



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:19 am GMT

PDB ID : 4ACQ
Title : Alpha-2 Macroglobulin
Authors : Marrero, A.; Duquerroy, S.; Trapani, S.; Goulas, T.; Guevara, T.; Andersen, G.R.; Navaza, J.; Sottrup-Jensen, L.; Gomis-Ruth, F.X.
Deposited on : 2011-12-17
Resolution : 4.30 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

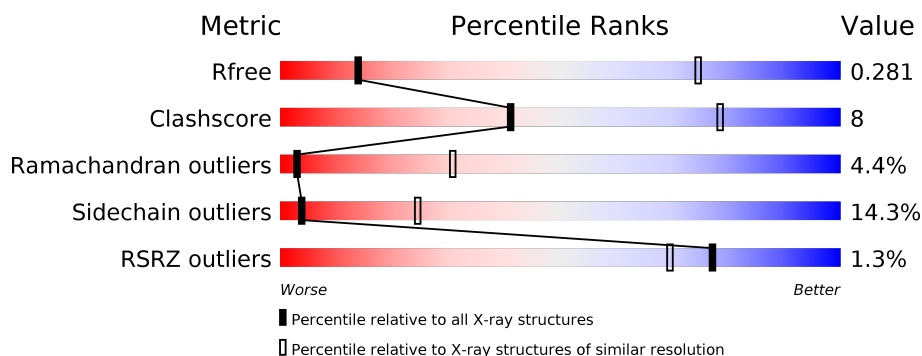
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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	1002 (4.92-3.62)
Clashscore	112137	1001 (4.92-3.68)
Ramachandran outliers	110173	1012 (4.92-3.64)
Sidechain outliers	110143	1021 (4.92-3.62)
RSRZ outliers	101464	1009 (4.92-3.62)

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	1451	<div> <div></div> <div>61% 22% 12%</div> </div>
1	B	1451	<div> <div></div> <div>61% 22% 12%</div> </div>
1	C	1451	<div> <div></div> <div>67% 25% 12%</div> </div>
1	D	1451	<div> <div></div> <div>61% 23% 12%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	2002	X	-	-	-
2	NAG	A	2401	-	-	-	X
2	NAG	A	2402	X	-	-	-
2	NAG	A	2502	X	-	-	-
2	NAG	B	2001	-	-	-	X
2	NAG	B	2002	X	-	-	-
2	NAG	B	2402	X	-	-	-
2	NAG	B	2502	X	-	-	-
2	NAG	C	2001	-	-	-	X
2	NAG	C	2002	X	-	-	-
2	NAG	C	2402	X	-	-	-
2	NAG	C	2502	X	-	-	-
2	NAG	D	2001	-	-	-	X
2	NAG	D	2002	X	-	-	-
2	NAG	D	2402	X	-	-	-
2	NAG	D	2502	X	-	-	-
4	NAG	A	2602	X	-	-	-
4	NAG	B	2602	X	-	-	-
4	MAN	B	2603	-	X	-	-
4	NAG	C	2602	X	-	-	-
4	MAN	C	2603	-	X	-	-
4	NAG	D	2602	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 39900 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 ALPHA-2-MACROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1270	Total	C	N	O	S	0	0	0
			9548	6067	1606	1833	42			
1	B	1270	Total	C	N	O	S	0	0	0
			9548	6067	1606	1833	42			
1	C	1403	Total	C	N	O	S	0	0	0
			10582	6729	1774	2032	47			
1	D	1270	Total	C	N	O	S	0	0	0
			9548	6067	1606	1833	42			

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

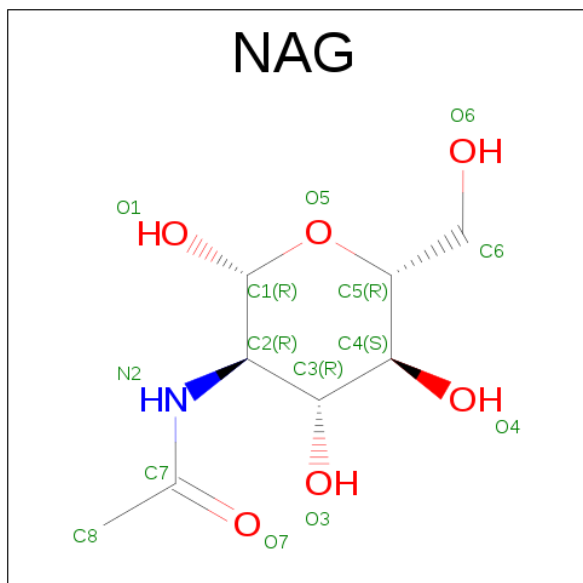
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16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

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

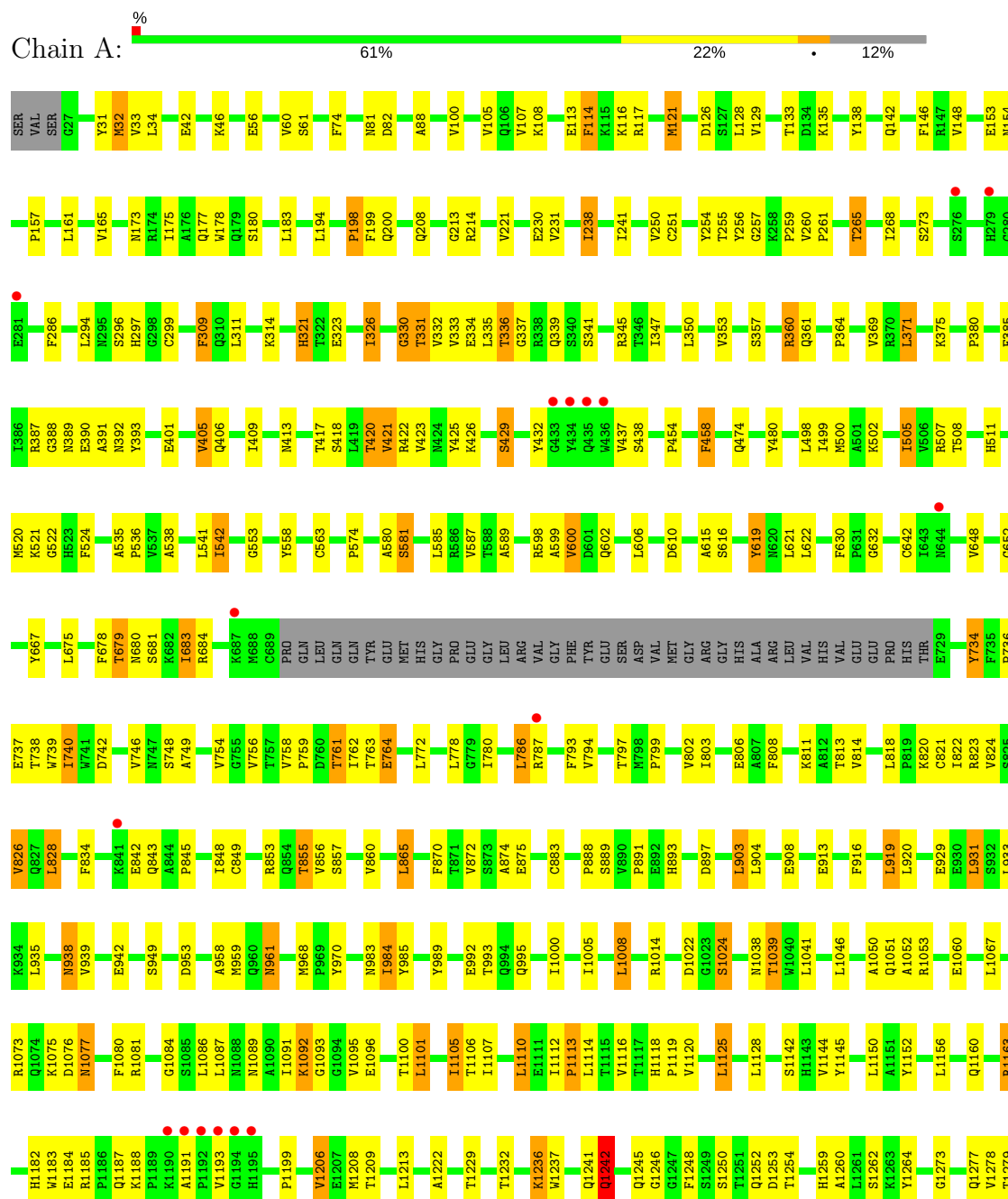
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

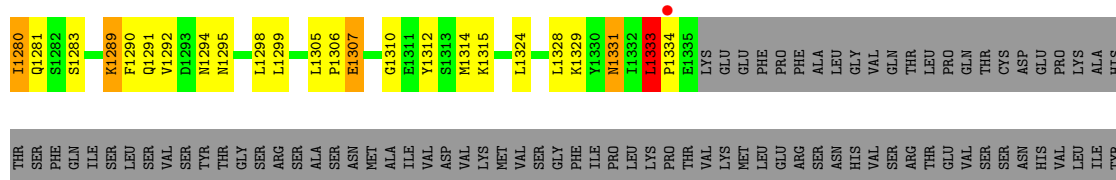
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	B	3	Total	C	N	O	0	0
			39	22	2	15		
4	C	3	Total	C	N	O	0	0
			39	22	2	15		
4	D	3	Total	C	N	O	0	0
			39	22	2	15		

3 Residue-property plots

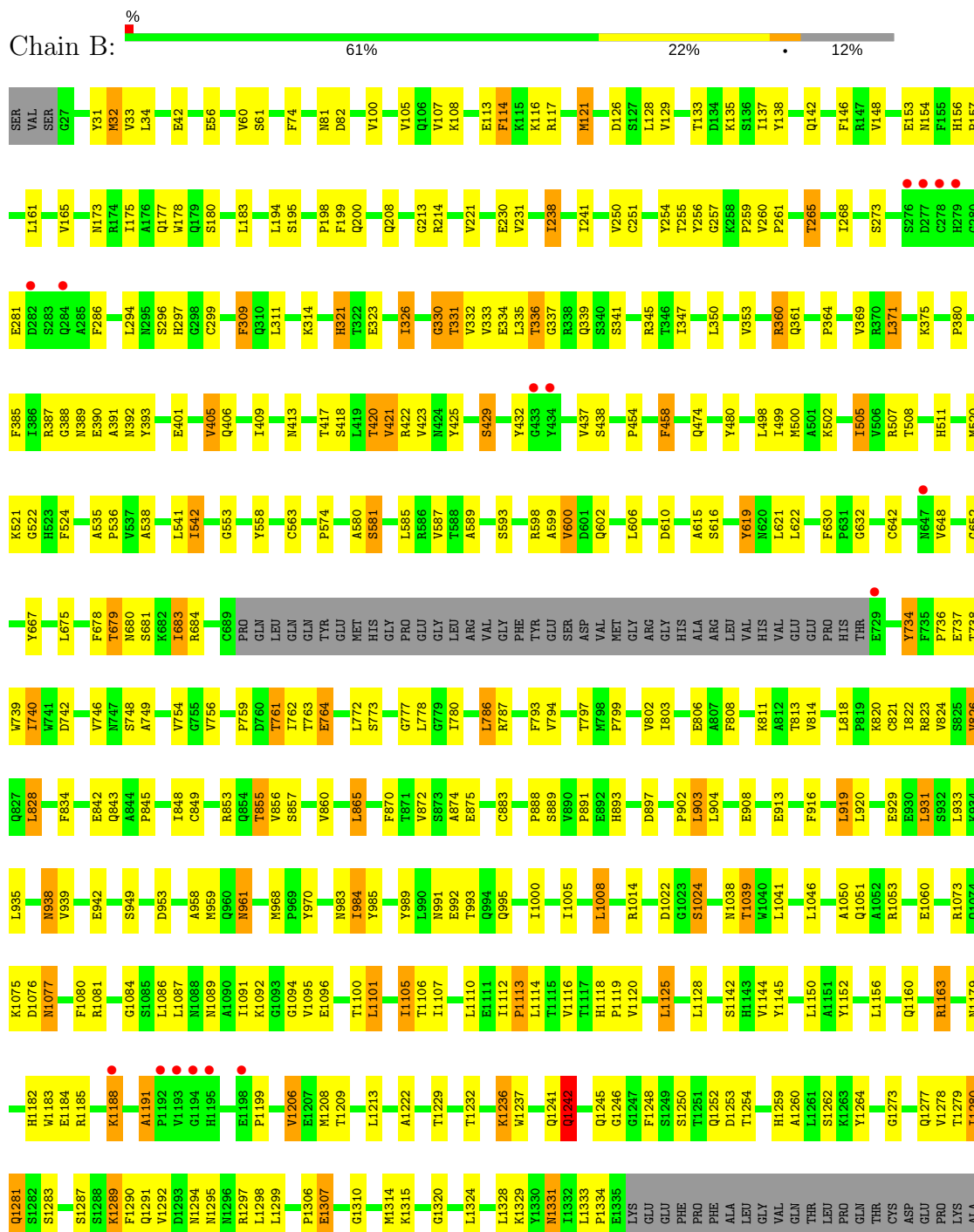
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: ALPHA-2-MACROGLOBULIN





• Molecule 1: ALPHA-2-MACROGLOBULIN



HIS	THR	SER	THR	SER	PHE	GLN	ILE	LEU	SER	SER	SER	THR	THR	GLY	SER	ARG	ALA	ALA	ASN	ASP	VAL	VAL	LYS	VAL	VAL	LEU	LYS	PRO	THR	VAL	VAL	LYS	VAL	LEU	GLU	ARG	SER	ASN	HIS	HIS	VAL	VAL	LEU	ILE
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TYR	LEU	ASP	LYS	VAL	SER	ASN	GLN	THR	LEU	SER	PHE	PHE	THR	VAL	LEU	LEU	GLN	ASP	VAL	PRO	VAL	ARG	ASP	LEU	LYS	PRO	ALA	ILE	VAL	LYS	VAL	TYR	TYR	TYR	GLU	THR	ASP	PHE	GLU	ALA	ILE	ALA	ASN	TYR	ASN	PRO	CYS	SER	LYS	ASP	LEU	GLY	ASN
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- Molecule 1: ALPHA-2-MACROGLOBULIN



SER	VAL	SER
G27		
X31		
M32		
V33		
L34		
E42		
K46		
E56		
V60		
S61		
F74		
N81		
D82		
A88		
V105		
I106		
V107		
K108		
E113		
F114		
K115		
K116		
R117		
M121		
D126		
V129		
T133		
D134		
K135		
S136		
L137		
V138		
Q142		
F146		
A147		
V148		
M154		
F155		
H156		
V157		

1161	1162	1163	1164	1165	1166	1167	1168	1169	1170	1171	1172	1173	1174	1175	1176	1177	1178	1179	1180	1181	1182	1183	1184	1185	1186	1187	1188	1189	1190	1191	1192	1193	1194	1195	1196	1197	1198	1199	1200	1201	1202	1203	1204	1205	1206	1207	1208	1209	1210	1211	1212	1213	1214	1215	1216	1217	1218	1219	1220	1221	1222	1223	1224	1225	1226	1227	1228	1229	1230	1231	1232	1233	1234	1235	1236	1237	1238	1239	1240	1241	1242	1243	1244	1245	1246	1247	1248	1249	1250	1251	1252	1253	1254	1255	1256	1257	1258	1259	1260	1261	1262	1263	1264	1265	1266	1267	1268	1269	1270	1271	1272	1273	1274	1275	1276	1277	1278	1279	1280	1281	1282	1283	1284	1285	1286	1287	1288	1289	1290	1291	1292	1293	1294	1295	1296	1297	1298	1299	1300	1301	1302	1303	1304	1305	1306	1307	1308	1309	1310	1311	1312	1313	1314	1315	1316	1317	1318	1319	1320	1321	1322	1323	1324	1325	1326	1327	1328	1329	1330	1331	1332	1333	1334	1335	1336	1337	1338	1339	1340	1341	1342	1343	1344	1345	1346	1347	1348	1349	1350	1351	1352	1353	1354	1355	1356	1357	1358	1359	1360	1361	1362	1363	1364	1365	1366	1367	1368	1369	1370	1371	1372	1373	1374	1375	1376	1377	1378	1379	1380	1381	1382	1383	1384	1385	1386	1387	1388	1389	1390	1391	1392	1393	1394	1395	1396	1397	1398	1399	1400	1401	1402	1403	1404	1405	1406	1407	1408	1409	1410	1411	1412	1413	1414	1415	1416	1417	1418	1419	1420	1421	1422	1423	1424	1425	1426	1427	1428	1429	1430	1431	1432	1433	1434	1435	1436	1437	1438	1439	1440	1441	1442	1443	1444	1445	1446	1447	1448	1449	1450	1451	1452	1453	1454	1455	1456	1457	1458	1459	1460	1461	1462	1463	1464	1465	1466	1467	1468	1469	1470	1471	1472	1473	1474	1475	1476	1477	1478	1479	1480	1481	1482	1483	1484	1485	1486	1487	1488	1489	1490	1491	1492	1493	1494	1495	1496	1497	1498	1499	1500	1501	1502	1503	1504	1505	1506	1507	1508	1509	1510	1511	1512	1513	1514	1515	1516	1517	1518	1519	1520	1521	1522	1523	1524	1525	1526	1527	1528	1529	1530	1531	1532	1533	1534	1535	1536	1537	1538	1539	1540	1541	1542	1543	1544	1545	1546	1547	1548	1549	1550	1551	1552	1553	1554	1555	1556	1557	1558	1559	1560	1561	1562	1563	1564	1565	1566	1567	1568	1569	1570	1571	1572	1573	1574	1575	1576	1577	1578	1579	1580	1581	1582	1583	1584	1585	1586	1587	1588	1589	1590	1591	1592	1593	1594	1595	1596	1597	1598	1599	1600	1601	1602	1603	1604	1605	1606	1607	1608	1609	1610	1611	1612	1613	1614
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G330
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V332
V333
E334
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C337
R338
Q339
S340
S341
R346
T346
I347
L350
V353
S357
R360
Q361
P364
V369
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K375
P380

F385
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 R387
 G388
 N389
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 A391
 K392
 Y393
 E401
 V405
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 V421
 R422
 V423
 M424
 V425
 S429
 Y432
 G433
 Y434
 Q435
 Q436
 V437
 S438
 P454
 F458
 L468
 Q474
 Y480
 L498
 I499
 M500
 A501
 K502
 I505
 V506
 R507
 T508

