



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:34 AM EDT

PDB ID : 2A74 / pdb_00002a74
Title : Human Complement Component C3c
Authors : Janssen, B.J.C.; Huizinga, E.G.; Raaijmakers, H.C.A.; Roos, A.; Daha, M.R.;
Nilsson-Ekdahl, K.; Nilsson, B.; Gros, P.
Deposited on : 2005-07-04
Resolution : 2.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

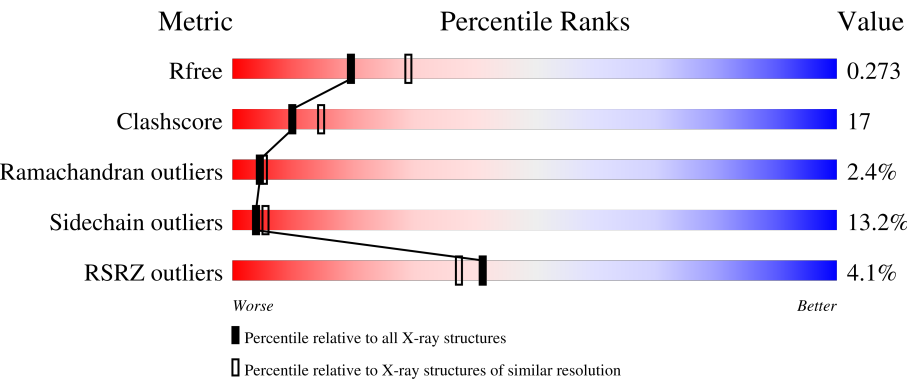
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	643	3% 64%26%7%..
1	D	643	6% 65%25%7%..
2	B	188	2% 77%14%6%.
2	E	188	7% 68%23%6%..
3	C	343	3% 55%22%7%.14%

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Mol	Chain	Length	Quality of chain
3	F	343	
4	G	2	
4	H	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NDG	G	2	X	-	-	-
4	NDG	H	2	X	-	-	-
5	GOL	A	712	-	-	X	-
5	GOL	D	711	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 18389 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 Component C3c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	630	Total	C	N	O	S	0	0	0
			4907	3127	828	937	15			
1	D	633	Total	C	N	O	S	0	0	0
			4933	3144	833	941	15			

- Molecule 2 is a protein called Complement Component C3c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	0	0
			1480	950	249	276	5			
2	E	184	Total	C	N	O	S	0	0	0
			1484	954	250	275	5			

- Molecule 3 is a protein called Complement Component C3c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	296	Total	C	N	O	S	0	0	0
			2407	1517	395	475	20			
3	F	298	Total	C	N	O	S	0	0	0
			2421	1524	397	480	20			

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



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

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



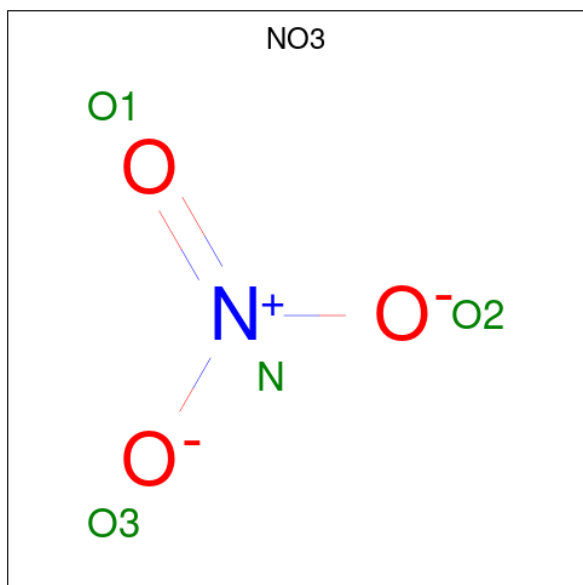
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	N	O	0	0
			4	1	3		
6	F	1	Total	N	O	0	0
			4	1	3		
6	F	1	Total	N	O	0	0
			4	1	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	188	Total	O	0	0
			188	188		
7	B	58	Total	O	0	0
			58	58		
7	C	71	Total	O	0	0
			71	71		

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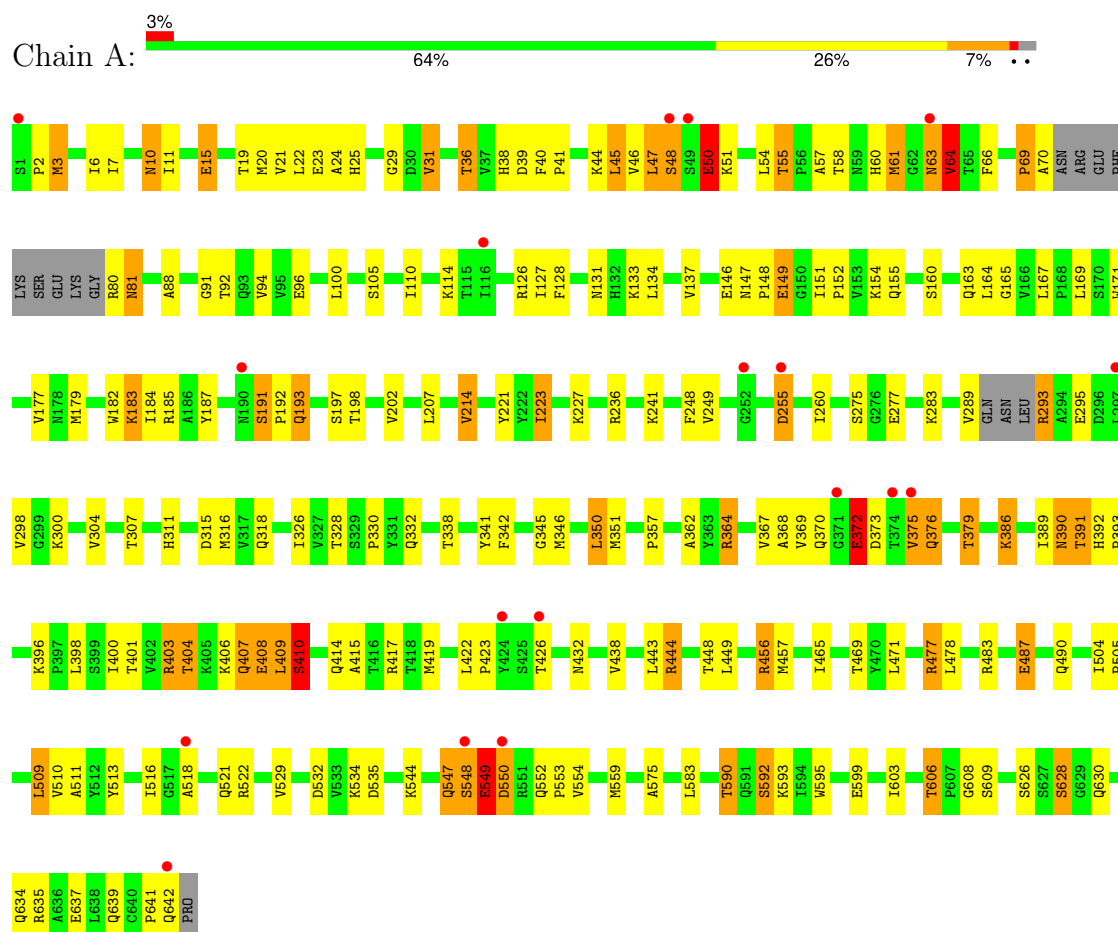
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	148	Total 148	O 148	0	0
7	E	53	Total 53	O 53	0	0
7	F	93	Total 93	O 93	0	0

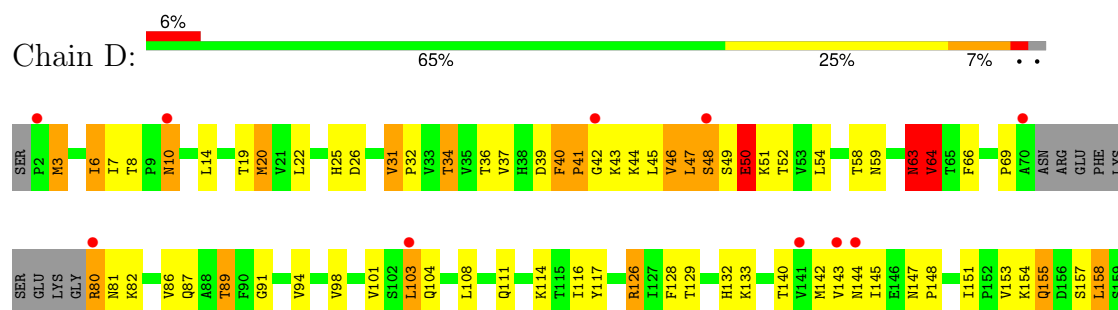
3 Residue-property plots [i](#)

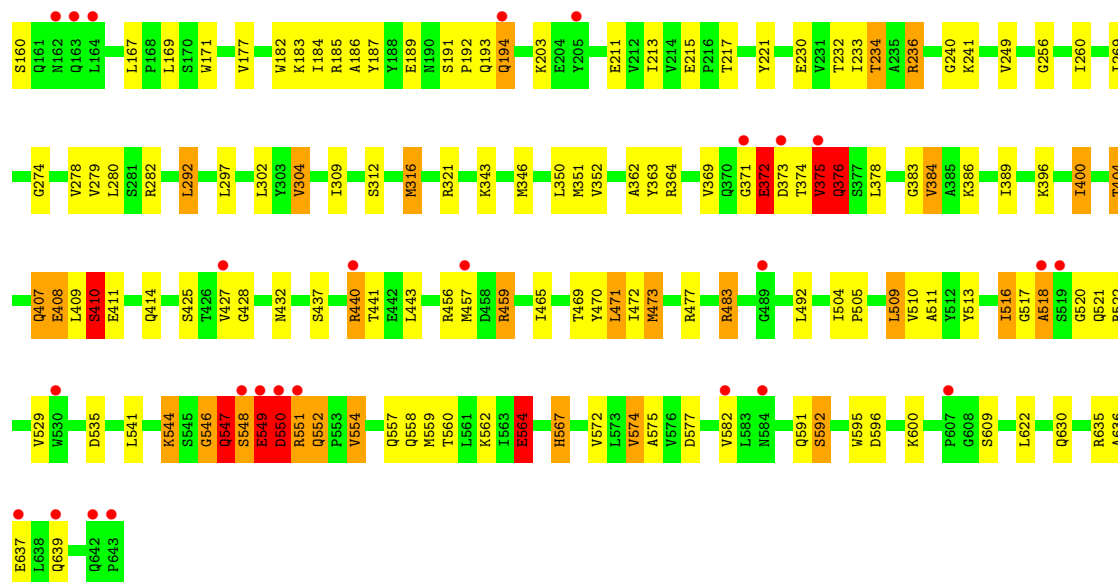
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 Component C3c

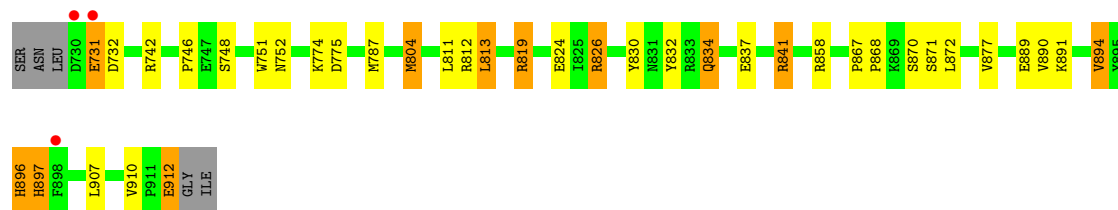
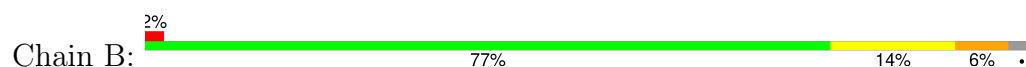


