Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 07:11 PM BST

PDB ID	:	1V0F
Title	:	Endosialidase of Bacteriophage K1F in complex with oligomeric alpha-2,8-sialic acid
Authors	:	Stummeyer, K.; Dickmanns, A.; Muehlenhoff, M.; Gerady-Schahn, R.; Ficner, R.
Deposited on	:	2004-03-28
Resolution	:	2.55 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:

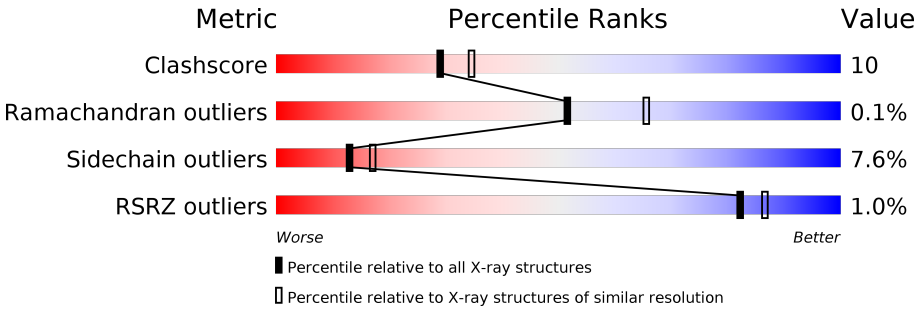
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.55 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))
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	666	76% 21%
1	B	666	76% 20%
1	C	666	72% 24%
1	D	666	76% 20%
1	E	666	74% 21%
1	F	666	76% 21%
2	G	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	2	50% 50%
2	I	2	50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32580 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.

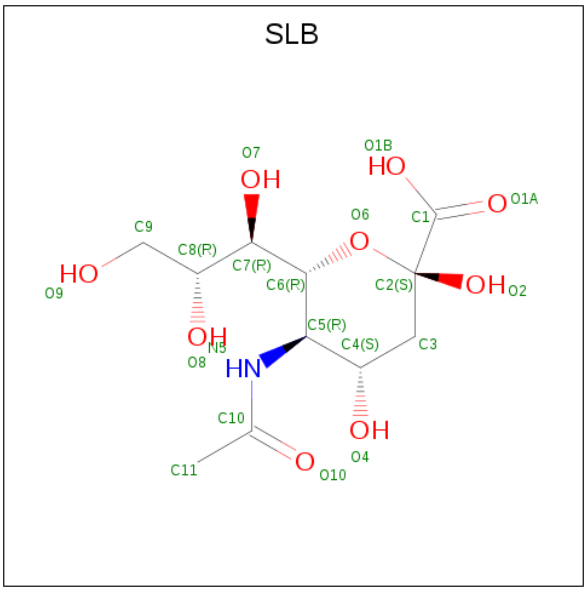
- Molecule 1 is a protein called ENDO-ALPHA-SIALIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	B	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	C	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	D	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	E	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			
1	F	666	Total	C	N	O	S	0	0	0
			5230	3293	908	1010	19			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha -neuraminic acid.

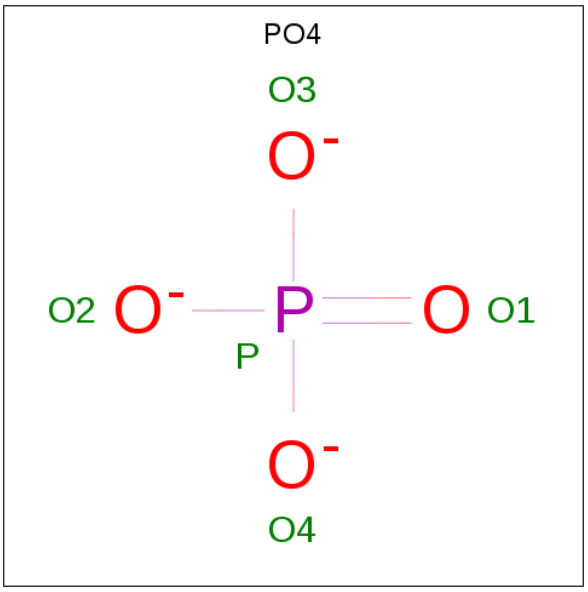
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	2	Total	C	N	O	0	0	0
			41	22	2	17			
2	H	2	Total	C	N	O	0	0	0
			41	22	2	17			
2	I	2	Total	C	N	O	0	0	0
			41	22	2	17			

- Molecule 3 is N-acetyl-beta-neuraminic acid (three-letter code: SLB) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	B	1	Total	C	N	O	0	0
			21	11	1	9		
3	C	1	Total	C	N	O	0	0
			21	11	1	9		
3	D	1	Total	C	N	O	0	0
			21	11	1	9		
3	E	1	Total	C	N	O	0	0
			21	11	1	9		
3	F	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

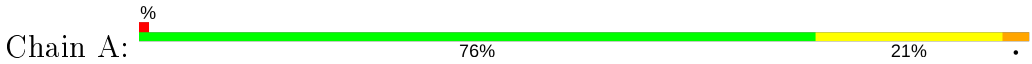
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	176	Total O 176 176	0	0
5	B	178	Total O 178 178	0	0
5	C	130	Total O 130 130	0	0
5	D	167	Total O 167 167	0	0
5	E	130	Total O 130 130	0	0
5	F	140	Total O 140 140	0	0

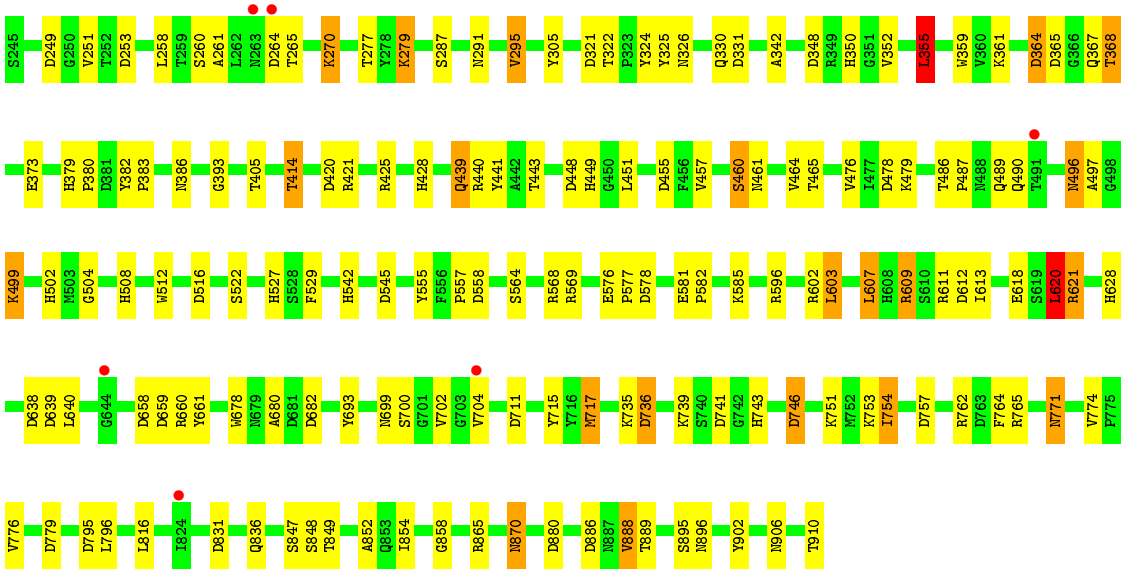
3 Residue-property plots (i)

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: ENDO-ALPHA-SIALIDASE

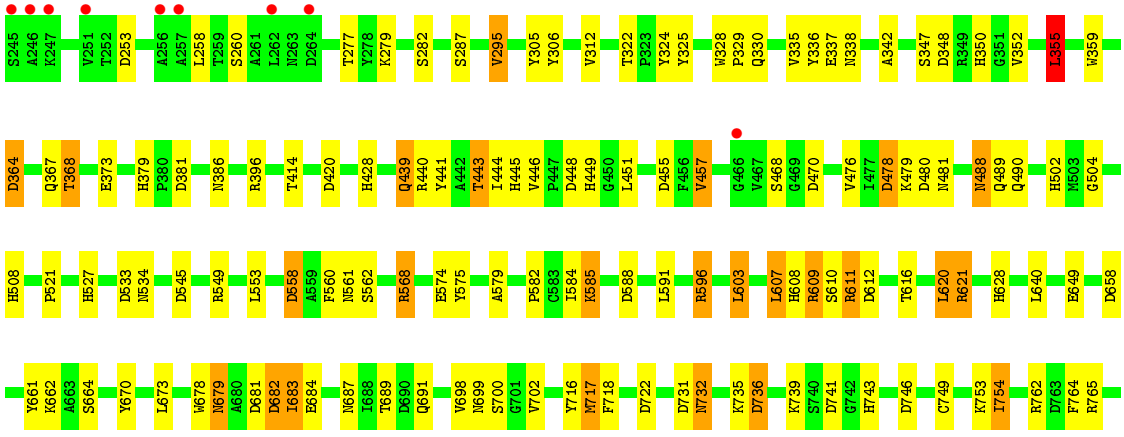
Chain A:

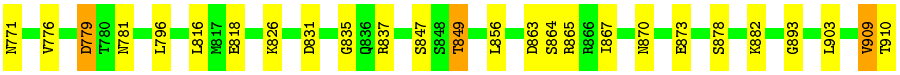




- Molecule 1: ENDO-ALPHA-SIALIDASE

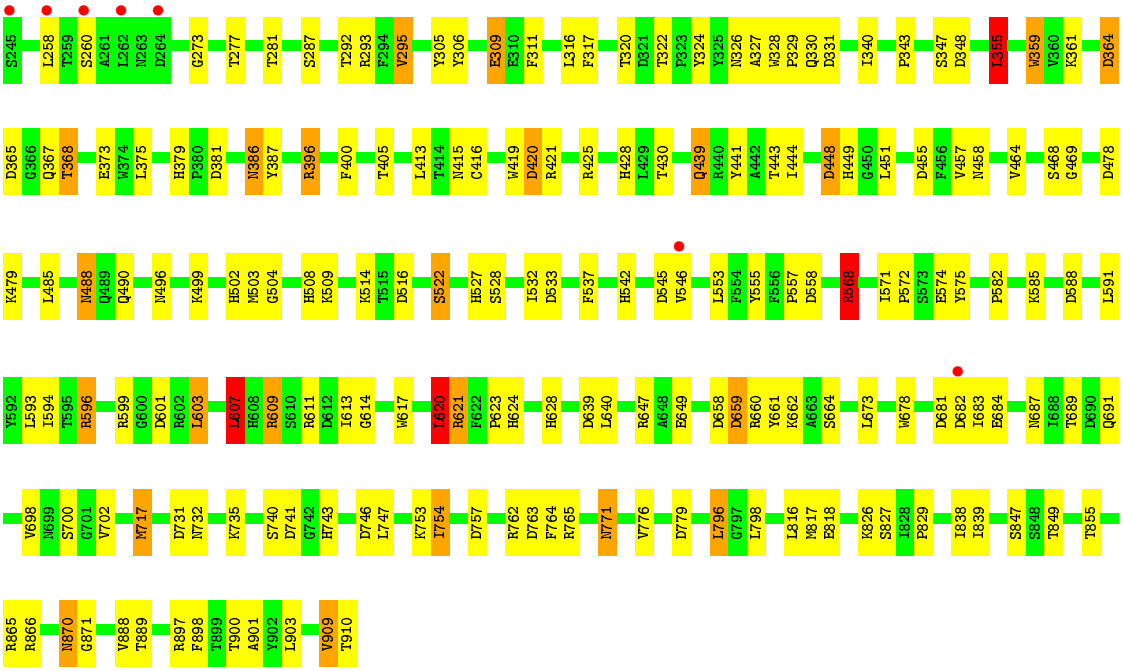
Chain B:





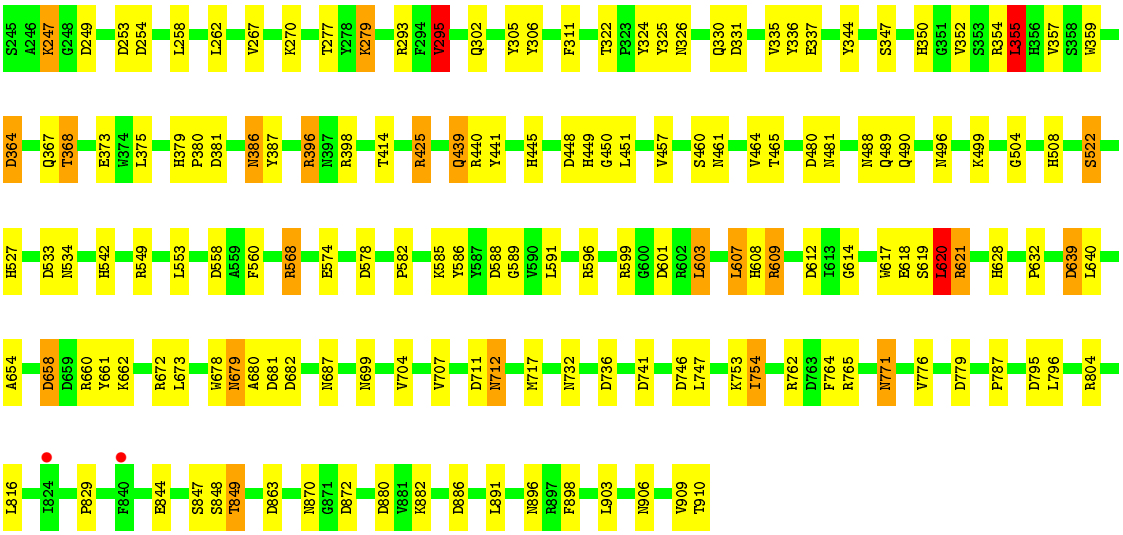
• Molecule 1: ENDO-ALPHA-SIALIDASE

Chain C:



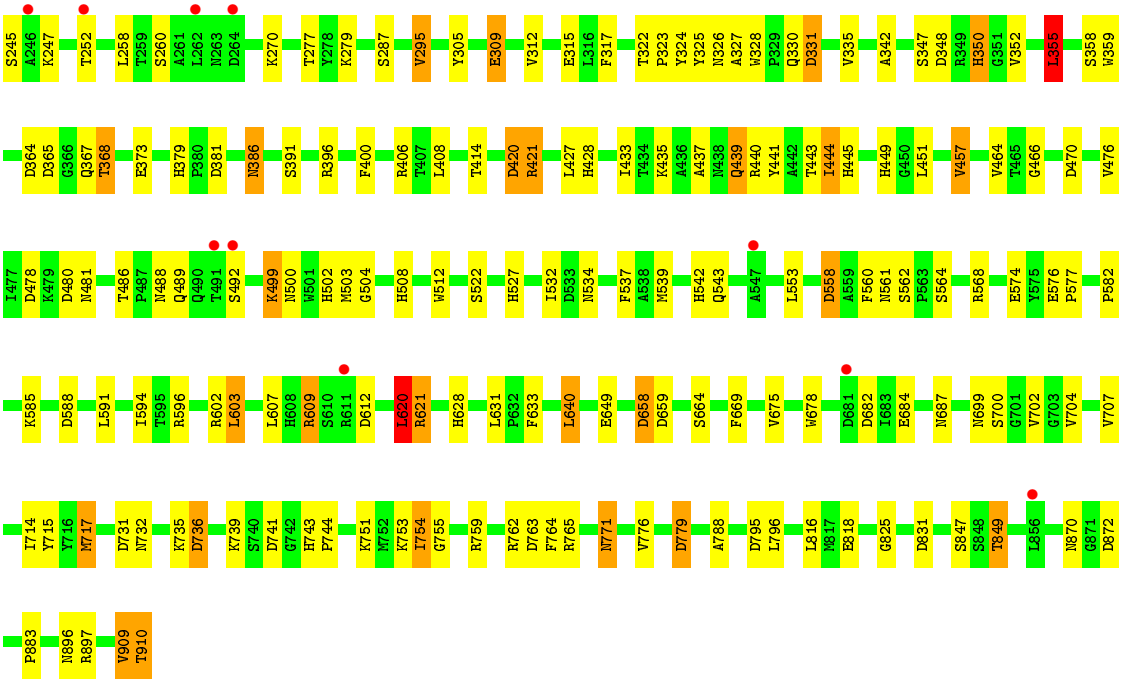
• Molecule 1: ENDO-ALPHA-SIALIDASE

Chain D:



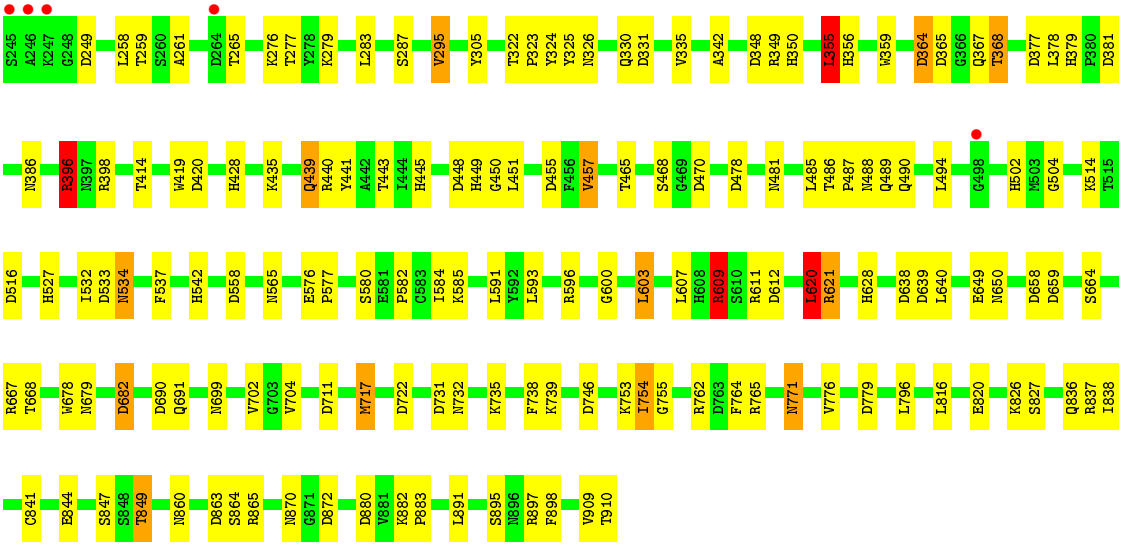
• Molecule 1: ENDO-ALPHA-SIALIDASE

Chain E:



• Molecule 1: ENDO-ALPHA-SIALIDASE

Chain F:



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid

Chain G:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid

Chain H:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	99.54Å 131.40Å 346.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.55 30.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	88.4 (30.00-2.55) 88.1 (30.00-2.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.28 (at 2.54Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.180 , 0.232 0.198 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 18.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	32580	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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: PO4, SIA, SLB

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	0.72	0/5376	0.94	31/7325 (0.4%)
1	B	0.72	0/5376	0.94	28/7325 (0.4%)
1	C	0.70	0/5376	0.94	29/7325 (0.4%)
1	D	0.73	0/5376	0.95	31/7325 (0.4%)
1	E	0.69	0/5376	0.92	23/7325 (0.3%)
1	F	0.71	0/5376	0.94	33/7325 (0.5%)
All	All	0.71	0/32256	0.94	175/43950 (0.4%)

There are no bond length outliers.