H51.1	M520	K521	G522	H523	P524	A535	A536	P537	A538	L541	T542	G553	P558	C563	P574	A580	S581	L585	R586	P587	T588	A589	A598	A599	V600	D601	Q602	L606	D610	A615	S616	Y619	L622	P630	P631	G632	V648	G652	V657
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L675	F678	T679	M680	S681	A682	R684	C689	PRO	GLN	LEU	GLN	GLN	GLN	TYR	GLU	MET	GLY	GLY	PRO	PRO	GLY	LEU	ARG	ARG	VAL	VAL	GLY	PHE	TYR	GLU	GLU	SER	ASP	VAL	VAL	MET	GLY	GLY	GLY	GLY	HIS	HIS	ALA	ALA	ARG	ARG	VAL	VAL	LEU	HIS	HIS	VAL	VAL	GLU	GLU	PRO	HIS	HIS	THR	E729	Y734	F735	P736	E737	T738	W739	W740
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W741	W742	W746	W747	W748	W749	W754	W755	W756	W757	W758	W759	W760	W761	W762	W763	W764	L772	G777	L778	G779	W780	W786	W787	F793	W794	W797	W796	P799	R802	R803	E806	A807	F808	K811	A812	T813	W814	L818	P819	K820	C821	I822	R823	W824	S825	W826	P827	W828
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F834 F842 F843 F844 F845 F848 F853 F854 F855 F856 F857 F860 F865 F870 F871 F872 F873 F874 F875 F883 F887 F888 F889 F890 F891 F892 F893 F897 F903 F904 F908 F913 F916 F919 F920 F929 F930 F931 F932 F933 F934 F935 F938

Y939
E942
S949
D953
A958
W959
O960
I961
E968
P969
T970
N983
E984
Y985
Y989
E992
T993
O994
Y995
I1000
I1005
L1008
R1014
D1022
G1023
S1024
W1035
L1036
G1037
N1038
T1039
O1040
L1041
L1046
A1050
R1053
E1060
I1073
G1074
L1075
O1076

LI1077	LI1080	LI1081	LI1084	LI1086	LI1087	LI1088	LI1089	LI1090	LI1091	LI1092	LI1093	LI1094	LI1095	LI1096	LI1100	LI1101	LI1105	LI1106	LI1107	LI1110	LI1111	LI1112	LI1113	LI1114	LI1115	LI1116	LI1117	LI1118	LI1119	LI1120	LI1124	LI1125	LI1128	LI1142	LI1143	LI1144	LI1145	LI1150	LI1151	LI1152	LI1155	LI1156	LI1160	LI1163	LI1175	LI1176	LI1177
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[illegible]

Year	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032	2033	2034	2035	2036	2037	2038	2039	2040	2041	2042	2043	2044	2045	2046	2047	2048	2049	2050	2051	2052	2053	2054	2055	2056	2057	2058	2059	2060	2061	2062	2063	2064	2065	2066	2067	2068	2069	2070	2071	2072	2073	2074	2075	2076	2077	2078	2079	2080	2081	2082	2083	2084	2085	2086	2087	2088	2089	2090	2091	2092	2093	2094	2095	2096	2097	2098	2099	2100					
Population	279	280	281	281	282	282	283				287	288	289	290	291	292	293	294	295				306	307			310		314	315		324		328	329	330	331	332	333	334			338		343		366			360	361	362	363	364	365	366	367	368	369			372			376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400

79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.69Å 260.30Å 281.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 4.30 24.95 – 4.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.00-4.30) 99.0 (24.95-4.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 4.24Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.238 , 0.260 0.263 , 0.281	Depositor DCC
R_{free} test set	3303 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	205.8	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 157.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	39900	wwPDB-VP
Average B, all atoms (Å ²)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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: MEQ, 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	0.42	0/9743	0.72	0/13275
1	B	0.42	0/9743	0.72	0/13275
1	C	0.44	0/10801	0.73	0/14718
1	D	0.41	0/9743	0.72	0/13275
All	All	0.43	0/40030	0.72	0/54543

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
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
2	A	3	0
2	B	3	0
2	C	3	0
2	D	3	0
4	A	1	0
4	B	1	0
4	C	4	0
4	D	1	0
All	All	19	8

There are no bond length outliers.

There are no bond angle outliers.

All (19) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2002	NAG	C1
2	A	2402	NAG	C1
2	A	2502	NAG	C1
4	A	2602	NAG	C1
2	B	2002	NAG	C1
2	B	2402	NAG	C1
2	B	2502	NAG	C1
4	B	2602	NAG	C1
2	C	2002	NAG	C1
2	C	2402	NAG	C1
2	C	2502	NAG	C1
4	C	2602	NAG	C2,C5,C1,C4
2	D	2002	NAG	C1
2	D	2402	NAG	C1
2	D	2502	NAG	C1
4	D	2602	NAG	C1

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	429	SER	Mainchain,Peptide
1	B	429	SER	Mainchain,Peptide
1	C	429	SER	Mainchain,Peptide
1	D	429	SER	Mainchain,Peptide

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	9548	0	9181	153	0
1	B	9548	0	9181	152	0
1	C	10582	0	10201	174	0
1	D	9548	0	9181	153	0
2	A	84	0	75	3	0
2	B	84	0	75	3	0
2	C	84	0	75	3	0
2	D	84	0	75	2	0
3	A	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	42	0	39	0	0
3	C	56	0	52	0	0
3	D	42	0	39	0	0
4	A	39	0	34	1	0
4	B	39	0	34	2	0
4	C	39	0	32	1	0
4	D	39	0	34	1	0
All	All	39900	0	38347	633	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 8.

