



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 21, 2022 – 01:27 PM EDT

PDB ID : 7TV9
Title : HUMAN COMPLEMENT COMPONENT C3B IN COMPLEX WITH APL-1030
Authors : Fontano, E.; Nadupalli, A.; Lakshminarasimhan, D.; White, A.; Garlish, J.; Cinier, M.; Chevrel, A.; Perrocheau, A.; Eyerman, D.; Orme, M.; Kitten, O.; Scheibler, L.
Deposited on : 2022-02-04
Resolution : 3.40 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

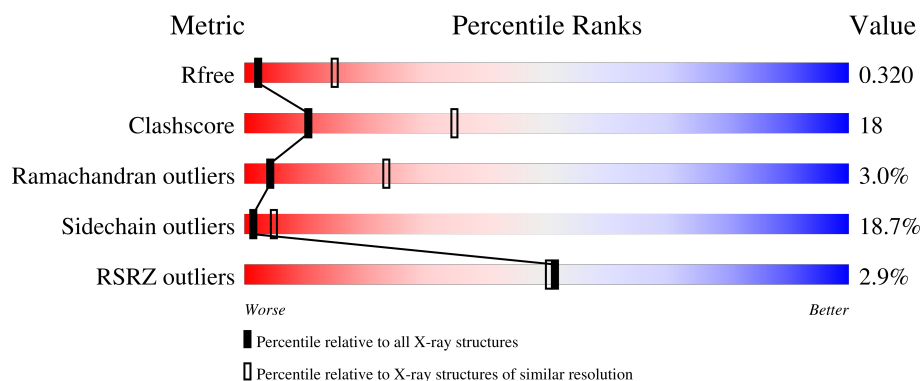
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




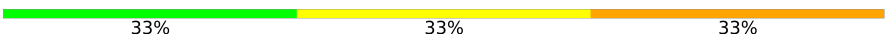
The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	645	
2	B	915	
3	C	65	
4	D	3	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12679 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Complement C3 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	636	Total	C	N	O	S	0	0	0
			4944	3148	836	945	15			

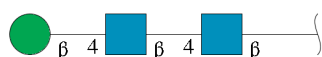
- Molecule 2 is a protein called Complement C3b alpha' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	902	Total	C	N	O	S	0	0	0
			7182	4548	1212	1384	38			

- Molecule 3 is a protein called APL-1030 Nanofitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	63	Total	C	N	O	S	0	0	0
			500	317	82	100	1			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

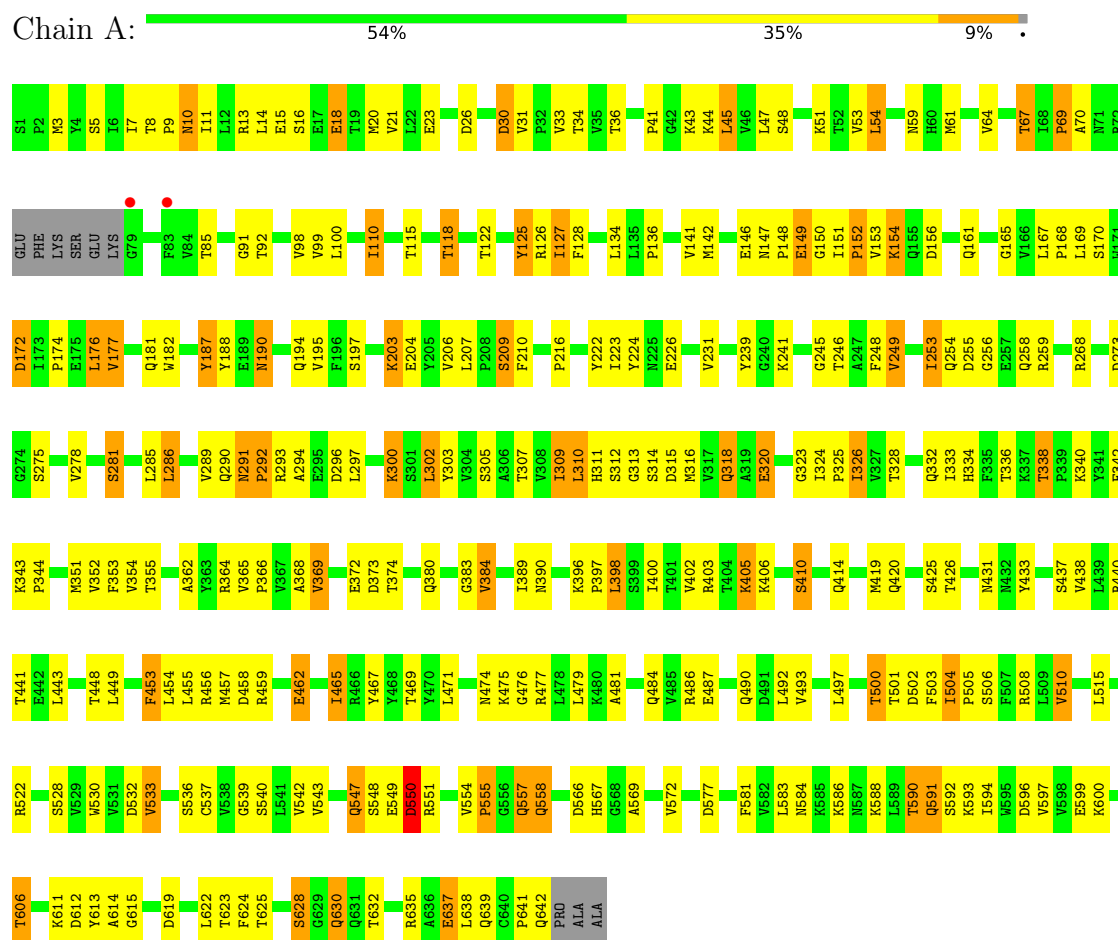


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	14	8	1	5	0	0

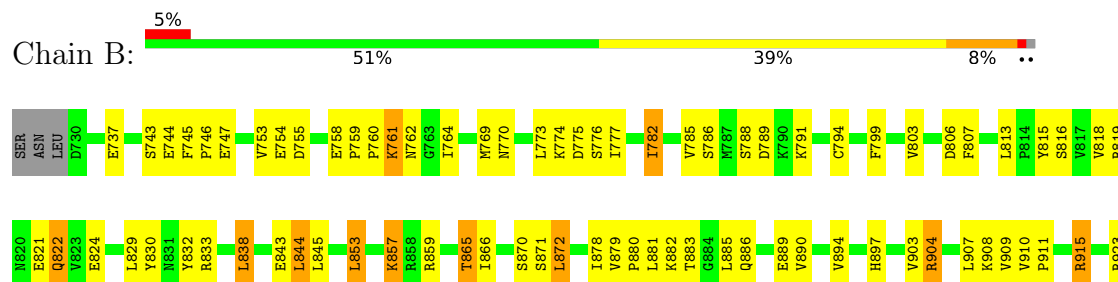
3 Residue-property plots

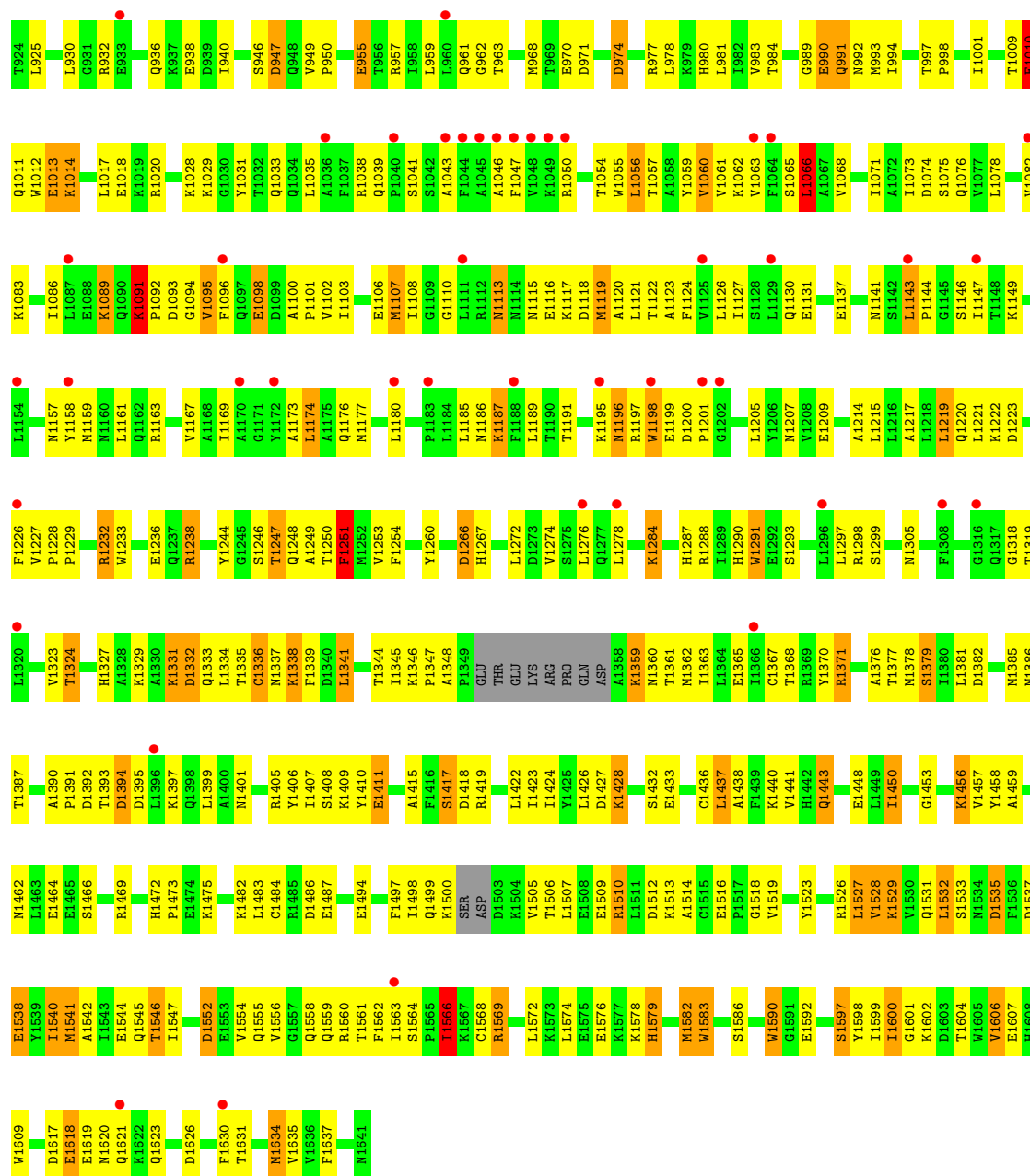
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Complement C3 beta chain



