



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 04:21 AM BST

PDB ID : 2C5D  
Title : Structure of a minimal Gas6-Axl complex  
Authors : Sasaki, T.; Knyazev, P.G.; Clout, N.J.; Cheburkin, Y.; Goehring, W.; Ullrich, A.; Timpl, R.; Hohenester, E.  
Deposited on : 2005-10-26  
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

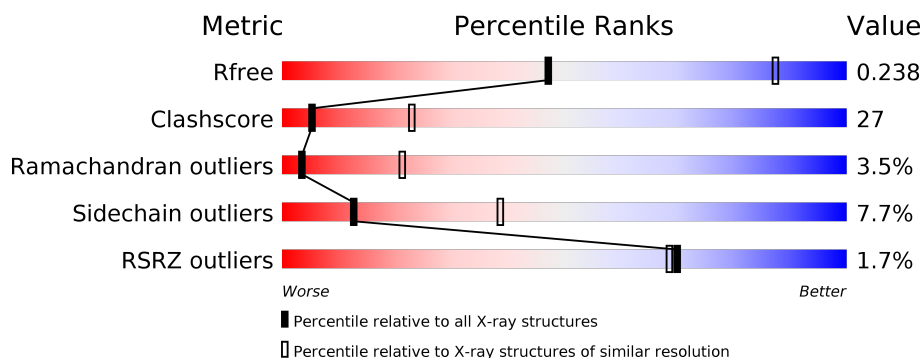
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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  $\geq 3$ , 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	422	<div> <div>0%</div> <div> <div>48%</div> <div>35%</div> <div>7%</div> <div>10%</div> </div> </div>
1	B	422	<div> <div>0%</div> <div> <div>47%</div> <div>36%</div> <div>7%</div> <div>10%</div> </div> </div>
2	C	195	<div> <div>2%</div> <div> <div>53%</div> <div>39%</div> <div>5%</div> <div>...</div> </div> </div>
2	D	195	<div> <div>2%</div> <div> <div>54%</div> <div>38%</div> <div>6%</div> <div>...</div> </div> </div>
3	E	2	<div> <div>100%</div> </div>
3	F	2	<div> <div>50%</div> <div>50%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8879 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 GROWTH-ARREST-SPECIFIC PROTEIN 6 PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	1
			2953	1882	518	539	14			
1	B	381	Total	C	N	O	S	0	0	1
			2953	1882	518	539	14			

- Molecule 2 is a protein called TYROSINE-PROTEIN KINASE RECEPTOR UFO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	192	Total	C	N	O	S	0	0	1
			1454	911	251	288	4			
2	D	192	Total	C	N	O	S	0	0	1
			1454	911	251	288	4			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

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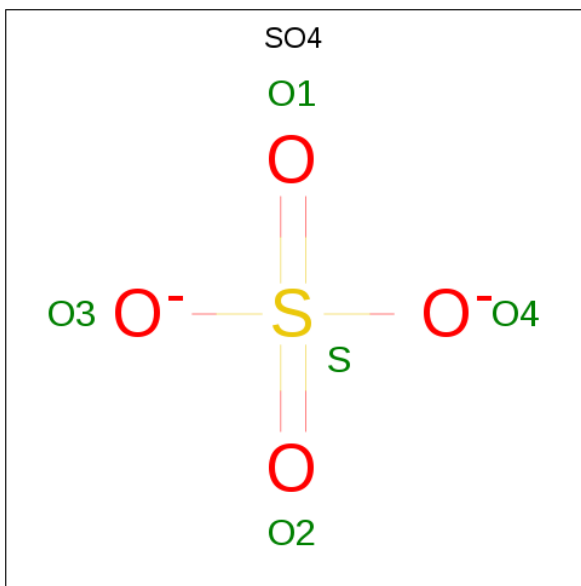
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Ni	0	0
			1	1		
5	C	1	Total	Ni	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

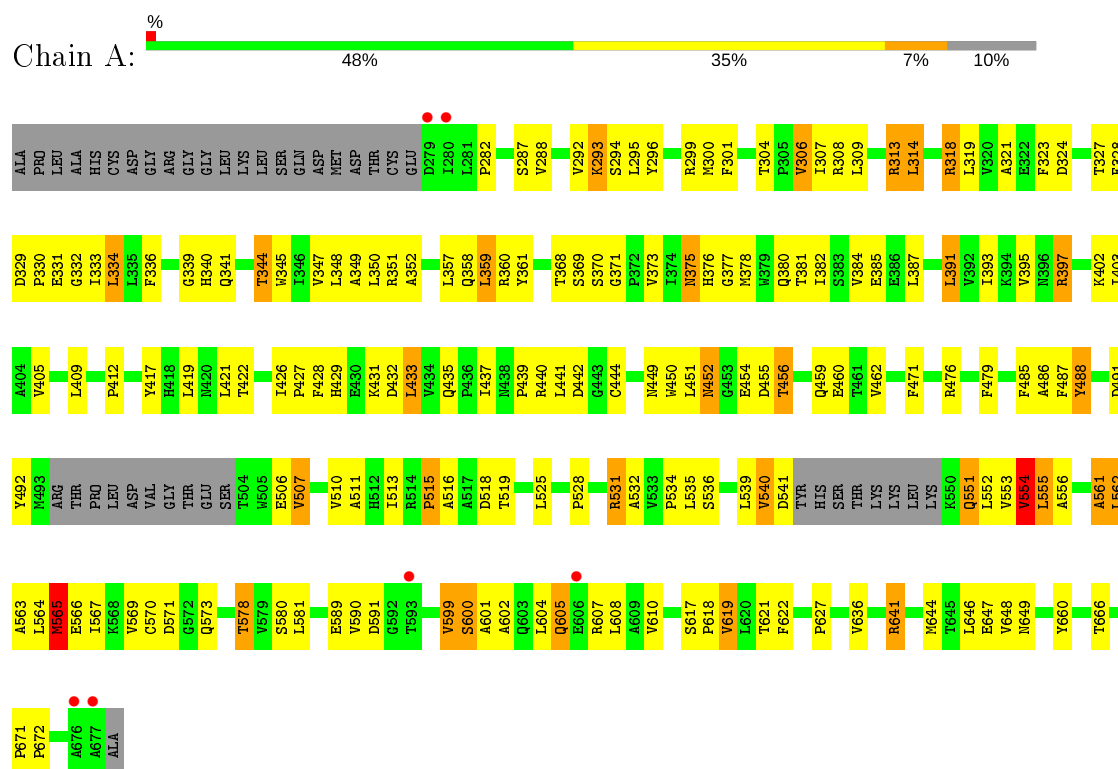


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		

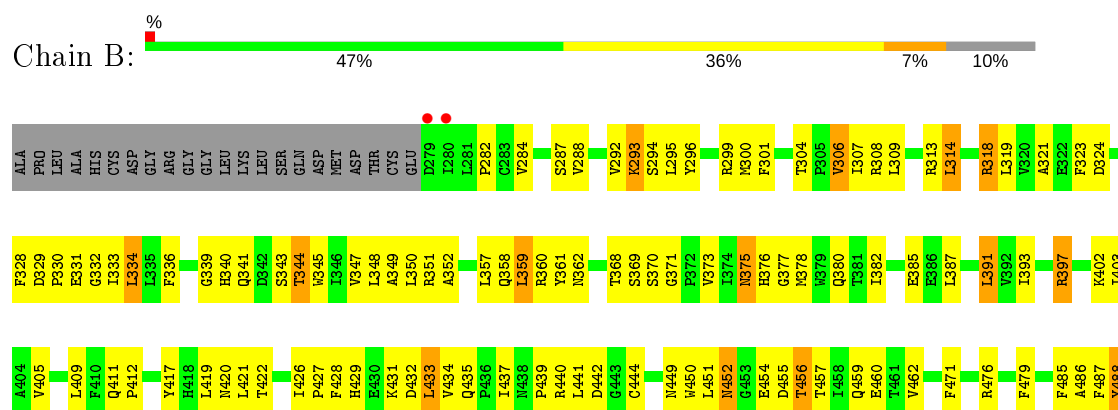
### 3 Residue-property plots

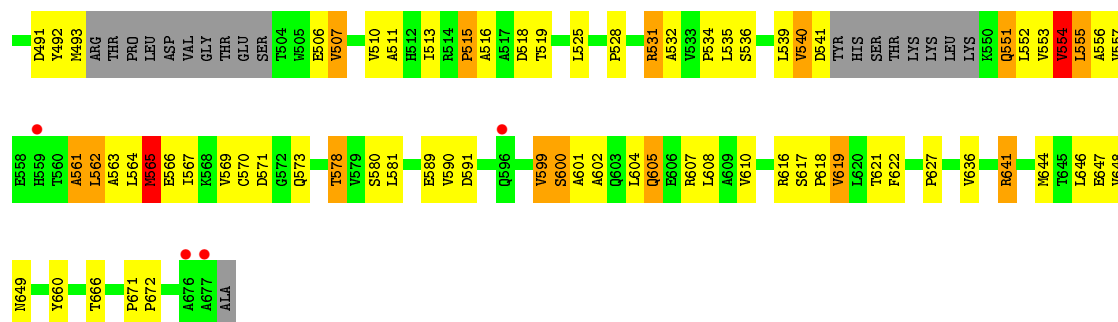
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: GROWTH-ARREST-SPECIFIC PROTEIN 6 PRECURSOR