All (633) 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)
2:D:2501:NAG:H83	2:D:2502:NAG:H82	1.65	0.79
2:C:2501:NAG:H83	2:C:2502:NAG:H82	1.65	0.78
2:B:2501:NAG:H83	2:B:2502:NAG:H82	1.65	0.78
1:C:280:GLY:HA3	1:D:429:SER:HA	1.65	0.77
1:C:535:ALA:HB1	1:C:536:PRO:HD2	1.65	0.76
2:A:2501:NAG:H83	2:A:2502:NAG:H82	1.66	0.76
1:C:1280:ILE:HG23	1:C:1314:MET:HB3	1.69	0.74
1:A:1280:ILE:HG23	1:A:1314:MET:HB3	1.70	0.74
1:D:535:ALA:HB1	1:D:536:PRO:HD2	1.68	0.74
1:D:1280:ILE:HG23	1:D:1314:MET:HB3	1.69	0.74
1:B:535:ALA:HB1	1:B:536:PRO:HD2	1.68	0.73
1:B:1280:ILE:HG23	1:B:1314:MET:HB3	1.70	0.73
1:A:535:ALA:HB1	1:A:536:PRO:HD2	1.71	0.71
1:B:502:LYS:HG3	1:B:535:ALA:HB2	1.72	0.71
1:D:502:LYS:HG3	1:D:535:ALA:HB2	1.73	0.70
1:C:502:LYS:HG3	1:C:535:ALA:HB2	1.71	0.70
1:A:502:LYS:HG3	1:A:535:ALA:HB2	1.73	0.70
1:A:919:LEU:H	1:A:1229:THR:HG22	1.57	0.70
1:B:919:LEU:H	1:B:1229:THR:HG22	1.57	0.69
1:C:865:LEU:H	1:C:865:LEU:HD13	1.60	0.67
1:C:938:ASN:HD22	1:C:1334:PRO:HG2	1.59	0.67
1:A:616:SER:HA	1:A:619:TYR:CE2	2.30	0.67
1:D:574:PRO:HA	1:D:786:LEU:HD12	1.76	0.67
1:C:574:PRO:HA	1:C:786:LEU:HD12	1.77	0.67
1:B:679:THR:HG22	1:B:681:SER:H	1.61	0.66
1:A:865:LEU:HD13	1:A:865:LEU:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:865:LEU:HD13	1:D:865:LEU:H	1.61	0.66
1:B:865:LEU:HD13	1:B:865:LEU:H	1.61	0.66
1:B:260:VAL:HG23	1:B:853:ARG:HH22	1.61	0.65
1:C:616:SER:HA	1:C:619:TYR:CE2	2.31	0.65
1:A:574:PRO:HA	1:A:786:LEU:HD12	1.78	0.65
1:B:574:PRO:HA	1:B:786:LEU:HD12	1.79	0.65
1:D:679:THR:HG22	1:D:681:SER:H	1.62	0.65
1:A:250:VAL:O	1:A:299:CYS:HB3	1.97	0.65
1:B:107:VAL:HB	1:B:114:PHE:HB2	1.78	0.65
1:B:157:PRO:HB3	1:B:772:LEU:HD23	1.78	0.65
1:B:616:SER:HA	1:B:619:TYR:CE2	2.32	0.65
1:C:1118:HIS:CD2	1:C:1120:VAL:HG22	2.32	0.64
1:D:157:PRO:HB3	1:D:772:LEU:HD23	1.79	0.64
1:A:931:LEU:HD11	1:A:1314:MET:SD	2.38	0.64
1:A:679:THR:HG22	1:A:681:SER:H	1.62	0.64
1:B:938:ASN:HD22	1:B:1334:PRO:HG2	1.61	0.64
1:D:616:SER:HA	1:D:619:TYR:CE2	2.32	0.64
1:D:260:VAL:HG23	1:D:853:ARG:HH22	1.62	0.64
1:C:165:VAL:HG13	1:C:178:TRP:HB2	1.79	0.64
1:B:1118:HIS:CD2	1:B:1120:VAL:HG22	2.33	0.63
1:D:107:VAL:HB	1:D:114:PHE:HB2	1.80	0.63
1:C:679:THR:HG22	1:C:681:SER:H	1.61	0.63
1:C:260:VAL:HG23	1:C:853:ARG:HH22	1.62	0.63
1:A:107:VAL:HB	1:A:114:PHE:HB2	1.80	0.63
1:D:799:PRO:HD2	1:D:903:LEU:HD11	1.81	0.63
1:B:364:PRO:HG3	2:B:2401:NAG:H81	1.80	0.63
1:A:1118:HIS:CD2	1:A:1120:VAL:HG22	2.34	0.63
1:C:919:LEU:H	1:C:1229:THR:HG22	1.64	0.63
1:A:499:ILE:HD12	1:A:507:ARG:HB3	1.82	0.62
1:B:250:VAL:O	1:B:299:CYS:HB3	1.98	0.62
1:A:260:VAL:HG23	1:A:853:ARG:HH22	1.64	0.62
1:C:157:PRO:HB3	1:C:772:LEU:HD23	1.80	0.62
1:D:165:VAL:HG13	1:D:178:TRP:HB2	1.81	0.62
1:C:799:PRO:HD2	1:C:903:LEU:HD11	1.81	0.62
1:D:1118:HIS:CD2	1:D:1120:VAL:HG22	2.34	0.62
1:B:165:VAL:HG13	1:B:178:TRP:HB2	1.80	0.62
1:C:107:VAL:HB	1:C:114:PHE:HB2	1.80	0.62
1:C:250:VAL:O	1:C:299:CYS:HB3	2.00	0.62
1:D:499:ILE:HD12	1:D:507:ARG:HB3	1.81	0.62
1:A:938:ASN:HD22	1:A:1334:PRO:HG2	1.65	0.62
1:A:165:VAL:HG13	1:A:178:TRP:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:ILE:HD12	1:B:507:ARG:HB3	1.81	0.62
1:D:250:VAL:O	1:D:299:CYS:HB3	2.00	0.62
1:A:157:PRO:HB3	1:A:772:LEU:HD23	1.80	0.61
1:A:1182:HIS:NE2	1:A:1237:TRP:HB3	2.16	0.61
1:C:33:VAL:HG11	1:C:105:VAL:HG11	1.82	0.61
1:A:117:ARG:HH22	1:D:1119:PRO:HB2	1.65	0.61
1:D:931:LEU:HD11	1:D:1314:MET:SD	2.41	0.61
1:C:364:PRO:HG3	2:C:2401:NAG:H81	1.82	0.61
1:A:364:PRO:HG3	2:A:2401:NAG:H81	1.82	0.61
1:B:117:ARG:HH22	1:C:1119:PRO:HB2	1.66	0.61
1:D:364:PRO:HG3	2:D:2401:NAG:H81	1.81	0.61
1:D:938:ASN:HD22	1:D:1334:PRO:HG2	1.64	0.61
1:B:799:PRO:HD2	1:B:903:LEU:HD11	1.83	0.61
1:C:499:ILE:HD12	1:C:507:ARG:HB3	1.82	0.61
1:C:931:LEU:HD11	1:C:1314:MET:SD	2.41	0.61
1:A:426:LYS:HA	1:B:1191:ALA:HB3	1.83	0.61
1:C:32:MET:HG2	1:C:679:THR:HG23	1.83	0.61
1:A:32:MET:HG2	1:A:679:THR:HG23	1.81	0.60
1:D:919:LEU:H	1:D:1229:THR:HG22	1.65	0.60
1:D:32:MET:HG2	1:D:679:THR:HG23	1.82	0.60
1:A:799:PRO:HD2	1:A:903:LEU:HD11	1.83	0.60
1:B:989:TYR:HA	1:B:1262:SER:HB3	1.83	0.60
1:D:764:GLU:HB3	1:D:787:ARG:HG3	1.84	0.60
1:B:32:MET:HG2	1:B:679:THR:HG23	1.82	0.60
1:D:989:TYR:HA	1:D:1262:SER:HB3	1.83	0.60
1:B:931:LEU:HD11	1:B:1314:MET:SD	2.42	0.59
1:D:1182:HIS:NE2	1:D:1237:TRP:HB3	2.17	0.59
1:B:1182:HIS:NE2	1:B:1237:TRP:HB3	2.17	0.59
1:C:1182:HIS:NE2	1:C:1237:TRP:HB3	2.16	0.59
1:A:989:TYR:HA	1:A:1262:SER:HB3	1.85	0.59
1:C:989:TYR:HA	1:C:1262:SER:HB3	1.83	0.59
1:D:33:VAL:HG11	1:D:105:VAL:HG11	1.85	0.59
1:C:600:VAL:HG12	1:C:738:THR:HA	1.84	0.58
1:C:616:SER:HA	1:C:619:TYR:CD2	2.38	0.58
1:A:764:GLU:HB3	1:A:787:ARG:HG3	1.85	0.58
1:C:764:GLU:HB3	1:C:787:ARG:HG3	1.85	0.58
1:D:273:SER:HB2	1:D:314:LYS:HA	1.85	0.58
1:C:138:TYR:HB2	1:C:221:VAL:HG22	1.85	0.58
1:D:600:VAL:HG12	1:D:738:THR:HA	1.86	0.58
1:B:33:VAL:HG11	1:B:105:VAL:HG11	1.86	0.58
1:B:764:GLU:HB3	1:B:787:ARG:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:SER:HB2	1:C:314:LYS:HA	1.85	0.58
1:A:138:TYR:HB2	1:A:221:VAL:HG22	1.85	0.58
1:A:33:VAL:HG11	1:A:105:VAL:HG11	1.85	0.57
1:C:385:PHE:HB2	1:C:422:ARG:HB2	1.86	0.57
1:A:1119:PRO:HB2	1:D:117:ARG:HH22	1.69	0.57
1:A:616:SER:HA	1:A:619:TYR:CD2	2.40	0.57
1:B:958:ALA:HA	1:B:961:ASN:HD21	1.69	0.57
1:A:273:SER:HB2	1:A:314:LYS:HA	1.86	0.57
1:B:385:PHE:HB2	1:B:422:ARG:HB2	1.86	0.57
1:C:1248:PHE:HB2	1:C:1254:THR:HG23	1.85	0.57
1:D:1248:PHE:HB2	1:D:1254:THR:HG23	1.86	0.57
1:A:385:PHE:HB2	1:A:422:ARG:HB2	1.86	0.57
1:B:600:VAL:HG12	1:B:738:THR:HA	1.87	0.56
1:C:667:TYR:HB2	1:C:684:ARG:HA	1.87	0.56
1:C:1391:PRO:HG2	1:C:1410:VAL:HG11	1.87	0.56
1:B:1242:GLN:HB2	1:B:1246:GLY:HA2	1.87	0.56
1:D:385:PHE:HB2	1:D:422:ARG:HB2	1.85	0.56
1:B:138:TYR:HB2	1:B:221:VAL:HG22	1.87	0.56
1:D:1242:GLN:HB2	1:D:1246:GLY:HA2	1.88	0.56
1:B:1038:ASN:HD22	1:B:1041:LEU:H	1.54	0.56
1:D:138:TYR:HB2	1:D:221:VAL:HG22	1.86	0.56
1:A:1242:GLN:HB2	1:A:1246:GLY:HA2	1.87	0.56
1:C:1038:ASN:HD22	1:C:1041:LEU:H	1.53	0.56
1:C:1367:VAL:HG21	1:C:1449:VAL:HG21	1.87	0.56
1:C:1391:PRO:HA	1:C:1433:VAL:HG12	1.86	0.56
1:C:1242:GLN:HB2	1:C:1246:GLY:HA2	1.88	0.56
1:A:1038:ASN:HD22	1:A:1041:LEU:H	1.54	0.56
1:A:389:ASN:HB2	1:A:418:SER:HB2	1.87	0.56
1:C:389:ASN:HB2	1:C:418:SER:HB2	1.88	0.56
1:A:600:VAL:HG12	1:A:738:THR:HA	1.86	0.55
1:C:814:VAL:HG11	1:C:824:VAL:HG11	1.89	0.55
1:D:389:ASN:HB2	1:D:418:SER:HB2	1.88	0.55
1:A:667:TYR:HB2	1:A:684:ARG:HA	1.89	0.55
1:B:273:SER:HB2	1:B:314:LYS:HA	1.87	0.55
1:D:958:ALA:HA	1:D:961:ASN:HD21	1.70	0.55
1:B:1248:PHE:HB2	1:B:1254:THR:HG23	1.88	0.55
1:C:958:ALA:HA	1:C:961:ASN:HD21	1.70	0.55
1:B:389:ASN:HB2	1:B:418:SER:HB2	1.87	0.55
1:B:667:TYR:HB2	1:B:684:ARG:HA	1.89	0.55
1:D:616:SER:HA	1:D:619:TYR:CD2	2.42	0.55
1:A:1248:PHE:HB2	1:A:1254:THR:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:SER:HA	1:B:619:TYR:CD2	2.42	0.55
1:D:1038:ASN:HD22	1:D:1041:LEU:H	1.54	0.55
1:A:794:VAL:HG12	1:A:814:VAL:HA	1.89	0.54
1:D:208:GLN:HG3	1:D:214:ARG:HG2	1.90	0.54
1:C:794:VAL:HG12	1:C:814:VAL:HA	1.89	0.54
1:D:667:TYR:HB2	1:D:684:ARG:HA	1.89	0.54
1:B:814:VAL:HG11	1:B:824:VAL:HG11	1.90	0.54
1:C:1038:ASN:HA	1:C:1084:GLY:HA3	1.89	0.54
1:C:1369:TYR:HE2	1:C:1372:SER:HA	1.73	0.54
1:A:813:THR:HB	1:A:855:THR:HG23	1.89	0.54
1:A:261:PRO:O	1:A:326:ILE:HG23	2.08	0.54
1:B:498:LEU:HD23	1:B:508:THR:HA	1.89	0.54
1:C:1369:TYR:CD2	1:C:1422:VAL:HB	2.43	0.54
1:C:1365:LEU:HD22	1:C:1447:VAL:HG11	1.89	0.54
1:C:498:LEU:HD23	1:C:508:THR:HA	1.88	0.54
1:A:958:ALA:HA	1:A:961:ASN:HD21	1.73	0.54
1:D:803:ILE:HB	1:D:806:GLU:HB2	1.90	0.54
1:A:498:LEU:HD23	1:A:508:THR:HA	1.90	0.54
1:B:500:MET:HG2	1:B:505:ILE:HA	1.90	0.54
1:A:1038:ASN:HA	1:A:1084:GLY:HA3	1.90	0.53
1:A:177:GLN:HB2	1:A:1299:LEU:HD13	1.90	0.53
1:A:814:VAL:HG11	1:A:824:VAL:HG11	1.89	0.53
1:B:1038:ASN:HA	1:B:1084:GLY:HA3	1.90	0.53
1:C:803:ILE:HB	1:C:806:GLU:HB2	1.90	0.53
1:D:148:VAL:HG23	1:D:183:LEU:HD21	1.91	0.53
1:C:813:THR:HB	1:C:855:THR:HG23	1.90	0.53
1:D:500:MET:HG2	1:D:505:ILE:HA	1.89	0.53
1:D:794:VAL:HG12	1:D:814:VAL:HA	1.89	0.53
1:C:208:GLN:HG3	1:C:214:ARG:HG2	1.90	0.53
1:C:500:MET:HG2	1:C:505:ILE:HA	1.91	0.53
1:C:993:THR:HB	1:C:995:GLN:HE21	1.74	0.53
1:A:273:SER:HB3	1:A:314:LYS:HG3	1.91	0.53
1:B:256:TYR:HA	1:B:787:ARG:HG2	1.90	0.53
1:C:273:SER:HB3	1:C:314:LYS:HG3	1.91	0.53
1:A:803:ILE:HB	1:A:806:GLU:HB2	1.90	0.53
1:C:261:PRO:O	1:C:326:ILE:HG23	2.08	0.53
1:D:813:THR:HB	1:D:855:THR:HG23	1.89	0.53
1:B:177:GLN:HB2	1:B:1299:LEU:HD13	1.91	0.53
1:D:1038:ASN:HA	1:D:1084:GLY:HA3	1.90	0.53
1:D:1160:GLN:HA	1:D:1163:ARG:HG2	1.91	0.53
1:D:286:PHE:HE2	1:D:309:PHE:HA	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:814:VAL:HG11	1:D:824:VAL:HG11	1.90	0.53
1:B:135:LYS:HE2	1:B:142:GLN:HE22	1.73	0.53
1:B:813:THR:HB	1:B:855:THR:HG23	1.90	0.53
1:B:1160:GLN:HA	1:B:1163:ARG:HG2	1.91	0.52
1:C:1392:LEU:HG	1:C:1394:PRO:HD2	1.92	0.52
1:C:256:TYR:HA	1:C:787:ARG:HG2	1.91	0.52
1:C:589:ALA:HB3	1:C:746:VAL:HG21	1.91	0.52
1:C:1182:HIS:CD2	1:C:1237:TRP:HB3	2.44	0.52
1:C:1363:ILE:HD11	1:C:1433:VAL:HG22	1.92	0.52
1:C:286:PHE:HE2	1:C:309:PHE:HA	1.74	0.52
1:D:261:PRO:O	1:D:326:ILE:HG23	2.09	0.52
1:B:261:PRO:O	1:B:326:ILE:HG23	2.09	0.52
1:B:371:LEU:HD11	1:B:423:VAL:HG21	1.91	0.52
1:B:794:VAL:HG12	1:B:814:VAL:HA	1.91	0.52
1:C:177:GLN:HB2	1:C:1299:LEU:HD13	1.92	0.52
1:D:256:TYR:HA	1:D:787:ARG:HG2	1.91	0.52
1:B:208:GLN:HG3	1:B:214:ARG:HG2	1.92	0.52
1:C:1160:GLN:HA	1:C:1163:ARG:HG2	1.91	0.52
1:A:500:MET:HG2	1:A:505:ILE:HA	1.92	0.52
1:B:133:THR:HG22	1:B:146:PHE:HB3	1.91	0.52
1:C:148:VAL:HG23	1:C:183:LEU:HD21	1.92	0.52
1:A:1182:HIS:CD2	1:A:1237:TRP:HB3	2.45	0.52
1:D:498:LEU:HD23	1:D:508:THR:HA	1.92	0.52
1:D:993:THR:HB	1:D:995:GLN:HE21	1.73	0.52
1:D:273:SER:HB3	1:D:314:LYS:HG3	1.92	0.51
1:A:135:LYS:HE2	1:A:142:GLN:HE22	1.74	0.51
1:D:1242:GLN:HB3	1:D:1248:PHE:CE1	2.45	0.51
1:B:589:ALA:HB3	1:B:746:VAL:HG21	1.93	0.51
1:C:345:ARG:HD3	1:C:438:SER:HA	1.92	0.51
1:A:1160:GLN:HA	1:A:1163:ARG:HG2	1.91	0.51
1:B:148:VAL:HG23	1:B:183:LEU:HD21	1.93	0.51
1:B:826:VAL:HG13	1:B:874:ALA:HB2	1.93	0.51
1:A:1022:ASP:OD1	1:A:1024:SER:HB2	2.10	0.51
1:D:265:THR:HG23	1:D:323:GLU:HB2	1.93	0.51
1:B:1182:HIS:CD2	1:B:1237:TRP:HB3	2.45	0.51
1:B:350:LEU:HD13	1:B:421:VAL:HB	1.93	0.51
1:A:286:PHE:HE2	1:A:309:PHE:HA	1.76	0.51
1:B:345:ARG:HD3	1:B:438:SER:HA	1.93	0.51
1:C:1125:LEU:HA	1:C:1128:LEU:HD12	1.92	0.51
1:A:826:VAL:HG13	1:A:874:ALA:HB2	1.93	0.51
1:B:286:PHE:HE2	1:B:309:PHE:HA	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:LYS:HE2	1:D:142:GLN:HE22	1.76	0.51
1:A:208:GLN:HG3	1:A:214:ARG:HG2	1.92	0.51
1:B:273:SER:HB3	1:B:314:LYS:HG3	1.93	0.51
1:C:1022:ASP:OD1	1:C:1024:SER:HB2	2.11	0.51
1:A:371:LEU:HD11	1:A:423:VAL:HG21	1.91	0.51
1:B:1022:ASP:OD1	1:B:1024:SER:HB2	2.11	0.51
1:B:1242:GLN:HB3	1:B:1248:PHE:CE1	2.46	0.51
1:B:820:LYS:HD2	1:B:891:PRO:HB3	1.93	0.50
1:D:1125:LEU:HA	1:D:1128:LEU:HD12	1.93	0.50
1:D:133:THR:HG22	1:D:146:PHE:HB3	1.93	0.50
1:A:256:TYR:HA	1:A:787:ARG:HG2	1.92	0.50
1:A:589:ALA:HB3	1:A:746:VAL:HG21	1.93	0.50
1:B:1125:LEU:HA	1:B:1128:LEU:HD12	1.93	0.50
1:A:148:VAL:HG23	1:A:183:LEU:HD21	1.93	0.50
1:B:803:ILE:HB	1:B:806:GLU:HB2	1.91	0.50
1:B:1053:ARG:HH12	1:B:1113:PRO:HD2	1.77	0.50
1:C:1242:GLN:HB3	1:C:1248:PHE:CE1	2.46	0.50
1:D:1182:HIS:CD2	1:D:1237:TRP:HB3	2.46	0.50
1:D:345:ARG:HD3	1:D:438:SER:HA	1.92	0.50
1:A:345:ARG:HD3	1:A:438:SER:HA	1.94	0.50
1:A:993:THR:HB	1:A:995:GLN:HE21	1.75	0.50
1:A:1242:GLN:HB3	1:A:1248:PHE:CE1	2.46	0.50
1:B:993:THR:HB	1:B:995:GLN:HE21	1.76	0.50
1:A:1080:PHE:CE1	1:A:1105:ILE:HD11	2.47	0.50
1:A:387:ARG:HB2	1:A:420:THR:HB	1.94	0.50
1:A:390:GLU:HG3	1:A:417:THR:HA	1.94	0.50
1:C:1053:ARG:HH12	1:C:1113:PRO:HD2	1.77	0.50
1:C:1385:MET:HB2	1:C:1413:ASN:HB3	1.93	0.50
1:D:589:ALA:HB3	1:D:746:VAL:HG21	1.93	0.50
1:A:1125:LEU:HA	1:A:1128:LEU:HD12	1.93	0.49
1:B:828:LEU:HD21	1:B:834:PHE:HE1	1.77	0.49
1:C:1175:VAL:HG22	1:C:1453:TYR:HA	1.93	0.49
1:C:1383:VAL:HG13	1:C:1447:VAL:HG22	1.94	0.49
1:D:371:LEU:HD11	1:D:423:VAL:HG21	1.94	0.49
1:C:498:LEU:HB3	1:C:505:ILE:HD11	1.94	0.49
1:D:1053:ARG:HH12	1:D:1113:PRO:HD2	1.77	0.49
1:A:828:LEU:HD21	1:A:834:PHE:HE1	1.77	0.49
1:B:116:LYS:HB3	1:B:678:PHE:HD2	1.78	0.49
1:C:135:LYS:HE2	1:C:142:GLN:HE22	1.76	0.49
1:C:133:THR:HG22	1:C:146:PHE:HB3	1.94	0.49
1:C:826:VAL:HG13	1:C:874:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1022:ASP:OD1	1:D:1024:SER:HB2	2.11	0.49
1:D:177:GLN:HB2	1:D:1299:LEU:HD13	1.93	0.49
1:C:1408:THR:HG22	1:C:1417:ILE:HG12	1.93	0.49
1:C:371:LEU:HD11	1:C:423:VAL:HG21	1.93	0.49
1:A:1183:TRP:HE3	1:A:1209:THR:HG22	1.77	0.49
1:A:1206:VAL:HG11	1:A:1241:GLN:HG3	1.94	0.49
1:B:265:THR:HG23	1:B:323:GLU:HB2	1.94	0.49
1:D:826:VAL:HG13	1:D:874:ALA:HB2	1.94	0.49
1:B:1106:THR:HG21	1:B:1128:LEU:HD11	1.94	0.49
1:B:230:GLU:HB2	1:B:606:LEU:HD22	1.95	0.49
1:D:350:LEU:HD13	1:D:421:VAL:HB	1.93	0.49
1:A:920:LEU:HD12	1:A:1324:LEU:HD13	1.95	0.49
1:A:133:THR:HG22	1:A:146:PHE:HB3	1.95	0.49
1:B:1206:VAL:HG11	1:B:1241:GLN:HG3	1.95	0.49
1:B:913:GLU:HG3	1:B:1329:LYS:HG3	1.94	0.49
1:C:820:LYS:HD2	1:C:891:PRO:HB3	1.94	0.49
1:A:1053:ARG:HH12	1:A:1113:PRO:HD2	1.78	0.49
1:C:828:LEU:HD21	1:C:834:PHE:HE1	1.78	0.49
1:A:1075:LYS:C	1:A:1077:ASN:H	2.16	0.49
1:B:321:HIS:CD2	1:B:337:GLY:HA3	2.48	0.49
1:C:1399:LEU:HB3	1:C:1405:VAL:HG21	1.94	0.49
1:B:1119:PRO:HB2	1:C:117:ARG:HH22	1.77	0.49
1:C:390:GLU:HG3	1:C:417:THR:HA	1.95	0.49
1:D:116:LYS:HB3	1:D:678:PHE:HD2	1.77	0.49
1:B:498:LEU:HB3	1:B:505:ILE:HD11	1.96	0.48
1:C:265:THR:HG23	1:C:323:GLU:HB2	1.94	0.48
1:C:350:LEU:HD13	1:C:421:VAL:HB	1.94	0.48
1:D:391:ALA:HB2	1:D:413:ASN:HD21	1.78	0.48
1:D:230:GLU:HB2	1:D:606:LEU:HD22	1.95	0.48
1:C:1183:TRP:HE3	1:C:1209:THR:HG22	1.78	0.48
1:C:823:ARG:HG2	1:C:845:PRO:HB2	1.95	0.48
1:D:1206:VAL:HG11	1:D:1241:GLN:HG3	1.95	0.48
1:D:498:LEU:HB3	1:D:505:ILE:HD11	1.95	0.48
1:A:265:THR:HG23	1:A:323:GLU:HB2	1.94	0.48
1:A:230:GLU:HB2	1:A:606:LEU:HD22	1.94	0.48
1:B:387:ARG:HB2	1:B:420:THR:HB	1.95	0.48
1:B:390:GLU:HG3	1:B:417:THR:HA	1.95	0.48
1:C:1075:LYS:C	1:C:1077:ASN:H	2.16	0.48
1:D:820:LYS:HD2	1:D:891:PRO:HB3	1.96	0.48
1:D:920:LEU:HD12	1:D:1324:LEU:HD13	1.96	0.48
1:A:1119:PRO:HB2	1:D:117:ARG:HH12	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:TYR:CZ	1:C:522:GLY:HA3	2.49	0.48
1:A:350:LEU:HD13	1:A:421:VAL:HB	1.95	0.48
1:B:1183:TRP:HE3	1:B:1209:THR:HG22	1.77	0.48
1:C:116:LYS:HB3	1:C:678:PHE:HD2	1.78	0.48