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	364	ASP	CB-CG-OD2	9.56	126.91	118.30
1	E	355	LEU	CA-CB-CG	9.49	137.13	115.30
1	F	638	ASP	CB-CG-OD2	8.38	125.84	118.30
1	D	682	ASP	CB-CG-OD2	8.26	125.74	118.30
1	C	545	ASP	CB-CG-OD2	8.15	125.64	118.30
1	A	620	LEU	CA-CB-CG	8.15	134.04	115.30
1	E	558	ASP	CB-CG-OD2	8.15	125.63	118.30
1	E	612	ASP	CB-CG-OD2	8.07	125.57	118.30
1	B	355	LEU	CA-CB-CG	8.00	133.70	115.30
1	C	355	LEU	CA-CB-CG	8.00	133.69	115.30
1	C	639	ASP	CB-CG-OD2	7.99	125.49	118.30
1	B	478	ASP	CB-CG-OD2	7.96	125.46	118.30
1	B	620	LEU	CA-CB-CG	7.85	133.35	115.30
1	D	253	ASP	CB-CG-OD2	7.83	125.35	118.30
1	E	348	ASP	CB-CG-OD2	7.77	125.29	118.30
1	C	731	ASP	CB-CG-OD2	7.71	125.24	118.30
1	F	746	ASP	CB-CG-OD2	7.69	125.22	118.30
1	B	420	ASP	CB-CG-OD2	7.59	125.14	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	872	ASP	CB-CG-OD2	7.58	125.12	118.30
1	D	795	ASP	CB-CG-OD2	7.52	125.07	118.30
1	B	558	ASP	CB-CG-OD2	7.44	125.00	118.30
1	A	355	LEU	CA-CB-CG	7.43	132.38	115.30
1	A	558	ASP	CB-CG-OD2	7.32	124.89	118.30
1	C	620	LEU	CA-CB-CG	7.30	132.08	115.30
1	F	722	ASP	CB-CG-OD2	7.17	124.75	118.30
1	D	620	LEU	CA-CB-CG	7.15	131.74	115.30
1	D	639	ASP	CB-CG-OD2	7.12	124.71	118.30
1	F	478	ASP	CB-CG-OD2	7.09	124.69	118.30
1	F	355	LEU	CA-CB-CG	7.07	131.57	115.30
1	B	253	ASP	CB-CG-OD2	7.03	124.63	118.30
1	D	711	ASP	CB-CG-OD2	6.98	124.58	118.30
1	C	558	ASP	CB-CG-OD2	6.92	124.53	118.30
1	F	455	ASP	CB-CG-OD2	6.90	124.51	118.30
1	B	480	ASP	CB-CG-OD2	6.88	124.50	118.30
1	D	578	ASP	CB-CG-OD2	6.86	124.47	118.30
1	A	348	ASP	CB-CG-OD2	6.83	124.45	118.30
1	E	736	ASP	CB-CG-OD1	6.74	124.36	118.30
1	E	682	ASP	CB-CG-OD2	6.68	124.32	118.30
1	C	533	ASP	CB-CG-OD2	6.67	124.30	118.30
1	F	731	ASP	CB-CG-OD2	6.65	124.29	118.30
1	D	355	LEU	CA-CB-CG	6.63	130.54	115.30
1	E	620	LEU	CA-CB-CG	6.62	130.54	115.30
1	A	249	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	253	ASP	CB-CG-OD2	6.59	124.24	118.30
1	B	863	ASP	CB-CG-OD2	6.56	124.21	118.30
1	F	711	ASP	CB-CG-OD2	6.56	124.20	118.30
1	D	658	ASP	CB-CG-OD2	6.56	124.20	118.30
1	A	478	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	865	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	741	ASP	CB-CG-OD2	6.51	124.16	118.30
1	F	639	ASP	CB-CG-OD2	6.46	124.11	118.30
1	B	731	ASP	CB-CG-OD2	6.46	124.11	118.30
1	A	455	ASP	CB-CG-OD2	6.44	124.10	118.30
1	D	872	ASP	CB-CG-OD2	6.44	124.10	118.30
1	F	863	ASP	CB-CG-OD2	6.43	124.09	118.30
1	D	746	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	545	ASP	CB-CG-OD2	6.42	124.08	118.30
1	E	478	ASP	CB-CG-OD2	6.41	124.07	118.30
1	E	420	ASP	CB-CG-OD2	6.39	124.05	118.30
1	B	381	ASP	CB-CG-OD2	6.37	124.03	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	448	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	795	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	639	ASP	CB-CG-OD2	6.32	123.99	118.30
1	E	365	ASP	CB-CG-OD2	6.32	123.99	118.30
1	C	746	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	612	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	741	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	588	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	757	ASP	CB-CG-OD2	6.27	123.95	118.30
1	F	364	ASP	CB-CG-OD2	6.25	123.93	118.30
1	B	545	ASP	CB-CG-OD2	6.25	123.92	118.30
1	D	558	ASP	CB-CG-OD2	6.25	123.92	118.30
1	F	558	ASP	CB-CG-OD2	6.24	123.91	118.30
1	D	480	ASP	CB-CG-OD2	6.17	123.85	118.30
1	E	588	ASP	CB-CG-OD2	6.15	123.83	118.30
1	E	831	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	420	ASP	CB-CG-OD2	6.14	123.83	118.30
1	C	364	ASP	CB-CG-OD2	6.12	123.80	118.30
1	C	659	ASP	CB-CG-OD2	6.08	123.78	118.30
1	B	736	ASP	CB-CG-OD1	6.08	123.77	118.30
1	F	348	ASP	CB-CG-OD2	6.04	123.74	118.30
1	F	377	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	746	ASP	CB-CG-OD2	6.03	123.72	118.30
1	D	381	ASP	CB-CG-OD2	6.02	123.72	118.30
1	F	381	ASP	CB-CG-OD2	6.02	123.72	118.30
1	F	620	LEU	CA-CB-CG	6.02	129.14	115.30
1	B	607	LEU	CA-CB-CG	6.01	129.12	115.30
1	D	601	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	365	ASP	CB-CG-OD2	5.98	123.68	118.30
1	D	612	ASP	CB-CG-OD2	5.97	123.67	118.30
1	F	880	ASP	CB-CG-OD2	5.94	123.65	118.30
1	C	607	LEU	CA-CB-CG	5.94	128.95	115.30
1	F	331	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	588	ASP	CB-CG-OD2	5.87	123.58	118.30
1	D	364	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	682	ASP	CB-CG-OD2	5.83	123.54	118.30
1	B	533	ASP	CB-CG-OD2	5.83	123.54	118.30
1	C	455	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	264	ASP	CB-CG-OD2	5.81	123.53	118.30
1	D	863	ASP	CB-CG-OD2	5.79	123.52	118.30
1	C	348	ASP	CB-CG-OD2	5.76	123.49	118.30
1	B	348	ASP	CB-CG-OD2	5.75	123.47	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	448	ASP	CB-CG-OD2	5.68	123.41	118.30
1	E	331	ASP	CB-CG-OD2	5.67	123.41	118.30
1	B	746	ASP	CB-CG-OD2	5.65	123.38	118.30
1	E	470	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	321	ASP	CB-CG-OD2	5.62	123.36	118.30
1	F	396	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	C	568	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	D	331	ASP	CB-CG-OD2	5.61	123.35	118.30
1	D	588	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	831	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	364	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	638	ASP	CB-CG-OD2	5.58	123.33	118.30
1	D	804	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	E	731	ASP	CB-CG-OD2	5.55	123.29	118.30
1	B	455	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	596	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	C	865	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	831	ASP	CB-CG-OD2	5.51	123.26	118.30
1	D	354	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	F	516	ASP	CB-CG-OD2	5.51	123.25	118.30
1	A	516	ASP	CB-CG-OD1	5.50	123.25	118.30
1	C	601	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	381	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	865	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	420	ASP	CB-CG-OD2	5.49	123.24	118.30
1	E	381	ASP	CB-CG-OD2	5.49	123.24	118.30
1	F	609	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	F	249	ASP	CB-CG-OD2	5.47	123.23	118.30
1	E	659	ASP	CB-CG-OD2	5.45	123.21	118.30
1	C	681	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	611	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	F	779	ASP	CB-CG-OD2	5.43	123.19	118.30
1	E	779	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	682	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	470	ASP	CB-CG-OD2	5.39	123.16	118.30
1	E	658	ASP	CB-CG-OD2	5.38	123.14	118.30
1	E	480	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	516	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	736	ASP	CB-CG-OD2	5.32	123.09	118.30
1	F	682	ASP	CB-CG-OD2	5.31	123.08	118.30
1	D	249	ASP	CB-CG-OD2	5.31	123.08	118.30
1	F	365	ASP	CB-CG-OD2	5.29	123.06	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	448	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	612	ASP	CB-CG-OD2	5.28	123.06	118.30
1	E	795	ASP	CB-CG-OD2	5.28	123.05	118.30
1	F	420	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	578	ASP	CB-CG-OD2	5.25	123.02	118.30
1	D	295	VAL	CB-CA-C	-5.23	101.47	111.40
1	F	659	ASP	CB-CG-OD2	5.23	123.00	118.30
1	F	612	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	722	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	880	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	421	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	711	ASP	CB-CG-OD2	5.18	122.97	118.30
1	D	533	ASP	CB-CG-OD2	5.17	122.96	118.30
1	F	690	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	779	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	659	ASP	CB-CG-OD2	5.15	122.94	118.30
1	F	448	ASP	CB-CG-OD2	5.15	122.93	118.30
1	E	741	ASP	CB-CG-OD2	5.14	122.93	118.30
1	C	478	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	787	PRO	N-CD-CG	-5.11	95.53	103.20
1	C	757	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	596	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	A	880	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	254	ASP	CB-CG-OD2	5.04	122.84	118.30
1	D	425	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	A	682	ASP	CB-CG-OD2	5.04	122.83	118.30
1	F	533	ASP	CB-CG-OD2	5.04	122.84	118.30
1	F	470	ASP	CB-CG-OD2	5.04	122.83	118.30
1	E	872	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	365	ASP	CB-CG-OD2	5.01	122.81	118.30
1	D	741	ASP	CB-CG-OD2	5.01	122.81	118.30

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	5230	0	4942	104	0
1	B	5230	0	4942	110	0
1	C	5230	0	4942	113	0
1	D	5230	0	4942	103	0
1	E	5230	0	4942	117	0
1	F	5230	0	4942	95	0
2	G	41	0	34	0	0
2	H	41	0	34	2	0
2	I	41	0	34	1	0
3	A	21	0	18	0	0
3	B	21	0	18	0	0
3	C	21	0	18	0	0
3	D	21	0	18	0	0
3	E	21	0	18	0	0
3	F	21	0	18	1	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
4	F	10	0	0	0	0
5	A	176	0	0	11	0
5	B	178	0	0	12	0
5	C	130	0	0	6	0
5	D	167	0	0	11	0
5	E	130	0	0	15	0
5	F	140	0	0	15	0
All	All	32580	0	29862	590	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 10.