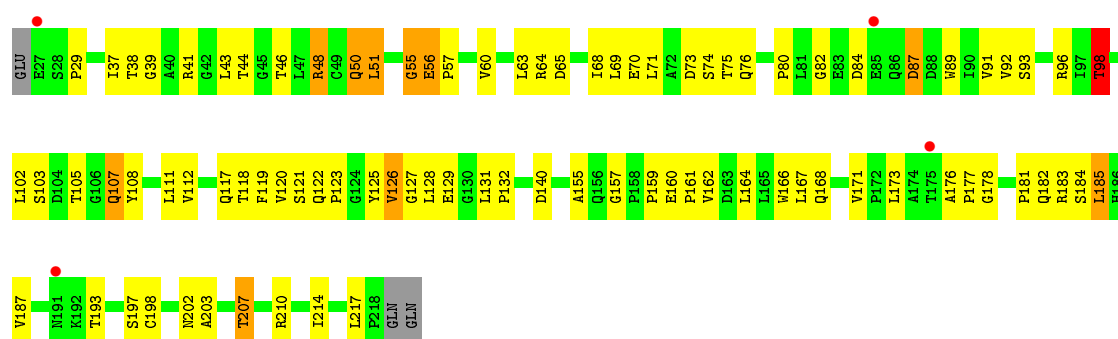


#### • Molecule 1: GROWTH-ARREST-SPECIFIC PROTEIN 6 PRECURSOR

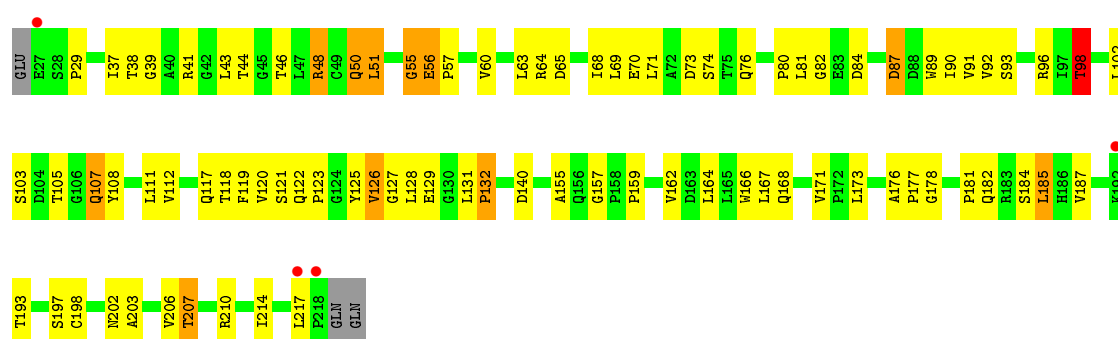




• Molecule 2: TYROSINE-PROTEIN KINASE RECEPTOR UFO



• Molecule 2: TYROSINE-PROTEIN KINASE RECEPTOR UFO



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	292.95Å 292.95Å 63.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.30 19.89 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-3.30) 99.9 (19.89-3.30)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 3.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.241 , 0.265 0.212 , 0.238	Depositor DCC
$R_{free}$ test set	2383 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.0	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 36.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, CA, NAG, SO4

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	0.45	0/3017	0.70	0/4107
1	B	0.45	0/3017	0.70	0/4107
2	C	0.52	0/1489	0.69	0/2041
2	D	0.52	0/1489	0.69	0/2041
All	All	0.48	0/9012	0.70	0/12296

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2953	0	2951	151	0
1	B	2953	0	2951	156	0
2	C	1454	0	1401	86	0
2	D	1454	0	1401	85	0
3	E	28	0	25	1	0
3	F	28	0	25	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
6	C	5	0	0	0	0
All	All	8879	0	8754	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 27.