• Molecule 2: Complement C3b alpha' chain





• Molecule 3: APL-1030 Nanofitin

Chain C: 68% 20% 9%



• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 33% 33% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.48Å 104.70Å 103.11Å 90.00° 97.46° 90.00°	Depositor
Resolution (Å)	98.83 – 3.40 98.64 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (98.83-3.40) 99.1 (98.64-3.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.41Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.239 , 0.328 0.236 , 0.320	Depositor DCC
R_{free} test set	1347 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	107.0	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12679	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.69	0/5043	0.67	0/6855
2	B	0.71	0/7322	0.67	0/9912
3	C	0.74	0/507	0.68	0/679
All	All	0.70	0/12872	0.67	0/17446

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	5
2	B	0	5
3	C	0	1
All	All	0	11

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	LYS	Peptide
1	A	384	VAL	Peptide
1	A	431	ASN	Peptide
1	A	550	ASP	Peptide
1	A	69	PRO	Peptide
2	B	1066	LEU	Peptide
2	B	1098	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	B	1436	CYS	Peptide
2	B	1523	TYR	Peptide
2	B	1578	LYS	Peptide
3	C	34	TYR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4944	0	4997	192	0
2	B	7182	0	7110	293	0
3	C	500	0	502	15	0
4	D	39	0	34	1	0
5	B	14	0	13	0	0
All	All	12679	0	12656	468	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 18.

