



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:48 PM UTC

PDB ID : 1QKC / pdb_00001qkc
Title : ESCHERICHIA COLI FERRIC HYDROXAMATE UPTAKE RECEPTOR (FHUA) IN COMPLEX DELTA TWO-ALBOMYCIN
Authors : Ferguson, A.D.; Braun, V.; Fiedler, H.-P.; Coulton, J.W.; Diederichs, K.; Welte, W.
Deposited on : 1999-07-18
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

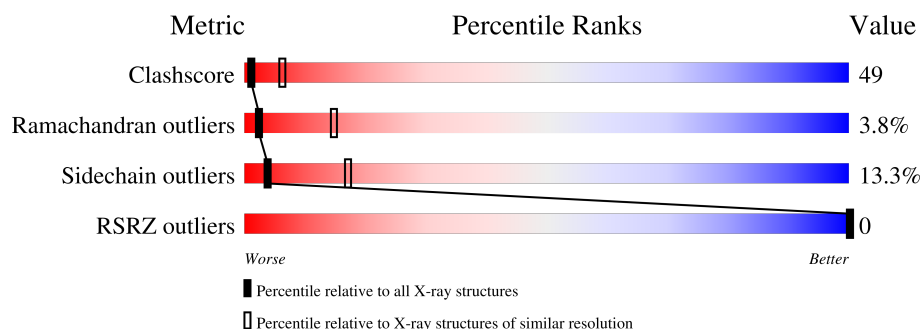
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	725	
2	B	11	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GMH	B	10	X	-	-	-
2	GCN	B	2	X	-	-	-
2	GMH	B	5	X	-	-	-
3	FTT	A	1006	X	-	-	-
5	PO4	A	1014	-	-	X	-
7	ALB	A	1022[A]	X	-	-	-
7	ALB	A	1022[B]	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6195 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.

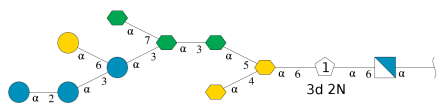
- Molecule 1 is a protein called FERRIC HYDROXAMATE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	707	5523	3475	944	1090	14	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

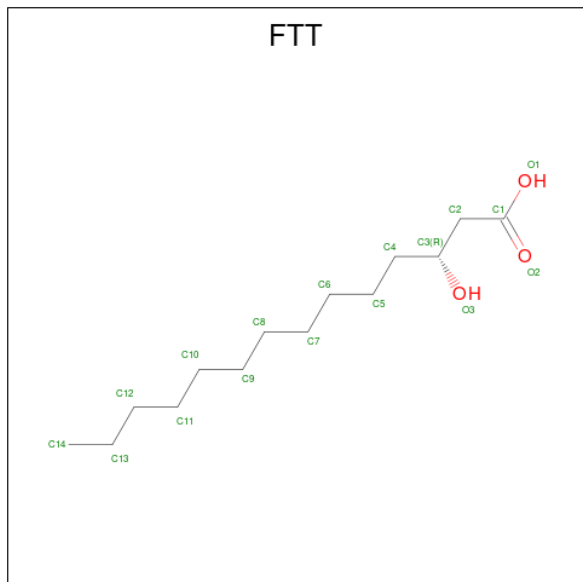
Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	insertion	UNP P06971
A	407	SER	-	insertion	UNP P06971
A	408	HIS	-	insertion	UNP P06971
A	409	HIS	-	insertion	UNP P06971
A	410	HIS	-	insertion	UNP P06971
A	411	HIS	-	insertion	UNP P06971
A	412	HIS	-	insertion	UNP P06971
A	413	HIS	-	insertion	UNP P06971
A	414	GLY	-	insertion	UNP P06971
A	415	SER	-	insertion	UNP P06971
A	416	SER	-	insertion	UNP P06971

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-[L-glycero-alpha-D-manno-o-heptopyranose-(1-7)]L-glycero-alpha-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2,3-dideoxy-alpha-D-glucopyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose.



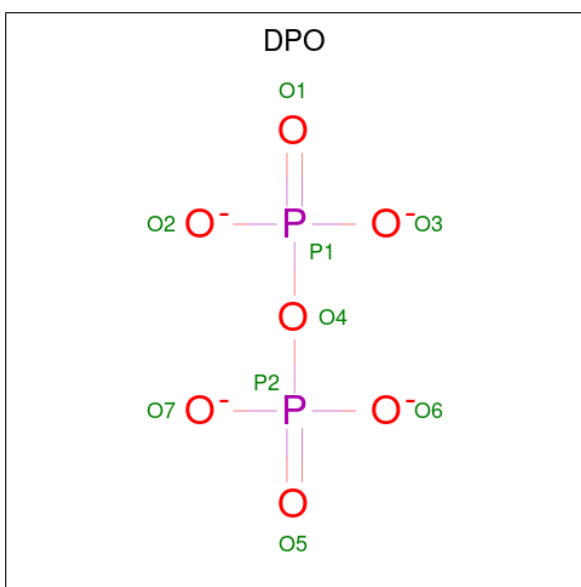
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	11	134	73	2	59	0	0	0

- Molecule 3 is 3-HYDROXY-TETRADECANOIC ACID (CCD ID: FTT) (formula: $C_{14}H_{28}O_3$).



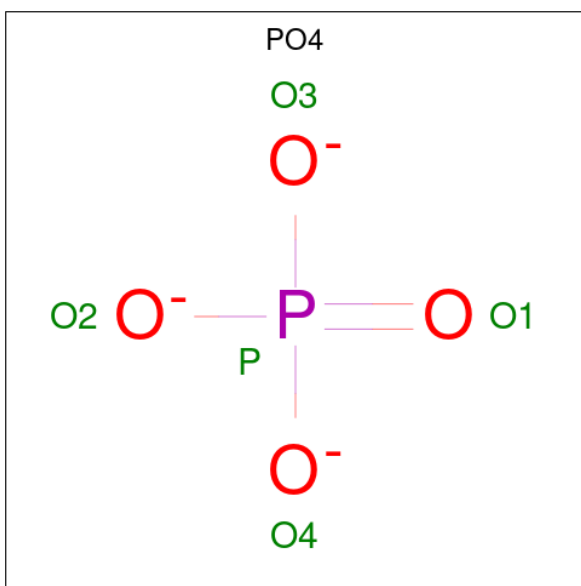
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	14	2		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			16	14	2		
3	A	1	Total	C	O	0	0
			13	12	1		
3	A	1	Total	C	O	0	0
			17	14	3		
3	A	1	Total	C	O	0	0
			15	14	1		

- Molecule 4 is DIPHOSPHATE (CCD ID: DPO) (formula: O_7P_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			8	6	2		
4	A	1	Total	O	P	0	0
			8	6	2		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

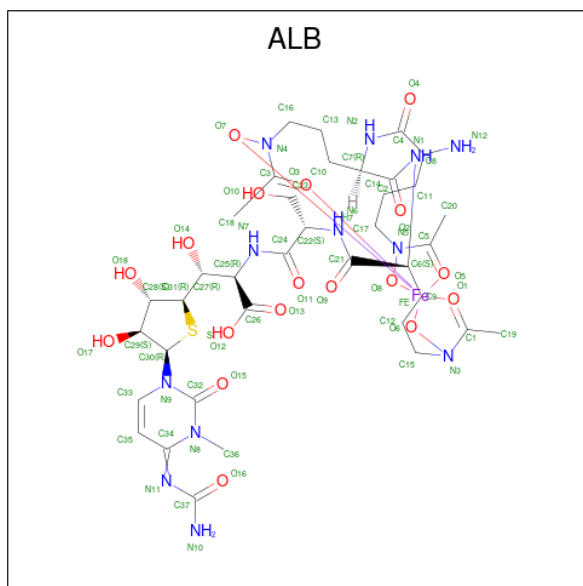


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			4	3	1		
5	A	1	Total	O	P	0	0
			4	3	1		

- Molecule 6 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ni 1 1	0	0

- Molecule 7 is DELTA-2-ALBOMYCIN A1 (CCD ID: ALB) (formula: $C_{37}H_{57}FeN_{12}O_{18}S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	Fe	N	O	S	0	1
			97	51	1	17	26	2		