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)
1:A:622:PHE:CE2	1:A:627:PRO:HD3	2.02	0.94
2:D:51:LEU:HD23	2:D:51:LEU:H	1.32	0.94
2:C:51:LEU:H	2:C:51:LEU:HD23	1.33	0.93
1:B:622:PHE:CE2	1:B:627:PRO:HD3	2.04	0.93
1:B:332:GLY:HA3	1:B:441:LEU:HB2	1.54	0.89
1:B:519:THR:HG22	1:B:540:VAL:HA	1.54	0.87
1:A:519:THR:HG22	1:A:540:VAL:HA	1.55	0.86
1:A:332:GLY:HA3	1:A:441:LEU:HB2	1.56	0.86
1:A:555:LEU:HD11	1:A:581:LEU:HD21	1.61	0.82
1:A:397:ARG:HH11	1:A:397:ARG:HG2	1.45	0.82
2:D:44:THR:HG22	2:D:98:THR:O	1.79	0.82
1:A:429:HIS:HD2	1:A:431:LYS:HB2	1.44	0.82
2:C:44:THR:HG22	2:C:98:THR:O	1.80	0.81
1:B:397:ARG:HH11	1:B:397:ARG:HG2	1.46	0.81
1:B:429:HIS:HD2	1:B:431:LYS:HB2	1.44	0.80
1:B:555:LEU:HD11	1:B:581:LEU:HD21	1.61	0.80
1:A:376:HIS:HD2	1:A:378:MET:H	1.29	0.80
1:A:555:LEU:HD23	1:A:556:ALA:H	1.49	0.78
2:D:60:VAL:HG11	2:D:93:SER:HB2	1.66	0.77
1:B:376:HIS:HD2	1:B:378:MET:H	1.29	0.77
1:B:555:LEU:HD23	1:B:556:ALA:H	1.50	0.76
1:B:300:MET:HE3	1:B:304:THR:HB	1.68	0.76
2:C:60:VAL:HG11	2:C:93:SER:HB2	1.68	0.75
1:A:300:MET:HE3	1:A:304:THR:HB	1.69	0.73
2:D:51:LEU:CD2	2:D:51:LEU:H	2.02	0.73
1:B:397:ARG:CG	1:B:397:ARG:HH11	2.01	0.72
1:A:397:ARG:HH11	1:A:397:ARG:CG	2.01	0.72
2:C:51:LEU:H	2:C:51:LEU:CD2	2.03	0.71
2:C:168:GLN:HB2	2:C:173:LEU:HD11	1.72	0.70
2:D:181:PRO:O	2:D:182:GLN:HG2	1.91	0.70
2:C:181:PRO:O	2:C:182:GLN:HG2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:50:GLN:HB2	2:C:92:VAL:HG22	1.73	0.70
1:A:319:LEU:HD12	1:A:451:LEU:HD11	1.73	0.70
2:D:168:GLN:HB2	2:D:173:LEU:HD11	1.74	0.70
1:A:607:ARG:HA	1:A:607:ARG:HE	1.58	0.69
1:B:319:LEU:HD12	1:B:451:LEU:HD11	1.74	0.68
1:A:314:LEU:HB2	2:C:73:ASP:OD1	1.92	0.68
2:D:50:GLN:HB2	2:D:92:VAL:HG22	1.75	0.67
1:B:507:VAL:HG11	1:B:535:LEU:CD2	2.25	0.67
1:A:507:VAL:HG11	1:A:535:LEU:CD2	2.24	0.67
2:D:166:TRP:C	2:D:167:LEU:HD12	2.15	0.67
1:A:599:VAL:HG21	1:A:604:LEU:HB2	1.76	0.67
1:A:299:ARG:NH2	2:C:80:PRO:O	2.29	0.66
1:A:344:THR:HB	1:A:361:TYR:HA	1.76	0.66
1:B:607:ARG:HE	1:B:607:ARG:HA	1.60	0.66
1:B:600:SER:C	1:B:602:ALA:H	1.98	0.66
1:A:531:ARG:HH11	1:A:531:ARG:HG3	1.60	0.65
1:B:599:VAL:HG21	1:B:604:LEU:HB2	1.78	0.65
2:C:166:TRP:C	2:C:167:LEU:HD12	2.16	0.65
1:B:344:THR:HB	1:B:361:TYR:HA	1.77	0.65
1:B:454:GLU:O	1:B:456:THR:N	2.30	0.65
1:A:454:GLU:O	1:A:456:THR:N	2.31	0.64
1:A:563:ALA:O	1:A:564:LEU:HD23	1.98	0.64
1:A:511:ALA:O	1:A:513:ILE:HG23	1.98	0.64
1:B:531:ARG:HH11	1:B:531:ARG:HG3	1.62	0.63
2:C:44:THR:HG22	2:C:98:THR:C	2.18	0.63
1:A:300:MET:CE	1:A:304:THR:HB	2.27	0.63
2:C:50:GLN:HG3	2:C:50:GLN:O	1.99	0.63
1:A:600:SER:C	1:A:602:ALA:H	1.99	0.63
2:D:44:THR:HG22	2:D:98:THR:C	2.17	0.63
1:B:318:ARG:HH11	1:B:318:ARG:CB	2.12	0.62
1:B:563:ALA:O	1:B:564:LEU:HD23	1.98	0.62
1:A:318:ARG:HH11	1:A:318:ARG:CB	2.12	0.62
1:B:357:LEU:HD13	1:B:393:ILE:HD11	1.80	0.62
1:B:336:PHE:HB3	1:B:422:THR:OG1	1.99	0.62
1:A:336:PHE:HB3	1:A:422:THR:OG1	2.00	0.62
1:A:553:VAL:CG2	1:A:567:ILE:HD12	2.29	0.62
1:B:553:VAL:CG2	1:B:567:ILE:HD12	2.30	0.62
1:A:357:LEU:HD13	1:A:393:ILE:HD11	1.82	0.61
1:B:300:MET:CE	1:B:304:THR:HB	2.30	0.61
1:B:301:PHE:O	1:B:440:ARG:NH1	2.33	0.61
2:C:181:PRO:C	2:C:182:GLN:HG2	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:LEU:C	2:D:43:LEU:HD23	2.20	0.61
1:B:299:ARG:NH2	2:D:80:PRO:O	2.34	0.61
1:B:578:THR:HG23	1:B:589:GLU:HB2	1.83	0.61
2:D:166:TRP:O	2:D:167:LEU:HD12	2.01	0.60
2:D:181:PRO:C	2:D:182:GLN:HG2	2.21	0.60
1:B:555:LEU:HD23	1:B:556:ALA:N	2.16	0.60
1:B:345:TRP:CZ3	1:B:347:VAL:HG23	2.37	0.60
2:D:50:GLN:HG3	2:D:50:GLN:O	2.00	0.60
1:B:604:LEU:O	1:B:608:LEU:HG	2.02	0.60
2:C:102:LEU:O	2:C:105:THR:HG22	2.02	0.60
2:C:132:PRO:O	2:C:207:THR:HG21	2.02	0.60
1:B:607:ARG:HH21	1:B:610:VAL:HG21	1.67	0.60
2:C:43:LEU:HD23	2:C:43:LEU:C	2.22	0.60
1:A:555:LEU:HD23	1:A:556:ALA:N	2.15	0.60
1:B:516:ALA:HB3	1:B:641:ARG:O	2.02	0.59
1:B:541:ASP:HA	1:B:551:GLN:H	1.68	0.59
1:A:552:LEU:HD12	1:A:564:LEU:HB3	1.84	0.59
1:A:604:LEU:O	1:A:608:LEU:HG	2.02	0.59
2:D:162:VAL:HG12	2:D:202:ASN:HB3	1.85	0.59
1:B:535:LEU:HD11	1:B:555:LEU:HD21	1.83	0.59
1:A:607:ARG:HH21	1:A:610:VAL:HG21	1.67	0.59
1:A:344:THR:HA	1:A:360:ARG:O	2.03	0.58
1:B:552:LEU:HD12	1:B:564:LEU:HB3	1.86	0.58
1:A:578:THR:HG23	1:A:589:GLU:HB2	1.85	0.58
1:B:331:GLU:HA	1:B:350:LEU:O	2.02	0.58
1:A:402:LYS:HB3	2:D:207:THR:HB	1.83	0.58
1:B:295:LEU:HD21	1:B:307:ILE:HD12	1.85	0.58
1:A:301:PHE:O	1:A:440:ARG:NH1	2.37	0.58
1:B:314:LEU:HB2	2:D:73:ASP:OD1	2.04	0.58
1:A:535:LEU:HD11	1:A:555:LEU:HD21	1.86	0.58
2:C:51:LEU:N	2:C:51:LEU:HD23	2.13	0.58
1:A:541:ASP:HA	1:A:551:GLN:H	1.69	0.58
2:D:132:PRO:O	2:D:207:THR:HG21	2.03	0.58
1:B:345:TRP:CE3	1:B:347:VAL:HG23	2.39	0.57
2:C:166:TRP:O	2:C:167:LEU:HD12	2.04	0.57
1:A:506:GLU:O	1:A:507:VAL:HG23	2.04	0.57
1:B:293:LYS:H	1:B:293:LYS:HD2	1.68	0.57
1:A:295:LEU:HD21	1:A:307:ILE:HD12	1.85	0.57
2:D:102:LEU:O	2:D:105:THR:HG22	2.05	0.57
1:A:293:LYS:HD2	1:A:293:LYS:H	1.68	0.57
1:A:345:TRP:CZ3	1:A:347:VAL:HG23	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:SER:O	1:A:581:LEU:HD23	2.05	0.57
1:B:429:HIS:CD2	1:B:431:LYS:H	2.23	0.57
1:A:456:THR:O	1:A:456:THR:HG22	2.05	0.57
1:B:580:SER:O	1:B:581:LEU:HD23	2.05	0.57
2:C:162:VAL:HG12	2:C:202:ASN:HB3	1.86	0.57
1:B:511:ALA:O	1:B:513:ILE:HG23	2.04	0.57
1:A:429:HIS:CD2	1:A:431:LYS:HB2	2.33	0.57
1:A:507:VAL:HG12	1:A:507:VAL:O	2.05	0.57
2:D:107:GLN:NE2	2:D:125:TYR:HE2	2.03	0.56
1:A:429:HIS:CD2	1:A:431:LYS:H	2.24	0.56
1:B:429:HIS:CD2	1:B:431:LYS:HB2	2.33	0.56
2:C:44:THR:HA	2:C:98:THR:O	2.06	0.56
1:A:345:TRP:CE3	1:A:347:VAL:HG23	2.40	0.56
1:A:569:VAL:HG23	1:A:570:CYS:SG	2.46	0.56
1:B:391:LEU:HD12	1:B:405:VAL:HG11	1.87	0.56
2:D:44:THR:HA	2:D:98:THR:O	2.06	0.56
1:A:426:ILE:HD12	1:A:428:PHE:CE1	2.41	0.56
1:A:516:ALA:HB3	1:A:641:ARG:O	2.06	0.56
1:B:456:THR:HG22	1:B:456:THR:O	2.06	0.55
1:B:525:LEU:HD12	1:B:535:LEU:HB3	1.87	0.55
1:B:552:LEU:HB2	1:B:565:MET:O	2.06	0.55
1:A:391:LEU:HD12	1:A:405:VAL:HG11	1.88	0.55
1:A:525:LEU:HD12	1:A:535:LEU:HB3	1.88	0.55
1:B:426:ILE:HD12	1:B:428:PHE:CE1	2.42	0.55
2:D:51:LEU:HD23	2:D:51:LEU:N	2.12	0.55
1:A:331:GLU:HA	1:A:350:LEU:O	2.06	0.55
1:A:513:ILE:HG13	1:A:515:PRO:HD3	1.86	0.55
1:A:552:LEU:HB2	1:A:565:MET:O	2.05	0.55
1:B:324:ASP:HA	1:B:380:GLN:O	2.06	0.55
2:C:46:THR:HG22	2:C:96:ARG:HG3	1.89	0.55
2:D:182:GLN:C	2:D:184:SER:H	2.08	0.55
1:B:553:VAL:HG12	1:B:554:VAL:N	2.22	0.55
1:B:344:THR:HA	1:B:360:ARG:O	2.06	0.55
1:B:648:VAL:O	1:B:649:ASN:HB2	2.06	0.54
2:C:129:GLU:HG3	2:C:159:PRO:HD3	1.88	0.54
2:C:182:GLN:C	2:C:184:SER:H	2.09	0.54
1:A:339:GLY:HA2	3:E:1:NAG:O7	2.07	0.54
1:A:552:LEU:N	1:A:552:LEU:HD23	2.23	0.54
2:D:46:THR:HG22	2:D:96:ARG:HG3	1.90	0.54
1:A:403:ILE:N	1:A:403:ILE:HD12	2.22	0.54
1:B:397:ARG:CG	1:B:397:ARG:NH1	2.67	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:129:GLU:HG3	2:D:159:PRO:HD3	1.90	0.54
1:A:590:VAL:O	1:A:591:ASP:HB2	2.08	0.54
1:B:426:ILE:HD12	1:B:428:PHE:CD1	2.43	0.54
1:A:648:VAL:O	1:A:649:ASN:HB2	2.08	0.53
2:C:69:LEU:HD11	2:C:108:TYR:HE2	1.74	0.53
1:A:373:VAL:HG13	1:A:375:ASN:ND2	2.23	0.53
1:B:457:THR:CG2	2:D:92:VAL:HG11	2.38	0.53
1:B:507:VAL:O	1:B:507:VAL:HG12	2.07	0.53
1:B:513:ILE:HG13	1:B:515:PRO:HD3	1.89	0.53
1:B:555:LEU:CD2	1:B:556:ALA:N	2.71	0.53
1:B:644:MET:HE3	1:B:646:LEU:HD11	1.90	0.53
1:A:306:VAL:O	1:A:307:ILE:HG13	2.09	0.53
2:C:48:ARG:HG3	2:C:48:ARG:O	2.09	0.53
1:B:552:LEU:HD23	1:B:552:LEU:N	2.24	0.53
1:A:324:ASP:HA	1:A:380:GLN:O	2.09	0.53
1:B:532:ALA:C	1:B:534:PRO:HD3	2.29	0.53
1:B:569:VAL:HG23	1:B:570:CYS:SG	2.49	0.53
1:A:553:VAL:HG12	1:A:554:VAL:N	2.24	0.53
1:A:375:ASN:HD22	1:A:375:ASN:N	2.07	0.53
1:A:555:LEU:CD2	1:A:556:ALA:N	2.72	0.53
1:A:471:PHE:CE1	1:A:671:PRO:HD3	2.44	0.53
1:B:561:ALA:O	1:B:562:LEU:HD23	2.09	0.53
1:A:426:ILE:HD12	1:A:428:PHE:CD1	2.44	0.53
1:B:605:GLN:C	1:B:607:ARG:H	2.11	0.53
2:C:122:GLN:HG3	2:C:123:PRO:HD2	1.91	0.53
1:B:373:VAL:HG13	1:B:375:ASN:ND2	2.25	0.52
1:A:385:GLU:OE1	1:A:387:LEU:HG	2.09	0.52
1:B:385:GLU:OE1	1:B:387:LEU:HG	2.09	0.52
2:D:60:VAL:CG1	2:D:93:SER:HB2	2.37	0.52
1:B:306:VAL:O	1:B:307:ILE:HG13	2.09	0.52
1:B:506:GLU:O	1:B:507:VAL:HG23	2.08	0.52
1:B:402:LYS:HB3	2:C:207:THR:HB	1.91	0.52
2:D:122:GLN:HG3	2:D:123:PRO:HD2	1.91	0.52
1:A:561:ALA:O	1:A:562:LEU:HD23	2.09	0.52
1:B:449:ASN:HD21	1:B:452:ASN:HA	1.74	0.52
1:A:535:LEU:HD12	1:A:536:SER:H	1.74	0.52
1:B:403:ILE:HD12	1:B:403:ILE:N	2.24	0.52
1:B:294:SER:O	1:B:462:VAL:HG11	2.09	0.52
1:A:644:MET:HE3	1:A:646:LEU:HD11	1.90	0.52
1:A:294:SER:O	1:A:462:VAL:HG11	2.09	0.52
1:B:590:VAL:O	1:B:591:ASP:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:ARG:HH11	2:C:41:ARG:HG3	1.75	0.52
2:C:60:VAL:CG1	2:C:93:SER:HB2	2.38	0.52
2:C:185:LEU:HD23	2:C:185:LEU:O	2.09	0.52
2:D:193:THR:HG23	2:D:214:ILE:O	2.09	0.52
1:A:449:ASN:HD21	1:A:452:ASN:HA	1.75	0.51
2:C:107:GLN:NE2	2:C:125:TYR:HE2	2.07	0.51
2:D:185:LEU:O	2:D:185:LEU:HD23	2.10	0.51
1:A:605:GLN:C	1:A:607:ARG:H	2.13	0.51
1:B:336:PHE:CE2	1:B:427:PRO:HG2	2.46	0.51
1:B:471:PHE:CE1	1:B:671:PRO:HD3	2.45	0.51
1:A:318:ARG:HB2	1:A:318:ARG:HH11	1.75	0.51
2:D:48:ARG:O	2:D:48:ARG:HG3	2.09	0.51
1:A:571:ASP:O	1:A:573:GLN:HG2	2.10	0.51
2:D:69:LEU:HD11	2:D:108:TYR:HE2	1.75	0.51
1:B:528:PRO:O	1:B:531:ARG:HD2	2.10	0.51
2:C:178:GLY:HA2	2:C:182:GLN:HE22	1.76	0.51
1:B:607:ARG:NE	1:B:607:ARG:HA	2.25	0.51
1:A:370:SER:OG	1:A:371:GLY:N	2.44	0.50
2:C:155:ALA:O	2:C:162:VAL:HG21	2.11	0.50
2:C:193:THR:HG23	2:C:214:ILE:O	2.11	0.50
1:A:532:ALA:C	1:A:534:PRO:HD3	2.31	0.50
1:B:318:ARG:HH11	1:B:318:ARG:HB2	1.76	0.50
1:B:375:ASN:N	1:B:375:ASN:HD22	2.09	0.50
1:B:535:LEU:HD12	1:B:536:SER:H	1.76	0.50
1:B:510:VAL:HB	1:B:647:GLU:HB2	1.93	0.50
1:A:318:ARG:NH1	1:A:318:ARG:HB2	2.27	0.50
1:B:339:GLY:HA2	3:F:1:NAG:H81	1.93	0.50
1:B:318:ARG:HB2	1:B:318:ARG:NH1	2.27	0.50
2:D:131:LEU:HB3	2:D:207:THR:HG22	1.94	0.50
1:B:487:PHE:HA	1:B:621:THR:O	2.12	0.50
1:B:294:SER:HB2	1:B:444:CYS:SG	2.52	0.49
1:B:351:ARG:O	1:B:352:ALA:HB3	2.10	0.49
1:A:607:ARG:NE	1:A:607:ARG:HA	2.24	0.49
1:B:555:LEU:CD2	1:B:556:ALA:H	2.23	0.49
1:B:571:ASP:O	1:B:573:GLN:HG2	2.11	0.49
1:A:555:LEU:CD2	1:A:556:ALA:H	2.23	0.49
1:B:456:THR:HG22	1:B:460:GLU:HG3	1.94	0.49
1:A:294:SER:HB2	1:A:444:CYS:SG	2.52	0.49
1:A:599:VAL:CG2	1:A:604:LEU:HB2	2.43	0.49
1:B:513:ILE:HD12	1:B:515:PRO:HG3	1.95	0.49
2:D:39:GLY:HA3	2:D:43:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:SER:C	1:A:602:ALA:N	2.65	0.49
