Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 02:58 AM BST

PDB ID	:	4AY5
Title	:	Human O-GlcNAc transferase (OGT) in complex with UDP and glycopeptide
Authors	:	Schimpl, M.; Zheng, X.; Blair, D.E.; Schuettelkopf, A.W.; Navratilova, I.; Aristotelous, T.; Ferenbach, A.T.; Macnaughtan, M.A.; Borodkin, V.S.; van Aalten, D.M.F.
Deposited on	:	2012-06-18
Resolution	:	3.15 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

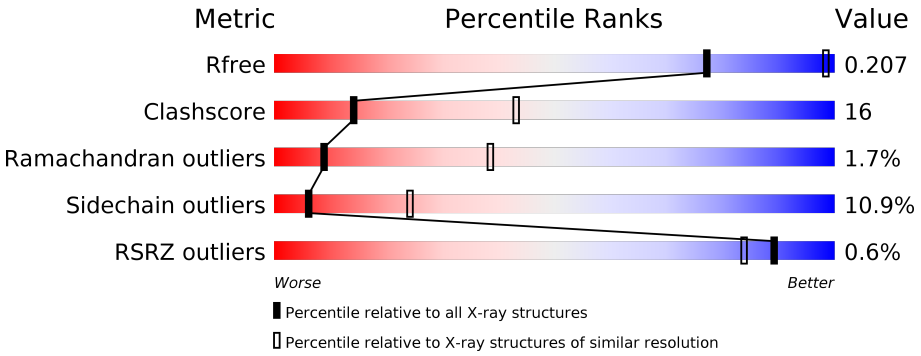
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=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	723	% 63% 29% 5% ·
1	B	723	61% 29% 6% ·
1	C	723	63% 28% 5% ·
1	D	723	% 63% 29% · ·
2	I	11	27% 55% 18%
2	J	11	18% 18% 55% 27%

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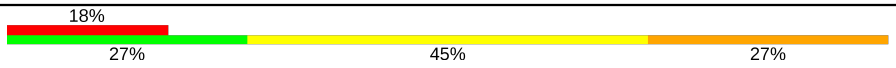
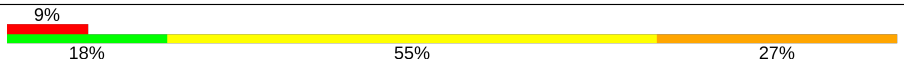
Mol	Chain	Length	Quality of chain
2	K	11	
2	L	11	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22524 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 UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYL TRANSFERASE 110 KDA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	698	Total	C	N	O	S	0	0	0
			5514	3499	964	1013	38			
1	B	698	Total	C	N	O	S	0	0	0
			5514	3499	964	1013	38			
1	C	698	Total	C	N	O	S	0	0	0
			5514	3499	964	1013	38			
1	D	698	Total	C	N	O	S	0	0	0
			5514	3499	964	1013	38			

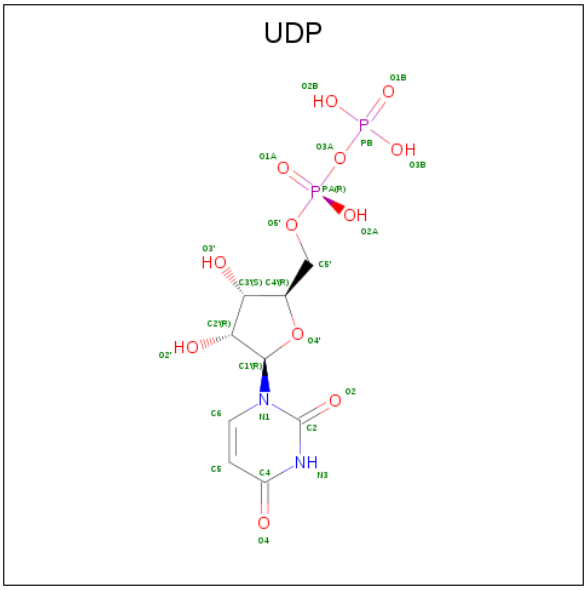
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	GLY	-	expression tag	UNP O15294
A	310	PRO	-	expression tag	UNP O15294
A	311	GLY	-	expression tag	UNP O15294
A	312	SER	-	expression tag	UNP O15294
B	309	GLY	-	expression tag	UNP O15294
B	310	PRO	-	expression tag	UNP O15294
B	311	GLY	-	expression tag	UNP O15294
B	312	SER	-	expression tag	UNP O15294
C	309	GLY	-	expression tag	UNP O15294
C	310	PRO	-	expression tag	UNP O15294
C	311	GLY	-	expression tag	UNP O15294
C	312	SER	-	expression tag	UNP O15294
D	309	GLY	-	expression tag	UNP O15294
D	310	PRO	-	expression tag	UNP O15294
D	311	GLY	-	expression tag	UNP O15294
D	312	SER	-	expression tag	UNP O15294

- Molecule 2 is a protein called GTAB1TIDE.

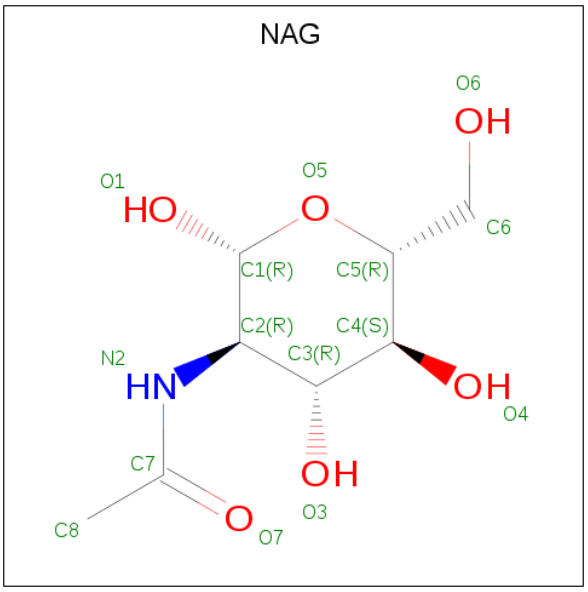
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	I	11	Total C N O 78 49 12 17	0	0	0
2	J	11	Total C N O 78 49 12 17	0	0	0
2	K	11	Total C N O 78 49 12 17	0	0	0
2	L	11	Total C N O 78 49 12 17	0	0	0

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 25 9 2 12 2	0	0
3	B	1	Total C N O P 25 9 2 12 2	0	0
3	C	1	Total C N O P 25 9 2 12 2	0	0
3	D	1	Total C N O P 25 9 2 12 2	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



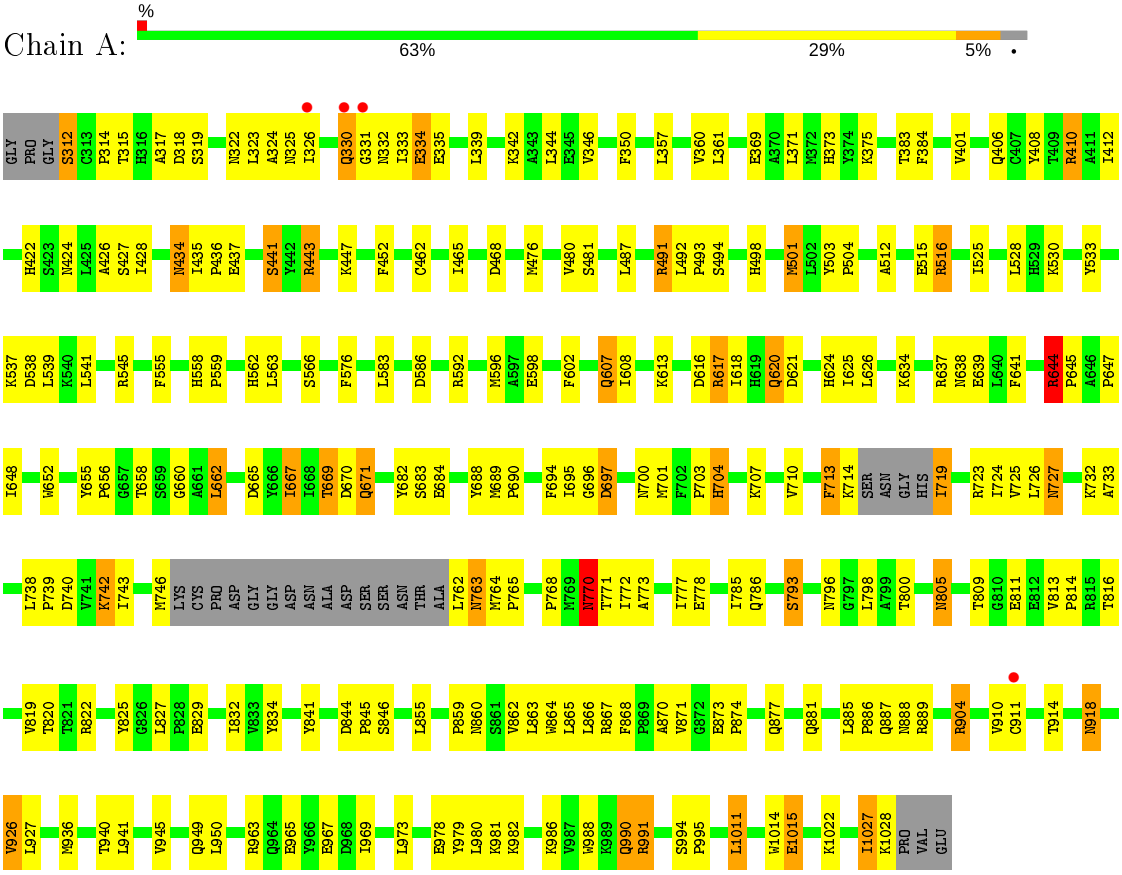
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total C N O 14 8 1 5	0	0
4	J	1	Total C N O 14 8 1 5	0	0
4	K	1	Total C N O 14 8 1 5	0	0
4	L	1	Total C N O 14 8 1 5	0	0

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.

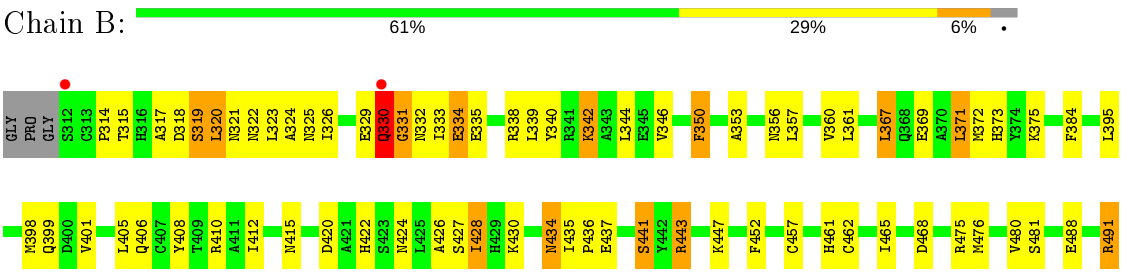
• Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYL TRANSFERASE 110 KDA SUBUNIT

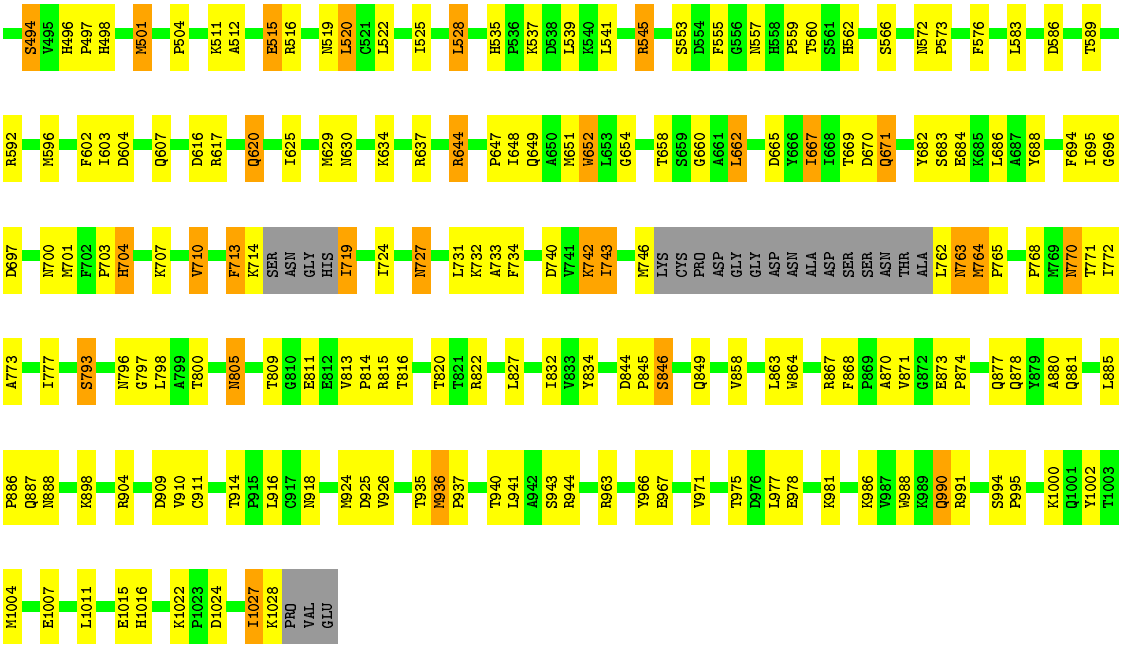
Chain A:



• Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYL TRANSFERASE 110 KDA SUBUNIT

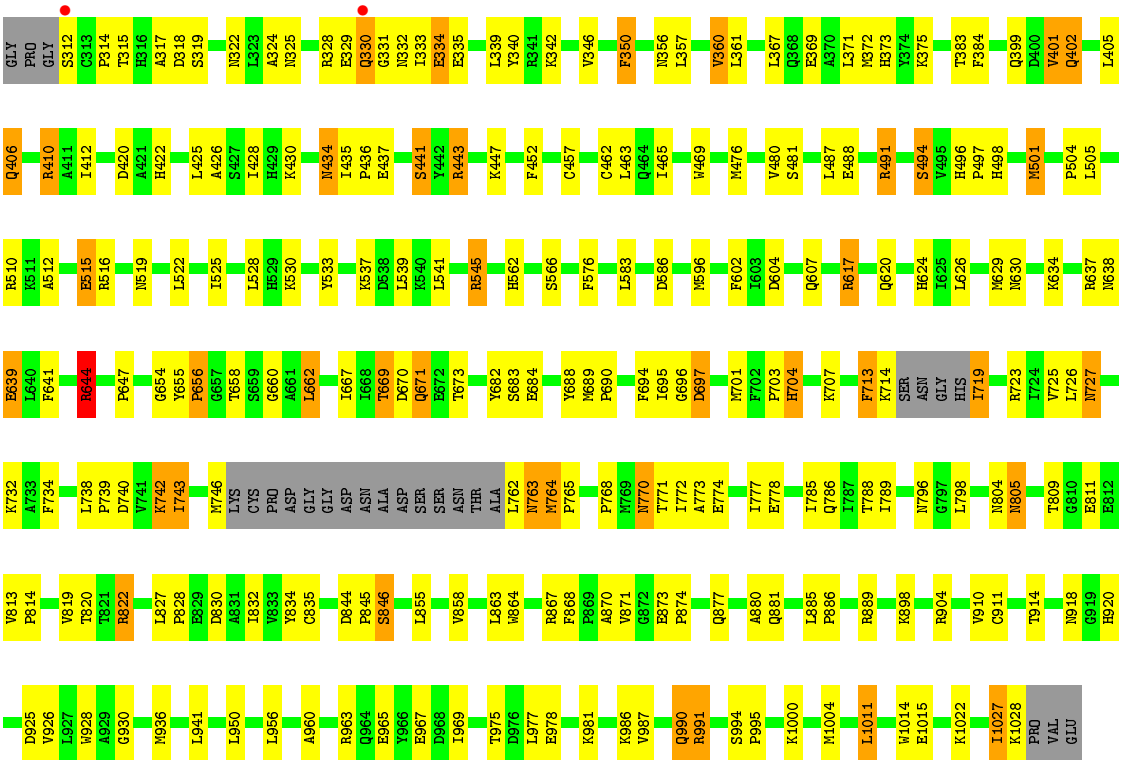
Chain B:





