.69
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.74	0.69
2:B:1473:PRO:O	2:B:1474:GLU:HB2	1.92	0.69
2:B:1419:ARG:HH11	2:B:1419:ARG:HG3	1.58	0.68
2:B:998:PRO:HG3	2:B:1251:PHE:CE1	2.29	0.67
2:B:1496:CYS:O	2:B:1497:PHE:HB3	1.92	0.67
1:A:554:VAL:CG2	1:A:555:PRO:HD2	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:HG21	1:A:278:VAL:HG21	1.77	0.65
2:B:813:LEU:HD22	2:B:907:LEU:HB3	1.79	0.64
2:B:1392:ASP:OD2	2:B:1394:ASP:HB2	1.98	0.64
1:A:554:VAL:HG22	1:A:555:PRO:CD	2.27	0.64
1:A:580:VAL:HG13	2:B:745:PHE:CD1	2.33	0.64
2:B:1014:LYS:O	2:B:1294:ALA:HB2	1.98	0.64
2:B:710:THR:O	2:B:714:ARG:HB2	1.98	0.63
2:B:686:GLN:O	2:B:689:THR:HG22	1.99	0.62
2:B:1320:LEU:HG	2:B:1320:LEU:O	1.98	0.62
2:B:1501:SER:C	2:B:1503:ASP:H	2.03	0.62
2:B:1116:GLU:HA	2:B:1119:MET:HB2	1.80	0.62
2:B:657:ARG:HD3	2:B:676:MET:HB3	1.81	0.62
2:B:1001:ILE:HD11	2:B:1254:PHE:CD1	2.35	0.62
2:B:1237:GLN:OE1	2:B:1239:TYR:OH	2.18	0.62
2:B:956:THR:HG23	2:B:1324:THR:HG22	1.82	0.61
2:B:1008:GLU:HG3	2:B:1262:LYS:HE3	1.82	0.60
2:B:823:VAL:HG23	2:B:878:ILE:HG13	1.82	0.60
2:B:1325:MET:HE1	3:B:1:NAG:H5	1.84	0.60
2:B:929:ARG:C	2:B:931:GLY:H	2.02	0.60
2:B:1291:TRP:O	2:B:1292:GLU:HB2	2.01	0.60
1:A:213:ILE:HG13	1:A:234:THR:HB	1.84	0.60
1:A:6:ILE:HG23	1:A:625:THR:HB	1.82	0.59
2:B:1228:PRO:CB	2:B:1229:PRO:HD3	2.32	0.59
2:B:991:GLN:HG2	2:B:1460:TYR:CZ	2.37	0.59
2:B:809:ILE:HD11	2:B:892:ALA:HB3	1.85	0.59
2:B:680:PRO:HB2	2:B:1438:ALA:O	2.02	0.59
2:B:1380:ILE:CD1	2:B:1460:TYR:HD1	2.15	0.59
2:B:1325:MET:HE3	3:B:1:NAG:H5	1.85	0.59
1:A:202:VAL:O	1:A:204:GLU:N	2.34	0.59
2:B:965:VAL:HG11	2:B:1254:PHE:HE1	1.68	0.59
1:A:24:ALA:HB2	1:A:54:LEU:HD13	1.84	0.59
2:B:965:VAL:CG1	2:B:1254:PHE:HE1	2.16	0.59
2:B:714:ARG:HH12	2:B:718:ARG:NH2	2.02	0.58
2:B:675:GLY:O	2:B:706:CYS:HB3	2.04	0.58
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.84	0.57
2:B:1484:CYS:O	2:B:1486:ASP:N	2.37	0.57
2:B:821:GLU:OE1	2:B:1387:THR:HG21	2.04	0.57
1:A:374:THR:O	1:A:376:GLN:N	2.38	0.57
2:B:742:ARG:HG2	2:B:745:PHE:CZ	2.40	0.57
2:B:818:VAL:HG11	2:B:1451:GLN:HG3	1.86	0.57
2:B:1408:SER:OG	2:B:1427:ASP:OD1	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:706:CYS:HA	2:B:709:ILE:HG22	1.87	0.57