2:C:51:LEU:CD1	2:C:112:VAL:HG11	2.43	0.49
1:A:528:PRO:O	1:A:531:ARG:HD2	2.12	0.49
2:D:178:GLY:HA2	2:D:182:GLN:HE22	1.78	0.48
1:A:513:ILE:HD12	1:A:515:PRO:HG3	1.95	0.48
1:B:532:ALA:O	1:B:534:PRO:HD3	2.13	0.48
1:B:567:ILE:HD11	1:B:590:VAL:CG1	2.43	0.48
1:B:518:ASP:OD1	1:B:519:THR:HG23	2.13	0.48
1:B:486:ALA:HA	1:B:660:TYR:O	2.13	0.48
1:A:567:ILE:HD11	1:A:590:VAL:CG1	2.44	0.48
1:A:510:VAL:HB	1:A:647:GLU:HB2	1.93	0.48
1:A:351:ARG:O	1:A:352:ALA:HB3	2.14	0.48
1:B:516:ALA:HB3	1:B:641:ARG:HD3	1.95	0.48
2:C:39:GLY:HA3	2:C:43:LEU:HD13	1.95	0.48
1:B:600:SER:C	1:B:602:ALA:N	2.65	0.48
2:D:63:LEU:CD2	2:D:68:ILE:HD13	2.44	0.48
1:A:336:PHE:CE2	1:A:427:PRO:HG2	2.48	0.48
1:B:359:LEU:HD12	1:B:359:LEU:N	2.28	0.48
1:B:331:GLU:HG3	1:B:437:ILE:HD11	1.96	0.48
1:B:599:VAL:CG2	1:B:604:LEU:HB2	2.44	0.48
1:A:456:THR:HG22	1:A:460:GLU:HG3	1.94	0.48
2:C:132:PRO:HB2	2:C:207:THR:HG23	1.95	0.48
1:B:457:THR:HG23	2:D:92:VAL:HG11	1.96	0.48
1:A:375:ASN:H	1:A:375:ASN:ND2	2.12	0.47
2:D:51:LEU:CD1	2:D:112:VAL:HG11	2.44	0.47
1:A:309:LEU:HD12	1:A:421:LEU:HD22	1.96	0.47
2:C:131:LEU:HB3	2:C:207:THR:HG22	1.96	0.47
2:D:164:LEU:HD22	2:D:198:CYS:SG	2.55	0.47
2:D:55:GLY:O	2:D:56:GLU:C	2.51	0.47
2:D:70:GLU:C	2:D:71:LEU:HD23	2.34	0.47
1:A:456:THR:HG23	1:A:459:GLN:HB3	1.96	0.47
1:A:487:PHE:HA	1:A:621:THR:O	2.15	0.47
1:B:309:LEU:HD12	1:B:421:LEU:HD22	1.96	0.47
1:A:486:ALA:HA	1:A:660:TYR:O	2.15	0.47
2:C:117:GLN:HG2	2:C:119:PHE:CE1	2.49	0.47
2:D:43:LEU:O	2:D:43:LEU:HD23	2.15	0.47
1:A:516:ALA:HB3	1:A:641:ARG:HD3	1.96	0.47
1:A:518:ASP:OD1	1:A:519:THR:HG23	2.15	0.47
1:B:476:ARG:HG2	1:B:476:ARG:HH11	1.79	0.47
2:C:29:PRO:HD2	2:C:119:PHE:CD2	2.50	0.47
2:D:126:VAL:O	2:D:126:VAL:CG2	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:ILE:O	2:D:37:ILE:HG13	2.14	0.47
2:D:41:ARG:HG3	2:D:41:ARG:HH11	1.79	0.47
2:C:64:ARG:HG3	2:C:108:TYR:CZ	2.50	0.47
2:C:41:ARG:HG2	2:C:128:LEU:HD21	1.97	0.47
2:C:70:GLU:C	2:C:71:LEU:HD23	2.35	0.47
1:A:532:ALA:O	1:A:534:PRO:HD3	2.15	0.47
2:D:41:ARG:NH2	2:D:157:GLY:O	2.48	0.47
1:A:333:ILE:HD13	1:A:426:ILE:HG23	1.96	0.47
1:B:332:GLY:O	1:B:349:ALA:HB1	2.15	0.47
1:B:456:THR:HG23	1:B:459:GLN:HB3	1.95	0.47
2:C:37:ILE:HG13	2:C:37:ILE:O	2.13	0.47
1:A:476:ARG:HH11	1:A:476:ARG:HG2	1.80	0.46
1:A:567:ILE:HG12	1:A:590:VAL:HG11	1.98	0.46
1:B:411:GLN:HA	1:B:412:PRO:HD3	1.75	0.46
2:C:140:ASP:CG	2:C:210:ARG:HH22	2.18	0.46
2:C:55:GLY:O	2:C:56:GLU:C	2.54	0.46
2:D:41:ARG:HG2	2:D:128:LEU:HD21	1.97	0.46
1:B:351:ARG:HG3	1:B:351:ARG:HH11	1.81	0.46
1:B:479:PHE:HB3	1:B:666:THR:OG1	2.15	0.46
1:B:437:ILE:O	1:B:439:PRO:HD3	2.15	0.46
2:D:167:LEU:HB2	2:D:197:SER:HB2	1.97	0.46
2:D:64:ARG:HG3	2:D:108:TYR:CZ	2.51	0.46
2:D:111:LEU:HD12	2:D:119:PHE:O	2.16	0.46
2:D:132:PRO:HB2	2:D:207:THR:HG23	1.96	0.46
1:A:437:ILE:O	1:A:439:PRO:HD3	2.16	0.46
1:B:412:PRO:HG3	1:B:417:TYR:CE2	2.50	0.46
2:C:178:GLY:CA	2:C:182:GLN:HE22	2.28	0.46
1:A:375:ASN:ND2	1:A:375:ASN:N	2.64	0.46
1:B:476:ARG:HG2	1:B:476:ARG:NH1	2.31	0.46
1:B:368:THR:HG22	1:B:369:SER:N	2.31	0.46
1:B:333:ILE:HD13	1:B:426:ILE:HG23	1.98	0.46
2:C:185:LEU:HD21	2:C:187:VAL:HG22	1.97	0.46
2:C:41:ARG:NH1	2:C:41:ARG:HG3	2.31	0.46
2:D:82:GLY:HA3	2:D:87:ASP:HB2	1.98	0.45
2:D:162:VAL:O	2:D:162:VAL:HG23	2.16	0.45
1:A:359:LEU:N	1:A:359:LEU:HD12	2.31	0.45
2:C:132:PRO:HD2	2:C:207:THR:CG2	2.46	0.45
2:C:43:LEU:HD23	2:C:43:LEU:O	2.17	0.45
2:D:182:GLN:O	2:D:184:SER:N	2.49	0.45
1:A:282:PRO:HA	1:A:516:ALA:O	2.16	0.45
1:A:567:ILE:CG1	1:A:590:VAL:HG11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:140:ASP:CG	2:D:210:ARG:HH22	2.19	0.45
1:A:479:PHE:HB3	1:A:666:THR:OG1	2.15	0.45
1:B:375:ASN:H	1:B:375:ASN:ND2	2.14	0.45
2:C:63:LEU:CD2	2:C:68:ILE:HD13	2.46	0.45
2:D:60:VAL:HG12	2:D:76:GLN:OE1	2.17	0.45
1:A:332:GLY:O	1:A:349:ALA:HB1	2.17	0.45
1:B:567:ILE:HG12	1:B:590:VAL:HG11	1.98	0.45
2:C:82:GLY:HA3	2:C:87:ASP:HB2	1.98	0.45
2:D:155:ALA:O	2:D:162:VAL:HG21	2.16	0.45
1:A:368:THR:HG22	1:A:369:SER:N	2.31	0.45
2:D:178:GLY:CA	2:D:182:GLN:HE22	2.30	0.45
1:A:412:PRO:HG3	1:A:417:TYR:CE2	2.51	0.45
1:A:331:GLU:HG3	1:A:437:ILE:HD11	1.98	0.44
1:B:567:ILE:CG1	1:B:590:VAL:HG11	2.47	0.44
2:C:57:PRO:HD3	2:C:89:TRP:CD1	2.51	0.44
1:B:370:SER:OG	1:B:371:GLY:N	2.47	0.44
1:B:488:TYR:CD1	1:B:488:TYR:N	2.86	0.44
2:C:103:SER:C	2:C:105:THR:H	2.20	0.44
1:A:340:HIS:CD2	1:A:341:GLN:N	2.85	0.44
1:A:519:THR:HA	1:A:539:LEU:O	2.17	0.44
2:C:38:THR:HA	2:C:127:GLY:O	2.17	0.44
1:A:358:GLN:C	1:A:359:LEU:HD12	2.38	0.44
1:B:420:ASN:ND2	3:F:1:NAG:H82	2.32	0.44
2:C:60:VAL:HG12	2:C:76:GLN:OE1	2.17	0.44
2:D:38:THR:HA	2:D:127:GLY:O	2.17	0.44
1:A:351:ARG:HG3	1:A:351:ARG:HH11	1.82	0.44
1:A:476:ARG:NH1	1:A:476:ARG:HG2	2.32	0.44
1:B:321:ALA:HB1	1:B:450:TRP:CZ3	2.53	0.44
2:D:140:ASP:OD2	2:D:210:ARG:NH2	2.51	0.44
1:A:617:SER:O	1:A:619:VAL:HG22	2.17	0.44
1:B:358:GLN:C	1:B:359:LEU:HD12	2.38	0.44
2:C:167:LEU:HB2	2:C:197:SER:HB2	1.99	0.44
1:B:340:HIS:CD2	1:B:341:GLN:N	2.86	0.44
2:C:46:THR:CG2	2:C:96:ARG:HG3	2.48	0.44
1:B:287:SER:HB2	1:B:672:PRO:HG2	2.00	0.43
2:C:167:LEU:HA	2:C:171:VAL:O	2.18	0.43
2:D:117:GLN:HG2	2:D:119:PHE:CE1	2.53	0.43
2:D:185:LEU:HD21	2:D:187:VAL:HG22	1.99	0.43
2:C:140:ASP:OD2	2:C:210:ARG:NH2	2.51	0.43
2:C:80:PRO:HD3	2:C:89:TRP:CZ3	2.53	0.43
2:D:57:PRO:HD3	2:D:89:TRP:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ARG:NH1	1:A:397:ARG:CG	2.67	0.43
1:A:308:ARG:HG2	1:A:422:THR:HG22	1.98	0.43
2:C:57:PRO:HD3	2:C:89:TRP:CG	2.53	0.43
2:D:103:SER:C	2:D:105:THR:H	2.22	0.43
2:D:64:ARG:O	2:D:65:ASP:HB2	2.19	0.43
1:A:432:ASP:O	1:A:433:LEU:O	2.37	0.43
1:B:336:PHE:HB2	1:B:426:ILE:HG22	1.99	0.43
2:C:162:VAL:HG23	2:C:162:VAL:O	2.18	0.43
2:C:182:GLN:O	2:C:184:SER:N	2.51	0.43
2:D:29:PRO:HD2	2:D:119:PHE:CD2	2.54	0.43
1:A:321:ALA:HB1	1:A:450:TRP:CZ3	2.53	0.43
1:B:329:ASP:HA	1:B:330:PRO:HD3	1.80	0.43
1:B:328:PHE:CE2	1:B:377:GLY:HA3	2.53	0.43
1:A:562:LEU:O	1:A:563:ALA:HB2	2.18	0.43
2:C:51:LEU:N	2:C:51:LEU:CD2	2.76	0.43
1:B:433:LEU:HB3	1:B:434:VAL:H	1.56	0.43
1:B:590:VAL:HG12	1:B:590:VAL:O	2.19	0.43
2:D:80:PRO:HD3	2:D:89:TRP:CZ3	2.54	0.43
1:B:375:ASN:N	1:B:375:ASN:ND2	2.66	0.42
1:B:562:LEU:O	1:B:563:ALA:HB2	2.19	0.42
2:C:41:ARG:NH2	2:C:157:GLY:O	2.50	0.42
2:D:107:GLN:HE21	2:D:125:TYR:HE2	1.66	0.42
1:A:601:ALA:HA	1:A:604:LEU:HB3	2.01	0.42
1:B:540:VAL:HG13	1:B:636:VAL:HG22	2.01	0.42
1:A:488:TYR:CD1	1:A:488:TYR:N	2.86	0.42
2:C:111:LEU:HD12	2:C:119:PHE:O	2.18	0.42
2:D:57:PRO:HD3	2:D:89:TRP:CG	2.53	0.42
1:A:492:TYR:CD2	1:A:507:VAL:HG22	2.54	0.42
1:A:287:SER:HB2	1:A:672:PRO:HG2	2.01	0.42
1:B:282:PRO:HA	1:B:516:ALA:O	2.18	0.42
1:A:323:PHE:CE1	1:A:382:ILE:HB	2.55	0.42
1:A:336:PHE:HB2	1:A:426:ILE:HG22	2.01	0.42
1:A:590:VAL:HG12	1:A:590:VAL:O	2.18	0.42
1:B:432:ASP:O	1:B:433:LEU:O	2.38	0.42
1:A:329:ASP:HA	1:A:330:PRO:HD3	1.81	0.42
1:B:601:ALA:HA	1:B:604:LEU:HB3	2.00	0.42
1:A:350:LEU:HA	1:A:350:LEU:HD12	1.88	0.42
1:B:308:ARG:HG2	1:B:422:THR:HG22	2.02	0.42
1:B:329:ASP:OD1	1:B:331:GLU:O	2.37	0.42
1:B:557:VAL:HG23	1:B:562:LEU:HD11	2.00	0.42
1:B:617:SER:HB3	1:B:618:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:185:LEU:HD21	2:C:187:VAL:CG2	2.50	0.42
2:D:167:LEU:HA	2:D:171:VAL:O	2.20	0.42
2:D:51:LEU:HD21	2:D:91:VAL:HB	2.02	0.42
1:A:334:LEU:HD23	1:A:348:LEU:CD2	2.50	0.42
1:A:334:LEU:HD23	1:A:348:LEU:HD23	2.02	0.42
2:D:125:TYR:N	2:D:125:TYR:CD1	2.88	0.42
2:D:80:PRO:HB3	2:D:89:TRP:CH2	2.55	0.42
1:A:336:PHE:CE1	1:A:345:TRP:HB2	2.55	0.42
1:A:552:LEU:HB3	1:A:566:GLU:HA	2.01	0.42
1:A:617:SER:HB3	1:A:618:PRO:CD	2.49	0.42
1:B:519:THR:HA	1:B:539:LEU:O	2.20	0.42
1:B:617:SER:O	1:B:619:VAL:HG22	2.18	0.42
1:B:341:GLN:HA	1:B:428:PHE:CE2	2.55	0.41
1:B:492:TYR:CD2	1:B:507:VAL:HG22	2.55	0.41
2:C:125:TYR:N	2:C:125:TYR:CD1	2.87	0.41
2:D:176:ALA:HB1	2:D:177:PRO:HD2	2.02	0.41
2:C:126:VAL:CG2	2:C:126:VAL:O	2.68	0.41
2:C:51:LEU:HD11	2:C:112:VAL:HG11	2.02	0.41
2:D:51:LEU:HD11	2:D:112:VAL:HG11	2.02	0.41
1:B:328:PHE:O	1:B:375:ASN:HB2	2.19	0.41
1:B:485:PHE:CD1	1:B:485:PHE:C	2.94	0.41
1:B:552:LEU:HB3	1:B:566:GLU:HA	2.01	0.41
2:C:29:PRO:CD	2:C:119:PHE:CD2	3.03	0.41
1:A:296:TYR:CE2	1:A:299:ARG:HA	2.55	0.41
1:A:328:PHE:CE2	1:A:377:GLY:HA3	2.55	0.41
2:C:164:LEU:HD22	2:C:198:CYS:SG	2.60	0.41
2:D:81:LEU:HD11	2:D:90:ILE:HG13	2.02	0.41
1:A:660:TYR:C	1:A:660:TYR:CD2	2.93	0.41
1:B:296:TYR:CE2	1:B:299:ARG:HA	2.55	0.41
1:B:336:PHE:CE1	1:B:345:TRP:HB2	2.56	0.41
2:D:41:ARG:NH1	2:D:41:ARG:HG3	2.36	0.41
1:A:531:ARG:NH1	1:A:531:ARG:HG3	2.30	0.41
1:A:617:SER:HB3	1:A:618:PRO:HD2	2.01	0.41
1:B:334:LEU:HD23	1:B:348:LEU:CD2	2.50	0.41
1:B:409:LEU:HA	1:B:409:LEU:HD23	1.85	0.41
1:B:284:VAL:HG21	1:B:570:CYS:HA	2.03	0.41
1:A:485:PHE:CD1	1:A:485:PHE:C	2.93	0.41
2:C:182:GLN:O	2:C:183:ARG:HB2	2.21	0.41
2:C:48:ARG:CG	2:C:48:ARG:O	2.69	0.41
2:C:64:ARG:O	2:C:65:ASP:HB2	2.20	0.41
2:D:126:VAL:O	2:D:126:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:185:LEU:HD21	2:D:187:VAL:CG2	2.51	0.41
1:B:343:SER:O	1:B:362:ASN:HA	2.21	0.41
2:D:56:GLU:HA	2:D:57:PRO:HD2	1.80	0.41
1:A:296:TYR:HE1	1:A:442:ASP:OD1	2.04	0.41
2:D:182:GLN:C	2:D:184:SER:N	2.73	0.41
1:A:409:LEU:HA	1:A:409:LEU:HD23	1.85	0.41
1:B:323:PHE:CE1	1:B:382:ILE:HB	2.56	0.41
2:C:185:LEU:C	2:C:185:LEU:HD23	2.41	0.41
1:A:314:LEU:N	2:C:73:ASP:OD1	2.54	0.41
2:C:51:LEU:HD21	2:C:91:VAL:HB	2.03	0.41
1:A:540:VAL:HG13	1:A:636:VAL:HG22	2.03	0.40
1:B:296:TYR:HE1	1:B:442:ASP:OD1	2.04	0.40
2:D:120:VAL:HG12	2:D:121:SER:O	2.21	0.40
1:B:600:SER:O	1:B:602:ALA:N	2.55	0.40
2:C:160:GLU:HB3	2:C:161:PRO:HA	2.02	0.40
2:D:51:LEU:CD2	2:D:91:VAL:HB	2.51	0.40
1:A:327:THR:O	1:A:375:ASN:HA	2.21	0.40
2:D:206:VAL:CG2	2:D:207:THR:N	2.83	0.40
2:D:63:LEU:HD23	2:D:68:ILE:HD13	2.02	0.40
1:B:493:MET:HE2	1:B:616:ARG:HA	2.03	0.40
1:A:381:THR:O	1:A:395:VAL:HA	2.21	0.40
1:B:617:SER:HB3	1:B:618:PRO:HD2	2.03	0.40
2:C:120:VAL:HG12	2:C:121:SER:O	2.21	0.40
2:C:176:ALA:HB1	2:C:177:PRO:HD2	2.04	0.40
2:C:202:ASN:OD1	2:C:202:ASN:C	2.60	0.40
2:C:63:LEU:HD23	2:C:68:ILE:HD13	2.03	0.40
1:A:313:ARG:NH2	2:C:75:THR:OG1	2.51	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	375/422 (89%)	296 (79%)	64 (17%)	15 (4%)	3	18
1	B	375/422 (89%)	297 (79%)	63 (17%)	15 (4%)	3	18
2	C	190/195 (97%)	171 (90%)	14 (7%)	5 (3%)	5	27
2	D	190/195 (97%)	171 (90%)	14 (7%)	5 (3%)	5	27
All	All	1130/1234 (92%)	935 (83%)	155 (14%)	40 (4%)	3	21