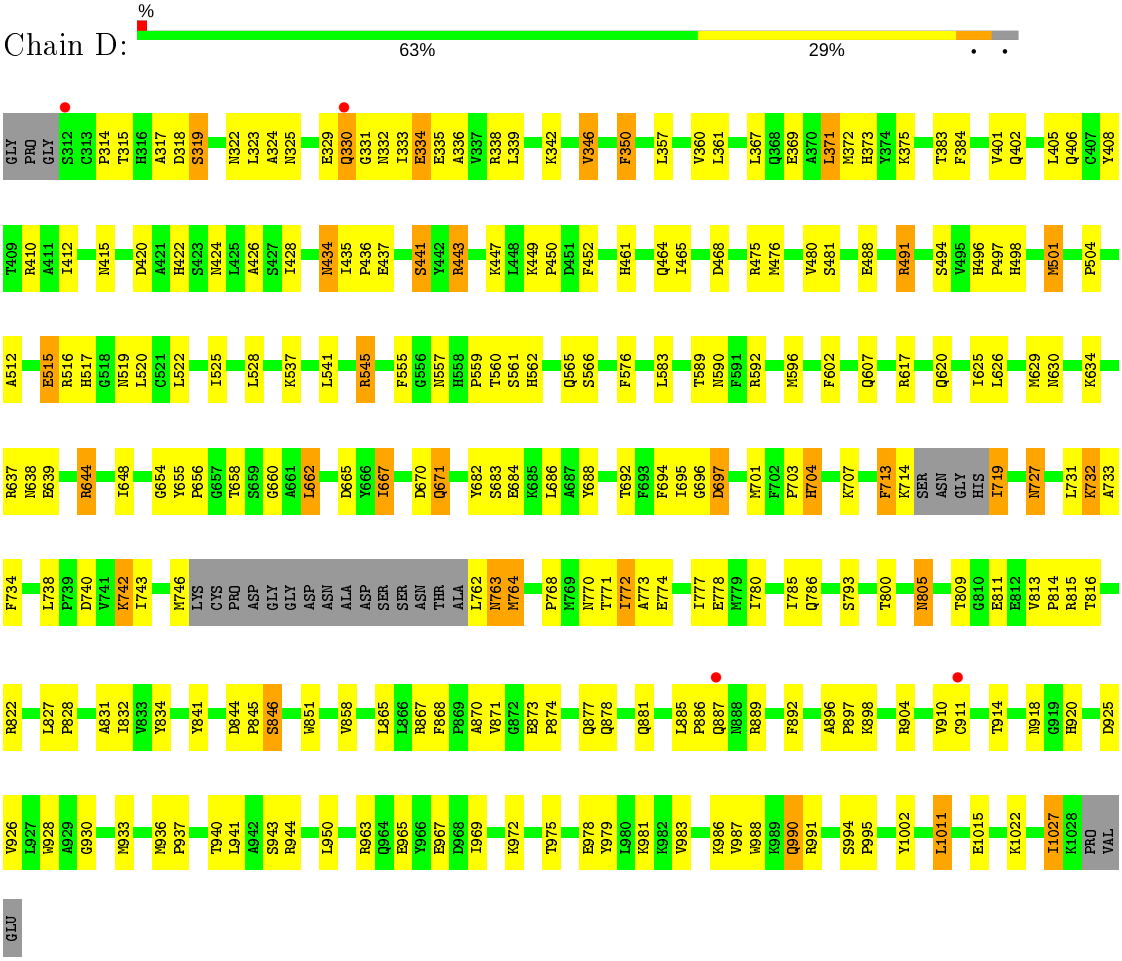
• Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYL TRANSFERASE 110 KDA SUBUNIT

Chain C:



• Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYL TRANSFERASE 110 KDA SUBUNIT

Chain D:

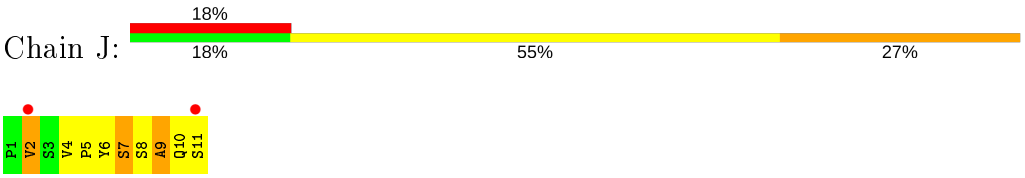


- Molecule 2: GTAB1TIDE

Chain I:

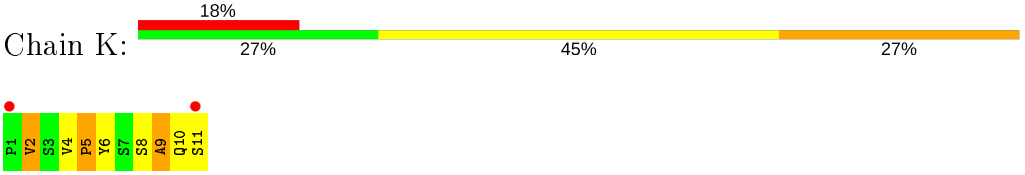
- Molecule 2: GTAB1TIDE

Chain J:



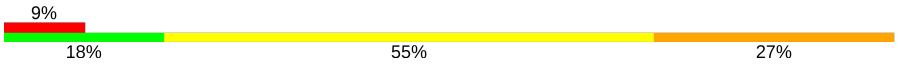
- Molecule 2: GTAB1TIDE

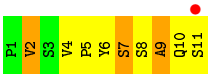
Chain K:



- Molecule 2: GTAB1TIDE

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	274.17Å 274.17Å 142.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	237.44 – 3.15 29.91 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (237.44-3.15) 99.7 (29.91-3.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.174 , 0.204 0.173 , 0.207	Depositor DCC
R_{free} test set	501 reflections (0.47%)	wwPDB-VP
Wilson B-factor (Å^2)	67.1	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 58.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22524	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.93	3/5641 (0.1%)	1.03	11/7650 (0.1%)
1	B	0.91	2/5641 (0.0%)	1.01	10/7650 (0.1%)
1	C	0.91	2/5641 (0.0%)	1.01	10/7650 (0.1%)
1	D	0.80	3/5641 (0.1%)	0.92	5/7650 (0.1%)
2	I	1.59	2/80 (2.5%)	1.63	0/109
2	J	1.67	1/80 (1.2%)	1.59	0/109
2	K	1.57	1/80 (1.2%)	1.61	0/109
2	L	1.50	1/80 (1.2%)	1.55	0/109
All	All	0.90	15/22884 (0.1%)	1.01	36/31036 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	6	TYR	CB-CG	-6.71	1.41	1.51
1	A	988	TRP	CD2-CE2	6.64	1.49	1.41
1	B	652	TRP	CD2-CE2	6.36	1.49	1.41
2	J	6	TYR	CB-CG	-6.16	1.42	1.51
1	A	598	GLU	CD-OE1	6.13	1.32	1.25
1	C	864	TRP	CD2-CE2	5.91	1.48	1.41
2	K	6	TYR	CB-CG	-5.69	1.43	1.51
1	D	928	TRP	CD2-CE2	5.68	1.48	1.41
1	A	652	TRP	CD2-CE2	5.56	1.48	1.41
1	C	469	TRP	CD2-CE2	5.41	1.47	1.41
1	B	988	TRP	CD2-CE2	5.25	1.47	1.41
1	D	988	TRP	CD2-CE2	5.24	1.47	1.41
1	D	851	TRP	CD2-CE2	5.14	1.47	1.41
2	I	6	TYR	CB-CG	-5.13	1.44	1.51
2	I	5	PRO	CA-C	-5.08	1.42	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	904	ARG	NE-CZ-NH2	-9.25	115.68	120.30
1	A	904	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	B	925	ASP	CB-CG-OD1	7.52	125.07	118.30
1	A	855	LEU	CB-CG-CD1	-7.24	98.70	111.00
1	B	904	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	644	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	C	925	ASP	CB-CG-OD1	6.53	124.17	118.30
1	C	925	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	1011	LEU	CA-CB-CG	-6.48	100.40	115.30
1	A	991	ARG	CG-CD-NE	-6.44	98.28	111.80
1	B	1011	LEU	CA-CB-CG	-6.43	100.50	115.30
1	C	1011	LEU	CA-CB-CG	-6.11	101.25	115.30
1	D	904	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	586	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	617	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	B	520	LEU	CA-CB-CG	-5.84	101.86	115.30
1	D	925	ASP	CB-CG-OD1	5.75	123.48	118.30
1	C	410	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	528	LEU	CB-CG-CD2	-5.63	101.43	111.00
1	C	904	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	D	371	LEU	CB-CG-CD2	-5.58	101.51	111.00
1	C	855	LEU	CB-CG-CD1	-5.54	101.58	111.00
1	B	916	LEU	CB-CG-CD1	5.54	120.41	111.00
1	A	586	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	410	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	980	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	B	586	ASP	CB-CG-OD1	5.42	123.17	118.30
1	D	925	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	B	428	ILE	CG1-CB-CG2	-5.33	99.66	111.40
1	B	320	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	D	1011	LEU	CA-CB-CG	-5.19	103.36	115.30
1	C	644	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	516	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	516	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	C	822	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	B	395	LEU	CB-CG-CD1	-5.10	102.33	111.00

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	5514	0	5489	169	0
1	B	5514	0	5489	191	0
1	C	5514	0	5489	167	0
1	D	5514	0	5489	165	0
2	I	78	0	75	4	0
2	J	78	0	75	5	0
2	K	78	0	75	4	0
2	L	78	0	75	5	0
3	A	25	0	11	2	0
3	B	25	0	11	2	0
3	C	25	0	11	2	0
3	D	25	0	11	3	0
4	I	14	0	13	0	0
4	J	14	0	13	0	0
4	K	14	0	13	0	0
4	L	14	0	13	0	0
All	All	22524	0	22352	701	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 16.