2:B:850:PHE:HB3	2:B:880:PRO:HA	1.87	0.56
2:B:997:THR:O	2:B:1001:ILE:HG23	2.05	0.56
2:B:991:GLN:O	2:B:994:ILE:HG13	2.06	0.56
1:A:334:HIS:HB2	1:A:353:PHE:HB3	1.86	0.56
2:B:657:ARG:HA	2:B:676:MET:HE1	1.87	0.56
1:A:588:LYS:O	1:A:593:LYS:HD2	2.06	0.56
2:B:1448:GLU:O	2:B:1449:LEU:HB2	2.06	0.56
1:A:434:LEU:HB2	1:A:513:TYR:HE2	1.70	0.56
2:B:663:LYS:O	2:B:664:TYR:HB2	2.06	0.56
2:B:1498:ILE:HD12	2:B:1605:TRP:HB2	1.87	0.56
1:A:584:ASN:ND2	1:A:587:ASN:H	2.03	0.55
2:B:894:VAL:CG2	2:B:897:HIS:HB2	2.36	0.55
2:B:908:LYS:O	2:B:908:LYS:HG3	2.06	0.55
2:B:1126:LEU:HD11	2:B:1147:ILE:HG23	1.87	0.55
2:B:955:GLU:O	2:B:955:GLU:HG3	2.06	0.55
2:B:1341:LEU:HB3	2:B:1469:ARG:HD3	1.87	0.55
2:B:1593:LYS:HB2	2:B:1594:PRO:CA	2.31	0.55
2:B:826:ARG:NH2	2:B:1444:TYR:O	2.40	0.55
1:A:30:ASP:HB3	1:A:56:PRO:HD3	1.89	0.55
2:B:778:THR:OG1	2:B:779:THR:N	2.39	0.55
2:B:990:GLU:HG2	2:B:1461:TYR:OH	2.06	0.55
2:B:679:ASN:HB2	2:B:688:ARG:HH21	1.71	0.55
2:B:1276:LEU:HB2	2:B:1285:ILE:HB	1.88	0.55
2:B:818:VAL:HB	2:B:821:GLU:CD	2.28	0.55
2:B:1484:CYS:C	2:B:1486:ASP:H	2.10	0.54
2:B:851:CYS:SG	2:B:881:LEU:HD11	2.47	0.54
2:B:927:PRO:O	2:B:928:GLU:CB	2.55	0.54
2:B:1408:SER:O	2:B:1409:LYS:HB3	2.08	0.54
2:B:985:PRO:HG3	2:B:1423:ILE:HG21	1.90	0.54
1:A:374:THR:HG22	1:A:375:VAL:H	1.74	0.53
2:B:1390:ALA:HB3	2:B:1444:TYR:HE1	1.74	0.53
2:B:1501:SER:O	2:B:1503:ASP:N	2.42	0.53
2:B:1180:LEU:HD23	2:B:1221:LEU:HD11	1.90	0.53
2:B:910:VAL:HG11	2:B:1418:ASP:HA	1.90	0.53
2:B:1121:LEU:O	2:B:1125:VAL:HG23	2.08	0.53
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.39	0.53
2:B:1479:LYS:HD2	2:B:1566:ILE:HD11	1.91	0.52
2:B:919:THR:HG21	2:B:1238:ARG:O	2.09	0.52
2:B:1380:ILE:HD11	2:B:1460:TYR:HD1	1.74	0.52
2:B:1385:MET:O	2:B:1419:ARG:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:VAL:O	1:A:582:VAL:HG12	2.10	0.52
2:B:1001:ILE:HG13	2:B:1002:ALA:N	2.24	0.52
2:B:734:ILE:HG22	2:B:736:GLU:H	1.74	0.52
2:B:1001:ILE:HD11	2:B:1254:PHE:CE1	2.45	0.52
2:B:915:ARG:HD2	2:B:1325:MET:HE2	1.92	0.52
2:B:1338:LYS:HZ2	2:B:1338:LYS:N	2.08	0.52
2:B:750:LEU:HD11	2:B:771:ILE:HG21	1.92	0.52
2:B:1419:ARG:NH1	2:B:1419:ARG:HG3	2.19	0.51
2:B:1555:GLN:H	2:B:1558:GLN:NE2	2.08	0.51
2:B:1130:GLN:HA	2:B:1133:LYS:HG3	1.92	0.51