• Molecule 1: Complement Component C3c

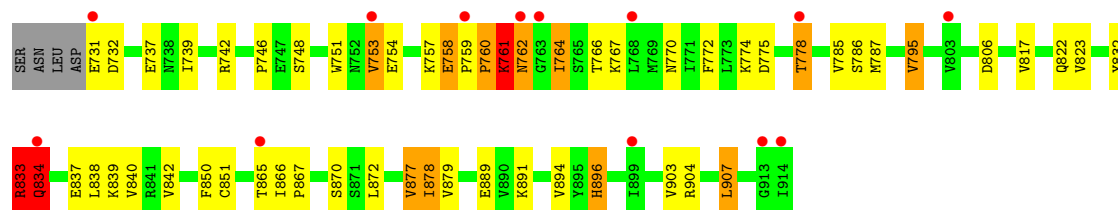




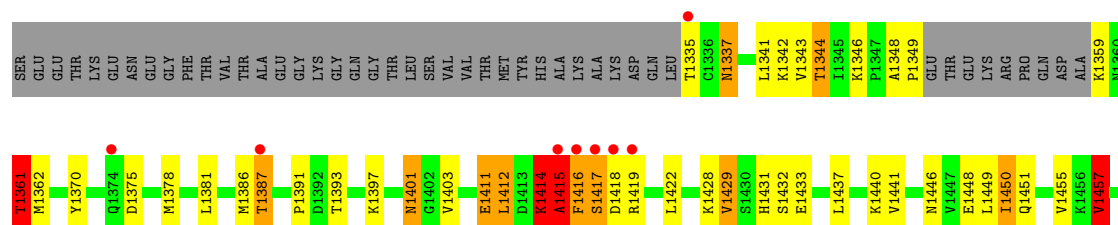
• Molecule 2: Complement Component C3c

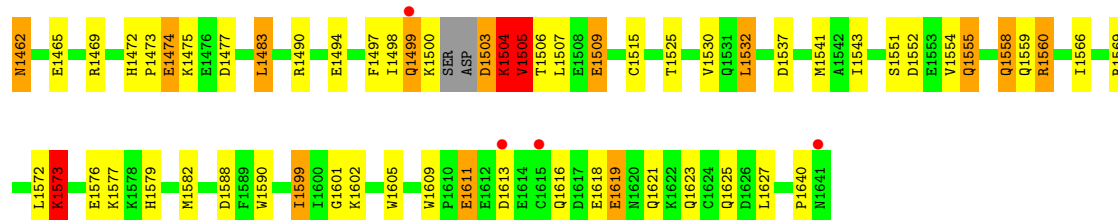


• Molecule 2: Complement Component C3c

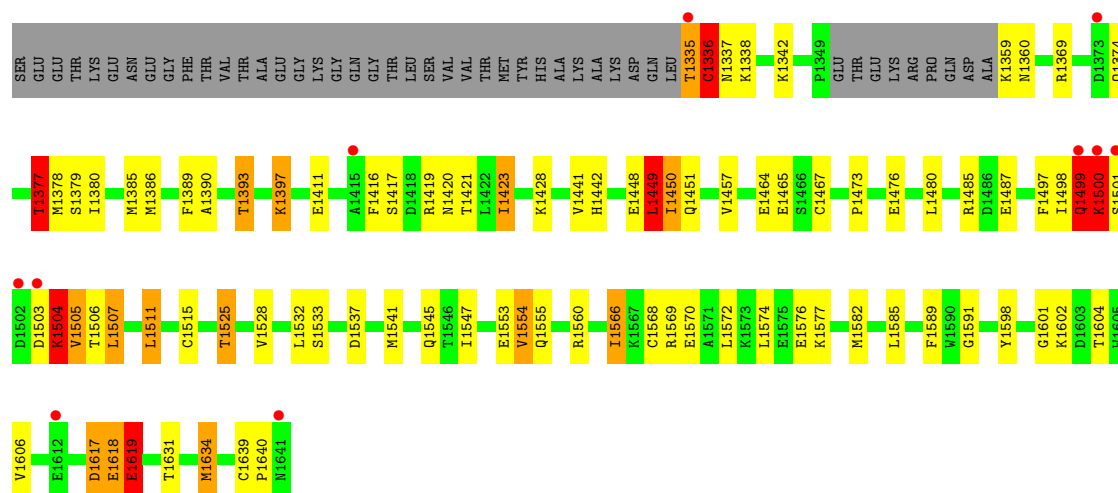


• Molecule 3: Complement Component C3c





• Molecule 3: Complement Component C3c



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.87Å 246.86Å 87.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40 40.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.00-2.40) 97.3 (40.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.31Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.215 , 0.275 0.213 , 0.273	Depositor DCC
R_{free} test set	3471 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtrriage
Anisotropy	0.511	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18389	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7203e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDG, GOL, NO3

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	0.55	1/5004 (0.0%)	0.86	2/6799 (0.0%)
1	D	0.73	15/5032 (0.3%)	0.85	3/6839 (0.0%)
2	B	0.72	3/1512 (0.2%)	0.83	1/2055 (0.0%)
2	E	1.53	24/1516 (1.6%)	0.91	2/2060 (0.1%)
3	C	0.49	0/2453	0.82	2/3305 (0.1%)
3	F	0.64	4/2468 (0.2%)	0.84	1/3327 (0.0%)
All	All	0.75	47/17985 (0.3%)	0.85	11/24385 (0.0%)

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
1	D	0	8
3	C	0	1
3	F	0	3
All	All	0	17

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	896	HIS	CE1-NE2	23.95	1.56	1.32
2	E	896	HIS	CG-CD2	17.07	1.54	1.35
2	E	761	LYS	C-O	15.95	1.42	1.24
2	E	896	HIS	CG-ND1	12.83	1.52	1.38
2	E	759	PRO	CA-C	12.61	1.63	1.52
2	B	896	HIS	CE1-NE2	12.28	1.44	1.32
1	D	564	GLU	CG-CD	11.95	1.81	1.52
1	D	559	MET	C-O	11.00	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	761	LYS	CE-NZ	10.81	1.81	1.49
3	F	1397	LYS	CE-NZ	10.25	1.80	1.49
1	D	544	LYS	CE-NZ	9.97	1.79	1.49
2	B	896	HIS	CG-ND1	9.66	1.48	1.38
1	D	567	HIS	CE1-NE2	9.49	1.42	1.32
2	E	837	GLU	CD-OE1	9.48	1.43	1.25
2	E	767	LYS	C-O	8.89	1.34	1.24
2	E	834	GLN	C-O	8.58	1.34	1.24
2	E	761	LYS	C-N	8.46	1.45	1.33
2	E	766	THR	CA-CB	8.19	1.65	1.53
2	E	834	GLN	C-N	7.65	1.44	1.33
2	E	764	ILE	CB-CG1	7.62	1.68	1.53
3	F	1617	ASP	CG-OD1	7.58	1.39	1.25
1	D	567	HIS	CG-CD2	7.57	1.44	1.35
2	E	758	GLU	CD-OE2	7.38	1.39	1.25
2	E	762	ASN	C-N	7.16	1.42	1.33
2	E	761	LYS	CA-C	7.15	1.61	1.52
1	D	559	MET	C-N	6.99	1.43	1.33
1	D	546	GLY	C-O	6.98	1.33	1.23
2	E	837	GLU	CD-OE2	6.93	1.38	1.25
3	F	1617	ASP	CG-OD2	6.72	1.38	1.25
2	E	760	PRO	C-N	6.41	1.44	1.33
2	E	764	ILE	C-O	6.32	1.31	1.24
2	E	896	HIS	CD2-NE2	6.31	1.44	1.37
2	E	762	ASN	CG-OD1	6.24	1.35	1.23
2	E	761	LYS	CD-CE	6.03	1.70	1.52
2	B	896	HIS	CG-CD2	5.93	1.42	1.35
1	D	546	GLY	C-N	5.84	1.41	1.33
1	D	544	LYS	CD-CE	5.84	1.70	1.52
1	A	149	GLU	CD-OE2	5.73	1.36	1.25
1	D	562	LYS	CD-CE	5.71	1.69	1.52
3	F	1618	GLU	CG-CD	5.42	1.65	1.52
1	D	151	ILE	CB-CG1	5.34	1.64	1.53
1	D	547	GLN	CG-CD	5.21	1.65	1.52
1	D	562	LYS	CG-CD	5.19	1.68	1.52
1	D	547	GLN	C-O	5.17	1.30	1.23
1	D	549	GLU	CD-OE1	5.14	1.35	1.25
2	E	762	ASN	CA-C	5.12	1.59	1.53
2	E	896	HIS	ND1-CE1	5.05	1.37	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	804	MET	N-CA-C	7.09	118.86	108.86
1	A	48	SER	N-CA-C	-6.01	107.77	114.62
3	C	1415	ALA	N-CA-C	5.87	116.30	108.38
3	C	1457	VAL	CB-CA-C	-5.82	102.77	110.98
1	D	562	LYS	CG-CD-CE	-5.30	99.12	111.30
1	D	384	VAL	N-CA-C	5.26	116.16	108.53
2	E	761	LYS	CD-CE-NZ	-5.23	95.16	111.90
1	D	48	SER	N-CA-C	-5.21	105.59	112.94
1	A	96	GLU	N-CA-C	5.16	117.65	109.50
3	F	1337	ASN	N-CA-C	5.15	119.72	113.38
2	E	760	PRO	CA-C-O	-5.01	115.46	121.48

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	ASP	Peptide
1	A	403	ARG	Peptide
1	A	549	GLU	Peptide
1	A	63	ASN	Peptide
1	A	69	PRO	Peptide
3	C	1415	ALA	Peptide
1	D	374	THR	Peptide
1	D	40	PHE	Peptide
1	D	428	GLY	Peptide
1	D	44	LYS	Peptide
1	D	548	SER	Peptide
1	D	549	GLU	Peptide
1	D	63	ASN	Peptide
1	D	80	ARG	Peptide
3	F	1417	SER	Peptide
3	F	1500	LYS	Peptide
3	F	1640	PRO	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	4907	0	4970	214	0
1	D	4933	0	4996	197	0
2	B	1480	0	1501	31	0
2	E	1484	0	1511	48	0
3	C	2407	0	2316	99	0
3	F	2421	0	2326	67	0
4	G	28	0	23	2	0
4	H	28	0	19	1	0
5	A	18	0	24	6	0
5	B	12	0	16	2	0
5	C	12	0	16	0	0
5	D	6	0	8	5	0
5	E	18	0	24	2	0
5	F	12	0	16	4	0
6	C	4	0	0	0	0
6	F	8	0	0	0	0
7	A	188	0	0	12	0
7	B	58	0	0	0	0
7	C	71	0	0	6	0
7	D	148	0	0	3	0
7	E	53	0	0	2	0
7	F	93	0	0	1	0
All	All	18389	0	17766	621	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 17.