All (701) 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:443:ARG:HH11	1:A:443:ARG:HG2	1.26	1.01
1:A:773:ALA:O	1:A:777:ILE:HG22	1.61	1.00
1:D:713:PHE:H	1:D:713:PHE:HD1	1.03	0.99
1:A:713:PHE:HD1	1:A:713:PHE:H	1.02	0.96
1:B:662:LEU:HD12	1:B:662:LEU:H	1.30	0.95
1:C:443:ARG:HG2	1:C:443:ARG:HH11	1.30	0.95
1:B:713:PHE:H	1:B:713:PHE:HD1	1.00	0.95
1:B:671:GLN:HG2	1:B:688:TYR:CE2	2.05	0.92
1:C:713:PHE:HD1	1:C:713:PHE:H	1.00	0.91
1:D:773:ALA:O	1:D:777:ILE:HG22	1.71	0.91
1:D:443:ARG:HH11	1:D:443:ARG:HG2	1.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:ARG:HH11	1:B:443:ARG:HG2	1.37	0.90
1:A:994:SER:HB2	1:A:995:PRO:HD3	1.54	0.89
1:B:644:ARG:CG	1:B:644:ARG:HH11	1.85	0.89
1:D:671:GLN:HG2	1:D:688:TYR:CE2	2.08	0.88
1:D:805:ASN:HD22	1:D:805:ASN:H	1.19	0.87
1:C:773:ALA:O	1:C:777:ILE:HG22	1.73	0.87
1:D:644:ARG:HH11	1:D:644:ARG:CG	1.89	0.85
1:D:662:LEU:HD12	1:D:662:LEU:H	1.40	0.85
1:B:714:LYS:HZ3	1:B:719:ILE:N	1.76	0.84
1:B:773:ALA:O	1:B:777:ILE:HG22	1.77	0.84
1:C:671:GLN:HG2	1:C:688:TYR:CE2	2.13	0.84
1:A:1015:GLU:OE1	1:A:1015:GLU:HA	1.78	0.83
1:A:662:LEU:HD12	1:A:662:LEU:H	1.42	0.83
1:B:994:SER:HB2	1:B:995:PRO:CD	2.10	0.82
1:A:714:LYS:HZ3	1:A:719:ILE:N	1.77	0.81
1:C:994:SER:HB2	1:C:995:PRO:CD	2.12	0.80
1:C:662:LEU:H	1:C:662:LEU:HD12	1.47	0.80
1:D:443:ARG:HH11	1:D:443:ARG:CG	1.93	0.80
1:C:1015:GLU:OE1	1:C:1015:GLU:HA	1.82	0.79
1:D:994:SER:HB2	1:D:995:PRO:HD3	1.65	0.78
1:B:994:SER:HB2	1:B:995:PRO:HD3	1.65	0.78
1:B:317:ALA:HB2	1:B:346:VAL:HB	1.64	0.78
1:C:443:ARG:HH11	1:C:443:ARG:CG	1.97	0.78
1:C:805:ASN:H	1:C:805:ASN:HD22	1.30	0.77
1:C:644:ARG:HH11	1:C:644:ARG:CG	1.96	0.77
1:B:443:ARG:HH11	1:B:443:ARG:CG	1.98	0.76
1:C:740:ASP:HB2	1:C:768:PRO:HG3	1.67	0.76
1:B:476:MET:O	1:B:480:VAL:HG23	1.86	0.76
1:B:367:LEU:HD23	1:B:367:LEU:N	2.01	0.75
1:A:740:ASP:HB2	1:A:768:PRO:HG3	1.69	0.74
1:A:426:ALA:HB2	1:A:441:SER:HB3	1.70	0.74
1:D:740:ASP:HB2	1:D:768:PRO:HG3	1.70	0.74
1:B:809:THR:OG1	1:B:811:GLU:HG3	1.88	0.73
1:A:713:PHE:N	1:A:713:PHE:CD1	2.56	0.73
3:D:1201:UDP:O2	2:L:4:VAL:HG11	1.89	0.73
1:A:644:ARG:CG	1:A:644:ARG:HH11	2.01	0.73
1:D:707:LYS:HE2	1:D:762:LEU:HD22	1.72	0.72
1:B:644:ARG:HH11	1:B:644:ARG:HG2	1.55	0.72
1:D:361:LEU:HD13	1:D:369:GLU:HG2	1.70	0.72
1:D:713:PHE:CD1	1:D:713:PHE:N	2.58	0.72
1:B:1015:GLU:HA	1:B:1015:GLU:OE1	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:GLN:HG2	1:A:688:TYR:CE2	2.26	0.71
1:D:1015:GLU:OE1	1:D:1015:GLU:HA	1.88	0.71
1:B:367:LEU:HD23	1:B:367:LEU:H	1.54	0.71
1:A:844:ASP:HB2	1:A:845:PRO:HD2	1.72	0.71
1:C:713:PHE:CD1	1:C:713:PHE:N	2.55	0.70
1:B:426:ALA:HB2	1:B:441:SER:HB3	1.73	0.70
1:B:662:LEU:CD1	1:B:662:LEU:H	2.03	0.70
1:C:809:THR:OG1	1:C:811:GLU:HG3	1.92	0.70
1:D:476:MET:O	1:D:480:VAL:HG23	1.91	0.70
1:D:644:ARG:HH11	1:D:644:ARG:HG3	1.55	0.70
3:C:1201:UDP:O2	2:K:4:VAL:HG11	1.92	0.70
1:A:667:ILE:HG22	1:A:684:GLU:HB2	1.73	0.69
1:B:644:ARG:HG3	1:B:644:ARG:NH1	2.06	0.69
1:A:994:SER:HB2	1:A:995:PRO:CD	2.22	0.69
1:B:704:HIS:CD2	1:B:814:PRO:HG2	2.28	0.69
1:D:994:SER:HB2	1:D:995:PRO:CD	2.22	0.68
1:B:434:ASN:HB2	1:B:437:GLU:CG	2.23	0.68
1:D:426:ALA:HB2	1:D:441:SER:HB3	1.75	0.68
1:A:607:GLN:HA	1:A:607:GLN:OE1	1.92	0.68
1:A:859:PRO:HG2	1:B:1016:HIS:ND1	2.09	0.68
1:A:669:THR:OG1	1:A:670:ASP:N	2.24	0.67
1:A:793:SER:HB2	1:A:816:THR:HG22	1.76	0.67
1:D:644:ARG:NH1	1:D:644:ARG:HG3	2.06	0.67
1:B:324:ALA:HB2	1:B:339:LEU:HB2	1.77	0.67
1:A:434:ASN:HB2	1:A:437:GLU:CG	2.24	0.67
1:B:361:LEU:HD13	1:B:369:GLU:HG2	1.76	0.67
2:I:4:VAL:HG12	2:I:5:PRO:HD2	1.76	0.67
1:D:793:SER:HB2	1:D:816:THR:HG22	1.76	0.67
1:A:707:LYS:HE2	1:A:762:LEU:HD22	1.77	0.67
1:A:877:GLN:OE1	1:A:877:GLN:HA	1.95	0.66
1:B:805:ASN:H	1:B:805:ASN:HD22	1.43	0.66
1:A:443:ARG:HH11	1:A:443:ARG:CG	2.04	0.66
1:C:714:LYS:HZ3	1:C:719:ILE:N	1.94	0.66
1:D:805:ASN:ND2	1:D:805:ASN:H	1.87	0.66
1:A:714:LYS:NZ	1:A:719:ILE:N	2.43	0.66
1:B:660:GLY:HA2	1:B:683:SER:HB3	1.78	0.66
1:A:918:ASN:N	1:A:918:ASN:HD22	1.92	0.65
1:B:746:MET:HG3	1:B:763:ASN:HA	1.78	0.65
1:B:793:SER:HB2	1:B:816:THR:HG22	1.80	0.64
1:D:877:GLN:OE1	1:D:877:GLN:HA	1.98	0.64
1:B:963:ARG:O	1:B:967:GLU:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:LEU:HD13	1:C:369:GLU:HG2	1.79	0.64
1:C:994:SER:HB2	1:C:995:PRO:HD3	1.80	0.64
1:A:476:MET:O	1:A:480:VAL:HG23	1.99	0.63
1:D:805:ASN:ND2	1:D:805:ASN:N	2.45	0.63
1:B:350:PHE:CD1	1:B:350:PHE:C	2.72	0.63
1:B:671:GLN:HG2	1:B:688:TYR:HE2	1.63	0.63
1:B:644:ARG:HG3	1:B:644:ARG:HH11	1.58	0.63
1:D:746:MET:HG3	1:D:763:ASN:HA	1.81	0.63
1:B:658:THR:HB	1:B:682:TYR:HA	1.81	0.63
1:C:644:ARG:HH11	1:C:644:ARG:HG3	1.64	0.63
1:B:583:LEU:HD22	1:B:637:ARG:HD3	1.82	0.62
1:D:324:ALA:HB2	1:D:339:LEU:HB2	1.82	0.62
1:A:743:ILE:HG22	1:A:743:ILE:O	2.00	0.62
1:B:714:LYS:NZ	1:B:719:ILE:N	2.47	0.62
1:B:740:ASP:HB2	1:B:768:PRO:HG3	1.81	0.62
1:C:324:ALA:HB2	1:C:339:LEU:HB2	1.80	0.62
1:A:768:PRO:HG2	1:A:770:ASN:OD1	1.98	0.61
1:A:644:ARG:HH11	1:A:644:ARG:HG2	1.65	0.61
1:B:644:ARG:CG	1:B:644:ARG:NH1	2.50	0.61
1:C:335:GLU:OE1	1:C:335:GLU:HA	1.99	0.61
1:C:660:GLY:HA2	1:C:683:SER:HB3	1.82	0.61
1:A:965:GLU:O	1:A:969:ILE:HG13	2.00	0.61
1:C:805:ASN:N	1:C:805:ASN:HD22	1.98	0.61
1:B:695:ILE:HG13	1:B:696:GLY:N	2.15	0.61
1:A:867:ARG:HB3	1:A:870:ALA:HA	1.82	0.61
1:C:426:ALA:HB2	1:C:441:SER:HB3	1.83	0.61
1:C:671:GLN:HG2	1:C:688:TYR:HE2	1.65	0.61
1:B:688:TYR:CD2	1:B:1027:ILE:HG22	2.36	0.61
1:C:322:ASN:HA	1:C:325:ASN:HD22	1.65	0.61
1:C:867:ARG:HB3	1:C:870:ALA:HA	1.83	0.61
1:D:434:ASN:HB2	1:D:437:GLU:CG	2.31	0.60
1:B:994:SER:CB	1:B:995:PRO:CD	2.77	0.60
1:C:746:MET:HG3	1:C:763:ASN:HA	1.83	0.60
1:B:350:PHE:HD1	1:B:350:PHE:C	2.05	0.60
1:A:881:GLN:HG3	1:A:885:LEU:O	2.00	0.60
1:D:844:ASP:HB2	1:D:845:PRO:HD2	1.83	0.60
1:C:367:LEU:N	1:C:367:LEU:HD23	2.17	0.60
1:D:324:ALA:HA	1:D:339:LEU:HD12	1.84	0.60
1:D:357:LEU:HD23	1:D:373:HIS:CE1	2.36	0.60
3:B:1201:UDP:O2	2:J:4:VAL:HG11	2.02	0.60
1:A:361:LEU:HD13	1:A:369:GLU:HG2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:ILE:HG13	1:C:696:GLY:N	2.17	0.60
1:D:671:GLN:HG2	1:D:688:TYR:HE2	1.65	0.59
1:B:426:ALA:HB2	1:B:441:SER:CB	2.32	0.59
1:A:335:GLU:HA	1:A:335:GLU:OE1	2.02	0.59
1:A:822:ARG:HB3	1:A:827:LEU:HB2	1.84	0.59
1:B:324:ALA:HB2	1:B:339:LEU:CB	2.32	0.59
1:C:644:ARG:NH1	1:C:644:ARG:HG3	2.15	0.59
1:A:324:ALA:HB2	1:A:339:LEU:HB2	1.83	0.59
1:C:314:PRO:O	1:C:318:ASP:HB2	2.03	0.59
1:D:805:ASN:HD22	1:D:805:ASN:N	1.94	0.59
1:C:329:GLU:HA	1:C:329:GLU:OE1	2.02	0.59
1:C:986:LYS:O	1:C:990:GLN:HG2	2.03	0.59
1:A:703:PRO:HD2	1:A:813:VAL:HG22	1.85	0.59
1:B:844:ASP:HB2	1:B:845:PRO:CD	2.33	0.59
1:C:435:ILE:HB	1:C:436:PRO:HD3	1.84	0.59
1:A:583:LEU:HD22	1:A:637:ARG:HD3	1.85	0.59
1:A:644:ARG:CG	1:A:644:ARG:NH1	2.63	0.59
1:C:476:MET:O	1:C:480:VAL:HG23	2.02	0.59
1:C:644:ARG:NH1	1:C:644:ARG:CG	2.61	0.59
1:D:714:LYS:HZ3	1:D:719:ILE:N	2.00	0.59
1:A:785:ILE:HG22	1:A:786:GLN:HG2	1.85	0.59
1:D:408:TYR:CE1	1:D:424:ASN:HB3	2.38	0.59
1:A:994:SER:CB	1:A:995:PRO:HD3	2.30	0.58
1:A:695:ILE:HG13	1:A:696:GLY:N	2.18	0.58
1:C:638:ASN:O	1:C:641:PHE:N	2.36	0.58
1:A:805:ASN:H	1:A:805:ASN:HD22	1.49	0.58
1:C:317:ALA:HB2	1:C:346:VAL:HB	1.85	0.58
1:D:963:ARG:O	1:D:967:GLU:HG3	2.03	0.58
2:J:4:VAL:HG12	2:J:5:PRO:HD2	1.84	0.58
1:A:314:PRO:O	1:A:318:ASP:HB2	2.03	0.58
1:A:844:ASP:HB2	1:A:845:PRO:CD	2.33	0.58
1:C:805:ASN:H	1:C:805:ASN:ND2	2.01	0.58
1:C:877:GLN:HA	1:C:877:GLN:OE1	2.04	0.58
1:D:644:ARG:HH11	1:D:644:ARG:HG2	1.65	0.58
1:B:318:ASP:O	1:B:322:ASN:ND2	2.36	0.57
1:C:805:ASN:N	1:C:805:ASN:ND2	2.52	0.57
1:D:660:GLY:HA2	1:D:683:SER:HB3	1.85	0.57
1:C:638:ASN:O	1:C:639:GLU:C	2.43	0.57
1:B:324:ALA:HA	1:B:339:LEU:HD12	1.87	0.57
1:A:994:SER:CB	1:A:995:PRO:CD	2.81	0.57
1:B:434:ASN:HB2	1:B:437:GLU:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:ILE:HB	1:B:436:PRO:HD3	1.86	0.57
1:A:660:GLY:HA2	1:A:683:SER:HB3	1.85	0.57
1:D:498:HIS:O	1:D:501:MET:HE3	2.05	0.57
1:D:846:SER:HB2	1:D:963:ARG:HH21	1.69	0.57
1:C:669:THR:OG1	1:C:670:ASP:N	2.34	0.57
1:C:994:SER:HB2	1:C:995:PRO:HD2	1.86	0.56
1:D:944:ARG:HG2	1:D:944:ARG:HH11	1.70	0.56
1:A:330:GLN:O	1:A:332:ASN:N	2.39	0.56
1:B:844:ASP:HB2	1:B:845:PRO:HD2	1.86	0.56
1:D:525:ILE:HA	1:D:528:LEU:HD12	1.87	0.56
1:A:435:ILE:HB	1:A:436:PRO:HD3	1.86	0.56
1:D:704:HIS:CD2	1:D:814:PRO:HG2	2.40	0.56
1:A:1015:GLU:CA	1:A:1015:GLU:OE1	2.53	0.56
1:A:809:THR:OG1	1:A:811:GLU:HG3	2.05	0.56
1:A:860:ASN:HB2	1:B:1016:HIS:HE1	1.70	0.56
1:C:704:HIS:O	1:C:727:ASN:HB3	2.05	0.56
1:D:367:LEU:N	1:D:367:LEU:HD23	2.20	0.56
1:B:321:ASN:HD21	1:B:356:ASN:HD22	1.53	0.56
1:C:941:LEU:HD23	1:C:941:LEU:C	2.26	0.56
1:B:986:LYS:O	1:B:990:GLN:HG2	2.06	0.55
1:C:443:ARG:CG	1:C:443:ARG:NH1	2.63	0.55
1:A:324:ALA:HA	1:A:339:LEU:HD12	1.88	0.55
1:A:607:GLN:CA	1:A:607:GLN:OE1	2.54	0.55
1:A:859:PRO:HG2	1:B:1016:HIS:CE1	2.41	0.55
1:D:314:PRO:O	1:D:318:ASP:HB2	2.05	0.55
1:A:608:ILE:HG22	1:A:608:ILE:O	2.05	0.55
1:B:322:ASN:HA	1:B:325:ASN:HD22	1.71	0.55
1:C:886:PRO:HG2	1:C:889:ARG:HG2	1.87	0.55
1:D:317:ALA:HB2	1:D:346:VAL:HB	1.88	0.55
1:D:994:SER:CB	1:D:995:PRO:CD	2.84	0.55
2:J:8:SER:O	2:J:9:ALA:O	2.25	0.55
1:C:525:ILE:HA	1:C:528:LEU:HD12	1.89	0.55
1:D:583:LEU:HD22	1:D:637:ARG:HD3	1.88	0.55
1:D:809:THR:OG1	1:D:811:GLU:HG3	2.06	0.55
1:C:496:HIS:CG	1:C:497:PRO:HD2	2.41	0.55
1:C:434:ASN:HB2	1:C:437:GLU:CG	2.37	0.55
1:C:624:HIS:O	1:C:647:PRO:HG2	2.07	0.54
1:A:719:ILE:CG2	1:A:719:ILE:O	2.55	0.54
1:D:335:GLU:OE1	1:D:335:GLU:HA	2.07	0.54
1:D:443:ARG:NH1	1:D:443:ARG:CG	2.61	0.54
2:L:4:VAL:HG12	2:L:5:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:877:GLN:OE1	1:B:877:GLN:HA	2.07	0.54
1:D:443:ARG:NH1	1:D:443:ARG:HG2	2.13	0.54
1:D:607:GLN:OE1	1:D:607:GLN:HA	2.06	0.54
1:B:443:ARG:NH1	1:B:443:ARG:CG	2.65	0.54
1:B:873:GLU:N	1:B:874:PRO:HD2	2.23	0.54
1:D:350:PHE:C	1:D:350:PHE:CD1	2.81	0.54
2:K:4:VAL:HG12	2:K:5:PRO:HD2	1.90	0.54
1:B:329:GLU:HA	1:B:329:GLU:OE1	2.06	0.54
1:D:662:LEU:H	1:D:662:LEU:CD1	2.16	0.54
1:A:707:LYS:HE2	1:A:762:LEU:CD2	2.38	0.53
1:B:512:ALA:O	1:B:516:ARG:HG2	2.08	0.53
1:B:713:PHE:CD1	1:B:713:PHE:N	2.55	0.53
1:D:658:THR:HB	1:D:682:TYR:HA	1.90	0.53
1:A:424:ASN:O	1:A:427:SER:HB2	2.09	0.53
1:C:785:ILE:HG22	1:C:786:GLN:HG2	1.91	0.53
1:A:644:ARG:HG3	1:A:644:ARG:NH1	2.24	0.53
1:B:977:LEU:HD23	1:B:977:LEU:N	2.24	0.53
1:C:994:SER:CB	1:C:995:PRO:CD	2.79	0.53
1:D:986:LYS:O	1:D:990:GLN:HG2	2.09	0.53