2:B:1276:LEU:HD23	2:B:1310:VAL:HG22	1.92	0.51
1:A:126:ARG:NH2	1:A:573:LEU:O	2.44	0.51
1:A:166:VAL:HG11	1:A:572:VAL:HG11	1.92	0.51
1:A:366:PRO:HD2	1:A:406:LYS:HG2	1.92	0.51
2:B:689:THR:HG23	2:B:690:ARG:HG2	1.93	0.51
1:A:262:LEU:HD22	1:A:288:GLY:HA3	1.93	0.51
1:A:584:ASN:HD21	1:A:587:ASN:HB2	1.76	0.51
1:A:404:THR:CG2	1:A:415:ALA:H	2.24	0.50
2:B:922:VAL:O	2:B:923:ARG:O	2.28	0.50
2:B:1591:GLY:O	2:B:1596:LEU:HD12	2.11	0.50
1:A:338:THR:HG21	1:A:350:LEU:HD23	1.93	0.50
1:A:215:GLU:HB3	1:A:321:ARG:NH2	2.27	0.49
2:B:1248:GLN:O	2:B:1252:MET:HB2	2.11	0.49
2:B:663:LYS:HD2	2:B:663:LYS:H	1.77	0.49
1:A:577:ASP:HB2	2:B:746:PRO:HG2	1.94	0.49
2:B:1496:CYS:O	2:B:1497:PHE:CB	2.60	0.49
2:B:1105:GLN:O	2:B:1106:GLU:C	2.50	0.49
2:B:1270:LEU:HB2	2:B:1291:TRP:HB2	1.94	0.49
1:A:572:VAL:HG12	2:B:753:VAL:HG22	1.94	0.49
2:B:1278:LEU:HD22	2:B:1302:THR:HG21	1.95	0.49
1:A:443:LEU:H	1:A:443:LEU:HD23	1.77	0.49
2:B:733:ILE:HG22	2:B:734:ILE:H	1.78	0.49
2:B:950:PRO:HB3	2:B:1599:ILE:HD12	1.95	0.48
2:B:888:VAL:HG23	2:B:907:LEU:HD22	1.95	0.48
2:B:1091:LYS:HE3	2:B:1095:VAL:HB	1.95	0.48
2:B:657:ARG:O	2:B:658:MET:HB3	2.14	0.48
1:A:332:GLN:HE21	1:A:357:PRO:HA	1.78	0.48
1:A:567:HIS:HB2	2:B:760:PRO:HB3	1.96	0.48
2:B:1014:LYS:HZ2	2:B:1292:GLU:H	1.62	0.48
1:A:554:VAL:CG2	1:A:555:PRO:CD	2.90	0.47
2:B:1448:GLU:HB2	2:B:1482:LYS:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1228:PRO:HB2	2:B:1229:PRO:CD	2.39	0.47
1:A:398:LEU:HD22	1:A:400:ILE:HG13	1.96	0.47
2:B:1065:SER:HB2	2:B:1131:GLU:HB3	1.96	0.47
2:B:1014:LYS:HD2	2:B:1292:GLU:HA	1.96	0.47
2:B:1516:GLU:HB3	2:B:1519:VAL:HG23	1.97	0.46
1:A:126:ARG:HG3	2:B:751:TRP:CH2	2.51	0.46
2:B:1593:LYS:CB	2:B:1594:PRO:CA	2.92	0.46
1:A:22:LEU:HD13	1:A:33:VAL:HG11	1.98	0.46
2:B:1095:VAL:HG12	2:B:1096:PHE:N	2.30	0.46
1:A:161:GLN:O	1:A:162:ASN:HB2	2.16	0.46
2:B:1157:ASN:HD22	2:B:1157:ASN:N	2.12	0.46
2:B:818:VAL:O	2:B:821:GLU:HB2	2.15	0.46
1:A:108:LEU:HB2	1:A:196:PHE:CD1	2.51	0.46
2:B:1215:LEU:HD23	2:B:1256:ALA:HB1	1.98	0.46
1:A:179:MET:HA	1:A:202:VAL:HG23	1.98	0.46
1:A:547:GLN:HE22	1:A:559:MET:HA	1.81	0.46
2:B:1336:CYS:HB3	2:B:1339:PHE:O	2.16	0.46
2:B:1414:LYS:O	2:B:1415:ALA:C	2.54	0.46
2:B:1516:GLU:HG3	2:B:1518:GLY:H	1.79	0.46