All (590) 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:B:490:GLN:HG3	5:B:2041:HOH:O	1.51	1.09
1:E:499:LYS:HE2	1:E:500:ASN:H	1.21	1.04
1:A:765:ARG:HH12	1:C:367:GLN:HE21	1.07	0.98
1:F:449:HIS:HD2	1:F:451:LEU:H	1.07	0.98
1:C:449:HIS:HD2	1:C:451:LEU:H	1.00	0.96
1:B:367:GLN:HE21	1:C:765:ARG:HH12	1.12	0.95
1:A:449:HIS:HD2	1:A:451:LEU:H	1.10	0.94
1:C:449:HIS:CD2	1:C:451:LEU:H	1.86	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:GLN:HE21	1:B:765:ARG:HH12	0.93	0.91
1:A:771:ASN:HD21	1:A:776:VAL:H	1.18	0.90
1:D:449:HIS:HD2	1:D:451:LEU:H	1.20	0.89
1:E:449:HIS:HD2	1:E:451:LEU:H	1.21	0.88
1:F:449:HIS:CD2	1:F:451:LEU:H	1.91	0.88
1:B:449:HIS:HD2	1:B:451:LEU:H	1.22	0.88
1:E:542:HIS:HD2	5:E:2038:HOH:O	1.56	0.87
1:B:682:ASP:HB2	5:B:2107:HOH:O	1.75	0.87
1:D:347:SER:HB3	1:D:355:LEU:HB2	1.57	0.87
1:B:771:ASN:HD21	1:B:776:VAL:H	1.20	0.86
1:D:765:ARG:NH1	1:E:367:GLN:HE21	1.74	0.86
1:D:765:ARG:HH12	1:E:367:GLN:HE21	0.89	0.86
1:E:765:ARG:HH12	1:F:367:GLN:HE21	1.25	0.83
1:B:440:ARG:HE	1:B:489:GLN:HE21	1.25	0.82
1:A:367:GLN:NE2	1:B:765:ARG:HH12	1.77	0.82
1:C:609:ARG:HG2	1:C:678:TRP:CH2	2.15	0.81
1:F:322:THR:HG21	5:F:2012:HOH:O	1.80	0.81
1:C:322:THR:HG22	1:C:324:TYR:H	1.46	0.81
1:E:440:ARG:HD2	5:E:2031:HOH:O	1.79	0.80
1:A:368:THR:HG22	5:A:2028:HOH:O	1.81	0.80
1:A:449:HIS:CD2	1:A:451:LEU:H	1.96	0.80
1:D:771:ASN:HD21	1:D:776:VAL:H	1.28	0.80
1:E:449:HIS:CD2	1:E:451:LEU:H	1.99	0.80
1:D:490:GLN:HG3	5:D:2042:HOH:O	1.83	0.79
1:B:611:ARG:HD3	5:B:2093:HOH:O	1.82	0.79
1:D:322:THR:HG22	1:D:324:TYR:H	1.47	0.79
1:B:449:HIS:CD2	1:B:451:LEU:H	2.01	0.78
1:C:779:ASP:HB2	5:C:2102:HOH:O	1.82	0.78
1:D:295:VAL:HG13	1:D:305:TYR:CE2	2.19	0.78
1:A:439:GLN:HE22	1:A:441:TYR:HB2	1.48	0.78
1:D:440:ARG:HE	1:D:489:GLN:HE21	1.32	0.78
1:D:882:LYS:HE3	5:D:2158:HOH:O	1.84	0.78
1:E:499:LYS:HE2	1:E:500:ASN:N	1.98	0.77
1:A:542:HIS:HD2	5:A:2063:HOH:O	1.68	0.77
1:D:765:ARG:HH12	1:E:367:GLN:NE2	1.75	0.77
1:C:295:VAL:HG13	1:C:305:TYR:CE2	2.19	0.77
1:D:542:HIS:HD2	5:D:2059:HOH:O	1.68	0.77
1:A:771:ASN:ND2	1:A:776:VAL:H	1.83	0.76
1:D:368:THR:HG21	5:E:2005:HOH:O	1.84	0.76
1:D:367:GLN:HE22	1:D:764:PHE:H	1.32	0.76
1:A:270:LYS:HE2	5:A:2002:HOH:O	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:ARG:HH11	1:A:602:ARG:HG3	1.51	0.75
1:E:714:ILE:HG22	1:E:754:ILE:HD13	1.68	0.75
1:F:440:ARG:HE	1:F:489:GLN:HE21	1.34	0.74
1:E:609:ARG:HG2	1:E:678:TRP:CH2	2.22	0.74
1:F:295:VAL:HG13	1:F:305:TYR:CE2	2.22	0.74
1:F:322:THR:HG22	1:F:324:TYR:H	1.53	0.74
1:E:499:LYS:CE	1:E:500:ASN:H	1.98	0.74
1:A:367:GLN:HE21	1:B:765:ARG:NH1	1.79	0.72
1:A:448:ASP:OD2	1:A:479:LYS:NZ	2.22	0.72
1:E:364:ASP:OD1	1:E:368:THR:HB	1.89	0.72
1:C:673:LEU:HD12	1:C:683:ILE:HD12	1.71	0.72
1:C:449:HIS:HD2	1:C:451:LEU:N	1.84	0.72
1:C:364:ASP:OD1	1:C:368:THR:HB	1.90	0.72
1:F:771:ASN:HD21	1:F:776:VAL:H	1.38	0.71
1:B:743:HIS:HD2	5:B:2131:HOH:O	1.74	0.71
1:C:870:ASN:HD22	1:C:870:ASN:C	1.94	0.71
1:B:609:ARG:HG2	1:B:678:TRP:CH2	2.26	0.70
1:B:771:ASN:ND2	1:B:776:VAL:H	1.89	0.70
1:B:439:GLN:HE22	1:B:441:TYR:HB2	1.56	0.70
1:E:322:THR:HG22	1:E:324:TYR:H	1.54	0.70
1:C:448:ASP:OD2	1:C:479:LYS:NZ	2.23	0.69
1:E:367:GLN:HE22	1:E:764:PHE:H	1.37	0.69
1:B:379:HIS:H	1:B:386:ASN:ND2	1.91	0.69
1:D:844:GLU:HG2	5:D:2149:HOH:O	1.91	0.69
1:F:367:GLN:HE22	1:F:764:PHE:H	1.37	0.69
5:A:2012:HOH:O	1:B:368:THR:HG21	1.93	0.69
1:C:740:SER:OG	1:C:741:ASP:N	2.26	0.69
1:A:295:VAL:HG13	1:A:305:TYR:CE2	2.27	0.68
1:D:679:ASN:ND2	1:D:681:ASP:H	1.92	0.68
1:F:753:LYS:HE2	1:F:755:GLY:O	1.93	0.68
1:E:779:ASP:HB2	5:E:2094:HOH:O	1.93	0.68
1:B:364:ASP:OD1	1:B:368:THR:HB	1.94	0.68
1:D:779:ASP:HB2	5:D:2131:HOH:O	1.94	0.68
1:A:440:ARG:HE	1:A:489:GLN:HE21	1.42	0.67
1:E:350:HIS:CE1	1:E:699:ASN:HB3	2.29	0.67
1:D:367:GLN:HE21	1:F:765:ARG:HH12	1.40	0.67
1:A:367:GLN:HE22	1:A:764:PHE:H	1.42	0.67
1:C:689:THR:HG23	1:C:691:GLN:HE22	1.59	0.67
1:E:421:ARG:HD2	1:E:512:TRP:CD2	2.29	0.67
1:A:322:THR:HG22	1:A:324:TYR:H	1.60	0.66
1:E:532:ILE:HG12	1:E:537:PHE:HA	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:628:HIS:HD2	5:F:2066:HOH:O	1.77	0.66
1:F:330:GLN:HE21	1:F:527:HIS:HE1	1.44	0.66
1:A:527:HIS:HD2	1:A:582:PRO:O	1.79	0.66
1:D:771:ASN:ND2	1:D:776:VAL:H	1.94	0.66
1:A:291:ASN:HB2	5:C:2002:HOH:O	1.95	0.66
1:E:603:LEU:HG	1:E:621:ARG:HD3	1.78	0.66
1:A:886:ASP:OD2	1:C:897:ARG:NH1	2.29	0.65
1:D:847:SER:OG	1:D:849:THR:HB	1.95	0.65
1:E:373:GLU:OE2	1:E:508:HIS:HE1	1.78	0.65
1:A:486:THR:HB	1:A:487:PRO:HD3	1.79	0.65
1:F:330:GLN:HE21	1:F:527:HIS:CE1	2.14	0.65
1:D:662:LYS:HE3	5:D:2084:HOH:O	1.97	0.65
5:D:2010:HOH:O	1:F:368:THR:HG21	1.97	0.65
1:F:449:HIS:HD2	1:F:451:LEU:N	1.89	0.65
1:B:373:GLU:OE2	1:B:508:HIS:HE1	1.80	0.64
1:D:765:ARG:HD3	5:D:2126:HOH:O	1.97	0.64
1:C:322:THR:HB	1:C:326:ASN:OD1	1.97	0.64
1:E:427:LEU:N	1:E:503:MET:O	2.23	0.64
1:D:712:ASN:HD22	1:D:712:ASN:H	1.46	0.64
1:B:322:THR:HG22	1:B:324:TYR:H	1.62	0.64
1:D:609:ARG:HG2	1:D:678:TRP:CH2	2.33	0.64
1:B:443:THR:HG22	5:B:2045:HOH:O	1.96	0.64
1:F:609:ARG:HG2	1:F:678:TRP:CH2	2.33	0.63
1:B:558:ASP:OD1	1:B:561:ASN:HB2	1.98	0.63
1:A:368:THR:HG21	5:C:2006:HOH:O	1.98	0.63
1:A:906:ASN:OD1	1:C:909:VAL:HG11	1.98	0.63
1:D:886:ASP:OD2	1:E:897:ARG:NH1	2.32	0.63
1:E:309:GLU:OE1	1:E:309:GLU:HA	1.97	0.63
1:D:449:HIS:CD2	1:D:451:LEU:H	2.09	0.62
1:A:364:ASP:OD1	1:A:368:THR:HB	1.99	0.62
1:B:322:THR:HG21	5:B:2012:HOH:O	1.98	0.62
1:C:771:ASN:HD21	1:C:776:VAL:H	1.47	0.62
1:B:527:HIS:HD2	1:B:582:PRO:O	1.82	0.62
1:A:896:ASN:HB2	1:B:882:LYS:HD2	1.81	0.62
1:B:440:ARG:HE	1:B:489:GLN:NE2	1.98	0.62
1:A:373:GLU:OE2	1:A:508:HIS:HE1	1.83	0.61
1:E:439:GLN:HE22	1:E:441:TYR:HB2	1.64	0.61
1:B:818:GLU:HB3	4:B:1686:PO4:O2	2.00	0.61
1:D:553:LEU:HD22	1:D:591:LEU:HD21	1.81	0.61
1:E:714:ILE:CG2	1:E:754:ILE:HD13	2.30	0.61
1:C:373:GLU:OE2	1:C:508:HIS:HE1	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:580:SER:HB3	5:F:2058:HOH:O	2.02	0.60
1:C:439:GLN:NE2	1:C:441:TYR:H	1.99	0.60
1:A:847:SER:OG	1:A:849:THR:HB	2.02	0.60
1:A:609:ARG:HG2	1:A:678:TRP:CH2	2.36	0.60
1:B:835:GLY:O	1:B:837:ARG:HG2	2.01	0.60
1:B:367:GLN:NE2	1:C:765:ARG:HH12	1.93	0.60
1:D:632:PRO:HB2	1:D:707:VAL:HG23	1.84	0.60
1:B:396:ARG:HB3	1:B:560:PHE:CZ	2.37	0.60
1:D:527:HIS:HD2	1:D:582:PRO:O	1.85	0.59
1:E:368:THR:HG21	5:F:2009:HOH:O	2.03	0.59
1:A:277:THR:HG22	1:A:295:VAL:HG22	1.85	0.59
1:B:396:ARG:NH2	1:B:534:ASN:O	2.32	0.59
1:D:439:GLN:HE22	1:D:441:TYR:HB2	1.67	0.59
1:C:273:GLY:HA3	1:C:292:THR:OG1	2.03	0.59
1:A:486:THR:HB	1:A:487:PRO:CD	2.33	0.59
1:E:759:ARG:HD3	5:F:2080:HOH:O	2.03	0.58
1:A:886:ASP:OD1	1:C:897:ARG:NH1	2.37	0.58
1:F:668:THR:OG1	1:F:691:GLN:NE2	2.36	0.58
1:F:628:HIS:HE1	1:F:658:ASP:OD1	1.87	0.58
1:C:488:ASN:ND2	1:C:490:GLN:HE22	2.02	0.58
1:C:439:GLN:HE22	1:C:441:TYR:HB2	1.67	0.58
1:C:700:SER:OG	1:C:702:VAL:HG13	2.04	0.58
1:E:527:HIS:HD2	1:E:582:PRO:O	1.86	0.58
1:F:295:VAL:HG13	1:F:305:TYR:CD2	2.39	0.58
1:C:330:GLN:HE21	1:C:527:HIS:CE1	2.21	0.57
1:C:607:LEU:HB3	1:C:620:LEU:HD22	1.87	0.57
1:C:735:LYS:O	1:C:743:HIS:HE1	1.86	0.57
1:A:854:ILE:HD12	1:B:856:LEU:HD21	1.85	0.57
1:B:295:VAL:HG13	1:B:305:TYR:CE2	2.40	0.57
1:B:277:THR:CG2	1:B:295:VAL:HG22	2.35	0.57
1:B:350:HIS:CE1	1:B:699:ASN:HB3	2.39	0.57
1:A:576:GLU:N	1:A:577:PRO:HD2	2.20	0.57
1:A:325:TYR:OH	1:A:350:HIS:HE1	1.87	0.57
1:B:428:HIS:ND1	1:B:502:HIS:HD2	2.03	0.57
1:E:277:THR:HG22	1:E:295:VAL:HG22	1.86	0.57
1:C:367:GLN:HE22	1:C:764:PHE:H	1.53	0.57
1:C:419:TRP:CE2	1:C:514:LYS:HD3	2.39	0.57
1:E:305:TYR:CZ	1:E:684:GLU:HG2	2.40	0.57
1:F:603:LEU:HB3	1:F:621:ARG:CZ	2.35	0.56
2:H:2:SIA:H6	2:H:2:SIA:O1B	2.05	0.56
1:D:396:ARG:HB3	1:D:560:PHE:CZ	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:SER:HB2	1:B:616:THR:O	2.06	0.56
1:B:488:ASN:C	1:B:488:ASN:HD22	2.08	0.56
1:D:553:LEU:CD2	1:D:591:LEU:HD21	2.36	0.56
1:A:779:ASP:HB2	5:A:2155:HOH:O	2.06	0.56
1:B:444:ILE:HG22	1:B:446:VAL:HG23	1.88	0.56
1:E:457:VAL:HA	1:E:504:GLY:O	2.05	0.56
1:F:325:TYR:OH	1:F:350:HIS:HE1	1.89	0.56
1:A:352:VAL:HB	1:A:386:ASN:HB3	1.88	0.56
1:A:428:HIS:ND1	1:A:502:HIS:HD2	2.04	0.56
1:A:736:ASP:HB3	1:A:739:LYS:HG3	1.88	0.56
1:B:445:HIS:HD2	1:B:481:ASN:ND2	2.04	0.56
1:A:440:ARG:HE	1:A:489:GLN:NE2	2.03	0.56
1:F:439:GLN:HE22	1:F:441:TYR:HB2	1.71	0.56
1:B:445:HIS:CD2	1:B:481:ASN:HD21	2.23	0.55
1:A:602:ARG:NH1	1:A:602:ARG:HG3	2.21	0.55
1:B:287:SER:OG	1:C:753:LYS:HE3	2.05	0.55
1:A:628:HIS:HE1	1:A:658:ASP:OD1	1.88	0.55
1:C:818:GLU:HB3	4:C:1687:PO4:O4	2.05	0.55
1:E:277:THR:CG2	1:E:295:VAL:HG22	2.36	0.55
1:C:888:VAL:HG12	1:C:889:THR:HG23	1.87	0.55
1:F:765:ARG:HD2	5:F:2112:HOH:O	2.05	0.55
1:C:277:THR:HG22	1:C:295:VAL:HG22	1.87	0.55
1:D:586:TYR:OH	1:D:589:GLY:HA2	2.05	0.55
1:E:327:ALA:HB3	1:E:328:TRP:CE3	2.42	0.55
1:B:732:ASN:HD21	1:B:736:ASP:H	1.53	0.55
1:D:490:GLN:CG	5:D:2042:HOH:O	2.47	0.55
1:D:373:GLU:OE2	1:D:508:HIS:HE1	1.89	0.55
1:A:379:HIS:H	1:A:386:ASN:ND2	2.05	0.54
1:A:602:ARG:NE	5:A:2082:HOH:O	2.37	0.54
1:B:847:SER:OG	1:B:849:THR:HB	2.07	0.54
1:D:330:GLN:HE21	1:D:527:HIS:CE1	2.25	0.54
1:F:457:VAL:HA	1:F:504:GLY:O	2.07	0.54
1:A:607:LEU:HB3	1:A:620:LEU:HD22	1.90	0.54
1:B:909:VAL:HA	1:C:903:LEU:O	2.08	0.54
1:E:466:GLY:HA3	1:E:486:THR:HB	1.90	0.54
1:E:342:ALA:HB2	1:E:717:MET:HE2	1.89	0.54
1:D:460:SER:OG	2:H:2:SIA:H4	2.07	0.54
1:B:445:HIS:HD2	1:B:481:ASN:HD21	1.55	0.54
1:A:613:ILE:O	1:A:613:ILE:HG22	2.08	0.54
1:E:715:TYR:CE1	1:E:751:LYS:HG3	2.42	0.54
1:F:486:THR:HB	1:F:487:PRO:HD2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:532:ILE:HG12	1:F:537:PHE:HA	1.89	0.54
1:B:367:GLN:HE22	1:B:764:PHE:H	1.56	0.54
1:C:386:ASN:ND2	1:C:387:TYR:H	2.06	0.54
1:D:277:THR:HG22	1:D:295:VAL:HG22	1.90	0.53
1:E:440:ARG:HE	1:E:489:GLN:HE21	1.56	0.53
1:B:277:THR:HG22	1:B:295:VAL:HG22	1.89	0.53
1:C:405:THR:HB	1:C:415:ASN:HB3	1.91	0.53
1:E:433:ILE:HG12	1:E:444:ILE:HG23	1.90	0.53
5:E:2110:HOH:O	1:F:844:GLU:HG2	2.07	0.53
1:C:628:HIS:HE1	1:C:658:ASP:OD1	1.90	0.53
1:E:910:THR:HG22	1:F:897:ARG:HH11	1.74	0.53
1:A:465:THR:HB	1:A:490:GLN:HE22	1.73	0.53
1:A:342:ALA:HB2	1:A:717:MET:HE2	1.90	0.53
1:D:306:TYR:HD1	1:D:687:ASN:HD22	1.54	0.53
1:F:650:ASN:HA	1:F:667:ARG:NH2	2.24	0.53
1:D:367:GLN:HE21	1:F:765:ARG:NH1	2.07	0.53
1:E:379:HIS:H	1:E:386:ASN:ND2	2.06	0.53
1:E:352:VAL:HA	1:E:355:LEU:HD23	1.91	0.52
1:F:368:THR:HG22	5:F:2024:HOH:O	2.07	0.52
1:A:522:SER:HB3	1:A:568:ARG:HH22	1.74	0.52
1:A:287:SER:OG	1:B:753:LYS:HE3	2.09	0.52
1:C:771:ASN:ND2	1:C:776:VAL:H	2.07	0.52
1:A:464:VAL:HG23	1:A:496:ASN:HB3	1.91	0.52
1:A:771:ASN:HD21	1:A:776:VAL:N	1.96	0.52
1:D:352:VAL:HA	1:D:355:LEU:HD23	1.90	0.52
1:C:293:ARG:HD3	1:C:311:PHE:CE2	2.45	0.52
1:E:330:GLN:HB2	1:E:527:HIS:HE1	1.75	0.52
1:F:330:GLN:HB2	1:F:527:HIS:HE1	1.74	0.52
1:B:700:SER:OG	1:B:702:VAL:HG13	2.09	0.51
1:A:693:TYR:HE1	5:A:2105:HOH:O	1.91	0.51
1:B:903:LEU:HA	1:C:898:PHE:O	2.10	0.51
1:D:379:HIS:ND1	1:D:380:PRO:HD2	2.25	0.51
1:E:400:PHE:CD1	1:E:420:ASP:HB3	2.45	0.51
1:E:620:LEU:HD23	1:E:620:LEU:C	2.31	0.51
1:C:522:SER:HB3	1:C:568:ARG:NH2	2.25	0.51
1:E:322:THR:HG21	5:E:2009:HOH:O	2.09	0.51
1:A:261:ALA:O	1:A:265:THR:HG23	2.10	0.51
1:A:555:TYR:O	1:A:557:PRO:HD3	2.10	0.51
1:F:398:ARG:HD2	1:F:450:GLY:O	2.10	0.51
1:A:393:GLY:HA3	1:A:529:PHE:CD2	2.46	0.51
1:A:774:VAL:O	1:A:776:VAL:HG23	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:TRP:CE3	1:C:375:LEU:HD11	2.46	0.51
1:E:373:GLU:OE2	1:E:508:HIS:CE1	2.62	0.51
1:E:396:ARG:HD3	1:E:534:ASN:O	2.10	0.51
1:C:305:TYR:CZ	1:C:684:GLU:HG2	2.45	0.51
1:E:322:THR:HB	1:E:326:ASN:OD1	2.11	0.51
1:C:396:ARG:CG	1:C:396:ARG:O	2.58	0.51
1:D:330:GLN:HG3	1:D:330:GLN:O	2.10	0.51
1:F:765:ARG:CD	5:F:2112:HOH:O	2.58	0.51
1:F:379:HIS:H	1:F:386:ASN:ND2	2.09	0.51
1:C:527:HIS:HD2	1:C:582:PRO:O	1.94	0.50
1:E:433:ILE:HG22	1:E:464:VAL:HG21	1.92	0.50
1:F:439:GLN:NE2	1:F:441:TYR:H	2.09	0.50
1:E:347:SER:HB3	1:E:355:LEU:HB2	1.94	0.50
5:A:2032:HOH:O	1:B:779:ASP:HB2	2.10	0.50
1:D:732:ASN:HD21	1:D:736:ASP:H	1.60	0.50
1:A:449:HIS:HD2	1:A:451:LEU:N	1.93	0.50
1:B:743:HIS:CD2	5:B:2131:HOH:O	2.55	0.50
1:D:325:TYR:OH	1:D:350:HIS:HE1	1.94	0.50
1:C:870:ASN:HD22	1:C:871:GLY:N	2.09	0.50
1:A:277:THR:CG2	1:A:295:VAL:HG22	2.42	0.50
1:A:660:ARG:O	1:A:661:TYR:HB2	2.11	0.50
1:A:765:ARG:HH12	1:C:367:GLN:NE2	1.91	0.50
1:B:373:GLU:OE2	1:B:508:HIS:CE1	2.64	0.50
1:D:440:ARG:NE	1:D:489:GLN:HE21	2.06	0.50
1:C:628:HIS:HD2	5:C:2058:HOH:O	1.95	0.50
1:E:594:ILE:HD12	1:E:633:PHE:CD2	2.47	0.50
1:A:522:SER:HB3	1:A:568:ARG:NH2	2.26	0.50
1:D:322:THR:HB	1:D:326:ASN:OD1	2.12	0.50
1:D:386:ASN:ND2	1:D:387:TYR:H	2.10	0.50
1:E:628:HIS:HE1	1:E:658:ASP:OD1	1.95	0.50
1:F:837:ARG:NH2	3:F:1685:SLB:H111	2.26	0.50
1:D:896:ASN:HB2	1:F:882:LYS:HD2	1.94	0.50
1:E:771:ASN:HD21	1:E:776:VAL:H	1.58	0.49
1:A:888:VAL:HG12	1:A:889:THR:HG23	1.94	0.49
1:D:352:VAL:HB	1:D:386:ASN:HB3	1.94	0.49
5:A:2012:HOH:O	1:B:368:THR:CG2	2.56	0.49
1:D:465:THR:HG21	1:D:490:GLN:HE21	1.77	0.49
1:E:669:PHE:CE1	1:E:687:ASN:HB2	2.47	0.49
1:C:413:LEU:HD21	1:C:416:CYS:SG	2.53	0.49
1:A:527:HIS:CD2	1:A:582:PRO:O	2.60	0.49
1:A:700:SER:OG	1:A:702:VAL:HG13	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:SER:HB3	1:B:355:LEU:HD22	1.95	0.49
1:B:603:LEU:HB3	1:B:621:ARG:CZ	2.42	0.49
1:F:428:HIS:ND1	1:F:502:HIS:HD2	2.11	0.49
1:C:367:GLN:HE22	1:C:763:ASP:HA	1.77	0.49