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	LEU
1	A	455	ASP
1	A	456	THR
1	B	433	LEU
1	B	455	ASP
1	B	456	THR
1	A	507	VAL
1	A	599	VAL
1	B	507	VAL
1	B	599	VAL
2	C	55	GLY
2	C	98	THR
2	C	203	ALA
2	D	55	GLY
2	D	98	THR
2	D	203	ALA
1	B	600	SER
1	A	292	VAL
1	A	551	GLN
1	A	561	ALA
1	A	562	LEU
1	A	600	SER
1	B	562	LEU
1	A	452	ASN
1	A	515	PRO
1	A	565	MET
1	B	292	VAL
1	B	452	ASN
1	B	551	GLN
1	B	565	MET
2	C	56	GLU
2	D	56	GLU
1	B	515	PRO

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Mol	Chain	Res	Type
1	B	561	ALA
2	C	217	LEU
2	D	217	LEU
1	A	554	VAL
1	B	554	VAL
1	A	288	VAL
1	B	288	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	320/356 (90%)	295 (92%)	25 (8%)	12	38
1	B	320/356 (90%)	296 (92%)	24 (8%)	13	39
2	C	162/166 (98%)	150 (93%)	12 (7%)	13	40
2	D	162/166 (98%)	149 (92%)	13 (8%)	12	37
All	All	964/1044 (92%)	890 (92%)	74 (8%)	13	38