1:A:553:PRO:HG3	2:B:801:VAL:HG12	1.98	0.45
1:A:584:ASN:CB	1:A:585:LYS:CA	2.65	0.45
2:B:1227:VAL:N	2:B:1228:PRO:CD	2.79	0.45
2:B:1482:LYS:HA	2:B:1483:LEU:HA	1.69	0.45
2:B:669:ARG:O	2:B:673:GLU:HB2	2.17	0.45
1:A:134:LEU:HD12	1:A:595:TRP:CZ3	2.51	0.45
1:A:606:THR:HA	1:A:607:PRO:HD3	1.82	0.45
2:B:1052:PRO:O	2:B:1100:ALA:HB2	2.16	0.45
2:B:1337:ASN:C	2:B:1338:LYS:HD3	2.37	0.45
1:A:55:THR:HG22	1:A:57:ALA:H	1.80	0.45
2:B:1043:ALA:O	2:B:1057:THR:OG1	2.27	0.45
1:A:495:LEU:HD12	1:A:496:PRO:HD2	1.98	0.45
2:B:1411:GLU:HB3	2:B:1423:ILE:HB	1.99	0.45
1:A:504:ILE:CG2	1:A:505:PRO:HA	2.47	0.45
2:B:1380:ILE:O	2:B:1457:VAL:HA	2.16	0.45
2:B:908:LYS:CE	2:B:1417:SER:HA	2.28	0.45
2:B:929:ARG:C	2:B:931:GLY:N	2.66	0.45
1:A:175:GLU:H	1:A:175:GLU:CD	2.20	0.45
1:A:437:SER:OG	1:A:452:ASN:HB2	2.17	0.45
1:A:589:LEU:O	2:B:795:VAL:HG11	2.17	0.45
2:B:1079:CYS:O	2:B:1083:LYS:HB2	2.17	0.44
2:B:817:VAL:O	2:B:909:VAL:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:956:THR:OG1	2:B:1324:THR:HG22	2.17	0.44
2:B:1065:SER:CB	2:B:1131:GLU:HB3	2.47	0.44
2:B:1005:TYR:HA	2:B:1262:LYS:HD2	1.99	0.44
1:A:249:VAL:CG2	1:A:278:VAL:HG21	2.46	0.44
2:B:998:PRO:HG3	2:B:1251:PHE:CD1	2.53	0.44
1:A:356:ASN:HB3	1:A:357:PRO:HD2	2.00	0.44
2:B:931:GLY:O	2:B:932:ARG:HB2	2.16	0.44
1:A:356:ASN:HB3	1:A:357:PRO:CD	2.48	0.44
2:B:1208:VAL:HG12	2:B:1253:VAL:CG2	2.48	0.44
2:B:940:ILE:HD13	2:B:1322:VAL:HG21	1.99	0.44
2:B:1501:SER:C	2:B:1503:ASP:N	2.70	0.44
2:B:668:LEU:HG	2:B:701:VAL:HG21	2.00	0.43
2:B:965:VAL:HG13	2:B:1254:PHE:CE1	2.53	0.43
2:B:689:THR:O	2:B:690:ARG:HB2	2.19	0.43
2:B:915:ARG:HG2	2:B:1327:HIS:CE1	2.54	0.43
2:B:996:MET:O	2:B:1000:VAL:HG23	2.18	0.43
2:B:1143:LEU:N	2:B:1144:PRO:CD	2.81	0.43
2:B:818:VAL:HG23	2:B:1419:ARG:HH21	1.83	0.43
2:B:965:VAL:CG1	2:B:1254:PHE:CE1	2.99	0.43
2:B:1103:ILE:HG23	2:B:1378:MET:HG3	1.99	0.43
2:B:949:VAL:HG23	2:B:1327:HIS:O	2.18	0.43
2:B:953:GLU:HG3	2:B:953:GLU:H	1.51	0.43
1:A:6:ILE:HD13	1:A:88:ALA:HB2	2.00	0.43
2:B:1354:ARG:CZ	2:B:1361:THR:HG22	2.48	0.43
2:B:672:CYS:HB2	2:B:701:VAL:CG1	2.49	0.43
2:B:1008:GLU:HG3	2:B:1262:LYS:CE	2.49	0.43
2:B:1380:ILE:HD11	2:B:1460:TYR:CD1	2.52	0.43
2:B:1632:GLU:C	2:B:1634:MET:H	2.23	0.43