1:A:609:ARG:HG2	1:A:678:TRP:CZ2	2.47	0.49
1:A:620:LEU:HD21	1:A:680:ALA:HB2	1.94	0.49
1:B:396:ARG:HD3	1:B:534:ASN:O	2.13	0.49
1:D:765:ARG:NH1	5:D:2126:HOH:O	2.25	0.49
1:B:568:ARG:HD2	5:B:2082:HOH:O	2.12	0.49
1:D:293:ARG:HD3	1:D:311:PHE:CE2	2.48	0.49
1:E:352:VAL:HB	1:E:386:ASN:HB3	1.94	0.49
1:E:736:ASP:HB3	1:E:739:LYS:HG2	1.94	0.49
1:A:497:ALA:HB2	5:A:2057:HOH:O	2.13	0.49
1:B:649:GLU:HB3	1:B:664:SER:HB2	1.94	0.49
1:C:295:VAL:HG13	1:C:305:TYR:CD2	2.47	0.49
1:D:753:LYS:HE3	1:E:287:SER:OG	2.12	0.49
1:E:449:HIS:HD2	1:E:451:LEU:N	2.01	0.49
1:B:661:TYR:CZ	1:B:698:VAL:HB	2.48	0.48
1:D:603:LEU:HB3	1:D:621:ARG:CZ	2.43	0.48
1:E:558:ASP:OD1	1:E:561:ASN:HB2	2.13	0.48
1:C:571:ILE:HB	1:C:572:PRO:HD2	1.95	0.48
1:D:460:SER:HB3	1:D:461:ASN:ND2	2.28	0.48
1:E:277:THR:HG22	1:E:295:VAL:CG2	2.43	0.48
1:F:603:LEU:HG	1:F:621:ARG:HD3	1.94	0.48
1:E:628:HIS:HD2	5:E:2045:HOH:O	1.96	0.48
1:F:350:HIS:CE1	1:F:699:ASN:HB3	2.48	0.48
1:C:614:GLY:HA2	1:C:617:TRP:CZ2	2.48	0.48
1:A:352:VAL:O	1:A:355:LEU:HB3	2.13	0.48
1:C:532:ILE:HG12	1:C:537:PHE:HA	1.95	0.48
1:A:753:LYS:HE3	1:C:287:SER:OG	2.14	0.48
1:D:357:VAL:HG12	1:D:375:LEU:HD12	1.96	0.48
1:D:679:ASN:HD22	1:D:680:ALA:N	2.11	0.48
1:E:700:SER:OG	1:E:702:VAL:HG13	2.13	0.48
1:F:342:ALA:HB2	1:F:717:MET:HE2	1.96	0.48
1:B:305:TYR:CE1	1:B:684:GLU:HB3	2.49	0.48
1:B:521:PRO:HA	5:B:2071:HOH:O	2.14	0.48
1:D:906:ASN:OD1	1:E:909:VAL:HG11	2.14	0.48
1:E:342:ALA:HB2	1:E:717:MET:CE	2.44	0.48
1:E:609:ARG:HG2	1:E:678:TRP:CZ2	2.48	0.48
1:E:744:PRO:HD2	5:E:2087:HOH:O	2.14	0.48
1:E:428:HIS:ND1	1:E:502:HIS:HD2	2.11	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:433:ILE:CG2	1:E:464:VAL:HG21	2.44	0.47
1:F:379:HIS:H	1:F:386:ASN:HD22	1.63	0.47
1:B:673:LEU:HD12	1:B:683:ILE:HD12	1.95	0.47
1:F:419:TRP:CD1	1:F:514:LYS:HG2	2.48	0.47
1:B:330:GLN:HB2	1:B:527:HIS:HE1	1.80	0.47
1:B:527:HIS:CD2	1:B:582:PRO:O	2.66	0.47
1:B:673:LEU:HD12	1:B:683:ILE:CD1	2.45	0.47
1:C:503:MET:HG2	1:C:504:GLY:HA3	1.96	0.47
1:E:788:ALA:HB2	1:F:738:PHE:CD1	2.50	0.47
1:B:328:TRP:N	1:B:329:PRO:HD3	2.29	0.47
1:D:396:ARG:HD3	1:D:534:ASN:O	2.15	0.47
1:E:735:LYS:O	1:E:743:HIS:HE1	1.97	0.47
1:B:689:THR:HG23	1:B:691:GLN:HE22	1.79	0.47
1:E:649:GLU:HB2	1:E:664:SER:HB2	1.96	0.47
1:F:435:LYS:HB3	1:F:494:LEU:HB2	1.96	0.47
1:D:848:SER:O	1:F:865:ARG:NE	2.47	0.47
1:A:405:THR:HB	1:A:414:THR:HG22	1.96	0.47
1:B:771:ASN:HD21	1:B:776:VAL:N	2.02	0.47
1:D:712:ASN:ND2	1:D:712:ASN:H	2.11	0.47
1:E:753:LYS:HE2	1:E:755:GLY:O	2.15	0.47
1:B:878:SER:HB2	1:C:871:GLY:O	2.15	0.47
1:D:440:ARG:HE	1:D:489:GLN:NE2	2.05	0.47
1:E:847:SER:OG	1:E:849:THR:HB	2.15	0.47
1:B:325:TYR:OH	1:B:350:HIS:HE1	1.97	0.46
1:B:457:VAL:HA	1:B:504:GLY:O	2.15	0.46
1:B:379:HIS:HB2	1:B:386:ASN:HD22	1.79	0.46
1:F:682:ASP:HB2	5:F:2082:HOH:O	2.15	0.46
1:F:847:SER:OG	1:F:849:THR:HB	2.14	0.46
1:A:852:ALA:HB1	1:B:867:ILE:HG12	1.96	0.46
1:B:549:ARG:HD3	1:B:579:ALA:O	2.16	0.46
1:A:870:ASN:ND2	1:B:865:ARG:HH22	2.13	0.46
1:C:320:THR:HG23	1:C:747:LEU:HB2	1.96	0.46
1:C:428:HIS:ND1	1:C:502:HIS:HD2	2.14	0.46
1:C:661:TYR:CZ	1:C:698:VAL:HB	2.50	0.46
1:E:445:HIS:HD2	1:E:481:ASN:HD21	1.62	0.46
1:C:306:TYR:HD1	1:C:687:ASN:HD22	1.62	0.46
1:A:886:ASP:CG	1:C:897:ARG:NH1	2.69	0.46
1:D:398:ARG:HD2	1:D:450:GLY:O	2.15	0.46
1:B:445:HIS:CD2	1:B:481:ASN:ND2	2.82	0.46
1:D:464:VAL:HG23	1:D:496:ASN:HB3	1.97	0.46
1:D:754:ILE:HA	1:D:754:ILE:HD12	1.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:743:HIS:O	5:E:2085:HOH:O	2.20	0.46
1:E:367:GLN:NE2	1:E:763:ASP:HA	2.31	0.46
1:A:322:THR:HB	1:A:326:ASN:OD1	2.16	0.46
1:C:607:LEU:HD13	1:C:678:TRP:CH2	2.50	0.46
1:C:340:ILE:CG2	1:C:717:MET:HE1	2.46	0.46
1:E:440:ARG:HE	1:E:489:GLN:NE2	2.14	0.46
1:C:347:SER:HB3	1:C:355:LEU:HB2	1.97	0.46
1:E:771:ASN:ND2	1:E:776:VAL:H	2.13	0.46
1:F:439:GLN:HE22	1:F:441:TYR:H	1.62	0.46
1:F:440:ARG:HG2	1:F:489:GLN:HB3	1.96	0.46
1:A:382:TYR:CG	1:A:383:PRO:HA	2.51	0.46
1:A:460:SER:HB3	1:A:461:ASN:ND2	2.31	0.46
1:D:367:GLN:NE2	1:F:765:ARG:HH12	2.12	0.46
1:C:464:VAL:HG23	1:C:496:ASN:HB3	1.98	0.46
1:C:826:LYS:HB2	1:C:838:ILE:HG13	1.97	0.46
1:F:527:HIS:HD2	1:F:582:PRO:O	1.98	0.46
1:A:852:ALA:HB1	1:B:867:ILE:CG1	2.46	0.45
1:D:620:LEU:C	1:D:620:LEU:HD23	2.36	0.45
1:E:391:SER:OG	1:E:539:MET:HG2	2.16	0.45
1:F:295:VAL:CG1	1:F:305:TYR:CE2	2.98	0.45
1:F:609:ARG:HG2	1:F:678:TRP:CZ3	2.51	0.45
1:C:441:TYR:CZ	1:C:485:LEU:HD13	2.52	0.45
1:C:827:SER:O	1:C:829:PRO:HD3	2.16	0.45
1:C:661:TYR:OH	1:C:698:VAL:HB	2.16	0.45
1:F:325:TYR:OH	1:F:350:HIS:CE1	2.69	0.45
1:F:620:LEU:HD23	1:F:620:LEU:C	2.37	0.45
1:C:322:THR:HG22	1:C:324:TYR:N	2.23	0.45
1:F:679:ASN:C	1:F:679:ASN:OD1	2.55	0.45
1:E:553:LEU:HD22	1:E:591:LEU:HD21	1.98	0.45
1:F:322:THR:HG23	1:F:323:PRO:HD2	1.99	0.45
1:C:659:ASP:OD1	1:C:662:LYS:HE3	2.17	0.45
1:D:712:ASN:HB3	5:D:2122:HOH:O	2.16	0.45
1:F:739:LYS:CD	5:F:2098:HOH:O	2.65	0.45
1:F:826:LYS:HB2	1:F:838:ILE:HG13	1.99	0.45
1:E:883:PRO:HD3	1:F:898:PHE:CZ	2.51	0.45
1:C:870:ASN:ND2	1:C:870:ASN:C	2.61	0.45
1:B:584:ILE:O	1:B:585:LYS:HD2	2.17	0.44
1:B:739:LYS:HE3	5:B:2126:HOH:O	2.15	0.44
1:C:458:ASN:HA	1:C:469:GLY:O	2.17	0.44
1:C:305:TYR:CE1	1:C:684:GLU:HG2	2.52	0.44
1:C:754:ILE:HA	1:C:754:ILE:HD12	1.59	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:796:LEU:HG	1:C:798:LEU:HD21	1.99	0.44
1:D:457:VAL:HA	1:D:504:GLY:O	2.17	0.44
1:E:553:LEU:CD2	1:E:591:LEU:HD21	2.47	0.44
1:E:910:THR:HB	5:E:2126:HOH:O	2.18	0.44
1:A:836:GLN:HG2	1:A:858:GLY:HA3	1.98	0.44
1:A:848:SER:O	1:B:865:ARG:NE	2.50	0.44
1:C:343:PRO:HA	1:C:359:TRP:HB3	1.99	0.44
1:C:430:THR:HA	1:C:499:LYS:O	2.17	0.44
1:F:322:THR:HB	1:F:326:ASN:OD1	2.18	0.44
1:B:449:HIS:HE1	1:B:478:ASP:O	2.00	0.44
1:C:613:ILE:O	1:C:613:ILE:HG22	2.18	0.44
1:E:732:ASN:HA	5:E:2081:HOH:O	2.17	0.44
1:A:428:HIS:ND1	1:A:502:HIS:CD2	2.84	0.44
1:C:574:GLU:HG3	1:C:575:TYR:CD2	2.52	0.44
1:C:593:LEU:HD23	1:C:593:LEU:C	2.38	0.44
1:B:826:LYS:HD2	1:C:817:MET:O	2.16	0.44
1:A:279:LYS:HA	1:A:295:VAL:HG23	1.99	0.44
1:C:379:HIS:H	1:C:386:ASN:ND2	2.14	0.44
1:D:247:LYS:HA	1:D:247:LYS:HD3	1.73	0.44
1:F:364:ASP:OD1	1:F:368:THR:HB	2.16	0.44
1:F:378:LEU:HA	1:F:386:ASN:HD21	1.83	0.44
1:A:603:LEU:HB3	1:A:621:ARG:CZ	2.48	0.44
1:A:902:TYR:CD1	1:B:893:GLY:HA2	2.52	0.44
1:E:322:THR:HG23	1:E:323:PRO:HD2	1.98	0.44
1:B:305:TYR:CD1	1:B:305:TYR:N	2.86	0.44
1:B:306:TYR:HD1	1:B:687:ASN:HD22	1.66	0.44
1:A:848:SER:HB2	1:B:865:ARG:NH2	2.33	0.44
1:D:898:PHE:CE1	1:F:883:PRO:HD3	2.53	0.44
1:E:247:LYS:HG3	1:E:252:THR:HG21	2.00	0.44
1:F:326:ASN:ND2	5:F:2012:HOH:O	2.51	0.44
1:F:771:ASN:ND2	1:F:776:VAL:H	2.12	0.44
1:B:379:HIS:H	1:B:386:ASN:HD22	1.65	0.44
1:C:330:GLN:HA	1:C:331:ASP:HA	1.82	0.44
1:D:330:GLN:HB2	1:D:527:HIS:HE1	1.83	0.44
1:F:277:THR:HG22	1:F:295:VAL:HG22	2.00	0.44
1:A:457:VAL:HA	1:A:504:GLY:O	2.17	0.43
1:A:735:LYS:O	1:A:743:HIS:HE1	2.00	0.43
1:C:330:GLN:HB2	1:C:527:HIS:HE1	1.83	0.43
1:D:614:GLY:HA2	1:D:617:TRP:CZ2	2.53	0.43
1:D:350:HIS:CE1	1:D:699:ASN:HB3	2.53	0.43
1:F:445:HIS:HD2	1:F:481:ASN:HD21	1.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:HIS:HD2	1:B:451:LEU:N	2.03	0.43
1:C:400:PHE:CD1	1:C:420:ASP:HB3	2.53	0.43
1:C:542:HIS:HD2	5:C:2047:HOH:O	2.00	0.43
1:C:839:ILE:HG12	1:C:855:THR:HG23	2.00	0.43
1:C:847:SER:OG	1:C:849:THR:HB	2.17	0.43
1:F:754:ILE:HA	1:F:754:ILE:HD12	1.62	0.43
1:D:445:HIS:HD2	1:D:481:ASN:HD21	1.66	0.43
1:E:367:GLN:HE22	1:E:763:ASP:HA	1.82	0.43
1:A:342:ALA:HB2	1:A:717:MET:CE	2.49	0.43
1:C:457:VAL:HA	1:C:504:GLY:O	2.19	0.43
1:D:267:VAL:HB	5:F:2007:HOH:O	2.18	0.43
1:B:277:THR:HG22	1:B:295:VAL:CG2	2.49	0.43
1:B:649:GLU:CB	1:B:664:SER:HB2	2.49	0.43
1:D:522:SER:HB3	1:D:568:ARG:NH2	2.33	0.43
1:D:609:ARG:HD2	1:D:618:GLU:OE1	2.19	0.43
1:E:315:GLU:HB3	5:E:2004:HOH:O	2.18	0.43
1:F:283:LEU:HA	1:F:283:LEU:HD23	1.86	0.43
1:D:903:LEU:HA	1:F:898:PHE:O	2.19	0.43
1:A:325:TYR:OH	1:A:350:HIS:CE1	2.70	0.43
1:A:576:GLU:N	1:A:577:PRO:CD	2.81	0.43
1:C:735:LYS:O	1:C:743:HIS:CE1	2.71	0.43
1:E:771:ASN:HA	1:E:771:ASN:HD22	1.70	0.43
1:F:396:ARG:HD3	1:F:534:ASN:O	2.19	0.43
1:F:542:HIS:HD2	5:F:2057:HOH:O	2.01	0.43
1:B:679:ASN:HD21	1:B:681:ASP:CG	2.21	0.43
1:D:364:ASP:OD1	1:D:368:THR:HB	2.19	0.43
1:D:882:LYS:HD2	1:E:896:ASN:HB2	2.01	0.43
1:D:765:ARG:O	1:E:317:PHE:HA	2.19	0.43
1:E:352:VAL:HG11	1:E:406:ARG:HB2	2.01	0.43
1:E:542:HIS:CD2	5:E:2038:HOH:O	2.44	0.43
1:E:707:VAL:HA	1:E:715:TYR:O	2.19	0.43
1:F:576:GLU:N	1:F:577:PRO:CD	2.82	0.43
1:F:349:ARG:HB3	1:F:735:LYS:HD3	2.01	0.43
1:A:715:TYR:CE1	1:A:751:LYS:HD2	2.54	0.43
1:C:367:GLN:NE2	1:C:763:ASP:HA	2.34	0.43
1:A:421:ARG:HD2	1:A:512:TRP:CD2	2.54	0.42
1:C:327:ALA:HB3	1:C:328:TRP:CE3	2.53	0.42
1:C:649:GLU:HB2	1:C:664:SER:HB2	2.01	0.42
1:D:603:LEU:HG	1:D:621:ARG:HD3	2.01	0.42
1:F:836:GLN:OE1	1:F:860:ASN:HB2	2.18	0.42
1:D:607:LEU:HB3	1:D:620:LEU:HD22	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:818:GLU:HA	1:F:827:SER:OG	2.19	0.42
1:A:754:ILE:HA	1:A:754:ILE:HD12	1.51	0.42
1:B:338:ASN:HB2	5:B:2017:HOH:O	2.18	0.42
1:B:754:ILE:HA	1:B:754:ILE:HD12	1.88	0.42
1:C:316:LEU:HD22	1:C:689:THR:OG1	2.19	0.42
1:E:330:GLN:HA	1:E:331:ASP:HA	1.82	0.42
1:E:437:ALA:HB2	1:E:492:SER:C	2.39	0.42
1:E:270:LYS:HD3	1:E:270:LYS:HA	1.92	0.42
1:E:435:LYS:HB3	5:E:2029:HOH:O	2.19	0.42
1:E:576:GLU:N	1:E:577:PRO:CD	2.83	0.42
2:I:2:SIA:O1B	2:I:2:SIA:H6	2.18	0.42
1:E:883:PRO:HD3	1:F:898:PHE:CE1	2.55	0.42
1:A:379:HIS:ND1	1:A:380:PRO:HD2	2.35	0.42
1:A:870:ASN:HD22	1:A:870:ASN:C	2.23	0.42
1:B:396:ARG:HB3	1:B:560:PHE:HZ	1.82	0.42
1:C:660:ARG:O	1:C:661:TYR:HB2	2.20	0.42
1:C:900:THR:OG1	1:C:901:ALA:N	2.52	0.42
1:F:649:GLU:HB3	1:F:664:SER:HB2	2.02	0.42
1:C:594:ILE:HG12	1:C:607:LEU:HD23	2.02	0.42
1:D:330:GLN:HE21	1:D:527:HIS:HE1	1.68	0.42
1:D:586:TYR:CZ	1:D:589:GLY:HA2	2.55	0.42
1:F:440:ARG:NE	1:F:489:GLN:HE21	2.09	0.42
1:F:600:GLY:HA3	5:F:2077:HOH:O	2.19	0.42
1:D:639:ASP:OD1	1:D:672:ARG:HD3	2.19	0.42
1:A:379:HIS:CG	1:A:380:PRO:HD2	2.54	0.42
1:A:326:ASN:HB2	1:A:746:ASP:HA	2.01	0.42
1:E:640:LEU:HD22	1:E:675:VAL:HG12	2.02	0.42
1:A:569:ARG:HD2	1:A:613:ILE:O	2.20	0.41
1:A:765:ARG:O	1:C:317:PHE:HA	2.20	0.41
1:B:336:TYR:CE2	1:B:337:GLU:HG3	2.55	0.41
1:B:628:HIS:HE1	1:B:658:ASP:OD1	2.03	0.41
1:C:647:ARG:HH11	1:C:647:ARG:HG3	1.83	0.41
1:D:608:HIS:CE1	1:D:619:SER:HG	2.30	0.41
1:D:891:LEU:HD22	1:F:891:LEU:HD21	2.02	0.41
1:B:352:VAL:HA	1:B:355:LEU:HD23	2.02	0.41
1:C:468:SER:HA	5:C:2130:HOH:O	2.19	0.41
1:D:628:HIS:HE1	1:D:658:ASP:OD1	2.03	0.41
1:E:368:THR:HG22	5:E:2019:HOH:O	2.21	0.41
1:E:445:HIS:CD2	1:E:481:ASN:HD21	2.38	0.41
1:F:277:THR:CG2	1:F:295:VAL:HG22	2.50	0.41
1:A:324:TYR:HB2	1:A:326:ASN:HD21	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ALA:HB2	1:B:717:MET:CE	2.51	0.41
1:B:553:LEU:HD22	1:B:591:LEU:HD21	2.01	0.41
1:C:555:TYR:CZ	1:C:557:PRO:HA	2.55	0.41
1:C:647:ARG:NH1	1:C:647:ARG:HG3	2.35	0.41
1:E:305:TYR:N	1:E:305:TYR:CD1	2.89	0.41
1:E:631:LEU:HA	1:E:631:LEU:HD23	1.89	0.41
1:A:350:HIS:CE1	1:A:699:ASN:HB3	2.54	0.41
1:D:279:LYS:HA	1:D:295:VAL:HG23	2.02	0.41
1:D:325:TYR:OH	1:D:350:HIS:CE1	2.72	0.41
1:B:779:ASP:OD1	1:B:781:ASN:N	2.53	0.41
5:A:2170:HOH:O	1:B:864:SER:HB3	2.20	0.41
1:D:336:TYR:CE2	1:D:337:GLU:HG3	2.55	0.41
1:A:330:GLN:HA	1:A:331:ASP:HA	1.82	0.41
1:B:628:HIS:HD2	5:B:2088:HOH:O	2.04	0.41
1:E:295:VAL:HG13	1:E:305:TYR:CE2	2.55	0.41
1:E:325:TYR:OH	1:E:350:HIS:HE1	2.03	0.41
1:B:873:GLU:OE2	1:C:866:ARG:HB2	2.21	0.41
1:C:553:LEU:HD22	1:C:591:LEU:HD21	2.02	0.41
1:D:439:GLN:NE2	1:D:441:TYR:H	2.19	0.41
1:E:825:GLY:HA2	1:F:841:CYS:O	2.21	0.41
1:F:261:ALA:O	1:F:265:THR:HG23	2.20	0.41
1:B:330:GLN:HB2	1:B:527:HIS:CE1	2.56	0.41
1:B:771:ASN:HD22	1:B:771:ASN:HA	1.74	0.41
1:C:309:GLU:HA	1:C:309:GLU:OE1	2.20	0.41
1:D:262:LEU:HD23	1:D:262:LEU:HA	1.89	0.41
1:E:640:LEU:HD12	1:E:640:LEU:HA	1.95	0.41
1:C:603:LEU:HB3	1:C:621:ARG:CZ	2.51	0.41
1:C:623:PRO:HB2	1:C:624:HIS:CD2	2.56	0.41
1:E:367:GLN:HE22	1:E:764:PHE:N	2.12	0.41
1:E:765:ARG:HH12	1:F:367:GLN:NE2	2.05	0.41
1:F:593:LEU:C	1:F:593:LEU:HD23	2.41	0.40
1:D:673:LEU:HA	1:D:673:LEU:HD23	1.86	0.40
1:A:542:HIS:CD2	1:A:581:GLU:H	2.39	0.40
1:B:735:LYS:O	1:B:743:HIS:HE1	2.04	0.40
1:B:716:TYR:O	1:B:749:CYS:HA	2.20	0.40
1:C:328:TRP:N	1:C:329:PRO:HD3	2.36	0.40
1:D:553:LEU:CD2	1:D:591:LEU:CD2	2.99	0.40
1:D:660:ARG:O	1:D:661:TYR:HB2	2.20	0.40
1:D:829:PRO:HB3	1:F:820:GLU:HA	2.03	0.40
1:E:396:ARG:HB3	1:E:560:PHE:CZ	2.56	0.40
1:E:753:LYS:HE3	1:F:287:SER:OG	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:355:LEU:HD13	1:F:356:HIS:N	2.35	0.40
1:F:490:GLN:HG2	5:F:2049:HOH:O	2.21	0.40
1:D:522:SER:HB3	1:D:568:ARG:HH21	1.86	0.40
1:E:522:SER:HB2	1:E:568:ARG:NH2	2.37	0.40
1:A:499:LYS:HD2	1:A:499:LYS:HA	1.90	0.40
1:B:575:TYR:CG	1:B:608:HIS:HE1	2.39	0.40
1:D:302:GLN:HE22	1:D:654:ALA:HB3	1.87	0.40
1:D:344:TYR:CD2	1:D:747:LEU:HD11	2.56	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	664/666 (100%)	631 (95%)	31 (5%)	2 (0%)	41	51
1	B	664/666 (100%)	630 (95%)	34 (5%)	0	100	100
1	C	664/666 (100%)	629 (95%)	35 (5%)	0	100	100
1	D	664/666 (100%)	631 (95%)	32 (5%)	1 (0%)	47	60
1	E	664/666 (100%)	634 (96%)	28 (4%)	2 (0%)	41	51
1	F	664/666 (100%)	630 (95%)	34 (5%)	0	100	100
All	All	3984/3996 (100%)	3785 (95%)	194 (5%)	5 (0%)	51	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	496	ASN
1	D	704	VAL
1	E	350	HIS
1	E	704	VAL
1	A	704	VAL