All (468) 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:B:853:LEU:H	2:B:853:LEU:HD22	1.28	0.99
3:C:8:ALA:O	3:C:9:THR:OG1	1.79	0.98
2:B:1379:SER:OG	2:B:1459:ALA:HA	1.63	0.98
2:B:1336:CYS:O	2:B:1336:CYS:SG	2.30	0.89
2:B:1199:GLU:HB3	2:B:1207:ASN:HB3	1.59	0.84
1:A:176:LEU:H	1:A:176:LEU:HD22	1.43	0.83
1:A:623:THR:HA	1:A:632:THR:HG21	1.64	0.80
2:B:1541:MET:HG2	2:B:1582:MET:HE1	1.65	0.78
1:A:369:VAL:O	1:A:374:THR:HG21	1.82	0.77
2:B:978:LEU:HD21	2:B:1254:PHE:CE1	2.20	0.77
2:B:1532:LEU:HA	2:B:1537:ASP:HB2	1.68	0.76
1:A:141:VAL:HG22	1:A:188:TYR:HA	1.68	0.75
2:B:857:LYS:HE3	2:B:857:LYS:HA	1.69	0.74
3:C:40:ILE:HG23	3:C:40:ILE:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1537:ASP:O	2:B:1537:ASP:OD1	2.07	0.73
2:B:1590:TRP:HA	2:B:1590:TRP:CE3	2.23	0.73
2:B:1535:ASP:O	2:B:1566:ILE:HG23	1.88	0.73
1:A:115:THR:HB	1:A:584:ASN:OD1	1.89	0.73
2:B:1562:PHE:HA	2:B:1598:TYR:O	1.88	0.73
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.70	0.72
2:B:1091:LYS:CB	2:B:1092:PRO:HD2	2.20	0.72
2:B:1056:LEU:O	2:B:1060:VAL:HG12	1.90	0.71
1:A:477:ARG:HB3	1:A:477:ARG:HH11	1.55	0.71
2:B:806:ASP:HB3	2:B:833:ARG:HD3	1.71	0.71
2:B:844:LEU:HD12	2:B:845:LEU:N	2.07	0.70
1:A:457:MET:O	3:C:40:ILE:HG22	1.92	0.69
2:B:1071:ILE:O	2:B:1073:ILE:HG23	1.92	0.69
2:B:1287:HIS:CG	2:B:1298:ARG:HD2	2.27	0.69
2:B:1381:LEU:HB2	2:B:1424:ILE:O	1.93	0.69
2:B:1335:THR:HG23	2:B:1335:THR:O	1.92	0.68
1:A:41:PRO:HB3	2:B:1020:ARG:CZ	2.22	0.68
1:A:255:ASP:HB2	1:A:300:LYS:HG3	1.76	0.68
2:B:1379:SER:OG	2:B:1459:ALA:CA	2.41	0.68
2:B:1091:LYS:CB	2:B:1092:PRO:CD	2.72	0.67
1:A:149:GLU:OE2	1:A:149:GLU:HA	1.93	0.67
1:A:313:GLY:CA	2:B:1423:ILE:HD11	2.25	0.67
1:A:44:LYS:O	1:A:45:LEU:HG	1.95	0.67
1:A:110:ILE:HA	1:A:126:ARG:O	1.94	0.67
1:A:309:ILE:HG23	1:A:316:MET:HB3	1.78	0.66
2:B:1126:LEU:O	2:B:1130:GLN:HG2	1.95	0.66
2:B:1124:PHE:O	2:B:1127:ILE:HB	1.96	0.66
1:A:3:MET:HG3	1:A:628:SER:OG	1.96	0.65
2:B:889:GLU:HG3	2:B:904:ARG:HB3	1.78	0.65
2:B:853:LEU:H	2:B:853:LEU:CD2	2.05	0.65
1:A:291:ASN:N	1:A:292:PRO:HD3	2.12	0.65
1:A:147:ASN:OD1	1:A:151:ILE:HB	1.97	0.64
2:B:853:LEU:HD22	2:B:853:LEU:N	2.08	0.64
2:B:1472:HIS:CD2	2:B:1473:PRO:HD2	2.32	0.64
2:B:1012:TRP:CE2	2:B:1020:ARG:HD2	2.33	0.64
2:B:1583:TRP:CD1	2:B:1583:TRP:C	2.71	0.64
1:A:255:ASP:HB2	1:A:300:LYS:CG	2.29	0.63
1:A:487:GLU:O	1:A:490:GLN:HB2	1.97	0.63
2:B:1291:TRP:HA	2:B:1291:TRP:CE3	2.34	0.63
2:B:1392:ASP:OD1	2:B:1394:ASP:N	2.29	0.63
2:B:758:GLU:H	2:B:758:GLU:CD	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:SER:HB2	1:A:624:PHE:CE1	2.35	0.62
1:A:13:ARG:NH1	1:A:476:GLY:O	2.33	0.62
1:A:368:ALA:HB1	1:A:374:THR:HG23	1.81	0.62
1:A:311:HIS:HB3	2:B:1410:TYR:CE2	2.33	0.62
1:A:150:GLY:O	1:A:151:ILE:HG13	2.00	0.62
2:B:1590:TRP:HA	2:B:1590:TRP:HE3	1.63	0.62
2:B:998:PRO:O	2:B:1001:ILE:HG22	2.00	0.61
2:B:782:ILE:N	2:B:782:ILE:HD13	2.15	0.61
2:B:1113:ASN:HB2	2:B:1163:ARG:NH1	2.15	0.61
2:B:1276:LEU:HG	2:B:1276:LEU:O	2.02	0.60
2:B:843:GLU:OE2	2:B:859:ARG:HD2	2.01	0.60
2:B:981:LEU:HD23	2:B:981:LEU:N	2.17	0.60
2:B:1091:LYS:HB3	2:B:1092:PRO:CD	2.32	0.60
1:A:612:ASP:OD1	1:A:615:GLY:N	2.32	0.60
2:B:974:ASP:OD1	2:B:974:ASP:N	2.32	0.60
2:B:1035:LEU:O	2:B:1038:ARG:HB3	2.01	0.60
2:B:1462:ASN:HB2	2:B:1464:GLU:OE1	2.01	0.60
2:B:1126:LEU:HD22	2:B:1173:ALA:HB1	1.82	0.60
2:B:1039:GLN:N	2:B:1043:ALA:O	2.34	0.59
2:B:1198:TRP:N	2:B:1198:TRP:CE3	2.69	0.59
1:A:313:GLY:HA2	2:B:1423:ILE:HD11	1.84	0.59
1:A:34:THR:HG22	1:A:51:LYS:HG3	1.83	0.59
1:A:248:PHE:CD1	2:B:1378:MET:HE3	2.37	0.59
1:A:285:LEU:O	1:A:289:VAL:HG23	2.02	0.59
2:B:1514:ALA:O	2:B:1519:VAL:HG21	2.02	0.59
2:B:1579:HIS:HB3	2:B:1609:TRP:HB3	1.84	0.59
1:A:477:ARG:HB3	1:A:477:ARG:NH1	2.16	0.59
2:B:1176:GLN:HA	2:B:1220:GLN:HG2	1.84	0.59
2:B:1272:LEU:HB3	2:B:1274:VAL:HG23	1.83	0.59
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.84	0.59
1:A:253:ILE:HD13	1:A:289:VAL:HG22	1.84	0.59
2:B:1091:LYS:HB2	2:B:1092:PRO:HD2	1.83	0.59
1:A:222:TYR:CE2	1:A:224:TYR:HB2	2.38	0.58
2:B:1119:MET:O	2:B:1119:MET:SD	2.60	0.58
1:A:474:ASN:O	1:A:477:ARG:NH1	2.36	0.58
1:A:465:ILE:HG22	1:A:486:ARG:NH1	2.18	0.58
2:B:1544:GLU:O	2:B:1556:VAL:HB	2.03	0.58
2:B:830:TYR:CD1	2:B:871:SER:HB3	2.38	0.58
1:A:146:GLU:HB3	1:A:150:GLY:HA2	1.83	0.58
1:A:530:TRP:CH2	1:A:532:ASP:HB2	2.39	0.58
1:A:36:THR:HA	1:A:48:SER:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:994:ILE:HG22	2:B:1247:THR:HG21	1.85	0.57
1:A:248:PHE:HD1	2:B:1378:MET:CE	2.16	0.57
1:A:323:GLY:O	1:A:325:PRO:HD3	2.04	0.57
1:A:581:PHE:CE1	1:A:588:LYS:HD3	2.39	0.57
2:B:1378:MET:HA	2:B:1426:LEU:O	2.04	0.57
2:B:1115:ASN:HB3	2:B:1163:ARG:NH1	2.20	0.57
1:A:522:ARG:HB3	1:A:630:GLN:OE1	2.05	0.57
1:A:438:VAL:HG23	1:A:449:LEU:HD11	1.85	0.56
2:B:1541:MET:HG2	2:B:1582:MET:CE	2.33	0.56
1:A:438:VAL:CG2	1:A:449:LEU:HD11	2.35	0.56
2:B:1091:LYS:HB3	2:B:1092:PRO:HD2	1.85	0.56
1:A:438:VAL:HG21	1:A:449:LEU:HD21	1.86	0.56
2:B:947:ASP:O	2:B:1329:LYS:HG3	2.04	0.56
2:B:992:ASN:OD1	2:B:1033:GLN:NE2	2.37	0.56
2:B:1365:GLU:HA	2:B:1438:ALA:HB2	1.87	0.56
2:B:1617:ASP:HB3	2:B:1620:ASN:HB2	1.87	0.56
1:A:168:PRO:O	1:A:169:LEU:HD23	2.06	0.56
2:B:955:GLU:O	2:B:955:GLU:HG3	2.06	0.56
1:A:67:THR:O	1:A:69:PRO:HD3	2.06	0.56
1:A:492:LEU:HD23	1:A:492:LEU:C	2.27	0.55
2:B:754:GLU:HG3	2:B:769:MET:SD	2.46	0.55
2:B:894:VAL:HG23	2:B:897:HIS:HB2	1.87	0.55
2:B:1266:ASP:OD1	2:B:1266:ASP:N	2.39	0.55
2:B:1362:MET:O	2:B:1441:VAL:HG22	2.05	0.55
2:B:745:PHE:N	2:B:746:PRO:CD	2.69	0.55
1:A:210:PHE:CE1	1:A:310:LEU:CD2	2.89	0.55
2:B:1547:ILE:HG21	2:B:1634:MET:HG2	1.88	0.55
2:B:1198:TRP:N	2:B:1198:TRP:HE3	2.05	0.55
2:B:1527:LEU:HB3	2:B:1576:GLU:HA	1.88	0.55
2:B:1047:PHE:HB2	2:B:1050:ARG:HD2	1.89	0.55
1:A:302:LEU:CD2	1:A:326:ILE:HG22	2.37	0.54
2:B:1059:TYR:O	2:B:1062:LYS:N	2.40	0.54
2:B:1532:LEU:HA	2:B:1537:ASP:CB	2.35	0.54
1:A:176:LEU:HD22	1:A:176:LEU:N	2.14	0.54
1:A:302:LEU:N	1:A:302:LEU:HD23	2.22	0.54
2:B:1457:VAL:HG13	2:B:1457:VAL:O	2.08	0.54
2:B:1276:LEU:N	2:B:1276:LEU:HD23	2.23	0.54
2:B:1078:LEU:O	2:B:1082:VAL:HG23	2.07	0.54
1:A:474:ASN:HB3	1:A:479:LEU:HB2	1.90	0.54
1:A:465:ILE:HG22	1:A:465:ILE:O	2.07	0.54
2:B:1209:GLU:HB3	2:B:1249:ALA:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1291:TRP:HA	2:B:1291:TRP:HE3	1.70	0.53
2:B:1618:GLU:HA	2:B:1621:GLN:HG2	1.89	0.53
1:A:362:ALA:HB1	1:A:365:VAL:HG21	1.90	0.53
2:B:1232:ARG:N	2:B:1232:ARG:HD2	2.22	0.53
1:A:291:ASN:N	1:A:292:PRO:CD	2.71	0.53
2:B:1331:LYS:O	2:B:1333:GLN:N	2.40	0.53
2:B:1061:VAL:O	2:B:1065:SER:HB3	2.08	0.53
2:B:1110:GLY:O	2:B:1163:ARG:NH2	2.42	0.53
1:A:128:PHE:HA	1:A:165:GLY:O	2.07	0.53
1:A:30:ASP:OD1	1:A:30:ASP:N	2.42	0.53
2:B:866:ILE:HG13	2:B:872:LEU:HD23	1.90	0.53
2:B:1393:THR:HG22	2:B:1419:ARG:HH22	1.74	0.53
1:A:122:THR:HA	1:A:172:ASP:HA	1.91	0.52
1:A:248:PHE:CE1	1:A:268:ARG:HG3	2.44	0.52
1:A:486:ARG:NE	1:A:490:GLN:O	2.43	0.52
2:B:961:GLN:O	2:B:1319:THR:N	2.42	0.52
1:A:100:LEU:HD21	1:A:638:LEU:HG	1.92	0.52
1:A:309:ILE:HG23	1:A:316:MET:CB	2.38	0.52
2:B:894:VAL:CG2	2:B:897:HIS:HB2	2.39	0.52
2:B:1116:GLU:O	2:B:1120:ALA:N	2.41	0.52