1:A:746:MET:HG3	1:A:763:ASN:HA	1.90	0.53
1:B:719:ILE:O	1:B:719:ILE:CG2	2.57	0.53
1:C:324:ALA:HB2	1:C:339:LEU:CB	2.38	0.53
1:A:625:ILE:HG12	1:A:648:ILE:HB	1.90	0.53
1:A:941:LEU:HD23	1:A:941:LEU:C	2.30	0.53
1:A:498:HIS:O	1:A:501:MET:HE3	2.09	0.53
1:C:644:ARG:HG2	1:C:644:ARG:HH11	1.70	0.52
1:C:707:LYS:HE2	1:C:762:LEU:HD22	1.91	0.52
1:D:772:ILE:H	1:D:772:ILE:HD12	1.75	0.52
1:B:525:ILE:HA	1:B:528:LEU:HD12	1.92	0.52
1:C:873:GLU:N	1:C:874:PRO:HD2	2.23	0.52
1:B:805:ASN:HD22	1:B:805:ASN:N	2.06	0.52
1:A:332:ASN:HD21	1:A:335:GLU:HB2	1.75	0.52
1:A:834:TYR:O	1:A:863:LEU:HD12	2.08	0.52
1:D:415:ASN:C	1:D:415:ASN:OD1	2.47	0.52
1:B:881:GLN:HG3	1:B:885:LEU:O	2.10	0.52
1:C:918:ASN:HD22	1:C:918:ASN:N	2.08	0.52
1:D:545:ARG:NH1	1:D:576:PHE:O	2.43	0.52
1:A:563:LEU:HA	1:A:696:GLY:HA2	1.92	0.52
1:C:658:THR:HB	1:C:682:TYR:HA	1.92	0.52
1:C:726:LEU:HD22	1:C:819:VAL:HG22	1.91	0.52
1:C:920:HIS:HB2	3:C:1201:UDP:O2B	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:688:TYR:CD2	1:D:1027:ILE:HG22	2.45	0.52
1:A:318:ASP:O	1:A:322:ASN:ND2	2.43	0.51
1:A:443:ARG:NH1	1:A:443:ARG:HG2	2.06	0.51
1:A:658:THR:HB	1:A:682:TYR:HA	1.90	0.51
1:B:314:PRO:O	1:B:318:ASP:HB2	2.10	0.51
1:B:772:ILE:HD12	1:B:772:ILE:H	1.76	0.51
1:B:335:GLU:OE1	1:B:335:GLU:HA	2.11	0.51
1:D:844:ASP:HB2	1:D:845:PRO:CD	2.40	0.51
3:A:1201:UDP:O2	2:I:4:VAL:HG11	2.10	0.51
1:A:644:ARG:N	1:A:645:PRO:HD3	2.25	0.51
1:C:515:GLU:HA	1:C:660:GLY:O	2.11	0.51
1:D:350:PHE:C	1:D:350:PHE:HD1	2.14	0.51
1:D:557:ASN:O	2:L:5:PRO:HG3	2.11	0.51
1:A:624:HIS:O	1:A:647:PRO:HG2	2.10	0.51
1:D:590:ASN:HD22	1:D:811:GLU:HB3	1.76	0.51
1:B:344:LEU:HD21	1:B:353:ALA:HB3	1.93	0.51
1:D:333:ILE:O	1:D:334:GLU:C	2.49	0.51
1:D:519:ASN:HA	1:D:522:LEU:HD12	1.92	0.51
1:D:743:ILE:HG22	1:D:743:ILE:O	2.10	0.51
1:A:725:VAL:O	1:A:726:LEU:HD23	2.11	0.50
1:D:667:ILE:HG22	1:D:684:GLU:HB2	1.93	0.50
1:D:703:PRO:HD2	1:D:813:VAL:HG22	1.93	0.50
1:D:881:GLN:HG3	1:D:885:LEU:O	2.11	0.50
1:B:762:LEU:O	1:B:763:ASN:HB3	2.11	0.50
1:C:719:ILE:CG2	1:C:719:ILE:O	2.59	0.50
1:A:333:ILE:O	1:A:334:GLU:C	2.49	0.50
1:A:963:ARG:O	1:A:967:GLU:HG3	2.12	0.50
1:B:662:LEU:N	1:B:662:LEU:HD12	2.13	0.50
1:D:426:ALA:HB2	1:D:441:SER:CB	2.38	0.50
1:B:457:CYS:SG	1:B:494:SER:HB3	2.51	0.50
1:D:731:LEU:O	1:D:734:PHE:HB3	2.11	0.50
1:D:822:ARG:HB3	1:D:827:LEU:HB2	1.93	0.50
1:A:434:ASN:HB2	1:A:437:GLU:HG2	1.91	0.50
1:B:822:ARG:HB3	1:B:827:LEU:HB2	1.94	0.50
1:B:367:LEU:N	1:B:367:LEU:CD2	2.74	0.50
1:B:805:ASN:N	1:B:805:ASN:ND2	2.59	0.50
1:C:788:THR:O	1:C:789:ILE:HG13	2.11	0.50
1:C:318:ASP:O	1:C:322:ASN:ND2	2.45	0.50
1:D:318:ASP:O	1:D:322:ASN:ND2	2.45	0.50
1:D:515:GLU:HA	1:D:660:GLY:O	2.11	0.50
1:D:742:LYS:HE3	1:D:768:PRO:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:PHE:O	1:A:592:ARG:HD3	2.11	0.50
1:A:566:SER:HB2	1:A:697:ASP:OD1	2.12	0.50
1:A:825:TYR:CE2	1:A:904:ARG:HD2	2.46	0.50
1:A:465:ILE:HA	1:A:841:TYR:HB3	1.94	0.50
1:B:1002:TYR:CD1	1:B:1002:TYR:C	2.85	0.50
1:D:435:ILE:HB	1:D:436:PRO:HD3	1.93	0.50
1:A:559:PRO:HA	1:A:562:HIS:ND1	2.27	0.49
1:C:673:THR:HG22	1:C:941:LEU:HG	1.93	0.49
1:D:512:ALA:O	1:D:516:ARG:HG2	2.12	0.49
1:A:324:ALA:HB2	1:A:339:LEU:CB	2.42	0.49
1:C:704:HIS:CD2	1:C:814:PRO:HG2	2.47	0.49
1:C:835:CYS:SG	1:C:911:CYS:HB2	2.53	0.49
1:D:324:ALA:HB2	1:D:339:LEU:CB	2.41	0.49
1:A:911:CYS:HB2	1:A:926:VAL:HG21	1.94	0.49
1:D:468:ASP:O	1:D:475:ARG:NH2	2.39	0.49
1:A:539:LEU:HD21	1:A:1014:TRP:CE2	2.48	0.49
1:B:742:LYS:HE3	1:B:768:PRO:HB3	1.93	0.49
1:C:689:MET:HB3	1:C:690:PRO:HD2	1.95	0.49
1:C:742:LYS:HE3	1:C:768:PRO:HB3	1.95	0.49
1:D:704:HIS:O	1:D:727:ASN:HB3	2.13	0.49
1:B:576:PHE:CE2	1:B:1007:GLU:HG2	2.48	0.49
1:B:707:LYS:HE2	1:B:762:LEU:HD22	1.95	0.49
1:B:967:GLU:O	1:B:971:VAL:HG23	2.13	0.49
1:C:834:TYR:HA	1:C:910:VAL:O	2.13	0.49
1:D:342:LYS:O	1:D:346:VAL:HG23	2.13	0.49
1:A:738:LEU:HD22	1:A:739:PRO:HD2	1.93	0.49
1:B:333:ILE:O	1:B:334:GLU:C	2.51	0.49
1:C:457:CYS:SG	1:C:494:SER:HB3	2.52	0.49
1:D:322:ASN:HA	1:D:325:ASN:HD22	1.76	0.49
1:D:465:ILE:HG22	1:D:465:ILE:O	2.12	0.49
1:D:707:LYS:HE2	1:D:762:LEU:CD2	2.42	0.49
1:D:873:GLU:N	1:D:874:PRO:HD2	2.26	0.49
1:B:703:PRO:HD2	1:B:813:VAL:HG22	1.94	0.49
1:A:492:LEU:HD12	1:A:493:PRO:HD2	1.95	0.48
1:B:342:LYS:O	1:B:346:VAL:HG23	2.12	0.48
1:C:714:LYS:NZ	1:C:719:ILE:N	2.60	0.48
1:D:319:SER:O	1:D:323:LEU:HG	2.13	0.48
1:D:562:HIS:ND1	1:D:898:LYS:HE2	2.28	0.48
1:A:408:TYR:CE1	1:A:424:ASN:HB3	2.48	0.48
1:A:864:TRP:O	1:A:865:LEU:HD23	2.13	0.48
1:C:412:ILE:HD13	1:C:422:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:HIS:O	1:B:501:MET:HE3	2.13	0.48
1:B:846:SER:HB2	1:B:963:ARG:HH21	1.77	0.48
1:D:329:GLU:HA	1:D:329:GLU:OE1	2.12	0.48
1:D:772:ILE:O	1:D:773:ALA:C	2.51	0.48
1:B:719:ILE:O	1:B:719:ILE:HG22	2.13	0.48
1:C:1000:LYS:O	1:C:1004:MET:HG3	2.13	0.48
1:C:434:ASN:HB2	1:C:437:GLU:HG2	1.95	0.48
1:B:667:ILE:HG22	1:B:684:GLU:HB2	1.94	0.48
1:A:796:ASN:O	1:A:798:LEU:N	2.44	0.48
1:C:607:GLN:HA	1:C:607:GLN:OE1	2.13	0.48
1:C:956:LEU:HD12	1:C:956:LEU:H	1.78	0.48
1:A:312:SER:O	1:A:314:PRO:HD3	2.14	0.48
1:B:340:TYR:CZ	1:B:356:ASN:HB3	2.48	0.48
1:B:822:ARG:NH2	1:B:909:ASP:OD2	2.45	0.48
3:D:1201:UDP:O2A	2:L:7:SER:HB2	2.14	0.48
1:A:697:ASP:HB3	1:A:701:MET:HG3	1.95	0.48
1:B:881:GLN:NE2	1:B:887:GLN:HA	2.28	0.48
1:D:330:GLN:O	1:D:332:ASN:N	2.46	0.48
1:A:704:HIS:O	1:A:727:ASN:HB3	2.14	0.47
1:B:519:ASN:HA	1:B:522:LEU:HD12	1.95	0.47
1:C:510:ARG:NH1	1:C:510:ARG:HG3	2.28	0.47
1:D:815:ARG:NH1	1:D:815:ARG:HG3	2.29	0.47
1:A:785:ILE:CG2	1:A:786:GLN:HG2	2.45	0.47
1:B:697:ASP:HB3	1:B:701:MET:HG3	1.96	0.47
1:D:697:ASP:HB3	1:D:701:MET:HG3	1.95	0.47
1:A:860:ASN:HB2	1:B:1016:HIS:CE1	2.49	0.47
1:D:660:GLY:HA2	1:D:683:SER:CB	2.43	0.47
1:D:714:LYS:NZ	1:D:719:ILE:N	2.63	0.47
1:D:937:PRO:HA	1:D:943:SER:O	2.15	0.47
1:A:443:ARG:NH1	1:A:443:ARG:CG	2.70	0.47
1:C:333:ILE:O	1:C:334:GLU:C	2.53	0.47
1:C:342:LYS:O	1:C:346:VAL:HG23	2.15	0.47
1:A:805:ASN:N	1:A:805:ASN:HD22	2.13	0.47
1:D:525:ILE:O	1:D:528:LEU:HB2	2.13	0.47
1:A:545:ARG:NH1	1:A:576:PHE:O	2.47	0.47
1:A:688:TYR:CD2	1:A:1027:ILE:HG22	2.49	0.47
1:B:616:ASP:O	1:B:620:GLN:HB2	2.15	0.47
1:B:669:THR:OG1	1:B:670:ASP:N	2.47	0.47
1:C:350:PHE:C	1:C:350:PHE:CD1	2.86	0.47
1:C:743:ILE:HG22	1:C:743:ILE:O	2.14	0.47
1:D:465:ILE:CG2	1:D:465:ILE:O	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:566:SER:HB2	1:D:697:ASP:OD1	2.14	0.47
1:B:435:ILE:N	1:B:436:PRO:CD	2.77	0.47
1:A:408:TYR:O	1:A:412:ILE:HG13	2.15	0.47
1:C:324:ALA:HA	1:C:339:LEU:HD12	1.95	0.47
1:C:443:ARG:HG2	1:C:443:ARG:NH1	2.11	0.47
1:A:613:LYS:O	1:A:616:ASP:HB2	2.14	0.47
1:B:468:ASP:O	1:B:475:ARG:NH2	2.35	0.47
1:B:660:GLY:HA2	1:B:683:SER:CB	2.44	0.47
1:C:688:TYR:CD2	1:C:1027:ILE:HG22	2.50	0.47
1:C:734:PHE:HE1	1:C:789:ILE:HG22	1.80	0.47
1:A:725:VAL:C	1:A:726:LEU:HD23	2.35	0.47
1:B:695:ILE:HB	1:B:1002:TYR:CE2	2.50	0.47
1:B:319:SER:HA	1:B:322:ASN:HD22	1.79	0.46
1:C:764:MET:HA	1:C:765:PRO:HD2	1.79	0.46
1:C:844:ASP:HB2	1:C:845:PRO:HD2	1.95	0.46
1:D:941:LEU:C	1:D:941:LEU:HD23	2.35	0.46
1:A:596:MET:HG2	1:A:602:PHE:CG	2.50	0.46
1:B:695:ILE:HG13	1:B:696:GLY:H	1.79	0.46
1:B:713:PHE:N	1:B:713:PHE:HD1	1.83	0.46
3:B:1201:UDP:O2A	2:J:7:SER:HB2	2.14	0.46
1:A:638:ASN:O	1:A:641:PHE:N	2.48	0.46
1:B:329:GLU:C	1:B:331:GLY:H	2.19	0.46
1:B:415:ASN:C	1:B:415:ASN:OD1	2.51	0.46
1:C:465:ILE:CG2	1:C:465:ILE:O	2.63	0.46
1:C:512:ALA:O	1:C:516:ARG:HG2	2.15	0.46
2:I:4:VAL:CG1	2:I:5:PRO:HD2	2.43	0.46
1:A:772:ILE:O	1:A:773:ALA:C	2.50	0.46
1:D:785:ILE:HG22	1:D:786:GLN:HG2	1.96	0.46
1:A:342:LYS:O	1:A:346:VAL:HG23	2.15	0.46
1:D:896:ALA:HB1	1:D:897:PRO:HD2	1.97	0.46
1:D:911:CYS:O	1:D:933:MET:HA	2.16	0.46
1:B:357:LEU:HD23	1:B:373:HIS:CE1	2.51	0.46
1:D:629:MET:O	1:D:654:GLY:HA3	2.16	0.46
1:A:426:ALA:HB2	1:A:441:SER:CB	2.40	0.46
1:A:719:ILE:HG22	1:A:719:ILE:O	2.16	0.46
1:C:530:LYS:HE2	1:C:533:TYR:OH	2.16	0.46
1:A:428:ILE:HD12	1:A:428:ILE:HG23	1.43	0.46
1:A:655:TYR:HA	1:A:656:PRO:HD3	1.70	0.46
1:A:969:ILE:O	1:A:973:LEU:HD12	2.16	0.46
1:B:330:GLN:H	1:B:330:GLN:HG3	1.58	0.46
1:B:496:HIS:CG	1:B:497:PRO:HD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:LEU:HD22	1:C:637:ARG:HD3	1.98	0.46
1:D:764:MET:HB3	1:D:764:MET:HE3	1.83	0.46
1:A:512:ALA:O	1:A:516:ARG:HG2	2.16	0.46
1:B:461:HIS:O	1:B:465:ILE:HG13	2.15	0.46
1:C:519:ASN:HA	1:C:522:LEU:HD12	1.97	0.46
2:K:8:SER:O	2:K:9:ALA:O	2.34	0.46
1:B:629:MET:O	1:B:654:GLY:HA3	2.16	0.46
1:D:1011:LEU:HA	1:D:1011:LEU:HD23	1.72	0.46
1:B:562:HIS:ND1	1:B:898:LYS:HE2	2.31	0.45
1:C:357:LEU:HD23	1:C:373:HIS:CE1	2.51	0.45
1:C:402:GLN:HE21	1:C:406:GLN:NE2	2.14	0.45
1:A:950:LEU:HD23	1:A:950:LEU:HA	1.67	0.45
1:B:607:GLN:HA	1:B:607:GLN:OE1	2.16	0.45
1:C:330:GLN:O	1:C:332:ASN:N	2.49	0.45
1:C:703:PRO:HD2	1:C:813:VAL:HG22	1.98	0.45
1:C:844:ASP:HB2	1:C:845:PRO:CD	2.46	0.45
1:D:434:ASN:HB2	1:D:437:GLU:HG2	1.96	0.45
1:A:689:MET:HB3	1:A:690:PRO:HD2	1.98	0.45
1:C:545:ARG:NH1	1:C:576:PHE:O	2.49	0.45
1:C:965:GLU:O	1:C:969:ILE:HG13	2.16	0.45
1:A:979:TYR:O	1:A:982:LYS:HB3	2.16	0.45
1:B:994:SER:CB	1:B:995:PRO:HD3	2.36	0.45
1:D:496:HIS:CG	1:D:497:PRO:HD2	2.51	0.45
1:A:462:CYS:O	1:A:465:ILE:HB	2.15	0.45
1:A:525:ILE:HA	1:A:528:LEU:HD12	1.98	0.45
1:A:638:ASN:O	1:A:639:GLU:C	2.54	0.45
1:A:918:ASN:N	1:A:918:ASN:ND2	2.62	0.45
1:D:555:PHE:O	1:D:592:ARG:HD3	2.17	0.45
1:B:330:GLN:O	1:B:332:ASN:N	2.49	0.45
1:B:704:HIS:NE2	1:B:814:PRO:HG2	2.32	0.45
1:C:963:ARG:O	1:C:967:GLU:HG3	2.16	0.45
1:B:617:ARG:HD2	1:B:617:ARG:HA	1.79	0.45
1:C:704:HIS:ND1	1:C:704:HIS:N	2.61	0.45
1:D:412:ILE:HD13	1:D:422:HIS:CE1	2.52	0.45
1:D:468:ASP:OD1	1:D:468:ASP:C	2.54	0.45
1:A:644:ARG:HH22	1:A:665:ASP:CG	2.20	0.45
1:A:723:ARG:O	1:A:724:ILE:HG13	2.16	0.45
1:A:885:LEU:HA	1:A:886:PRO:HD2	1.79	0.45
1:B:553:SER:HA	1:B:583:LEU:HB2	1.99	0.45
1:B:704:HIS:O	1:B:727:ASN:HB3	2.16	0.45
1:C:498:HIS:O	1:C:501:MET:HE3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:596:MET:HG2	1:C:602:PHE:CG	2.51	0.45
1:D:655:TYR:HA	1:D:656:PRO:HD3	1.74	0.45
1:D:617:ARG:HD2	1:D:617:ARG:HA	1.77	0.45
1:A:412:ILE:HD13	1:A:422:HIS:CE1	2.52	0.45
1:A:503:TYR:HB3	1:A:504:PRO:HD2	1.99	0.45
1:D:867:ARG:HB3	1:D:870:ALA:HA	1.98	0.45
1:D:846:SER:HB2	1:D:963:ARG:NH2	2.30	0.45
1:A:772:ILE:HD12	1:A:772:ILE:H	1.81	0.44
1:C:437:GLU:CD	1:C:437:GLU:H	2.19	0.44
1:D:596:MET:HG2	1:D:602:PHE:CG	2.51	0.44
1:D:695:ILE:HG13	1:D:696:GLY:N	2.31	0.44
1:D:774:GLU:HA	1:D:777:ILE:CG2	2.48	0.44