1:C:860:VAL:HG11	1:C:870:PHE:HE2	1.78	0.48
1:D:261:PRO:HD2	1:D:853:ARG:NH2	2.28	0.48
1:A:116:LYS:HB3	1:A:678:PHE:HD2	1.79	0.48
1:A:498:LEU:HB3	1:A:505:ILE:HD11	1.96	0.48
1:A:261:PRO:HD2	1:A:853:ARG:NH2	2.28	0.48
1:C:321:HIS:CD2	1:C:337:GLY:HA3	2.49	0.48
1:D:387:ARG:HB2	1:D:420:THR:HB	1.96	0.48
1:C:1206:VAL:HG11	1:C:1241:GLN:HG3	1.96	0.48
1:C:1379:ALA:HB2	1:C:1422:VAL:HG13	1.96	0.48
1:D:321:HIS:CD2	1:D:337:GLY:HA3	2.48	0.48
1:B:920:LEU:HD12	1:B:1324:LEU:HD13	1.95	0.47
1:C:1080:PHE:CE1	1:C:1105:ILE:HD11	2.49	0.47
1:C:538:ALA:HB3	1:C:558:TYR:HB2	1.96	0.47
1:B:1306:PRO:O	1:B:1307:GLU:HB2	2.15	0.47
1:A:619:TYR:CD1	1:A:619:TYR:N	2.82	0.47
1:D:1080:PHE:CE1	1:D:1105:ILE:HD11	2.49	0.47
1:D:1232:THR:HG22	1:D:1264:TYR:OH	2.14	0.47
1:B:1075:LYS:C	1:B:1077:ASN:H	2.17	0.47
1:B:823:ARG:HG2	1:B:845:PRO:HB2	1.97	0.47
1:C:261:PRO:HD2	1:C:853:ARG:NH2	2.30	0.47
1:D:619:TYR:N	1:D:619:TYR:CD1	2.83	0.47
1:D:828:LEU:HD21	1:D:834:PHE:HE1	1.78	0.47
1:C:1343:LEU:HD13	1:C:1449:VAL:HB	1.97	0.47
1:D:1145:TYR:HB3	1:D:1185:ARG:HH21	1.79	0.47
1:A:823:ARG:HG2	1:A:845:PRO:HB2	1.96	0.47
1:A:820:LYS:HD2	1:A:891:PRO:HB3	1.95	0.47
1:B:619:TYR:CD1	1:B:619:TYR:N	2.83	0.47
1:A:1106:THR:HG21	1:A:1128:LEU:HD11	1.95	0.47
1:A:581:SER:HA	1:A:756:VAL:HG13	1.97	0.47
1:C:1232:THR:HG22	1:C:1264:TYR:OH	2.15	0.47
1:A:321:HIS:CD2	1:A:337:GLY:HA3	2.49	0.47
1:B:1118:HIS:CD2	1:B:1120:VAL:H	2.33	0.47
1:B:238:ILE:HG12	1:B:375:LYS:HG2	1.97	0.47
1:C:1399:LEU:HD22	1:C:1429:LEU:HD23	1.97	0.47
1:D:1183:TRP:HE3	1:D:1209:THR:HG22	1.80	0.47
1:D:390:GLU:HG3	1:D:417:THR:HA	1.96	0.47
1:B:538:ALA:HB3	1:B:558:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1080:PHE:CE1	1:B:1105:ILE:HD11	2.50	0.47
1:D:984:ILE:HB	1:D:1008:LEU:HD11	1.97	0.47
1:D:480:TYR:CZ	1:D:522:GLY:HA3	2.50	0.47
1:D:823:ARG:HG2	1:D:845:PRO:HB2	1.97	0.47
1:A:480:TYR:CZ	1:A:522:GLY:HA3	2.50	0.46
1:B:480:TYR:CZ	1:B:522:GLY:HA3	2.50	0.46
1:B:860:VAL:HG11	1:B:870:PHE:HE2	1.80	0.46
1:C:1118:HIS:CD2	1:C:1120:VAL:H	2.34	0.46
1:D:1075:LYS:C	1:D:1077:ASN:H	2.17	0.46
1:A:615:ALA:O	1:A:619:TYR:CE1	2.69	0.46
1:C:1106:THR:HG21	1:C:1128:LEU:HD11	1.97	0.46
1:C:231:VAL:HB	1:C:336:THR:HG21	1.97	0.46
1:C:387:ARG:HB2	1:C:420:THR:HB	1.96	0.46
1:D:860:VAL:HG11	1:D:870:PHE:HE2	1.80	0.46
1:A:913:GLU:HG3	1:A:1329:LYS:HG3	1.96	0.46
1:C:985:TYR:CE2	1:C:1259:HIS:HB2	2.50	0.46
1:C:984:ILE:HB	1:C:1008:LEU:HD11	1.96	0.46
1:D:935:LEU:HB3	1:D:939:VAL:HG21	1.98	0.46
1:A:1145:TYR:HB3	1:A:1185:ARG:HH21	1.80	0.46
1:A:117:ARG:HH12	1:D:1119:PRO:HB2	1.80	0.46
2:B:2501:NAG:C8	2:B:2502:NAG:H82	2.42	0.46
1:B:261:PRO:HD2	1:B:853:ARG:NH2	2.29	0.46
1:B:391:ALA:HB2	1:B:413:ASN:HD21	1.81	0.46
1:D:1118:HIS:CD2	1:D:1120:VAL:H	2.34	0.46
1:A:1145:TYR:HD1	1:A:1208:MET:HB3	1.80	0.46
1:C:1145:TYR:HB3	1:C:1185:ARG:HH21	1.80	0.46
1:C:581:SER:HA	1:C:756:VAL:HG13	1.97	0.46
1:A:538:ALA:HB3	1:A:558:TYR:HB2	1.98	0.46
1:B:1232:THR:HG22	1:B:1264:TYR:OH	2.15	0.46
1:C:913:GLU:HG3	1:C:1329:LYS:HG3	1.98	0.46
1:C:230:GLU:HB2	1:C:606:LEU:HD22	1.97	0.46
1:A:860:VAL:HG11	1:A:870:PHE:HE2	1.81	0.46
1:C:391:ALA:HB2	1:C:413:ASN:HD21	1.80	0.46
1:A:1306:PRO:O	1:A:1307:GLU:HB2	2.16	0.46
1:A:369:VAL:HG23	1:A:405:VAL:HG23	1.98	0.46
1:A:391:ALA:HB2	1:A:413:ASN:HD21	1.80	0.46
1:B:581:SER:HA	1:B:756:VAL:HG13	1.98	0.46
1:C:108:LYS:HA	1:C:113:GLU:HG3	1.98	0.46
1:C:1306:PRO:O	1:C:1307:GLU:HB2	2.16	0.46
1:C:920:LEU:HD12	1:C:1324:LEU:HD13	1.97	0.46
1:C:1381:VAL:HG22	1:C:1449:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1106:THR:HG21	1:D:1128:LEU:HD11	1.97	0.46
1:C:1145:TYR:HD1	1:C:1208:MET:HB3	1.81	0.46
1:C:1213:LEU:HD23	1:C:1260:ALA:HB1	1.98	0.46
1:D:1306:PRO:O	1:D:1307:GLU:HB2	2.16	0.46
1:D:913:GLU:HG3	1:D:1329:LYS:HG3	1.98	0.46
1:A:1118:HIS:CD2	1:A:1120:VAL:H	2.33	0.46
1:B:984:ILE:HB	1:B:1008:LEU:HD11	1.97	0.46
1:C:615:ALA:O	1:C:619:TYR:CE1	2.69	0.46
1:A:238:ILE:HG12	1:A:375:LYS:HG2	1.97	0.45
1:C:1417:ILE:HD13	1:C:1429:LEU:HD22	1.98	0.45
1:A:984:ILE:HB	1:A:1008:LEU:HD11	1.97	0.45
1:B:1145:TYR:HB3	1:B:1185:ARG:HH21	1.80	0.45
1:C:1250:SER:HB2	1:C:1253:ASP:OD1	2.15	0.45
1:D:31:TYR:H	1:D:680:ASN:CB	2.30	0.45
1:B:958:ALA:HB1	1:B:1248:PHE:HZ	1.81	0.45
1:D:1278:VAL:HB	1:D:1290:PHE:HB2	1.99	0.45
1:D:369:VAL:HG23	1:D:405:VAL:HG23	1.98	0.45
1:D:238:ILE:HG12	1:D:375:LYS:HG2	1.98	0.45
1:D:581:SER:HA	1:D:756:VAL:HG13	1.97	0.45
1:D:958:ALA:HB1	1:D:1248:PHE:HZ	1.80	0.45
1:C:1038:ASN:ND2	1:C:1041:LEU:H	2.15	0.45
1:C:61:SER:HB3	1:C:74:PHE:CE1	2.52	0.45
1:D:1145:TYR:HD1	1:D:1208:MET:HB3	1.81	0.45
1:D:538:ALA:HB3	1:D:558:TYR:HB2	1.98	0.45
1:C:958:ALA:HB1	1:C:1248:PHE:HZ	1.81	0.45
1:B:985:TYR:CE2	1:B:1259:HIS:HB2	2.52	0.45
1:D:1250:SER:HB2	1:D:1253:ASP:OD1	2.17	0.45
1:A:1152:TYR:O	1:A:1156:LEU:HB2	2.17	0.45
1:B:1250:SER:HB2	1:B:1253:ASP:OD1	2.16	0.45
1:D:1092:LYS:HB3	1:D:1093:GLY:H	1.63	0.45
1:A:1232:THR:HG22	1:A:1264:TYR:OH	2.16	0.44
1:B:1213:LEU:HD23	1:B:1260:ALA:HB1	1.99	0.44
1:C:369:VAL:HG23	1:C:405:VAL:HG23	1.99	0.44
1:C:619:TYR:CD1	1:C:619:TYR:N	2.84	0.44
1:A:985:TYR:CE2	1:A:1259:HIS:HB2	2.52	0.44
1:A:935:LEU:HB3	1:A:939:VAL:HG21	1.99	0.44
1:C:387:ARG:HG3	1:C:422:ARG:HD2	2.00	0.44
1:D:108:LYS:HA	1:D:113:GLU:HG3	1.99	0.44
1:D:387:ARG:HG3	1:D:422:ARG:HD2	1.99	0.44
1:D:128:LEU:HD23	1:D:621:LEU:HB3	2.00	0.44
2:A:2501:NAG:C8	2:A:2502:NAG:H82	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:TYR:H	1:A:680:ASN:CB	2.31	0.44
1:B:615:ALA:O	1:B:619:TYR:CE1	2.69	0.44
1:D:1038:ASN:ND2	1:D:1041:LEU:H	2.15	0.44
1:D:615:ALA:O	1:D:619:TYR:CE1	2.70	0.44
1:A:380:PRO:HB3	1:A:401:GLU:HA	2.00	0.44
1:B:1038:ASN:ND2	1:B:1041:LEU:H	2.16	0.44
1:B:259:PRO:HG2	1:B:297:HIS:HA	2.00	0.44
1:B:231:VAL:HB	1:B:336:THR:HG21	2.00	0.44
1:A:1193:VAL:HB	1:B:387:ARG:NH1	2.33	0.44
2:C:2501:NAG:C8	2:C:2502:NAG:H82	2.43	0.44
1:C:388:GLY:HA3	1:C:393:TYR:H	1.83	0.44
1:C:599:ALA:HB3	1:C:740:ILE:H	1.82	0.44
1:B:581:SER:O	1:B:756:VAL:HA	2.18	0.44
1:C:238:ILE:HG12	1:C:375:LYS:HG2	1.99	0.44
1:D:1281:GLN:HA	1:D:1287:SER:HB3	2.00	0.44
1:D:388:GLY:HA3	1:D:393:TYR:H	1.82	0.44
1:A:1110:LEU:HD22	1:A:1156:LEU:HG	1.99	0.44
1:A:958:ALA:HB1	1:A:1248:PHE:HZ	1.82	0.44
1:B:108:LYS:HA	1:B:113:GLU:HG3	1.99	0.44
1:B:1145:TYR:HD1	1:B:1208:MET:HB3	1.81	0.44
1:B:369:VAL:HG23	1:B:405:VAL:HG23	1.99	0.44
1:D:985:TYR:CE2	1:D:1259:HIS:HB2	2.53	0.44
4:A:2601:NAG:C8	4:A:2602:NAG:H83	2.48	0.44
1:A:599:ALA:HB3	1:A:740:ILE:H	1.83	0.44
1:B:935:LEU:HB3	1:B:939:VAL:HG21	1.99	0.44
1:C:1177:LYS:HG3	1:C:1455:THR:HG21	1.98	0.44
1:C:31:TYR:H	1:C:680:ASN:CB	2.31	0.44
1:D:380:PRO:HB3	1:D:401:GLU:HA	1.99	0.44
1:A:1250:SER:HB2	1:A:1253:ASP:OD1	2.18	0.44
1:B:380:PRO:HB3	1:B:401:GLU:HA	2.00	0.44
1:B:128:LEU:HD23	1:B:621:LEU:HB3	1.99	0.44
1:B:602:GLN:HB3	1:B:763:THR:HG23	2.00	0.44
1:B:797:THR:HB	1:B:811:LYS:HB2	2.00	0.44
1:C:1152:TYR:O	1:C:1156:LEU:HB2	2.17	0.44
1:D:581:SER:O	1:D:756:VAL:HA	2.18	0.44
1:A:1101:LEU:O	1:A:1105:ILE:HG23	2.18	0.43
1:A:108:LYS:HA	1:A:113:GLU:HG3	1.99	0.43
1:A:1213:LEU:HD23	1:A:1260:ALA:HB1	2.00	0.43
1:D:61:SER:HB3	1:D:74:PHE:CE1	2.53	0.43
1:C:380:PRO:HB3	1:C:401:GLU:HA	2.00	0.43
1:A:984:ILE:HD12	1:A:1051:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1279:THR:HG22	1:B:1289:LYS:HG3	2.01	0.43
1:B:388:GLY:HA3	1:B:393:TYR:H	1.82	0.43
1:B:31:TYR:H	1:B:680:ASN:CB	2.30	0.43
1:C:1448:LYS:HA	1:C:1460:ILE:HG12	2.01	0.43
1:C:156:HIS:HB3	1:C:777:GLY:HA2	2.00	0.43
1:D:231:VAL:HB	1:D:336:THR:HG21	1.99	0.43
1:D:602:GLN:HB3	1:D:763:THR:HG23	2.00	0.43
1:A:1038:ASN:ND2	1:A:1041:LEU:H	2.15	0.43
1:A:231:VAL:HB	1:A:336:THR:HG21	2.00	0.43
1:B:822:ILE:HG22	1:B:889:SER:HA	2.01	0.43
1:C:1278:VAL:HB	1:C:1290:PHE:HB2	2.01	0.43
1:A:1279:THR:HG22	1:A:1289:LYS:HG3	2.01	0.43
1:D:1101:LEU:O	1:D:1105:ILE:HG23	2.18	0.43
1:B:100:VAL:HG22	1:B:121:MET:HG2	2.00	0.43
1:B:599:ALA:HB3	1:B:740:ILE:H	1.84	0.43
4:D:2601:NAG:C8	4:D:2602:NAG:H83	2.48	0.43
1:C:1182:HIS:ND1	1:C:1237:TRP:HE3	2.17	0.43
4:C:2601:NAG:C8	4:C:2602:NAG:H83	2.48	0.43
1:D:1152:TYR:O	1:D:1156:LEU:HB2	2.18	0.43
1:D:903:LEU:HD23	1:D:904:LEU:H	1.84	0.43
1:C:970:TYR:HA	1:C:1014:ARG:HH21	1.84	0.43
1:D:822:ILE:HG22	1:D:889:SER:HA	2.00	0.43
1:A:1305:LEU:HA	1:A:1306:PRO:HD3	1.95	0.43
1:B:1278:VAL:HB	1:B:1290:PHE:HB2	2.00	0.43
4:B:2601:NAG:C8	4:B:2602:NAG:H83	2.49	0.43
1:B:970:TYR:HA	1:B:1014:ARG:HH21	1.84	0.43
1:C:797:THR:HB	1:C:811:LYS:HB2	2.00	0.43
1:A:1182:HIS:ND1	1:A:1237:TRP:HE3	2.16	0.43
1:A:581:SER:O	1:A:756:VAL:HA	2.19	0.43
1:C:935:LEU:HB3	1:C:939:VAL:HG21	2.01	0.43
1:B:933:LEU:H	1:B:1310:GLY:HA2	1.84	0.42
1:C:46:LYS:HA	1:C:88:ALA:HA	2.01	0.42
1:D:933:LEU:H	1:D:1310:GLY:HA2	1.84	0.42
1:D:167:ILE:HG22	1:D:175:ILE:HD12	2.01	0.42
1:A:259:PRO:HG2	1:A:297:HIS:HA	2.01	0.42
1:A:797:THR:HB	1:A:811:LYS:HB2	2.01	0.42
1:A:822:ILE:HG22	1:A:889:SER:HA	2.00	0.42
1:D:599:ALA:HB3	1:D:740:ILE:H	1.83	0.42
1:A:1278:VAL:HB	1:A:1290:PHE:HB2	2.00	0.42
1:C:933:LEU:H	1:C:1310:GLY:HA2	1.84	0.42
1:D:46:LYS:HA	1:D:88:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLY:HA3	1:A:393:TYR:H	1.83	0.42
1:A:61:SER:HB3	1:A:74:PHE:CE1	2.54	0.42
1:B:1281:GLN:HA	1:B:1287:SER:HB3	2.00	0.42
1:B:156:HIS:HB3	1:B:777:GLY:HA2	2.01	0.42
1:D:1182:HIS:ND1	1:D:1237:TRP:HE3	2.16	0.42
1:D:360:ARG:HH11	1:D:458:PHE:HB2	1.85	0.42
1:D:970:TYR:HA	1:D:1014:ARG:HH21	1.84	0.42
1:A:1092:LYS:HB3	1:A:1093:GLY:H	1.63	0.42
1:B:1152:TYR:O	1:B:1156:LEU:HB2	2.18	0.42
1:B:61:SER:HB3	1:B:74:PHE:CE1	2.54	0.42
1:A:903:LEU:HD23	1:A:904:LEU:H	1.85	0.42
1:B:1101:LEU:O	1:B:1105:ILE:HG23	2.20	0.42
1:B:820:LYS:HD3	1:B:888:PRO:HB2	2.01	0.42
1:C:1281:GLN:HA	1:C:1287:SER:HB3	2.02	0.42
1:C:1376:SER:HB3	1:C:1422:VAL:HG21	2.01	0.42
1:D:797:THR:HB	1:D:811:LYS:HB2	2.01	0.42
1:D:820:LYS:HD3	1:D:888:PRO:HB2	2.01	0.42
1:A:46:LYS:HA	1:A:88:ALA:HA	2.02	0.42
1:B:1206:VAL:HG23	1:B:1253:ASP:OD2	2.19	0.42
1:B:360:ARG:HH11	1:B:458:PHE:HB2	1.85	0.42
1:C:360:ARG:HH11	1:C:458:PHE:HB2	1.83	0.42
1:D:734:TYR:H	1:D:759:PRO:HB2	1.85	0.42
1:A:970:TYR:HA	1:A:1014:ARG:HH21	1.84	0.42
1:C:1377:ASN:O	1:C:1421:LYS:HG3	2.19	0.42
1:D:100:VAL:HG22	1:D:121:MET:HG2	2.02	0.42
1:A:1050:ALA:O	1:A:1053:ARG:HD3	2.20	0.42
1:B:1182:HIS:ND1	1:B:1237:TRP:HE3	2.17	0.42
1:C:1101:LEU:O	1:C:1105:ILE:HG23	2.19	0.42
1:C:422:ARG:NE	1:D:1193:VAL:HG21	2.35	0.42
1:C:820:LYS:HD3	1:C:888:PRO:HB2	2.02	0.42
1:D:1206:VAL:HG23	1:D:1253:ASP:OD2	2.20	0.42
1:D:49:VAL:HG21	1:D:60:VAL:HG21	2.02	0.42
1:D:61:SER:HB3	1:D:74:PHE:HE1	1.85	0.42
1:B:984:ILE:HD12	1:B:1051:GLN:HG3	2.02	0.41
1:C:1039:THR:HG21	1:C:1081:ARG:O	2.20	0.41
1:C:1206:VAL:HG23	1:C:1253:ASP:OD2	2.20	0.41
1:A:128:LEU:HD23	1:A:621:LEU:HB3	2.01	0.41
1:A:360:ARG:HH11	1:A:458:PHE:HB2	1.84	0.41
1:B:1094:GLY:HA2	1:B:1145:TYR:HE2	1.86	0.41
1:B:1331:ASN:HD22	1:B:1331:ASN:N	2.18	0.41
1:B:330:GLY:C	1:B:332:VAL:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:TYR:H	1:B:759:PRO:HB2	1.86	0.41
1:D:1039:THR:HG21	1:D:1081:ARG:O	2.20	0.41
1:A:602:GLN:HB3	1:A:763:THR:HG23	2.02	0.41
1:C:802:VAL:HG21	1:C:808:PHE:CD1	2.55	0.41
1:A:820:LYS:HD3	1:A:888:PRO:HB2	2.01	0.41
1:B:260:VAL:HA	1:B:261:PRO:HD3	1.94	0.41
1:C:167:ILE:HG22	1:C:175:ILE:HD12	2.03	0.41
1:D:156:HIS:HB3	1:D:777:GLY:HA2	2.03	0.41
1:A:933:LEU:H	1:A:1310:GLY:HA2	1.84	0.41
1:A:387:ARG:HG3	1:A:422:ARG:HD2	2.02	0.41
1:A:734:TYR:H	1:A:759:PRO:HB2	1.85	0.41
1:C:822:ILE:HG22	1:C:889:SER:HA	2.01	0.41
1:A:388:GLY:O	1:A:392:ASN:HA	2.21	0.41
1:B:137:ILE:H	1:B:137:ILE:HG13	1.76	0.41
1:D:259:PRO:HG2	1:D:297:HIS:HA	2.02	0.41
1:A:1333:LEU:H	1:A:1334:PRO:HD2	1.86	0.41
1:A:542:ILE:O	1:A:553:GLY:HA3	2.21	0.41
1:C:1279:THR:HG22	1:C:1289:LYS:HG3	2.03	0.41
1:C:330:GLY:C	1:C:332:VAL:H	2.24	0.41
1:C:602:GLN:HB3	1:C:763:THR:HG23	2.02	0.41
1:C:734:TYR:H	1:C:759:PRO:HB2	1.85	0.41
1:D:330:GLY:C	1:D:332:VAL:H	2.24	0.41
1:D:802:VAL:HG21	1:D:808:PHE:CD1	2.55	0.41
1:A:758:VAL:HA	1:A:759:PRO:HD3	1.88	0.41
1:C:259:PRO:HG2	1:C:297:HIS:HA	2.02	0.41
1:C:581:SER:O	1:C:756:VAL:HA	2.20	0.41
1:B:961:ASN:HB2	1:B:1246:GLY:HA3	2.03	0.41
1:C:137:ILE:H	1:C:137:ILE:HG13	1.75	0.41
1:C:903:LEU:HD23	1:C:904:LEU:H	1.85	0.41
1:B:903:LEU:HD23	1:B:904:LEU:H	1.86	0.41
1:B:991:ASN:O	4:B:2601:NAG:H61	2.21	0.41
1:C:961:ASN:HB2	1:C:1246:GLY:HA3	2.03	0.41
1:C:1333:LEU:H	1:C:1334:PRO:HD2	1.85	0.41
1:D:192:PHE:HA	1:D:193:PRO:HD3	1.99	0.41
1:D:388:GLY:O	1:D:392:ASN:HA	2.21	0.41
1:A:1039:THR:HG21	1:A:1081:ARG:O	2.20	0.41
1:A:1331:ASN:N	1:A:1331:ASN:HD22	2.19	0.41
1:B:1050:ALA:O	1:B:1053:ARG:HD3	2.21	0.41
1:B:1183:TRP:H	1:B:1209:THR:CG2	2.34	0.41
1:B:1297:ARG:HH22	1:B:1320:GLY:HA3	1.86	0.41
1:C:1050:ALA:HA	1:C:1053:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1118:HIS:HD2	1:C:1120:VAL:HG22	1.84	0.41
1:C:1094:GLY:HA2	1:C:1145:TYR:HE2	1.86	0.41
1:D:468:LEU:HA	1:D:469:PRO:HD3	2.00	0.41
1:A:1206:VAL:HG23	1:A:1253:ASP:OD2	2.22	0.40
1:A:330:GLY:C	1:A:332:VAL:H	2.24	0.40
1:A:802:VAL:HG21	1:A:808:PHE:CD1	2.56	0.40
1:C:542:ILE:O	1:C:553:GLY:HA3	2.21	0.40
1:C:758:VAL:HA	1:C:759:PRO:HD3	1.87	0.40
1:A:100:VAL:HG22	1:A:121:MET:HG2	2.02	0.40
1:B:1039:THR:HG21	1:B:1081:ARG:O	2.21	0.40
1:B:388:GLY:O	1:B:392:ASN:HA	2.21	0.40
1:C:1106:THR:HG22	1:C:1124:ALA:HB1	2.03	0.40
1:D:1110:LEU:HD22	1:D:1156:LEU:HG	2.03	0.40
1:D:758:VAL:HA	1:D:759:PRO:HD3	1.88	0.40
1:D:984:ILE:HD12	1:D:1051:GLN:HG3	2.03	0.40
1:B:542:ILE:O	1:B:553:GLY:HA3	2.21	0.40
1:C:204:LYS:HD2	1:C:216:GLU:HG2	2.03	0.40
1:C:388:GLY:O	1:C:392:ASN:HA	2.21	0.40
1:D:1050:ALA:O	1:D:1053:ARG:HD3	2.21	0.40
1:D:1279:THR:HG22	1:D:1289:LYS:HG3	2.03	0.40
1:D:593:SER:HB3	1:D:773:SER:HB2	2.03	0.40
1:A:1305:LEU:HD13	1:A:1312:TYR:CD1	2.57	0.40
1:A:61:SER:HB3	1:A:74:PHE:HE1	1.87	0.40
1:A:961:ASN:HB2	1:A:1246:GLY:HA3	2.03	0.40
1:B:61:SER:HB3	1:B:74:PHE:HE1	1.86	0.40
1:B:593:SER:HB3	1:B:773:SER:HB2	2.02	0.40
1:A:984:ILE:HG13	1:A:1052:ALA:HA	2.04	0.40
1:B:1118:HIS:HD2	1:B:1120:VAL:HG22	1.84	0.40
1:B:802:VAL:HG21	1:B:808:PHE:CD1	2.57	0.40
1:C:1183:TRP:H	1:C:1209:THR:CG2	2.34	0.40
1:C:1331:ASN:N	1:C:1331:ASN:HD22	2.19	0.40
1:C:468:LEU:HD22	1:C:474:GLN:HG3	2.03	0.40
1:D:542:ILE:O	1:D:553:GLY:HA3	2.21	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	1265/1451 (87%)	1061 (84%)	147 (12%)	57 (4%)	3	30
1	B	1265/1451 (87%)	1058 (84%)	149 (12%)	58 (5%)	3	30
1	C	1398/1451 (96%)	1162 (83%)	177 (13%)	59 (4%)	3	31
1	D	1265/1451 (87%)	1059 (84%)	149 (12%)	57 (4%)	3	30
All	All	5193/5804 (90%)	4340 (84%)	622 (12%)	231 (4%)	3	31