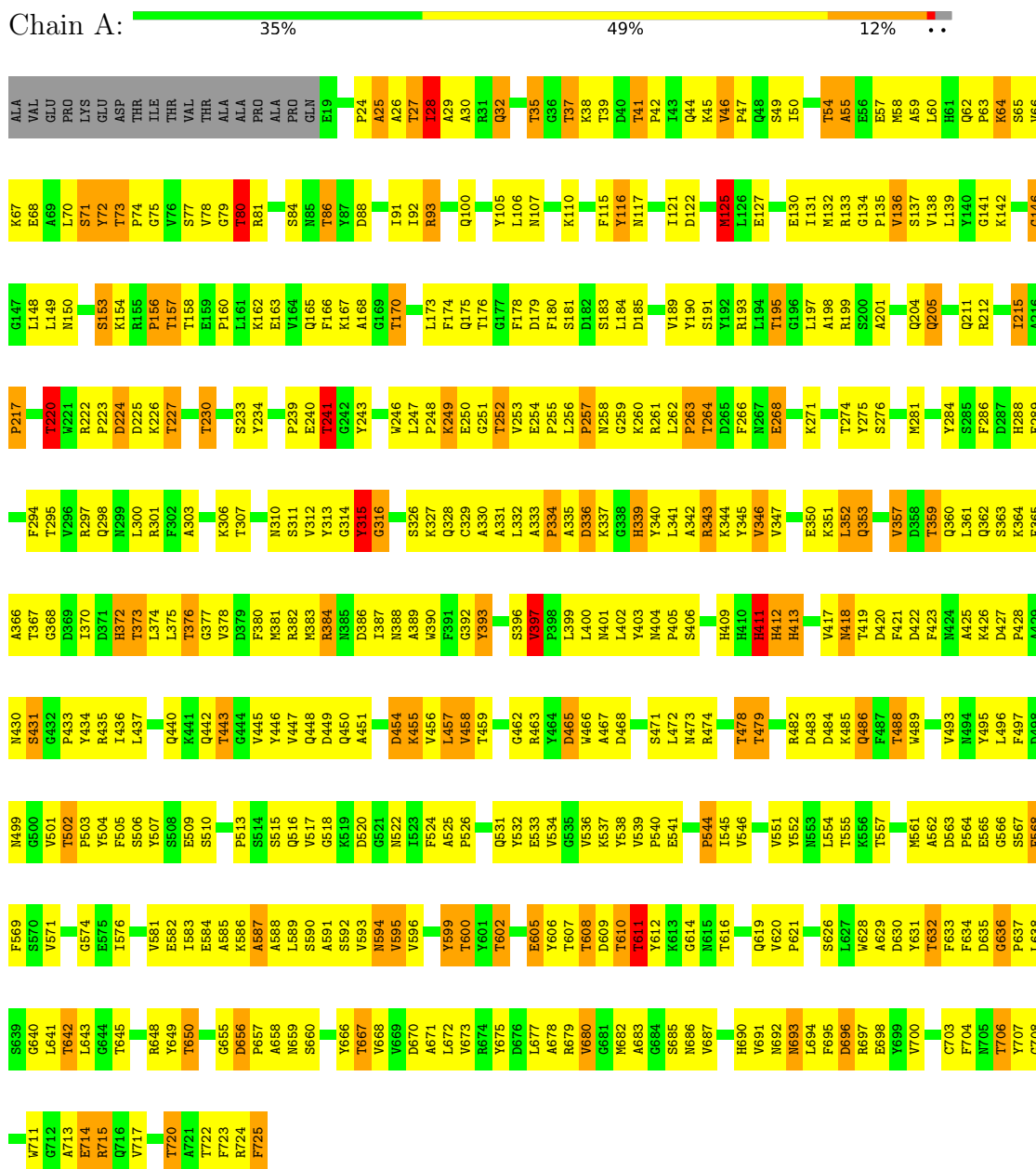
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	332	Total O 332 332	0	0

3 Residue-property plots

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

• Molecule 1: FERRIC HYDROXAMATE RECEPTOR



- Molecule 2: alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-[L-glycero-alpha-D-manno-heptopyranose-(1-7)]L-glycero-alpha-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2,3-dideoxy-alpha-D-glucopyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	171.80Å 171.80Å 86.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-3.10) 94.3 (50.00-3.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.69Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.222 , 0.283 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6195	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GCN, PO4, KDO, GMH, GLA, PA1, ALB, NI, GLC, FTT, DPO

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	1.10	7/5663 (0.1%)	1.16	35/7696 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	ALA	CA-CB	-6.93	1.44	1.53
1	A	263	PRO	CA-C	5.86	1.59	1.52
1	A	166	PHE	CA-C	-5.56	1.46	1.52
1	A	397	VAL	CA-CB	5.49	1.61	1.54
1	A	215	ILE	CA-CB	-5.21	1.47	1.54
1	A	346	VAL	CA-CB	-5.16	1.49	1.55
1	A	217	PRO	CA-C	5.04	1.58	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	SER	N-CA-C	8.12	118.98	108.34
1	A	249	LYS	N-CA-C	-7.57	103.01	111.71
1	A	595	VAL	N-CA-C	7.34	119.39	108.46
1	A	46	VAL	CA-C-N	7.22	128.87	119.84
1	A	46	VAL	C-N-CA	7.22	128.87	119.84
1	A	406	SER	CB-CA-C	-7.22	106.00	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	ALA	N-CA-C	-6.70	104.04	111.82
1	A	515	SER	N-CA-C	-6.69	104.25	112.88
1	A	693	ASN	N-CA-C	-6.44	102.51	111.52
1	A	71	SER	N-CA-C	-6.42	106.40	114.56
1	A	311	SER	N-CA-C	6.34	119.06	109.23
1	A	605	GLU	N-CA-C	6.32	118.91	108.99
1	A	656	ASP	CA-C-N	6.26	126.45	119.32
1	A	656	ASP	C-N-CA	6.26	126.45	119.32
1	A	66	VAL	N-CA-C	-6.04	103.50	111.05
1	A	241	THR	N-CA-C	5.88	120.30	113.18
1	A	220	THR	N-CA-C	5.76	117.91	108.52
1	A	591	ALA	N-CA-C	-5.68	106.44	113.19
1	A	704	PHE	N-CA-C	-5.54	105.88	113.30
1	A	32	GLN	N-CA-C	5.41	117.79	109.07
1	A	88	ASP	N-CA-C	-5.39	103.19	110.68
1	A	64	LYS	N-CA-C	-5.38	105.86	112.90
1	A	377	GLY	N-CA-C	5.33	118.86	110.91
1	A	331	ALA	N-CA-C	-5.33	105.75	113.21
1	A	457	LEU	N-CA-C	-5.31	100.65	109.46
1	A	372	HIS	N-CA-C	5.30	118.20	109.72
1	A	77	SER	N-CA-C	-5.30	102.20	110.42
1	A	136	VAL	CB-CA-C	-5.26	105.49	110.70
1	A	506	SER	N-CA-C	5.26	116.52	108.42
1	A	251	GLY	N-CA-C	-5.22	107.59	114.95
1	A	315	TYR	N-CA-C	-5.21	101.38	109.72
1	A	125	MET	N-CA-C	-5.20	106.34	113.30
1	A	72	TYR	N-CA-C	-5.12	106.88	112.72
1	A	154	LYS	N-CA-C	-5.08	102.96	110.48
1	A	587	ALA	N-CA-C	5.07	115.74	108.74

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	599	TYR	Sidechain

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5523	0	5223	528	0
2	B	134	0	102	11	0
3	A	84	0	126	8	0
4	A	16	0	0	1	0
5	A	8	0	0	2	0
6	A	1	0	0	0	0
7	A	97	0	36	14	0
8	A	332	0	0	67	0
All	All	6195	0	5487	554	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 49.