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	564/564 (100%)	527 (93%)	37 (7%)	16	22
1	B	564/564 (100%)	519 (92%)	45 (8%)	12	15
1	C	564/564 (100%)	523 (93%)	41 (7%)	14	18
1	D	564/564 (100%)	523 (93%)	41 (7%)	14	18
1	E	564/564 (100%)	518 (92%)	46 (8%)	11	14
1	F	564/564 (100%)	518 (92%)	46 (8%)	11	14
All	All	3384/3384 (100%)	3128 (92%)	256 (8%)	13	17

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	VAL
1	A	258	LEU
1	A	260	SER
1	A	270	LYS
1	A	279	LYS
1	A	295	VAL
1	A	355	LEU
1	A	359	TRP
1	A	361	LYS
1	A	368	THR
1	A	414	THR
1	A	425	ARG
1	A	439	GLN
1	A	443	THR
1	A	460	SER
1	A	476	VAL
1	A	499	LYS
1	A	564	SER
1	A	585	LYS
1	A	596	ARG
1	A	603	LEU
1	A	607	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	609	ARG
1	A	618	GLU
1	A	620	LEU
1	A	621	ARG
1	A	640	LEU
1	A	717	MET
1	A	754	ILE
1	A	762	ARG
1	A	771	ASN
1	A	796	LEU
1	A	816	LEU
1	A	870	ASN
1	A	888	VAL
1	A	895	SER
1	A	910	THR
1	B	258	LEU
1	B	260	SER
1	B	279	LYS
1	B	282	SER
1	B	295	VAL
1	B	312	VAL
1	B	335	VAL
1	B	355	LEU
1	B	359	TRP
1	B	368	THR
1	B	414	THR
1	B	439	GLN
1	B	443	THR
1	B	457	VAL
1	B	468	SER
1	B	476	VAL
1	B	479	LYS
1	B	488	ASN
1	B	562	SER
1	B	568	ARG
1	B	574	GLU
1	B	585	LYS
1	B	596	ARG
1	B	603	LEU
1	B	607	LEU
1	B	609	ARG
1	B	611	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	620	LEU
1	B	621	ARG
1	B	640	LEU
1	B	662	LYS
1	B	670	TYR
1	B	679	ASN
1	B	683	ILE
1	B	717	MET
1	B	718	PHE
1	B	732	ASN
1	B	754	ILE
1	B	762	ARG
1	B	796	LEU
1	B	816	LEU
1	B	849	THR
1	B	870	ASN
1	B	909	VAL
1	B	910	THR
1	C	258	LEU
1	C	260	SER
1	C	281	THR
1	C	295	VAL
1	C	309	GLU
1	C	355	LEU
1	C	359	TRP
1	C	361	LYS
1	C	368	THR
1	C	386	ASN
1	C	396	ARG
1	C	425	ARG
1	C	439	GLN
1	C	443	THR
1	C	444	ILE
1	C	488	ASN
1	C	509	LYS
1	C	522	SER
1	C	528	SER
1	C	546	VAL
1	C	568	ARG
1	C	585	LYS
1	C	596	ARG
1	C	599	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	603	LEU
1	C	607	LEU
1	C	609	ARG
1	C	611	ARG
1	C	620	LEU
1	C	621	ARG
1	C	640	LEU
1	C	717	MET
1	C	732	ASN
1	C	754	ILE
1	C	762	ARG
1	C	771	ASN
1	C	796	LEU
1	C	816	LEU
1	C	870	ASN
1	C	909	VAL
1	C	910	THR
1	D	247	LYS
1	D	258	LEU
1	D	270	LYS
1	D	279	LYS
1	D	295	VAL
1	D	335	VAL
1	D	355	LEU
1	D	359	TRP
1	D	368	THR
1	D	386	ASN
1	D	396	ARG
1	D	414	THR
1	D	425	ARG
1	D	439	GLN
1	D	488	ASN
1	D	499	LYS
1	D	522	SER
1	D	549	ARG
1	D	568	ARG
1	D	574	GLU
1	D	585	LYS
1	D	596	ARG
1	D	599	ARG
1	D	603	LEU
1	D	607	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	609	ARG
1	D	620	LEU
1	D	621	ARG
1	D	640	LEU
1	D	679	ASN
1	D	712	ASN
1	D	717	MET
1	D	754	ILE
1	D	762	ARG
1	D	771	ASN
1	D	796	LEU
1	D	816	LEU
1	D	849	THR
1	D	870	ASN
1	D	909	VAL
1	D	910	THR
1	E	245	SER
1	E	258	LEU
1	E	260	SER
1	E	279	LYS
1	E	295	VAL
1	E	309	GLU
1	E	312	VAL
1	E	335	VAL
1	E	355	LEU
1	E	358	SER
1	E	359	TRP
1	E	368	THR
1	E	386	ASN
1	E	408	LEU
1	E	414	THR
1	E	421	ARG
1	E	439	GLN
1	E	443	THR
1	E	444	ILE
1	E	457	VAL
1	E	476	VAL
1	E	488	ASN
1	E	499	LYS
1	E	543	GLN
1	E	562	SER
1	E	564	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	574	GLU
1	E	585	LYS
1	E	596	ARG
1	E	602	ARG
1	E	603	LEU
1	E	607	LEU
1	E	609	ARG
1	E	620	LEU
1	E	621	ARG
1	E	640	LEU
1	E	717	MET
1	E	754	ILE
1	E	762	ARG
1	E	771	ASN
1	E	796	LEU
1	E	816	LEU
1	E	849	THR
1	E	870	ASN
1	E	909	VAL
1	E	910	THR
1	F	258	LEU
1	F	259	THR
1	F	276	LYS
1	F	279	LYS
1	F	295	VAL
1	F	335	VAL
1	F	355	LEU
1	F	359	TRP
1	F	368	THR
1	F	396	ARG
1	F	414	THR
1	F	439	GLN
1	F	443	THR
1	F	457	VAL
1	F	465	THR
1	F	468	SER
1	F	485	LEU
1	F	488	ASN
1	F	534	ASN
1	F	565	ASN
1	F	584	ILE
1	F	585	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	591	LEU
1	F	596	ARG
1	F	603	LEU
1	F	607	LEU
1	F	609	ARG
1	F	611	ARG
1	F	620	LEU
1	F	621	ARG
1	F	640	LEU
1	F	702	VAL
1	F	704	VAL
1	F	717	MET
1	F	732	ASN
1	F	754	ILE
1	F	762	ARG
1	F	771	ASN
1	F	796	LEU
1	F	816	LEU
1	F	849	THR
1	F	864	SER
1	F	870	ASN
1	F	895	SER
1	F	909	VAL
1	F	910	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (163) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
1	A	338	ASN
1	A	350	HIS
1	A	367	GLN
1	A	386	ASN
1	A	439	GLN
1	A	445	HIS
1	A	449	HIS
1	A	461	ASN
1	A	481	ASN
1	A	489	GLN
1	A	490	GLN
1	A	502	HIS
1	A	508	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	527	HIS
1	A	542	HIS
1	A	561	ASN
1	A	625	ASN
1	A	628	HIS
1	A	650	ASN
1	A	691	GLN
1	A	732	ASN
1	A	743	HIS
1	A	771	ASN
1	A	832	ASN
1	A	853	GLN
1	A	860	ASN
1	A	870	ASN
1	B	263	ASN
1	B	350	HIS
1	B	367	GLN
1	B	386	ASN
1	B	397	ASN
1	B	439	GLN
1	B	445	HIS
1	B	449	HIS
1	B	461	ASN
1	B	481	ASN
1	B	488	ASN
1	B	489	GLN
1	B	502	HIS
1	B	508	HIS
1	B	527	HIS
1	B	625	ASN
1	B	628	HIS
1	B	677	ASN
1	B	679	ASN
1	B	691	GLN
1	B	732	ASN
1	B	743	HIS
1	B	771	ASN
1	B	832	ASN
1	B	853	GLN
1	B	870	ASN
1	C	263	ASN
1	C	350	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	367	GLN
1	C	386	ASN
1	C	397	ASN
1	C	439	GLN
1	C	445	HIS
1	C	449	HIS
1	C	461	ASN
1	C	481	ASN
1	C	488	ASN
1	C	489	GLN
1	C	502	HIS
1	C	508	HIS
1	C	527	HIS
1	C	542	HIS
1	C	624	HIS
1	C	625	ASN
1	C	628	HIS
1	C	650	ASN
1	C	676	ASN
1	C	691	GLN
1	C	732	ASN
1	C	743	HIS
1	C	771	ASN
1	C	832	ASN
1	C	853	GLN
1	C	870	ASN
1	D	263	ASN
1	D	338	ASN
1	D	350	HIS
1	D	367	GLN
1	D	386	ASN
1	D	397	ASN
1	D	439	GLN
1	D	445	HIS
1	D	449	HIS
1	D	461	ASN
1	D	481	ASN
1	D	488	ASN
1	D	489	GLN
1	D	490	GLN
1	D	502	HIS
1	D	508	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	527	HIS
1	D	542	HIS
1	D	625	ASN
1	D	628	HIS
1	D	650	ASN
1	D	679	ASN
1	D	691	GLN
1	D	712	ASN
1	D	732	ASN
1	D	743	HIS
1	D	771	ASN
1	D	832	ASN
1	D	853	GLN
1	D	870	ASN
1	E	263	ASN
1	E	350	HIS
1	E	367	GLN
1	E	386	ASN
1	E	439	GLN
1	E	449	HIS
1	E	461	ASN
1	E	481	ASN
1	E	488	ASN
1	E	489	GLN
1	E	502	HIS
1	E	508	HIS
1	E	527	HIS
1	E	561	ASN
1	E	625	ASN
1	E	628	HIS
1	E	650	ASN
1	E	676	ASN
1	E	691	GLN
1	E	732	ASN
1	E	743	HIS
1	E	771	ASN
1	E	832	ASN
1	E	853	GLN
1	E	860	ASN
1	E	870	ASN
1	F	263	ASN
1	F	350	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	367	GLN
1	F	386	ASN
1	F	397	ASN
1	F	439	GLN
1	F	445	HIS
1	F	449	HIS
1	F	461	ASN
1	F	481	ASN
1	F	489	GLN
1	F	502	HIS
1	F	508	HIS
1	F	527	HIS
1	F	542	HIS
1	F	625	ASN
1	F	628	HIS
1	F	650	ASN
1	F	691	GLN
1	F	732	ASN
1	F	743	HIS
1	F	771	ASN
1	F	832	ASN
1	F	853	GLN
1	F	870	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

6 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	$\#\|Z\| > 2$
2	SIA	G	1	2	18,21,21	2.65	7 (38%)	21,31,31	1.53	2 (9%)
2	SIA	G	2	2	17,20,21	1.79	4 (23%)	21,28,31	1.25	3 (14%)
2	SIA	H	1	2	18,21,21	3.04	6 (33%)	21,31,31	1.84	4 (19%)
2	SIA	H	2	2	17,20,21	1.64	4 (23%)	21,28,31	1.11	2 (9%)
2	SIA	I	1	2	18,21,21	3.57	6 (33%)	21,31,31	1.24	0
2	SIA	I	2	2	17,20,21	1.62	3 (17%)	21,28,31	1.39	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	G	1	2	-	3/14/38/38	0/1/1/1
2	SIA	G	2	2	-	0/14/34/38	0/1/1/1
2	SIA	H	1	2	-	4/14/38/38	0/1/1/1
2	SIA	H	2	2	-	3/14/34/38	0/1/1/1
2	SIA	I	1	2	-	2/14/38/38	0/1/1/1
2	SIA	I	2	2	-	2/14/34/38	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	SIA	O6-C2	10.83	1.53	1.43
2	H	1	SIA	C4-C5	6.99	1.59	1.53
2	H	1	SIA	C3-C2	6.33	1.59	1.51
2	G	1	SIA	O6-C2	5.82	1.48	1.43
2	I	1	SIA	O2-C2	5.53	1.47	1.39
2	H	1	SIA	O2-C2	5.46	1.47	1.39
2	I	1	SIA	O6-C6	5.17	1.52	1.44
2	I	1	SIA	C3-C2	4.92	1.57	1.51
2	G	1	SIA	C3-C2	4.65	1.57	1.51
2	H	1	SIA	C3-C4	4.29	1.59	1.53
2	G	1	SIA	O2-C2	4.18	1.45	1.39
2	G	2	SIA	C4-C5	4.09	1.56	1.53
2	I	2	SIA	C4-C5	4.04	1.56	1.53
2	G	1	SIA	C4-C5	3.55	1.56	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	SIA	O6-C6	3.48	1.49	1.44
2	G	1	SIA	C3-C4	3.42	1.58	1.53
2	G	2	SIA	O6-C6	3.42	1.49	1.44
2	H	2	SIA	O6-C2	3.21	1.51	1.43
2	H	2	SIA	C4-C5	2.97	1.55	1.53
2	I	1	SIA	C3-C4	2.93	1.57	1.53
2	G	2	SIA	O6-C2	2.81	1.50	1.43
2	H	1	SIA	O6-C6	2.80	1.48	1.44
2	H	2	SIA	C7-C6	2.80	1.56	1.53
2	H	1	SIA	C5-N5	2.56	1.49	1.45
2	G	2	SIA	C7-C6	2.51	1.56	1.53
2	I	2	SIA	C7-C6	2.48	1.56	1.53
2	I	2	SIA	O6-C2	2.43	1.49	1.43
2	G	1	SIA	C5-N5	2.27	1.49	1.45
2	I	1	SIA	C5-N5	2.24	1.49	1.45
2	H	2	SIA	C9-C8	2.02	1.57	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	SIA	O6-C6-C5	-4.95	104.94	109.78
2	G	1	SIA	O6-C6-C7	4.50	114.24	107.29
2	H	1	SIA	O2-C2-C3	3.67	114.48	109.35
2	H	1	SIA	C3-C4-C5	3.44	115.27	109.98
2	I	2	SIA	C4-C5-C6	3.07	116.86	109.10
2	G	2	SIA	C6-O6-C2	2.73	117.18	111.34
2	I	2	SIA	C5-N5-C10	-2.68	116.67	123.18
2	H	1	SIA	C4-C5-N5	2.35	115.03	110.38
2	I	2	SIA	C3-C4-C5	2.33	114.28	111.46
2	H	2	SIA	C11-C10-N5	-2.27	112.26	116.10
2	G	2	SIA	O6-C2-C3	2.13	113.61	109.87
2	G	2	SIA	C6-C5-N5	-2.11	107.40	110.91
2	H	2	SIA	C8-C7-C6	2.06	116.94	113.03
2	G	1	SIA	O2-C2-C3	2.03	112.19	109.35

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	SIA	O6-C6-C7-O7
2	H	1	SIA	C7-C8-C9-O9
2	H	1	SIA	O8-C8-C9-O9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	I	2	SIA	C7-C8-C9-O9
2	I	1	SIA	C7-C8-C9-O9
2	I	2	SIA	O8-C8-C9-O9
2	G	1	SIA	C7-C8-C9-O9
2	G	1	SIA	O8-C8-C9-O9
2	I	1	SIA	O8-C8-C9-O9
2	H	1	SIA	C6-C7-C8-C9
2	H	2	SIA	C5-C6-C7-O7
2	H	2	SIA	C6-C7-C8-O8
2	G	1	SIA	C6-C7-C8-C9
2	H	2	SIA	O7-C7-C8-O8

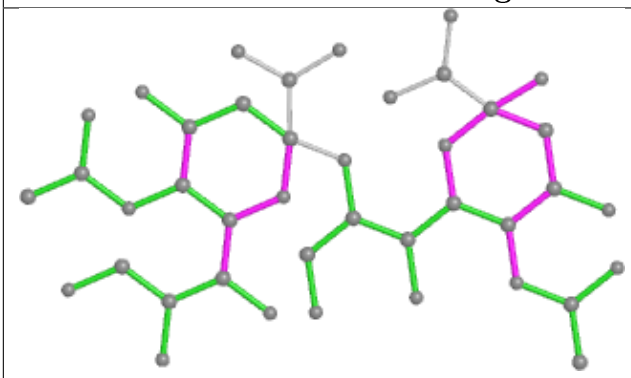
There are no ring outliers.

2 monomers are involved in 3 short contacts:

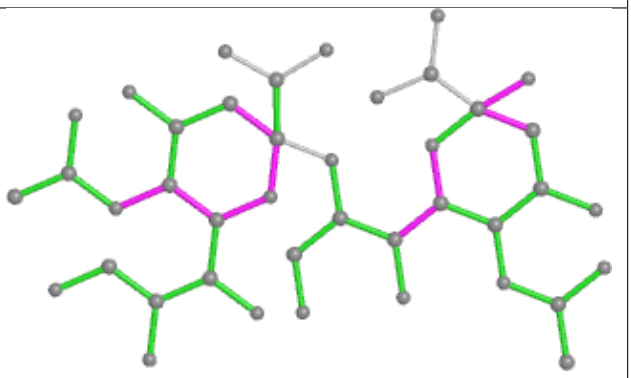
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	SIA	2	0
2	I	2	SIA	1	0