All (231) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	PRO
1	A	425	TYR
1	A	429	SER
1	A	580	ALA
1	A	736	PRO
1	A	761	THR
1	A	953	ASP
1	A	1095	VAL
1	A	1199	PRO
1	A	1307	GLU
1	B	425	TYR
1	B	429	SER
1	B	580	ALA
1	B	736	PRO
1	B	761	THR
1	B	953	ASP
1	B	1095	VAL
1	B	1199	PRO
1	B	1307	GLU
1	C	429	SER
1	C	580	ALA
1	C	736	PRO

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Mol	Chain	Res	Type
1	C	761	THR
1	C	953	ASP
1	C	1095	VAL
1	C	1199	PRO
1	C	1307	GLU
1	D	429	SER
1	D	580	ALA
1	D	736	PRO
1	D	761	THR
1	D	953	ASP
1	D	1095	VAL
1	D	1199	PRO
1	D	1307	GLU
1	A	81	ASN
1	A	255	THR
1	A	296	SER
1	A	309	PHE
1	A	331	THR
1	A	581	SER
1	A	739	TRP
1	A	748	SER
1	A	1076	ASP
1	A	1096	GLU
1	B	81	ASN
1	B	198	PRO
1	B	255	THR
1	B	296	SER
1	B	581	SER
1	B	739	TRP
1	B	748	SER
1	B	1076	ASP
1	B	1096	GLU
1	C	81	ASN
1	C	198	PRO
1	C	255	THR
1	C	296	SER
1	C	330	GLY
1	C	425	TYR
1	C	581	SER
1	C	739	TRP
1	C	1076	ASP
1	C	1096	GLU

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Mol	Chain	Res	Type
1	D	81	ASN
1	D	198	PRO
1	D	255	THR
1	D	296	SER
1	D	309	PHE
1	D	425	TYR
1	D	581	SER
1	D	739	TRP
1	D	1076	ASP
1	D	1096	GLU
1	A	311	LEU
1	A	330	GLY
1	A	734	TYR
1	A	762	ILE
1	A	883	CYS
1	A	1060	GLU
1	A	1116	VAL
1	A	1142	SER
1	A	1191	ALA
1	A	1236	LYS
1	B	309	PHE
1	B	311	LEU
1	B	330	GLY
1	B	331	THR
1	B	734	TYR
1	B	762	ILE
1	B	1060	GLU
1	B	1116	VAL
1	B	1142	SER
1	B	1191	ALA
1	B	1236	LYS
1	C	309	PHE
1	C	311	LEU
1	C	331	THR
1	C	630	PHE
1	C	734	TYR
1	C	748	SER
1	C	762	ILE
1	C	883	CYS
1	C	1060	GLU
1	C	1116	VAL
1	C	1142	SER

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Mol	Chain	Res	Type
1	C	1187	GLN
1	C	1387	SER
1	C	1460	ILE
1	D	311	LEU
1	D	330	GLY
1	D	331	THR
1	D	734	TYR
1	D	748	SER
1	D	762	ILE
1	D	883	CYS
1	D	1060	GLU
1	D	1116	VAL
1	D	1142	SER
1	D	1187	GLN
1	D	1236	LYS
1	A	180	SER
1	A	241	ILE
1	A	254	TYR
1	A	630	PHE
1	A	1092	LYS
1	A	1144	VAL
1	A	1187	GLN
1	A	1222	ALA
1	A	1283	SER
1	A	1333	LEU
1	B	180	SER
1	B	241	ILE
1	B	254	TYR
1	B	454	PRO
1	B	630	PHE
1	B	883	CYS
1	B	1092	LYS
1	B	1144	VAL
1	B	1222	ALA
1	B	1283	SER
1	B	1333	LEU
1	C	180	SER
1	C	241	ILE
1	C	254	TYR
1	C	737	GLU
1	C	749	ALA
1	C	1092	LYS

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Mol	Chain	Res	Type
1	C	1144	VAL
1	C	1191	ALA
1	C	1222	ALA
1	C	1236	LYS
1	C	1333	LEU
1	C	1338	GLU
1	D	180	SER
1	D	241	ILE
1	D	254	TYR
1	D	454	PRO
1	D	630	PHE
1	D	642	CYS
1	D	1092	LYS
1	D	1144	VAL
1	D	1191	ALA
1	D	1222	ALA
1	D	1333	LEU
1	A	454	PRO
1	A	642	CYS
1	A	648	VAL
1	A	737	GLU
1	A	749	ALA
1	A	1113	PRO
1	A	1242	GLN
1	B	281	GLU
1	B	521	LYS
1	B	642	CYS
1	B	737	GLU
1	B	749	ALA
1	B	1113	PRO
1	B	1242	GLN
1	B	1273	GLY
1	C	281	GLU
1	C	339	GLN
1	C	454	PRO
1	C	632	GLY
1	C	648	VAL
1	C	1113	PRO
1	C	1242	GLN
1	D	281	GLU
1	D	339	GLN
1	D	632	GLY

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Mol	Chain	Res	Type
1	D	737	GLU
1	D	749	ALA
1	D	1113	PRO
1	D	1242	GLN
1	A	339	GLN
1	A	521	LYS
1	A	632	GLY
1	B	339	GLN
1	B	632	GLY
1	B	648	VAL
1	B	1179	ASN
1	C	521	LYS
1	C	683	ILE
1	C	1273	GLY
1	C	1283	SER
1	D	521	LYS
1	D	648	VAL
1	D	1283	SER
1	A	683	ILE
1	A	1273	GLY
1	B	683	ILE
1	D	683	ILE
1	D	1273	GLY
1	A	257	GLY
1	B	213	GLY
1	B	257	GLY
1	C	213	GLY
1	C	257	GLY
1	D	257	GLY
1	A	213	GLY
1	A	652	GLY
1	B	652	GLY
1	B	1188	LYS
1	C	652	GLY
1	D	652	GLY
1	C	437	VAL
1	D	213	GLY
1	D	437	VAL
1	A	437	VAL
1	A	1188	LYS
1	B	437	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1013/1268 (80%)	868 (86%)	145 (14%)	4	24
1	B	1013/1268 (80%)	869 (86%)	144 (14%)	4	25
1	C	1132/1268 (89%)	970 (86%)	162 (14%)	4	24
1	D	1013/1268 (80%)	868 (86%)	145 (14%)	4	24
All	All	4171/5072 (82%)	3575 (86%)	596 (14%)	4	24

All (596) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	MET
1	A	34	LEU
1	A	42	GLU
1	A	56	GLU
1	A	60	VAL
1	A	82	ASP
1	A	114	PHE
1	A	121	MET
1	A	126	ASP
1	A	129	VAL
1	A	153	GLU
1	A	154	ASN
1	A	161	LEU
1	A	173	ASN
1	A	175	ILE
1	A	194	LEU
1	A	198	PRO
1	A	199	PHE
1	A	200	GLN
1	A	238	ILE
1	A	251	CYS
1	A	265	THR
1	A	268	ILE
1	A	294	LEU

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Mol	Chain	Res	Type
1	A	321	HIS
1	A	326	ILE
1	A	331	THR
1	A	333	VAL
1	A	334	GLU
1	A	335	LEU
1	A	336	THR
1	A	341	SER
1	A	347	ILE
1	A	353	VAL
1	A	357	SER
1	A	360	ARG
1	A	361	GLN
1	A	371	LEU
1	A	405	VAL
1	A	406	GLN
1	A	409	ILE
1	A	420	THR
1	A	421	VAL
1	A	432	TYR
1	A	458	PHE
1	A	474	GLN
1	A	505	ILE
1	A	511	HIS
1	A	520	MET
1	A	524	PHE
1	A	541	LEU
1	A	542	ILE
1	A	563	CYS
1	A	585	LEU
1	A	587	VAL
1	A	598	ARG
1	A	600	VAL
1	A	610	ASP
1	A	619	TYR
1	A	622	LEU
1	A	675	LEU
1	A	679	THR
1	A	683	ILE
1	A	740	ILE
1	A	742	ASP
1	A	754	VAL

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Mol	Chain	Res	Type
1	A	761	THR
1	A	764	GLU
1	A	778	LEU
1	A	780	ILE
1	A	786	LEU
1	A	793	PHE
1	A	818	LEU
1	A	821	CYS
1	A	826	VAL
1	A	828	LEU
1	A	842	GLU
1	A	843	GLN
1	A	848	ILE
1	A	849	CYS
1	A	855	THR
1	A	856	VAL
1	A	857	SER
1	A	865	LEU
1	A	872	VAL
1	A	875	GLU
1	A	893	HIS
1	A	897	ASP
1	A	903	LEU
1	A	908	GLU
1	A	916	PHE
1	A	919	LEU
1	A	929	GLU
1	A	931	LEU
1	A	938	ASN
1	A	942	GLU
1	A	949	SER
1	A	959	MET
1	A	961	ASN
1	A	968	MET
1	A	983	ASN
1	A	984	ILE
1	A	992	GLU
1	A	1000	ILE
1	A	1005	ILE
1	A	1008	LEU
1	A	1024	SER
1	A	1039	THR

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Mol	Chain	Res	Type
1	A	1046	LEU
1	A	1067	LEU
1	A	1073	ARG
1	A	1077	ASN
1	A	1086	LEU
1	A	1087	LEU
1	A	1089	ASN
1	A	1091	ILE
1	A	1100	THR
1	A	1101	LEU
1	A	1105	ILE
1	A	1107	ILE
1	A	1110	LEU
1	A	1112	ILE
1	A	1114	LEU
1	A	1125	LEU
1	A	1150	LEU
1	A	1163	ARG
1	A	1184	GLU
1	A	1206	VAL
1	A	1236	LYS
1	A	1242	GLN
1	A	1245	GLN
1	A	1252	GLN
1	A	1277	GLN
1	A	1280	ILE
1	A	1281	GLN
1	A	1289	LYS
1	A	1291	GLN
1	A	1292	VAL
1	A	1294	ASN
1	A	1295	ASN
1	A	1298	LEU
1	A	1315	LYS
1	A	1328	LEU
1	A	1331	ASN
1	A	1333	LEU
1	B	32	MET
1	B	34	LEU
1	B	42	GLU
1	B	56	GLU
1	B	60	VAL

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Mol	Chain	Res	Type
1	B	82	ASP
1	B	114	PHE
1	B	121	MET
1	B	126	ASP
1	B	129	VAL
1	B	153	GLU
1	B	154	ASN
1	B	161	LEU
1	B	173	ASN
1	B	175	ILE
1	B	194	LEU
1	B	195	SER
1	B	199	PHE
1	B	200	GLN
1	B	238	ILE
1	B	251	CYS
1	B	265	THR
1	B	268	ILE
1	B	294	LEU
1	B	321	HIS
1	B	326	ILE
1	B	331	THR
1	B	333	VAL
1	B	334	GLU
1	B	335	LEU
1	B	336	THR
1	B	341	SER
1	B	347	ILE
1	B	353	VAL
1	B	360	ARG
1	B	361	GLN
1	B	371	LEU
1	B	405	VAL
1	B	406	GLN
1	B	409	ILE
1	B	420	THR
1	B	421	VAL
1	B	432	TYR
1	B	458	PHE
1	B	474	GLN
1	B	505	ILE
1	B	511	HIS

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Mol	Chain	Res	Type
1	B	520	MET
1	B	524	PHE
1	B	541	LEU
1	B	542	ILE
1	B	563	CYS
1	B	585	LEU
1	B	587	VAL
1	B	598	ARG
1	B	600	VAL
1	B	610	ASP
1	B	619	TYR
1	B	622	LEU
1	B	675	LEU
1	B	679	THR
1	B	683	ILE
1	B	740	ILE
1	B	742	ASP
1	B	754	VAL
1	B	761	THR
1	B	764	GLU
1	B	778	LEU
1	B	780	ILE
1	B	786	LEU
1	B	793	PHE
1	B	818	LEU
1	B	821	CYS
1	B	826	VAL
1	B	828	LEU
1	B	842	GLU
1	B	843	GLN
1	B	848	ILE
1	B	849	CYS
1	B	855	THR
1	B	856	VAL
1	B	857	SER
1	B	865	LEU
1	B	872	VAL
1	B	875	GLU
1	B	893	HIS
1	B	897	ASP
1	B	902	PRO
1	B	903	LEU

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Mol	Chain	Res	Type
1	B	908	GLU
1	B	916	PHE
1	B	919	LEU
1	B	929	GLU
1	B	931	LEU
1	B	938	ASN
1	B	942	GLU
1	B	949	SER
1	B	959	MET
1	B	961	ASN
1	B	968	MET
1	B	983	ASN
1	B	984	ILE
1	B	992	GLU
1	B	1000	ILE
1	B	1005	ILE
1	B	1008	LEU
1	B	1024	SER
1	B	1039	THR
1	B	1046	LEU
1	B	1073	ARG
1	B	1077	ASN
1	B	1086	LEU
1	B	1087	LEU
1	B	1089	ASN
1	B	1091	ILE
1	B	1100	THR
1	B	1101	LEU
1	B	1105	ILE
1	B	1107	ILE
1	B	1110	LEU
1	B	1112	ILE
1	B	1114	LEU
1	B	1125	LEU
1	B	1150	LEU
1	B	1163	ARG
1	B	1184	GLU
1	B	1188	LYS
1	B	1206	VAL
1	B	1236	LYS
1	B	1242	GLN
1	B	1245	GLN