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	LYS
1	A	306	VAL
1	A	313	ARG
1	A	314	LEU
1	A	318	ARG
1	A	334	LEU
1	A	344	THR
1	A	359	LEU
1	A	375	ASN
1	A	384	VAL
1	A	391	LEU
1	A	397	ARG
1	A	419	LEU
1	A	435	GLN

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Mol	Chain	Res	Type
1	A	488	TYR
1	A	491	ASP
1	A	531	ARG
1	A	540	VAL
1	A	554	VAL
1	A	555	LEU
1	A	565	MET
1	A	578	THR
1	A	605	GLN
1	A	619	VAL
1	A	641	ARG
1	B	293	LYS
1	B	306	VAL
1	B	313	ARG
1	B	314	LEU
1	B	318	ARG
1	B	334	LEU
1	B	344	THR
1	B	359	LEU
1	B	375	ASN
1	B	391	LEU
1	B	397	ARG
1	B	419	LEU
1	B	435	GLN
1	B	488	TYR
1	B	491	ASP
1	B	531	ARG
1	B	540	VAL
1	B	554	VAL
1	B	555	LEU
1	B	565	MET
1	B	578	THR
1	B	605	GLN
1	B	619	VAL
1	B	641	ARG
2	C	48	ARG
2	C	50	GLN
2	C	51	LEU
2	C	74	SER
2	C	84	ASP
2	C	87	ASP
2	C	98	THR