All (621) 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:D:564:GLU:CG	1:D:564:GLU:CD	1.81	1.53
3:F:1397:LYS:CE	3:F:1397:LYS:NZ	1.80	1.44
1:D:544:LYS:CE	1:D:544:LYS:NZ	1.79	1.43
2:E:761:LYS:CE	2:E:761:LYS:NZ	1.81	1.42
1:A:6:ILE:HD11	1:A:20:MET:CG	1.53	1.39
1:A:6:ILE:CD1	1:A:20:MET:HG3	1.50	1.38
1:D:292:LEU:H	1:D:292:LEU:CD2	1.42	1.27
1:D:375:VAL:HG23	1:D:376:GLN:H	1.12	1.14
1:A:403:ARG:HB3	1:A:404:THR:HG22	1.16	1.14
1:D:6:ILE:HD11	1:D:20:MET:SD	1.88	1.14
1:A:404:THR:HG23	1:A:414:GLN:HB3	1.26	1.14
1:A:372:GLU:HA	1:A:373:ASP:HB3	1.13	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:LEU:HD23	1:D:292:LEU:N	1.63	1.11
1:D:20:MET:CE	1:D:86:VAL:CG1	2.29	1.10
1:A:375:VAL:HG12	1:A:376:GLN:H	0.99	1.09
1:D:20:MET:HE3	1:D:86:VAL:CG1	1.83	1.07
1:D:80:ARG:HD3	1:D:637:GLU:HA	1.13	1.07
1:A:36:THR:HG21	1:A:38:HIS:CE1	1.91	1.06
3:C:1525:THR:OG1	3:C:1541:MET:HE2	1.53	1.06
3:F:1533:SER:O	3:F:1566:ILE:HD11	1.56	1.04
1:A:606:THR:HG21	7:A:652:HOH:O	1.58	1.03
3:C:1411:GLU:HG2	3:C:1422:LEU:HD12	1.42	1.01
3:F:1504:LYS:HG2	3:F:1505:VAL:H	1.25	1.01
1:A:409:LEU:O	1:A:410:SER:HB3	1.61	1.00
1:D:20:MET:CE	1:D:86:VAL:HG11	1.90	1.00
3:C:1391:PRO:HG2	3:C:1419:ARG:HD2	1.40	1.00
1:D:160:SER:HB3	1:D:167:LEU:HD11	1.44	0.99
3:F:1504:LYS:HG2	3:F:1505:VAL:N	1.77	0.99
1:A:36:THR:HG21	1:A:38:HIS:HE1	1.27	0.98
1:A:315:ASP:HA	5:A:703:GOL:H31	1.41	0.98
1:A:293:ARG:HH21	1:A:295:GLU:HB2	1.30	0.97
1:D:292:LEU:H	1:D:292:LEU:HD23	0.81	0.97
1:A:20:MET:HE1	1:A:88:ALA:HB2	1.43	0.97
1:A:372:GLU:HA	1:A:373:ASP:CB	1.90	0.97
1:D:63:ASN:HA	7:D:781:HOH:O	1.65	0.97
1:A:36:THR:CG2	1:A:38:HIS:CE1	2.48	0.96
1:D:473:MET:CE	1:D:622:LEU:HD21	1.96	0.96
1:D:535:ASP:HB3	5:D:711:GOL:H32	1.48	0.96
1:A:426:THR:CG2	7:A:829:HOH:O	2.15	0.95
3:F:1386:MET:HB3	3:F:1450:ILE:HD12	1.48	0.95
1:A:375:VAL:HG12	1:A:376:GLN:N	1.82	0.95
1:A:404:THR:CG2	1:A:414:GLN:HB3	1.96	0.94
1:A:3:MET:HE3	1:A:522:ARG:HG2	1.50	0.94
1:A:338:THR:HG21	1:A:419:MET:HE1	1.47	0.93
3:F:1448:GLU:O	3:F:1449:LEU:HB2	1.68	0.93
1:A:403:ARG:CB	1:A:404:THR:HG22	1.98	0.93
3:C:1525:THR:CB	3:C:1541:MET:HE2	1.99	0.93
3:F:1386:MET:HB3	3:F:1450:ILE:CD1	1.98	0.93
1:A:372:GLU:CA	1:A:373:ASP:HB3	1.99	0.93
1:D:160:SER:HB3	1:D:167:LEU:CD1	1.98	0.92
1:A:404:THR:HG21	1:A:415:ALA:O	1.71	0.89
1:D:404:THR:HG22	1:D:414:GLN:OE1	1.73	0.89
3:F:1591:GLY:H	5:F:707:GOL:H31	1.35	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PHE:HD1	3:C:1378:MET:CE	1.87	0.87
1:D:20:MET:HE3	1:D:86:VAL:HG13	1.57	0.86
1:A:548:SER:O	1:A:549:GLU:HB2	1.73	0.86
1:A:375:VAL:CG1	1:A:376:GLN:H	1.84	0.86
1:A:362:ALA:O	1:A:379:THR:HG21	1.73	0.85
1:A:369:VAL:O	1:A:372:GLU:HG2	1.75	0.85
1:D:375:VAL:HG23	1:D:376:GLN:N	1.90	0.85
3:C:1415:ALA:HB3	3:C:1417:SER:HB3	1.56	0.85
1:D:375:VAL:CG2	1:D:376:GLN:H	1.88	0.85
1:D:549:GLU:HB3	1:D:550:ASP:CA	2.07	0.85
1:D:577:ASP:OD1	2:E:778:THR:HG21	1.77	0.85
1:A:31:VAL:HG13	1:A:54:LEU:HB2	1.59	0.85
1:D:6:ILE:CD1	1:D:20:MET:SD	2.65	0.84
1:A:477:ARG:HH11	1:A:477:ARG:CG	1.90	0.83
1:A:20:MET:HE2	1:A:22:LEU:HD21	1.58	0.83
3:C:1387:THR:CG2	3:C:1451:GLN:H	1.91	0.83
1:D:80:ARG:HD3	1:D:637:GLU:CA	2.04	0.83
1:D:47:LEU:HD13	1:D:66:PHE:HB2	1.59	0.82
3:C:1348:ALA:HB1	3:C:1349:PRO:HD2	1.62	0.82
1:D:549:GLU:CB	1:D:550:ASP:HB2	2.08	0.82
1:D:20:MET:HE2	1:D:86:VAL:HG11	1.60	0.82
2:B:824:GLU:OE1	2:B:826:ARG:NH1	2.12	0.81
1:A:248:PHE:HD1	3:C:1378:MET:HE3	1.46	0.80
1:A:404:THR:CG2	1:A:415:ALA:O	2.28	0.80
1:A:6:ILE:CG1	1:A:20:MET:HE3	2.11	0.80
1:A:403:ARG:HB3	1:A:404:THR:CG2	2.08	0.80
1:A:393:PRO:HD3	7:A:722:HOH:O	1.80	0.80
3:C:1525:THR:OG1	3:C:1541:MET:CE	2.30	0.80
1:D:47:LEU:CD1	1:D:66:PHE:HB2	2.10	0.80
1:D:473:MET:HE3	1:D:622:LEU:HD21	1.62	0.80
1:D:372:GLU:HG3	1:D:375:VAL:HG22	1.63	0.80
1:A:351:MET:HE1	1:A:386:LYS:HD3	1.64	0.79
1:A:20:MET:CE	1:A:88:ALA:HB2	2.10	0.79
1:A:248:PHE:CD1	3:C:1378:MET:HE3	2.19	0.78
1:D:292:LEU:CD2	1:D:292:LEU:N	2.24	0.78
1:A:362:ALA:O	1:A:379:THR:CG2	2.32	0.78
2:B:896:HIS:C	2:B:897:HIS:HD1	1.91	0.78
3:C:1362:MET:HE1	3:C:1473:PRO:HG3	1.65	0.78
1:A:606:THR:HG22	1:A:608:GLY:H	1.48	0.78
1:D:473:MET:HE1	1:D:622:LEU:HD21	1.65	0.77
1:A:6:ILE:CD1	1:A:20:MET:CG	2.30	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1498:ILE:HG22	3:C:1499:GLN:HG2	1.67	0.77
2:E:889:GLU:HG3	2:E:904:ARG:HB3	1.65	0.77
1:D:386:LYS:HB3	1:D:440:ARG:HD2	1.65	0.77
1:A:426:THR:HG22	7:A:829:HOH:O	1.78	0.76
1:D:144:ASN:ND2	1:D:155:GLN:HG3	2.01	0.76
1:D:386:LYS:CB	1:D:440:ARG:HD2	2.15	0.76
1:A:426:THR:HG23	7:A:829:HOH:O	1.78	0.76
2:B:819:ARG:HH11	2:B:819:ARG:HB3	1.51	0.76
1:D:3:MET:HE3	1:D:522:ARG:CD	2.15	0.76
1:D:6:ILE:HD11	1:D:20:MET:CG	2.16	0.75
1:D:58:THR:HG23	1:D:58:THR:O	1.86	0.75
1:D:549:GLU:OE1	1:D:549:GLU:HA	1.85	0.75
1:A:372:GLU:HB3	1:A:375:VAL:HB	1.67	0.75
1:A:6:ILE:HD13	1:A:20:MET:HE3	1.69	0.75
1:A:404:THR:HG23	1:A:404:THR:O	1.86	0.74
1:D:6:ILE:HD13	1:D:7:ILE:N	2.02	0.74
1:A:128:PHE:HB3	2:B:787:MET:HE1	1.68	0.74
3:C:1341:LEU:HD22	3:C:1457:VAL:HG22	1.68	0.74
1:D:80:ARG:CD	1:D:637:GLU:HA	2.07	0.74
1:A:6:ILE:CD1	1:A:20:MET:HE3	2.17	0.74
3:C:1525:THR:CB	3:C:1541:MET:CE	2.65	0.74
3:C:1361:THR:HA	3:C:1441:VAL:O	1.86	0.73
3:C:1490:ARG:NE	7:C:526:HOH:O	2.16	0.73
1:A:29:GLY:O	1:A:60:HIS:HE1	1.70	0.73
1:D:371:GLY:O	1:D:372:GLU:HB2	1.88	0.73
3:F:1448:GLU:O	3:F:1449:LEU:CB	2.35	0.73
3:F:1576:GLU:O	3:F:1577:LYS:HB2	1.87	0.73
1:D:549:GLU:HB3	1:D:550:ASP:HB2	1.71	0.73
1:A:6:ILE:HG12	1:A:20:MET:HE3	1.70	0.73
1:A:6:ILE:HG12	1:A:20:MET:CE	2.18	0.72
1:A:191:SER:HA	1:A:193:GLN:HE21	1.54	0.72
2:B:837:GLU:HB3	2:B:868:PRO:HD3	1.70	0.71
1:D:351:MET:HE1	1:D:386:LYS:HD2	1.73	0.71
1:A:367:VAL:HG12	1:A:404:THR:H	1.53	0.71
1:A:372:GLU:CA	1:A:373:ASP:CB	2.63	0.71
1:D:312:SER:O	7:D:786:HOH:O	2.07	0.71
1:A:350:LEU:HD21	1:A:400:ILE:HG21	1.73	0.71
1:D:111:GLN:OE1	1:D:126:ARG:HD3	1.90	0.71
1:D:473:MET:CE	1:D:622:LEU:CD2	2.69	0.71
1:D:3:MET:HE3	1:D:522:ARG:CG	2.20	0.71
2:B:858:ARG:NH2	3:C:1494:GLU:HA	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:549:GLU:HB3	1:D:550:ASP:HA	1.73	0.70
1:A:370:GLN:CG	1:A:401:THR:HB	2.22	0.70
1:D:549:GLU:HB3	1:D:550:ASP:CB	2.21	0.70
1:D:3:MET:CE	1:D:522:ARG:HG2	2.21	0.70
3:F:1449:LEU:N	3:F:1449:LEU:HD23	2.07	0.70
1:A:592:SER:HA	5:A:712:GOL:H32	1.74	0.70
2:B:819:ARG:HH11	2:B:819:ARG:CB	2.05	0.70
2:E:822:GLN:HE22	3:F:1480:LEU:H	1.38	0.69
1:A:69:PRO:HA	1:A:70:ALA:HB3	1.73	0.69
1:A:477:ARG:HH11	1:A:477:ARG:HG2	1.57	0.69
3:C:1337:ASN:H	3:C:1337:ASN:HD22	1.41	0.69
1:A:154:LYS:HD2	1:A:171:TRP:CD1	2.26	0.69
1:A:47:LEU:CD1	1:A:66:PHE:HB2	2.23	0.68
1:D:3:MET:HE3	1:D:522:ARG:HG2	1.73	0.68
1:A:3:MET:HE3	1:A:522:ARG:CG	2.21	0.68
1:A:370:GLN:HG2	1:A:401:THR:HB	1.76	0.68
3:C:1572:LEU:O	3:C:1573:LYS:HD2	1.94	0.68
3:F:1428:LYS:HE3	7:F:68:HOH:O	1.93	0.68
3:C:1465:GLU:O	3:C:1465:GLU:HG3	1.91	0.68
3:C:1525:THR:HB	3:C:1541:MET:CE	2.23	0.68
3:C:1411:GLU:HG2	3:C:1422:LEU:CD1	2.19	0.68
1:D:6:ILE:CG1	1:D:20:MET:SD	2.82	0.67
1:D:592:SER:HB3	5:D:711:GOL:H11	1.74	0.67
2:B:819:ARG:HH11	2:B:819:ARG:CG	2.07	0.66
1:D:369:VAL:HG22	1:D:400:ILE:HD11	1.77	0.66
3:C:1381:LEU:CD2	3:C:1457:VAL:HG13	2.25	0.66
1:A:23:GLU:HG2	1:A:61:MET:HG2	1.77	0.66
1:D:541:LEU:HD22	2:E:786:SER:HB3	1.78	0.66
3:C:1499:GLN:HG3	3:C:1500:LYS:N	2.10	0.66
1:D:409:LEU:O	1:D:410:SER:HB3	1.96	0.66
1:D:473:MET:HE1	1:D:622:LEU:CD2	2.26	0.65
3:F:1525:THR:CG2	3:F:1541:MET:SD	2.84	0.65
1:D:6:ILE:HD13	1:D:7:ILE:H	1.61	0.65
3:F:1385:MET:HE2	3:F:1390:ALA:N	2.11	0.65
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.27	0.65
1:D:20:MET:HE3	1:D:86:VAL:HG11	1.62	0.65
1:A:345:GLY:H	1:A:391:THR:HG22	1.62	0.65
2:E:761:LYS:NZ	2:E:761:LYS:CD	2.60	0.65
1:A:6:ILE:HD12	1:A:21:VAL:O	1.95	0.64
1:A:80:ARG:O	1:A:81:ASN:HB2	1.96	0.64
1:D:103:LEU:HD22	1:D:103:LEU:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:SER:CB	1:D:167:LEU:HD11	2.24	0.64
1:A:350:LEU:HD23	1:A:419:MET:CE	2.27	0.64
2:B:819:ARG:NH1	2:B:912:GLU:OE2	2.31	0.64
2:B:894:VAL:CG2	2:B:897:HIS:HB2	2.27	0.64
1:D:549:GLU:CB	1:D:550:ASP:CB	2.76	0.64
3:F:1397:LYS:NZ	3:F:1397:LYS:CD	2.60	0.64
3:C:1448:GLU:O	3:C:1449:LEU:HB2	1.97	0.64
1:D:40:PHE:CD2	1:D:41:PRO:HD3	2.33	0.64
1:D:20:MET:CE	1:D:86:VAL:HG12	2.27	0.63
2:E:785:VAL:HG22	2:E:795:VAL:HB	1.79	0.63
1:D:3:MET:CE	1:D:522:ARG:CG	2.77	0.63
1:D:6:ILE:HD11	1:D:20:MET:HG2	1.81	0.63
1:A:6:ILE:HG12	1:A:20:MET:SD	2.38	0.63
1:D:473:MET:HE3	1:D:622:LEU:CD2	2.29	0.63
2:B:858:ARG:HH22	3:C:1494:GLU:HA	1.64	0.63
3:F:1385:MET:HE2	3:F:1389:PHE:C	2.24	0.62
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.81	0.62
1:A:7:ILE:HG21	1:A:471:LEU:HD22	1.81	0.62
3:C:1537:ASP:OD2	3:C:1569:ARG:HD3	2.00	0.62
3:F:1386:MET:HB3	3:F:1450:ILE:HD11	1.82	0.62
1:A:293:ARG:HH21	1:A:295:GLU:CB	2.10	0.61
1:D:472:ILE:HD13	1:D:509:LEU:HD22	1.82	0.61
1:D:309:ILE:HG12	1:D:316:MET:HG3	1.82	0.61
1:D:577:ASP:CG	2:E:778:THR:HG21	2.25	0.61
3:C:1515:CYS:SG	3:C:1640:PRO:HD3	2.40	0.61
1:A:404:THR:CG2	1:A:404:THR:O	2.48	0.61
1:D:547:GLN:H	1:D:547:GLN:HE21	1.47	0.61
1:A:3:MET:HE2	1:A:630:GLN:OE1	2.01	0.61
1:D:233:ILE:HD13	1:D:269:ILE:HD11	1.83	0.61
1:D:472:ILE:CD1	1:D:509:LEU:HD22	2.31	0.61
1:A:6:ILE:HD11	1:A:20:MET:SD	2.40	0.60
1:A:47:LEU:HD13	1:A:66:PHE:HB2	1.82	0.60
1:A:535:ASP:HB3	5:A:712:GOL:H11	1.83	0.60
2:B:811:LEU:HG	2:B:813:LEU:HD13	1.84	0.60
3:C:1381:LEU:HD23	3:C:1457:VAL:HG13	1.83	0.60
3:C:1359:LYS:NZ	3:C:1446:ASN:HB2	2.17	0.60
1:A:47:LEU:HD21	1:A:50:GLU:HG2	1.81	0.60
1:D:564:GLU:CD	1:D:564:GLU:CB	2.71	0.60
1:D:558:GLN:NE2	2:E:770:ASN:OD1	2.33	0.60
1:A:6:ILE:CD1	1:A:20:MET:SD	2.89	0.60
3:C:1483:LEU:HD23	3:C:1599:ILE:HD12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ILE:HG12	1:D:22:LEU:HD23	1.83	0.60
1:D:19:THR:HG21	4:H:1:NDG:H8C1	1.83	0.60
3:F:1507:LEU:HD22	3:F:1511:LEU:HD22	1.84	0.59
1:A:477:ARG:HH11	1:A:477:ARG:HG3	1.66	0.59
1:D:45:LEU:HD21	1:D:48:SER:OG	2.02	0.59
3:F:1386:MET:SD	3:F:1473:PRO:HD3	2.42	0.59
1:D:549:GLU:HB2	1:D:550:ASP:HB2	1.83	0.59
1:A:6:ILE:HD12	1:A:7:ILE:H	1.68	0.59
3:F:1537:ASP:OD2	3:F:1569:ARG:HG2	2.02	0.59
1:D:409:LEU:O	1:D:410:SER:CB	2.50	0.59
1:D:80:ARG:HB3	1:D:636:ALA:O	2.02	0.59
1:D:108:LEU:CD2	1:D:129:THR:HG22	2.33	0.59
1:A:477:ARG:HG2	1:A:477:ARG:NH1	2.18	0.59
1:A:367:VAL:O	1:A:376:GLN:HA	2.03	0.58
1:D:143:VAL:HG11	1:D:169:LEU:CD1	2.33	0.58
3:F:1634:MET:HA	3:F:1634:MET:HE2	1.85	0.58
3:C:1613:ASP:HA	3:C:1616:GLN:HE21	1.68	0.58
1:A:6:ILE:HD11	1:A:20:MET:HG3	0.68	0.57
3:C:1387:THR:HG23	3:C:1451:GLN:H	1.66	0.57
1:A:15:GLU:HG2	1:A:70:ALA:HB2	1.85	0.57
1:D:8:THR:HG22	1:D:20:MET:HG2	1.86	0.57
3:C:1555:GLN:HG2	7:C:579:HOH:O	2.05	0.57
2:E:867:PRO:HG2	2:E:870:SER:OG	2.05	0.57
2:E:877:VAL:HG13	3:F:1451:GLN:CG	2.35	0.57
3:F:1515:CYS:SG	3:F:1634:MET:HE1	2.45	0.57
3:C:1588:ASP:OD2	7:C:561:HOH:O	2.17	0.57
2:E:877:VAL:HG13	3:F:1451:GLN:HG2	1.87	0.57
1:D:50:GLU:HB3	1:D:64:VAL:HB	1.86	0.57
1:D:386:LYS:H	1:D:440:ARG:CZ	2.17	0.57
1:D:386:LYS:HB2	1:D:440:ARG:HD2	1.87	0.56
3:C:1391:PRO:CG	3:C:1419:ARG:HD2	2.26	0.56
3:C:1543:ILE:HD12	3:C:1554:VAL:HG21	1.88	0.56
1:D:544:LYS:NZ	1:D:544:LYS:CD	2.66	0.56
1:A:6:ILE:CD1	1:A:20:MET:CE	2.83	0.56
1:A:255:ASP:HB2	1:A:300:LYS:HG2	1.88	0.56
2:E:907:LEU:HD12	2:E:907:LEU:H	1.70	0.56
1:A:69:PRO:CA	1:A:70:ALA:HB3	2.35	0.56
1:A:404:THR:HG21	1:A:415:ALA:N	2.20	0.56
1:A:487:GLU:H	1:A:490:GLN:NE2	2.04	0.56
2:B:837:GLU:HB2	2:B:867:PRO:HA	1.88	0.56
3:F:1338:LYS:HG3	3:F:1465:GLU:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:MET:HG3	1:A:483:ARG:CZ	2.36	0.55
1:D:470:TYR:C	1:D:471:LEU:HG	2.32	0.55
1:D:504:ILE:CG2	1:D:505:PRO:HA	2.35	0.55
1:D:147:ASN:HB2	1:D:148:PRO:CD	2.36	0.55
3:F:1335:THR:O	3:F:1335:THR:OG1	2.21	0.55
1:A:590:THR:HG23	7:A:724:HOH:O	2.06	0.55
3:C:1346:LYS:O	3:C:1362:MET:HB3	2.06	0.55
3:C:1525:THR:HB	3:C:1541:MET:HE3	1.88	0.55
1:A:400:ILE:HD13	1:A:419:MET:HE3	1.89	0.55
2:B:834:GLN:HE21	2:B:834:GLN:HA	1.72	0.55
1:D:6:ILE:HG13	1:D:20:MET:CE	2.37	0.55
2:B:858:ARG:CZ	3:C:1449:LEU:HD11	2.37	0.55
1:A:350:LEU:HD23	1:A:419:MET:HE2	1.88	0.55
1:A:409:LEU:O	1:A:410:SER:CB	2.44	0.55
1:A:444:ARG:NH2	1:A:534:LYS:HE2	2.21	0.55
1:A:504:ILE:HG23	1:A:505:PRO:HA	1.89	0.55
2:E:903:VAL:HG21	5:E:705:GOL:H11	1.88	0.55
3:C:1419:ARG:HD3	3:C:1422:LEU:HD13	1.89	0.55
3:C:1621:GLN:O	3:C:1625:GLN:HG3	2.07	0.54
3:F:1499:GLN:CG	3:F:1500:LYS:H	2.21	0.54
3:C:1499:GLN:CG	3:C:1500:LYS:H	2.20	0.54
1:D:128:PHE:HD1	2:E:787:MET:CE	2.19	0.54
1:D:160:SER:HB3	1:D:167:LEU:HD13	1.89	0.54
1:A:346:MET:O	1:A:391:THR:HB	2.07	0.54
3:F:1525:THR:HG23	3:F:1541:MET:SD	2.48	0.54
1:A:6:ILE:HD13	1:A:20:MET:CE	2.38	0.54
1:A:315:ASP:HA	5:A:703:GOL:C3	2.28	0.54
1:D:25:HIS:O	1:D:26:ASP:HB2	2.07	0.54
3:C:1370:TYR:HB2	3:C:1429:VAL:HG22	1.89	0.54
1:D:596:ASP:O	1:D:600:LYS:HG2	2.08	0.54
3:C:1506:THR:OG1	3:C:1509:GLU:HG2	2.06	0.54
1:D:504:ILE:HG23	1:D:505:PRO:HA	1.90	0.54
1:A:504:ILE:CG2	1:A:505:PRO:HA	2.38	0.53
3:C:1391:PRO:HG2	3:C:1419:ARG:CD	2.27	0.53
1:D:548:SER:O	1:D:549:GLU:HB2	2.06	0.53
3:F:1541:MET:HE3	3:F:1582:MET:SD	2.48	0.53
3:C:1504:LYS:O	3:C:1505:VAL:HG23	2.07	0.53
1:A:595:TRP:HD1	5:A:712:GOL:H12	1.72	0.53
3:C:1375:ASP:OD1	3:C:1431:HIS:HD2	1.91	0.53
3:F:1385:MET:HE2	3:F:1390:ALA:CA	2.39	0.53
1:A:487:GLU:H	1:A:490:GLN:HE21	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:GLN:HG3	7:A:795:HOH:O	2.09	0.53
3:C:1401:ASN:N	3:C:1401:ASN:HD22	2.05	0.53
2:E:834:GLN:HG3	7:E:577:HOH:O	2.08	0.53
1:A:20:MET:HE2	1:A:22:LEU:CD2	2.35	0.53
1:A:407:GLN:C	1:A:409:LEU:H	2.17	0.53
1:D:230:GLU:HG2	1:D:279:VAL:HG22	1.91	0.53
1:A:177:VAL:HG22	1:A:182:TRP:HZ2	1.73	0.53
3:C:1337:ASN:H	3:C:1337:ASN:ND2	2.04	0.53
1:D:37:VAL:N	1:D:47:LEU:O	2.32	0.53
1:D:103:LEU:HD22	1:D:103:LEU:N	2.23	0.53
1:D:407:GLN:O	1:D:408:GLU:HG2	2.08	0.53
1:A:69:PRO:HA	1:A:70:ALA:CB	2.38	0.53
1:A:248:PHE:HD1	3:C:1378:MET:HE2	1.69	0.53
3:C:1490:ARG:HD2	3:C:1590:TRP:CZ3	2.44	0.53