2:B:652:GLN:O	2:B:654:THR:N	2.49	0.43
1:A:487:GLU:O	1:A:490:GLN:HB2	2.19	0.42
2:B:677:ARG:HG3	2:B:734:ILE:HD11	2.01	0.42
1:A:19:THR:HA	1:A:65:THR:HG22	1.99	0.42
2:B:1340:ASP:OD2	2:B:1371:ARG:NH2	2.52	0.42
2:B:1414:LYS:HD3	2:B:1420:ASN:HB2	2.01	0.42
2:B:1380:ILE:HD12	2:B:1460:TYR:HD1	1.82	0.42
3:B:3:MAN:O4	3:B:5:MAN:C1	2.65	0.42
1:A:39:ASP:HB2	1:A:44:LYS:HD2	1.99	0.42
2:B:1294:ALA:O	2:B:1295:SER:HB3	2.20	0.42
2:B:1354:ARG:HB2	2:B:1355:PRO:HD2	2.00	0.42
2:B:1527:LEU:O	2:B:1577:LYS:HA	2.19	0.42
2:B:1346:LYS:HA	2:B:1347:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1381:LEU:HB2	2:B:1424:ILE:HB	2.00	0.42
2:B:1497:PHE:HE1	2:B:1500:LYS:HZ3	1.68	0.42
2:B:963:THR:HG22	2:B:965:VAL:H	1.84	0.42
1:A:611:LYS:HD2	1:A:611:LYS:H	1.84	0.42
2:B:1380:ILE:CD1	2:B:1460:TYR:CD1	3.01	0.42
2:B:888:VAL:CG2	2:B:907:LEU:HD22	2.49	0.42
1:A:603:ILE:HA	1:A:604:GLY:HA2	1.73	0.42
2:B:1040:PRO:HA	2:B:1041:SER:HA	1.44	0.42
2:B:1592:GLU:H	2:B:1592:GLU:HG2	1.56	0.42
2:B:1593:LYS:CD	2:B:1593:LYS:H	2.31	0.42
1:A:40:PHE:HA	1:A:41:PRO:HA	1.61	0.42
1:A:504:ILE:HG13	1:A:504:ILE:H	1.55	0.42
1:A:553:PRO:HA	1:A:557:GLN:HE22	1.85	0.42
1:A:606:THR:HB	1:A:619:ASP:HB3	2.01	0.42
2:B:1390:ALA:HB3	2:B:1444:TYR:CE1	2.52	0.42
2:B:1619:GLU:CD	2:B:1619:GLU:H	2.23	0.42
2:B:1341:LEU:O	2:B:1469:ARG:HD3	2.19	0.41
1:A:193:GLN:HG2	1:A:193:GLN:H	1.48	0.41
1:A:312:SER:HB2	2:B:1356:GLN:HG3	2.02	0.41
1:A:214:VAL:O	1:A:321:ARG:HB2	2.19	0.41
1:A:324:ILE:HA	1:A:325:PRO:HD3	1.83	0.41
2:B:1206:TYR:CE2	2:B:1462:ASN:HB2	2.55	0.41
2:B:1014:LYS:NZ	2:B:1292:GLU:H	2.19	0.41
2:B:750:LEU:CD1	2:B:771:ILE:HG21	2.50	0.41
2:B:1277:GLN:HB2	2:B:1284:LYS:HZ3	1.84	0.41
2:B:1482:LYS:HG3	2:B:1482:LYS:O	2.20	0.41
2:B:883:THR:HA	2:B:909:VAL:HB	2.00	0.41
2:B:1074:ASP:OD2	2:B:1076:GLN:HB2	2.19	0.41
1:A:178:ASN:O	1:A:202:VAL:HG21	2.21	0.41
1:A:422:LEU:HB3	1:A:423:PRO:HD2	2.02	0.41
1:A:614:ALA:HB1	1:A:632:THR:HG22	2.02	0.41
2:B:819:ARG:O	2:B:820:ASN:HB2	2.21	0.41
1:A:153:VAL:HG21	1:A:182:TRP:HZ3	1.84	0.41
2:B:1204:GLN:HG3	2:B:1464:GLU:HG2	2.02	0.41
1:A:454:LEU:HD13	1:A:454:LEU:HA	1.96	0.41
2:B:1227:VAL:HB	2:B:1228:PRO:HD3	2.01	0.41
1:A:10:ASN:HA	1:A:10:ASN:HD22	1.62	0.41