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Mol	Chain	Res	Type
2	C	107	GLN
2	C	118	THR
2	C	126	VAL
2	C	185	LEU
2	C	207	THR
2	D	48	ARG
2	D	50	GLN
2	D	51	LEU
2	D	74	SER
2	D	84	ASP
2	D	87	ASP
2	D	98	THR
2	D	107	GLN
2	D	118	THR
2	D	126	VAL
2	D	132	PRO
2	D	185	LEU
2	D	207	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	HIS
1	A	375	ASN
1	A	376	HIS
1	A	429	HIS
1	A	449	ASN
1	A	465	ASN
1	A	573	GLN
1	B	340	HIS
1	B	375	ASN
1	B	376	HIS
1	B	429	HIS
1	B	449	ASN
1	B	465	ASN
1	B	573	GLN
2	C	101	GLN
2	C	107	GLN
2	C	109	GLN
2	C	182	GLN
2	D	94	GLN
2	D	101	GLN

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Mol	Chain	Res	Type
2	D	107	GLN
2	D	109	GLN
2	D	182	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 ⓘ

4 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$
3	NAG	E	1	1,3	14,14,15	0.63	0	17,19,21	0.89	0
3	NAG	E	2	3	14,14,15	0.67	0	17,19,21	0.77	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.53	0	17,19,21	0.79	1 (5%)
3	NAG	F	2	3	14,14,15	0.77	0	17,19,21	0.98	2 (11%)

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	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C2-N2-C7	-2.59	119.22	122.90
3	F	2	NAG	C2-N2-C7	-2.47	119.38	122.90
3	E	2	NAG	C2-N2-C7	-2.31	119.61	122.90
3	F	2	NAG	C4-C3-C2	-2.18	107.82	111.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

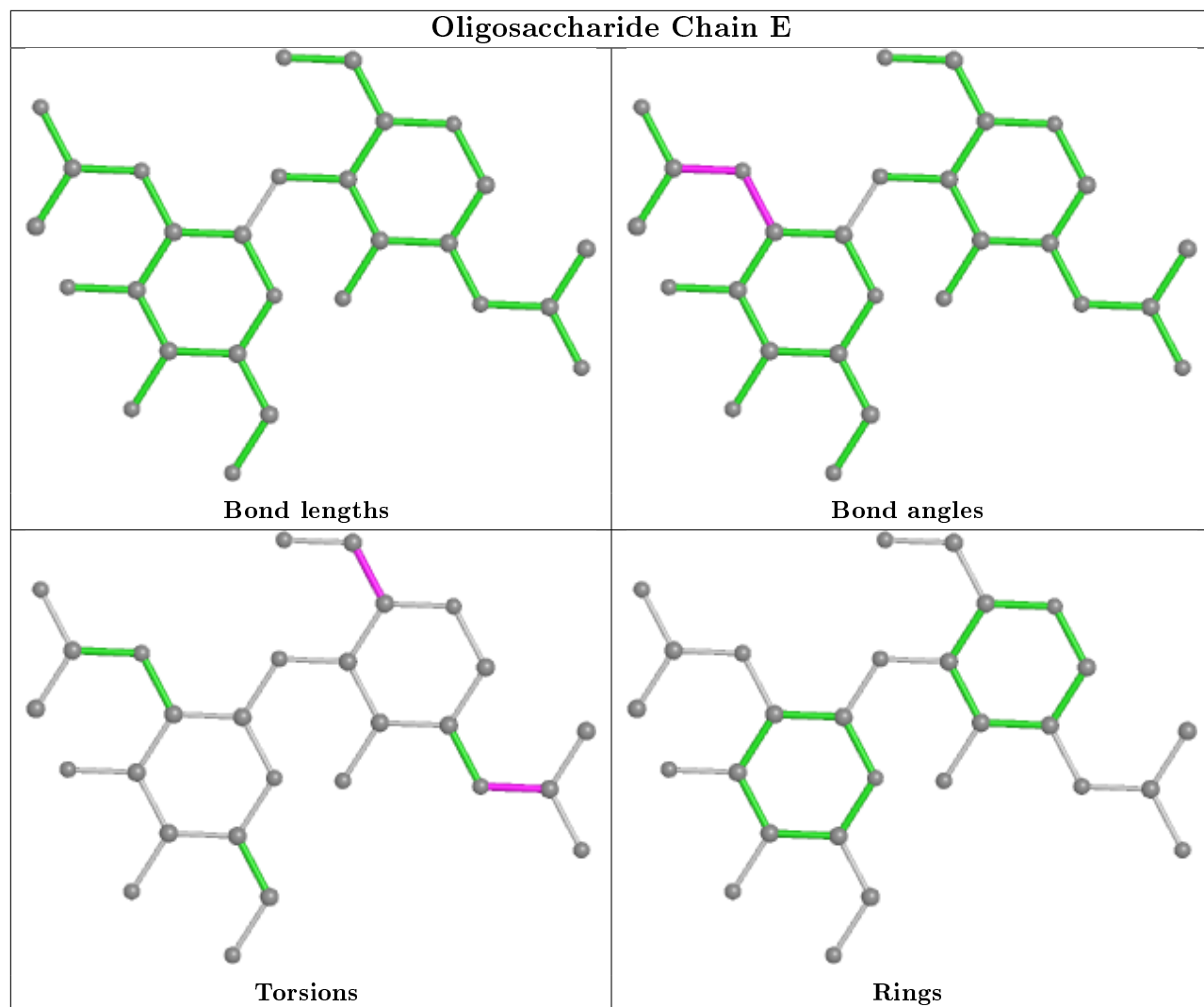
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6

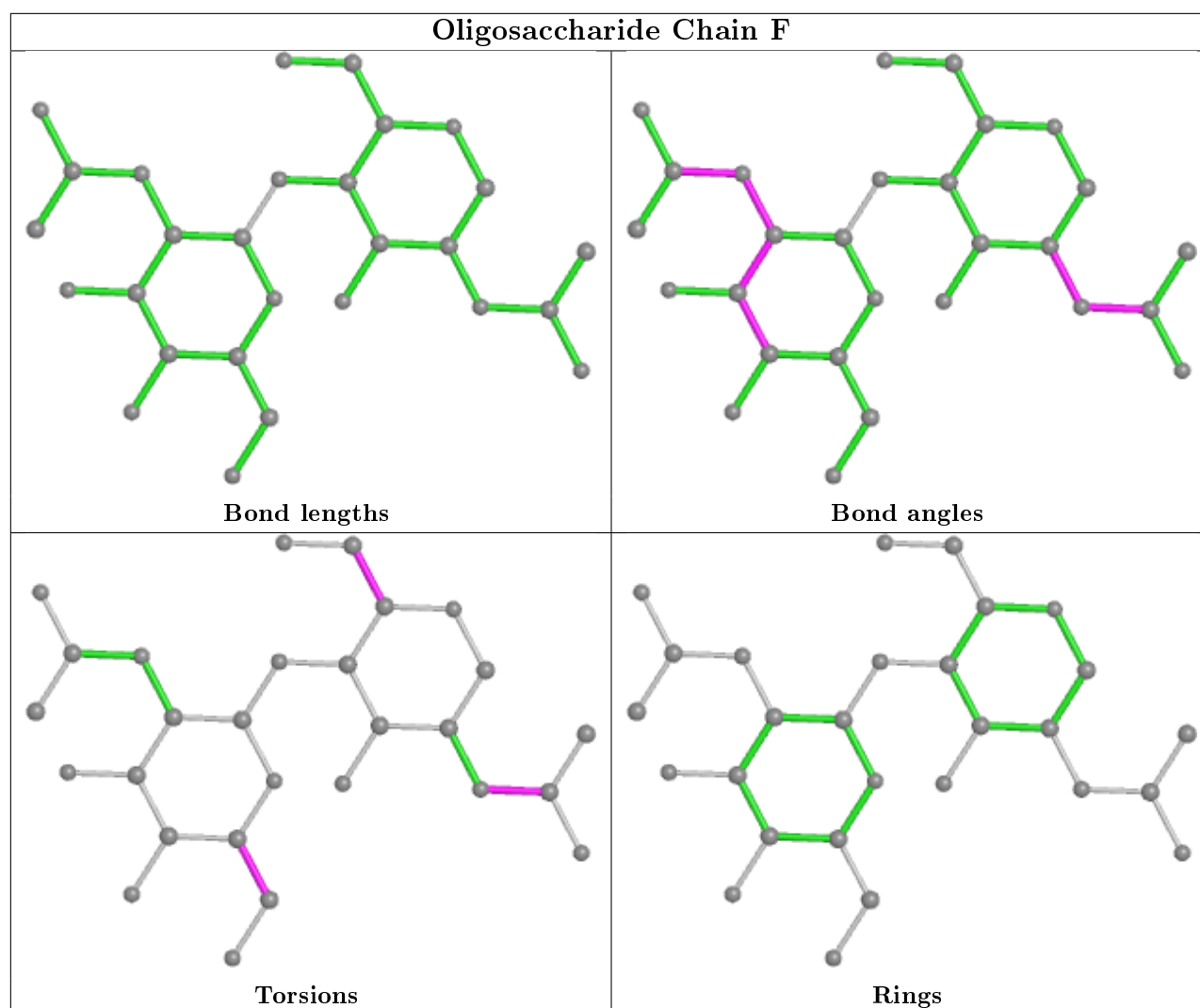
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	2	0
3	E	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 ⓘ

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
6	SO4	C	1219	-	4,4,4	0.31	0	6,6,6	0.15	0

There are no bond length outliers.