1:A:829:GLU:H	1:A:829:GLU:HG2	1.56	0.44
1:A:726:LEU:HD22	1:A:819:VAL:HG22	1.97	0.44
1:B:686:LEU:HD23	1:B:686:LEU:N	2.33	0.44
1:B:815:ARG:NH1	1:B:815:ARG:HG3	2.32	0.44
1:C:372:MET:HB2	1:C:372:MET:HE2	1.87	0.44
1:C:596:MET:HG2	1:C:602:PHE:CD1	2.52	0.44
1:D:972:LYS:HG2	1:D:979:TYR:CD2	2.52	0.44
1:B:557:ASN:HB2	1:B:589:THR:HG21	2.00	0.44
1:B:918:ASN:HD22	1:B:918:ASN:N	2.13	0.44
1:C:487:LEU:O	1:C:516:ARG:NH2	2.49	0.44
1:C:604:ASP:C	1:C:604:ASP:OD1	2.54	0.44
1:C:846:SER:HB2	1:C:963:ARG:HH21	1.81	0.44
1:B:320:LEU:HA	1:B:323:LEU:HD12	1.98	0.44
1:B:764:MET:HA	1:B:765:PRO:HD2	1.82	0.44
1:B:770:ASN:N	1:B:770:ASN:OD1	2.48	0.44
1:B:940:THR:O	1:B:941:LEU:C	2.56	0.44
1:C:1015:GLU:CA	1:C:1015:GLU:OE1	2.56	0.44
1:D:1002:TYR:CD1	1:D:1002:TYR:C	2.91	0.44
1:B:412:ILE:HD13	1:B:422:HIS:CE1	2.53	0.44
1:B:695:ILE:HD13	1:B:1002:TYR:CD2	2.53	0.44
1:D:896:ALA:HB1	1:D:897:PRO:CD	2.47	0.44
2:J:4:VAL:CG1	2:J:5:PRO:HD2	2.48	0.44
1:A:558:HIS:CG	1:A:559:PRO:HD2	2.53	0.44
1:A:859:PRO:CG	1:B:1016:HIS:ND1	2.80	0.44
1:B:877:GLN:O	1:B:880:ALA:HB3	2.18	0.44
1:C:350:PHE:C	1:C:350:PHE:HD1	2.21	0.44
1:C:430:LYS:HE2	1:C:462:CYS:SG	2.58	0.44
1:D:918:ASN:HD22	1:D:918:ASN:N	2.16	0.44
1:B:520:LEU:HA	1:B:520:LEU:HD23	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:725:VAL:O	1:C:726:LEU:HD23	2.17	0.44
1:D:461:HIS:O	1:D:464:GLN:HB3	2.18	0.44
1:B:1000:LYS:O	1:B:1004:MET:HG3	2.17	0.44
1:B:731:LEU:O	1:B:734:PHE:HB3	2.17	0.44
1:B:941:LEU:HD23	1:B:941:LEU:C	2.39	0.44
1:C:827:LEU:HA	1:C:828:PRO:HD2	1.78	0.44
1:C:990:GLN:CA	1:C:990:GLN:HE21	2.29	0.44
1:B:443:ARG:HG2	1:B:443:ARG:NH1	2.16	0.43
1:B:511:LYS:O	1:B:515:GLU:HB2	2.18	0.43
1:B:559:PRO:O	1:B:560:THR:C	2.55	0.43
1:B:743:ILE:O	1:B:743:ILE:HG22	2.18	0.43
1:B:867:ARG:HB3	1:B:870:ALA:HA	1.99	0.43
1:D:865:LEU:O	1:D:892:PHE:HA	2.18	0.43
1:A:322:ASN:HA	1:A:325:ASN:HD22	1.83	0.43
1:A:704:HIS:CD2	1:A:814:PRO:HG2	2.53	0.43
1:B:596:MET:HG2	1:B:602:PHE:CG	2.53	0.43
1:D:491:ARG:HA	1:D:491:ARG:HD2	1.74	0.43
1:A:487:LEU:O	1:A:516:ARG:NH2	2.50	0.43
1:A:539:LEU:N	1:A:539:LEU:HD23	2.32	0.43
1:A:618:ILE:O	1:A:621:ASP:N	2.43	0.43
1:C:738:LEU:HA	1:C:739:PRO:HD2	1.79	0.43
1:C:834:TYR:O	1:C:863:LEU:HD12	2.18	0.43
1:C:877:GLN:O	1:C:880:ALA:HB3	2.18	0.43
1:B:796:ASN:O	1:B:798:LEU:N	2.50	0.43
1:B:911:CYS:HB2	1:B:926:VAL:HG21	2.00	0.43
1:C:562:HIS:ND1	1:C:898:LYS:HE2	2.34	0.43
1:B:398:MET:O	1:B:399:GLN:HB2	2.18	0.43
1:B:535:HIS:HB3	1:B:647:PRO:HD3	1.99	0.43
1:C:629:MET:O	1:C:654:GLY:HA3	2.17	0.43
1:C:822:ARG:HB3	1:C:827:LEU:HB2	2.01	0.43
1:C:885:LEU:HA	1:C:886:PRO:HD2	1.72	0.43
1:D:686:LEU:HD23	1:D:686:LEU:N	2.34	0.43
1:D:780:ILE:HG23	1:D:780:ILE:HD12	1.73	0.43
1:A:357:LEU:HD23	1:A:373:HIS:CE1	2.53	0.43
1:D:858:VAL:HG22	1:D:975:THR:HG23	2.00	0.43
3:A:1201:UDP:O2A	2:I:7:SER:HB2	2.18	0.43
1:A:1011:LEU:HA	1:A:1011:LEU:HD23	1.60	0.43
1:A:317:ALA:HB2	1:A:346:VAL:HB	2.00	0.43
1:A:860:ASN:OD1	1:B:1024:ASP:HB2	2.19	0.43
1:A:945:VAL:O	1:A:949:GLN:HG3	2.19	0.43
1:C:340:TYR:CZ	1:C:356:ASN:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:ILE:HG22	1:C:465:ILE:O	2.18	0.43
1:D:965:GLU:O	1:D:969:ILE:HG13	2.19	0.43
1:C:667:ILE:HG22	1:C:684:GLU:HB2	2.01	0.43
1:C:858:VAL:HG22	1:C:975:THR:HG23	2.01	0.43
1:D:590:ASN:ND2	1:D:811:GLU:HB3	2.32	0.43
1:A:617:ARG:HD2	1:A:617:ARG:HA	1.86	0.43
1:A:805:ASN:ND2	1:A:805:ASN:N	2.67	0.43
1:B:371:LEU:O	1:B:371:LEU:HD12	2.18	0.43
1:B:399:GLN:HA	1:B:399:GLN:OE1	2.19	0.43
1:B:408:TYR:CE1	1:B:424:ASN:HB3	2.53	0.43
1:B:566:SER:HB2	1:B:697:ASP:OD1	2.19	0.43
1:B:710:VAL:HG12	1:B:724:ILE:O	2.19	0.43
1:B:937:PRO:HB2	1:B:944:ARG:NH1	2.34	0.43
1:B:936:MET:HB2	1:B:966:TYR:CD2	2.54	0.43
1:C:1011:LEU:HA	1:C:1011:LEU:HD23	1.65	0.43
1:C:399:GLN:HA	1:C:399:GLN:OE1	2.18	0.43
1:D:367:LEU:HD23	1:D:367:LEU:H	1.83	0.43
1:D:638:ASN:O	1:D:639:GLU:C	2.57	0.43
1:D:834:TYR:HA	1:D:910:VAL:O	2.19	0.43
1:A:859:PRO:O	1:B:1024:ASP:OD2	2.36	0.43
1:B:1027:ILE:H	1:B:1027:ILE:HG12	1.78	0.43
1:B:742:LYS:H	1:B:742:LYS:HG2	1.49	0.43
1:B:834:TYR:HA	1:B:910:VAL:O	2.19	0.42
1:C:501:MET:HB3	1:C:501:MET:HE3	1.75	0.42
1:C:697:ASP:HB3	1:C:701:MET:HG3	2.01	0.42
1:D:625:ILE:HG12	1:D:648:ILE:HB	2.01	0.42
1:B:625:ILE:HG12	1:B:648:ILE:HB	2.00	0.42
1:C:723:ARG:HH21	1:C:830:ASP:HA	1.84	0.42
1:D:714:LYS:HB2	1:D:714:LYS:HE2	1.95	0.42
1:A:873:GLU:N	1:A:874:PRO:HD2	2.34	0.42
1:A:860:ASN:HA	1:B:1024:ASP:OD2	2.19	0.42
1:B:424:ASN:O	1:B:427:SER:HB2	2.19	0.42
1:B:918:ASN:ND2	1:B:943:SER:HA	2.34	0.42
1:C:330:GLN:HG3	1:C:330:GLN:H	1.57	0.42
1:B:707:LYS:HE2	1:B:762:LEU:CD2	2.49	0.42
1:C:977:LEU:N	1:C:977:LEU:HD23	2.35	0.42
2:K:5:PRO:O	2:K:5:PRO:HG2	2.18	0.42
1:A:491:ARG:HD2	1:A:491:ARG:HA	1.78	0.42
1:A:660:GLY:HA2	1:A:683:SER:CB	2.50	0.42
1:C:361:LEU:HA	1:C:361:LEU:HD23	1.86	0.42
1:D:738:LEU:HD23	1:D:738:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:GLN:NE2	1:A:887:GLN:HA	2.33	0.42
1:B:522:LEU:HD23	1:B:525:ILE:HD11	2.02	0.42
1:C:525:ILE:O	1:C:528:LEU:HB2	2.20	0.42
1:D:742:LYS:CE	1:D:768:PRO:HB3	2.50	0.42
1:D:740:ASP:CB	1:D:768:PRO:HG3	2.45	0.42
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.85	0.42
1:A:926:VAL:CG1	1:A:927:LEU:N	2.82	0.42
1:D:405:LEU:HD12	1:D:405:LEU:HA	1.85	0.42
1:A:704:HIS:ND1	1:A:704:HIS:N	2.67	0.42
1:C:804:ASN:OD1	1:C:804:ASN:C	2.58	0.42
1:C:986:LYS:O	1:C:990:GLN:CG	2.68	0.42
1:D:561:SER:O	1:D:565:GLN:HG2	2.19	0.42
1:B:863:LEU:HD12	1:B:864:TRP:H	1.85	0.42
1:B:885:LEU:HA	1:B:886:PRO:HD2	1.77	0.42
1:C:774:GLU:O	1:C:778:GLU:HB2	2.19	0.42
1:A:617:ARG:O	1:A:620:GLN:HB3	2.20	0.42
1:B:405:LEU:HD12	1:B:405:LEU:HA	1.70	0.42
1:B:545:ARG:NH1	1:B:576:PHE:O	2.53	0.42
1:C:626:LEU:HD12	1:C:626:LEU:HA	1.80	0.42
1:D:330:GLN:H	1:D:330:GLN:HG3	1.68	0.42
1:A:525:ILE:O	1:A:528:LEU:HB2	2.20	0.41
1:B:936:MET:HB2	1:B:966:TYR:HD2	1.85	0.41
1:C:491:ARG:HD2	1:C:491:ARG:HA	1.68	0.41
1:C:539:LEU:HD21	1:C:1014:TRP:CE2	2.55	0.41
1:A:986:LYS:O	1:A:990:GLN:HG2	2.20	0.41
1:C:960:ALA:HB1	1:C:965:GLU:HB3	2.02	0.41
1:D:930:GLY:HA2	1:D:987:VAL:HG12	2.03	0.41
1:B:572:ASN:HA	1:B:573:PRO:HD2	1.81	0.41
1:D:335:GLU:O	1:D:336:ALA:C	2.57	0.41
1:D:405:LEU:HD13	1:D:428:ILE:HG21	2.01	0.41
1:D:815:ARG:HH11	1:D:815:ARG:CG	2.33	0.41
1:A:625:ILE:HD13	1:A:625:ILE:HG21	1.90	0.41
1:B:468:ASP:C	1:B:468:ASP:OD1	2.58	0.41
1:B:539:LEU:N	1:B:539:LEU:HD23	2.34	0.41
1:B:625:ILE:HG21	1:B:625:ILE:HD13	1.89	0.41
1:C:480:VAL:HG13	1:C:505:LEU:HD23	2.00	0.41
1:C:522:LEU:HD23	1:C:525:ILE:HD11	2.02	0.41
1:D:780:ILE:HA	1:D:780:ILE:HD13	1.94	0.41
1:B:813:VAL:HG13	1:B:814:PRO:HD2	2.03	0.41
1:C:566:SER:HB2	1:C:697:ASP:OD1	2.21	0.41
1:A:330:GLN:H	1:A:330:GLN:HG3	1.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:TYR:HA	1:A:910:VAL:O	2.20	0.41
1:A:940:THR:O	1:A:941:LEU:C	2.59	0.41
1:B:700:ASN:O	1:B:703:PRO:HD3	2.20	0.41
1:B:846:SER:HB2	1:B:963:ARG:NH2	2.36	0.41
1:C:426:ALA:HB2	1:C:441:SER:CB	2.48	0.41
1:C:719:ILE:HG22	1:C:719:ILE:O	2.20	0.41
1:C:928:TRP:O	1:C:991:ARG:NH1	2.48	0.41
1:D:886:PRO:HG2	1:D:889:ARG:HG2	2.02	0.41
1:A:530:LYS:HE2	1:A:533:TYR:OH	2.21	0.41
1:A:626:LEU:HD12	1:A:626:LEU:HA	1.76	0.41
1:C:428:ILE:HG23	1:C:428:ILE:HD12	1.71	0.41
1:C:930:GLY:HA2	1:C:987:VAL:HG12	2.03	0.41
1:D:557:ASN:HB2	1:D:589:THR:HG21	2.03	0.41
1:D:626:LEU:HD12	1:D:626:LEU:HA	1.87	0.41
1:D:920:HIS:HB2	3:D:1201:UDP:O2B	2.21	0.41
1:D:950:LEU:HA	1:D:950:LEU:HD23	1.90	0.41
1:B:326:ILE:O	1:B:329:GLU:HB2	2.21	0.41
1:B:555:PHE:O	1:B:592:ARG:HD3	2.21	0.41
1:B:604:ASP:OD1	1:B:604:ASP:C	2.59	0.41
1:B:935:THR:HG23	1:B:937:PRO:HD3	2.02	0.41
1:B:858:VAL:HG22	1:B:975:THR:HG23	2.03	0.41
1:D:670:ASP:OD2	1:D:692:THR:HA	2.20	0.41
1:D:940:THR:O	1:D:941:LEU:C	2.59	0.41
1:A:796:ASN:C	1:A:798:LEU:H	2.24	0.41
1:A:889:ARG:HG3	1:A:889:ARG:HH11	1.85	0.41
1:B:428:ILE:HD12	1:B:428:ILE:HG23	1.54	0.41
1:B:695:ILE:HB	1:B:1002:TYR:CD2	2.56	0.41
1:B:924:MET:H	1:B:924:MET:HG2	1.68	0.41
1:C:617:ARG:HA	1:C:617:ARG:HD2	1.74	0.41
1:C:655:TYR:HA	1:C:656:PRO:HD3	1.71	0.41
1:C:772:ILE:O	1:C:773:ALA:C	2.57	0.41
1:D:465:ILE:HA	1:D:841:TYR:HB3	2.03	0.41
1:D:517:HIS:O	1:D:520:LEU:HB2	2.20	0.41
1:D:815:ARG:HG3	1:D:815:ARG:HH11	1.86	0.41
1:D:881:GLN:NE2	1:D:887:GLN:HA	2.35	0.41
1:A:695:ILE:HG13	1:A:696:GLY:H	1.85	0.40
1:C:328:ARG:NH2	1:C:360:VAL:HG13	2.36	0.40
1:C:401:VAL:O	1:C:402:GLN:C	2.59	0.40
1:A:662:LEU:CD1	1:A:662:LEU:H	2.22	0.40
1:B:430:LYS:HE2	1:B:462:CYS:SG	2.61	0.40
1:B:603:ILE:HG12	1:B:617:ARG:NH2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:ARG:HH22	1:B:665:ASP:CG	2.24	0.40
1:C:405:LEU:HD12	1:C:405:LEU:HA	1.72	0.40
1:C:738:LEU:HD23	1:C:738:LEU:HA	1.81	0.40
1:D:1015:GLU:OE1	1:D:1015:GLU:CA	2.65	0.40
1:D:644:ARG:HH22	1:D:665:ASP:CG	2.25	0.40
1:D:937:PRO:HB2	1:D:944:ARG:NH1	2.35	0.40
1:A:468:ASP:OD1	1:A:468:ASP:C	2.60	0.40
1:A:538:ASP:C	1:A:539:LEU:HD23	2.40	0.40
1:A:697:ASP:OD2	1:A:700:ASN:HB3	2.21	0.40
1:A:866:LEU:HA	1:A:866:LEU:HD23	1.69	0.40
1:B:559:PRO:HA	1:B:562:HIS:ND1	2.36	0.40
1:B:651:MET:HE3	1:B:651:MET:HB3	1.96	0.40
1:C:425:LEU:O	1:C:426:ALA:C	2.59	0.40
1:C:950:LEU:HA	1:C:950:LEU:HD23	1.94	0.40
1:D:449:LYS:HA	1:D:450:PRO:HD3	1.85	0.40
1:D:559:PRO:O	1:D:560:THR:C	2.57	0.40
1:D:828:PRO:HG2	1:D:831:ALA:HB3	2.03	0.40
2:L:8:SER:O	2:L:9:ALA:O	2.40	0.40
1:A:323:LEU:O	1:A:326:ILE:HB	2.21	0.40
1:A:764:MET:HA	1:A:765:PRO:HD2	1.77	0.40
1:A:742:LYS:HE3	1:A:768:PRO:HB3	2.02	0.40
1:B:652:TRP:O	1:B:654:GLY:N	2.47	0.40
1:C:312:SER:O	1:C:314:PRO:HD3	2.20	0.40
1:C:510:ARG:HG3	1:C:510:ARG:HH11	1.86	0.40
1:C:785:ILE:CG2	1:C:786:GLN:HG2	2.51	0.40
1:D:435:ILE:N	1:D:436:PRO:CD	2.83	0.40
1:D:607:GLN:CA	1:D:607:GLN:OE1	2.68	0.40
1:B:491:ARG:HD2	1:B:491:ARG:HA	1.69	0.40
1:B:644:ARG:HA	1:B:649:GLN:OE1	2.22	0.40
1:B:846:SER:O	1:B:849:GLN:HB3	2.22	0.40
1:C:463:LEU:HA	1:C:463:LEU:HD23	1.83	0.40
1:C:772:ILE:HD12	1:C:772:ILE:H	1.87	0.40
1:C:796:ASN:O	1:C:798:LEU:N	2.54	0.40
1:D:983:VAL:O	1:D:986:LYS:HB3	2.21	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	692/723 (96%)	622 (90%)	63 (9%)	7 (1%)	15	51
1	B	692/723 (96%)	623 (90%)	59 (8%)	10 (1%)	11	43
1	C	692/723 (96%)	618 (89%)	65 (9%)	9 (1%)	12	44
1	D	692/723 (96%)	624 (90%)	58 (8%)	10 (1%)	11	43
2	I	9/11 (82%)	6 (67%)	0	3 (33%)	0	0
2	J	9/11 (82%)	6 (67%)	0	3 (33%)	0	0
2	K	9/11 (82%)	6 (67%)	0	3 (33%)	0	0
2	L	9/11 (82%)	6 (67%)	0	3 (33%)	0	0
All	All	2804/2936 (96%)	2511 (90%)	245 (9%)	48 (2%)	9	38