3:C:1:MET:SD	3:C:3:LYS:HE2	2.49	0.52
1:A:389:ILE:HG13	1:A:389:ILE:O	2.09	0.52
2:B:886:GLN:O	2:B:907:LEU:HD23	2.10	0.52
1:A:338:THR:OG1	1:A:351:MET:N	2.40	0.52
2:B:816:SER:HA	2:B:908:LYS:O	2.10	0.52
2:B:866:ILE:CG1	2:B:872:LEU:HD23	2.39	0.52
1:A:210:PHE:CE1	1:A:310:LEU:HD23	2.45	0.52
3:C:40:ILE:O	3:C:40:ILE:CG2	2.58	0.52
2:B:829:LEU:O	2:B:871:SER:HA	2.09	0.52
1:A:484:GLN:HA	1:A:484:GLN:OE1	2.09	0.52
2:B:1334:LEU:HD23	2:B:1334:LEU:H	1.75	0.52
2:B:1359:LYS:HE2	2:B:1359:LYS:HA	1.90	0.52
2:B:889:GLU:HG3	2:B:903:VAL:O	2.11	0.51
1:A:248:PHE:HD1	2:B:1378:MET:HE3	1.75	0.51
1:A:390:ASN:OD1	3:C:43:GLY:HA2	2.10	0.51
2:B:845:LEU:HB2	2:B:889:GLU:O	2.10	0.51
2:B:1057:THR:O	2:B:1061:VAL:HG23	2.10	0.51
2:B:1450:ILE:HD13	2:B:1450:ILE:H	1.74	0.51
1:A:127:ILE:HD12	1:A:167:LEU:HB2	1.92	0.51
1:A:254:GLN:CG	1:A:254:GLN:O	2.58	0.51
3:C:46:SER:O	3:C:49:ASP:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1215:LEU:HD23	2:B:1219:LEU:HD11	1.93	0.51
2:B:1361:THR:HG23	2:B:1361:THR:O	2.10	0.51
1:A:248:PHE:CD1	2:B:1378:MET:CE	2.94	0.50
2:B:1158:TYR:HA	2:B:1161:LEU:HD11	1.93	0.50
3:C:23:VAL:HG12	3:C:58:LEU:HD13	1.92	0.50
1:A:253:ILE:CD1	1:A:289:VAL:HG22	2.41	0.50
1:A:537:CYS:HB3	1:A:539:GLY:O	2.11	0.50
1:A:312:SER:OG	1:A:314:SER:OG	2.19	0.50
1:A:591:GLN:O	1:A:594:ILE:HB	2.11	0.50
2:B:990:GLU:O	2:B:994:ILE:HG23	2.11	0.50
2:B:1063:VAL:HG22	2:B:1251:PHE:CE2	2.47	0.50
1:A:302:LEU:HD21	1:A:326:ILE:HG22	1.93	0.50
1:A:398:LEU:HD22	1:A:400:ILE:HG13	1.94	0.50
2:B:1582:MET:HG3	2:B:1606:VAL:HG23	1.93	0.50
2:B:1562:PHE:CE1	2:B:1598:TYR:HB2	2.47	0.50
2:B:1011:GLN:HA	2:B:1014:LYS:HE2	1.94	0.50
2:B:1095:VAL:HG13	2:B:1096:PHE:N	2.26	0.50
1:A:606:THR:HB	1:A:619:ASP:HB3	1.94	0.49
2:B:746:PRO:HG2	2:B:774:LYS:HG2	1.94	0.49
1:A:390:ASN:ND2	3:C:44:TYR:O	2.45	0.49
1:A:628:SER:HB2	1:A:630:GLN:OE1	2.11	0.49
2:B:997:THR:HB	2:B:998:PRO:HD3	1.92	0.49
2:B:1063:VAL:HG22	2:B:1251:PHE:HE2	1.77	0.49
2:B:1236:GLU:O	2:B:1238:ARG:NE	2.45	0.49
2:B:1223:ASP:O	2:B:1227:VAL:HG23	2.13	0.49
2:B:1547:ILE:CG2	2:B:1634:MET:HG2	2.42	0.49
2:B:1583:TRP:CD1	2:B:1583:TRP:O	2.65	0.49
1:A:207:LEU:HD21	2:B:747:GLU:HG2	1.94	0.49
2:B:1066:LEU:HA	2:B:1068:VAL:HG12	1.95	0.49
2:B:1561:THR:HB	2:B:1597:SER:HB3	1.93	0.49
2:B:1290:HIS:ND1	2:B:1293:SER:HB3	2.28	0.49
2:B:1370:TYR:CD1	2:B:1376:ALA:HB2	2.47	0.49
1:A:153:VAL:O	1:A:154:LYS:HB2	2.13	0.49
1:A:455:LEU:HD12	1:A:456:ARG:H	1.76	0.49
2:B:1196:ASN:OD1	2:B:1197:ARG:N	2.46	0.49
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.42	0.49
1:A:293:ARG:O	1:A:296:ASP:HB2	2.13	0.49
2:B:1386:MET:HG2	2:B:1453:GLY:H	1.78	0.49
1:A:9:PRO:HG2	1:A:18:GLU:HG2	1.95	0.49
1:A:311:HIS:HB3	2:B:1410:TYR:HE2	1.78	0.49
1:A:606:THR:HG22	1:A:619:ASP:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:764:ILE:O	2:B:764:ILE:HG23	2.11	0.49
2:B:930:LEU:N	2:B:930:LEU:HD22	2.27	0.49
2:B:1554:VAL:HA	2:B:1558:GLN:NE2	2.28	0.49
2:B:1562:PHE:CZ	2:B:1598:TYR:HB2	2.47	0.49
2:B:1540:ILE:HD11	2:B:1559:GLN:HB2	1.95	0.48
1:A:456:ARG:HA	3:C:40:ILE:HG23	1.95	0.48
2:B:1054:THR:OG1	2:B:1089:LYS:HE2	2.13	0.48
2:B:1528:VAL:CG2	2:B:1542:ALA:HB2	2.43	0.48
1:A:557:GLN:NE2	1:A:558:GLN:O	2.43	0.48
1:A:572:VAL:HG12	2:B:753:VAL:HG13	1.95	0.48
2:B:1054:THR:H	2:B:1100:ALA:HB2	1.78	0.48
2:B:1555:GLN:CG	2:B:1556:VAL:H	2.26	0.48
2:B:1176:GLN:HA	2:B:1220:GLN:CG	2.44	0.48
2:B:1338:LYS:HA	2:B:1371:ARG:HB3	1.95	0.48
1:A:210:PHE:CE1	1:A:310:LEU:HD21	2.48	0.48
1:A:239:TYR:CE1	2:B:832:TYR:HE2	2.32	0.48
1:A:492:LEU:HD23	1:A:493:VAL:N	2.29	0.48
2:B:1385:MET:SD	2:B:1391:PRO:HD3	2.54	0.48
2:B:1392:ASP:OD1	2:B:1392:ASP:C	2.51	0.48
1:A:403:ARG:NH2	1:A:414:GLN:HB2	2.29	0.48
1:A:151:ILE:HG22	1:A:151:ILE:O	2.13	0.48
2:B:1532:LEU:HD11	2:B:1569:ARG:HG3	1.94	0.48
1:A:204:GLU:HG2	2:B:815:TYR:CE2	2.49	0.48
2:B:980:HIS:C	2:B:981:LEU:HD23	2.34	0.48
1:A:223:ILE:HG22	1:A:294:ALA:HB1	1.95	0.48
1:A:455:LEU:HD22	1:A:465:ILE:HG21	1.95	0.47
2:B:1195:LYS:HB2	2:B:1226:PHE:CZ	2.49	0.47
1:A:152:PRO:HD2	2:B:1297:LEU:HD22	1.95	0.47
1:A:448:THR:HA	1:A:497:LEU:O	2.14	0.47
2:B:1334:LEU:H	2:B:1334:LEU:CD2	2.27	0.47
1:A:594:ILE:O	1:A:597:VAL:HB	2.14	0.47
2:B:1013:GLU:HA	2:B:1017:LEU:CD1	2.44	0.47
2:B:1458:TYR:HB3	2:B:1466:SER:HB2	1.97	0.47
2:B:1579:HIS:C	2:B:1609:TRP:HB3	2.35	0.47
1:A:69:PRO:HB2	1:A:70:ALA:HB2	1.95	0.47
1:A:591:GLN:OE1	2:B:794:CYS:HA	2.14	0.47
2:B:962:GLY:HA2	2:B:1318:GLY:HA2	1.97	0.47
2:B:1174:LEU:O	2:B:1177:MET:N	2.48	0.47
1:A:297:LEU:O	1:A:300:LYS:HB2	2.14	0.47
2:B:1200:ASP:HB3	2:B:1201:PRO:HD2	1.95	0.47
1:A:396:LYS:HG3	1:A:397:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:VAL:HG11	1:A:622:LEU:HD12	1.97	0.47
2:B:923:ARG:HG3	2:B:940:ILE:HD11	1.96	0.47
2:B:777:ILE:HG22	2:B:777:ILE:O	2.15	0.47
2:B:1437:LEU:HD13	2:B:1438:ALA:H	1.79	0.47
2:B:807:PHE:HA	2:B:830:TYR:O	2.15	0.47
1:A:268:ARG:NH1	2:B:1427:ASP:OD1	2.46	0.47
2:B:991:GLN:HA	2:B:994:ILE:HG12	1.95	0.47
2:B:1098:GLU:HB2	2:B:1121:LEU:HD22	1.95	0.47
2:B:1510:ARG:HD3	2:B:1630:PHE:CD1	2.50	0.47
1:A:307:THR:HG23	1:A:318:GLN:HG3	1.97	0.46
1:A:334:HIS:HB3	1:A:336:THR:HG23	1.96	0.46
2:B:1531:GLN:HB2	2:B:1538:GLU:HG3	1.96	0.46
2:B:1533:SER:OG	2:B:1535:ASP:OD1	2.33	0.46
1:A:31:VAL:HB	1:A:54:LEU:CD1	2.46	0.46
1:A:255:ASP:HA	1:A:256:GLY:HA2	1.55	0.46
2:B:1095:VAL:HG22	2:B:1122:THR:OG1	2.15	0.46
2:B:1482:LYS:HD2	2:B:1484:CYS:SG	2.56	0.46
2:B:1323:VAL:HG12	2:B:1324:THR:N	2.30	0.46
1:A:332:GLN:O	1:A:354:VAL:HA	2.15	0.46
2:B:1526:ARG:HB2	2:B:1544:GLU:OE2	2.15	0.46
2:B:1529:LYS:O	2:B:1540:ILE:HG23	2.14	0.46
1:A:118:THR:HA	1:A:203:LYS:O	2.15	0.46
1:A:590:THR:O	1:A:592:SER:N	2.49	0.46
2:B:949:VAL:HG13	2:B:950:PRO:HD2	1.96	0.46
2:B:1093:ASP:OD1	2:B:1094:GLY:N	2.45	0.46
1:A:596:ASP:O	1:A:600:LYS:HG3	2.16	0.46
2:B:1055:TRP:CZ3	2:B:1107:MET:SD	3.09	0.46
2:B:1538:GLU:HB3	2:B:1563:ILE:HG22	1.97	0.46
1:A:456:ARG:O	1:A:456:ARG:HG3	2.16	0.45
2:B:989:GLY:HA3	2:B:1046:ALA:O	2.16	0.45
1:A:320:GLU:O	1:A:320:GLU:HG3	2.15	0.45
2:B:1209:GLU:OE1	2:B:1248:GLN:HG2	2.16	0.45
2:B:1335:THR:O	2:B:1335:THR:CG2	2.62	0.45
1:A:147:ASN:HB3	1:A:182:TRP:CH2	2.51	0.45
1:A:462:GLU:O	1:A:462:GLU:HG3	2.15	0.45
1:A:547:GLN:NE2	1:A:550:ASP:HB2	2.32	0.45
2:B:1117:LYS:O	2:B:1121:LEU:HB3	2.17	0.45
2:B:1513:LYS:O	2:B:1516:GLU:OE1	2.33	0.45
2:B:759:PRO:O	2:B:761:LYS:HG3	2.16	0.45
2:B:1535:ASP:OD1	2:B:1535:ASP:N	2.48	0.45
1:A:259:ARG:HD3	1:A:303:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1552:ASP:O	2:B:1554:VAL:HG22	2.16	0.45
1:A:255:ASP:CB	1:A:300:LYS:HG3	2.46	0.45
2:B:910:VAL:HG12	2:B:911:PRO:HD2	1.99	0.45
2:B:978:LEU:HD21	2:B:1254:PHE:CZ	2.51	0.45
1:A:454:LEU:HD11	3:C:31:LEU:HD11	1.98	0.45
1:A:475:LYS:HB2	1:A:477:ARG:HH12	1.82	0.45
1:A:147:ASN:O	1:A:149:GLU:N	2.50	0.45
2:B:1360:ASN:HB2	2:B:1443:GLN:HG3	1.99	0.45
2:B:1417:SER:O	2:B:1418:ASP:OD1	2.34	0.45
2:B:1527:LEU:HA	2:B:1541:MET:SD	2.56	0.45
2:B:1062:LYS:O	2:B:1065:SER:OG	2.23	0.45
2:B:1143:LEU:HD21	2:B:1147:ILE:HD11	1.99	0.45
2:B:1348:ALA:HB2	2:B:1363:ILE:HG13	1.99	0.45
1:A:425:SER:N	1:A:611:LYS:O	2.49	0.44