All (554) 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:220:THR:HG23	1:A:230:THR:HG23	1.26	1.17
1:A:378:VAL:HG12	1:A:445:VAL:HG12	1.39	1.04
1:A:132:MET:HE2	1:A:136:VAL:HG12	1.39	1.04
1:A:632:THR:HG23	1:A:642:THR:HG23	1.41	1.03
1:A:380:PHE:HD1	1:A:443:THR:HG23	1.22	1.02
7:A:1022[B]:ALB:H27	7:A:1022[B]:ALB:O11	1.54	1.02
1:A:668:VAL:HG13	1:A:693:ASN:HA	1.43	1.00
1:A:27:THR:HG21	1:A:588:ALA:HB2	1.44	0.99
1:A:35:THR:HG23	1:A:150:ASN:HD22	1.24	0.97
1:A:220:THR:CG2	1:A:230:THR:HG23	1.94	0.97
1:A:455:LYS:HE2	1:A:455:LYS:H	1.27	0.96
1:A:380:PHE:CD1	1:A:443:THR:HG23	2.03	0.94
1:A:446:TYR:HB3	1:A:463:ARG:HB2	1.49	0.94
1:A:691:VAL:HG22	1:A:717:VAL:HG12	1.47	0.93
1:A:134:GLY:C	1:A:146:GLY:HA2	1.93	0.92
1:A:365:PHE:HE1	1:A:372:HIS:HD1	1.18	0.92
1:A:531:GLN:HB2	1:A:554:LEU:HD13	1.49	0.91
1:A:544:PRO:HG2	1:A:588:ALA:HB3	1.52	0.90
1:A:205:GLN:HG3	1:A:243:TYR:CG	2.06	0.90
1:A:628:TRP:CH2	1:A:630:ASP:HB3	2.07	0.90
1:A:517:VAL:HG12	8:A:2253:HOH:O	1.71	0.90
1:A:274:THR:HG22	1:A:310:ASN:HB2	1.56	0.88
1:A:220:THR:HG23	1:A:230:THR:CG2	2.02	0.88
1:A:497:PHE:HB3	1:A:499:ASN:OD1	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:HB	8:A:2186:HOH:O	1.75	0.86
1:A:455:LYS:HE2	1:A:455:LYS:N	1.91	0.85
1:A:632:THR:HG23	1:A:642:THR:CG2	2.05	0.85
1:A:38:LYS:HG3	1:A:139:LEU:HD22	1.58	0.84
1:A:138:VAL:HG13	1:A:139:LEU:HG	1.56	0.84
1:A:189:VAL:HG13	1:A:190:TYR:CD2	2.13	0.84
1:A:488:THR:HG22	1:A:509:GLU:HB2	1.59	0.82
1:A:75:GLY:N	1:A:600:THR:HG21	1.95	0.82
1:A:184:LEU:HG	8:A:2098:HOH:O	1.77	0.82
1:A:632:THR:CG2	1:A:642:THR:HG23	2.09	0.81
2:B:7:GLC:H2	2:B:8:GLC:H3	1.63	0.81
3:A:1006:FTT:O2	2:B:2:GCN:O4	2.00	0.80
1:A:298:GLN:HG3	1:A:359:THR:HG23	1.64	0.80
1:A:568:PHE:O	7:A:1022[B]:ALB:C36	2.29	0.80
1:A:631:TYR:O	1:A:642:THR:HA	1.83	0.79
1:A:179:ASP:OD1	1:A:195:THR:HG23	1.82	0.79
1:A:125:MET:HG3	1:A:234:TYR:HE1	1.47	0.79
1:A:330:ALA:HA	1:A:337:LYS:HZ1	1.48	0.79
1:A:396:SER:HA	1:A:430:ASN:HB2	1.63	0.78
1:A:468:ASP:HB3	1:A:483:ASP:OD1	1.84	0.78
1:A:631:TYR:HD1	1:A:632:THR:N	1.82	0.78
1:A:330:ALA:HA	1:A:337:LYS:NZ	1.99	0.77
1:A:633:PHE:HB2	1:A:638:LEU:O	1.85	0.77
1:A:657:PRO:HD2	8:A:2310:HOH:O	1.84	0.77
1:A:35:THR:CG2	1:A:150:ASN:HD22	1.97	0.77
1:A:588:ALA:HA	1:A:594:ASN:ND2	2.00	0.76
1:A:298:GLN:HE21	1:A:359:THR:HG23	1.49	0.76
1:A:72:TYR:CE1	1:A:628:TRP:HB2	2.21	0.76
1:A:449:ASP:OD2	1:A:451:ALA:HB2	1.85	0.76
7:A:1022[B]:ALB:C24	7:A:1022[B]:ALB:H22	2.13	0.76
3:A:1004:FTT:H51	3:A:1006:FTT:H51	1.67	0.75
1:A:105:TYR:CE2	1:A:110:LYS:HB2	2.22	0.74
1:A:366:ALA:HB2	8:A:2188:HOH:O	1.88	0.74
1:A:586:LYS:HG2	1:A:596:VAL:HG22	1.67	0.74
1:A:693:ASN:O	1:A:715:ARG:HB2	1.88	0.73
1:A:70:LEU:HD13	1:A:131:ILE:HD11	1.71	0.73
1:A:217:PRO:HD2	1:A:233:SER:OG	1.89	0.73
1:A:495:TYR:O	1:A:503:PRO:HD2	1.88	0.72
1:A:28:ILE:HG22	1:A:54:THR:OG1	1.90	0.72
1:A:136:VAL:HG21	1:A:148:LEU:HD12	1.71	0.72
1:A:167:LYS:HG2	1:A:720:THR:HG23	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:THR:HG23	1:A:288:HIS:CD2	2.26	0.71
1:A:337:LYS:HE3	8:A:2168:HOH:O	1.90	0.71
1:A:298:GLN:HE21	1:A:359:THR:CG2	2.04	0.71
1:A:247:LEU:HD21	1:A:268:GLU:HG2	1.72	0.71
1:A:568:PHE:O	7:A:1022[B]:ALB:H361	1.89	0.71
1:A:247:LEU:CD2	1:A:268:GLU:HG2	2.20	0.70
1:A:42:PRO:HD2	1:A:45:LYS:HD2	1.72	0.70
1:A:27:THR:CG2	1:A:588:ALA:HB2	2.21	0.70
1:A:315:TYR:O	1:A:316:GLY:O	2.09	0.70
1:A:27:THR:HG21	1:A:588:ALA:CB	2.21	0.70
1:A:78:VAL:HG23	8:A:2032:HOH:O	1.93	0.69
1:A:609:ASP:HB3	1:A:612:TYR:O	1.93	0.68
1:A:412:HIS:O	1:A:413:HIS:HB2	1.93	0.68
1:A:588:ALA:HA	1:A:594:ASN:HD22	1.58	0.68
1:A:637:PRO:HA	8:A:2287:HOH:O	1.92	0.68
1:A:376:THR:HG23	1:A:447:VAL:HG22	1.75	0.68
1:A:148:LEU:HD23	1:A:149:LEU:N	2.09	0.67
1:A:341:LEU:HB2	1:A:402:LEU:HD21	1.77	0.67
1:A:457:LEU:HG	8:A:2224:HOH:O	1.94	0.67
1:A:628:TRP:HZ2	1:A:672:LEU:CD2	2.07	0.67
1:A:668:VAL:HG13	1:A:693:ASN:CA	2.23	0.67
1:A:141:GLY:HA3	1:A:442:GLN:HE22	1.60	0.67
1:A:361:LEU:HB3	8:A:2196:HOH:O	1.93	0.67
1:A:583:ILE:HD11	8:A:2116:HOH:O	1.93	0.66
1:A:133:ARG:HA	8:A:2071:HOH:O	1.95	0.66
1:A:365:PHE:O	1:A:372:HIS:HB2	1.95	0.66
1:A:544:PRO:CG	1:A:588:ALA:HB3	2.23	0.66
1:A:722:THR:HG22	8:A:2319:HOH:O	1.96	0.66
3:A:1004:FTT:H42	3:A:1006:FTT:H22	1.77	0.66
1:A:294:PHE:HE1	1:A:363:SER:HG	1.44	0.66
1:A:632:THR:HG23	1:A:642:THR:CB	2.25	0.66
1:A:692:ASN:O	1:A:715:ARG:HA	1.97	0.65
7:A:1022[A]:ALB:H362	7:A:1022[A]:ALB:N10	2.11	0.65
1:A:197:LEU:C	1:A:197:LEU:HD12	2.22	0.65
1:A:197:LEU:HD12	1:A:197:LEU:O	1.97	0.65
1:A:256:LEU:HB2	1:A:260:LYS:O	1.95	0.65
1:A:364:LYS:NZ	1:A:373:THR:HG23	2.11	0.64
1:A:493:VAL:HA	8:A:2242:HOH:O	1.95	0.64
1:A:29:ALA:HB1	1:A:546:VAL:HG23	1.79	0.64
1:A:274:THR:CG2	1:A:310:ASN:HB2	2.27	0.64
1:A:54:THR:HG22	8:A:2017:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LEU:HB2	1:A:384:ARG:O	1.98	0.63
1:A:376:THR:HB	8:A:2196:HOH:O	1.98	0.63
1:A:399:LEU:HD23	8:A:2205:HOH:O	1.97	0.63
1:A:632:THR:CB	1:A:642:THR:HG23	2.27	0.63
1:A:645:THR:HA	1:A:671:ALA:HA	1.80	0.63
1:A:513:PRO:HA	1:A:526:PRO:HB3	1.80	0.63
1:A:472:LEU:HD12	1:A:478:THR:O	1.97	0.63
1:A:298:GLN:CG	1:A:359:THR:HG23	2.27	0.62
1:A:390:TRP:CZ3	1:A:433:PRO:HB3	2.34	0.62
1:A:374:LEU:HG	8:A:2195:HOH:O	1.99	0.62
1:A:628:TRP:HZ2	1:A:672:LEU:HD22	1.64	0.62
1:A:65:SER:OG	1:A:67:LYS:HB3	1.99	0.62
1:A:695:PHE:O	1:A:697:ARG:N	2.32	0.62
1:A:75:GLY:H	1:A:600:THR:HG21	1.63	0.62
1:A:310:ASN:ND2	1:A:347:VAL:HG13	2.14	0.62
1:A:693:ASN:HB3	1:A:715:ARG:HA	1.82	0.62
1:A:339:HIS:ND1	1:A:403:TYR:HB2	2.15	0.62
1:A:411:HIS:O	1:A:413:HIS:N	2.32	0.62
1:A:695:PHE:O	1:A:696:ASP:C	2.43	0.62
1:A:226:LYS:NZ	8:A:2115:HOH:O	2.32	0.62
1:A:298:GLN:NE2	1:A:359:THR:HG23	2.15	0.62
1:A:462:GLY:HA2	1:A:489:TRP:HA	1.81	0.62
1:A:352:LEU:HD22	1:A:383:MET:SD	2.39	0.61
1:A:135:PRO:HB3	1:A:510:SER:HB3	1.83	0.61
1:A:505:PHE:HB2	1:A:534:VAL:HG12	1.82	0.61
1:A:35:THR:HG21	1:A:150:ASN:HB3	1.82	0.61
1:A:64:LYS:HB2	1:A:68:GLU:OE1	2.00	0.61
1:A:80:THR:HG21	1:A:91:ILE:CD1	2.31	0.61
1:A:531:GLN:NE2	8:A:2258:HOH:O	2.33	0.61
5:A:1014:PO4:O3	2:B:2:GCN:C6	2.49	0.61
1:A:484:ASP:HA	8:A:2240:HOH:O	2.00	0.61
1:A:79:GLY:C	1:A:81:ARG:H	2.09	0.61
1:A:333:ALA:O	1:A:336:ASP:N	2.34	0.61
1:A:376:THR:CG2	1:A:447:VAL:HG22	2.30	0.60
1:A:220:THR:CB	1:A:230:THR:HG23	2.31	0.60
1:A:134:GLY:O	1:A:146:GLY:HA2	2.01	0.60
3:A:1003:FTT:H21	3:A:1004:FTT:H22	1.83	0.60
1:A:390:TRP:CE2	1:A:426:LYS:HB3	2.37	0.60
1:A:592:SER:O	1:A:631:TYR:HA	2.02	0.60
1:A:93:ARG:NH1	1:A:582:GLU:OE1	2.35	0.60
1:A:167:LYS:HB2	1:A:175:GLN:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:PRO:HD3	8:A:2013:HOH:O	2.02	0.59
1:A:531:GLN:HB2	1:A:554:LEU:CD1	2.26	0.59
1:A:115:PHE:HA	8:A:2060:HOH:O	2.00	0.59
1:A:162:LYS:CB	1:A:725:PHE:HB2	2.33	0.59
1:A:134:GLY:CA	1:A:146:GLY:HA2	2.32	0.59
1:A:173:LEU:HA	1:A:201:ALA:HB2	1.83	0.59
1:A:628:TRP:HH2	1:A:630:ASP:HB3	1.67	0.59
1:A:50:ILE:N	1:A:50:ILE:HD12	2.18	0.59
1:A:107:ASN:HD21	1:A:153:SER:H	1.48	0.59
1:A:248:PRO:O	1:A:252:THR:OG1	2.20	0.59
1:A:332:LEU:HD13	1:A:340:TYR:CD2	2.38	0.59
1:A:224:ASP:OD1	1:A:225:ASP:N	2.36	0.59
5:A:1014:PO4:O3	2:B:2:GCN:H61	2.02	0.59
1:A:393:TYR:CD1	1:A:393:TYR:N	2.69	0.59
1:A:504:TYR:CE2	1:A:537:LYS:HE3	2.38	0.59
1:A:297:ARG:HD2	1:A:360:GLN:HE21	1.68	0.59
1:A:635:ASP:O	1:A:636:GLY:O	2.20	0.59
1:A:44:GLN:HG2	1:A:45:LYS:N	2.17	0.58
1:A:137:SER:HB2	1:A:510:SER:HA	1.84	0.58
1:A:402:LEU:O	1:A:405:PRO:HD2	2.03	0.58
1:A:364:LYS:HZ2	1:A:373:THR:HG23	1.69	0.58
1:A:72:TYR:HA	1:A:626:SER:OG	2.03	0.58
1:A:170:THR:OG1	1:A:717:VAL:HG22	2.02	0.58
1:A:576:ILE:HD11	1:A:606:TYR:CE1	2.38	0.58
1:A:27:THR:HG22	8:A:2019:HOH:O	2.04	0.58
1:A:258:ASN:HB3	1:A:403:TYR:HE1	1.67	0.58
1:A:602:THR:HG23	8:A:2265:HOH:O	2.03	0.58
1:A:240:GLU:HA	1:A:275:TYR:O	2.03	0.58
7:A:1022[A]:ALB:C36	7:A:1022[A]:ALB:C37	2.81	0.58
1:A:163:GLU:HG3	1:A:724:ARG:HD3	1.86	0.58
1:A:220:THR:HG23	1:A:230:THR:CB	2.33	0.58
1:A:153:SER:HB3	8:A:2068:HOH:O	2.04	0.57
1:A:655:GLY:O	1:A:656:ASP:HB3	2.03	0.57
1:A:396:SER:CA	1:A:430:ASN:HB2	2.34	0.57
1:A:333:ALA:O	1:A:336:ASP:HB2	2.03	0.57