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	2	VAL
2	I	9	ALA
2	J	2	VAL
2	J	9	ALA
2	K	2	VAL
2	K	9	ALA
2	L	2	VAL
2	L	9	ALA
1	A	331	GLY
1	A	334	GLU
1	B	331	GLY
1	B	334	GLU
1	B	763	ASN
1	B	797	GLY
1	C	331	GLY
1	C	334	GLU
1	C	620	GLN

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Mol	Chain	Res	Type
1	C	770	ASN
1	D	331	GLY
1	D	334	GLU
1	D	402	GLN
1	A	620	GLN
1	A	763	ASN
1	A	888	ASN
1	C	763	ASN
1	D	620	GLN
1	D	733	ALA
1	D	763	ASN
2	I	10	GLN
2	J	10	GLN
2	K	10	GLN
2	L	10	GLN
1	A	733	ALA
1	A	770	ASN
1	B	330	GLN
1	B	620	GLN
1	B	733	ALA
1	D	732	LYS
1	D	878	GLN
1	B	888	ASN
1	C	402	GLN
1	B	878	GLN
1	C	639	GLU
1	B	504	PRO
1	C	504	PRO
1	C	656	PRO
1	D	772	ILE
1	D	504	PRO

5.3.2 Protein sidechains (i)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	600/618 (97%)	535 (89%)	65 (11%)	6 25
1	B	600/618 (97%)	535 (89%)	65 (11%)	6 25
1	C	600/618 (97%)	537 (90%)	63 (10%)	7 26
1	D	600/618 (97%)	537 (90%)	63 (10%)	7 26
2	I	10/10 (100%)	8 (80%)	2 (20%)	1 6
2	J	10/10 (100%)	7 (70%)	3 (30%)	0 1
2	K	10/10 (100%)	7 (70%)	3 (30%)	0 1
2	L	10/10 (100%)	7 (70%)	3 (30%)	0 1
All	All	2440/2512 (97%)	2173 (89%)	267 (11%)	6 24

All (267) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	312	SER
1	A	315	THR
1	A	319	SER
1	A	330	GLN
1	A	350	PHE
1	A	360	VAL
1	A	371	LEU
1	A	375	LYS
1	A	383	THR
1	A	384	PHE
1	A	401	VAL
1	A	406	GLN
1	A	410	ARG
1	A	434	ASN
1	A	441	SER
1	A	443	ARG
1	A	447	LYS
1	A	452	PHE
1	A	481	SER
1	A	491	ARG
1	A	494	SER
1	A	501	MET
1	A	515	GLU
1	A	537	LYS

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Mol	Chain	Res	Type
1	A	541	LEU
1	A	607	GLN
1	A	634	LYS
1	A	644	ARG
1	A	662	LEU
1	A	667	ILE
1	A	669	THR
1	A	671	GLN
1	A	694	PHE
1	A	697	ASP
1	A	704	HIS
1	A	710	VAL
1	A	713	PHE
1	A	719	ILE
1	A	727	ASN
1	A	732	LYS
1	A	742	LYS
1	A	770	ASN
1	A	771	THR
1	A	778	GLU
1	A	793	SER
1	A	800	THR
1	A	805	ASN
1	A	820	THR
1	A	832	ILE
1	A	846	SER
1	A	862	VAL
1	A	868	PHE
1	A	871	VAL
1	A	914	THR
1	A	918	ASN
1	A	926	VAL
1	A	936	MET
1	A	978	GLU
1	A	981	LYS
1	A	990	GLN
1	A	991	ARG
1	A	1015	GLU
1	A	1022	LYS
1	A	1027	ILE
1	A	1028	LYS
1	B	315	THR

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Mol	Chain	Res	Type
1	B	319	SER
1	B	330	GLN
1	B	338	ARG
1	B	342	LYS
1	B	350	PHE
1	B	360	VAL
1	B	367	LEU
1	B	371	LEU
1	B	372	MET
1	B	375	LYS
1	B	384	PHE
1	B	401	VAL
1	B	406	GLN
1	B	410	ARG
1	B	420	ASP
1	B	434	ASN
1	B	441	SER
1	B	443	ARG
1	B	447	LYS
1	B	452	PHE
1	B	481	SER
1	B	488	GLU
1	B	491	ARG
1	B	494	SER
1	B	501	MET
1	B	515	GLU
1	B	537	LYS
1	B	541	LEU
1	B	545	ARG
1	B	630	ASN
1	B	634	LYS
1	B	644	ARG
1	B	662	LEU
1	B	667	ILE
1	B	671	GLN
1	B	694	PHE
1	B	704	HIS
1	B	710	VAL
1	B	713	PHE
1	B	719	ILE
1	B	727	ASN
1	B	732	LYS

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Mol	Chain	Res	Type
1	B	742	LYS
1	B	743	ILE
1	B	764	MET
1	B	770	ASN
1	B	771	THR
1	B	793	SER
1	B	800	THR
1	B	805	ASN
1	B	820	THR
1	B	832	ILE
1	B	846	SER
1	B	868	PHE
1	B	871	VAL
1	B	914	THR
1	B	936	MET
1	B	978	GLU
1	B	981	LYS
1	B	990	GLN
1	B	991	ARG
1	B	1022	LYS
1	B	1027	ILE
1	B	1028	LYS
1	C	315	THR
1	C	319	SER
1	C	330	GLN
1	C	350	PHE
1	C	360	VAL
1	C	371	LEU
1	C	375	LYS
1	C	383	THR
1	C	384	PHE
1	C	401	VAL
1	C	406	GLN
1	C	410	ARG
1	C	420	ASP
1	C	434	ASN
1	C	441	SER
1	C	443	ARG
1	C	447	LYS
1	C	452	PHE
1	C	481	SER
1	C	488	GLU

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Mol	Chain	Res	Type
1	C	491	ARG
1	C	494	SER
1	C	501	MET
1	C	515	GLU
1	C	537	LYS
1	C	541	LEU
1	C	545	ARG
1	C	617	ARG
1	C	630	ASN
1	C	634	LYS
1	C	644	ARG
1	C	662	LEU
1	C	669	THR
1	C	671	GLN
1	C	694	PHE
1	C	697	ASP
1	C	704	HIS
1	C	713	PHE
1	C	719	ILE
1	C	727	ASN
1	C	732	LYS
1	C	742	LYS
1	C	743	ILE
1	C	764	MET
1	C	770	ASN
1	C	771	THR
1	C	805	ASN
1	C	820	THR
1	C	832	ILE
1	C	846	SER
1	C	868	PHE
1	C	871	VAL
1	C	881	GLN
1	C	914	THR
1	C	926	VAL
1	C	936	MET
1	C	978	GLU
1	C	981	LYS
1	C	990	GLN
1	C	991	ARG
1	C	1022	LYS
1	C	1027	ILE

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Mol	Chain	Res	Type
1	C	1028	LYS
1	D	315	THR
1	D	319	SER
1	D	330	GLN
1	D	338	ARG
1	D	346	VAL
1	D	350	PHE
1	D	360	VAL
1	D	371	LEU
1	D	372	MET
1	D	375	LYS
1	D	383	THR
1	D	384	PHE
1	D	401	VAL
1	D	406	GLN
1	D	410	ARG
1	D	420	ASP
1	D	434	ASN
1	D	441	SER
1	D	443	ARG
1	D	447	LYS
1	D	452	PHE
1	D	481	SER
1	D	488	GLU
1	D	491	ARG
1	D	494	SER
1	D	501	MET
1	D	515	GLU
1	D	537	LYS
1	D	541	LEU
1	D	545	ARG
1	D	630	ASN
1	D	634	LYS
1	D	644	ARG
1	D	662	LEU
1	D	667	ILE
1	D	671	GLN
1	D	694	PHE
1	D	697	ASP
1	D	704	HIS
1	D	713	PHE
1	D	719	ILE

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Mol	Chain	Res	Type
1	D	727	ASN
1	D	732	LYS
1	D	742	LYS
1	D	764	MET
1	D	770	ASN
1	D	771	THR
1	D	778	GLU
1	D	800	THR
1	D	805	ASN
1	D	832	ILE
1	D	846	SER
1	D	868	PHE
1	D	871	VAL
1	D	914	THR
1	D	926	VAL
1	D	936	MET
1	D	978	GLU
1	D	981	LYS
1	D	990	GLN
1	D	991	ARG
1	D	1022	LYS
1	D	1027	ILE
2	I	2	VAL
2	I	11	SER
2	J	2	VAL
2	J	7	SER
2	J	11	SER
2	K	2	VAL
2	K	5	PRO
2	K	11	SER
2	L	2	VAL
2	L	7	SER
2	L	11	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	321	ASN
1	A	322	ASN
1	A	325	ASN
1	A	332	ASN
1	A	406	GLN

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Mol	Chain	Res	Type
1	A	434	ASN
1	A	727	ASN
1	A	805	ASN
1	A	878	GLN
1	A	881	GLN
1	A	906	GLN
1	A	990	GLN
1	B	321	ASN
1	B	322	ASN
1	B	325	ASN
1	B	406	GLN
1	B	424	ASN
1	B	805	ASN
1	B	878	GLN
1	B	881	GLN
1	B	990	GLN
1	C	321	ASN
1	C	322	ASN
1	C	325	ASN
1	C	406	GLN
1	C	434	ASN
1	C	517	HIS
1	C	784	GLN
1	C	805	ASN
1	C	878	GLN
1	C	881	GLN
1	C	990	GLN
1	D	321	ASN
1	D	322	ASN
1	D	325	ASN
1	D	362	GLN
1	D	406	GLN
1	D	434	ASN
1	D	590	ASN
1	D	784	GLN
1	D	805	ASN
1	D	878	GLN
1	D	881	GLN
1	D	990	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	UDP	C	1201	-	20,26,26	1.14	1 (5%)	25,40,40	1.44	3 (12%)
4	NAG	L	1202	2	14,14,15	1.59	4 (28%)	17,19,21	2.26	5 (29%)
4	NAG	K	1202	2	14,14,15	1.73	4 (28%)	17,19,21	2.32	6 (35%)
3	UDP	D	1201	-	20,26,26	0.87	1 (5%)	25,40,40	1.41	4 (16%)
4	NAG	J	1202	2	14,14,15	1.75	4 (28%)	17,19,21	2.66	5 (29%)
4	NAG	I	1202	2	14,14,15	1.81	3 (21%)	17,19,21	2.63	5 (29%)
3	UDP	B	1201	-	20,26,26	0.95	0	25,40,40	1.71	7 (28%)
3	UDP	A	1201	-	20,26,26	1.14	2 (10%)	25,40,40	1.46	7 (28%)