1:A:10:ASN:OD1	1:A:635:ARG:NH1	2.50	0.44
1:A:362:ALA:O	1:A:383:GLY:HA2	2.17	0.44
2:B:990:GLU:O	2:B:993:MET:HB3	2.17	0.44
2:B:1143:LEU:N	2:B:1144:PRO:HD2	2.31	0.44
1:A:323:GLY:O	1:A:325:PRO:CD	2.64	0.44
2:B:1226:PHE:CD1	2:B:1226:PHE:O	2.70	0.44
2:B:1546:THR:O	2:B:1546:THR:OG1	2.35	0.44
1:A:465:ILE:HG22	1:A:486:ARG:HH11	1.82	0.44
1:A:216:PRO:HA	1:A:231:VAL:HA	2.00	0.44
1:A:245:GLY:O	1:A:311:HIS:CE1	2.71	0.44
1:A:591:GLN:HA	1:A:594:ILE:HD12	1.99	0.44
1:A:41:PRO:HB3	2:B:1020:ARG:NH1	2.32	0.44
2:B:1095:VAL:CG2	2:B:1118:ASP:O	2.65	0.44
1:A:505:PRO:HG2	1:A:599:GLU:OE2	2.18	0.44
1:A:567:HIS:HB2	2:B:760:PRO:HB3	1.99	0.44
2:B:1528:VAL:HG23	2:B:1542:ALA:HB2	2.00	0.44
1:A:209:SER:HB3	1:A:315:ASP:OD2	2.18	0.44
2:B:1387:THR:HB	2:B:1450:ILE:HA	1.98	0.44
2:B:788:SER:HB3	2:B:791:LYS:HB2	1.99	0.43
2:B:1526:ARG:O	2:B:1542:ALA:HB3	2.18	0.43
2:B:1566:ILE:HD13	2:B:1566:ILE:H	1.83	0.43
1:A:449:LEU:N	1:A:497:LEU:O	2.49	0.43
1:A:606:THR:CG2	1:A:619:ASP:HB3	2.48	0.43
2:B:911:PRO:HG2	2:B:1327:HIS:ND1	2.33	0.43
2:B:1564:SER:HA	2:B:1600:ILE:HD12	2.00	0.43
2:B:822:GLN:HB2	2:B:879:VAL:HG22	2.01	0.43
2:B:915:ARG:H	2:B:915:ARG:HG2	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:31:LEU:C	3:C:31:LEU:CD2	2.87	0.43
1:A:149:GLU:O	1:A:151:ILE:HD12	2.18	0.43
1:A:453:PHE:N	1:A:453:PHE:CD1	2.86	0.43
2:B:1631:THR:O	2:B:1635:VAL:HG12	2.19	0.43
1:A:98:VAL:CG1	2:B:1017:LEU:HD23	2.48	0.43
1:A:402:VAL:HG12	1:A:403:ARG:N	2.33	0.43
2:B:1331:LYS:O	2:B:1332:ASP:C	2.56	0.43
2:B:1527:LEU:CA	2:B:1541:MET:SD	3.06	0.43
2:B:1562:PHE:CZ	2:B:1598:TYR:CB	3.01	0.43
1:A:8:THR:HG23	1:A:20:MET:HB2	2.00	0.43
1:A:497:LEU:HD12	1:A:497:LEU:HA	1.81	0.43
2:B:1117:LYS:HG3	2:B:1118:ASP:N	2.34	0.43
2:B:1564:SER:CB	2:B:1600:ILE:HD12	2.49	0.43
1:A:590:THR:O	1:A:593:LYS:N	2.52	0.43
2:B:997:THR:HG21	2:B:1247:THR:HG22	2.01	0.43
2:B:1601:GLY:H	2:B:1604:THR:HB	1.84	0.43
1:A:366:PRO:HB2	1:A:405:LYS:HB2	2.00	0.43
1:A:481:ALA:HB3	4:D:1:NAG:C8	2.49	0.43
2:B:1159:MET:SD	2:B:1187:LYS:HG3	2.59	0.43
2:B:1214:ALA:O	2:B:1217:ALA:HB3	2.18	0.43
2:B:1347:PRO:HA	2:B:1362:MET:HA	2.01	0.43
1:A:569:ALA:HB2	2:B:788:SER:HB2	2.00	0.43
2:B:838:LEU:O	2:B:865:THR:HA	2.19	0.43
2:B:1560:ARG:HA	2:B:1560:ARG:HD3	1.86	0.43
2:B:1341:LEU:HA	2:B:1367:CYS:O	2.18	0.42
2:B:1359:LYS:HG3	2:B:1360:ASN:H	1.83	0.42
1:A:23:GLU:OE1	1:A:469:THR:CG2	2.68	0.42
1:A:187:TYR:HB3	1:A:195:VAL:HA	2.00	0.42
2:B:843:GLU:OE2	2:B:859:ARG:CD	2.65	0.42
2:B:1031:TYR:CZ	2:B:1035:LEU:HD11	2.54	0.42
2:B:1382:ASP:HB3	2:B:1456:LYS:HG2	1.99	0.42
2:B:1390:ALA:HA	2:B:1391:PRO:HD3	1.89	0.42
2:B:1483:LEU:HD23	2:B:1563:ILE:HD12	2.00	0.42
1:A:154:LYS:HE2	1:A:156:ASP:OD1	2.19	0.42
2:B:1186:ASN:HA	2:B:1189:LEU:HB3	2.01	0.42
2:B:1197:ARG:HD2	2:B:1233:TRP:CZ2	2.54	0.42
2:B:1599:ILE:HG22	2:B:1600:ILE:O	2.19	0.42
1:A:344:PRO:HG2	1:A:433:TYR:OH	2.18	0.42
1:A:148:PRO:HG3	1:A:181:GLN:N	2.34	0.42
1:A:390:ASN:HD21	3:C:44:TYR:N	2.18	0.42
2:B:774:LYS:CD	2:B:774:LYS:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:910:VAL:CG1	2:B:911:PRO:HD2	2.49	0.42
2:B:1180:LEU:HD21	2:B:1185:LEU:HA	2.00	0.42
2:B:1505:VAL:O	2:B:1505:VAL:HG22	2.19	0.42
1:A:297:LEU:HB2	1:A:326:ILE:HD11	2.02	0.42
1:A:353:PHE:CE2	1:A:355:THR:CG2	3.03	0.42
2:B:1143:LEU:N	2:B:1144:PRO:CD	2.82	0.42
2:B:1221:LEU:HD11	2:B:1223:ASP:HB2	2.02	0.42
3:C:8:ALA:C	3:C:9:THR:OG1	2.54	0.42
2:B:818:VAL:HB	2:B:821:GLU:HB2	2.01	0.42
2:B:1411:GLU:HG2	2:B:1422:LEU:HD12	2.02	0.42
2:B:1399:LEU:HD23	2:B:1399:LEU:HA	1.90	0.42
2:B:1600:ILE:O	2:B:1600:ILE:HD13	2.20	0.42
1:A:7:ILE:HB	1:A:21:VAL:HB	2.02	0.42
1:A:286:LEU:HD22	1:A:286:LEU:HA	1.79	0.42
1:A:504:ILE:HG23	1:A:533:VAL:HG11	2.02	0.42
2:B:880:PRO:HB2	2:B:909:VAL:CG1	2.50	0.42
2:B:1513:LYS:HE2	2:B:1513:LYS:HB3	1.95	0.42
1:A:410:SER:O	1:A:414:GLN:HG2	2.20	0.41
2:B:1028:LYS:CG	2:B:1071:ILE:HD13	2.50	0.41
2:B:1344:THR:HG23	2:B:1346:LYS:HE3	2.02	0.41
2:B:1345:ILE:O	2:B:1345:ILE:HG23	2.20	0.41
2:B:997:THR:CG2	2:B:1059:TYR:OH	2.68	0.41
2:B:997:THR:HG23	2:B:1059:TYR:OH	2.19	0.41
1:A:23:GLU:CG	1:A:61:MET:HG2	2.50	0.41
2:B:904:ARG:O	2:B:904:ARG:HG3	2.20	0.41
2:B:1009:THR:O	2:B:1010:GLU:C	2.59	0.41
2:B:1407:ILE:HG12	2:B:1424:ILE:HG12	2.01	0.41
1:A:3:MET:HE3	1:A:522:ARG:HG2	2.02	0.41
1:A:125:TYR:N	1:A:125:TYR:CD1	2.88	0.41
1:A:136:PRO:HG2	2:B:789:ASP:HA	2.02	0.41
1:A:398:LEU:O	1:A:420:GLN:HA	2.20	0.41
1:A:456:ARG:HA	3:C:40:ILE:CG2	2.50	0.41
1:A:613:TYR:CG	1:A:614:ALA:N	2.89	0.41
2:B:904:ARG:O	2:B:904:ARG:CG	2.68	0.41
2:B:936:GLN:HE21	2:B:938:GLU:HG3	1.85	0.41
2:B:1039:GLN:C	2:B:1041:SER:H	2.24	0.41
2:B:1197:ARG:HE	2:B:1199:GLU:HG2	1.86	0.41
2:B:1323:VAL:HG12	2:B:1324:THR:H	1.83	0.41
2:B:1563:ILE:HD11	2:B:1599:ILE:HG12	2.02	0.41
1:A:174:PRO:O	1:A:177:VAL:HB	2.20	0.41
2:B:764:ILE:O	2:B:764:ILE:CG2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:773:LEU:HD13	2:B:803:VAL:HG22	2.01	0.41
2:B:1083:LYS:O	2:B:1086:ILE:HG13	2.20	0.41
2:B:1507:LEU:HD13	2:B:1507:LEU:C	2.41	0.41
1:A:151:ILE:O	1:A:153:VAL:HG23	2.21	0.41
1:A:249:VAL:HG21	1:A:278:VAL:HG11	2.03	0.41
1:A:572:VAL:HG22	2:B:785:VAL:HB	2.03	0.41
1:A:639:GLN:O	1:A:641:PRO:HD3	2.20	0.41
2:B:1209:GLU:CB	2:B:1249:ALA:HA	2.50	0.41
2:B:1219:LEU:HD22	2:B:1260:TYR:HA	2.03	0.41
2:B:1284:LYS:H	2:B:1284:LYS:HG3	1.66	0.41
1:A:125:TYR:CE2	1:A:169:LEU:HD12	2.56	0.41
1:A:190:ASN:OD1	1:A:190:ASN:N	2.48	0.41
1:A:503:PHE:O	1:A:506:SER:O	2.39	0.41
1:A:543:VAL:HG12	2:B:799:PHE:CD2	2.56	0.41
1:A:635:ARG:NE	1:A:637:GLU:O	2.48	0.41
2:B:1039:GLN:O	2:B:1041:SER:N	2.54	0.41
2:B:1113:ASN:OD1	2:B:1113:ASN:N	2.54	0.41
2:B:1167:VAL:HG11	2:B:1191:THR:HG21	2.02	0.41
2:B:1428:LYS:HG3	2:B:1428:LYS:O	2.20	0.41
1:A:313:GLY:HA3	2:B:1423:ILE:HD11	2.00	0.41
2:B:1227:VAL:HB	2:B:1228:PRO:HD3	2.02	0.41
2:B:1228:PRO:HB2	2:B:1229:PRO:HD3	2.02	0.41
2:B:1572:LEU:HB3	2:B:1574:LEU:HD13	2.02	0.41
2:B:1287:HIS:HB3	2:B:1298:ARG:HD2	2.03	0.40
1:A:577:ASP:C	1:A:577:ASP:OD1	2.60	0.40
2:B:806:ASP:HB3	2:B:833:ARG:CD	2.46	0.40
2:B:889:GLU:CG	2:B:904:ARG:HB3	2.47	0.40
2:B:1055:TRP:NE1	2:B:1124:PHE:CE2	2.90	0.40
2:B:1472:HIS:CG	2:B:1473:PRO:HD2	2.55	0.40
1:A:248:PHE:CE1	2:B:1378:MET:HE3	2.57	0.40
2:B:1100:ALA:N	2:B:1101:PRO:HD3	2.35	0.40
2:B:1123:ALA:CB	2:B:1169:ILE:HG22	2.51	0.40
2:B:1564:SER:OG	2:B:1568:CYS:HB2	2.22	0.40
1:A:187:TYR:CD1	1:A:187:TYR:N	2.89	0.40
1:A:333:ILE:HG23	1:A:352:VAL:HG13	2.04	0.40
1:A:342:PHE:CE2	1:A:398:LEU:HB2	2.56	0.40
1:A:500:THR:C	1:A:502:ASP:H	2.25	0.40
1:A:147:ASN:ND2	1:A:149:GLU:O	2.55	0.40
1:A:344:PRO:HD2	1:A:433:TYR:CE1	2.57	0.40
1:A:443:LEU:HD21	1:A:449:LEU:HD13	2.04	0.40
1:A:454:LEU:CD2	1:A:492:LEU:HD12	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1028:LYS:HG2	2:B:1071:ILE:HD13	2.04	0.40
2:B:1197:ARG:C	2:B:1198:TRP:CE3	2.95	0.40
2:B:1510:ARG:NH2	2:B:1607:GLU:OE1	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	632/645 (98%)	541 (86%)	70 (11%)	21 (3%)	4	22
2	B	896/915 (98%)	730 (82%)	143 (16%)	23 (3%)	5	26
3	C	61/65 (94%)	48 (79%)	10 (16%)	3 (5%)	2	14
All	All	1589/1625 (98%)	1319 (83%)	223 (14%)	47 (3%)	4	23