3:F:1634:MET:HE1	3:F:1639:CYS:SG	2.49	0.53
3:C:1344:THR:CG2	3:C:1346:LYS:HE2	2.38	0.52
1:D:58:THR:O	1:D:58:THR:CG2	2.57	0.52
1:D:554:VAL:HG12	1:D:557:GLN:HB2	1.91	0.52
1:A:248:PHE:CD1	3:C:1378:MET:CE	2.76	0.52
1:D:574:VAL:HG13	2:E:751:TRP:HE3	1.75	0.52
1:A:444:ARG:HH22	1:A:534:LYS:HE2	1.73	0.52
1:A:628:SER:HB2	1:A:630:GLN:OE1	2.10	0.52
3:C:1359:LYS:NZ	3:C:1446:ASN:CB	2.72	0.52
1:D:104:GLN:HE21	1:D:132:HIS:CE1	2.27	0.52
3:C:1381:LEU:HD21	3:C:1457:VAL:HG13	1.90	0.52
1:A:338:THR:CG2	1:A:419:MET:HE1	2.31	0.52
3:C:1462:ASN:HD22	3:C:1465:GLU:H	1.57	0.52
1:D:187:TYR:CD1	1:D:192:PRO:HA	2.44	0.52
1:A:469:THR:O	1:A:511:ALA:HA	2.10	0.52
1:D:3:MET:HE3	1:D:522:ARG:HD2	1.89	0.52
3:C:1344:THR:HG21	3:C:1346:LYS:HE2	1.91	0.52
1:D:157:SER:C	1:D:158:LEU:HG	2.35	0.52
1:A:187:TYR:CD1	1:A:192:PRO:HA	2.45	0.52
1:A:223:ILE:HD11	1:A:328:THR:HG22	1.90	0.52
3:C:1530:VAL:HG12	3:C:1532:LEU:HD13	1.92	0.52
3:F:1499:GLN:O	3:F:1500:LYS:HB3	2.08	0.51
3:C:1386:MET:HB3	3:C:1450:ILE:CD1	2.40	0.51
1:D:221:TYR:OH	1:D:282:ARG:HG3	2.10	0.51
3:C:1483:LEU:HD23	3:C:1599:ILE:CD1	2.40	0.51
1:D:104:GLN:HE21	1:D:132:HIS:HE1	1.57	0.51
1:D:372:GLU:OE1	1:D:372:GLU:HA	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1498:ILE:HG22	3:F:1499:GLN:HG3	1.93	0.51
1:A:19:THR:HG21	4:G:1:NDG:H8C1	1.91	0.51
2:E:746:PRO:CG	2:E:774:LYS:HG2	2.40	0.51
2:E:889:GLU:CG	2:E:904:ARG:HB3	2.39	0.51
1:A:149:GLU:OE2	1:D:363:TYR:OH	2.24	0.51
1:A:403:ARG:CA	1:A:404:THR:HG22	2.40	0.51
3:F:1525:THR:HG21	3:F:1541:MET:SD	2.50	0.51
3:F:1591:GLY:N	5:F:707:GOL:H31	2.15	0.51
1:A:160:SER:HA	1:A:167:LEU:HD21	1.91	0.51
1:D:591:GLN:NE2	2:E:795:VAL:H	2.08	0.51
2:E:822:GLN:NE2	3:F:1480:LEU:H	2.08	0.51
1:D:104:GLN:HG3	1:D:194:GLN:OE1	2.10	0.51
1:A:45:LEU:CG	1:A:48:SER:HB3	2.41	0.50
1:D:550:ASP:O	1:D:552:GLN:N	2.40	0.50
1:D:517:GLY:O	1:D:518:ALA:C	2.54	0.50
3:F:1537:ASP:OD2	3:F:1569:ARG:CG	2.60	0.50
3:C:1552:ASP:OD2	3:C:1560:ARG:HD2	2.12	0.50
1:A:128:PHE:HA	1:A:165:GLY:O	2.11	0.50
1:A:375:VAL:CG1	1:A:376:GLN:N	2.55	0.50
3:F:1606:VAL:O	5:F:710:GOL:H12	2.11	0.50
1:A:575:ALA:O	2:B:748:SER:HA	2.11	0.50
1:D:40:PHE:CD2	1:D:41:PRO:CD	2.95	0.50
3:F:1416:PHE:HZ	3:F:1442:HIS:HB2	1.77	0.50
3:C:1499:GLN:CG	3:C:1500:LYS:N	2.70	0.50
1:D:126:ARG:HA	1:D:167:LEU:O	2.12	0.50
1:A:133:LYS:O	1:A:134:LEU:HB2	2.11	0.50
1:A:547:GLN:OE1	1:A:559:MET:HB2	2.12	0.50
1:D:45:LEU:CD2	1:D:48:SER:OG	2.59	0.50
1:A:177:VAL:HG22	1:A:182:TRP:CZ2	2.47	0.49
2:B:819:ARG:HH11	2:B:819:ARG:HG2	1.76	0.49
3:C:1386:MET:HB3	3:C:1450:ILE:HD13	1.93	0.49
1:D:592:SER:CB	5:D:711:GOL:H11	2.43	0.49
2:B:841:ARG:HD2	5:B:701:GOL:O2	2.13	0.49
1:A:260:ILE:HD12	2:E:762:ASN:CG	2.37	0.49
3:C:1582:MET:HA	3:C:1605:TRP:O	2.12	0.49
2:E:737:GLU:CD	2:E:737:GLU:H	2.20	0.49
1:A:407:GLN:O	1:A:409:LEU:N	2.46	0.49
1:D:211:GLU:HB3	1:D:582:VAL:HG22	1.95	0.49
3:C:1344:THR:HG22	7:C:505:HOH:O	2.13	0.49
3:C:1362:MET:HE1	3:C:1473:PRO:CG	2.38	0.49
1:D:595:TRP:HD1	5:D:711:GOL:H31	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLN:HG3	1:A:401:THR:HB	1.92	0.49
1:A:375:VAL:O	1:A:376:GLN:HB2	2.12	0.49
3:F:1504:LYS:O	3:F:1505:VAL:HB	2.13	0.49
1:D:558:GLN:HB3	2:E:772:PHE:CE2	2.47	0.48
1:A:332:GLN:HE21	1:A:357:PRO:HA	1.78	0.48
1:A:595:TRP:CD1	5:A:712:GOL:H12	2.48	0.48
1:D:375:VAL:CG2	1:D:376:GLN:N	2.58	0.48
1:A:47:LEU:CD2	1:A:66:PHE:HB2	2.43	0.48
3:C:1359:LYS:HZ3	3:C:1446:ASN:HB2	1.78	0.48
3:C:1509:GLU:HB2	7:C:494:HOH:O	2.12	0.48
1:D:36:THR:HG22	1:D:48:SER:HA	1.95	0.48
1:A:599:GLU:HG3	7:A:690:HOH:O	2.13	0.48
3:C:1609:TRP:CG	3:C:1627:LEU:HD13	2.49	0.48
3:F:1393:THR:CG2	3:F:1419:ARG:HH12	2.25	0.48
1:A:6:ILE:HD13	1:A:22:LEU:HD23	1.94	0.48
1:A:183:LYS:HD3	1:A:197:SER:HB3	1.94	0.48
1:D:6:ILE:CD1	1:D:7:ILE:N	2.76	0.48
1:A:55:THR:HG22	1:A:58:THR:H	1.79	0.48
1:A:346:MET:HE3	1:A:456:ARG:HB2	1.96	0.48
3:C:1504:LYS:O	3:C:1505:VAL:CG2	2.62	0.48
1:D:241:LYS:HG3	2:E:832:TYR:CE1	2.49	0.48
1:D:350:LEU:HD21	1:D:400:ILE:HG12	1.94	0.48
1:A:63:ASN:O	1:A:64:VAL:HG22	2.14	0.48
1:D:47:LEU:HD11	1:D:66:PHE:HB2	1.95	0.48
1:D:177:VAL:CG2	1:D:182:TRP:CZ2	2.97	0.48
1:D:193:GLN:CD	1:D:193:GLN:H	2.22	0.48
3:F:1497:PHE:HA	3:F:1601:GLY:O	2.14	0.48
3:F:1532:LEU:HD22	3:F:1569:ARG:HD3	1.95	0.48
1:D:249:VAL:HG11	1:D:278:VAL:HG11	1.96	0.47
1:D:595:TRP:HD1	5:D:711:GOL:C3	2.27	0.47
1:A:341:TYR:HA	1:A:422:LEU:O	2.14	0.47
1:A:364:ARG:HG2	1:A:364:ARG:HH11	1.79	0.47
3:C:1555:GLN:HB2	3:C:1558:GLN:NE2	2.29	0.47
1:A:606:THR:HG22	1:A:608:GLY:N	2.24	0.47
3:F:1572:LEU:HB3	3:F:1574:LEU:HG	1.95	0.47
1:A:477:ARG:CG	1:A:477:ARG:NH1	2.60	0.47
1:D:215:GLU:HG2	7:D:712:HOH:O	2.14	0.47
1:A:532:ASP:OD1	7:A:812:HOH:O	2.20	0.47
2:B:731:GLU:CD	2:B:731:GLU:H	2.20	0.47
3:C:1497:PHE:HA	3:C:1601:GLY:O	2.15	0.47
1:A:432:ASN:CG	1:A:457:MET:HE2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:VAL:HG13	1:D:54:LEU:HB2	1.96	0.47
3:F:1547:ILE:HG12	3:F:1631:THR:HG23	1.96	0.47
1:D:183:LYS:HD2	1:D:185:ARG:CZ	2.44	0.47
1:A:330:PRO:O	1:A:357:PRO:HD3	2.15	0.46
1:D:279:VAL:HG12	1:D:280:LEU:C	2.40	0.46
1:D:547:GLN:HE21	1:D:547:GLN:N	2.13	0.46
3:C:1465:GLU:O	3:C:1465:GLU:CG	2.60	0.46
1:A:3:MET:HG3	1:A:628:SER:OG	2.15	0.46
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.50	0.46
1:D:126:ARG:HD2	2:E:751:TRP:CZ2	2.50	0.46
1:A:6:ILE:CG1	1:A:20:MET:SD	3.02	0.46
1:A:182:TRP:CD1	1:A:202:VAL:HG23	2.51	0.46
3:F:1335:THR:O	3:F:1336:CYS:C	2.57	0.46
3:F:1385:MET:HE1	3:F:1441:VAL:CG1	2.46	0.46
1:A:45:LEU:HG	1:A:48:SER:HB3	1.98	0.46
1:A:590:THR:HG22	1:A:593:LYS:H	1.81	0.46
1:D:59:ASN:O	1:D:483:ARG:NH2	2.49	0.46
1:D:509:LEU:C	1:D:509:LEU:CD1	2.88	0.46
1:D:20:MET:HE1	1:D:86:VAL:HG12	1.96	0.46
1:D:369:VAL:O	1:D:372:GLU:HG2	2.16	0.46
3:F:1499:GLN:O	3:F:1500:LYS:CB	2.63	0.46
1:D:34:THR:O	1:D:34:THR:HG22	2.15	0.46
1:D:465:ILE:HD12	1:D:513:TYR:CD1	2.49	0.46
2:E:758:GLU:CD	2:E:758:GLU:H	2.24	0.46
2:E:833:ARG:O	2:E:834:GLN:C	2.59	0.46
1:A:20:MET:CE	1:A:22:LEU:HD21	2.38	0.46
3:C:1579:HIS:HD2	3:C:1611:GLU:OE1	1.99	0.46
1:A:6:ILE:HD13	1:A:20:MET:CG	2.35	0.45
1:A:45:LEU:HD21	1:A:48:SER:HB3	1.98	0.45
1:D:46:VAL:HG12	1:D:69:PRO:HD2	1.97	0.45
1:A:11:ILE:HG12	1:A:100:LEU:HD23	1.98	0.45
2:B:841:ARG:CD	5:B:701:GOL:O2	2.64	0.45
1:D:304:VAL:HG13	1:D:321:ARG:HB3	1.98	0.45
1:D:567:HIS:CE1	2:E:760:PRO:HD3	2.51	0.45
1:A:407:GLN:C	1:A:408:GLU:HG3	2.41	0.45
2:E:877:VAL:HG13	3:F:1451:GLN:CD	2.41	0.45
3:F:1420:ASN:OD1	3:F:1421:THR:HG23	2.17	0.45
3:F:1554:VAL:HG13	3:F:1560:ARG:HE	1.81	0.45
3:C:1462:ASN:ND2	3:C:1465:GLU:H	2.13	0.45
3:F:1589:PHE:HE1	3:F:1598:TYR:CE2	2.34	0.45
1:A:3:MET:CE	1:A:630:GLN:OE1	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1437:LEU:HD12	3:C:1437:LEU:C	2.41	0.45
1:D:10:ASN:HD22	1:D:10:ASN:HA	1.59	0.45
1:A:50:GLU:HB3	1:A:64:VAL:HB	1.99	0.45
1:A:338:THR:HG23	1:A:350:LEU:HA	1.98	0.45
1:D:145:ILE:HG12	1:D:184:ILE:HG12	1.99	0.45
2:E:823:VAL:HG23	2:E:878:ILE:HG23	1.99	0.45
2:B:742:ARG:HB3	2:B:775:ASP:HB3	1.99	0.45
1:A:110:ILE:HB	1:A:198:THR:OG1	2.16	0.45
1:D:116:ILE:HD11	1:D:203:LYS:HD2	1.99	0.45
1:D:126:ARG:HD2	2:E:751:TRP:CH2	2.52	0.45
1:D:574:VAL:HG13	2:E:751:TRP:CE3	2.52	0.45
2:E:732:ASP:OD1	2:E:896:HIS:HA	2.15	0.45
3:F:1501:SER:HB2	3:F:1503:ASP:O	2.17	0.45
1:A:2:PRO:HA	1:A:25:HIS:O	2.17	0.45
1:A:641:PRO:O	1:A:642:GLN:HB2	2.15	0.45
1:A:40:PHE:HA	1:A:41:PRO:HA	1.72	0.45
1:A:184:ILE:O	1:A:197:SER:HA	2.17	0.45
3:F:1499:GLN:HG3	3:F:1500:LYS:H	1.81	0.45
1:A:147:ASN:CB	1:A:148:PRO:CD	2.94	0.44
1:D:516:ILE:HD11	1:D:520:GLY:HA2	1.97	0.44
3:F:1393:THR:HG23	3:F:1419:ARG:HH12	1.81	0.44
1:A:3:MET:SD	1:A:626:SER:HB2	2.57	0.44
2:B:746:PRO:CG	2:B:774:LYS:HG3	2.47	0.44
2:B:819:ARG:NH1	2:B:819:ARG:HG2	2.33	0.44
3:F:1497:PHE:HB2	3:F:1604:THR:O	2.17	0.44
1:A:55:THR:CG2	1:A:57:ALA:H	2.31	0.44
1:A:368:ALA:N	1:A:403:ARG:O	2.40	0.44
3:C:1472:HIS:CE1	3:C:1474:GLU:HG2	2.53	0.44
1:D:50:GLU:HA	1:D:50:GLU:OE1	2.17	0.44
1:A:61:MET:HE3	1:A:61:MET:HB3	1.68	0.44
1:A:422:LEU:HB3	1:A:423:PRO:HD2	2.00	0.44
3:C:1415:ALA:C	3:C:1417:SER:N	2.74	0.44
1:D:20:MET:HE1	1:D:86:VAL:CG1	2.39	0.44
2:E:851:CYS:HB3	2:E:879:VAL:HB	2.00	0.44
2:B:830:TYR:CD1	2:B:871:SER:HB3	2.53	0.44
3:C:1503:ASP:O	3:C:1504:LYS:HB3	2.18	0.44
1:D:49:SER:HB2	1:D:50:GLU:OE2	2.17	0.44
1:D:142:MET:HG3	1:D:187:TYR:CE1	2.53	0.44
3:C:1504:LYS:HG2	3:C:1505:VAL:N	2.32	0.43
2:E:806:ASP:HB3	2:E:833:ARG:HG2	2.00	0.43
3:F:1617:ASP:O	3:F:1619:GLU:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:ILE:HA	7:A:757:HOH:O	2.17	0.43
3:C:1415:ALA:CB	3:C:1417:SER:H	2.31	0.43
1:D:143:VAL:HG11	1:D:169:LEU:HD11	2.00	0.43
1:D:148:PRO:HD3	1:D:182:TRP:CE2	2.53	0.43
1:D:546:GLY:HA3	1:D:560:THR:HG22	2.01	0.43
1:D:575:ALA:O	2:E:748:SER:HA	2.18	0.43
3:C:1343:VAL:HG21	3:C:1455:VAL:HB	2.00	0.43
2:E:817:VAL:HG22	2:E:907:LEU:HD22	2.01	0.43
1:D:236:ARG:HH12	1:D:240:GLY:HA2	1.83	0.43
3:F:1485:ARG:HD2	5:F:707:GOL:O3	2.18	0.43
4:G:1:NDG:H6C1	4:G:2:NDG:C7	2.48	0.43
1:A:160:SER:CA	1:A:167:LEU:HD21	2.49	0.43
1:D:39:ASP:N	1:D:39:ASP:OD1	2.51	0.43
1:D:154:LYS:HD2	1:D:171:TRP:CD1	2.54	0.43
1:D:292:LEU:H	1:D:292:LEU:HD22	1.63	0.43
1:A:50:GLU:OE2	1:A:50:GLU:HA	2.18	0.43
1:A:177:VAL:CG2	1:A:182:TRP:CZ2	3.02	0.43
1:A:407:GLN:C	1:A:409:LEU:N	2.77	0.43
1:D:14:LEU:HD21	1:D:101:VAL:HG11	1.99	0.43
1:D:234:THR:HA	1:D:274:GLY:O	2.18	0.43
1:A:10:ASN:HB3	1:A:635:ARG:HD3	2.00	0.43
1:A:21:VAL:HG23	1:A:478:LEU:HD13	2.01	0.43
1:A:443:LEU:HD11	1:A:449:LEU:HD22	2.00	0.43
1:D:160:SER:CB	1:D:167:LEU:CD1	2.85	0.43
1:D:473:MET:HE3	1:D:473:MET:HB2	1.91	0.43
1:A:241:LYS:HG3	2:B:832:TYR:CE2	2.54	0.43
1:A:151:ILE:HA	1:A:152:PRO:HD3	1.93	0.43
3:C:1472:HIS:HB3	3:C:1475:LYS:HB2	2.00	0.43
1:D:427:VAL:HG12	1:D:521:GLN:NE2	2.34	0.43
1:A:432:ASN:OD1	1:A:457:MET:CB	2.67	0.42
1:D:89:THR:HB	1:D:94:VAL:HG22	2.02	0.42
2:E:907:LEU:HD12	2:E:907:LEU:N	2.32	0.42
3:C:1387:THR:CG2	3:C:1451:GLN:N	2.72	0.42
1:D:126:ARG:CZ	1:D:572:VAL:HB	2.49	0.42
1:A:24:ALA:HB3	1:A:60:HIS:HB3	2.01	0.42
1:A:552:GLN:HA	1:A:553:PRO:HD2	1.86	0.42
3:C:1359:LYS:HZ2	3:C:1446:ASN:HB2	1.84	0.42
1:D:6:ILE:HG13	1:D:20:MET:SD	2.57	0.42
3:C:1414:LYS:HB3	3:C:1415:ALA:H	1.76	0.42
3:F:1379:SER:C	3:F:1380:ILE:HD12	2.44	0.42
1:A:127:ILE:CD1	1:A:169:LEU:HD12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:739:ILE:HB	2:E:891:LYS:HD3	2.01	0.42
2:E:742:ARG:HB3	2:E:775:ASP:HB3	2.02	0.42
1:A:105:SER:O	1:A:131:ASN:HA	2.20	0.42
1:D:128:PHE:HB3	2:E:787:MET:HE1	2.00	0.42
1:D:177:VAL:CG2	1:D:182:TRP:HZ2	2.32	0.42
1:D:469:THR:O	1:D:511:ALA:HA	2.19	0.42
1:A:6:ILE:CG1	1:A:20:MET:CE	2.83	0.42
1:A:214:VAL:O	1:A:214:VAL:CG2	2.68	0.42
1:A:342:PHE:HD1	1:A:391:THR:HG21	1.83	0.42
1:A:390:ASN:HD22	1:A:391:THR:H	1.66	0.42
5:E:705:GOL:H32	7:E:510:HOH:O	2.20	0.42
1:A:128:PHE:HD1	2:B:787:MET:HE2	1.85	0.42
1:A:191:SER:HA	1:A:193:GLN:NE2	2.28	0.42
1:A:307:THR:OG1	1:A:318:GLN:NE2	2.47	0.42
3:C:1387:THR:HG21	3:C:1451:GLN:H	1.79	0.42
2:E:746:PRO:CD	2:E:774:LYS:HG2	2.50	0.42
3:F:1566:ILE:C	3:F:1568:CYS:H	2.28	0.42
1:A:114:LYS:NZ	7:A:718:HOH:O	2.45	0.41
1:A:465:ILE:HD12	1:A:513:TYR:CD1	2.55	0.41
3:C:1504:LYS:CG	3:C:1506:THR:HG23	2.50	0.41
1:D:3:MET:HE2	1:D:630:GLN:OE1	2.20	0.41
1:A:146:GLU:OE1	1:A:185:ARG:HD3	2.20	0.41
1:A:392:HIS:HA	1:A:393:PRO:HD3	1.91	0.41
1:D:236:ARG:NH1	1:D:240:GLY:HA2	2.35	0.41
1:A:221:TYR:O	1:A:326:ILE:HA	2.20	0.41
1:A:345:GLY:O	1:A:456:ARG:NH2	2.53	0.41
1:A:406:LYS:C	1:A:407:GLN:O	2.61	0.41
3:C:1341:LEU:HD22	3:C:1457:VAL:CG2	2.43	0.41
1:D:10:ASN:HB3	1:D:635:ARG:HD3	2.02	0.41
1:D:432:ASN:CG	1:D:457:MET:HE3	2.45	0.41
2:E:787:MET:HE2	2:E:787:MET:HB2	1.81	0.41
1:D:63:ASN:O	1:D:64:VAL:HG22	2.20	0.41
1:D:142:MET:O	1:D:186:ALA:HA	2.20	0.41
2:E:866:ILE:HA	2:E:867:PRO:HD2	1.90	0.41
1:A:154:LYS:HD2	1:A:171:TRP:HD1	1.81	0.41
1:A:223:ILE:HG12	1:A:298:VAL:HG22	2.02	0.41
2:B:897:HIS:HD1	2:B:897:HIS:N	2.17	0.41
3:C:1387:THR:HG23	3:C:1451:GLN:N	2.34	0.41
3:C:1412:LEU:HD12	3:C:1412:LEU:HA	1.89	0.41
1:D:49:SER:CB	1:D:50:GLU:OE2	2.68	0.41
1:A:39:ASP:OD1	1:A:44:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:LEU:CD1	1:A:509:LEU:C	2.93	0.41
1:D:147:ASN:HB2	1:D:148:PRO:HD2	2.01	0.41
2:E:753:VAL:C	2:E:754:GLU:HG2	2.45	0.41
3:F:1336:CYS:HB3	3:F:1467:CYS:HB2	1.89	0.41
3:C:1576:GLU:O	3:C:1577:LYS:HB2	2.21	0.41
1:D:241:LYS:HA	1:D:241:LYS:HD3	1.88	0.41
1:D:346:MET:HE3	1:D:456:ARG:HB2	2.02	0.41
1:A:148:PRO:HD3	1:A:182:TRP:CE2	2.55	0.41
1:A:164:LEU:O	2:B:787:MET:HG2	2.21	0.41
1:A:592:SER:HB2	7:A:724:HOH:O	2.20	0.41
2:B:837:GLU:CB	2:B:868:PRO:HD3	2.44	0.41
1:D:114:LYS:HE3	1:D:117:TYR:CE1	2.56	0.41
1:D:362:ALA:O	1:D:383:GLY:HA2	2.20	0.41
3:F:1385:MET:CE	3:F:1389:PHE:HB3	2.52	0.41
1:A:10:ASN:HD22	1:A:10:ASN:HA	1.69	0.40
1:D:459:ARG:H	1:D:459:ARG:HG2	1.62	0.40
1:A:15:GLU:CG	1:A:70:ALA:HB2	2.52	0.40
1:A:47:LEU:HD21	1:A:50:GLU:CG	2.48	0.40
3:C:1337:ASN:ND2	3:C:1337:ASN:N	2.67	0.40
1:D:128:PHE:CD1	2:E:787:MET:HE1	2.56	0.40
2:E:850:PHE:CE1	2:E:878:ILE:HD11	2.56	0.40
3:F:1377:THR:HB	3:F:1378:MET:H	1.70	0.40
2:B:889:GLU:OE2	2:B:891:LYS:HE3	2.22	0.40
3:C:1525:THR:HB	3:C:1541:MET:HE2	1.82	0.40
1:A:45:LEU:HD21	1:A:48:SER:CB	2.50	0.40
3:C:1450:ILE:O	3:C:1450:ILE:HG13	2.22	0.40
1:D:31:VAL:HA	1:D:32:PRO:HD2	1.98	0.40
1:D:42:GLY:O	1:D:43:LYS:HG3	2.22	0.40
3:F:1560:ARG:HD3	3:F:1560:ARG:HA	1.92	0.40
3:C:1403:VAL:HA	7:C:499:HOH:O	2.21	0.40
3:C:1541:MET:O	3:C:1559:GLN:HA	2.21	0.40
1:D:45:LEU:HG	1:D:48:SER:OG	2.21	0.40
1:D:343:LYS:HD2	1:D:343:LYS:N	2.36	0.40
3:F:1380:ILE:HG23	3:F:1423:ILE:HG23	2.04	0.40
3:F:1380:ILE:O	3:F:1457:VAL:HA	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	624/643 (97%)	582 (93%)	27 (4%)	15 (2%)	4	5
1	D	629/643 (98%)	593 (94%)	21 (3%)	15 (2%)	4	5
2	B	181/188 (96%)	172 (95%)	8 (4%)	1 (1%)	21	32
2	E	182/188 (97%)	167 (92%)	13 (7%)	2 (1%)	11	18
3	C	290/343 (84%)	270 (93%)	9 (3%)	11 (4%)	2	2
3	F	294/343 (86%)	274 (93%)	11 (4%)	9 (3%)	3	3
All	All	2200/2348 (94%)	2058 (94%)	89 (4%)	53 (2%)	4	5