2:B:1205:LEU:HA	2:B:1205:LEU:HD23	1.94	0.41
2:B:1338:LYS:HB2	2:B:1338:LYS:NZ	2.35	0.41
2:B:916:MET:O	2:B:1325:MET:HA	2.21	0.41
2:B:923:ARG:NH1	2:B:938:GLU:HG3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1583:TRP:C	2:B:1583:TRP:CD1	2.95	0.41
1:A:8:THR:HG23	1:A:623:THR:OG1	2.21	0.41
2:B:878:ILE:HG13	2:B:878:ILE:O	2.21	0.41
2:B:1227:VAL:N	2:B:1228:PRO:HD2	2.36	0.40
2:B:837:GLU:HB3	2:B:868:PRO:HD3	2.04	0.40
2:B:1029:LYS:O	2:B:1033:GLN:HG3	2.21	0.40
1:A:133:LYS:HG3	1:A:477:ARG:HH22	1.86	0.40
2:B:1113:ASN:OD1	2:B:1115:ASN:ND2	2.54	0.40
1:A:504:ILE:HG22	1:A:505:PRO:HA	2.04	0.40
2:B:1104:HIS:O	2:B:1105:GLN:C	2.59	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	629/643 (98%)	564 (90%)	54 (9%)	11 (2%)	11	42
2	B	970/991 (98%)	853 (88%)	87 (9%)	30 (3%)	5	30
All	All	1599/1634 (98%)	1417 (89%)	141 (9%)	41 (3%)	6	33

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	LYS
1	A	204	GLU
1	A	424	TYR
2	B	923	ARG
2	B	930	LEU
2	B	1295	SER
2	B	1330	ALA
1	A	64	VAL

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Mol	Chain	Res	Type
2	B	928	GLU
2	B	1268	GLN
2	B	1473	PRO
1	A	49	SER
1	A	425	SER
1	A	584	ASN
2	B	742	ARG
2	B	934	GLY
2	B	1105	GLN
2	B	1294	ALA
2	B	1331	LYS
2	B	1474	GLU
2	B	1475	LYS
2	B	1501	SER
1	A	81	ASN
1	A	628	SER
2	B	929	ARG
2	B	1044	PHE
2	B	1377	THR
2	B	1417	SER
2	B	1482	LYS
2	B	1497	PHE
1	A	45	LEU
1	A	549	GLU
2	B	664	TYR
2	B	678	GLU
2	B	857	LYS
2	B	1292	GLU
2	B	1315	LYS
2	B	1419	ARG
2	B	1314	GLY
2	B	1591	GLY
2	B	764	ILE

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	560/567 (99%)	525 (94%)	35 (6%)	21	56
2	B	867/878 (99%)	766 (88%)	101 (12%)	6	27
All	All	1427/1445 (99%)	1291 (90%)	136 (10%)	10	35

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	8	THR
1	A	10	ASN
1	A	36	THR
1	A	51	LYS
1	A	103	LEU
1	A	104	GLN
1	A	105	SER
1	A	115	THR
1	A	164	LEU
1	A	177	VAL
1	A	179	MET
1	A	193	GLN
1	A	197	SER
1	A	202	VAL
1	A	204	GLU
1	A	215	GLU
1	A	223	ILE
1	A	241	LYS
1	A	246	THR
1	A	277	GLU
1	A	289	VAL
1	A	310	LEU
1	A	398	LEU
1	A	404	THR
1	A	409	LEU
1	A	478	LEU
1	A	491	ASP
1	A	492	LEU
1	A	498	SER
1	A	580	VAL
1	A	584	ASN
1	A	611	LYS
1	A	623	THR
1	A	639	GLN

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Mol	Chain	Res	Type