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

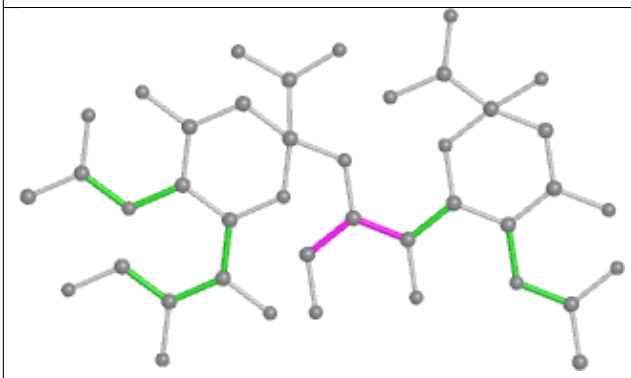
Oligosaccharide Chain G



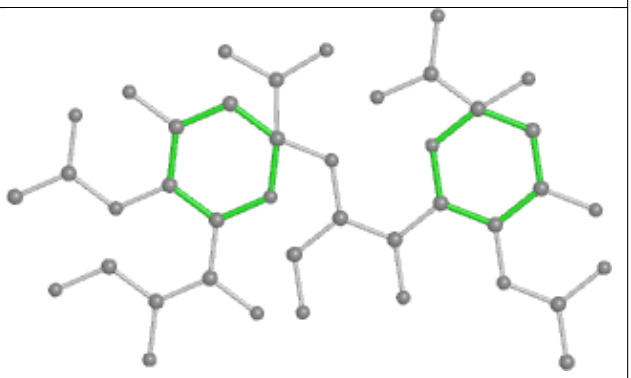
Bond lengths



Bond angles

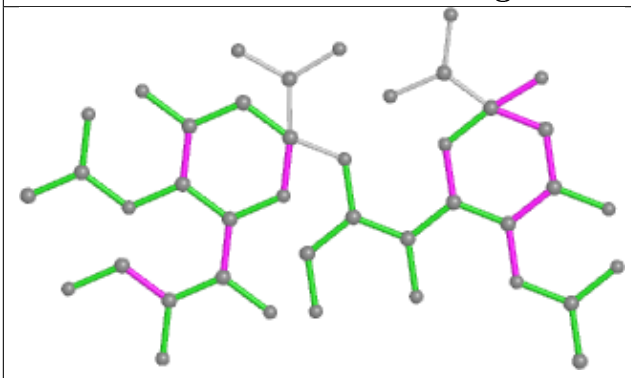


Torsions

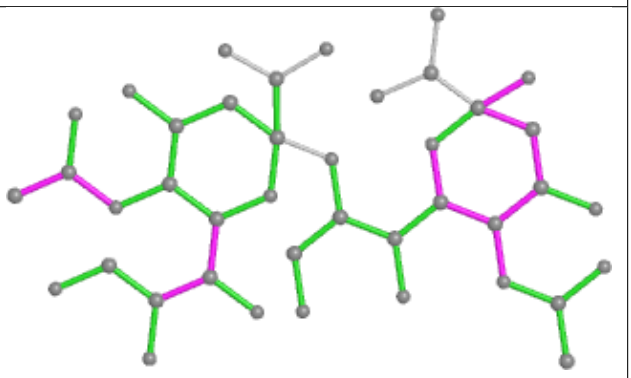


Rings

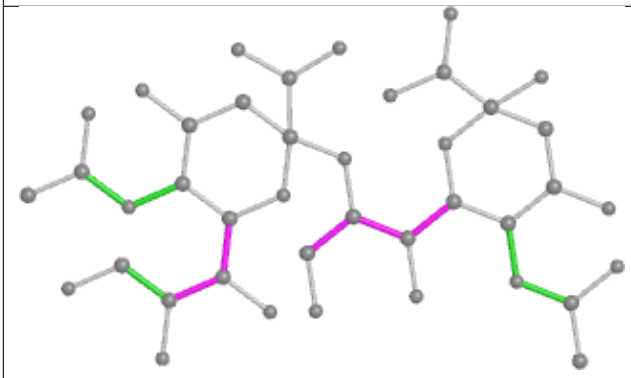
Oligosaccharide Chain H



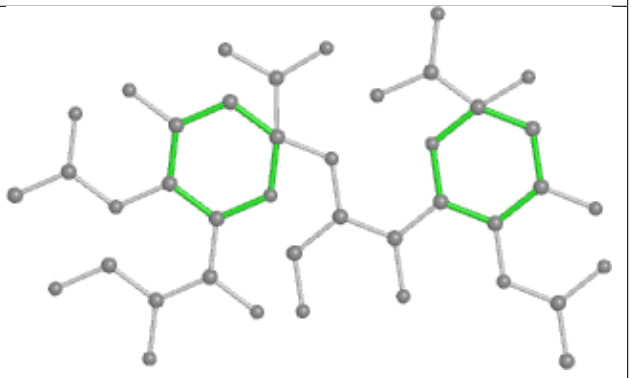
Bond lengths



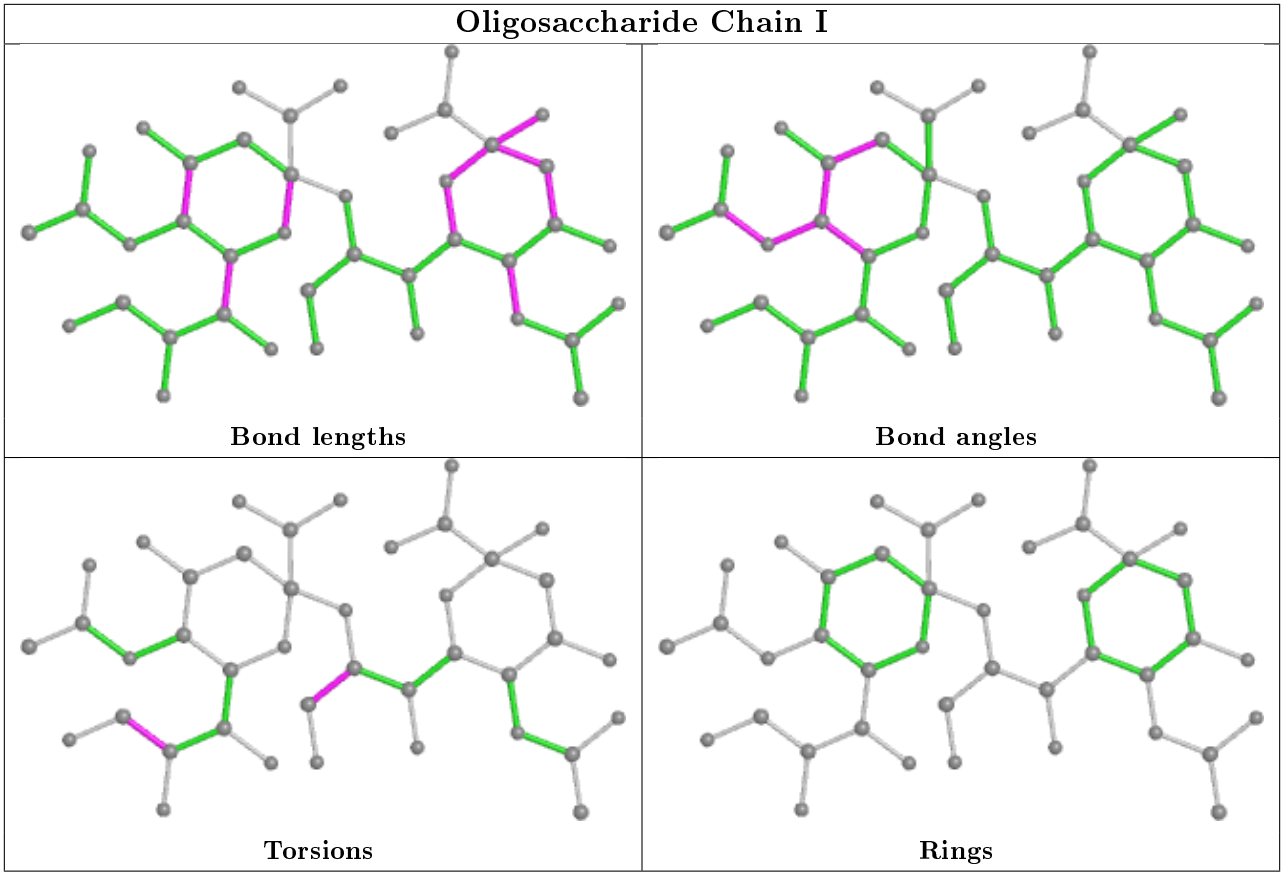
Bond angles



Torsions



Rings



5.6 Ligand geometry

12 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	$\#\|Z\| > 2$
4	PO4	A	1686	-	4,4,4	0.96	0	6,6,6	0.97	0
4	PO4	C	1687	-	4,4,4	0.85	0	6,6,6	0.68	0
4	PO4	D	1687	-	4,4,4	1.28	0	6,6,6	0.67	0
3	SLB	B	1685	-	18,21,21	2.77	6 (33%)	21,31,31	1.83	4 (19%)
3	SLB	A	1685	-	18,21,21	2.56	7 (38%)	21,31,31	1.91	3 (14%)
3	SLB	D	1685	-	18,21,21	2.62	7 (38%)	21,31,31	1.92	4 (19%)
3	SLB	C	1685	-	18,21,21	2.54	8 (44%)	21,31,31	1.52	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SLB	F	1685	-	18,21,21	2.27	6 (33%)	21,31,31	1.31	3 (14%)
3	SLB	E	1685	-	18,21,21	2.58	7 (38%)	21,31,31	1.64	3 (14%)
4	PO4	F	1687	-	4,4,4	0.91	0	6,6,6	0.90	0
4	PO4	F	1686	-	4,4,4	0.87	0	6,6,6	0.65	0
4	PO4	B	1686	-	4,4,4	1.39	0	6,6,6	0.97	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
3	SLB	B	1685	-	-	6/14/38/38	0/1/1/1
3	SLB	A	1685	-	-	3/14/38/38	0/1/1/1
3	SLB	D	1685	-	-	5/14/38/38	0/1/1/1
3	SLB	C	1685	-	-	6/14/38/38	0/1/1/1
3	SLB	F	1685	-	-	5/14/38/38	0/1/1/1
3	SLB	E	1685	-	-	2/14/38/38	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1685	SLB	O6-C2	7.32	1.50	1.43
3	C	1685	SLB	O2-C2	6.29	1.48	1.39
3	F	1685	SLB	O6-C2	6.01	1.49	1.43
3	D	1685	SLB	O6-C2	5.61	1.48	1.43
3	A	1685	SLB	O6-C6	5.55	1.52	1.44
3	A	1685	SLB	O6-C2	5.44	1.48	1.43
3	E	1685	SLB	O2-C2	5.02	1.46	1.39
3	B	1685	SLB	O6-C6	5.01	1.51	1.44
3	E	1685	SLB	O6-C2	4.56	1.47	1.43
3	E	1685	SLB	C3-C2	4.55	1.57	1.51
3	B	1685	SLB	O2-C2	4.21	1.45	1.39
3	A	1685	SLB	O2-C2	4.18	1.45	1.39
3	D	1685	SLB	C8-C7	4.17	1.61	1.53
3	D	1685	SLB	O2-C2	4.17	1.45	1.39
3	E	1685	SLB	C4-C5	3.97	1.56	1.53
3	C	1685	SLB	O6-C6	3.91	1.50	1.44
3	A	1685	SLB	C3-C2	3.80	1.56	1.51
3	D	1685	SLB	C4-C5	3.72	1.56	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1685	SLB	O6-C2	3.54	1.46	1.43
3	F	1685	SLB	O2-C2	3.36	1.44	1.39
3	B	1685	SLB	C3-C2	3.36	1.55	1.51
3	D	1685	SLB	C3-C2	3.31	1.55	1.51
3	D	1685	SLB	O6-C6	3.25	1.49	1.44
3	C	1685	SLB	C3-C2	3.22	1.55	1.51
3	F	1685	SLB	C7-C6	3.21	1.57	1.53
3	D	1685	SLB	C7-C6	3.10	1.56	1.53
3	F	1685	SLB	C8-C7	3.01	1.59	1.53
3	E	1685	SLB	C3-C4	2.93	1.57	1.53
3	E	1685	SLB	O6-C6	-2.90	1.39	1.44
3	F	1685	SLB	C6-C5	2.86	1.57	1.53
3	B	1685	SLB	C3-C4	2.79	1.57	1.53
3	C	1685	SLB	C7-C6	2.56	1.56	1.53
3	A	1685	SLB	C3-C4	2.52	1.56	1.53
3	C	1685	SLB	C6-C5	2.42	1.57	1.53
3	C	1685	SLB	C11-C10	2.37	1.55	1.50
3	C	1685	SLB	C4-C5	2.37	1.55	1.53
3	A	1685	SLB	C4-C5	2.24	1.55	1.53
3	B	1685	SLB	C6-C5	2.15	1.56	1.53
3	E	1685	SLB	C11-C10	2.14	1.55	1.50
3	A	1685	SLB	C11-C10	2.04	1.54	1.50
3	F	1685	SLB	C3-C2	2.00	1.54	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1685	SLB	O6-C6-C5	6.61	116.23	109.78
3	D	1685	SLB	O6-C6-C5	6.53	116.14	109.78
3	B	1685	SLB	O2-C2-C3	-4.92	102.48	109.35
3	B	1685	SLB	O6-C6-C7	4.59	114.38	107.29
3	C	1685	SLB	O6-C6-C5	4.31	113.98	109.78
3	E	1685	SLB	C6-C5-N5	-3.97	104.32	110.91
3	E	1685	SLB	O6-C6-C5	3.42	113.11	109.78
3	E	1685	SLB	C4-C5-N5	3.29	116.88	110.38
3	A	1685	SLB	C8-C7-C6	-2.96	107.42	113.03
3	D	1685	SLB	C9-C8-C7	2.77	118.42	112.41
3	F	1685	SLB	C8-C7-C6	2.65	118.05	113.03
3	D	1685	SLB	O7-C7-C8	2.47	114.78	108.81
3	F	1685	SLB	C4-C5-N5	2.46	115.25	110.38
3	B	1685	SLB	C8-C7-C6	2.42	117.62	113.03
3	C	1685	SLB	O2-C2-C3	2.39	112.69	109.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1685	SLB	C9-C8-C7	2.27	117.32	112.41
3	D	1685	SLB	C3-C4-C5	2.24	113.42	109.98
3	C	1685	SLB	O4-C4-C3	-2.19	104.81	109.91
3	B	1685	SLB	O6-C6-C5	2.17	111.89	109.78
3	C	1685	SLB	C4-C5-N5	2.15	114.63	110.38
3	A	1685	SLB	O10-C10-N5	2.10	125.81	121.95

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1685	SLB	C6-C7-C8-O8
3	B	1685	SLB	O7-C7-C8-O8
3	B	1685	SLB	O8-C8-C9-O9
3	C	1685	SLB	C6-C7-C8-O8
3	C	1685	SLB	O7-C7-C8-O8
3	C	1685	SLB	C7-C8-C9-O9
3	C	1685	SLB	O8-C8-C9-O9
3	F	1685	SLB	O8-C8-C9-O9
3	B	1685	SLB	C7-C8-C9-O9
3	F	1685	SLB	C7-C8-C9-O9
3	F	1685	SLB	C6-C7-C8-O8
3	B	1685	SLB	O7-C7-C8-C9
3	C	1685	SLB	O7-C7-C8-C9
3	B	1685	SLB	C6-C7-C8-C9
3	D	1685	SLB	C6-C7-C8-C9
3	C	1685	SLB	C6-C7-C8-C9
3	F	1685	SLB	C6-C7-C8-C9
3	D	1685	SLB	O7-C7-C8-C9
3	D	1685	SLB	O7-C7-C8-O8
3	E	1685	SLB	O8-C8-C9-O9
3	D	1685	SLB	C7-C8-C9-O9
3	E	1685	SLB	C7-C8-C9-O9
3	A	1685	SLB	O7-C7-C8-C9
3	A	1685	SLB	O8-C8-C9-O9
3	D	1685	SLB	O8-C8-C9-O9
3	A	1685	SLB	C6-C7-C8-C9
3	F	1685	SLB	O7-C7-C8-O8

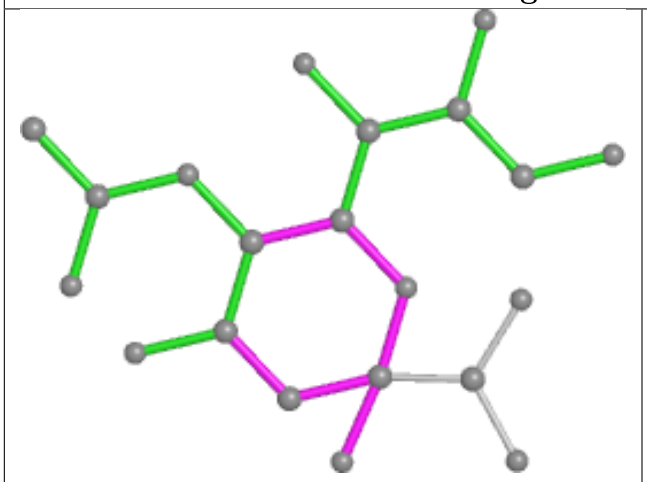
There are no ring outliers.

3 monomers are involved in 3 short contacts:

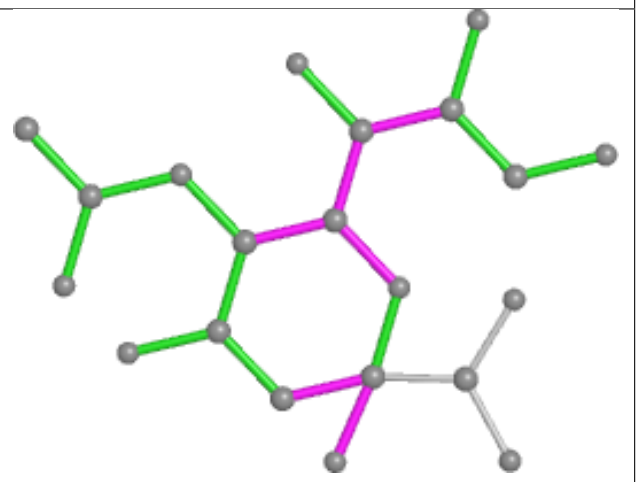
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1687	PO4	1	0
3	F	1685	SLB	1	0
4	B	1686	PO4	1	0