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	SER
1	A	550	ASP
3	C	1361	THR
1	D	41	PRO
1	D	372	GLU
1	D	549	GLU
1	D	550	ASP
2	E	834	GLN
3	F	1336	CYS
3	F	1500	LYS
1	A	91	GLY
1	A	375	VAL
1	A	518	ALA
2	B	732	ASP
3	C	1414	LYS
3	C	1504	LYS
3	C	1505	VAL
1	D	50	GLU
1	D	64	VAL
1	D	256	GLY

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Mol	Chain	Res	Type
1	D	375	VAL
1	D	518	ALA
1	D	551	ARG
1	D	609	SER
2	E	833	ARG
3	F	1449	LEU
3	F	1499	GLN
3	F	1618	GLU
3	F	1619	GLU
1	A	50	GLU
1	A	64	VAL
1	A	372	GLU
1	A	404	THR
1	A	407	GLN
1	A	548	SER
1	A	549	GLU
3	C	1477	ASP
3	C	1499	GLN
3	C	1619	GLU
1	D	410	SER
1	D	376	GLN
3	F	1504	LYS
3	F	1505	VAL
1	A	81	ASN
1	A	609	SER
3	C	1416	PHE
3	C	1417	SER
3	C	1573	LYS
3	C	1618	GLU
1	D	552	GLN
3	F	1377	THR
1	A	376	GLN
1	D	91	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	555/567 (98%)	483 (87%)	72 (13%)	4	5
1	D	558/567 (98%)	479 (86%)	79 (14%)	3	4
2	B	171/175 (98%)	153 (90%)	18 (10%)	6	10
2	E	171/175 (98%)	152 (89%)	19 (11%)	6	9
3	C	270/309 (87%)	228 (84%)	42 (16%)	2	3
3	F	272/309 (88%)	239 (88%)	33 (12%)	5	7
All	All	1997/2102 (95%)	1734 (87%)	263 (13%)	4	5