2	B	651	VAL
2	B	673	GLU
2	B	684	SER
2	B	686	GLN
2	B	687	ARG
2	B	689	THR
2	B	696	GLU
2	B	700	LYS
2	B	712	LEU
2	B	716	HIS
2	B	730	ASP
2	B	733	ILE
2	B	742	ARG
2	B	755	ASP
2	B	778	THR
2	B	789	ASP
2	B	804	MET
2	B	822	GLN
2	B	823	VAL
2	B	826	ARG
2	B	841	ARG
2	B	857	LYS
2	B	859	ARG
2	B	864	VAL
2	B	894	VAL
2	B	898	PHE
2	B	908	LYS
2	B	916	MET
2	B	922	VAL
2	B	937	LYS
2	B	953	GLU
2	B	955	GLU
2	B	970	GLU
2	B	974	ASP
2	B	980	HIS
2	B	982	ILE
2	B	983	VAL
2	B	988	CYS
2	B	990	GLU
2	B	1001	ILE
2	B	1018	GLU
2	B	1024	LEU

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Mol	Chain	Res	Type
2	B	1042	SER
2	B	1093	ASP
2	B	1114	ASN
2	B	1131	GLU
2	B	1133	LYS
2	B	1137	GLU
2	B	1143	LEU
2	B	1157	ASN
2	B	1169	ILE
2	B	1197	ARG
2	B	1226	PHE
2	B	1246	SER
2	B	1269	GLU
2	B	1278	LEU
2	B	1298	ARG
2	B	1302	THR
2	B	1332	ASP
2	B	1337	ASN
2	B	1338	LYS
2	B	1341	LEU
2	B	1345	ILE
2	B	1350	GLU
2	B	1351	THR
2	B	1371	ARG
2	B	1373	ASP
2	B	1378	MET
2	B	1387	THR
2	B	1393	THR
2	B	1404	ASP
2	B	1411	GLU
2	B	1412	LEU
2	B	1414	LYS
2	B	1416	PHE
2	B	1417	SER
2	B	1419	ARG
2	B	1420	ASN
2	B	1428	LYS
2	B	1433	GLU
2	B	1440	LYS
2	B	1448	GLU
2	B	1463	LEU
2	B	1469	ARG

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Mol	Chain	Res	Type
2	B	1480	LEU
2	B	1482	LYS
2	B	1483	LEU
2	B	1485	ARG
2	B	1496	CYS
2	B	1497	PHE
2	B	1503	ASP
2	B	1509	GLU
2	B	1532	LEU
2	B	1566	ILE
2	B	1568	CYS
2	B	1577	LYS
2	B	1592	GLU
2	B	1593	LYS
2	B	1602	LYS
2	B	1619	GLU
2	B	1626	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	178	ASN
1	A	181	GLN
1	A	332	GLN
1	A	334	HIS
1	A	490	GLN
1	A	547	GLN
1	A	557	GLN
1	A	584	ASN
2	B	679	ASN
2	B	686	GLN
2	B	1105	GLN
2	B	1157	ASN
2	B	1261	GLN
2	B	1277	GLN
2	B	1337	ASN
2	B	1472	HIS
2	B	1495	ASN
2	B	1558	GLN
2	B	1620	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 ⓘ

7 carbohydrates 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	A	644	1,4	14,14,15	0.54	0	15,19,21	0.60	0
4	NAG	A	645	4	14,14,15	0.51	0	15,19,21	0.60	0
3	NAG	B	1	3,2	14,14,15	0.62	0	15,19,21	1.25	2 (13%)
3	NAG	B	2	3	14,14,15	0.67	0	15,19,21	1.25	1 (6%)
3	MAN	B	3	3	11,11,12	0.83	0	13,15,17	0.70	0
3	BMA	B	4	3	11,11,12	0.63	0	13,15,17	0.71	0