There are no bond angle outliers.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	381/422 (90%)	-0.26	6 (1%) 72 70	25, 60, 118, 144	2 (0%)
1	B	381/422 (90%)	-0.31	6 (1%) 72 70	25, 60, 118, 144	2 (0%)
2	C	192/195 (98%)	-0.34	4 (2%) 63 62	28, 56, 86, 101	0
2	D	192/195 (98%)	-0.25	4 (2%) 63 62	27, 56, 86, 101	0
All	All	1146/1234 (92%)	-0.29	20 (1%) 70 68	25, 59, 112, 144	4 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	677	ALA	4.9
1	A	676	ALA	3.3
2	D	218	PRO	3.1
2	D	192	LYS	3.0
1	B	677	ALA	2.9
1	B	676	ALA	2.8
2	D	27	GLU	2.7
1	B	279	ASP	2.6
1	B	596	GLN	2.6
1	A	279	ASP	2.5
2	C	85	GLU	2.4
2	C	27	GLU	2.4
2	C	191	ASN	2.3
2	C	175	THR	2.3
1	A	280	ILE	2.3
1	B	559	HIS	2.2
1	A	606	GLU	2.2
1	B	280	ILE	2.2
1	A	593	THR	2.1
2	D	217	LEU	2.1

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

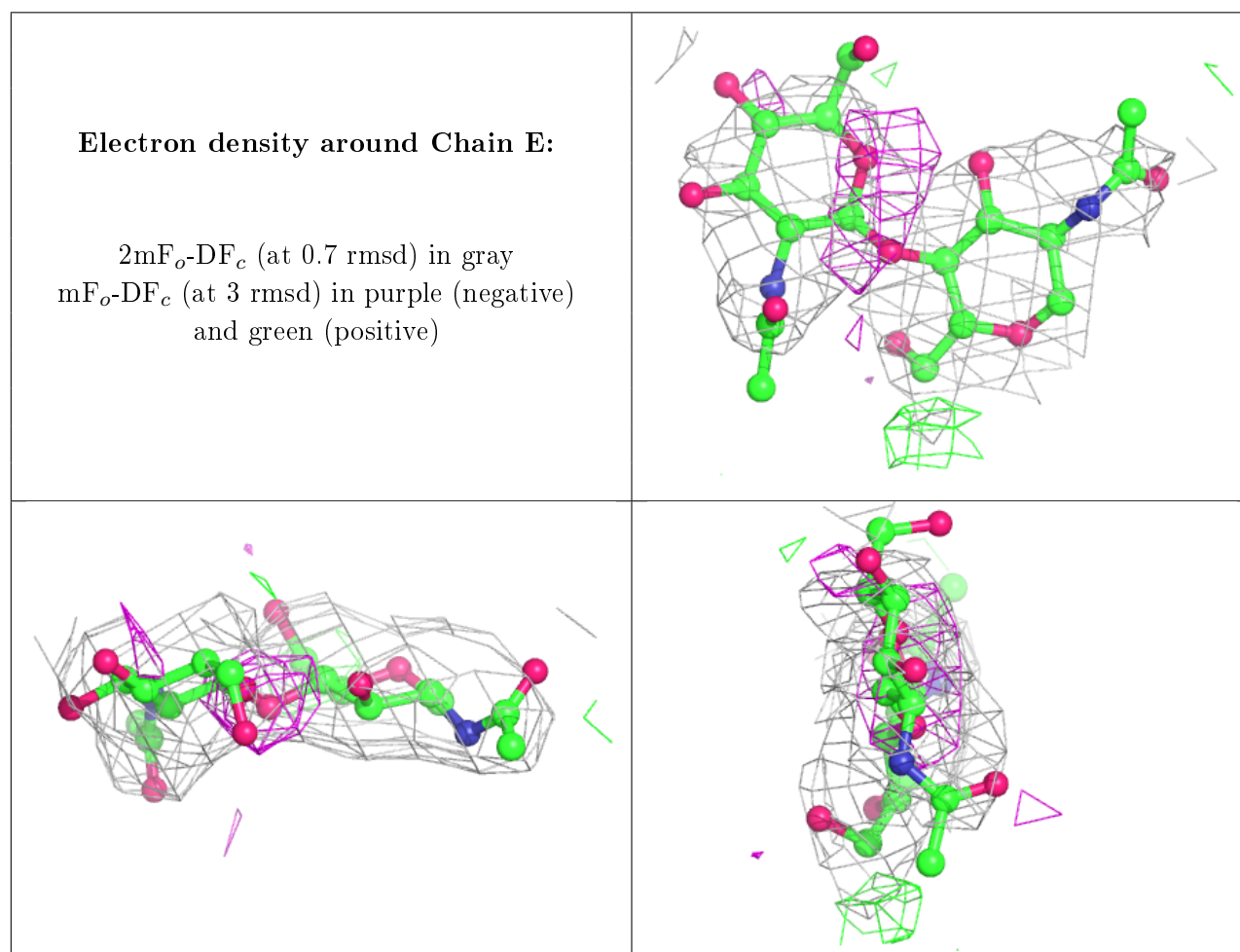
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

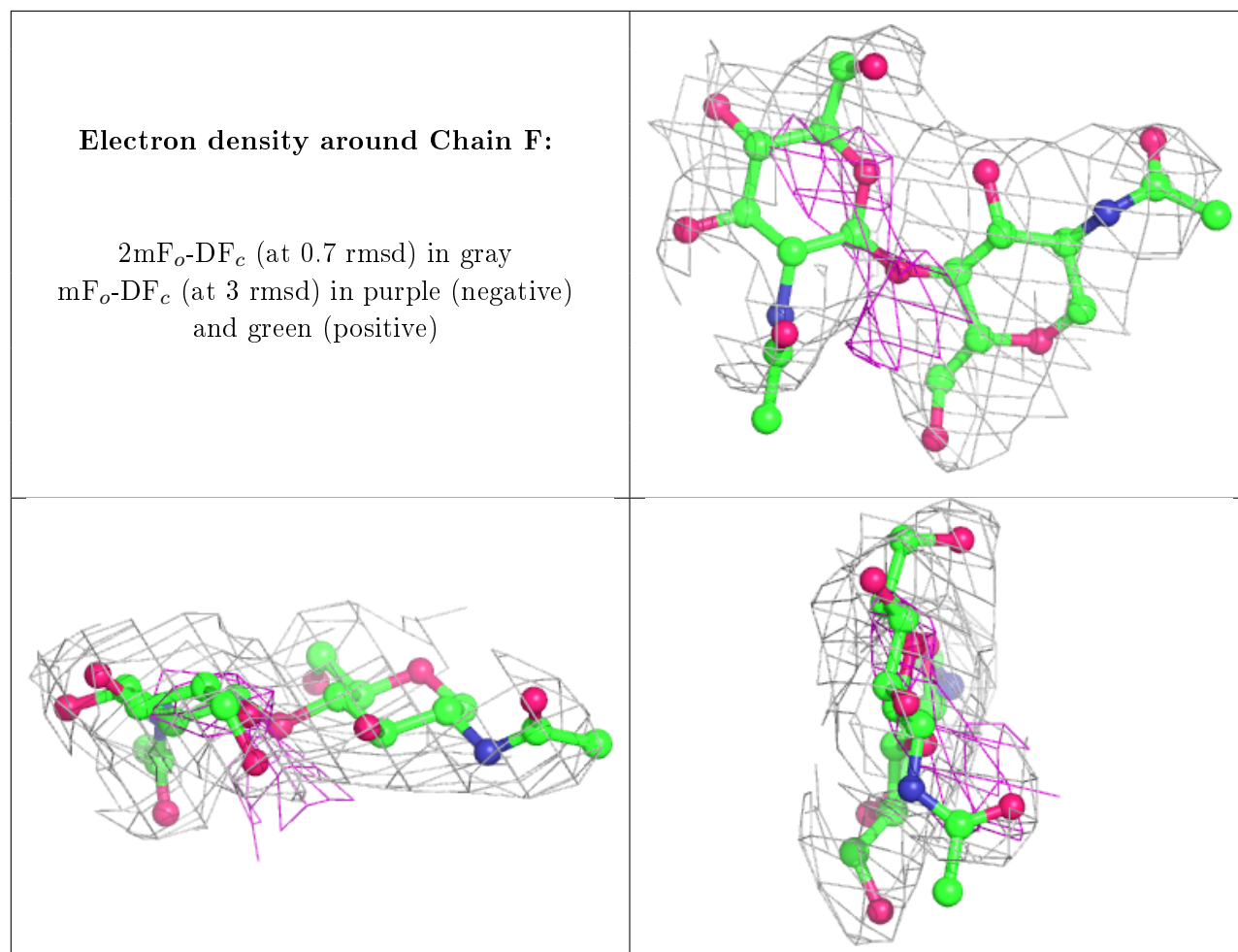
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	E	2	14/15	0.84	0.56	86,91,94,95	0
3	NAG	E	1	14/15	0.85	0.23	65,73,77,82	0
3	NAG	F	2	14/15	0.86	0.41	86,89,91,92	0
3	NAG	F	1	14/15	0.92	0.17	62,68,72,80	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NI	D	1218	1/1	0.91	0.06	134,134,134,134	0
6	SO4	C	1219	5/5	0.95	0.09	103,103,104,104	0
4	CA	A	1677	1/1	0.99	0.18	40,40,40,40	0
4	CA	B	1677	1/1	0.99	0.17	45,45,45,45	0
5	NI	C	1218	1/1	0.99	0.03	127,127,127,127	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.