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

Mol	Chain	Res	Type
1	A	3	MET
1	A	10	ASN
1	A	15	GLU
1	A	31	VAL
1	A	36	THR
1	A	45	LEU
1	A	46	VAL
1	A	47	LEU
1	A	50	GLU
1	A	51	LYS
1	A	55	THR
1	A	61	MET
1	A	64	VAL
1	A	92	THR
1	A	94	VAL
1	A	137	VAL
1	A	155	GLN
1	A	163	GLN
1	A	179	MET
1	A	183	LYS
1	A	191	SER
1	A	193	GLN
1	A	207	LEU
1	A	214	VAL
1	A	223	ILE
1	A	227	LYS
1	A	236	ARG
1	A	249	VAL
1	A	275	SER
1	A	277	GLU

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Mol	Chain	Res	Type
1	A	283	LYS
1	A	289	VAL
1	A	293	ARG
1	A	304	VAL
1	A	311	HIS
1	A	316	MET
1	A	350	LEU
1	A	364	ARG
1	A	372	GLU
1	A	379	THR
1	A	386	LYS
1	A	389	ILE
1	A	390	ASN
1	A	391	THR
1	A	396	LYS
1	A	398	LEU
1	A	408	GLU
1	A	409	LEU
1	A	410	SER
1	A	417	ARG
1	A	438	VAL
1	A	444	ARG
1	A	448	THR
1	A	456	ARG
1	A	477	ARG
1	A	487	GLU
1	A	509	LEU
1	A	510	VAL
1	A	516	ILE
1	A	521	GLN
1	A	529	VAL
1	A	544	LYS
1	A	547	GLN
1	A	550	ASP
1	A	554	VAL
1	A	583	LEU
1	A	590	THR
1	A	592	SER
1	A	606	THR
1	A	628	SER
1	A	637	GLU
1	A	639	GLN

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Mol	Chain	Res	Type
2	B	731	GLU
2	B	752	ASN
2	B	804	MET
2	B	812	ARG
2	B	813	LEU
2	B	819	ARG
2	B	826	ARG
2	B	834	GLN
2	B	841	ARG
2	B	870	SER
2	B	872	LEU
2	B	877	VAL
2	B	890	VAL
2	B	894	VAL
2	B	897	HIS
2	B	907	LEU
2	B	910	VAL
2	B	912	GLU
3	C	1335	THR
3	C	1337	ASN
3	C	1342	LYS
3	C	1344	THR
3	C	1361	THR
3	C	1387	THR
3	C	1393	THR
3	C	1397	LYS
3	C	1401	ASN
3	C	1411	GLU
3	C	1412	LEU
3	C	1414	LYS
3	C	1416	PHE
3	C	1418	ASP
3	C	1428	LYS
3	C	1429	VAL
3	C	1432	SER
3	C	1433	GLU
3	C	1440	LYS
3	C	1450	ILE
3	C	1457	VAL
3	C	1462	ASN
3	C	1469	ARG
3	C	1474	GLU

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Mol	Chain	Res	Type
3	C	1483	LEU
3	C	1503	ASP
3	C	1504	LYS
3	C	1505	VAL
3	C	1507	LEU
3	C	1509	GLU
3	C	1532	LEU
3	C	1551	SER
3	C	1555	GLN
3	C	1558	GLN
3	C	1560	ARG
3	C	1566	ILE
3	C	1573	LYS
3	C	1599	ILE
3	C	1602	LYS
3	C	1611	GLU
3	C	1619	GLU
3	C	1623	GLN
1	D	3	MET
1	D	6	ILE
1	D	10	ASN
1	D	20	MET
1	D	31	VAL
1	D	34	THR
1	D	46	VAL
1	D	47	LEU
1	D	50	GLU
1	D	51	LYS
1	D	52	THR
1	D	63	ASN
1	D	64	VAL
1	D	81	ASN
1	D	82	LYS
1	D	87	GLN
1	D	89	THR
1	D	98	VAL
1	D	103	LEU
1	D	126	ARG
1	D	133	LYS
1	D	140	THR
1	D	153	VAL
1	D	155	GLN

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Mol	Chain	Res	Type
1	D	158	LEU
1	D	189	GLU
1	D	191	SER
1	D	194	GLN
1	D	213	ILE
1	D	217	THR
1	D	232	THR
1	D	234	THR
1	D	236	ARG
1	D	260	ILE
1	D	292	LEU
1	D	297	LEU
1	D	302	LEU
1	D	304	VAL
1	D	316	MET
1	D	352	VAL
1	D	364	ARG
1	D	372	GLU
1	D	373	ASP
1	D	375	VAL
1	D	376	GLN
1	D	378	LEU
1	D	384	VAL
1	D	389	ILE
1	D	396	LYS
1	D	400	ILE
1	D	404	THR
1	D	407	GLN
1	D	408	GLU
1	D	410	SER
1	D	411	GLU
1	D	425	SER
1	D	437	SER
1	D	440	ARG
1	D	441	THR
1	D	443	LEU
1	D	459	ARG
1	D	471	LEU
1	D	473	MET
1	D	477	ARG
1	D	483	ARG
1	D	492	LEU

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Mol	Chain	Res	Type
1	D	509	LEU
1	D	510	VAL
1	D	516	ILE
1	D	529	VAL
1	D	547	GLN
1	D	549	GLU
1	D	550	ASP
1	D	551	ARG
1	D	554	VAL
1	D	564	GLU
1	D	574	VAL
1	D	592	SER
1	D	639	GLN
2	E	731	GLU
2	E	753	VAL
2	E	757	LYS
2	E	761	LYS
2	E	764	ILE
2	E	778	THR
2	E	795	VAL
2	E	833	ARG
2	E	834	GLN
2	E	838	LEU
2	E	839	LYS
2	E	840	VAL
2	E	842	VAL
2	E	865	THR
2	E	872	LEU
2	E	877	VAL
2	E	878	ILE
2	E	894	VAL
2	E	907	LEU
3	F	1335	THR
3	F	1336	CYS
3	F	1342	LYS
3	F	1359	LYS
3	F	1360	ASN
3	F	1369	ARG
3	F	1374	GLN
3	F	1377	THR
3	F	1393	THR
3	F	1411	GLU