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Mol	Chain	Res	Type
1	B	1252	GLN
1	B	1277	GLN
1	B	1280	ILE
1	B	1281	GLN
1	B	1289	LYS
1	B	1291	GLN
1	B	1292	VAL
1	B	1294	ASN
1	B	1295	ASN
1	B	1298	LEU
1	B	1315	LYS
1	B	1328	LEU
1	B	1331	ASN
1	C	32	MET
1	C	34	LEU
1	C	42	GLU
1	C	56	GLU
1	C	60	VAL
1	C	82	ASP
1	C	114	PHE
1	C	121	MET
1	C	126	ASP
1	C	129	VAL
1	C	154	ASN
1	C	161	LEU
1	C	173	ASN
1	C	175	ILE
1	C	194	LEU
1	C	199	PHE
1	C	200	GLN
1	C	238	ILE
1	C	251	CYS
1	C	265	THR
1	C	268	ILE
1	C	294	LEU
1	C	321	HIS
1	C	326	ILE
1	C	331	THR
1	C	333	VAL
1	C	334	GLU
1	C	335	LEU
1	C	336	THR

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Mol	Chain	Res	Type
1	C	341	SER
1	C	347	ILE
1	C	353	VAL
1	C	357	SER
1	C	360	ARG
1	C	361	GLN
1	C	371	LEU
1	C	405	VAL
1	C	406	GLN
1	C	408	SER
1	C	409	ILE
1	C	420	THR
1	C	421	VAL
1	C	432	TYR
1	C	458	PHE
1	C	474	GLN
1	C	505	ILE
1	C	511	HIS
1	C	520	MET
1	C	524	PHE
1	C	541	LEU
1	C	542	ILE
1	C	563	CYS
1	C	585	LEU
1	C	587	VAL
1	C	598	ARG
1	C	600	VAL
1	C	610	ASP
1	C	619	TYR
1	C	622	LEU
1	C	675	LEU
1	C	679	THR
1	C	683	ILE
1	C	740	ILE
1	C	742	ASP
1	C	754	VAL
1	C	761	THR
1	C	764	GLU
1	C	778	LEU
1	C	780	ILE
1	C	786	LEU
1	C	793	PHE

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Mol	Chain	Res	Type
1	C	818	LEU
1	C	821	CYS
1	C	826	VAL
1	C	828	LEU
1	C	842	GLU
1	C	843	GLN
1	C	848	ILE
1	C	849	CYS
1	C	855	THR
1	C	856	VAL
1	C	857	SER
1	C	865	LEU
1	C	872	VAL
1	C	875	GLU
1	C	893	HIS
1	C	897	ASP
1	C	903	LEU
1	C	908	GLU
1	C	916	PHE
1	C	919	LEU
1	C	929	GLU
1	C	931	LEU
1	C	938	ASN
1	C	942	GLU
1	C	949	SER
1	C	959	MET
1	C	961	ASN
1	C	968	MET
1	C	983	ASN
1	C	984	ILE
1	C	992	GLU
1	C	1000	ILE
1	C	1005	ILE
1	C	1008	LEU
1	C	1024	SER
1	C	1039	THR
1	C	1046	LEU
1	C	1073	ARG
1	C	1077	ASN
1	C	1086	LEU
1	C	1087	LEU
1	C	1089	ASN

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Mol	Chain	Res	Type
1	C	1091	ILE
1	C	1100	THR
1	C	1101	LEU
1	C	1105	ILE
1	C	1107	ILE
1	C	1110	LEU
1	C	1112	ILE
1	C	1114	LEU
1	C	1125	LEU
1	C	1150	LEU
1	C	1163	ARG
1	C	1184	GLU
1	C	1188	LYS
1	C	1206	VAL
1	C	1236	LYS
1	C	1242	GLN
1	C	1245	GLN
1	C	1252	GLN
1	C	1277	GLN
1	C	1280	ILE
1	C	1281	GLN
1	C	1289	LYS
1	C	1291	GLN
1	C	1292	VAL
1	C	1294	ASN
1	C	1295	ASN
1	C	1298	LEU
1	C	1315	LYS
1	C	1328	LEU
1	C	1331	ASN
1	C	1333	LEU
1	C	1356	LYS
1	C	1362	GLN
1	C	1363	ILE
1	C	1365	LEU
1	C	1384	LYS
1	C	1401	ARG
1	C	1402	SER
1	C	1408	THR
1	C	1422	VAL
1	C	1425	GLN
1	C	1426	THR

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Mol	Chain	Res	Type
1	C	1430	PHE
1	C	1434	LEU
1	C	1442	LEU
1	C	1446	ILE
1	C	1451	ASP
1	C	1457	GLU
1	C	1467	CYS
1	D	32	MET
1	D	34	LEU
1	D	42	GLU
1	D	56	GLU
1	D	60	VAL
1	D	82	ASP
1	D	114	PHE
1	D	121	MET
1	D	126	ASP
1	D	129	VAL
1	D	153	GLU
1	D	154	ASN
1	D	161	LEU
1	D	173	ASN
1	D	175	ILE
1	D	194	LEU
1	D	199	PHE
1	D	200	GLN
1	D	238	ILE
1	D	251	CYS
1	D	265	THR
1	D	268	ILE
1	D	294	LEU
1	D	321	HIS
1	D	326	ILE
1	D	331	THR
1	D	333	VAL
1	D	334	GLU
1	D	335	LEU
1	D	336	THR
1	D	341	SER
1	D	347	ILE
1	D	353	VAL
1	D	360	ARG
1	D	361	GLN

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Mol	Chain	Res	Type
1	D	371	LEU
1	D	382	LYS
1	D	405	VAL
1	D	406	GLN
1	D	409	ILE
1	D	420	THR
1	D	421	VAL
1	D	432	TYR
1	D	458	PHE
1	D	474	GLN
1	D	505	ILE
1	D	511	HIS
1	D	520	MET
1	D	524	PHE
1	D	541	LEU
1	D	542	ILE
1	D	563	CYS
1	D	585	LEU
1	D	587	VAL
1	D	598	ARG
1	D	600	VAL
1	D	610	ASP
1	D	619	TYR
1	D	622	LEU
1	D	675	LEU
1	D	679	THR
1	D	683	ILE
1	D	740	ILE
1	D	742	ASP
1	D	754	VAL
1	D	761	THR
1	D	764	GLU
1	D	778	LEU
1	D	780	ILE
1	D	786	LEU
1	D	793	PHE
1	D	818	LEU
1	D	821	CYS
1	D	826	VAL
1	D	828	LEU
1	D	829	GLU
1	D	842	GLU

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Mol	Chain	Res	Type
1	D	843	GLN
1	D	848	ILE
1	D	849	CYS
1	D	855	THR
1	D	856	VAL
1	D	857	SER
1	D	865	LEU
1	D	872	VAL
1	D	875	GLU
1	D	893	HIS
1	D	897	ASP
1	D	903	LEU
1	D	908	GLU
1	D	916	PHE
1	D	919	LEU
1	D	929	GLU
1	D	931	LEU
1	D	938	ASN
1	D	942	GLU
1	D	949	SER
1	D	959	MET
1	D	961	ASN
1	D	968	MET
1	D	983	ASN
1	D	984	ILE
1	D	992	GLU
1	D	999	GLU
1	D	1000	ILE
1	D	1005	ILE
1	D	1008	LEU
1	D	1024	SER
1	D	1039	THR
1	D	1046	LEU
1	D	1073	ARG
1	D	1077	ASN
1	D	1086	LEU
1	D	1087	LEU
1	D	1089	ASN
1	D	1091	ILE
1	D	1100	THR
1	D	1101	LEU
1	D	1105	ILE

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Mol	Chain	Res	Type
1	D	1107	ILE
1	D	1110	LEU
1	D	1112	ILE
1	D	1114	LEU
1	D	1125	LEU
1	D	1150	LEU
1	D	1163	ARG
1	D	1184	GLU
1	D	1188	LYS
1	D	1206	VAL
1	D	1236	LYS
1	D	1242	GLN
1	D	1245	GLN
1	D	1252	GLN
1	D	1277	GLN
1	D	1280	ILE
1	D	1281	GLN
1	D	1289	LYS
1	D	1291	GLN
1	D	1292	VAL
1	D	1294	ASN
1	D	1295	ASN
1	D	1298	LEU
1	D	1315	LYS
1	D	1328	LEU
1	D	1331	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	208	GLN
1	A	368	GLN
1	A	406	GLN
1	A	413	ASN
1	A	460	HIS
1	A	995	GLN
1	A	1038	ASN
1	A	1065	GLN
1	A	1118	HIS
1	A	1179	ASN
1	A	1233	ASN

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Mol	Chain	Res	Type
1	A	1242	GLN
1	A	1325	GLN
1	A	1331	ASN
1	B	112	GLN
1	B	208	GLN
1	B	368	GLN
1	B	406	GLN
1	B	413	ASN
1	B	460	HIS
1	B	995	GLN
1	B	1038	ASN
1	B	1065	GLN
1	B	1118	HIS
1	B	1179	ASN
1	B	1233	ASN
1	B	1242	GLN
1	B	1325	GLN
1	B	1331	ASN
1	C	106	GLN
1	C	112	GLN
1	C	208	GLN
1	C	368	GLN
1	C	406	GLN
1	C	413	ASN
1	C	995	GLN
1	C	1038	ASN
1	C	1065	GLN
1	C	1118	HIS
1	C	1179	ASN
1	C	1242	GLN
1	C	1325	GLN
1	C	1331	ASN
1	C	1435	GLN
1	D	112	GLN
1	D	208	GLN
1	D	368	GLN
1	D	406	GLN
1	D	413	ASN
1	D	917	ASN
1	D	995	GLN
1	D	1013	GLN
1	D	1038	ASN

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Mol	Chain	Res	Type
1	D	1065	GLN
1	D	1072	GLN
1	D	1118	HIS
1	D	1179	ASN
1	D	1242	GLN
1	D	1291	GLN
1	D	1331	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	MEQ	A	975	1	9,9,10	0.92	1 (11%)	7,10,12	1.01	1 (14%)
1	MEQ	B	975	1	9,9,10	0.91	1 (11%)	7,10,12	0.99	1 (14%)
1	MEQ	C	975	1	9,9,10	0.90	1 (11%)	7,10,12	1.02	1 (14%)
1	MEQ	D	975	1	9,9,10	0.88	1 (11%)	7,10,12	1.03	1 (14%)

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
1	MEQ	A	975	1	-	0/7/9/11	0/0/0/0
1	MEQ	B	975	1	-	0/7/9/11	0/0/0/0
1	MEQ	C	975	1	-	0/7/9/11	0/0/0/0
1	MEQ	D	975	1	-	0/7/9/11	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	975	MEQ	CA-C	2.02	1.52	1.50
1	D	975	MEQ	CA-C	2.11	1.53	1.50
1	B	975	MEQ	CA-C	2.15	1.53	1.50
1	A	975	MEQ	CA-C	2.21	1.53	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	975	MEQ	O-C-CA	-2.46	118.21	125.02
1	C	975	MEQ	O-C-CA	-2.44	118.28	125.02
1	A	975	MEQ	O-C-CA	-2.42	118.34	125.02
1	B	975	MEQ	O-C-CA	-2.39	118.41	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

36 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
2	NAG	A	2001	1,2	14,14,15	1.64	2 (14%)	15,19,21	1.16	1 (6%)
2	NAG	A	2002	2	14,14,15	1.53	1 (7%)	15,19,21	1.65	2 (13%)
2	NAG	A	2401	1,2	14,14,15	1.57	1 (7%)	15,19,21	1.98	3 (20%)
2	NAG	A	2402	2	14,14,15	1.70	1 (7%)	15,19,21	1.77	4 (26%)
2	NAG	A	2501	1,2	14,14,15	1.90	2 (14%)	15,19,21	2.15	4 (26%)
2	NAG	A	2502	2	14,14,15	1.40	1 (7%)	15,19,21	1.87	4 (26%)
4	NAG	A	2601	1,4	14,14,15	2.10	6 (42%)	15,19,21	2.84	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	2602	4	14,14,15	2.62	5 (35%)	15,19,21	2.58	4 (26%)
4	MAN	A	2603	4	11,11,12	3.97	10 (90%)	13,15,17	3.07	7 (53%)
2	NAG	B	2001	1,2	14,14,15	1.68	2 (14%)	15,19,21	1.17	1 (6%)
2	NAG	B	2002	2	14,14,15	1.55	1 (7%)	15,19,21	1.66	2 (13%)
2	NAG	B	2401	1,2	14,14,15	1.56	1 (7%)	15,19,21	1.98	3 (20%)
2	NAG	B	2402	2	14,14,15	1.75	2 (14%)	15,19,21	1.84	4 (26%)
2	NAG	B	2501	1,2	14,14,15	1.92	3 (21%)	15,19,21	2.07	5 (33%)
2	NAG	B	2502	2	14,14,15	1.71	2 (14%)	15,19,21	1.80	4 (26%)
4	NAG	B	2601	1,4	14,14,15	2.07	7 (50%)	15,19,21	2.90	6 (40%)
4	NAG	B	2602	4	14,14,15	2.57	5 (35%)	15,19,21	2.64	4 (26%)
4	MAN	B	2603	4	11,11,12	4.45	10 (90%)	13,15,17	3.13	9 (69%)
2	NAG	C	2001	1,2	14,14,15	1.86	2 (14%)	15,19,21	1.16	1 (6%)
2	NAG	C	2002	2	14,14,15	1.56	1 (7%)	15,19,21	1.63	2 (13%)
2	NAG	C	2401	1,2	14,14,15	1.66	1 (7%)	15,19,21	2.02	4 (26%)
2	NAG	C	2402	2	14,14,15	1.79	4 (28%)	15,19,21	1.68	4 (26%)
2	NAG	C	2501	1,2	14,14,15	1.96	3 (21%)	15,19,21	2.10	5 (33%)
2	NAG	C	2502	2	14,14,15	1.41	1 (7%)	15,19,21	1.89	4 (26%)
4	NAG	C	2601	1	14,14,15	2.28	9 (64%)	15,19,21	2.81	7 (46%)
4	NAG	C	2602	4	14,14,15	34.48	6 (42%)	16,19,21	18.67	9 (56%)
4	MAN	C	2603	4	11,11,12	2.91	10 (90%)	13,15,17	3.25	9 (69%)
2	NAG	D	2001	1,2	14,14,15	1.72	2 (14%)	15,19,21	1.16	1 (6%)
2	NAG	D	2002	2	14,14,15	1.52	1 (7%)	15,19,21	1.62	2 (13%)
2	NAG	D	2401	1,2	14,14,15	1.59	1 (7%)	15,19,21	2.01	4 (26%)
2	NAG	D	2402	2	14,14,15	1.79	2 (14%)	15,19,21	1.67	4 (26%)
2	NAG	D	2501	1,2	14,14,15	2.05	3 (21%)	15,19,21	1.98	3 (20%)
2	NAG	D	2502	2	14,14,15	1.43	1 (7%)	15,19,21	1.88	3 (20%)
4	NAG	D	2601	1,4	14,14,15	1.94	6 (42%)	15,19,21	2.80	7 (46%)
4	NAG	D	2602	4	14,14,15	2.40	6 (42%)	15,19,21	2.65	4 (26%)
4	MAN	D	2603	4	11,11,12	2.78	8 (72%)	13,15,17	3.25	6 (46%)

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
2	NAG	A	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2002	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	2401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2402	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	2501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2502	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	2601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2602	4	1/1/5/7	0/6/23/26	0/1/1/1
4	MAN	A	2603	4	-	0/2/19/22	0/1/1/1
2	NAG	B	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2002	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	2401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2402	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	2501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2502	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	2601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2602	4	1/1/5/7	0/6/23/26	0/1/1/1
4	MAN	B	2603	4	-	0/2/19/22	0/1/1/1
2	NAG	C	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2002	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	2401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2402	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	2501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2502	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	2601	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2602	4	4/4/5/7	0/6/22/26	1/1/1/1
4	MAN	C	2603	4	-	0/2/19/22	0/1/1/1
2	NAG	D	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2002	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	2401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2402	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	2501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2502	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	D	2601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2602	4	1/1/5/7	0/6/23/26	0/1/1/1
4	MAN	D	2603	4	-	0/2/19/22	0/1/1/1