1:A:333:ALA:O	1:A:335:ALA:N	2.38	0.57
1:A:222:ARG:C	1:A:224:ASP:H	2.13	0.57
1:A:362:GLN:HE21	1:A:364:LYS:HD3	1.69	0.57
1:A:474:ARG:HH11	1:A:474:ARG:HG2	1.69	0.57
1:A:605:GLU:HG3	1:A:614:GLY:HA2	1.87	0.57
1:A:353:GLN:HG3	8:A:2199:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:LEU:O	1:A:447:VAL:HA	2.04	0.57
1:A:300:LEU:C	1:A:300:LEU:HD23	2.29	0.57
1:A:482:ARG:CZ	1:A:525:ALA:HA	2.34	0.57
1:A:73:THR:HG23	8:A:2269:HOH:O	2.03	0.56
1:A:45:LYS:HD3	1:A:457:LEU:HD13	1.87	0.56
1:A:62:GLN:OE1	1:A:167:LYS:NZ	2.31	0.56
1:A:370:ILE:HG22	1:A:372:HIS:CD2	2.40	0.56
1:A:567:SER:C	1:A:569:PHE:H	2.12	0.56
1:A:25:ALA:O	1:A:26:ALA:HB3	2.06	0.56
1:A:27:THR:C	1:A:29:ALA:H	2.12	0.56
1:A:70:LEU:HD22	1:A:131:ILE:HD12	1.86	0.56
1:A:404:ASN:HB3	1:A:405:PRO:HD3	1.87	0.56
1:A:93:ARG:CZ	1:A:552:TYR:CD2	2.89	0.56
1:A:141:GLY:HA3	1:A:442:GLN:NE2	2.21	0.56
1:A:418:ASN:HB3	8:A:2211:HOH:O	2.06	0.56
1:A:436:ILE:HD13	1:A:473:ASN:HA	1.87	0.56
1:A:497:PHE:HB2	1:A:501:VAL:O	2.06	0.56
1:A:567:SER:O	1:A:569:PHE:N	2.34	0.56
1:A:249:LYS:HZ2	1:A:250:GLU:CD	2.14	0.55
1:A:167:LYS:HZ3	1:A:720:THR:HG21	1.70	0.55
1:A:306:LYS:HG2	1:A:351:LYS:HB2	1.87	0.55
1:A:589:LEU:HB2	1:A:593:VAL:HG12	1.88	0.55
1:A:71:SER:HB3	1:A:648:ARG:HG2	1.87	0.55
1:A:495:TYR:HB3	1:A:503:PRO:HD2	1.87	0.55
1:A:93:ARG:HD2	1:A:582:GLU:OE2	2.07	0.55
1:A:199:ARG:HH22	1:A:212:ARG:NH1	2.05	0.55
1:A:605:GLU:OE2	1:A:614:GLY:HA2	2.05	0.55
1:A:58:MET:C	1:A:60:LEU:H	2.15	0.55
1:A:585:ALA:O	1:A:596:VAL:HA	2.05	0.55
1:A:70:LEU:O	1:A:78:VAL:HG11	2.07	0.55
1:A:80:THR:HG21	1:A:91:ILE:HD11	1.89	0.55
1:A:422:ASP:O	1:A:423:PHE:HB2	2.06	0.55
1:A:502:THR:C	8:A:2245:HOH:O	2.50	0.55
1:A:592:SER:HB2	1:A:631:TYR:CE1	2.41	0.55
1:A:648:ARG:NH2	8:A:2290:HOH:O	2.38	0.55
1:A:78:VAL:HA	8:A:2033:HOH:O	2.08	0.54
1:A:397:VAL:HB	1:A:421:PHE:CE1	2.42	0.54
1:A:608:THR:HG23	8:A:2279:HOH:O	2.06	0.54
1:A:714:GLU:O	1:A:715:ARG:C	2.50	0.54
7:A:1022[A]:ALB:N10	7:A:1022[A]:ALB:C36	2.70	0.54
1:A:281:MET:HB3	1:A:303:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:SER:C	1:A:50:ILE:HD12	2.32	0.54
1:A:310:ASN:ND2	1:A:347:VAL:HG22	2.23	0.54
1:A:677:LEU:HD11	1:A:687:VAL:HG23	1.88	0.54
1:A:422:ASP:CG	1:A:425:ALA:H	2.16	0.54
1:A:62:GLN:N	1:A:63:PRO:HD3	2.22	0.54
1:A:75:GLY:CA	1:A:600:THR:HG21	2.37	0.54
1:A:448:GLN:NE2	1:A:450:GLN:HG3	2.23	0.54
1:A:239:PRO:O	1:A:276:SER:HB3	2.08	0.54
1:A:370:ILE:HG22	1:A:372:HIS:NE2	2.22	0.54
1:A:167:LYS:HD2	1:A:175:GLN:HB3	1.90	0.54
1:A:562:ALA:O	1:A:610:THR:OG1	2.18	0.54
1:A:694:LEU:O	1:A:715:ARG:HD3	2.08	0.54
1:A:268:GLU:OE1	1:A:314:GLY:N	2.42	0.53
1:A:458:VAL:HG23	1:A:493:VAL:HG22	1.88	0.53
1:A:341:LEU:CB	1:A:402:LEU:HD21	2.39	0.53
1:A:300:LEU:HB2	1:A:357:VAL:HG12	1.89	0.53
1:A:310:ASN:HD21	1:A:347:VAL:HG13	1.72	0.53
1:A:383:MET:CE	1:A:440:GLN:NE2	2.71	0.53
1:A:37:THR:HG22	1:A:448:GLN:CD	2.33	0.53
1:A:258:ASN:ND2	1:A:260:LYS:HD2	2.24	0.53
1:A:328:GLN:HE21	1:A:399:LEU:HG	1.73	0.53
1:A:505:PHE:HA	1:A:534:VAL:HA	1.91	0.53
1:A:341:LEU:HB2	1:A:402:LEU:HD11	1.90	0.53
1:A:446:TYR:CB	1:A:463:ARG:HB2	2.32	0.53
1:A:382:ARG:NH2	8:A:2199:HOH:O	2.36	0.53
1:A:365:PHE:CD1	1:A:365:PHE:C	2.87	0.52
1:A:373:THR:HB	1:A:450:GLN:HB2	1.90	0.52
1:A:352:LEU:C	1:A:352:LEU:HD12	2.34	0.52
1:A:456:VAL:HG12	1:A:456:VAL:O	2.09	0.52
1:A:690:HIS:HB3	8:A:2301:HOH:O	2.08	0.52
1:A:226:LYS:HD3	8:A:2151:HOH:O	2.08	0.52
1:A:421:PHE:CD2	1:A:422:ASP:N	2.78	0.52
1:A:249:LYS:NZ	1:A:250:GLU:CD	2.69	0.51
1:A:70:LEU:CD1	1:A:131:ILE:HD11	2.39	0.51
1:A:326:SER:HB3	1:A:329:CYS:HB2	1.92	0.51
1:A:545:ILE:HG22	1:A:587:ALA:HB1	1.91	0.51
1:A:222:ARG:O	1:A:224:ASP:N	2.44	0.51
1:A:142:LYS:HB2	1:A:513:PRO:HD2	1.92	0.51
1:A:496:LEU:HD23	1:A:502:THR:CG2	2.40	0.51
1:A:116:TYR:O	1:A:307:THR:HG21	2.10	0.51
1:A:605:GLU:CG	1:A:614:GLY:HA2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASP:CG	1:A:195:THR:HG23	2.35	0.51
1:A:286:PHE:CZ	1:A:288:HIS:HB2	2.46	0.51
1:A:298:GLN:NE2	1:A:359:THR:CG2	2.74	0.51
1:A:677:LEU:HD13	1:A:686:ASN:HA	1.91	0.51
1:A:696:ASP:C	1:A:696:ASP:OD1	2.54	0.51
1:A:271:LYS:HG3	1:A:417:VAL:HG21	1.93	0.51
1:A:360:GLN:HB2	1:A:375:LEU:HD11	1.93	0.51
1:A:520:ASP:OD2	1:A:522:ASN:HB2	2.11	0.51
1:A:93:ARG:HG3	1:A:552:TYR:OH	2.12	0.50
1:A:495:TYR:CD2	1:A:497:PHE:HE1	2.29	0.50
1:A:249:LYS:HE3	1:A:706:THR:CG2	2.42	0.50
1:A:649:TYR:HD1	1:A:667:THR:HG23	1.76	0.50
1:A:696:ASP:HA	1:A:715:ARG:HB2	1.91	0.50
7:A:1022[B]:ALB:O11	7:A:1022[B]:ALB:C27	2.33	0.50
1:A:79:GLY:C	1:A:81:ARG:N	2.68	0.50
1:A:135:PRO:HB3	1:A:509:GLU:C	2.36	0.50
1:A:551:VAL:HG23	1:A:581:VAL:HG22	1.94	0.50
1:A:586:LYS:HA	1:A:595:VAL:O	2.11	0.50
1:A:678:ALA:C	1:A:680:VAL:H	2.20	0.50
1:A:68:GLU:C	1:A:70:LEU:H	2.20	0.50
1:A:93:ARG:NH1	1:A:582:GLU:CD	2.69	0.50
1:A:595:VAL:HG12	1:A:629:ALA:HB2	1.93	0.50
8:A:2323:HOH:O	2:B:11:KDO:H7	2.12	0.50
1:A:176:THR:HG23	1:A:176:THR:O	2.10	0.50
1:A:632:THR:HG23	1:A:642:THR:OG1	2.10	0.50
7:A:1022[B]:ALB:O15	7:A:1022[B]:ALB:S	2.70	0.50
1:A:621:PRO:HG3	1:A:650:THR:HG22	1.94	0.49
8:A:2329:HOH:O	2:B:6:GLC:H61	2.13	0.49
1:A:300:LEU:HD12	1:A:357:VAL:CG1	2.43	0.49
1:A:167:LYS:HG2	1:A:720:THR:CG2	2.42	0.49
1:A:316:GLY:H	1:A:707:TYR:HB3	1.78	0.49
1:A:383:MET:CE	1:A:440:GLN:HE21	2.25	0.49
1:A:427:ASP:OD1	1:A:428:PRO:HD2	2.13	0.49
1:A:163:GLU:HG3	1:A:724:ARG:HE	1.77	0.49
1:A:648:ARG:HH11	1:A:670:ASP:CG	2.21	0.49
8:A:2219:HOH:O	2:B:10:GMH:H6	2.12	0.49
1:A:422:ASP:OD2	1:A:425:ALA:N	2.46	0.49
1:A:249:LYS:HE3	1:A:706:THR:HG22	1.94	0.49
1:A:352:LEU:HD12	1:A:352:LEU:O	2.13	0.49
1:A:608:THR:O	1:A:609:ASP:HB2	2.13	0.49
1:A:696:ASP:OD1	1:A:696:ASP:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:TRP:HZ3	1:A:315:TYR:CE1	2.31	0.49
1:A:590:SER:C	1:A:592:SER:H	2.19	0.49
1:A:44:GLN:HB2	1:A:502:THR:OG1	2.13	0.48
1:A:316:GLY:H	1:A:707:TYR:CB	2.26	0.48
1:A:715:ARG:HH11	1:A:715:ARG:HG2	1.77	0.48
1:A:281:MET:HB3	1:A:303:ALA:CB	2.43	0.48
1:A:342:ALA:HA	1:A:399:LEU:HD22	1.95	0.48
1:A:589:LEU:HB2	1:A:593:VAL:CG1	2.43	0.48
1:A:37:THR:O	1:A:38:LYS:HB2	2.13	0.48
1:A:185:ASP:CG	1:A:189:VAL:HG12	2.38	0.48
1:A:435:ARG:NH1	8:A:2219:HOH:O	2.46	0.48
1:A:561:MET:HE2	1:A:574:GLY:N	2.28	0.48
1:A:106:LEU:O	1:A:301:ARG:NH1	2.41	0.48
1:A:364:LYS:HD2	1:A:373:THR:HG23	1.94	0.48
1:A:446:TYR:HB3	1:A:463:ARG:CB	2.33	0.48
1:A:703:CYS:HA	1:A:708:GLY:O	2.12	0.48
1:A:364:LYS:NZ	1:A:373:THR:CG2	2.76	0.48
1:A:448:GLN:NE2	1:A:450:GLN:CG	2.77	0.48
1:A:673:VAL:HG23	1:A:673:VAL:O	2.13	0.48
1:A:678:ALA:HA	1:A:682:MET:C	2.39	0.48
1:A:284:TYR:CD1	1:A:284:TYR:C	2.92	0.48
1:A:401:ASN:OD1	1:A:403:TYR:HB3	2.13	0.48
1:A:173:LEU:O	1:A:174:PHE:CD1	2.67	0.48
1:A:294:PHE:HE1	1:A:363:SER:OG	1.95	0.48
1:A:507:TYR:CD1	1:A:532:TYR:CE1	3.02	0.48
1:A:160:PRO:HA	1:A:181:SER:O	2.14	0.47
1:A:435:ARG:HB2	1:A:474:ARG:HB2	1.96	0.47
1:A:105:TYR:CZ	1:A:110:LYS:HB2	2.48	0.47
1:A:165:GLN:HG3	1:A:722:THR:HB	1.96	0.47
1:A:247:LEU:HD23	1:A:268:GLU:HG2	1.94	0.47
1:A:148:LEU:HD23	1:A:148:LEU:C	2.39	0.47
1:A:343:ARG:CZ	1:A:400:LEU:HG	2.44	0.47
1:A:327:LYS:O	1:A:328:GLN:C	2.56	0.47
1:A:405:PRO:HA	1:A:409:HIS:HD2	1.79	0.47
1:A:632:THR:HA	1:A:641:LEU:O	2.14	0.47
1:A:141:GLY:HA2	1:A:465:ASP:OD2	2.15	0.47
1:A:538:TYR:CE1	1:A:540:PRO:HD3	2.50	0.47
3:A:1006:FTT:H102	3:A:1007:FTT:C9	2.45	0.47
1:A:344:LYS:HB3	1:A:392:GLY:O	2.14	0.47
1:A:35:THR:HG23	1:A:150:ASN:ND2	2.09	0.47
1:A:180:PHE:O	1:A:193:ARG:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ILE:HG22	1:A:437:LEU:N	2.30	0.47
1:A:631:TYR:CD1	1:A:632:THR:N	2.73	0.47
1:A:677:LEU:CD1	1:A:687:VAL:HG23	2.44	0.47
2:B:7:GLC:H2	2:B:8:GLC:C3	2.34	0.47
1:A:390:TRP:CD2	1:A:426:LYS:HD3	2.49	0.47
1:A:472:LEU:HD13	8:A:2236:HOH:O	2.14	0.47
1:A:496:LEU:HD23	1:A:502:THR:HG21	1.95	0.47
1:A:146:GLY:C	8:A:2071:HOH:O	2.58	0.47
7:A:1022[A]:ALB:H33	7:A:1022[A]:ALB:O14	2.15	0.47
1:A:133:ARG:NH1	1:A:133:ARG:HG3	2.30	0.47
1:A:257:PRO:HB2	8:A:2136:HOH:O	2.14	0.47
1:A:642:THR:O	1:A:673:VAL:HA	2.15	0.47
1:A:122:ASP:CG	1:A:197:LEU:HD21	2.40	0.46
1:A:262:LEU:HD13	1:A:266:PHE:CD2	2.50	0.46
1:A:634:PHE:HD1	8:A:2285:HOH:O	1.96	0.46