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	UDP	C	1201	-	-	6/14/32/32	0/2/2/2
4	NAG	L	1202	2	-	1/6/23/26	0/1/1/1
4	NAG	K	1202	2	-	2/6/23/26	0/1/1/1
3	UDP	D	1201	-	-	5/14/32/32	0/2/2/2
4	NAG	J	1202	2	-	1/6/23/26	0/1/1/1
4	NAG	I	1202	2	-	1/6/23/26	0/1/1/1
3	UDP	B	1201	-	-	5/14/32/32	0/2/2/2
3	UDP	A	1201	-	-	3/14/32/32	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1202	NAG	O3-C3	4.75	1.54	1.43
4	K	1202	NAG	O3-C3	4.32	1.53	1.43
4	J	1202	NAG	O5-C1	-3.94	1.37	1.43
4	L	1202	NAG	O3-C3	3.76	1.51	1.43
3	C	1201	UDP	O4'-C1'	3.51	1.46	1.41
4	J	1202	NAG	O3-C3	3.29	1.50	1.43
3	A	1201	UDP	O4'-C1'	3.04	1.45	1.41
4	K	1202	NAG	C3-C2	2.51	1.57	1.52
4	L	1202	NAG	O5-C1	-2.47	1.39	1.43
4	J	1202	NAG	C8-C7	2.42	1.55	1.50
4	I	1202	NAG	O5-C1	-2.32	1.40	1.43
4	K	1202	NAG	C4-C5	-2.31	1.48	1.53
4	I	1202	NAG	C3-C2	2.27	1.57	1.52
4	K	1202	NAG	O5-C1	-2.26	1.40	1.43
3	A	1201	UDP	C2-N3	-2.26	1.33	1.38
3	D	1201	UDP	O4'-C1'	2.24	1.44	1.41
4	L	1202	NAG	C3-C2	2.13	1.57	1.52
4	L	1202	NAG	C8-C7	2.12	1.54	1.50
4	J	1202	NAG	C1-C2	2.10	1.55	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	1202	NAG	C1-O5-C5	6.92	121.57	112.19
4	K	1202	NAG	C1-O5-C5	6.84	121.46	112.19
4	J	1202	NAG	O5-C5-C6	-6.52	96.98	107.20
4	J	1202	NAG	C1-O5-C5	6.23	120.63	112.19
4	L	1202	NAG	C1-O5-C5	6.15	120.53	112.19
4	I	1202	NAG	O5-C5-C6	-5.47	98.63	107.20
4	L	1202	NAG	O5-C5-C6	-4.57	100.04	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1201	UDP	O2B-PB-O3A	-3.68	92.29	104.64
3	B	1201	UDP	O2A-PA-O1A	3.59	129.98	112.24
4	J	1202	NAG	C2-N2-C7	-3.50	117.92	122.90
4	I	1202	NAG	O3-C3-C2	3.34	116.37	109.47
3	B	1201	UDP	O4'-C1'-C2'	-3.22	102.22	106.93
3	D	1201	UDP	O2B-PB-O3A	-3.18	93.97	104.64
3	A	1201	UDP	O2B-PB-O3A	-3.16	94.03	104.64
3	A	1201	UDP	PA-O3A-PB	-3.10	122.18	132.83
3	C	1201	UDP	PA-O3A-PB	-3.10	122.20	132.83
4	K	1202	NAG	O5-C5-C6	-3.05	102.42	107.20
3	C	1201	UDP	O2A-PA-O1A	2.75	125.84	112.24
3	D	1201	UDP	O2A-PA-O1A	2.75	125.83	112.24
3	A	1201	UDP	O3B-PB-O2B	2.68	117.87	107.64
3	B	1201	UDP	O3B-PB-O1B	2.66	121.10	110.68
3	D	1201	UDP	PA-O3A-PB	-2.63	123.80	132.83
4	I	1202	NAG	C2-N2-C7	-2.59	119.22	122.90
4	I	1202	NAG	C6-C5-C4	-2.55	107.03	113.00
3	A	1201	UDP	O4'-C1'-C2'	-2.52	103.24	106.93
4	L	1202	NAG	O3-C3-C2	2.51	114.67	109.47
4	K	1202	NAG	C2-N2-C7	-2.48	119.36	122.90
3	B	1201	UDP	O2B-PB-O1B	2.42	120.14	110.68
4	J	1202	NAG	O3-C3-C2	2.40	114.42	109.47
4	L	1202	NAG	C2-N2-C7	-2.33	119.59	122.90
4	K	1202	NAG	O3-C3-C2	2.31	114.25	109.47
3	A	1201	UDP	C3'-C2'-C1'	-2.28	97.55	100.98
3	B	1201	UDP	PA-O3A-PB	-2.26	125.08	132.83
4	K	1202	NAG	O5-C5-C4	-2.23	105.40	110.83
4	K	1202	NAG	O5-C1-C2	-2.22	107.78	111.29
3	D	1201	UDP	O2B-PB-O1B	2.18	119.22	110.68
3	A	1201	UDP	O2A-PA-O1A	2.17	122.95	112.24
3	B	1201	UDP	C3'-C2'-C1'	-2.16	97.72	100.98
4	L	1202	NAG	C1-C2-N2	-2.12	106.86	110.49
3	C	1201	UDP	O4'-C1'-C2'	-2.12	103.83	106.93
3	A	1201	UDP	O3B-PB-O1B	2.09	118.86	110.68
4	J	1202	NAG	O3-C3-C4	-2.04	105.63	110.35

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1201	UDP	C2'-C1'-N1-C6
3	C	1201	UDP	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
3	C	1201	UDP	C3'-C4'-C5'-O5'
3	C	1201	UDP	O4'-C4'-C5'-O5'
3	C	1201	UDP	PA-O3A-PB-O2B
3	C	1201	UDP	PA-O3A-PB-O3B
3	D	1201	UDP	C2'-C1'-N1-C6
3	D	1201	UDP	O4'-C1'-N1-C6
3	D	1201	UDP	C3'-C4'-C5'-O5'
3	D	1201	UDP	O4'-C4'-C5'-O5'
3	D	1201	UDP	PA-O3A-PB-O2B
3	B	1201	UDP	C2'-C1'-N1-C6
3	B	1201	UDP	O4'-C1'-N1-C6
3	B	1201	UDP	C3'-C4'-C5'-O5'
3	B	1201	UDP	O4'-C4'-C5'-O5'
3	A	1201	UDP	O4'-C1'-N1-C6
3	A	1201	UDP	C3'-C4'-C5'-O5'
3	A	1201	UDP	O4'-C4'-C5'-O5'
4	K	1202	NAG	O5-C5-C6-O6
3	B	1201	UDP	PA-O3A-PB-O2B
4	J	1202	NAG	O5-C5-C6-O6
4	L	1202	NAG	O5-C5-C6-O6
4	I	1202	NAG	O5-C5-C6-O6
4	K	1202	NAG	C4-C5-C6-O6

There are no ring outliers.

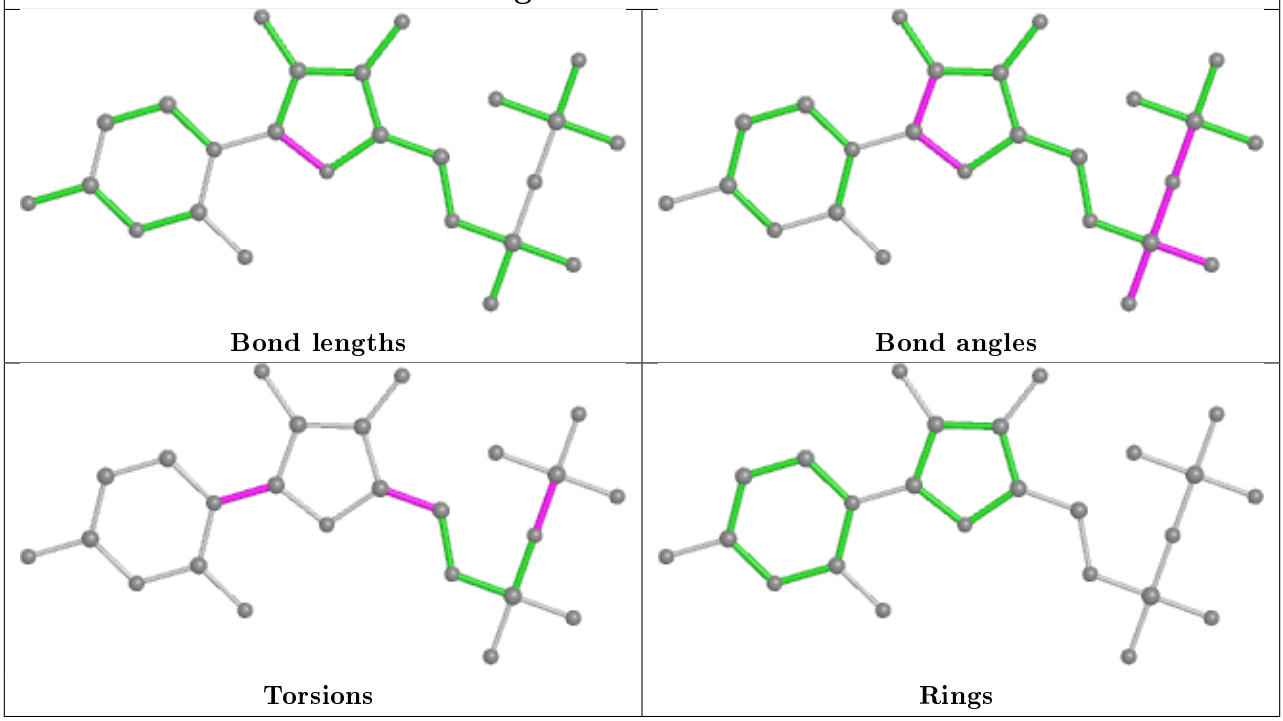
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1201	UDP	2	0
3	D	1201	UDP	3	0
3	B	1201	UDP	2	0
3	A	1201	UDP	2	0

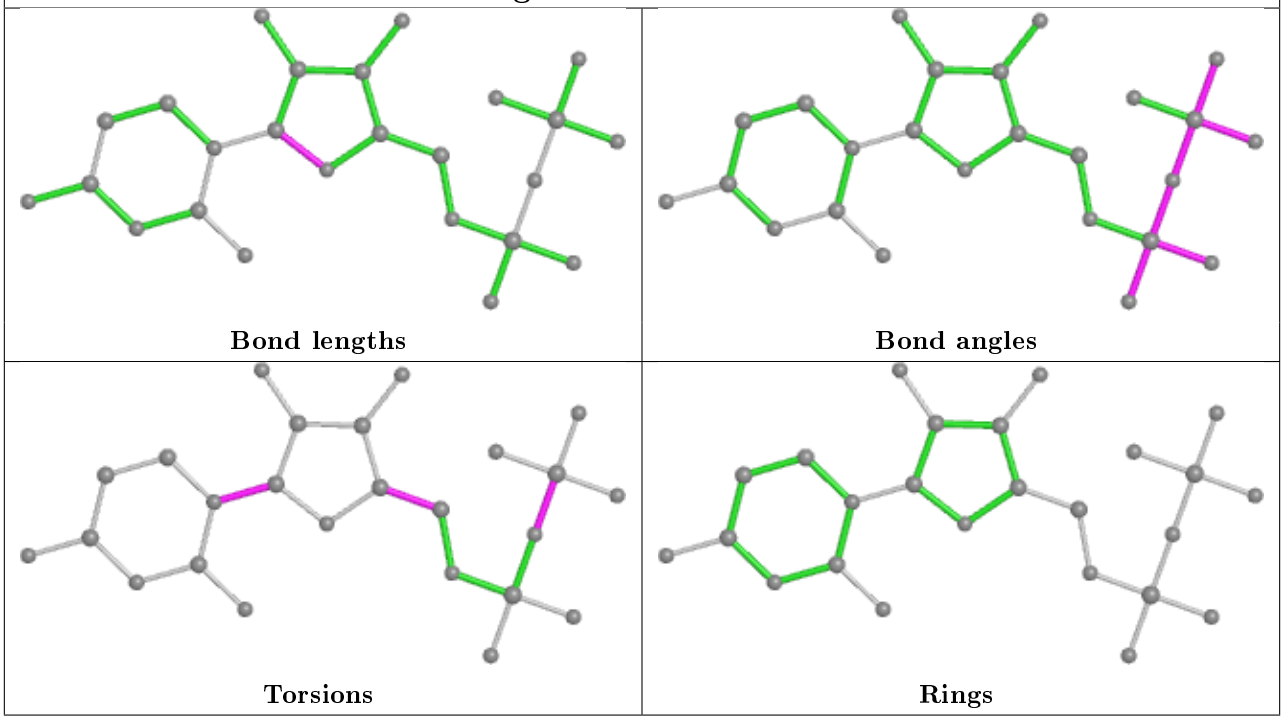
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

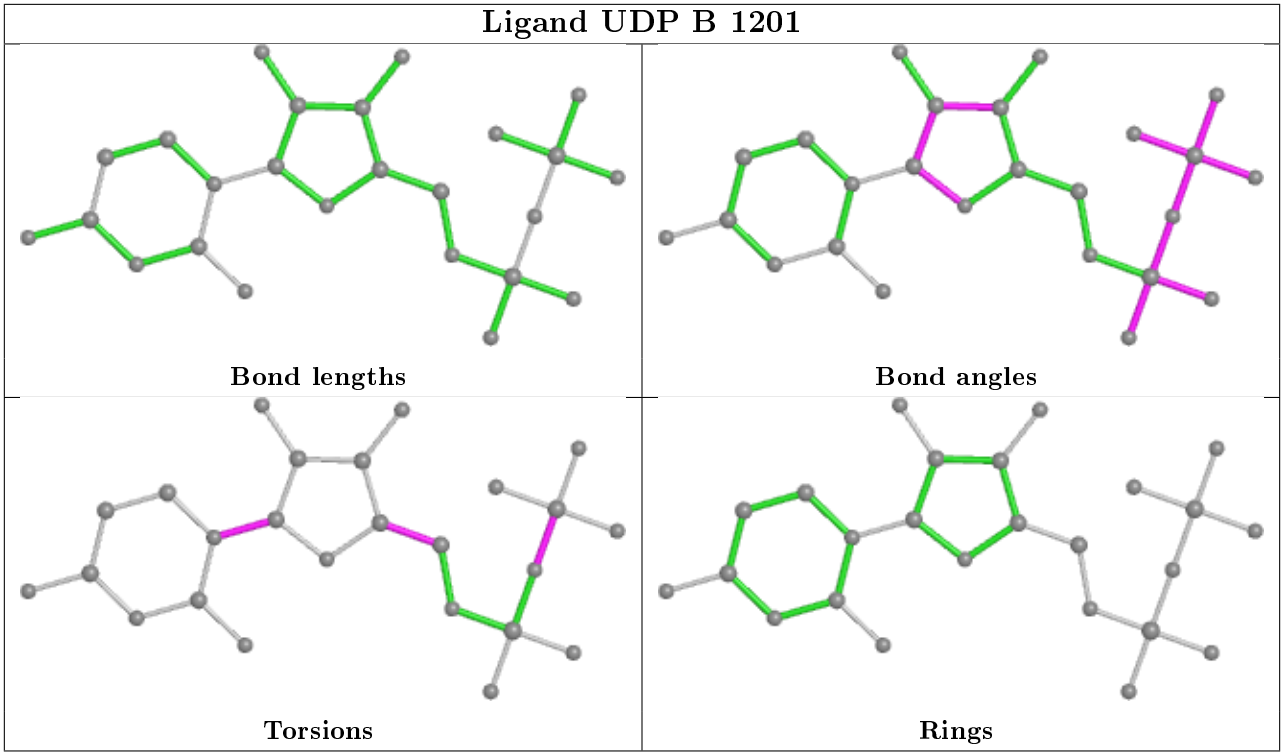
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