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

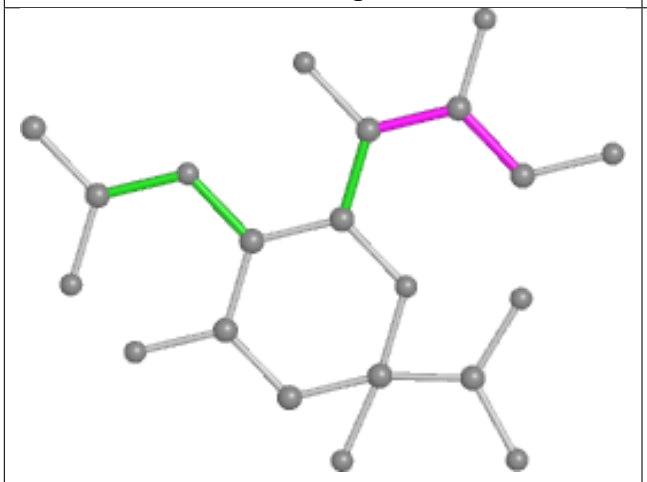
Ligand SLB B 1685



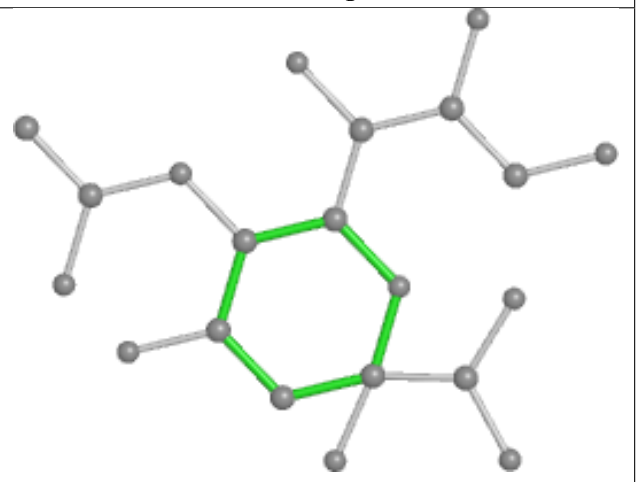
Bond lengths



Bond angles

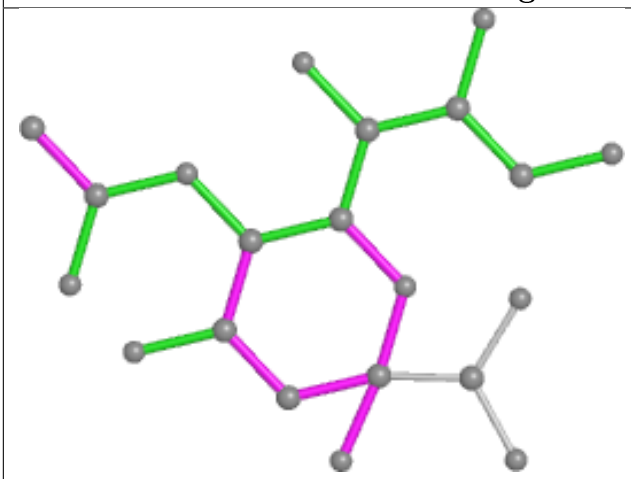


Torsions

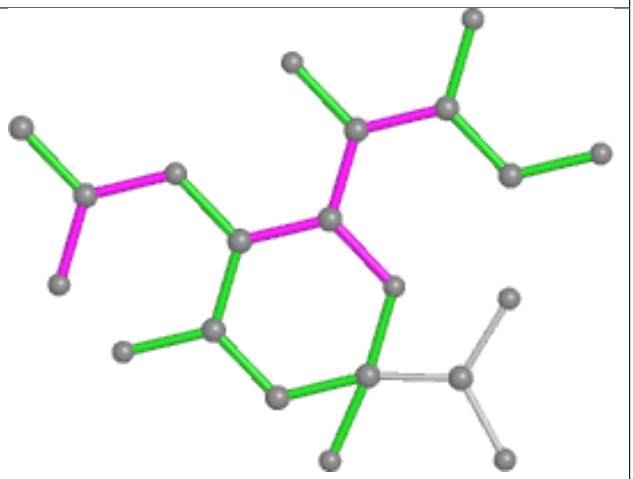


Rings

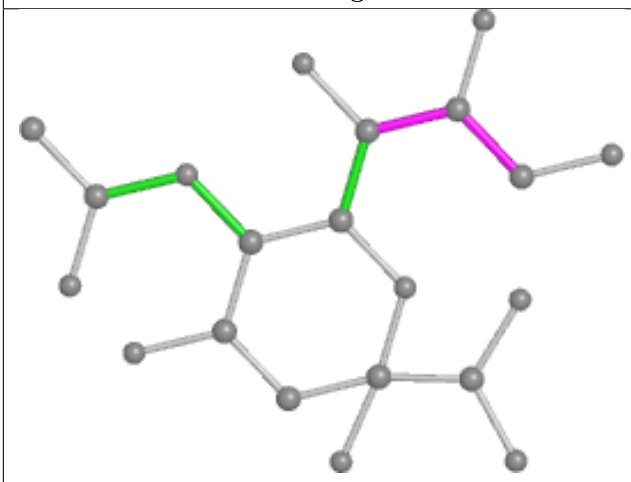
Ligand SLB A 1685



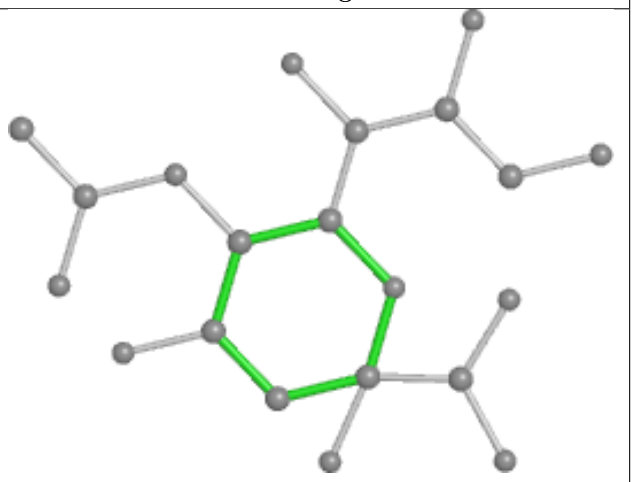
Bond lengths



Bond angles

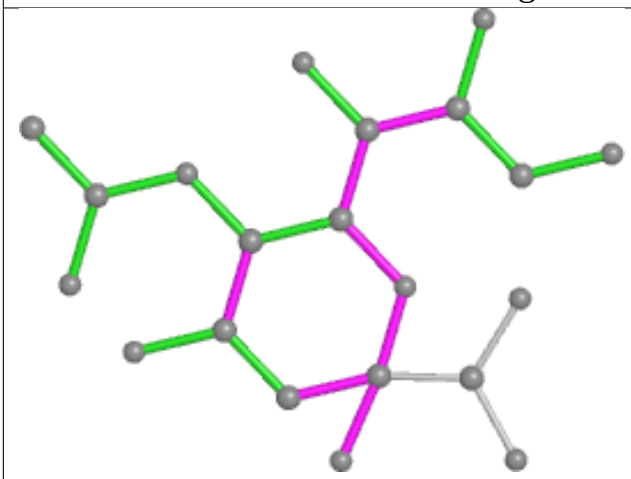


Torsions

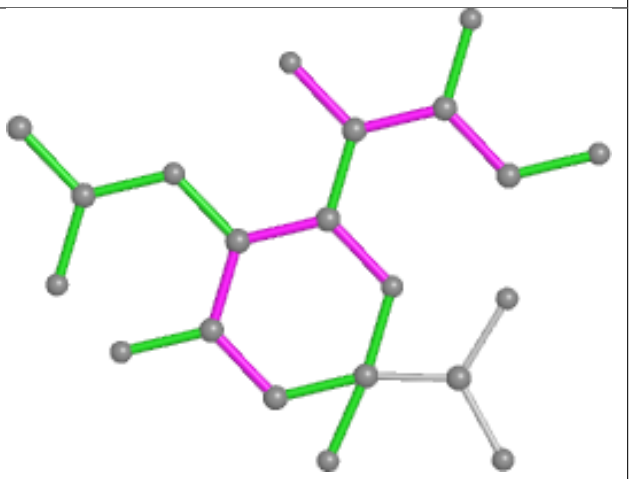


Rings

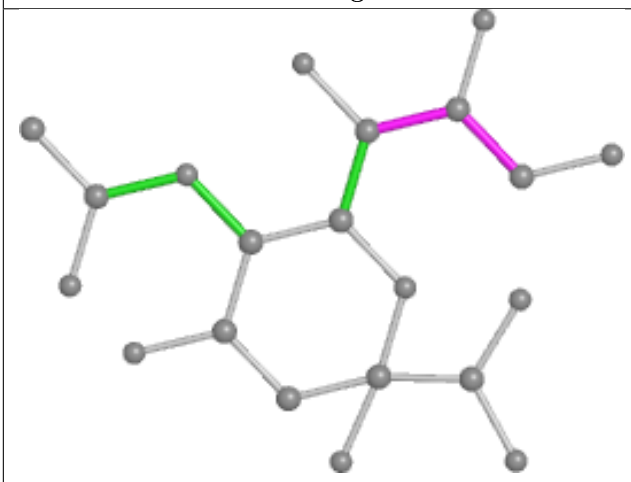
Ligand SLB D 1685



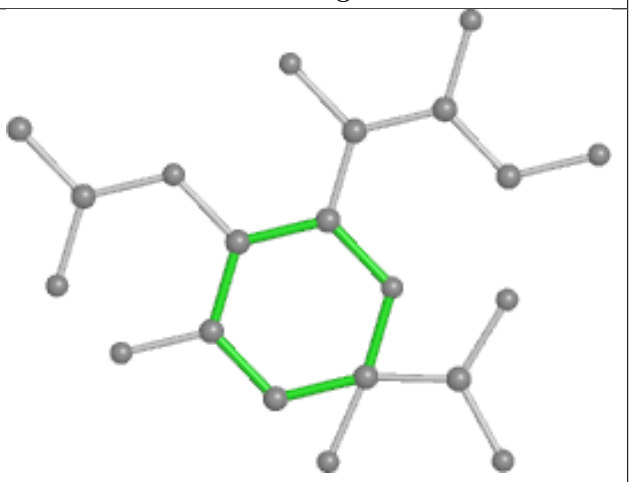
Bond lengths



Bond angles

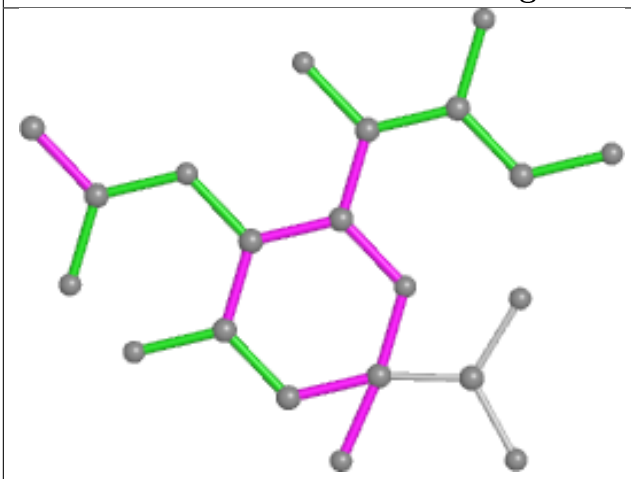


Torsions

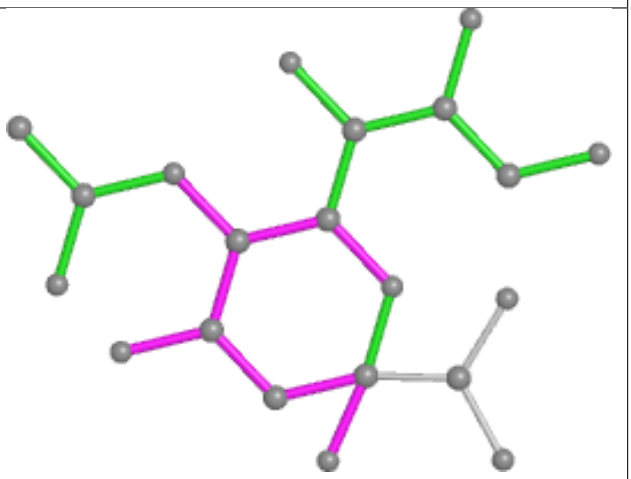


Rings

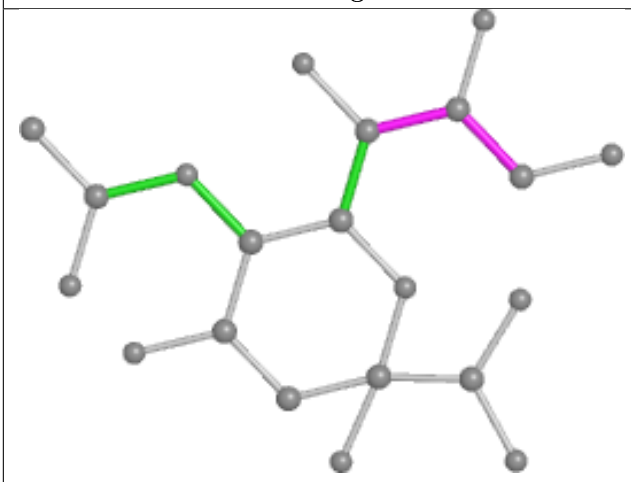
Ligand SLB C 1685



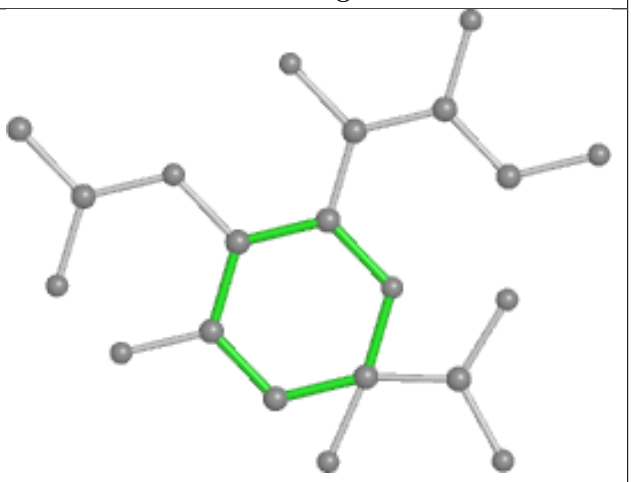
Bond lengths



Bond angles

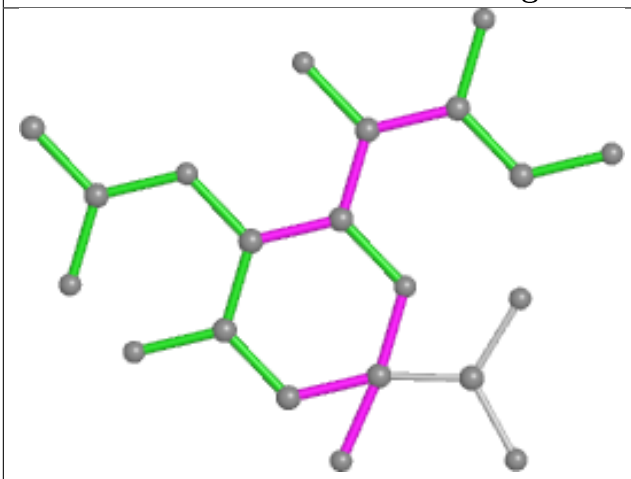


Torsions

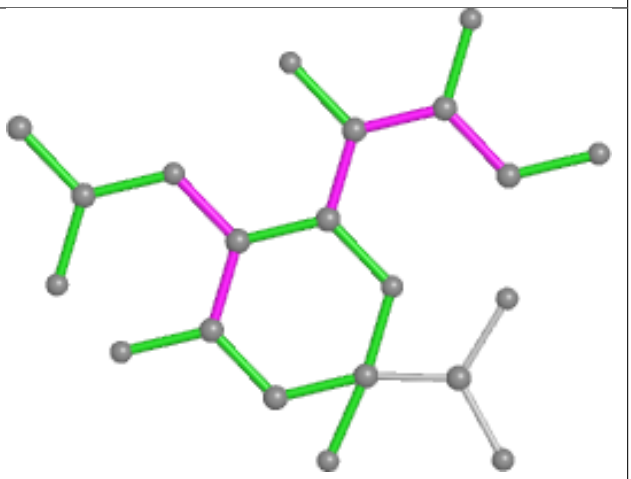


Rings

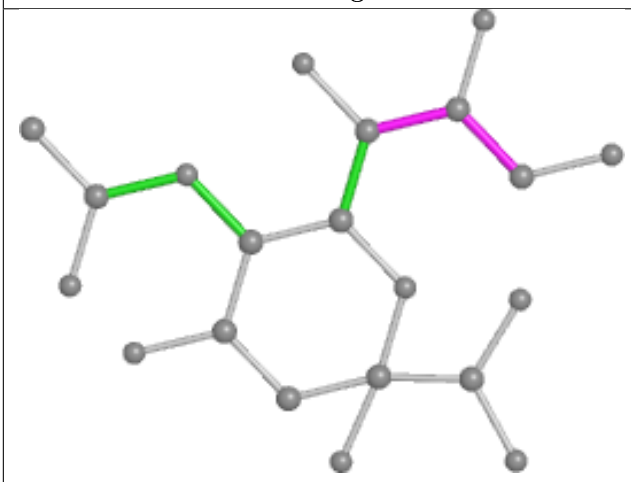
Ligand SLB F 1685



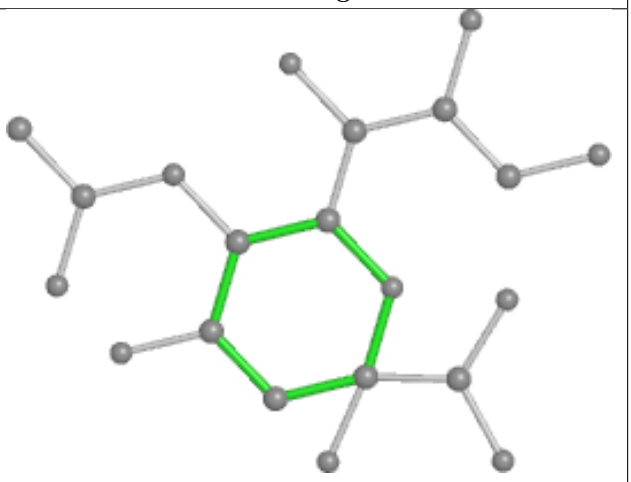
Bond lengths



Bond angles

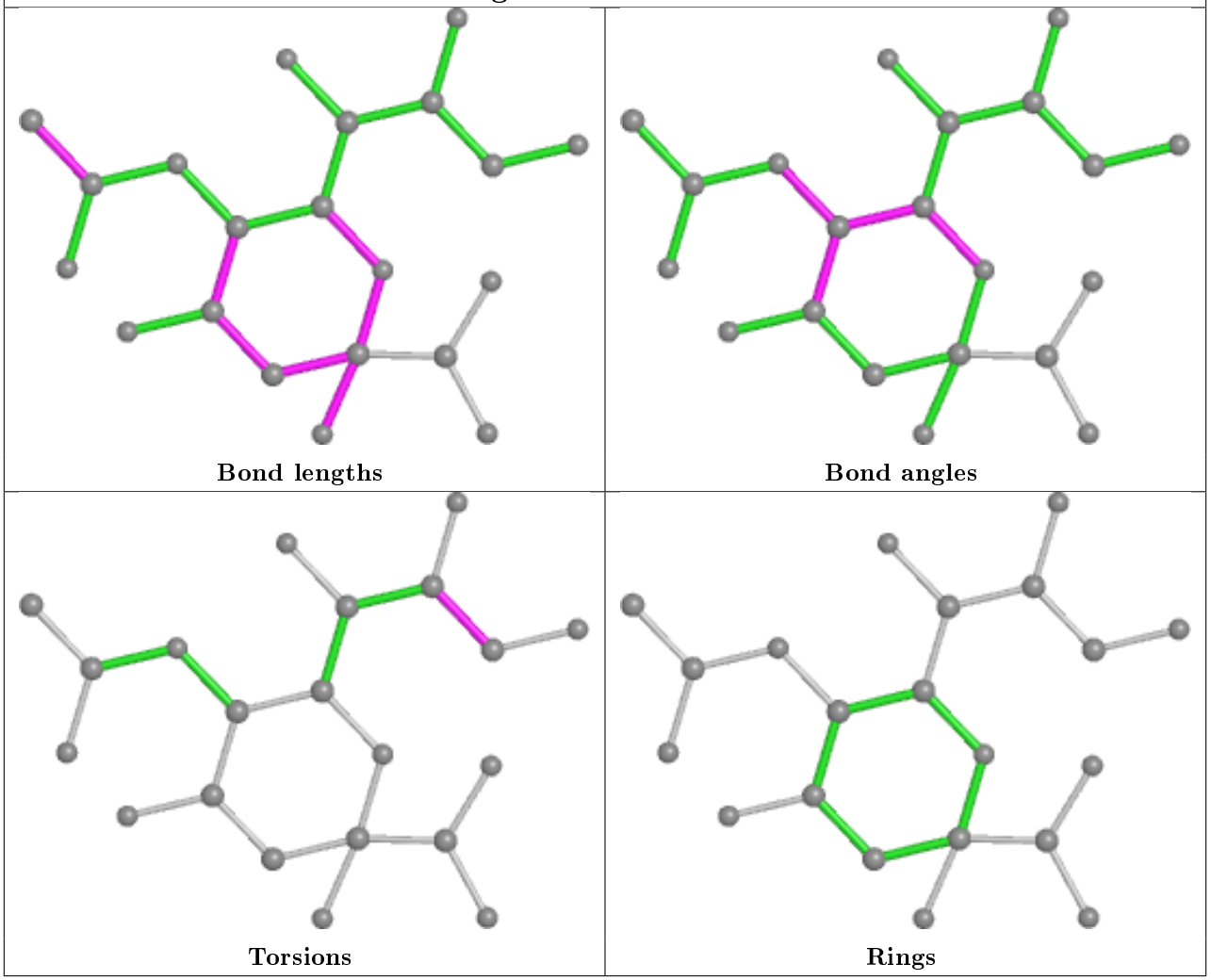


Torsions



Rings

Ligand SLB E 1685



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, 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	666/666 (100%)	-0.22	6 (0%) 84 88	17, 21, 24, 30	0
1	B	666/666 (100%)	-0.17	9 (1%) 75 81	17, 21, 23, 30	0
1	C	666/666 (100%)	-0.13	7 (1%) 80 85	17, 21, 23, 29	0
1	D	666/666 (100%)	-0.28	2 (0%) 94 96	18, 21, 23, 31	0
1	E	666/666 (100%)	-0.17	10 (1%) 73 79	18, 21, 23, 30	0
1	F	666/666 (100%)	-0.24	5 (0%) 86 89	18, 21, 23, 29	0
All	All	3996/3996 (100%)	-0.20	39 (0%) 82 86	17, 21, 23, 31	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	245	SER	4.9
1	F	245	SER	4.9
1	E	246	ALA	4.5
1	F	246	ALA	4.3
1	C	245	SER	3.5
1	C	682	ASP	3.2
1	B	246	ALA	3.1
1	E	262	LEU	3.1
1	F	247	LYS	2.9
1	A	491	THR	2.9
1	E	491	THR	2.9
1	B	262	LEU	2.8
1	B	466	GLY	2.7
1	B	251	VAL	2.7
1	C	262	LEU	2.6
1	B	264	ASP	2.6
1	E	492	SER	2.6
1	A	263	ASN	2.5
1	B	257	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	498	GLY	2.4
1	A	824	ILE	2.4
1	E	681	ASP	2.4
1	D	840	PHE	2.3
1	C	260	SER	2.3
1	E	252	THR	2.2
1	E	547	ALA	2.2
1	A	644	GLY	2.2
1	A	704	VAL	2.2
1	A	264	ASP	2.1
1	E	264	ASP	2.1
1	B	256	ALA	2.1
1	C	546	VAL	2.1
1	C	258	LEU	2.1
1	E	611	ARG	2.1
1	F	264	ASP	2.1
1	E	856	LEU	2.1
1	B	247	LYS	2.1
1	C	264	ASP	2.0
1	D	824	ILE	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, 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.

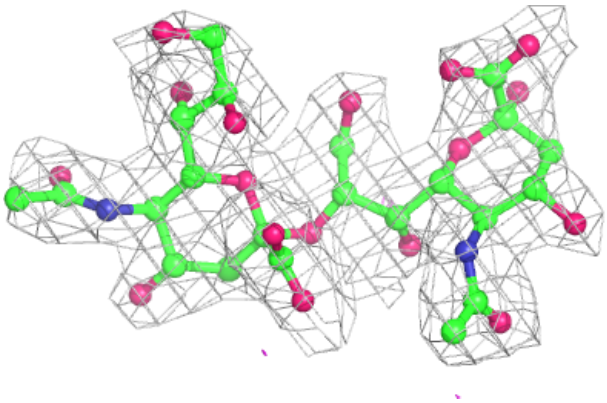
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SIA	H	1	21/21	0.82	0.33	43,45,49,51	0
2	SIA	G	1	21/21	0.85	0.28	36,40,43,44	0
2	SIA	I	1	21/21	0.85	0.27	38,41,47,49	0
2	SIA	H	2	20/21	0.93	0.20	35,40,42,44	0
2	SIA	G	2	20/21	0.94	0.18	35,38,43,45	0
2	SIA	I	2	20/21	0.94	0.16	31,38,44,46	0

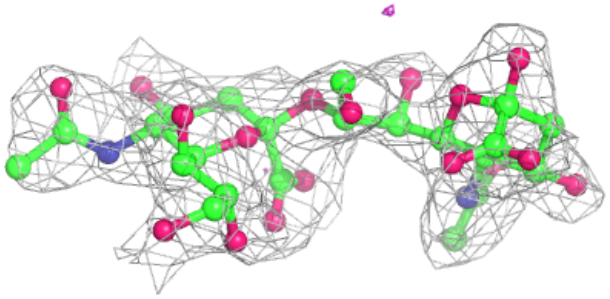
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

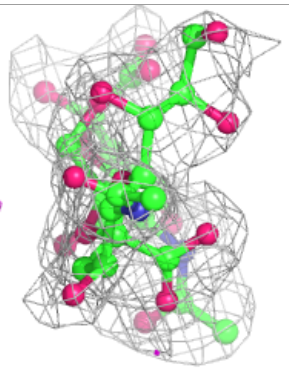
charide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

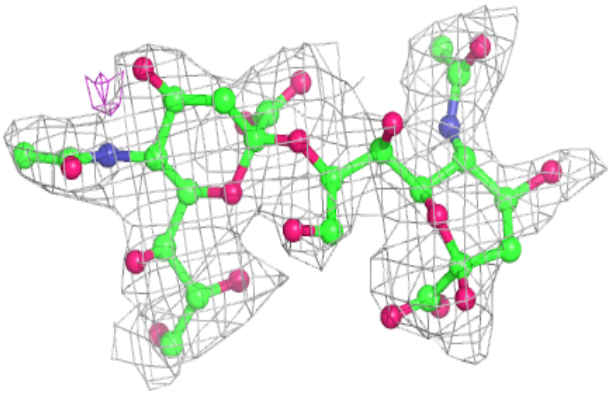


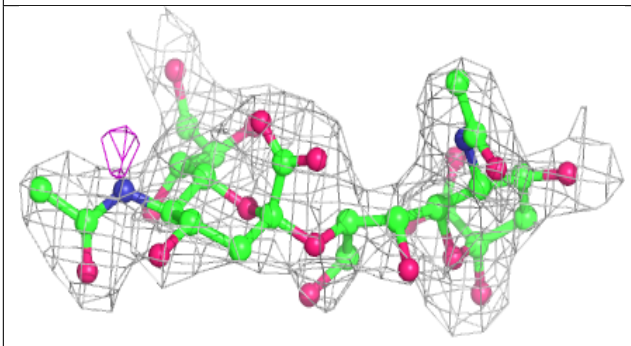


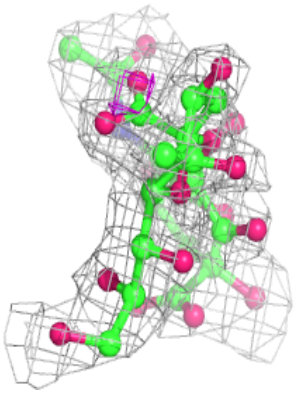


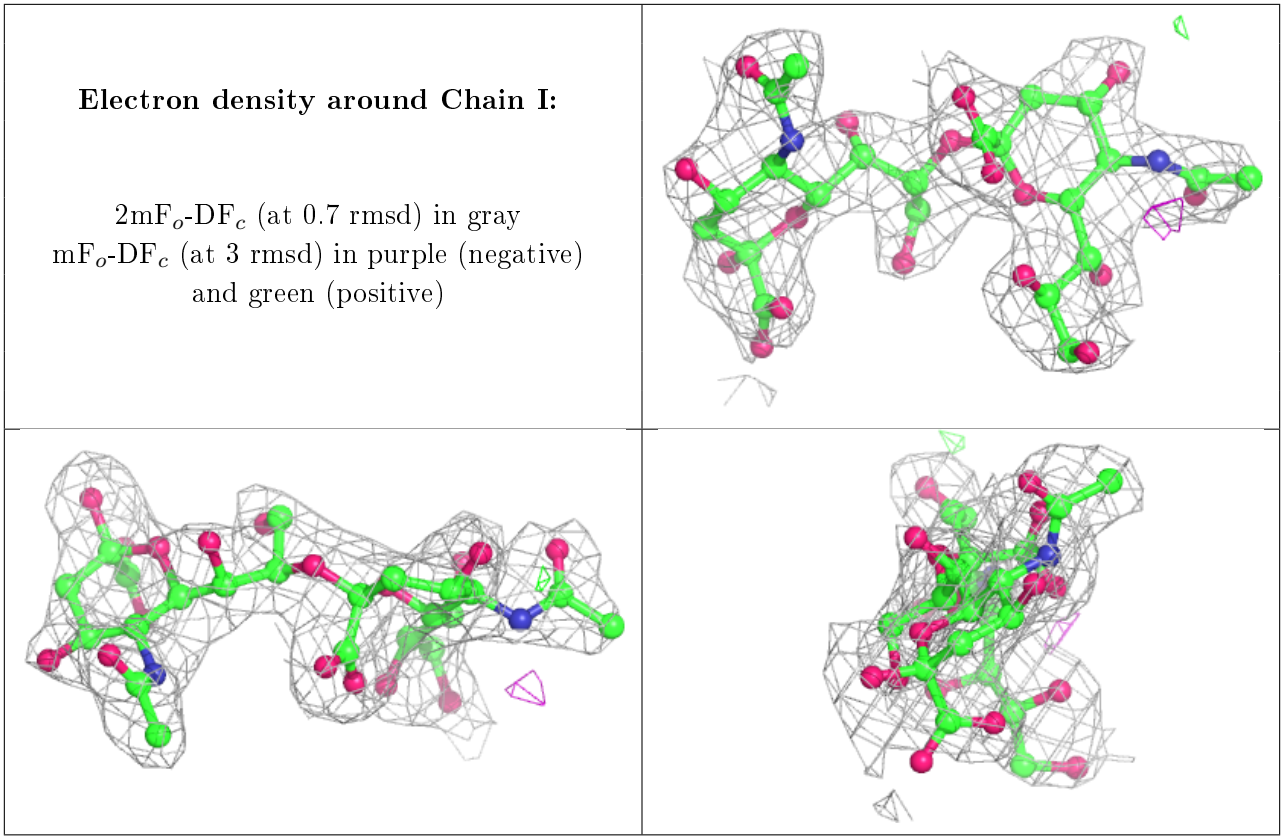
Electron density around Chain H:

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









6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

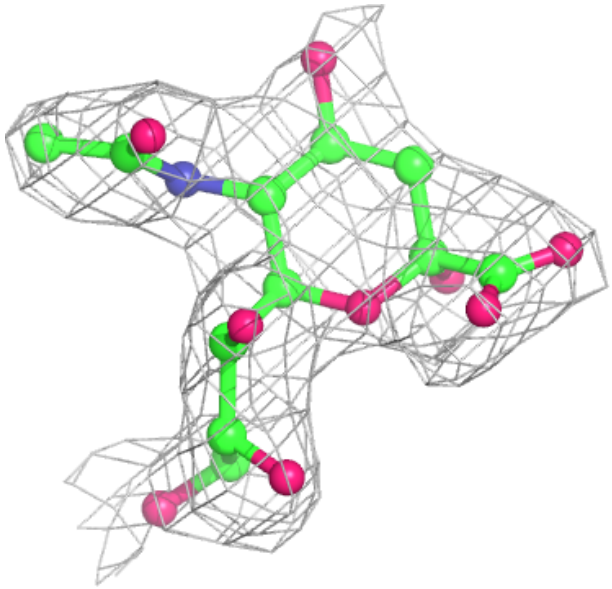
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SLB	F	1685	21/21	0.89	0.21	33,40,46,49	0
3	SLB	D	1685	21/21	0.91	0.15	33,39,42,46	0
3	SLB	A	1685	21/21	0.91	0.21	37,42,47,48	0
3	SLB	C	1685	21/21	0.92	0.16	37,39,43,44	0
3	SLB	B	1685	21/21	0.92	0.19	30,37,43,44	0
3	SLB	E	1685	21/21	0.93	0.21	32,37,44,50	0
4	PO4	A	1686	5/5	0.97	0.11	33,36,38,39	0
4	PO4	F	1687	5/5	0.97	0.13	34,36,37,39	0
4	PO4	D	1687	5/5	0.98	0.13	35,35,37,37	0
4	PO4	C	1687	5/5	0.98	0.10	36,37,38,40	0
4	PO4	F	1686	5/5	0.98	0.08	38,39,39,40	0
4	PO4	B	1686	5/5	0.98	0.12	30,33,34,34	0

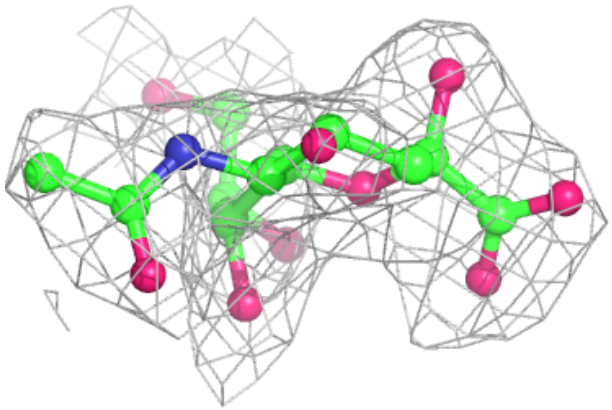
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

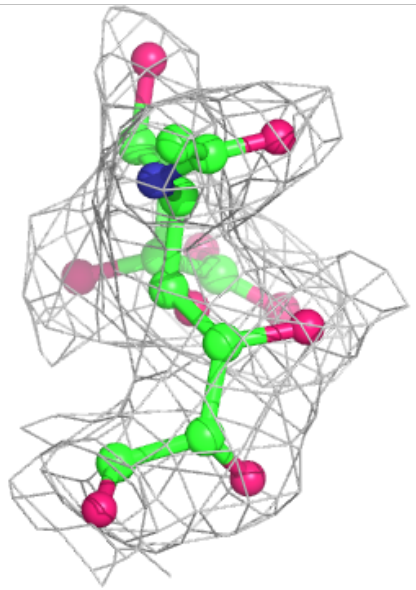
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SLB F 1685:

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

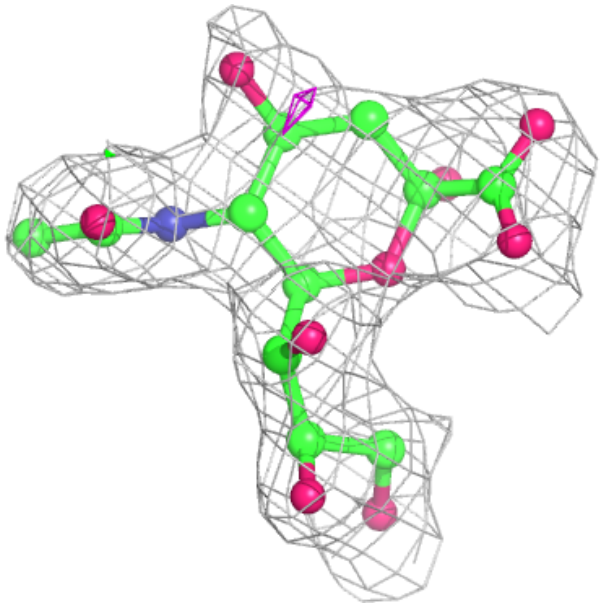


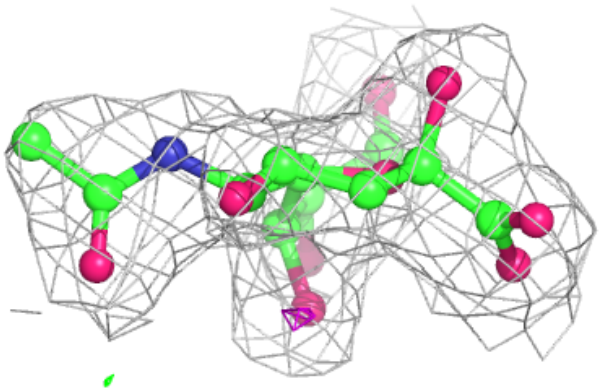


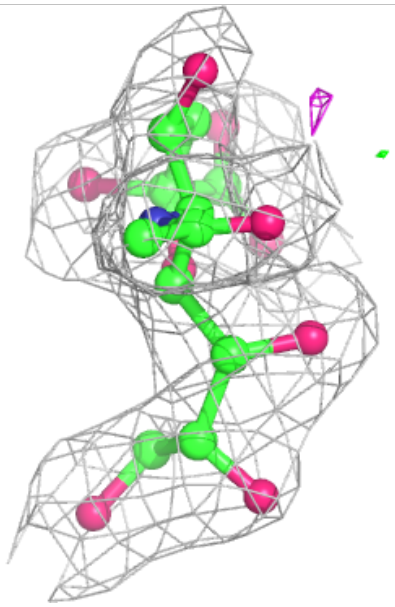


Electron density around SLB D 1685:

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

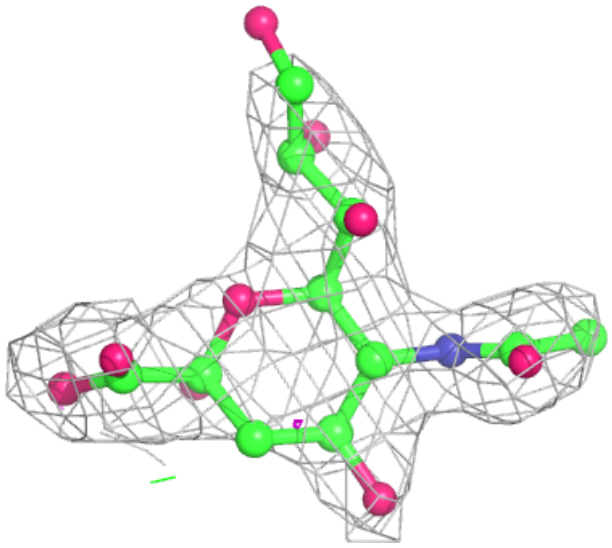


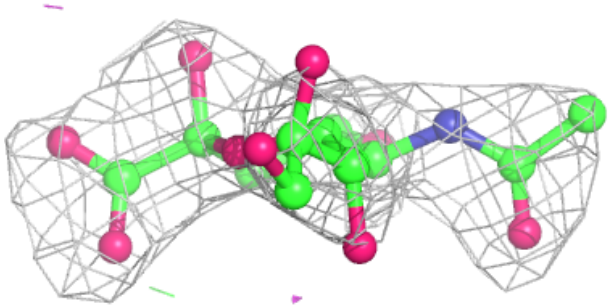


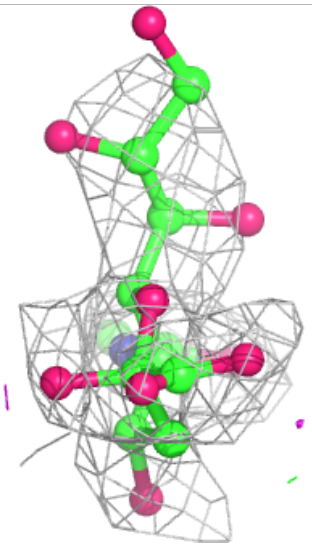


Electron density around SLB A 1685:

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

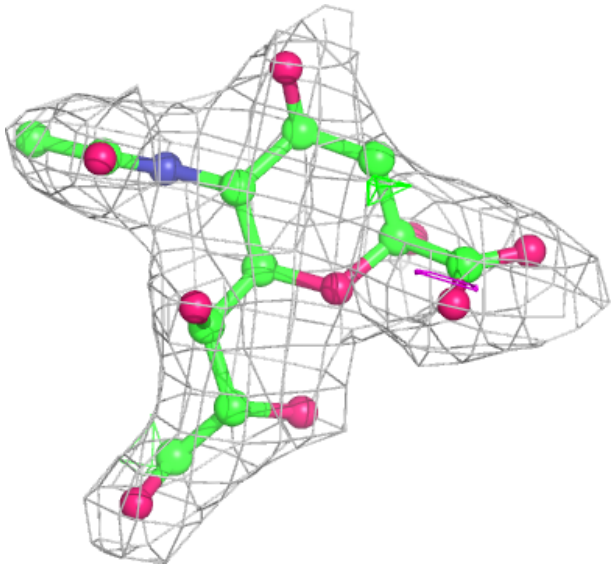


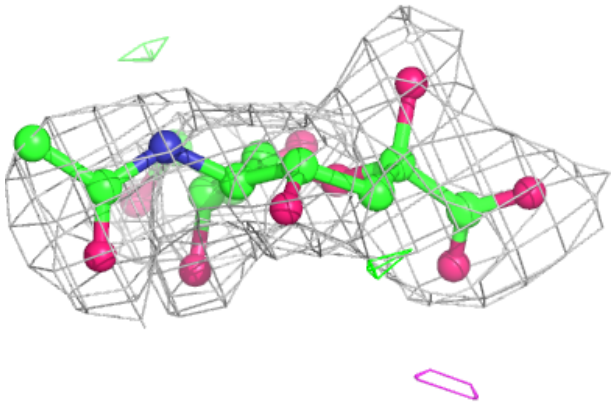


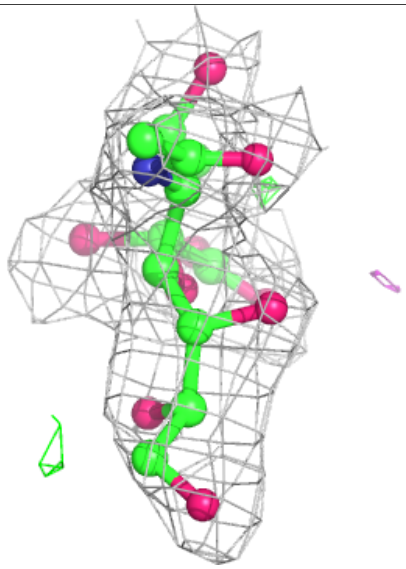


Electron density around SLB C 1685:

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

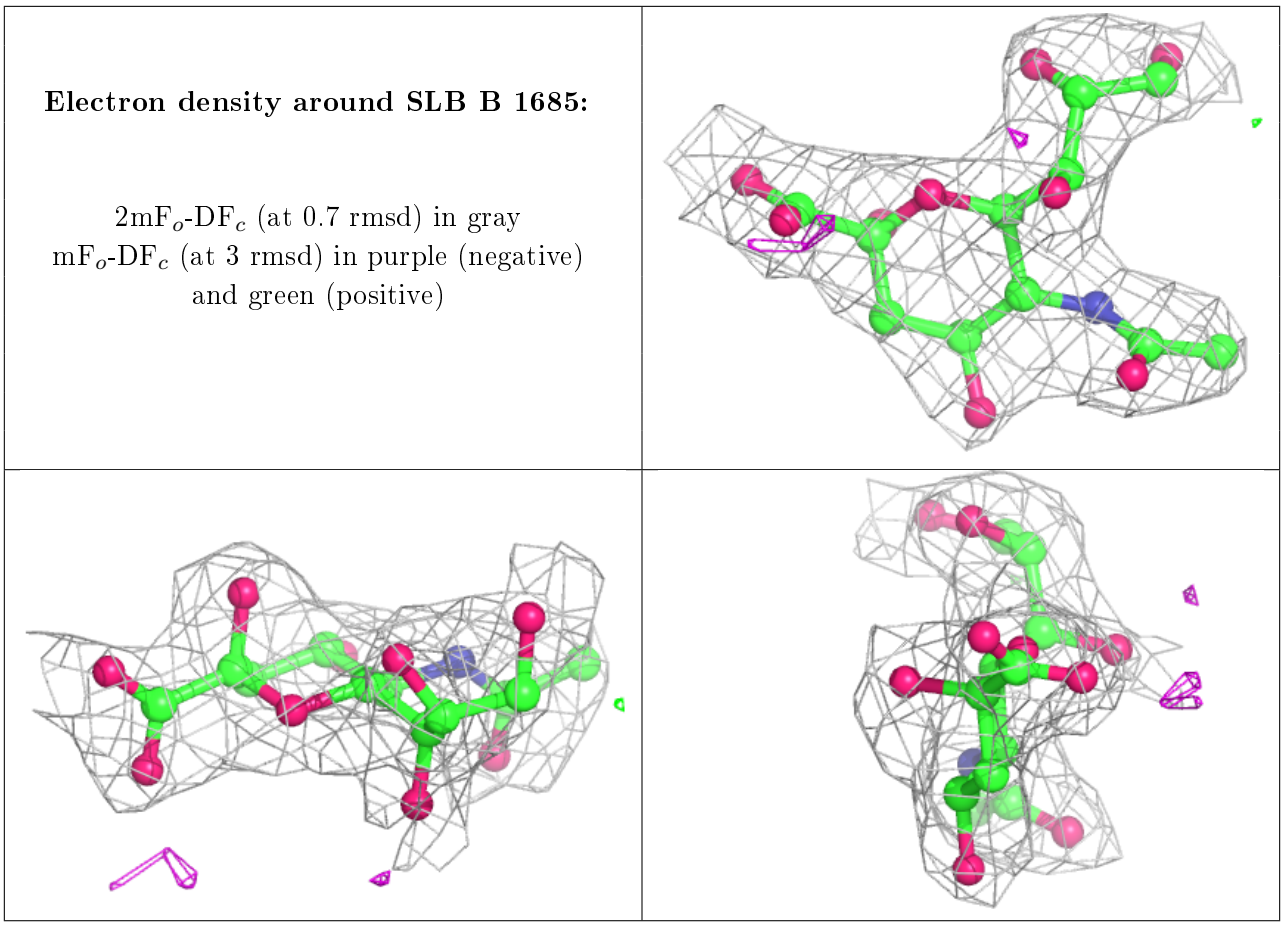






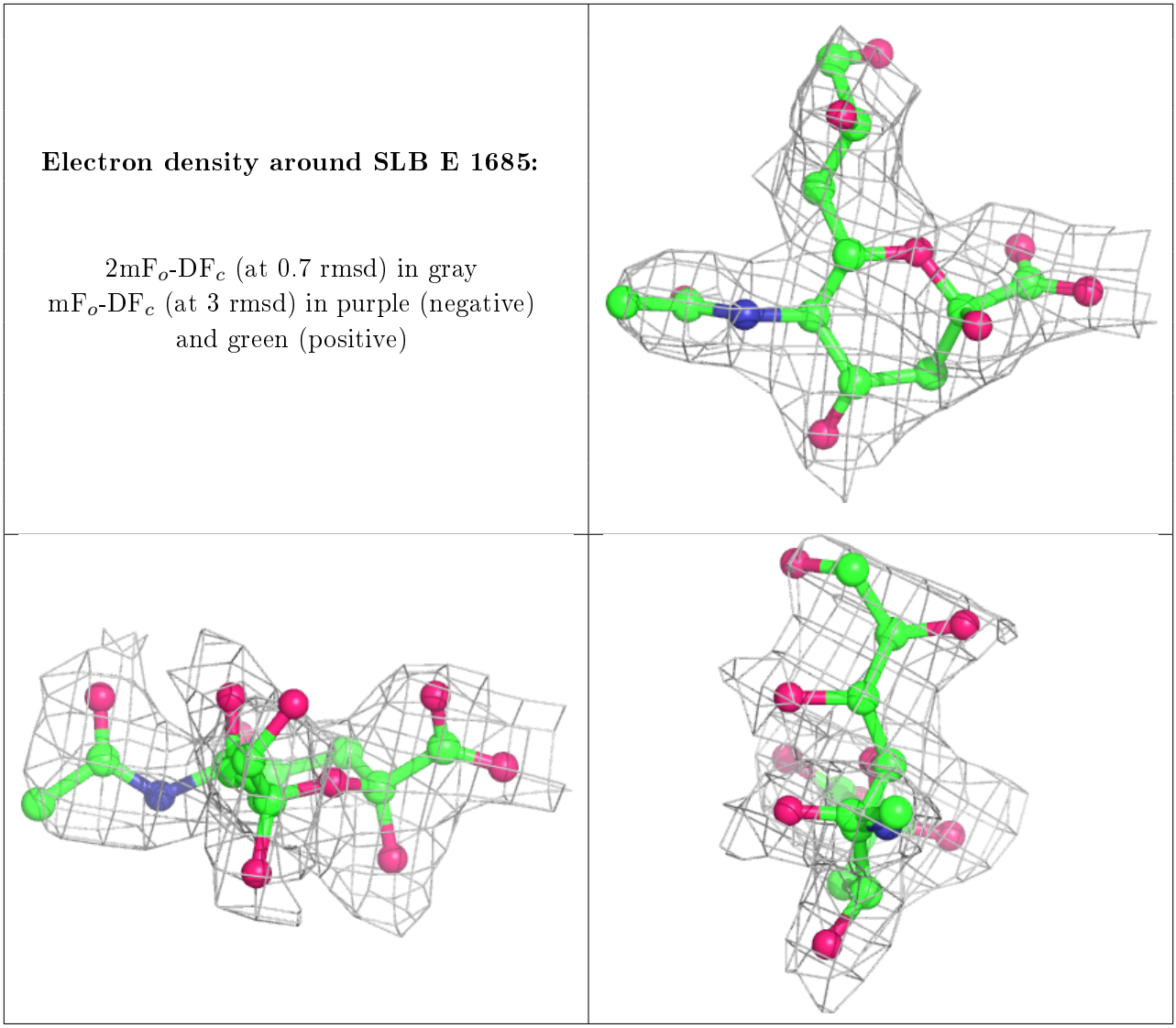
Electron density around SLB B 1685:

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



Electron density around SLB E 1685:

$2mF_o$-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.