1:A:38:LYS:HB2	1:A:375:LEU:CD2	2.45	0.46
1:A:105:TYR:O	1:A:150:ASN:HA	2.16	0.46
1:A:115:PHE:C	1:A:117:ASN:H	2.24	0.46
1:A:163:GLU:HG3	1:A:724:ARG:CD	2.45	0.46
1:A:222:ARG:C	1:A:224:ASP:N	2.73	0.46
1:A:175:GLN:HA	1:A:198:ALA:O	2.15	0.46
1:A:422:ASP:CG	1:A:425:ALA:HB3	2.41	0.46
1:A:541:GLU:N	8:A:2262:HOH:O	2.41	0.46
1:A:563:ASP:OD1	1:A:564:PRO:HD2	2.16	0.46
1:A:390:TRP:NE1	1:A:426:LYS:HB3	2.30	0.46
1:A:482:ARG:NH2	1:A:525:ALA:HA	2.30	0.46
1:A:668:VAL:HG11	8:A:2309:HOH:O	2.14	0.46
1:A:590:SER:HB3	1:A:593:VAL:HB	1.98	0.46
1:A:526:PRO:HD3	8:A:2256:HOH:O	2.15	0.46
1:A:28:ILE:HG22	1:A:57:GLU:HB2	1.97	0.46
1:A:167:LYS:HZ3	1:A:720:THR:CG2	2.28	0.46
1:A:364:LYS:CD	1:A:373:THR:HG23	2.45	0.46
1:A:396:SER:HA	1:A:430:ASN:CB	2.39	0.46
1:A:246:TRP:O	1:A:247:LEU:HD23	2.16	0.46
1:A:641:LEU:HD11	1:A:643:LEU:HD21	1.97	0.46
4:A:1015:DPO:O5	2:B:4:GMH:H6	2.16	0.46
1:A:448:GLN:HG3	8:A:2241:HOH:O	2.17	0.45
1:A:465:ASP:O	1:A:485:LYS:HA	2.16	0.45
1:A:178:PHE:N	1:A:178:PHE:CD1	2.84	0.45
1:A:253:VAL:HG22	1:A:700:VAL:HG11	1.99	0.45
1:A:539:VAL:HG13	8:A:2264:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ARG:CG	1:A:698:GLU:N	2.79	0.45
1:A:32:GLN:NE2	1:A:41:THR:C	2.75	0.45
1:A:93:ARG:HH11	1:A:582:GLU:CD	2.23	0.45
1:A:67:LYS:NZ	8:A:2027:HOH:O	2.49	0.45
1:A:162:LYS:HB2	1:A:725:PHE:HB2	1.97	0.45
1:A:211:GLN:HB2	1:A:239:PRO:HG2	1.99	0.45
1:A:561:MET:SD	1:A:609:ASP:HA	2.56	0.45
1:A:162:LYS:HB3	1:A:725:PHE:HB2	1.98	0.45
1:A:205:GLN:HG3	1:A:243:TYR:CB	2.45	0.45
1:A:636:GLY:C	1:A:638:LEU:H	2.24	0.45
1:A:658:ALA:O	1:A:659:ASN:HB2	2.15	0.45
1:A:725:PHE:CD1	1:A:725:PHE:N	2.82	0.45
1:A:37:THR:HG22	1:A:448:GLN:NE2	2.32	0.45
3:A:1006:FTT:H102	3:A:1007:FTT:H91	1.99	0.45
1:A:384:ARG:NH2	2:B:11:KDO:O1B	2.49	0.45
1:A:46:VAL:O	1:A:537:LYS:NZ	2.50	0.45
1:A:434:TYR:CZ	1:A:436:ILE:HG13	2.51	0.45
1:A:563:ASP:HB2	1:A:569:PHE:O	2.17	0.45
1:A:42:PRO:HB3	1:A:44:GLN:OE1	2.17	0.45
1:A:80:THR:HG22	1:A:619:GLN:CD	2.41	0.45
1:A:163:GLU:N	1:A:180:PHE:HE1	2.15	0.45
1:A:350:GLU:HA	1:A:386:ASP:O	2.17	0.45
1:A:373:THR:CB	1:A:450:GLN:HB2	2.47	0.45
1:A:421:PHE:CG	1:A:422:ASP:N	2.85	0.45
1:A:643:LEU:HD22	1:A:673:VAL:HG12	1.99	0.45
1:A:255:PRO:HG3	1:A:261:ARG:NH2	2.32	0.45
1:A:86:THR:HG23	1:A:241:THR:HB	2.00	0.44
1:A:45:LYS:HD3	1:A:457:LEU:CD1	2.47	0.44
1:A:92:ILE:CG2	8:A:2071:HOH:O	2.65	0.44
1:A:197:LEU:C	1:A:197:LEU:CD1	2.90	0.44
1:A:353:GLN:OE1	1:A:384:ARG:HD3	2.17	0.44
1:A:390:TRP:CE3	1:A:426:LYS:HD3	2.52	0.44
1:A:583:ILE:HG12	1:A:599:TYR:HB3	2.00	0.44
1:A:205:GLN:HG3	1:A:243:TYR:CD2	2.51	0.44
1:A:386:ASP:OD2	1:A:437:LEU:HD13	2.17	0.44
1:A:656:ASP:OD1	1:A:660:SER:N	2.50	0.44
1:A:183:SER:HA	1:A:191:SER:HA	1.99	0.44
1:A:346:VAL:HA	1:A:390:TRP:O	2.17	0.44
1:A:384:ARG:HD2	8:A:2199:HOH:O	2.18	0.44
1:A:628:TRP:CZ3	1:A:630:ASP:HB3	2.50	0.44
1:A:685:SER:O	1:A:686:ASN:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HD13	1:A:131:ILE:CD1	2.45	0.44
1:A:133:ARG:HG3	1:A:133:ARG:HH11	1.81	0.44
1:A:388:ASN:HD22	1:A:435:ARG:HG2	1.83	0.44
1:A:650:THR:OG1	1:A:666:TYR:CE1	2.61	0.44
3:A:1004:FTT:H92	3:A:1006:FTT:H82	2.00	0.44
2:B:1:PA1:H4	2:B:2:GCN:N2	2.33	0.44
1:A:163:GLU:HG3	1:A:724:ARG:NE	2.33	0.44
1:A:533:GLU:HG2	1:A:534:VAL:N	2.33	0.44
1:A:125:MET:HG3	1:A:234:TYR:CE1	2.39	0.43
1:A:536:VAL:HB	8:A:2245:HOH:O	2.18	0.43
1:A:640:GLY:O	1:A:675:TYR:HA	2.18	0.43
1:A:28:ILE:HD13	1:A:586:LYS:HB3	1.99	0.43
1:A:383:MET:HB3	1:A:440:GLN:HB2	1.98	0.43
1:A:427:ASP:OD1	1:A:428:PRO:CD	2.67	0.43
1:A:93:ARG:NH2	1:A:533:GLU:OE1	2.40	0.43
1:A:163:GLU:HA	1:A:723:PHE:O	2.18	0.43
1:A:370:ILE:CG2	1:A:372:HIS:NE2	2.81	0.43
1:A:467:ALA:O	1:A:484:ASP:N	2.50	0.43
1:A:75:GLY:N	1:A:600:THR:CG2	2.76	0.43
1:A:60:LEU:HD21	1:A:628:TRP:CH2	2.53	0.43
1:A:247:LEU:HD21	1:A:268:GLU:CG	2.42	0.43
1:A:264:THR:HA	1:A:711:TRP:CD1	2.53	0.43
1:A:649:TYR:CD1	1:A:667:THR:HG23	2.53	0.43
1:A:393:TYR:N	1:A:393:TYR:HD1	2.15	0.43
1:A:468:ASP:HA	1:A:483:ASP:HA	2.00	0.43
1:A:611:THR:HB	1:A:612:TYR:H	1.44	0.43
1:A:136:VAL:CG2	1:A:148:LEU:HD12	2.46	0.43
1:A:281:MET:CB	1:A:303:ALA:HB2	2.48	0.43
1:A:516:GLN:CD	7:A:1022[A]:ALB:H1N2	2.27	0.43
1:A:631:TYR:HD1	1:A:632:THR:H	1.63	0.43
1:A:454:ASP:C	1:A:456:VAL:H	2.26	0.43
1:A:58:MET:O	1:A:63:PRO:HD3	2.18	0.43
1:A:93:ARG:HG3	1:A:552:TYR:CZ	2.54	0.43
1:A:632:THR:OG1	1:A:642:THR:HG23	2.18	0.43
1:A:55:ALA:HB2	1:A:127:GLU:O	2.19	0.43
1:A:310:ASN:HD22	1:A:347:VAL:HG22	1.84	0.43
1:A:590:SER:C	1:A:592:SER:N	2.77	0.43
1:A:312:VAL:HG22	1:A:345:TYR:HB3	2.00	0.42
1:A:263:PRO:HG2	1:A:266:PHE:HB2	2.00	0.42
1:A:288:HIS:ND1	1:A:289:GLU:N	2.67	0.42
1:A:350:GLU:OE1	1:A:387:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:PRO:HA	1:A:409:HIS:CD2	2.54	0.42
1:A:422:ASP:OD2	1:A:425:ALA:HB3	2.19	0.42
1:A:635:ASP:C	1:A:636:GLY:O	2.62	0.42
1:A:74:PRO:HG3	1:A:584:GLU:HB2	2.02	0.42
1:A:86:THR:HG23	8:A:2125:HOH:O	2.18	0.42
1:A:226:LYS:O	1:A:288:HIS:HA	2.20	0.42
1:A:246:TRP:HB3	1:A:708:GLY:HA2	2.01	0.42
1:A:594:ASN:HD22	1:A:594:ASN:HA	1.53	0.42
1:A:100:GLN:HA	8:A:2043:HOH:O	2.18	0.42
1:A:594:ASN:HB2	1:A:630:ASP:OD1	2.20	0.42
1:A:596:VAL:O	1:A:628:TRP:N	2.44	0.42
1:A:390:TRP:HE1	1:A:431:SER:CB	2.32	0.42
1:A:412:HIS:CD2	1:A:412:HIS:N	2.87	0.42
1:A:471:SER:O	1:A:479:THR:HA	2.20	0.42
1:A:496:LEU:HA	1:A:502:THR:HG23	2.00	0.42
1:A:115:PHE:CZ	1:A:434:TYR:CE2	3.08	0.42
1:A:352:LEU:C	1:A:352:LEU:CD1	2.92	0.42
1:A:68:GLU:C	1:A:70:LEU:N	2.77	0.42
1:A:227:THR:CG2	1:A:288:HIS:CD2	2.98	0.42
1:A:680:VAL:HG12	1:A:680:VAL:O	2.20	0.42
1:A:37:THR:HG22	1:A:448:GLN:OE1	2.20	0.42
1:A:75:GLY:HA2	1:A:600:THR:HG21	2.02	0.42
1:A:274:THR:HB	8:A:2122:HOH:O	2.19	0.42
1:A:435:ARG:CB	1:A:474:ARG:HB2	2.49	0.42
1:A:465:ASP:N	1:A:486:GLN:O	2.46	0.42
1:A:567:SER:C	1:A:569:PHE:N	2.77	0.42
1:A:683:ALA:HA	8:A:2305:HOH:O	2.20	0.42
1:A:697:ARG:HG2	1:A:698:GLU:N	2.35	0.42
1:A:163:GLU:N	1:A:180:PHE:CE1	2.87	0.41
1:A:479:THR:HG21	8:A:2236:HOH:O	2.20	0.41
1:A:538:TYR:CD1	1:A:540:PRO:HD3	2.55	0.41
1:A:539:VAL:O	1:A:539:VAL:HG12	2.19	0.41
1:A:545:ILE:O	1:A:545:ILE:HG13	2.20	0.41
1:A:633:PHE:HD2	1:A:641:LEU:HD23	1.85	0.41
1:A:79:GLY:O	1:A:81:ARG:N	2.53	0.41
1:A:204:GLN:OE1	1:A:713:ALA:HA	2.21	0.41
1:A:274:THR:O	1:A:274:THR:HG23	2.20	0.41
1:A:365:PHE:C	1:A:365:PHE:HD1	2.28	0.41
1:A:595:VAL:HG12	1:A:629:ALA:CB	2.50	0.41
1:A:168:ALA:HA	1:A:173:LEU:O	2.20	0.41
1:A:215:ILE:O	1:A:215:ILE:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LYS:HA	1:A:496:LEU:HB2	2.02	0.41
1:A:516:GLN:NE2	7:A:1022[A]:ALB:H1N2	2.18	0.41
1:A:86:THR:CG2	8:A:2125:HOH:O	2.68	0.41
1:A:426:LYS:H	1:A:426:LYS:HG3	1.70	0.41
1:A:38:LYS:CE	1:A:139:LEU:HB3	2.51	0.41
1:A:92:ILE:HG22	8:A:2071:HOH:O	2.20	0.41
1:A:130:GLU:O	1:A:149:LEU:HD12	2.20	0.41
1:A:157:THR:OG1	1:A:181:SER:HB3	2.20	0.41
1:A:329:CYS:O	1:A:337:LYS:NZ	2.54	0.41
1:A:347:VAL:O	1:A:389:ALA:HA	2.21	0.41
1:A:649:TYR:HB2	1:A:667:THR:HG23	2.03	0.41
1:A:696:ASP:HA	1:A:715:ARG:CB	2.50	0.41
1:A:284:TYR:CE2	3:A:1005:FTT:H111	2.56	0.41
1:A:561:MET:HG2	1:A:571:VAL:O	2.21	0.41
1:A:249:LYS:HG3	1:A:250:GLU:OE1	2.20	0.41
1:A:466:TRP:CD1	1:A:485:LYS:HG2	2.56	0.41
1:A:631:TYR:CD1	1:A:631:TYR:C	2.99	0.41
1:A:722:THR:HG21	8:A:2091:HOH:O	2.20	0.41
1:A:724:ARG:HD2	8:A:2088:HOH:O	2.21	0.41
1:A:156:PRO:HD2	8:A:2109:HOH:O	2.20	0.41
1:A:458:VAL:N	8:A:2224:HOH:O	2.54	0.41
1:A:28:ILE:HA	1:A:54:THR:OG1	2.22	0.40
1:A:445:VAL:HG22	8:A:2228:HOH:O	2.21	0.40
1:A:121:ILE:HG23	1:A:234:TYR:CE1	2.55	0.40
1:A:205:GLN:H	1:A:205:GLN:HG2	1.58	0.40
1:A:268:GLU:H	1:A:268:GLU:HG3	1.71	0.40
1:A:518:GLY:HA2	1:A:524:PHE:CZ	2.56	0.40
1:A:638:LEU:O	1:A:641:LEU:HB3	2.21	0.40
1:A:32:GLN:HE22	1:A:41:THR:C	2.30	0.40
1:A:249:LYS:HD2	1:A:254:GLU:CD	2.46	0.40
1:A:360:GLN:NE2	8:A:2178:HOH:O	2.51	0.40
1:A:133:ARG:NH1	8:A:2070:HOH:O	2.55	0.40
1:A:313:TYR:CZ	1:A:344:LYS:HB2	2.57	0.40
1:A:341:LEU:HB2	1:A:402:LEU:CD2	2.48	0.40
1:A:388:ASN:ND2	1:A:435:ARG:CD	2.85	0.40
1:A:455:LYS:HE2	1:A:455:LYS:CA	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	705/725 (97%)	601 (85%)	77 (11%)	27 (4%)	2	15