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2602	NAG	C2-N2	2.01	1.49	1.46
2	C	2402	NAG	C3-C2	2.02	1.56	1.52
2	B	2501	NAG	C2-N2	2.02	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2601	NAG	O3-C3	2.04	1.47	1.43
2	C	2501	NAG	O5-C5	2.04	1.47	1.43
2	D	2501	NAG	C3-C2	2.05	1.57	1.52
2	C	2402	NAG	C2-N2	2.05	1.49	1.46
2	A	2501	NAG	C4-C3	2.05	1.57	1.52
4	D	2601	NAG	C7-N2	2.07	1.42	1.34
2	B	2501	NAG	C4-C5	2.07	1.57	1.53
4	C	2603	MAN	O3-C3	2.07	1.47	1.43
2	D	2402	NAG	C4-C5	2.07	1.57	1.53
2	B	2402	NAG	C3-C2	2.09	1.57	1.52
4	D	2602	NAG	O4-C4	2.10	1.47	1.43
4	C	2603	MAN	C6-C5	2.10	1.59	1.51
4	B	2601	NAG	O5-C1	2.11	1.47	1.43
4	B	2602	NAG	C2-N2	2.16	1.50	1.46
2	C	2501	NAG	C4-C3	2.17	1.57	1.52
4	D	2601	NAG	O4-C4	2.18	1.48	1.43
2	C	2402	NAG	C4-C5	2.19	1.57	1.53
4	D	2602	NAG	C4-C3	2.19	1.57	1.52
2	C	2001	NAG	C3-C2	2.21	1.57	1.52
4	B	2601	NAG	C3-C2	2.24	1.57	1.52
4	B	2601	NAG	O4-C4	2.24	1.48	1.43
4	A	2602	NAG	C2-N2	2.24	1.50	1.46
2	B	2502	NAG	C4-C3	2.25	1.58	1.52
4	A	2601	NAG	O5-C1	2.26	1.47	1.43
2	A	2001	NAG	C3-C2	2.26	1.57	1.52
4	D	2603	MAN	O5-C1	2.31	1.47	1.43
4	B	2601	NAG	C7-N2	2.32	1.42	1.34
4	C	2601	NAG	O4-C4	2.33	1.48	1.43
4	D	2603	MAN	O5-C5	2.36	1.48	1.43
4	C	2601	NAG	C7-N2	2.36	1.43	1.34
4	A	2601	NAG	C7-N2	2.36	1.43	1.34
4	C	2601	NAG	C3-C2	2.39	1.57	1.52
4	C	2603	MAN	O4-C4	2.40	1.48	1.43
4	B	2601	NAG	C4-C5	2.40	1.58	1.53
2	D	2001	NAG	C3-C2	2.44	1.57	1.52
4	C	2601	NAG	O5-C1	2.45	1.47	1.43
4	C	2602	NAG	C2-N2	2.46	1.50	1.46
4	C	2603	MAN	O2-C2	2.47	1.48	1.43
4	D	2603	MAN	C4-C3	2.48	1.58	1.52
4	C	2603	MAN	C4-C3	2.51	1.58	1.52
4	B	2602	NAG	C4-C3	2.51	1.58	1.52
4	D	2601	NAG	C4-C5	2.52	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2603	MAN	O4-C4	2.53	1.48	1.43
4	D	2601	NAG	C2-N2	2.53	1.50	1.46
4	D	2603	MAN	O2-C2	2.53	1.48	1.43
2	B	2001	NAG	C3-C2	2.54	1.58	1.52
2	D	2501	NAG	O5-C5	2.57	1.48	1.43
4	D	2602	NAG	C4-C5	2.57	1.58	1.53
4	A	2601	NAG	C4-C5	2.60	1.58	1.53
4	C	2603	MAN	O5-C5	2.63	1.49	1.43
4	C	2601	NAG	C1-C2	2.64	1.56	1.52
4	C	2601	NAG	C4-C5	2.68	1.58	1.53
4	A	2603	MAN	O3-C3	2.68	1.49	1.43
4	A	2601	NAG	C3-C2	2.70	1.58	1.52
4	D	2601	NAG	C3-C2	2.70	1.58	1.52
4	C	2603	MAN	O5-C1	2.72	1.48	1.43
4	A	2603	MAN	C6-C5	2.72	1.61	1.51
4	D	2602	NAG	C3-C2	2.75	1.58	1.52
4	A	2602	NAG	C4-C3	2.77	1.59	1.52
4	B	2602	NAG	C4-C5	2.81	1.59	1.53
4	A	2601	NAG	C2-N2	2.81	1.51	1.46
4	B	2603	MAN	C6-C5	2.85	1.61	1.51
4	A	2602	NAG	C4-C5	2.85	1.59	1.53
4	A	2602	NAG	C3-C2	2.93	1.58	1.52
4	B	2601	NAG	C2-N2	2.94	1.51	1.46
4	A	2603	MAN	O2-C2	2.96	1.49	1.43
4	B	2602	NAG	C3-C2	2.98	1.59	1.52
4	D	2603	MAN	C4-C5	2.99	1.59	1.53
2	A	2502	NAG	C1-C2	3.08	1.56	1.52
4	C	2603	MAN	C4-C5	3.09	1.59	1.53
4	B	2603	MAN	O4-C4	3.12	1.50	1.43
4	C	2601	NAG	C2-N2	3.20	1.52	1.46
4	D	2601	NAG	C4-C3	3.21	1.60	1.52
2	C	2502	NAG	C1-C2	3.28	1.57	1.52
4	B	2603	MAN	O3-C3	3.32	1.50	1.43
4	D	2603	MAN	C1-C2	3.35	1.60	1.52
4	A	2603	MAN	O4-C4	3.42	1.50	1.43
4	C	2603	MAN	C1-C2	3.45	1.60	1.52
4	A	2601	NAG	C4-C3	3.45	1.61	1.52
4	B	2601	NAG	C4-C3	3.47	1.61	1.52
2	D	2502	NAG	C1-C2	3.50	1.57	1.52
4	C	2602	NAG	C4-C5	3.54	1.58	1.52
2	B	2502	NAG	C1-C2	3.61	1.57	1.52
4	B	2603	MAN	O5-C1	3.66	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2603	MAN	C4-C3	3.71	1.61	1.52
4	A	2603	MAN	O5-C5	3.83	1.51	1.43
2	B	2001	NAG	C1-C2	3.85	1.57	1.52
4	C	2601	NAG	C4-C3	3.87	1.62	1.52
2	A	2001	NAG	C1-C2	3.89	1.57	1.52
2	A	2401	NAG	C1-C2	3.90	1.57	1.52
4	B	2603	MAN	O2-C2	3.95	1.52	1.43
2	D	2401	NAG	C1-C2	3.99	1.58	1.52
2	B	2401	NAG	C1-C2	4.00	1.58	1.52
4	B	2603	MAN	O5-C5	4.02	1.51	1.43
2	D	2001	NAG	C1-C2	4.14	1.58	1.52
2	D	2002	NAG	C1-C2	4.36	1.58	1.52
2	C	2002	NAG	C1-C2	4.39	1.58	1.52
2	A	2002	NAG	C1-C2	4.40	1.58	1.52
4	A	2603	MAN	C1-C2	4.44	1.62	1.52
2	B	2002	NAG	C1-C2	4.45	1.58	1.52
2	C	2401	NAG	C1-C2	4.48	1.58	1.52
4	A	2603	MAN	C4-C3	4.50	1.63	1.52
2	B	2501	NAG	C1-C2	4.60	1.58	1.52
2	C	2402	NAG	C1-C2	4.61	1.58	1.52
4	C	2602	NAG	C1-C2	4.65	1.58	1.52
2	A	2402	NAG	C1-C2	4.66	1.58	1.52
4	A	2603	MAN	C4-C5	4.67	1.63	1.53
2	A	2501	NAG	C1-C2	4.69	1.58	1.52
2	B	2402	NAG	C1-C2	4.84	1.59	1.52
4	A	2603	MAN	O5-C1	4.84	1.51	1.43
2	C	2001	NAG	C1-C2	4.90	1.59	1.52
2	D	2402	NAG	C1-C2	4.90	1.59	1.52
4	B	2603	MAN	C1-C2	4.90	1.63	1.52
2	C	2501	NAG	C1-C2	4.94	1.59	1.52
4	B	2603	MAN	C4-C5	5.00	1.63	1.53
4	C	2602	NAG	C3-C2	5.02	1.61	1.53
4	D	2603	MAN	C2-C3	5.11	1.59	1.52
4	C	2603	MAN	C2-C3	5.40	1.59	1.52
2	D	2501	NAG	C1-C2	5.51	1.60	1.52
4	A	2603	MAN	C2-C3	6.15	1.60	1.52
4	D	2602	NAG	C1-C2	6.60	1.61	1.52
4	B	2602	NAG	C1-C2	6.94	1.62	1.52
4	A	2602	NAG	C1-C2	7.06	1.62	1.52
4	B	2603	MAN	C2-C3	8.98	1.64	1.52
4	C	2602	NAG	O5-C1	83.58	2.95	1.43
4	C	2602	NAG	C3-C4	97.85	3.08	1.52

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2602	NAG	O5-C1-C2	-49.28	59.99	109.52
4	C	2602	NAG	C3-C4-C5	-45.92	50.56	110.82
4	C	2602	NAG	C1-O5-C5	-26.90	64.87	113.39
4	C	2602	NAG	O4-C4-C3	-11.20	82.91	110.02
2	C	2401	NAG	C8-C7-N2	-2.63	111.35	116.11
4	C	2601	NAG	C8-C7-N2	-2.54	111.52	116.11
4	D	2601	NAG	C8-C7-N2	-2.18	112.17	116.11
2	D	2401	NAG	C8-C7-N2	-2.16	112.21	116.11
4	A	2601	NAG	C8-C7-N2	-2.09	112.33	116.11
2	A	2401	NAG	C8-C7-N2	-2.09	112.34	116.11
4	C	2603	MAN	C3-C4-C5	2.01	113.76	110.22
2	C	2501	NAG	O3-C3-C4	2.01	114.73	110.36
4	C	2603	MAN	O6-C6-C5	2.02	118.14	111.34
2	A	2502	NAG	O5-C1-C2	2.03	114.29	111.47
4	A	2603	MAN	O4-C4-C5	2.03	114.39	109.28
2	B	2502	NAG	C4-C3-C2	2.07	114.05	111.02
4	D	2603	MAN	O4-C4-C5	2.08	114.52	109.28
2	B	2501	NAG	O3-C3-C4	2.09	114.90	110.36
2	C	2501	NAG	O5-C1-C2	2.10	114.39	111.47
2	C	2502	NAG	O5-C1-C2	2.10	114.40	111.47
4	C	2603	MAN	O4-C4-C5	2.12	114.64	109.28
2	A	2501	NAG	O3-C3-C4	2.15	115.04	110.36
2	D	2402	NAG	C1-O5-C5	2.15	115.13	112.17
2	C	2402	NAG	C1-O5-C5	2.17	115.15	112.17
4	C	2603	MAN	O3-C3-C2	2.20	114.03	110.02
4	B	2603	MAN	O2-C2-C3	2.21	114.52	110.17
2	D	2502	NAG	C4-C3-C2	2.22	114.27	111.02
4	B	2603	MAN	O3-C3-C2	2.22	114.07	110.02
2	C	2401	NAG	C1-C2-N2	2.25	114.33	110.49
2	D	2402	NAG	C2-N2-C7	2.26	126.24	122.94
4	B	2602	NAG	C3-C4-C5	2.26	114.21	110.22
2	A	2502	NAG	C4-C3-C2	2.27	114.34	111.02
2	C	2502	NAG	C4-C3-C2	2.28	114.36	111.02
2	B	2502	NAG	O5-C1-C2	2.32	114.70	111.47
2	B	2402	NAG	O5-C1-C2	2.33	114.72	111.47
4	A	2603	MAN	O3-C3-C4	2.34	115.46	110.36
4	B	2603	MAN	O2-C2-C1	2.35	113.96	109.18
2	A	2402	NAG	C2-N2-C7	2.36	126.38	122.94
4	D	2603	MAN	O2-C2-C1	2.36	113.98	109.18
2	C	2402	NAG	C2-N2-C7	2.36	126.39	122.94
4	B	2603	MAN	O6-C6-C5	2.37	119.33	111.34
2	D	2002	NAG	O5-C1-C2	2.39	114.80	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2401	NAG	C4-C3-C2	2.41	114.55	111.02
2	B	2401	NAG	C4-C3-C2	2.42	114.56	111.02
2	C	2002	NAG	O5-C1-C2	2.47	114.91	111.47
2	A	2402	NAG	O5-C1-C2	2.56	115.04	111.47
4	C	2603	MAN	O2-C2-C1	2.56	114.39	109.18
2	A	2002	NAG	O5-C1-C2	2.58	115.06	111.47
2	B	2002	NAG	O5-C1-C2	2.58	115.07	111.47
2	D	2402	NAG	O5-C1-C2	2.59	115.08	111.47
2	D	2001	NAG	C2-N2-C7	2.60	126.74	122.94
2	C	2401	NAG	C4-C3-C2	2.63	114.88	111.02
2	B	2402	NAG	C2-N2-C7	2.64	126.79	122.94
2	B	2001	NAG	C2-N2-C7	2.70	126.89	122.94
2	A	2402	NAG	C1-O5-C5	2.72	115.92	112.17
4	D	2602	NAG	C3-C4-C5	2.73	115.02	110.22
2	C	2001	NAG	C2-N2-C7	2.75	126.95	122.94
4	C	2601	NAG	C4-C3-C2	2.78	115.09	111.02
4	D	2601	NAG	C4-C3-C2	2.78	115.10	111.02
4	B	2603	MAN	O4-C4-C5	2.80	116.34	109.28
2	D	2401	NAG	C4-C3-C2	2.80	115.12	111.02
2	A	2001	NAG	C2-N2-C7	2.81	127.04	122.94
2	B	2501	NAG	O5-C1-C2	2.82	115.40	111.47
2	C	2402	NAG	O5-C1-C2	2.82	115.40	111.47
4	A	2603	MAN	O2-C2-C1	2.82	114.92	109.18
2	A	2502	NAG	C1-C2-N2	2.88	115.40	110.49
4	C	2602	NAG	O5-C5-C6	2.92	113.40	106.41
2	B	2502	NAG	C1-C2-N2	2.92	115.48	110.49
2	D	2502	NAG	C1-C2-N2	2.93	115.49	110.49
4	A	2603	MAN	C1-O5-C5	2.94	116.22	112.17
4	A	2601	NAG	C4-C3-C2	2.95	115.33	111.02
2	A	2501	NAG	C4-C3-C2	2.99	115.40	111.02
2	B	2401	NAG	C1-C2-N2	3.01	115.63	110.49
2	C	2502	NAG	C1-C2-N2	3.01	115.63	110.49
2	B	2402	NAG	C1-O5-C5	3.15	116.51	112.17
4	A	2602	NAG	C3-C4-C5	3.16	115.79	110.22
2	D	2401	NAG	C1-C2-N2	3.20	115.95	110.49
4	B	2601	NAG	C4-C3-C2	3.26	115.80	111.02
4	D	2601	NAG	O4-C4-C3	3.30	117.54	110.36
2	C	2501	NAG	C4-C3-C2	3.32	115.89	111.02
4	C	2601	NAG	O7-C7-N2	3.37	128.40	121.92
4	C	2601	NAG	C1-O5-C5	3.39	116.84	112.17
4	A	2601	NAG	O7-C7-N2	3.40	128.46	121.92
4	D	2601	NAG	O7-C7-N2	3.41	128.49	121.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2601	NAG	O4-C4-C3	3.48	117.92	110.36
4	B	2601	NAG	O7-C7-N2	3.48	128.61	121.92
4	B	2601	NAG	O4-C4-C3	3.49	117.94	110.36
2	D	2501	NAG	C1-O5-C5	3.50	116.99	112.17
2	B	2501	NAG	C4-C3-C2	3.50	116.15	111.02
4	C	2602	NAG	O4-C4-C5	3.54	117.33	109.91
4	B	2603	MAN	C1-O5-C5	3.60	117.12	112.17
4	B	2603	MAN	C2-C3-C4	3.61	117.17	110.88
4	C	2601	NAG	O4-C4-C3	3.71	118.42	110.36
2	D	2501	NAG	C4-C3-C2	3.73	116.48	111.02
2	C	2501	NAG	C1-O5-C5	3.75	117.34	112.17
4	A	2603	MAN	C2-C3-C4	3.81	117.51	110.88
4	D	2601	NAG	C1-O5-C5	3.82	117.43	112.17
4	A	2601	NAG	C1-O5-C5	3.84	117.46	112.17
2	B	2501	NAG	C1-O5-C5	3.89	117.53	112.17
2	B	2501	NAG	C1-C2-N2	3.96	117.25	110.49
4	C	2601	NAG	C3-C4-C5	3.99	117.25	110.22
4	B	2601	NAG	C1-O5-C5	4.01	117.70	112.17
4	D	2601	NAG	C3-C4-C5	4.04	117.34	110.22
4	B	2601	NAG	C3-C4-C5	4.05	117.35	110.22
4	C	2603	MAN	C2-C3-C4	4.12	118.05	110.88
4	A	2601	NAG	C3-C4-C5	4.13	117.49	110.22
2	D	2501	NAG	C1-C2-N2	4.17	117.61	110.49
2	C	2402	NAG	C1-C2-N2	4.18	117.62	110.49
4	D	2603	MAN	C2-C3-C4	4.18	118.16	110.88
2	D	2402	NAG	C1-C2-N2	4.19	117.65	110.49
4	D	2603	MAN	O5-C1-C2	4.23	117.42	110.79
4	A	2602	NAG	C2-N2-C7	4.35	129.29	122.94
4	C	2603	MAN	O5-C1-C2	4.38	117.65	110.79
2	A	2501	NAG	C1-O5-C5	4.40	118.23	112.17
4	D	2602	NAG	C2-N2-C7	4.45	129.44	122.94
2	A	2402	NAG	C1-C2-N2	4.46	118.11	110.49
4	B	2602	NAG	C2-N2-C7	4.52	129.53	122.94
2	B	2402	NAG	C1-C2-N2	4.54	118.25	110.49
4	C	2602	NAG	C2-N2-C7	4.55	129.58	122.94
2	A	2501	NAG	C1-C2-N2	4.62	118.38	110.49
2	C	2501	NAG	C1-C2-N2	4.69	118.51	110.49
2	D	2002	NAG	C1-C2-N2	4.74	118.59	110.49
2	A	2002	NAG	C1-C2-N2	4.78	118.66	110.49
2	B	2002	NAG	C1-C2-N2	4.80	118.68	110.49
2	C	2002	NAG	C1-C2-N2	4.84	118.75	110.49
2	B	2502	NAG	C1-O5-C5	4.97	119.02	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2603	MAN	C1-O5-C5	4.97	119.02	112.17
4	A	2602	NAG	C1-C2-N2	5.14	119.26	110.49
4	C	2602	NAG	C3-C2-N2	5.15	119.24	110.65
4	D	2603	MAN	C1-O5-C5	5.29	119.45	112.17
2	A	2502	NAG	C1-O5-C5	5.33	119.51	112.17
4	D	2602	NAG	C1-C2-N2	5.34	119.61	110.49
2	C	2502	NAG	C1-O5-C5	5.36	119.55	112.17
2	D	2401	NAG	C1-O5-C5	5.37	119.57	112.17
2	D	2502	NAG	C1-O5-C5	5.38	119.59	112.17
4	B	2602	NAG	C1-C2-N2	5.40	119.71	110.49
2	C	2401	NAG	C1-O5-C5	5.50	119.75	112.17
4	B	2603	MAN	O5-C1-C2	5.51	119.43	110.79
2	B	2401	NAG	C1-O5-C5	5.62	119.91	112.17
4	A	2602	NAG	C4-C3-C2	5.65	119.30	111.02
4	A	2603	MAN	O5-C1-C2	5.70	119.72	110.79
4	A	2603	MAN	C1-C2-C3	5.81	117.01	109.65
4	B	2603	MAN	C1-C2-C3	5.91	117.14	109.65
2	A	2401	NAG	C1-O5-C5	6.07	120.53	112.17
4	D	2602	NAG	C4-C3-C2	6.10	119.96	111.02
4	B	2602	NAG	C4-C3-C2	6.25	120.17	111.02
4	C	2601	NAG	C2-N2-C7	6.46	132.37	122.94
4	A	2601	NAG	C2-N2-C7	6.54	132.49	122.94
4	D	2603	MAN	C1-C2-C3	6.62	118.05	109.65
4	D	2601	NAG	C2-N2-C7	6.65	132.65	122.94
4	B	2601	NAG	C2-N2-C7	6.68	132.68	122.94
4	C	2603	MAN	C1-C2-C3	6.68	118.12	109.65
4	C	2602	NAG	O1-C1-O5	10.89	142.41	110.20