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Mol	Chain	Res	Type
3	F	1423	ILE
3	F	1449	LEU
3	F	1450	ILE
3	F	1464	GLU
3	F	1476	GLU
3	F	1487	GLU
3	F	1499	GLN
3	F	1504	LYS
3	F	1506	THR
3	F	1507	LEU
3	F	1511	LEU
3	F	1525	THR
3	F	1528	VAL
3	F	1545	GLN
3	F	1553	GLU
3	F	1554	VAL
3	F	1555	GLN
3	F	1566	ILE
3	F	1570	GLU
3	F	1585	LEU
3	F	1602	LYS
3	F	1619	GLU
3	F	1634	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	38	HIS
1	A	60	HIS
1	A	87	GLN
1	A	104	GLN
1	A	181	GLN
1	A	193	GLN
1	A	318	GLN
1	A	332	GLN
1	A	334	HIS
1	A	390	ASN
1	A	490	GLN
1	A	567	HIS
1	A	587	ASN
1	A	639	GLN

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Mol	Chain	Res	Type
1	A	642	GLN
2	B	738	ASN
2	B	752	ASN
2	B	805	GLN
2	B	820	ASN
2	B	834	GLN
2	B	836	GLN
2	B	846	HIS
2	B	861	GLN
2	B	862	GLN
3	C	1337	ASN
3	C	1401	ASN
3	C	1431	HIS
3	C	1451	GLN
3	C	1462	ASN
3	C	1531	GLN
3	C	1534	ASN
3	C	1555	GLN
3	C	1579	HIS
3	C	1616	GLN
3	C	1620	ASN
1	D	10	ASN
1	D	38	HIS
1	D	81	ASN
1	D	104	GLN
1	D	132	HIS
1	D	144	ASN
1	D	155	GLN
1	D	163	GLN
1	D	190	ASN
1	D	291	ASN
1	D	318	GLN
1	D	356	ASN
1	D	376	GLN
1	D	521	GLN
1	D	547	GLN
1	D	558	GLN
1	D	591	GLN
2	E	738	ASN
2	E	770	ASN
2	E	805	GLN
2	E	822	GLN

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Mol	Chain	Res	Type
2	E	834	GLN
2	E	846	HIS
2	E	897	HIS
3	F	1337	ASN
3	F	1401	ASN
3	F	1431	HIS
3	F	1462	ASN
3	F	1616	GLN
3	F	1620	ASN
3	F	1641	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
4	NDG	G	1	4	14,14,15	0.60	0	17,19,21	0.66	0
4	NDG	G	2	4	14,14,15	0.54	0	17,19,21	0.76	0
4	NDG	H	1	4	14,14,15	0.55	0	17,19,21	1.07	1 (5%)
4	NDG	H	2	4	14,14,15	0.92	1 (7%)	17,19,21	0.72	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	NDG	G	1	4	-	0/6/23/26	0/1/1/1
4	NDG	G	2	4	1/1/5/7	2/6/23/26	0/1/1/1
4	NDG	H	1	4	-	2/6/23/26	0/1/1/1
4	NDG	H	2	4	1/1/5/7	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	NDG	C1-C2	-2.91	1.48	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NDG	O4-C4-C5	2.71	116.00	109.32

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	2	NDG	C1
4	H	2	NDG	C1

All (8) torsion outliers are listed below:

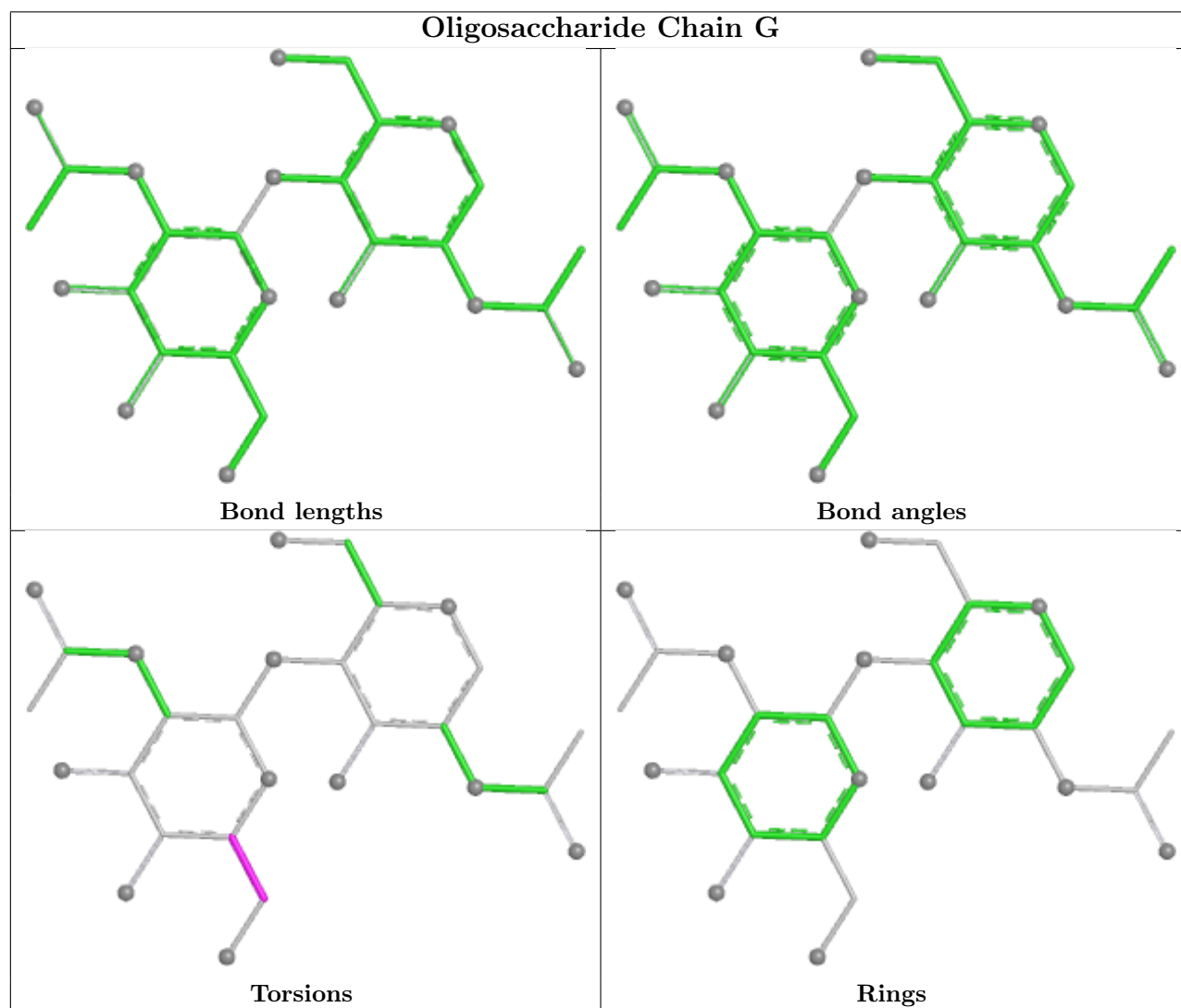
Mol	Chain	Res	Type	Atoms
4	H	2	NDG	C8-C7-N2-C2
4	H	2	NDG	O7-C7-N2-C2
4	G	2	NDG	O5-C5-C6-O6
4	H	1	NDG	O5-C5-C6-O6
4	H	2	NDG	O5-C5-C6-O6
4	H	1	NDG	C4-C5-C6-O6
4	H	2	NDG	C4-C5-C6-O6
4	G	2	NDG	C4-C5-C6-O6

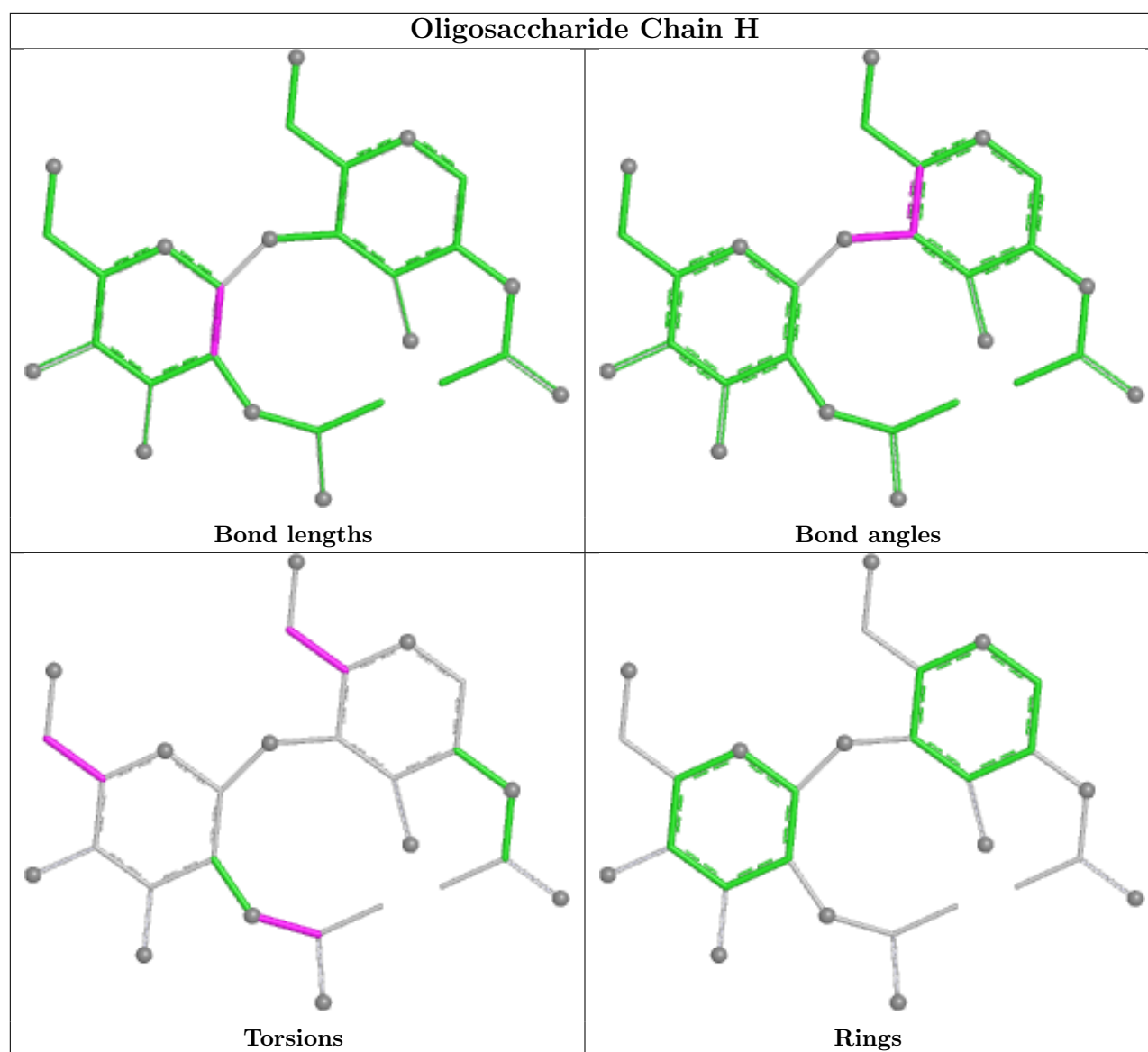
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NDG	1	0
4	G	1	NDG	2	0
4	G	2	NDG	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](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	E	705	-	5,5,5	0.38	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	E	706	-	5,5,5	0.38	0	5,5,5	0.50	0
5	GOL	A	703	-	5,5,5	0.35	0	5,5,5	0.23	0
5	GOL	E	704	-	5,5,5	0.43	0	5,5,5	0.50	0
5	GOL	C	708	-	5,5,5	0.31	0	5,5,5	0.44	0
5	GOL	B	701	-	5,5,5	0.40	0	5,5,5	0.54	0
5	GOL	F	710	-	5,5,5	0.36	0	5,5,5	0.25	0
5	GOL	B	702	-	5,5,5	0.41	0	5,5,5	0.24	0
5	GOL	F	707	-	5,5,5	0.38	0	5,5,5	0.29	0
5	GOL	A	712	-	5,5,5	0.33	0	5,5,5	0.43	0
5	GOL	A	713	-	5,5,5	0.44	0	5,5,5	0.40	0
6	NO3	F	802	-	1,3,3	3.33	1 (100%)	0,3,3	-	-
6	NO3	F	803	-	1,3,3	3.26	1 (100%)	0,3,3	-	-
5	GOL	D	711	-	5,5,5	0.39	0	5,5,5	0.39	0
6	NO3	C	801	-	1,3,3	3.33	1 (100%)	0,3,3	-	-
5	GOL	C	709	-	5,5,5	0.32	0	5,5,5	0.45	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	E	705	-	-	2/4/4/4	-
5	GOL	E	706	-	-	2/4/4/4	-
5	GOL	A	703	-	-	2/4/4/4	-
5	GOL	E	704	-	-	1/4/4/4	-
5	GOL	C	708	-	-	2/4/4/4	-
5	GOL	B	701	-	-	4/4/4/4	-
5	GOL	F	710	-	-	3/4/4/4	-
5	GOL	B	702	-	-	3/4/4/4	-
5	GOL	F	707	-	-	3/4/4/4	-
5	GOL	A	712	-	-	0/4/4/4	-
5	GOL	A	713	-	-	1/4/4/4	-
5	GOL	D	711	-	-	0/4/4/4	-
5	GOL	C	709	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	801	NO3	O1-N	3.33	1.40	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	802	NO3	O1-N	3.33	1.40	1.24
6	F	803	NO3	O1-N	3.26	1.40	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	703	GOL	C1-C2-C3-O3
5	B	701	GOL	O1-C1-C2-C3
5	B	701	GOL	C1-C2-C3-O3
5	B	701	GOL	O2-C2-C3-O3
5	B	702	GOL	O1-C1-C2-C3
5	C	708	GOL	C1-C2-C3-O3
5	E	705	GOL	O1-C1-C2-C3
5	F	707	GOL	O1-C1-C2-C3
5	F	710	GOL	O1-C1-C2-C3
5	B	702	GOL	O1-C1-C2-O2
5	E	705	GOL	O1-C1-C2-O2
5	F	707	GOL	O1-C1-C2-O2
5	A	703	GOL	O2-C2-C3-O3
5	B	701	GOL	O1-C1-C2-O2
5	C	708	GOL	O2-C2-C3-O3
5	F	710	GOL	O1-C1-C2-O2
5	E	706	GOL	O2-C2-C3-O3
5	F	707	GOL	O2-C2-C3-O3
5	E	704	GOL	O1-C1-C2-O2
5	A	713	GOL	O2-C2-C3-O3
5	B	702	GOL	C1-C2-C3-O3
5	E	706	GOL	C1-C2-C3-O3
5	F	710	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	705	GOL	2	0
5	A	703	GOL	2	0
5	B	701	GOL	2	0
5	F	710	GOL	1	0
5	F	707	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	712	GOL	4	0
5	D	711	GOL	5	0