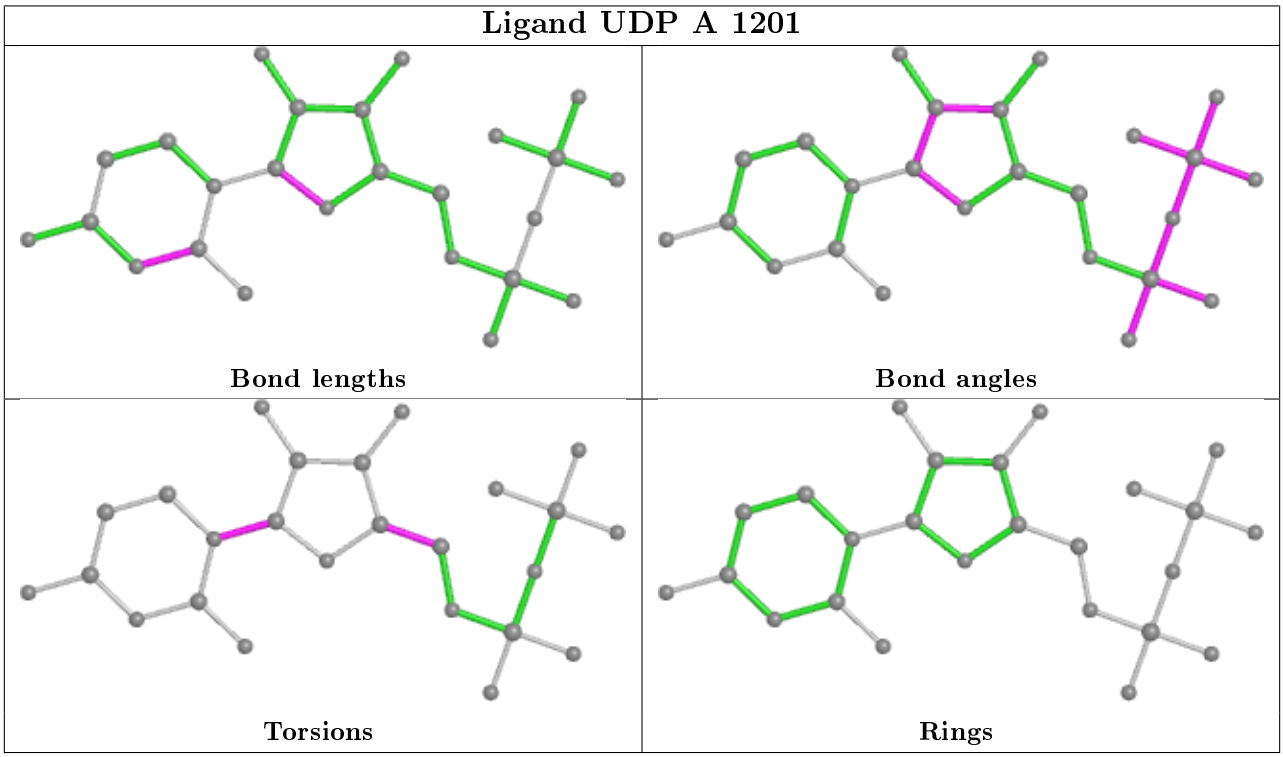
Ligand UDP C 1201



Ligand UDP D 1201







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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	698/723 (96%)	-0.53	4 (0%) 89 84	30, 53, 95, 148	0
1	B	698/723 (96%)	-0.54	2 (0%) 94 92	27, 54, 91, 137	0
1	C	698/723 (96%)	-0.59	2 (0%) 94 92	30, 51, 88, 122	0
1	D	698/723 (96%)	-0.41	4 (0%) 89 84	36, 66, 97, 134	0
2	I	11/11 (100%)	0.08	0 100 100	67, 82, 106, 108	0
2	J	11/11 (100%)	0.53	2 (18%) 1 1	74, 85, 121, 140	0
2	K	11/11 (100%)	0.51	2 (18%) 1 1	66, 86, 111, 142	0
2	L	11/11 (100%)	0.02	1 (9%) 9 5	82, 101, 121, 129	0
All	All	2836/2936 (96%)	-0.50	17 (0%) 89 84	27, 56, 97, 148	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	11	SER	4.9
1	B	312	SER	4.3
2	J	11	SER	4.0
1	D	911	CYS	3.2
2	L	11	SER	3.1
1	C	330	GLN	2.9
1	A	331	GLY	2.9
1	D	330	GLN	2.8
1	B	330	GLN	2.7
1	A	330	GLN	2.7
2	J	2	VAL	2.6
1	C	312	SER	2.6
1	D	887	GLN	2.4
1	A	326	ILE	2.3
1	D	312	SER	2.1
1	A	911	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	K	1	PRO	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)

There are no monosaccharides in this entry.

6.4 Ligands (i)

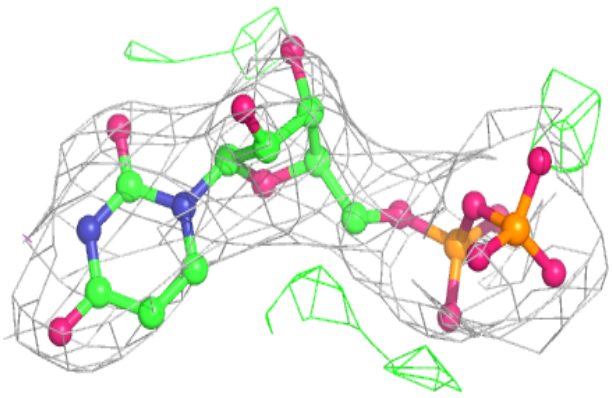
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

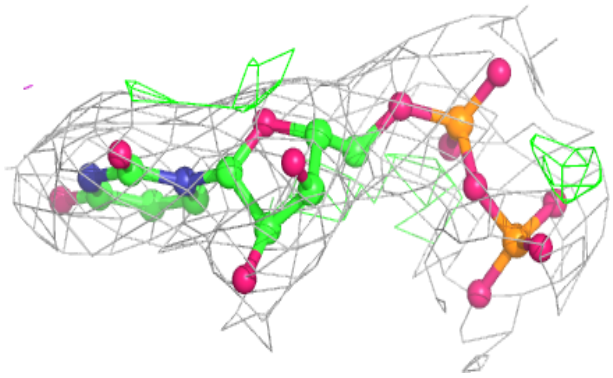
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	L	1202	14/15	0.95	0.19	63,79,93,94	0
4	NAG	J	1202	14/15	0.96	0.23	56,69,83,85	0
4	NAG	I	1202	14/15	0.97	0.17	57,67,77,81	0
3	UDP	B	1201	25/25	0.97	0.17	35,62,72,76	0
3	UDP	A	1201	25/25	0.97	0.16	32,55,61,64	0
4	NAG	K	1202	14/15	0.98	0.23	54,59,76,81	0
3	UDP	D	1201	25/25	0.98	0.17	60,76,83,85	0
3	UDP	C	1201	25/25	0.98	0.17	44,57,63,64	0

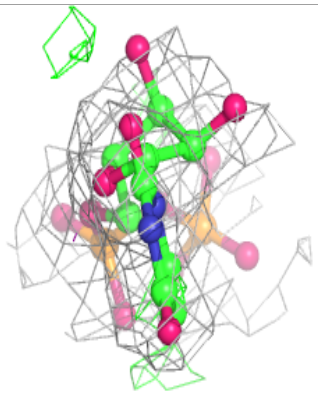
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UDP B 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

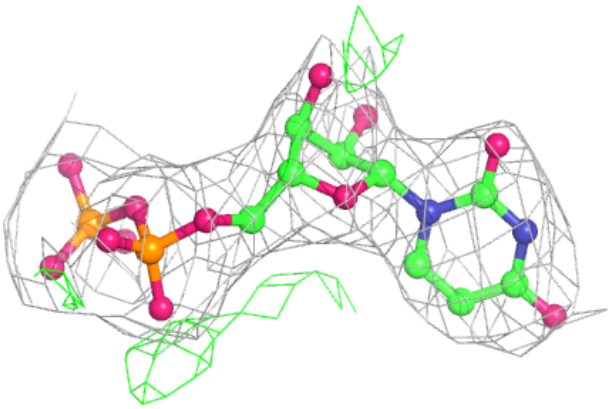


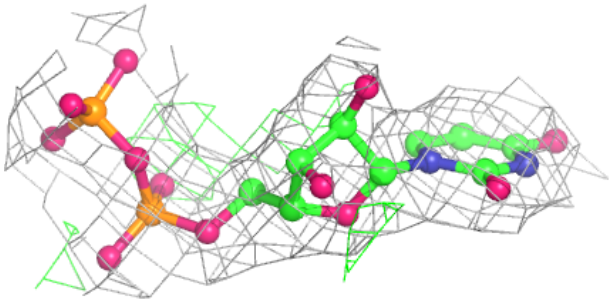


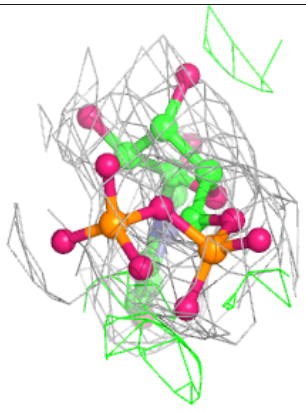


Electron density around UDP A 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

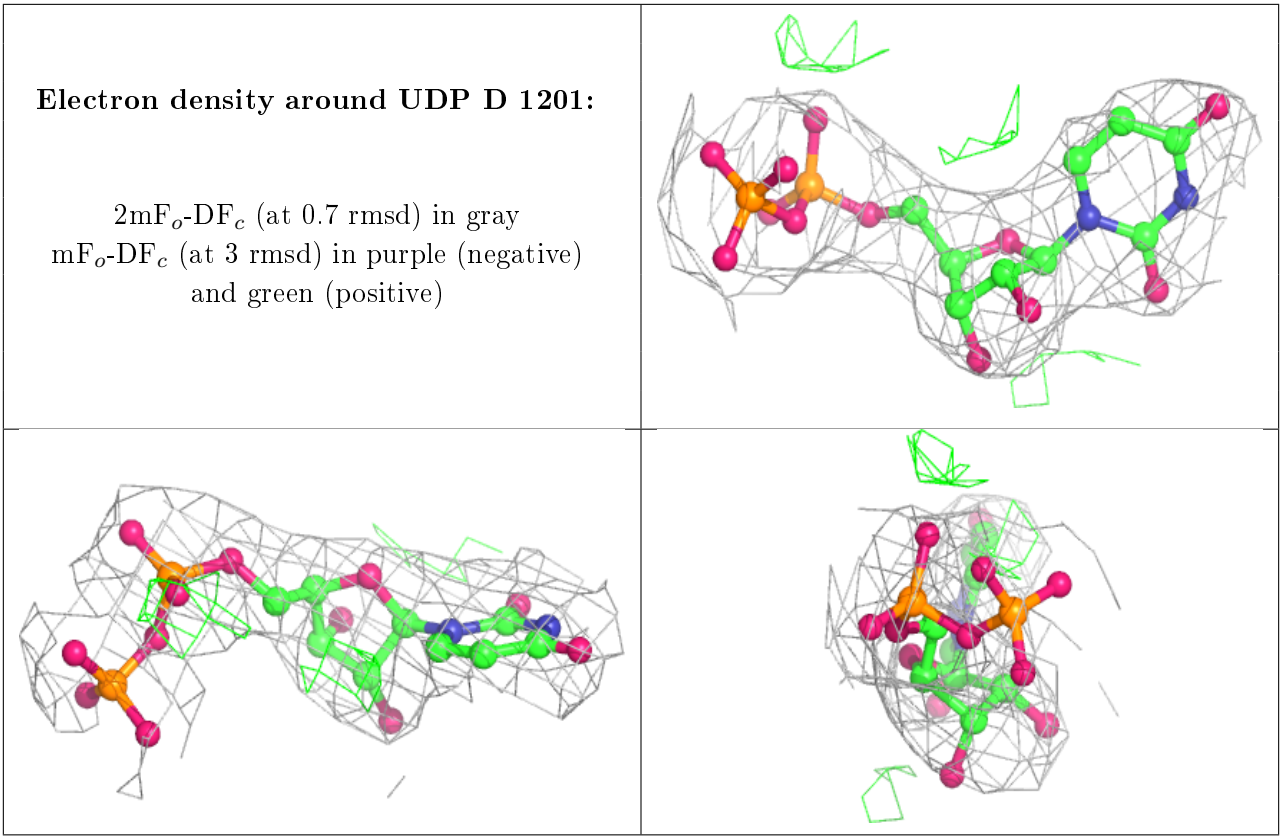






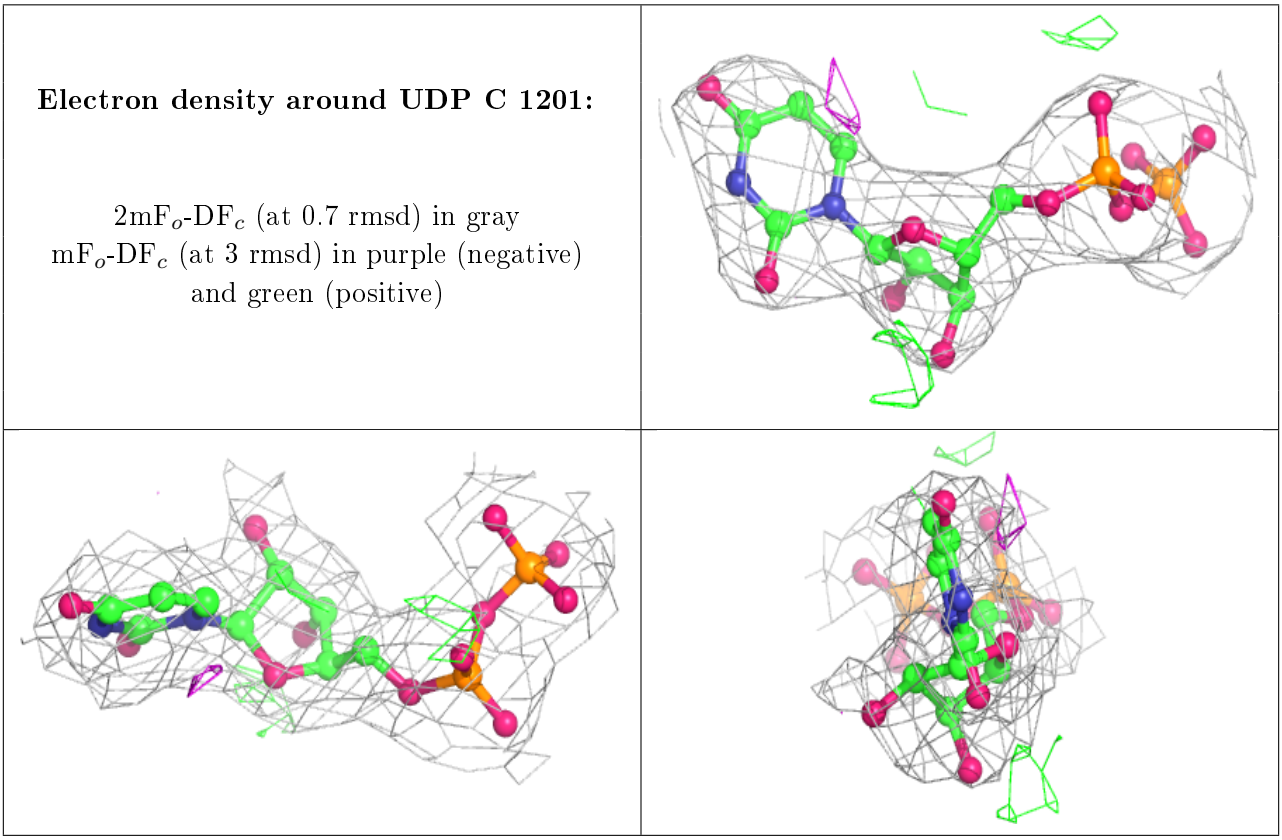
Electron density around UDP D 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around UDP C 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.