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	ASN
1	A	441	THR
2	B	1332	ASP
2	B	1417	SER
1	A	15	GLU
1	A	91	GLY
1	A	154	LYS
1	A	290	GLN
1	A	292	PRO
1	A	536	SER
2	B	1010	GLU
2	B	1103	ILE
2	B	1267	HIS
2	B	1448	GLU

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Mol	Chain	Res	Type
2	B	1528	VAL
2	B	1535	ASP
3	C	36	ASP
1	A	194	GLN
1	A	300	LYS
1	A	380	GLN
1	A	501	THR
1	A	591	GLN
2	B	1013	GLU
2	B	1089	LYS
2	B	1244	TYR
2	B	1250	THR
2	B	1377	THR
2	B	1415	ALA
2	B	1579	HIS
1	A	152	PRO
1	A	549	GLU
2	B	1251	PHE
2	B	1494	GLU
2	B	1566	ILE
1	A	161	GLN
1	A	281	SER
1	A	324	ILE
1	A	550	ASP
1	A	555	PRO
2	B	1486	ASP
3	C	9	THR
3	C	47	GLU
1	A	465	ILE
2	B	1091	LYS
2	B	1102	VAL
2	B	1253	VAL
2	B	1518	GLY

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	558/567 (98%)	459 (82%)	99 (18%)	2	6
2	B	794/810 (98%)	639 (80%)	155 (20%)	1	4
3	C	53/55 (96%)	44 (83%)	9 (17%)	2	8
All	All	1405/1432 (98%)	1142 (81%)	263 (19%)	1	5