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(Å²)	Q<0.9
1	A	630/643 (97%)	0.49	18 (2%)	53	50	30, 44, 55, 73	0
1	D	633/643 (98%)	0.68	36 (5%)	29	25	33, 44, 56, 78	0
2	B	183/188 (97%)	0.30	3 (1%)	70	66	32, 44, 52, 59	0
2	E	184/188 (97%)	0.79	13 (7%)	22	18	37, 44, 51, 71	0
3	C	296/343 (86%)	0.42	12 (4%)	41	37	33, 45, 56, 65	0
3	F	298/343 (86%)	0.54	10 (3%)	48	44	30, 45, 57, 68	0
All	All	2224/2348 (94%)	0.55	92 (4%)	41	37	30, 44, 55, 78	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	1501	SER	4.8
3	F	1502	ASP	4.8
3	C	1416	PHE	4.8
3	F	1335	THR	4.0
3	C	1417	SER	3.7
2	E	759	PRO	3.6
1	D	143	VAL	3.6
1	D	194	GLN	3.4
1	A	548	SER	3.4
1	D	643	PRO	3.2
1	D	48	SER	3.1
2	E	899	ILE	3.1
1	D	440	ARG	3.1
3	F	1499	GLN	3.1
1	A	371	GLY	3.1
2	E	913	GLY	3.1
2	E	834	GLN	3.0
2	E	914	ILE	3.0
2	E	763	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	778	THR	3.0
1	D	2	PRO	3.0
2	E	731	GLU	3.0
1	A	518	ALA	3.0
1	A	48	SER	2.9
1	A	426	THR	2.9
1	D	70	ALA	2.9
1	D	373	ASP	2.8
3	F	1641	ASN	2.8
1	D	164	LEU	2.8
3	C	1613	ASP	2.7
3	C	1374	GLN	2.7
3	C	1499	GLN	2.7
1	D	489	GLY	2.6
3	C	1641	ASN	2.6
1	A	252	GLY	2.6
3	F	1503	ASP	2.6
2	B	898	PHE	2.6
2	E	768	LEU	2.6
2	E	753	VAL	2.5
3	C	1418	ASP	2.5
2	B	731	GLU	2.5
1	D	637	GLU	2.5
1	D	550	ASP	2.5
1	D	551	ARG	2.5
1	A	374	THR	2.5
1	D	371	GLY	2.4
1	A	550	ASP	2.4
1	A	297	LEU	2.4
3	C	1415	ALA	2.4
1	A	63	ASN	2.4
1	D	144	ASN	2.4
1	D	584	ASN	2.4
1	D	457	MET	2.4
1	D	375	VAL	2.3
1	D	427	VAL	2.3
1	A	375	VAL	2.3
1	A	642	GLN	2.3
1	D	163	GLN	2.3
1	D	642	GLN	2.3
2	B	730	ASP	2.2
1	D	549	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	803	VAL	2.2
1	D	518	ALA	2.2
2	E	865	THR	2.2
1	D	519	SER	2.2
1	D	530	TRP	2.2
1	A	190	ASN	2.2
1	A	116	ILE	2.2
1	A	49	SER	2.2
1	D	548	SER	2.2
3	C	1335	THR	2.2
3	C	1615	CYS	2.2
1	D	141	VAL	2.1
1	D	10	ASN	2.1
3	C	1387	THR	2.1
3	F	1612	GLU	2.1
1	A	255	ASP	2.1
1	D	607	PRO	2.1
3	F	1415	ALA	2.1
1	A	1	SER	2.1
1	D	42	GLY	2.1
1	D	80	ARG	2.1
1	A	424	TYR	2.1
1	D	639	GLN	2.0
3	F	1500	LYS	2.0
1	D	205	TYR	2.0
1	D	582	VAL	2.0
3	C	1419	ARG	2.0
1	D	103	LEU	2.0
1	D	162	ASN	2.0
2	E	762	ASN	2.0
3	F	1373	ASP	2.0

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

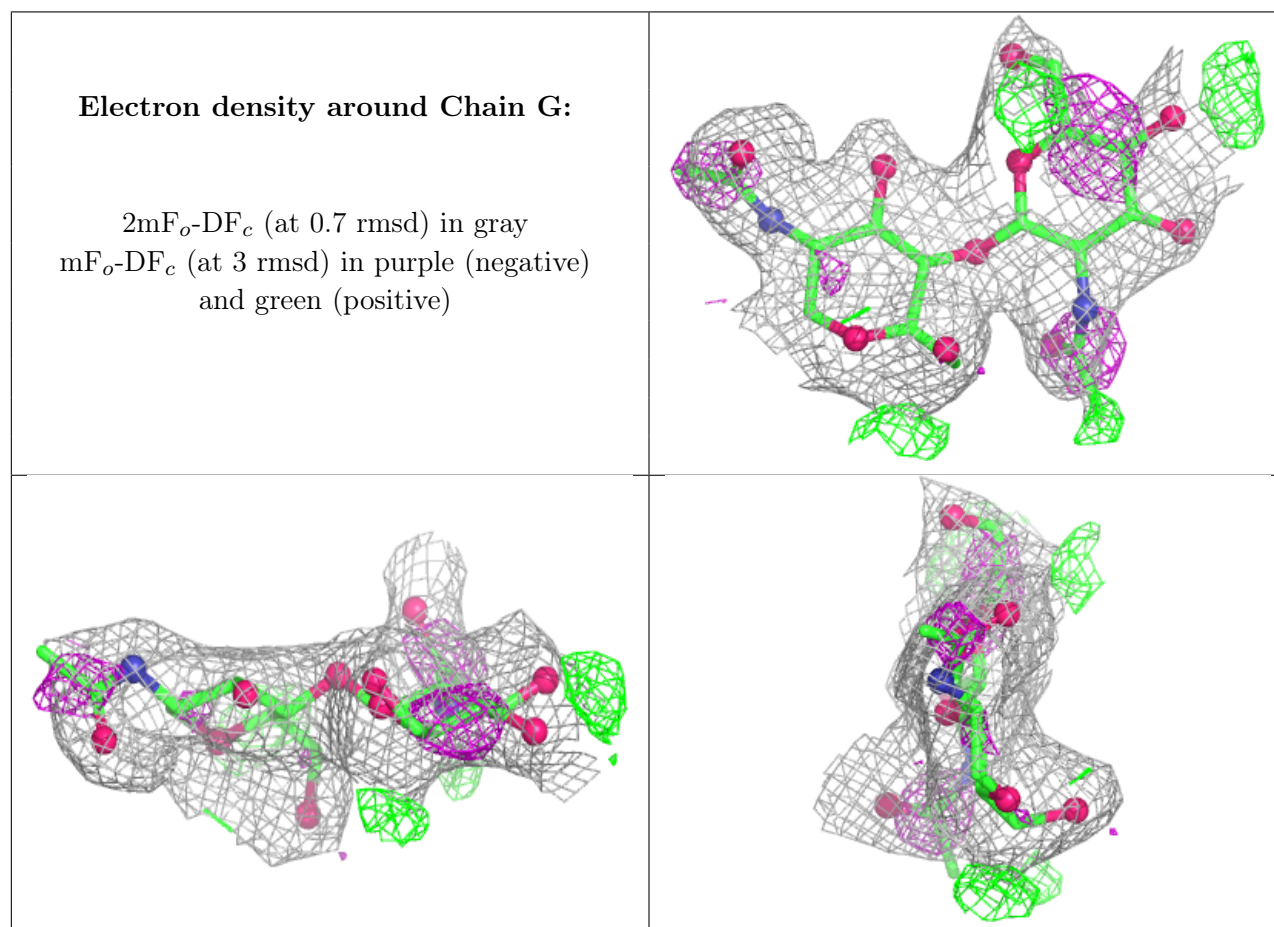
There are no non-standard protein/DNA/RNA residues in this entry.

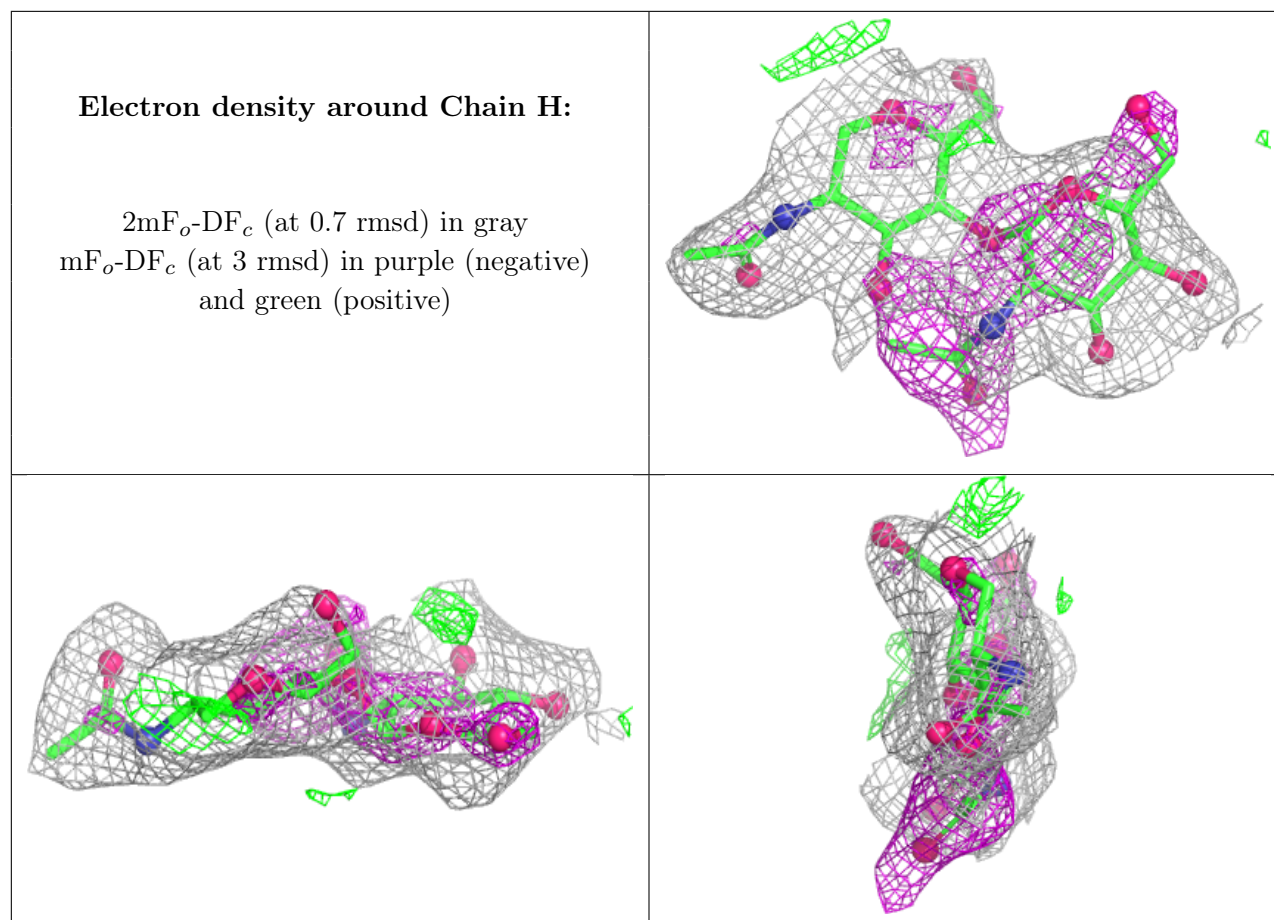
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
4	NDG	H	2	14/15	0.24	0.19	75,76,78,79	0
4	NDG	G	2	14/15	0.54	0.17	64,66,69,69	0
4	NDG	H	1	14/15	0.70	0.14	61,66,70,73	0
4	NDG	G	1	14/15	0.79	0.12	54,57,59,62	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(Å ²)	Q<0.9
5	GOL	F	707	6/6	0.62	0.16	86,88,88,89	0
5	GOL	A	712	6/6	0.65	0.18	78,81,82,85	0
5	GOL	C	708	6/6	0.70	0.23	66,72,73,75	0
5	GOL	E	706	6/6	0.72	0.27	57,60,63,64	0
5	GOL	A	703	6/6	0.73	0.23	60,62,63,65	0
5	GOL	B	702	6/6	0.75	0.15	87,88,88,89	0
5	GOL	C	709	6/6	0.75	0.17	90,90,91,91	0
5	GOL	F	710	6/6	0.75	0.20	72,73,73,74	0
5	GOL	D	711	6/6	0.76	0.15	81,83,84,88	0
5	GOL	A	713	6/6	0.77	0.20	61,65,66,68	0
6	NO3	F	802	4/4	0.79	0.22	89,89,89,90	0
6	NO3	F	803	4/4	0.79	0.18	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NO3	C	801	4/4	0.82	0.17	77,77,77,77	0
5	GOL	E	705	6/6	0.84	0.26	62,66,66,67	0
5	GOL	E	704	6/6	0.86	0.19	45,49,51,52	0
5	GOL	B	701	6/6	0.87	0.15	45,46,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.