3	MAN	B	5	3	11,11,12	0.63	0	13,15,17	0.60	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
4	NAG	A	644	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	645	4	-	2/6/23/26	0/1/1/1
3	NAG	B	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	MAN	B	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	BMA	B	4	3	-	0/2/19/22	0/1/1/1
3	MAN	B	5	3	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	1	NAG	C3-C4-C5	2.41	114.47	110.22
3	B	1	NAG	C4-C3-C2	2.96	115.36	111.02
3	B	2	NAG	C4-C3-C2	4.04	116.94	111.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	3	MAN	C1
3	B	5	MAN	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	645	NAG	C8-C7-N2-C2
4	A	645	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	NAG	3	0
3	B	3	MAN	1	0
3	B	5	MAN	1	0

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, 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	635/643 (98%)	0.33	27 (4%) 36 34	79, 97, 116, 123	0
2	B	976/991 (98%)	0.05	8 (0%) 86 85	71, 91, 108, 129	0
All	All	1611/1634 (98%)	0.16	35 (2%) 62 60	71, 93, 113, 129	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	739	ILE	3.7
1	A	101	VAL	3.7
1	A	20	MET	3.7
1	A	427	VAL	3.4
1	A	61	MET	3.1
1	A	300	LYS	3.1
2	B	762	ASN	3.1
1	A	326	ILE	3.1
1	A	105	SER	3.1
1	A	377	SER	3.0
2	B	1481	ASN	2.9
2	B	1485	ARG	2.8
1	A	1	SER	2.7
2	B	1594	PRO	2.7
1	A	520	GLY	2.5
1	A	103	LEU	2.5
1	A	408	GLU	2.5
2	B	763	GLY	2.5
1	A	378	LEU	2.5
1	A	167	LEU	2.5
2	B	930	LEU	2.4
1	A	84	VAL	2.4
1	A	459	ARG	2.3
1	A	392	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	52	THR	2.2
1	A	229	LEU	2.2
1	A	43	LYS	2.2
2	B	1337	ASN	2.2
1	A	523	GLU	2.2
1	A	159	SER	2.1
1	A	221	TYR	2.1
1	A	442	GLU	2.1
1	A	28	GLN	2.1
1	A	519	SER	2.1
1	A	606	THR	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](#)

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
4	NAG	A	645	14/15	0.62	0.32	-	106,106,106,107	0
3	NAG	B	2	14/15	0.89	0.19	-	126,129,132,138	0
3	BMA	B	4	11/12	0.60	0.31	-	150,151,152,152	0
3	MAN	B	3	11/12	0.84	0.19	-	141,144,147,149	0
3	NAG	B	1	14/15	0.90	0.22	-	109,113,116,121	0
4	NAG	A	644	14/15	0.71	0.30	-	107,108,108,109	0
3	MAN	B	5	11/12	0.68	0.33	-	147,148,148,149	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.