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	PRO
1	A	224	ASP
1	A	412	HIS
1	A	696	ASP
1	A	25	ALA
1	A	146	GLY
1	A	259	GLY
1	A	316	GLY
1	A	334	PRO
1	A	418	ASN
1	A	454	ASP
1	A	566	GLY
1	A	611	THR
1	A	636	GLY
1	A	679	ARG
1	A	715	ARG
1	A	368	GLY
1	A	413	HIS
1	A	420	ASP
1	A	568	PHE
1	A	59	ALA
1	A	80	THR
1	A	116	TYR
1	A	411	HIS
1	A	223	PRO
1	A	680	VAL
1	A	28	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	587/601 (98%)	509 (87%)	78 (13%)	4 17

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	28	ILE
1	A	35	THR
1	A	37	THR
1	A	39	THR
1	A	41	THR
1	A	54	THR
1	A	73	THR
1	A	80	THR
1	A	84	SER
1	A	86	THR
1	A	93	ARG
1	A	125	MET
1	A	153	SER
1	A	156	PRO
1	A	157	THR
1	A	158	THR
1	A	170	THR
1	A	195	THR
1	A	205	GLN
1	A	220	THR
1	A	227	THR
1	A	230	THR
1	A	241	THR
1	A	252	THR
1	A	257	PRO
1	A	264	THR
1	A	268	GLU
1	A	295	THR
1	A	315	TYR