All (19) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2002	NAG	C1
2	B	2402	NAG	C1
2	A	2402	NAG	C1
2	A	2502	NAG	C1
2	D	2502	NAG	C1
2	C	2002	NAG	C1
2	D	2402	NAG	C1
2	C	2402	NAG	C1
2	A	2002	NAG	C1
2	C	2502	NAG	C1
4	C	2602	NAG	C2

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Mol	Chain	Res	Type	Atom
4	C	2602	NAG	C5
4	C	2602	NAG	C1
4	C	2602	NAG	C4
4	B	2602	NAG	C1
4	D	2602	NAG	C1
2	B	2502	NAG	C1
4	A	2602	NAG	C1
2	D	2002	NAG	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2602	NAG	C1-C2-C3-C4-C5-O5

20 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2401	NAG	1	0
2	A	2501	NAG	2	0
2	A	2502	NAG	2	0
4	A	2601	NAG	1	0
4	A	2602	NAG	1	0
2	B	2401	NAG	1	0
2	B	2501	NAG	2	0
2	B	2502	NAG	2	0
4	B	2601	NAG	2	0
4	B	2602	NAG	1	0
2	C	2401	NAG	1	0
2	C	2501	NAG	2	0
2	C	2502	NAG	2	0
4	C	2601	NAG	1	0
4	C	2602	NAG	1	0
2	D	2401	NAG	1	0
2	D	2501	NAG	1	0
2	D	2502	NAG	1	0
4	D	2601	NAG	1	0
4	D	2602	NAG	1	0

5.6 Ligand geometry

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	A	2101	1	14,14,15	1.85	3 (21%)	15,19,21	2.43	5 (33%)
3	NAG	A	2201	1	14,14,15	1.81	3 (21%)	15,19,21	1.44	2 (13%)
3	NAG	A	2301	1	14,14,15	1.78	3 (21%)	15,19,21	2.41	4 (26%)
3	NAG	B	2101	1	14,14,15	1.98	3 (21%)	15,19,21	2.39	5 (33%)
3	NAG	B	2201	1	14,14,15	1.72	2 (14%)	15,19,21	1.61	2 (13%)
3	NAG	B	2301	1	14,14,15	1.83	3 (21%)	15,19,21	2.37	5 (33%)
3	NAG	C	2101	1	14,14,15	2.30	3 (21%)	15,19,21	2.42	7 (46%)
3	NAG	C	2201	1	14,14,15	1.84	1 (7%)	15,19,21	2.00	3 (20%)
3	NAG	C	2301	1	14,14,15	2.18	5 (35%)	15,19,21	2.40	5 (33%)
3	NAG	C	2701	1	14,14,15	1.56	2 (14%)	15,19,21	1.29	2 (13%)
3	NAG	D	2101	1	14,14,15	1.76	3 (21%)	15,19,21	2.44	5 (33%)
3	NAG	D	2201	1	14,14,15	1.71	2 (14%)	15,19,21	1.42	2 (13%)
3	NAG	D	2301	1	14,14,15	1.72	2 (14%)	15,19,21	2.41	5 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	2101	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2201	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2301	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2101	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2201	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2101	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2201	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	2301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2701	1	-	0/6/23/26	0/1/1/1
3	NAG	D	2101	1	-	0/6/23/26	0/1/1/1
3	NAG	D	2201	1	-	0/6/23/26	0/1/1/1
3	NAG	D	2301	1	-	0/6/23/26	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2301	NAG	C3-C2	2.03	1.56	1.52
3	D	2301	NAG	C3-C2	2.04	1.57	1.52
3	A	2201	NAG	O5-C5	2.05	1.47	1.43
3	A	2301	NAG	C3-C2	2.07	1.57	1.52
3	D	2201	NAG	C3-C2	2.08	1.57	1.52
3	B	2201	NAG	C3-C2	2.08	1.57	1.52
3	A	2201	NAG	C3-C2	2.15	1.57	1.52
3	C	2301	NAG	C2-N2	2.18	1.50	1.46
3	C	2301	NAG	C4-C3	2.19	1.57	1.52
3	C	2701	NAG	C3-C2	2.27	1.57	1.52
3	B	2301	NAG	C2-N2	2.33	1.50	1.46
3	A	2301	NAG	C2-N2	2.38	1.50	1.46
3	D	2101	NAG	C3-C2	2.41	1.57	1.52
3	B	2101	NAG	C3-C2	2.41	1.57	1.52
3	D	2101	NAG	C2-N2	2.42	1.50	1.46
3	A	2101	NAG	C3-C2	2.49	1.57	1.52
3	C	2301	NAG	C3-C2	2.59	1.58	1.52
3	C	2101	NAG	C3-C2	2.67	1.58	1.52
3	A	2101	NAG	C2-N2	2.88	1.51	1.46
3	C	2301	NAG	O5-C1	3.07	1.48	1.43
3	C	2101	NAG	C2-N2	3.25	1.52	1.46
3	B	2101	NAG	C2-N2	3.43	1.52	1.46
3	C	2701	NAG	C1-C2	4.38	1.58	1.52
3	A	2301	NAG	C1-C2	4.44	1.58	1.52
3	D	2301	NAG	C1-C2	4.44	1.58	1.52
3	D	2101	NAG	C1-C2	4.50	1.58	1.52
3	B	2201	NAG	C1-C2	4.55	1.58	1.52
3	B	2301	NAG	C1-C2	4.56	1.58	1.52
3	A	2101	NAG	C1-C2	4.69	1.58	1.52
3	D	2201	NAG	C1-C2	4.74	1.59	1.52
3	A	2201	NAG	C1-C2	4.95	1.59	1.52
3	B	2101	NAG	C1-C2	5.16	1.59	1.52
3	C	2201	NAG	C1-C2	5.26	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2301	NAG	C1-C2	5.33	1.59	1.52
3	C	2101	NAG	C1-C2	6.23	1.61	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2301	NAG	C8-C7-N2	-2.55	111.51	116.11
3	C	2301	NAG	C8-C7-N2	-2.31	111.94	116.11
3	B	2301	NAG	C8-C7-N2	-2.16	112.20	116.11
3	C	2101	NAG	C6-C5-C4	-2.13	108.02	113.00
3	C	2101	NAG	C8-C7-N2	-2.00	112.49	116.11
3	C	2201	NAG	O7-C7-N2	2.03	125.83	121.92
3	C	2701	NAG	C2-N2-C7	2.17	126.10	122.94
3	D	2301	NAG	O7-C7-N2	2.41	126.56	121.92
3	D	2201	NAG	C1-C2-N2	2.52	114.80	110.49
3	B	2301	NAG	O7-C7-N2	2.53	126.79	121.92
3	B	2101	NAG	C1-O5-C5	2.53	115.65	112.17
3	A	2201	NAG	C1-C2-N2	2.56	114.87	110.49
3	A	2301	NAG	O7-C7-N2	2.60	126.93	121.92
3	A	2101	NAG	C1-O5-C5	2.63	115.79	112.17
3	D	2101	NAG	C1-O5-C5	2.70	115.89	112.17
3	D	2101	NAG	O5-C1-C2	2.74	115.28	111.47
3	C	2301	NAG	O7-C7-N2	2.84	127.38	121.92
3	B	2101	NAG	O5-C1-C2	3.04	115.70	111.47
3	B	2201	NAG	C1-C2-N2	3.11	115.81	110.49
3	C	2701	NAG	C4-C3-C2	3.25	115.77	111.02
3	A	2101	NAG	O5-C1-C2	3.30	116.07	111.47
3	C	2101	NAG	O5-C1-C2	3.33	116.11	111.47
3	A	2301	NAG	C1-C2-N2	3.34	116.20	110.49
3	C	2101	NAG	C1-O5-C5	3.35	116.79	112.17
3	C	2301	NAG	C1-C2-N2	3.37	116.24	110.49
3	C	2101	NAG	C4-C3-C2	3.56	116.23	111.02
3	D	2101	NAG	C1-C2-N2	3.67	116.75	110.49
3	D	2201	NAG	C1-O5-C5	3.69	117.25	112.17
3	B	2301	NAG	C1-C2-N2	3.69	116.80	110.49
3	B	2101	NAG	C1-C2-N2	3.77	116.93	110.49
3	A	2101	NAG	C1-C2-N2	3.80	116.97	110.49
3	C	2101	NAG	C1-C2-N2	3.81	117.00	110.49
3	C	2201	NAG	C1-O5-C5	3.88	117.51	112.17
3	A	2201	NAG	C1-O5-C5	3.90	117.53	112.17
3	B	2101	NAG	C4-C3-C2	3.95	116.81	111.02
3	D	2301	NAG	C1-C2-N2	4.05	117.41	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2101	NAG	C4-C3-C2	4.09	117.02	111.02
3	B	2301	NAG	C1-O5-C5	4.10	117.82	112.17
3	A	2101	NAG	C4-C3-C2	4.10	117.03	111.02
3	C	2301	NAG	C1-O5-C5	4.20	117.95	112.17
3	B	2201	NAG	C1-O5-C5	4.37	118.19	112.17
3	D	2301	NAG	C1-O5-C5	4.40	118.23	112.17
3	A	2301	NAG	C1-O5-C5	4.46	118.31	112.17
3	C	2101	NAG	C2-N2-C7	4.83	129.99	122.94
3	C	2201	NAG	C1-C2-N2	5.14	119.28	110.49
3	D	2301	NAG	C2-N2-C7	5.16	130.47	122.94
3	C	2301	NAG	C2-N2-C7	5.44	130.88	122.94
3	B	2301	NAG	C2-N2-C7	5.51	130.98	122.94
3	A	2101	NAG	C2-N2-C7	5.62	131.14	122.94
3	A	2301	NAG	C2-N2-C7	5.73	131.30	122.94
3	B	2101	NAG	C2-N2-C7	5.74	131.31	122.94
3	D	2101	NAG	C2-N2-C7	6.00	131.70	122.94

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 [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	1269/1451 (87%)	-0.31	18 (1%) 75 67	81, 159, 293, 300	0
1	B	1269/1451 (87%)	-0.29	16 (1%) 77 69	65, 153, 297, 300	0
1	C	1402/1451 (96%)	-0.31	18 (1%) 77 69	60, 148, 292, 300	0
1	D	1269/1451 (87%)	-0.21	17 (1%) 77 69	91, 182, 300, 300	0
All	All	5209/5804 (89%)	-0.28	69 (1%) 77 69	60, 161, 299, 300	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1192	PRO	7.0
1	C	433	GLY	6.0
1	A	1191	ALA	4.7
1	D	633	PRO	4.5
1	B	277	ASP	4.4
1	C	435	GLN	4.1
1	A	1193	VAL	4.0
1	D	1192	PRO	3.8
1	C	434	TYR	3.5
1	C	1360	SER	3.4
1	B	1193	VAL	3.4
1	A	1194	GLY	3.4
1	B	729	GLU	3.4
1	B	276	SER	3.3
1	D	1189	PRO	3.1
1	A	434	TYR	3.1
1	A	433	GLY	3.0
1	A	281	GLU	3.0
1	A	435	GLN	3.0
1	B	433	GLY	3.0
1	D	1191	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	432	TYR	2.9
1	B	1194	GLY	2.8
1	D	1081	ARG	2.8
1	C	1191	ALA	2.8
1	D	71	ARG	2.7
1	C	1035	ASN	2.6
1	C	1192	PRO	2.6
1	A	1195	HIS	2.6
1	A	436	TRP	2.6
1	D	1193	VAL	2.6
1	D	1190	LYS	2.5
1	B	279	HIS	2.5
1	C	820	LYS	2.5
1	B	284	GLN	2.5
1	A	1190	LYS	2.5
1	B	1192	PRO	2.4
1	A	1334	PRO	2.4
1	A	279	HIS	2.4
1	C	1036	GLN	2.4
1	B	434	TYR	2.4
1	A	276	SER	2.3
1	C	1198	GLU	2.3
1	A	644	ASN	2.3
1	D	889	SER	2.3
1	B	282	ASP	2.3
1	B	1188	LYS	2.3
1	D	1197	TYR	2.2
1	D	1330	TYR	2.2
1	B	1195	HIS	2.2
1	C	1375	ALA	2.2
1	D	553	GLY	2.2
1	C	889	SER	2.2
1	B	1198	GLU	2.2
1	B	278	CYS	2.2
1	A	787	ARG	2.2
1	C	1195	HIS	2.1
1	C	1441	ASP	2.1
1	A	687	LYS	2.1
1	A	841	LYS	2.1
1	C	1377	ASN	2.1
1	D	1335	GLU	2.1
1	C	888	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	27	GLY	2.1
1	D	1332	ILE	2.1
1	D	689	CYS	2.1
1	B	647	ASN	2.1
1	D	276	SER	2.0
1	C	1190	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	MEQ	B	975	10/11	0.90	0.20	-	164,187,254,273	0
1	MEQ	A	975	10/11	0.89	0.44	-	156,174,185,253	0
1	MEQ	D	975	10/11	0.85	0.35	-	190,274,288,289	0
1	MEQ	C	975	10/11	0.76	0.30	-	136,153,165,173	0

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
2	NAG	A	2401	14/15	0.72	0.32	2.78	208,291,293,294	0
2	NAG	C	2001	14/15	0.69	0.64	1.89	200,206,300,300	0
2	NAG	D	2001	14/15	0.77	0.69	1.62	287,288,290,291	0
2	NAG	B	2001	14/15	0.78	0.45	0.76	299,300,300,300	0
2	NAG	C	2401	14/15	0.76	0.26	0.53	156,171,244,254	0
2	NAG	A	2001	14/15	0.81	0.28	-0.16	292,292,294,295	0
4	MAN	C	2603	11/12	0.46	0.58	-	186,200,293,296	0
2	NAG	B	2002	14/15	0.77	0.65	-	296,298,300,300	0
2	NAG	D	2502	14/15	0.72	0.64	-	300,300,300,300	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	C	2002	14/15	0.72	0.68	-	194,299,300,300	0
2	NAG	D	2402	14/15	0.71	0.71	-	300,300,300,300	0
2	NAG	D	2501	14/15	0.78	0.56	-	193,295,300,300	0
2	NAG	C	2402	14/15	0.76	0.41	-	259,262,266,267	0
4	NAG	B	2601	14/15	0.96	0.24	-	143,166,224,228	0
4	MAN	D	2603	11/12	0.66	0.55	-	295,297,299,300	0
2	NAG	C	2501	14/15	0.89	0.41	-	186,209,298,300	0
2	NAG	B	2501	14/15	0.92	0.39	-	126,141,148,151	0
2	NAG	A	2002	14/15	0.72	0.42	-	292,293,295,295	0
2	NAG	C	2502	14/15	0.93	0.38	-	267,300,300,300	0
4	MAN	B	2603	11/12	0.82	0.48	-	100,100,100,100	0
4	NAG	C	2602	14/15	0.87	0.50	-	139,163,178,180	0
2	NAG	A	2501	14/15	0.90	0.51	-	180,196,251,259	0
4	NAG	B	2602	14/15	0.82	0.36	-	154,221,227,228	0
4	NAG	D	2601	14/15	0.77	0.38	-	167,210,263,270	0
2	NAG	D	2401	14/15	0.64	0.44	-	300,300,300,300	0
2	NAG	B	2401	14/15	0.57	0.39	-	300,300,300,300	0
4	NAG	D	2602	14/15	0.73	0.59	-	181,277,288,294	0
2	NAG	B	2402	14/15	0.80	0.79	-	300,300,300,300	0
2	NAG	B	2502	14/15	0.89	0.40	-	154,162,183,190	0
4	NAG	C	2601	14/15	0.90	0.36	-	119,140,154,161	0
4	NAG	A	2601	14/15	0.91	0.31	-	128,148,165,169	0
4	MAN	A	2603	11/12	0.60	0.62	-	100,100,100,100	0
4	NAG	A	2602	14/15	0.79	0.57	-	140,166,182,185	0
2	NAG	D	2002	14/15	0.64	0.52	-	286,288,291,291	0
2	NAG	A	2402	14/15	0.80	0.50	-	289,292,295,296	0
2	NAG	A	2502	14/15	0.77	0.56	-	211,286,300,300	0

6.4 Ligands

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(\AA^2)	Q<0.9
3	NAG	A	2101	14/15	0.57	0.65	-	198,290,291,291	0
3	NAG	B	2201	14/15	0.74	0.59	-	190,197,262,265	0
3	NAG	D	2201	14/15	0.60	0.39	-	215,300,300,300	0
3	NAG	C	2201	14/15	0.32	0.65	-	202,298,300,300	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	C	2701	14/15	0.72	0.55	-	300,300,300,300	0
3	NAG	B	2101	14/15	0.80	0.41	-	180,203,294,295	0
3	NAG	C	2301	14/15	0.81	0.25	-	158,176,251,258	0
3	NAG	A	2201	14/15	0.69	0.30	-	183,192,270,280	0
3	NAG	D	2101	14/15	0.62	0.65	-	287,297,300,300	0
3	NAG	C	2101	14/15	0.70	0.49	-	129,154,175,189	0
3	NAG	B	2301	14/15	0.74	0.23	-	300,300,300,300	0
3	NAG	A	2301	14/15	0.87	0.15	-	278,290,292,292	0
3	NAG	D	2301	14/15	0.82	0.28	-	300,300,300,300	0

6.5 Other polymers [i](#)

There are no such residues in this entry.