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	11	ILE
1	A	14	LEU
1	A	16	SER
1	A	18	GLU
1	A	26	ASP
1	A	30	ASP
1	A	33	VAL
1	A	43	LYS
1	A	45	LEU
1	A	47	LEU
1	A	53	VAL
1	A	54	LEU
1	A	59	ASN
1	A	64	VAL
1	A	67	THR
1	A	85	THR
1	A	92	THR
1	A	99	VAL
1	A	110	ILE
1	A	118	THR
1	A	125	TYR
1	A	127	ILE
1	A	134	LEU
1	A	142	MET
1	A	149	GLU
1	A	170	SER
1	A	172	ASP
1	A	176	LEU
1	A	177	VAL
1	A	187	TYR
1	A	190	ASN
1	A	197	SER
1	A	206	VAL

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Mol	Chain	Res	Type
1	A	209	SER
1	A	226	GLU
1	A	241	LYS
1	A	246	THR
1	A	249	VAL
1	A	253	ILE
1	A	258	GLN
1	A	273	ASP
1	A	275	SER
1	A	281	SER
1	A	286	LEU
1	A	302	LEU
1	A	305	SER
1	A	309	ILE
1	A	310	LEU
1	A	318	GLN
1	A	320	GLU
1	A	326	ILE
1	A	328	THR
1	A	338	THR
1	A	340	LYS
1	A	343	LYS
1	A	364	ARG
1	A	369	VAL
1	A	372	GLU
1	A	373	ASP
1	A	384	VAL
1	A	398	LEU
1	A	405	LYS
1	A	406	LYS
1	A	410	SER
1	A	419	MET
1	A	426	THR
1	A	437	SER
1	A	440	ARG
1	A	453	PHE
1	A	458	ASP
1	A	459	ARG
1	A	462	GLU
1	A	467	TYR
1	A	471	LEU
1	A	500	THR

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Mol	Chain	Res	Type
1	A	504	ILE
1	A	508	ARG
1	A	510	VAL
1	A	515	LEU
1	A	528	SER
1	A	533	VAL
1	A	540	SER
1	A	542	VAL
1	A	547	GLN
1	A	548	SER
1	A	551	ARG
1	A	557	GLN
1	A	558	GLN
1	A	566	ASP
1	A	583	LEU
1	A	586	LYS
1	A	590	THR
1	A	606	THR
1	A	625	THR
1	A	628	SER
1	A	630	GLN
1	A	637	GLU
1	A	642	GLN
2	B	737	GLU
2	B	743	SER
2	B	744	GLU
2	B	755	ASP
2	B	761	LYS
2	B	762	ASN
2	B	770	ASN
2	B	775	ASP
2	B	776	SER
2	B	782	ILE
2	B	786	SER
2	B	813	LEU
2	B	819	ARG
2	B	822	GLN
2	B	824	GLU
2	B	838	LEU
2	B	844	LEU
2	B	853	LEU
2	B	857	LYS

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Mol	Chain	Res	Type
2	B	865	THR
2	B	870	SER
2	B	872	LEU
2	B	878	ILE
2	B	881	LEU
2	B	882	LYS
2	B	883	THR
2	B	885	LEU
2	B	890	VAL
2	B	904	ARG
2	B	915	ARG
2	B	925	LEU
2	B	932	ARG
2	B	946	SER
2	B	947	ASP
2	B	955	GLU
2	B	957	ARG
2	B	959	LEU
2	B	963	THR
2	B	968	MET
2	B	970	GLU
2	B	971	ASP
2	B	974	ASP
2	B	977	ARG
2	B	983	VAL
2	B	984	THR
2	B	990	GLU
2	B	991	GLN
2	B	1010	GLU
2	B	1014	LYS
2	B	1018	GLU
2	B	1029	LYS
2	B	1056	LEU
2	B	1060	VAL
2	B	1066	LEU
2	B	1074	ASP
2	B	1075	SER
2	B	1076	GLN
2	B	1091	LYS
2	B	1095	VAL
2	B	1106	GLU
2	B	1107	MET

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Mol	Chain	Res	Type
2	B	1108	ILE
2	B	1113	ASN
2	B	1119	MET
2	B	1131	GLU
2	B	1137	GLU
2	B	1141	ASN
2	B	1143	LEU
2	B	1146	SER
2	B	1149	LYS
2	B	1157	ASN
2	B	1174	LEU
2	B	1187	LYS
2	B	1196	ASN
2	B	1198	TRP
2	B	1205	LEU
2	B	1219	LEU
2	B	1222	LYS
2	B	1232	ARG
2	B	1238	ARG
2	B	1246	SER
2	B	1247	THR
2	B	1251	PHE
2	B	1266	ASP
2	B	1278	LEU
2	B	1284	LYS
2	B	1288	ARG
2	B	1291	TRP
2	B	1299	SER
2	B	1305	ASN
2	B	1324	THR
2	B	1331	LYS
2	B	1336	CYS
2	B	1337	ASN
2	B	1338	LYS
2	B	1339	PHE
2	B	1341	LEU
2	B	1359	LYS
2	B	1368	THR
2	B	1371	ARG
2	B	1379	SER
2	B	1394	ASP
2	B	1395	ASP

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Mol	Chain	Res	Type
2	B	1397	LYS
2	B	1401	ASN
2	B	1405	ARG
2	B	1406	TYR
2	B	1408	SER
2	B	1409	LYS
2	B	1411	GLU
2	B	1428	LYS
2	B	1432	SER
2	B	1433	GLU
2	B	1437	LEU
2	B	1440	LYS
2	B	1443	GLN
2	B	1450	ILE
2	B	1456	LYS
2	B	1469	ARG
2	B	1475	LYS
2	B	1487	GLU
2	B	1497	PHE
2	B	1498	ILE
2	B	1499	GLN
2	B	1500	LYS
2	B	1506	THR
2	B	1509	GLU
2	B	1510	ARG
2	B	1512	ASP
2	B	1527	LEU
2	B	1529	LYS
2	B	1532	LEU
2	B	1538	GLU
2	B	1540	ILE
2	B	1541	MET
2	B	1545	GLN
2	B	1546	THR
2	B	1552	ASP
2	B	1566	ILE
2	B	1569	ARG
2	B	1582	MET
2	B	1583	TRP
2	B	1586	SER
2	B	1590	TRP
2	B	1592	GLU

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Mol	Chain	Res	Type
2	B	1597	SER
2	B	1600	ILE
2	B	1602	LYS
2	B	1606	VAL
2	B	1618	GLU
2	B	1619	GLU
2	B	1623	GLN
2	B	1626	ASP
2	B	1634	MET
2	B	1637	PHE
3	C	12	GLU
3	C	14	GLU
3	C	31	LEU
3	C	34	TYR
3	C	35	ASP
3	C	40	ILE
3	C	46	SER
3	C	47	GLU
3	C	63	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
2	B	1039	GLN
2	B	1105	GLN
2	B	1248	GLN
2	B	1337	ASN
2	B	1558	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

3 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	D	1	4,1	14,14,15	1.03	1 (7%)	17,19,21	1.27	2 (11%)
4	NAG	D	2	4	14,14,15	1.21	1 (7%)	17,19,21	0.76	0
4	BMA	D	3	4	11,11,12	0.75	0	15,15,17	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	NAG	C1-C2	3.43	1.57	1.52
4	D	1	NAG	C1-C2	-2.29	1.48	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C4-C3-C2	-3.92	105.27	111.02
4	D	1	NAG	C2-N2-C7	-2.15	119.85	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