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Mol	Chain	Res	Type
1	A	334	PRO
1	A	336	ASP
1	A	339	HIS
1	A	343	ARG
1	A	352	LEU
1	A	353	GLN
1	A	357	VAL
1	A	359	THR
1	A	367	THR
1	A	373	THR
1	A	376	THR
1	A	381	MET
1	A	384	ARG
1	A	393	TYR
1	A	397	VAL
1	A	411	HIS
1	A	419	THR
1	A	443	THR
1	A	455	LYS
1	A	458	VAL
1	A	459	THR
1	A	465	ASP
1	A	478	THR
1	A	479	THR
1	A	486	GLN
1	A	488	THR
1	A	502	THR
1	A	544	PRO
1	A	555	THR
1	A	557	THR
1	A	565	GLU
1	A	594	ASN
1	A	600	THR
1	A	602	THR
1	A	607	THR
1	A	608	THR
1	A	610	THR
1	A	611	THR
1	A	616	THR
1	A	620	VAL
1	A	632	THR
1	A	642	THR

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Mol	Chain	Res	Type
1	A	650	THR
1	A	667	THR
1	A	706	THR
1	A	714	GLU
1	A	720	THR
1	A	725	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	150	ASN
1	A	165	GLN
1	A	211	GLN
1	A	298	GLN
1	A	299	ASN
1	A	310	ASN
1	A	328	GLN
1	A	354	ASN
1	A	360	GLN
1	A	362	GLN
1	A	388	ASN
1	A	404	ASN
1	A	410	HIS
1	A	412	HIS
1	A	418	ASN
1	A	438	ASN
1	A	448	GLN
1	A	522	ASN
1	A	531	GLN
1	A	594	ASN
1	A	716	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 ⓘ

11 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	PA1	B	1	2,3,4	11,11,12	2.67	4 (36%)	15,15,17	2.75	6 (40%)
2	GMH	B	10	2	13,13,14	1.38	3 (23%)	16,18,20	0.60	0
2	KDO	B	11	2	15,15,16	1.04	1 (6%)	17,21,24	1.25	2 (11%)
2	GCN	B	2	5,2,3	10,10,11	2.29	5 (50%)	13,13,15	5.99	5 (38%)
2	KDO	B	3	2	15,15,16	0.99	1 (6%)	17,21,24	1.16	1 (5%)
2	GMH	B	4	2,4	13,13,14	0.85	1 (7%)	16,18,20	0.89	1 (6%)
2	GMH	B	5	5,2	13,13,14	0.76	0	16,18,20	0.97	1 (6%)
2	GLC	B	6	2	11,11,12	0.44	0	15,15,17	1.00	1 (6%)
2	GLC	B	7	2	11,11,12	0.77	0	15,15,17	0.60	0
2	GLC	B	8	2	11,11,12	1.61	3 (27%)	15,15,17	1.13	1 (6%)
2	GLA	B	9	2	11,11,12	0.68	0	15,15,17	0.66	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
2	PA1	B	1	2,3,4	-	0/2/18/22	0/1/1/1
2	GMH	B	10	2	1/1/5/6	2/6/23/26	0/1/1/1
2	KDO	B	11	2	-	5/10/26/30	0/1/1/1
2	GCN	B	2	5,2,3	2/2/3/4	2/2/15/18	0/1/1/1
2	KDO	B	3	2	-	2/10/26/30	0/1/1/1
2	GMH	B	4	2,4	-	0/6/23/26	0/1/1/1
2	GMH	B	5	5,2	1/1/5/6	0/6/23/26	1/1/1/1
2	GLC	B	6	2	-	2/2/19/22	0/1/1/1
2	GLC	B	7	2	-	1/2/19/22	0/1/1/1
2	GLC	B	8	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLA	B	9	2	-	1/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	PA1	C1-C2	7.12	1.61	1.52
2	B	2	GCN	C3-C4	4.23	1.60	1.52
2	B	2	GCN	C3-C2	-3.37	1.46	1.53
2	B	2	GCN	C1-C2	-3.30	1.48	1.52
2	B	10	GMH	O5-C5	3.14	1.47	1.43
2	B	1	PA1	O5-C1	3.04	1.50	1.42
2	B	8	GLC	C2-C3	2.97	1.57	1.52
2	B	1	PA1	O1-C1	-2.60	1.31	1.39
2	B	1	PA1	C3-C4	-2.57	1.47	1.52
2	B	8	GLC	O5-C5	2.57	1.48	1.43
2	B	2	GCN	O4-C4	2.42	1.48	1.43
2	B	2	GCN	C4-C5	2.39	1.56	1.52
2	B	11	KDO	C3-C2	2.32	1.56	1.52
2	B	8	GLC	C1-C2	2.27	1.57	1.52
2	B	3	KDO	O1A-C1	2.26	1.28	1.22
2	B	4	GMH	C2-C3	2.11	1.55	1.52
2	B	10	GMH	C2-C3	2.09	1.55	1.52
2	B	10	GMH	C1-C2	2.08	1.57	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	GCN	C3-C2-C1	19.69	125.80	109.87
2	B	1	PA1	C1-C2-N2	7.61	124.43	110.49
2	B	2	GCN	O4-C4-C5	5.38	121.25	110.08
2	B	2	GCN	C1-C2-N2	4.32	118.55	111.61
2	B	1	PA1	C3-C4-C5	-3.86	105.83	110.76
2	B	2	GCN	C6-C5-C4	3.78	118.69	113.53
2	B	5	GMH	C1-O5-C5	3.56	117.31	111.48
2	B	1	PA1	C4-C3-C2	3.51	119.84	112.65
2	B	8	GLC	C1-O5-C5	3.48	116.85	112.19
2	B	1	PA1	C3-C2-N2	-3.25	98.66	110.78
2	B	11	KDO	C3-C4-C5	-3.02	106.31	110.67
2	B	6	GLC	C1-O5-C5	2.75	115.87	112.19
2	B	1	PA1	C3-C2-C1	2.69	115.98	109.56
2	B	2	GCN	C3-C4-C5	-2.53	107.53	110.76
2	B	4	GMH	C1-O5-C5	2.35	115.33	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	KDO	O6-C6-C7	2.33	111.13	106.60
2	B	11	KDO	O1A-C1-C2	-2.14	118.22	122.85
2	B	1	PA1	O1-C1-O5	-2.01	104.44	110.41