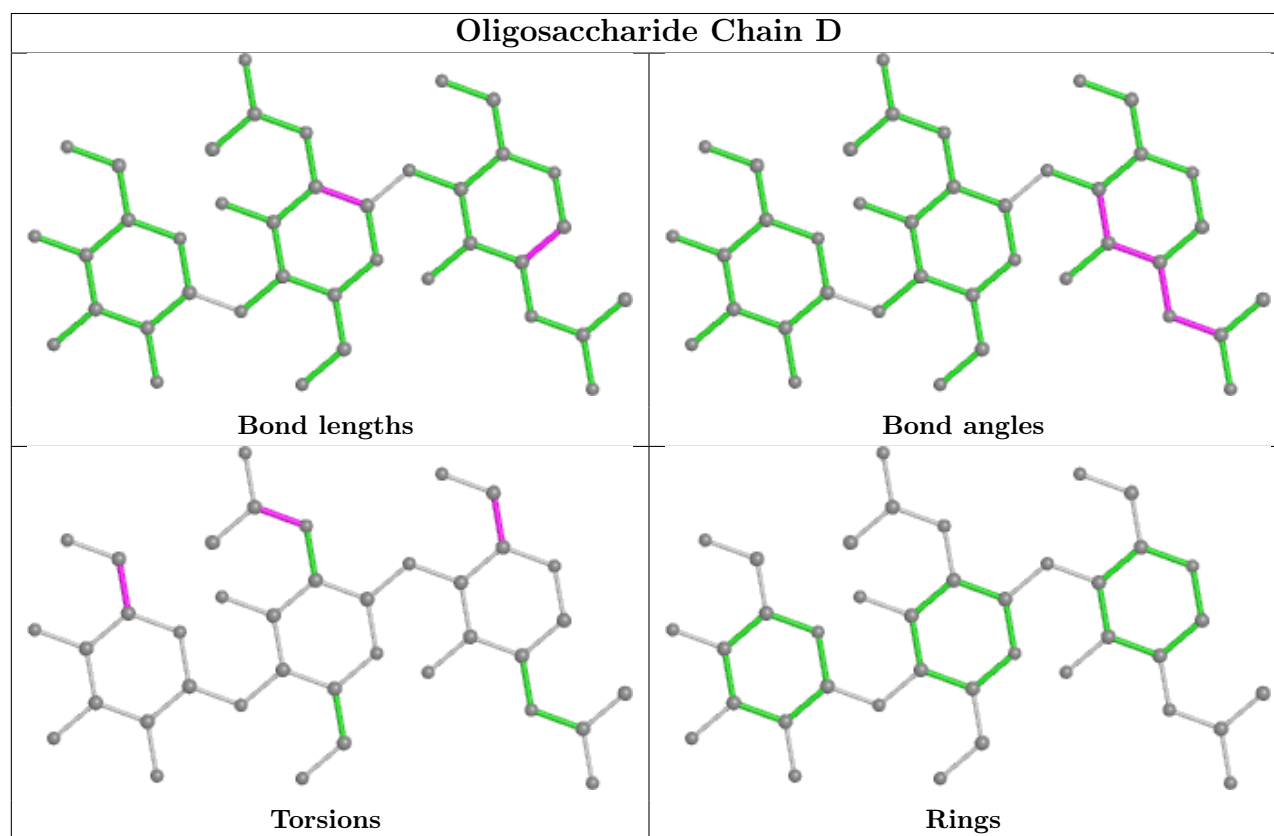
Mol	Chain	Res	Type	Atoms
4	D	3	BMA	C4-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	3	BMA	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	B	1701	2	14,14,15	0.44	0	17,19,21	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1701	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1701	NAG	C4-C5-C6-O6
5	B	1701	NAG	O5-C5-C6-O6

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	636/645 (98%)	0.10	2 (0%) 94 93	90, 116, 149, 172	0
2	B	902/915 (98%)	0.27	45 (4%) 28 29	94, 146, 192, 217	0
3	C	63/65 (96%)	0.02	0 100 100	97, 127, 150, 162	0
All	All	1601/1625 (98%)	0.19	47 (2%) 51 50	90, 134, 186, 217	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1044	PHE	6.1
2	B	1045	ALA	4.1
2	B	1316	GLY	3.7
2	B	1047	PHE	3.4
2	B	1096	PHE	3.3
2	B	1621	GLN	3.2
2	B	1202	GLY	3.2
2	B	1048	VAL	3.1
2	B	1147	ILE	3.1
2	B	1158	TYR	3.0
2	B	1040	PRO	2.9
2	B	1198	TRP	2.8
2	B	1049	LYS	2.8
2	B	933	GLU	2.8
2	B	1630	PHE	2.7
2	B	1050	ARG	2.7
2	B	1183	PRO	2.7
2	B	1125	VAL	2.6
2	B	1087	LEU	2.6
2	B	1276	LEU	2.5
2	B	1063	VAL	2.5
2	B	1170	ALA	2.5
2	B	960	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	1296	LEU	2.4
1	A	79	GLY	2.4
2	B	1188	PHE	2.4
2	B	1226	PHE	2.4
2	B	1036	ALA	2.4
2	B	1064	PHE	2.3
2	B	1320	LEU	2.3
1	A	83	PHE	2.3
2	B	1366	ILE	2.3
2	B	1111	LEU	2.3
2	B	1563	ILE	2.2
2	B	1043	ALA	2.2
2	B	1278	LEU	2.2
2	B	1201	PRO	2.2
2	B	1143	LEU	2.2
2	B	1129	LEU	2.2
2	B	1154	LEU	2.1
2	B	1046	ALA	2.1
2	B	1082	VAL	2.1
2	B	1396	LEU	2.1
2	B	1180	LEU	2.1
2	B	1172	TYR	2.1
2	B	1195	LYS	2.0
2	B	1308	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

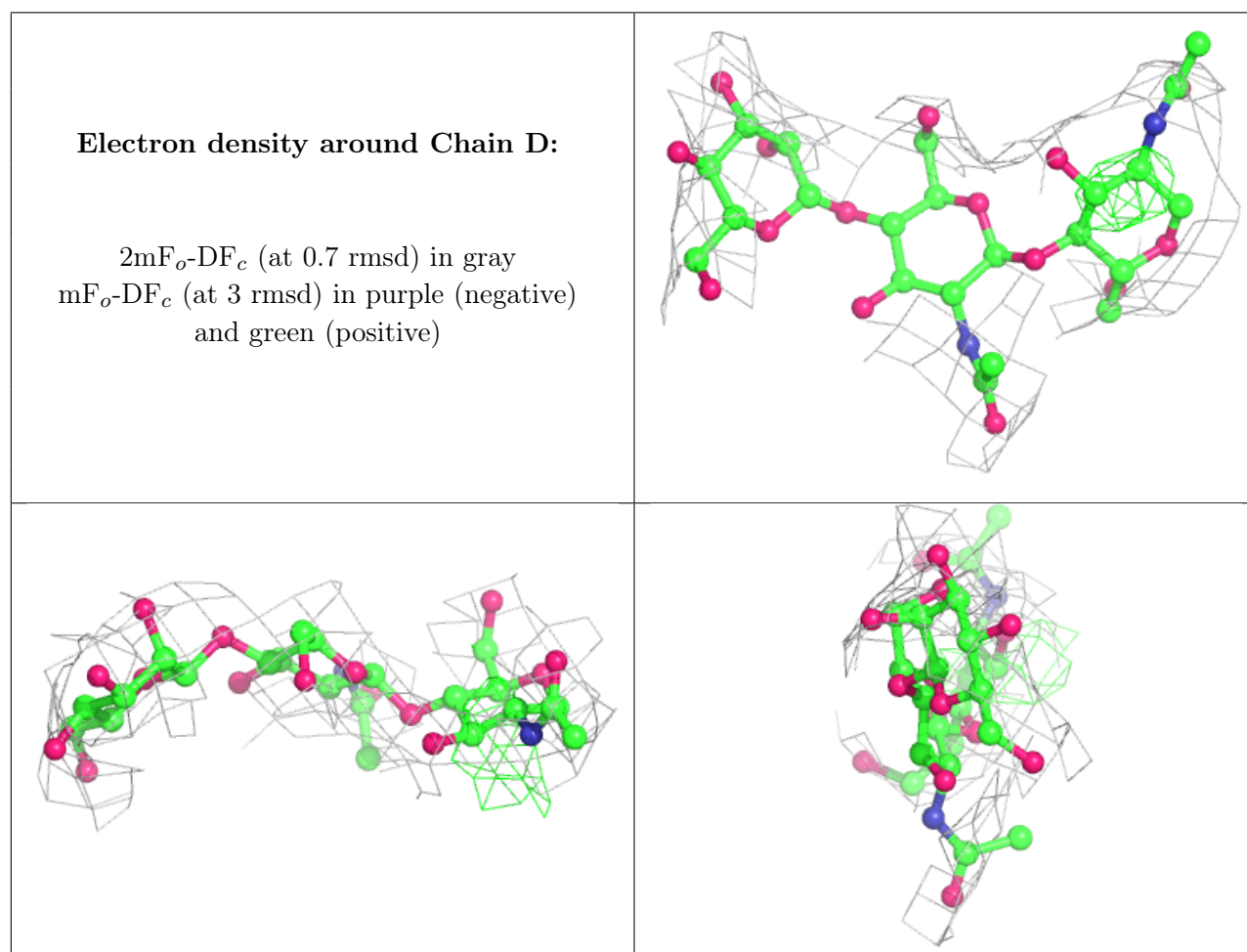
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	D	3	11/12	0.68	0.29	190,194,195,196	0
4	NAG	D	2	14/15	0.83	0.26	177,180,184,192	0
4	NAG	D	1	14/15	0.85	0.29	155,159,171,171	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	B	1701	14/15	0.81	0.31	126,134,141,143	0

6.5 Other polymers [i](#)

There are no such residues in this entry.