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2	GCN	C2
2	B	2	GCN	C1
2	B	5	GMH	C6
2	B	10	GMH	C6

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	11	KDO	O6-C6-C7-O7
2	B	11	KDO	O6-C6-C7-C8
2	B	8	GLC	O5-C5-C6-O6
2	B	2	GCN	O5-C5-C6-O6
2	B	8	GLC	C4-C5-C6-O6
2	B	9	GLA	O5-C5-C6-O6
2	B	7	GLC	O5-C5-C6-O6
2	B	3	KDO	O7-C7-C8-O8
2	B	10	GMH	C4-C5-C6-C7
2	B	11	KDO	C5-C6-C7-C8
2	B	10	GMH	O5-C5-C6-C7
2	B	11	KDO	C5-C6-C7-O7
2	B	6	GLC	C4-C5-C6-O6
2	B	11	KDO	O1A-C1-C2-O6
2	B	6	GLC	O5-C5-C6-O6
2	B	3	KDO	C6-C7-C8-O8
2	B	2	GCN	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5	GMH	C1-C2-C3-C4-C5-O5

8 monomers are involved in 11 short contacts:

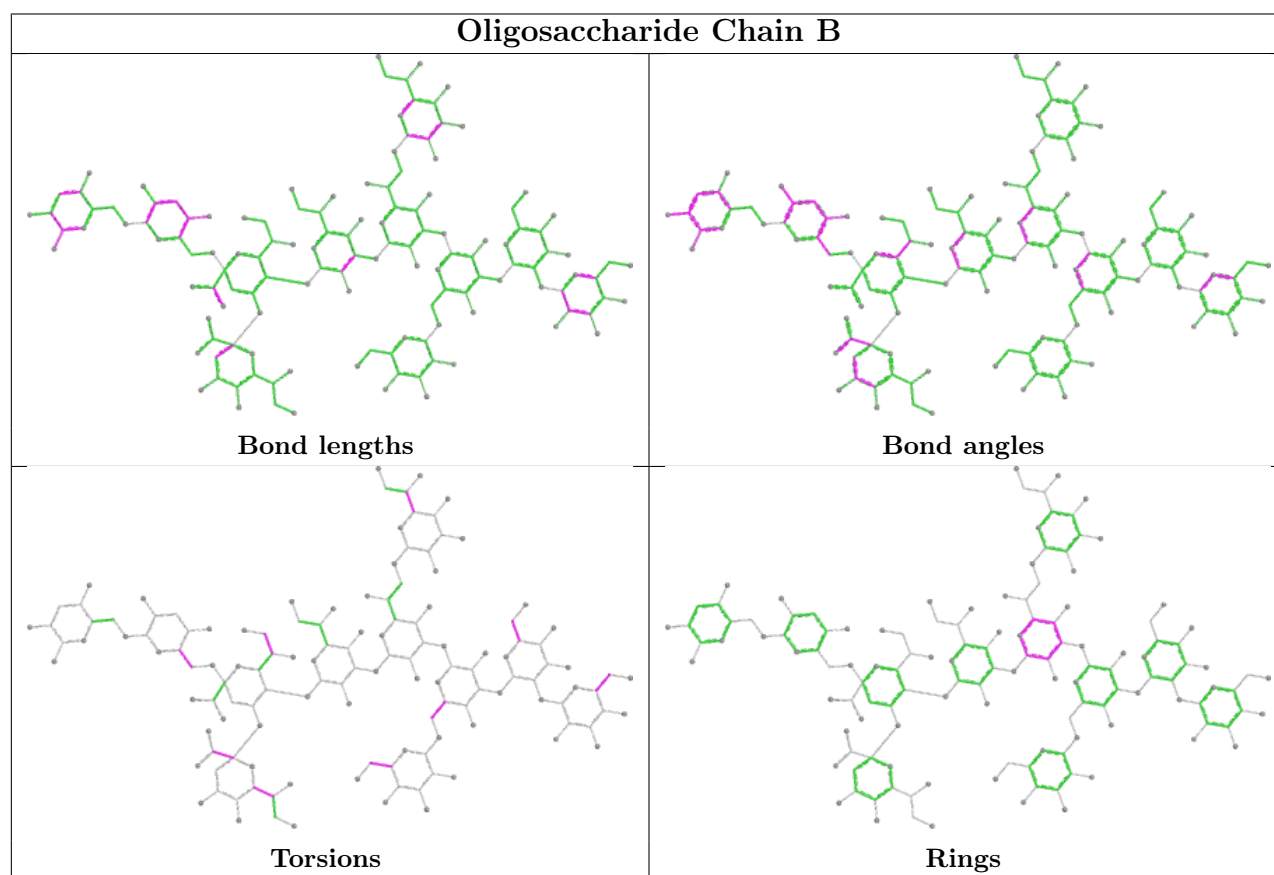
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	8	GLC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	PA1	1	0
2	B	6	GLC	1	0
2	B	4	GMH	1	0
2	B	11	KDO	2	0
2	B	10	GMH	1	0
2	B	2	GCN	4	0
2	B	7	GLC	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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	ALB	A	1022[B]	-	72,75,75	2.47	14 (19%)	78,117,117	4.36	27 (34%)
3	FTT	A	1002	2	14,15,16	2.11	2 (14%)	15,15,17	2.91	1 (6%)
3	FTT	A	1007	3	13,14,16	0.43	0	12,13,17	0.61	0
3	FTT	A	1005	3	11,12,16	0.39	0	10,11,17	0.68	0
3	FTT	A	1006	2,3	16,16,16	1.34	1 (6%)	16,17,17	1.07	1 (6%)
3	FTT	A	1004	2,3	14,15,16	1.20	1 (7%)	15,15,17	3.19	3 (20%)
4	DPO	A	1013	2	3,7,8	1.38	0	6,10,13	1.34	1 (16%)
3	FTT	A	1003	2	6,6,16	2.08	1 (16%)	6,7,17	2.11	2 (33%)
5	PO4	A	1016	6,2	0,3,4	-	-	0,3,6	-	-
5	PO4	A	1014	2	0,3,4	-	-	0,3,6	-	-
7	ALB	A	1022[A]	-	72,75,75	2.37	17 (23%)	78,117,117	4.48	30 (38%)
4	DPO	A	1015	2	3,7,8	1.22	0	6,10,13	0.89	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
7	ALB	A	1022[B]	-	7/7/23/27	33/70/142/142	0/5/7/7
3	FTT	A	1002	2	-	2/14/14/15	-
3	FTT	A	1007	3	-	1/12/12/15	-
3	FTT	A	1005	3	-	0/10/10/15	-
3	FTT	A	1006	2,3	1/1/2/2	1/15/15/15	-
3	FTT	A	1004	2,3	-	1/14/14/15	-
4	DPO	A	1013	2	-	0/2/5/6	-
3	FTT	A	1003	2	-	1/4/4/15	-
7	ALB	A	1022[A]	-	5/5/23/27	39/70/142/142	0/5/7/7
4	DPO	A	1015	2	-	0/2/5/6	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1022[B]	ALB	C30-C29	9.77	1.66	1.54
7	A	1022[B]	ALB	C22-C24	9.57	1.77	1.52
7	A	1022[A]	ALB	C22-C24	8.48	1.74	1.52
7	A	1022[A]	ALB	C36-N8	-7.81	1.33	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	FTT	C2-C1	7.25	1.69	1.50
7	A	1022[A]	ALB	C30-N9	6.13	1.56	1.47
7	A	1022[B]	ALB	C35-C34	-5.68	1.31	1.41
7	A	1022[B]	ALB	C32-N9	-5.59	1.30	1.38
7	A	1022[A]	ALB	C30-C29	5.25	1.60	1.54
7	A	1022[A]	ALB	C6-C21	5.05	1.65	1.52
7	A	1022[B]	ALB	C6-C21	5.05	1.65	1.52
3	A	1006	FTT	O1-C1	5.00	1.47	1.30
7	A	1022[B]	ALB	C29-C28	4.86	1.66	1.53
7	A	1022[A]	ALB	C32-N9	-4.70	1.32	1.38
3	A	1003	FTT	O1-C1	4.67	1.46	1.30
3	A	1004	FTT	C2-C1	4.16	1.60	1.50
7	A	1022[A]	ALB	C31-S	-3.72	1.78	1.83
7	A	1022[A]	ALB	C33-N9	-3.67	1.29	1.38
7	A	1022[A]	ALB	C25-N7	3.65	1.53	1.45
7	A	1022[B]	ALB	C30-N9	3.65	1.52	1.47
7	A	1022[A]	ALB	C8-N12	-3.38	1.31	1.48
7	A	1022[B]	ALB	C8-N12	-3.38	1.31	1.48
7	A	1022[B]	ALB	C37-N11	-3.37	1.33	1.39
7	A	1022[A]	ALB	O15-C32	3.29	1.28	1.22
7	A	1022[B]	ALB	C33-N9	-3.28	1.30	1.38
7	A	1022[B]	ALB	C32-N8	-3.21	1.32	1.39
7	A	1022[A]	ALB	C29-C28	3.01	1.61	1.53
7	A	1022[A]	ALB	C37-N11	-2.85	1.33	1.39
3	A	1002	FTT	O2-C1	2.73	1.35	1.20
7	A	1022[B]	ALB	C27-C25	2.69	1.63	1.54
7	A	1022[A]	ALB	C27-C25	2.59	1.63	1.54
7	A	1022[A]	ALB	C25-C26	2.53	1.56	1.52
7	A	1022[A]	ALB	O4-C4	2.17	1.27	1.23
7	A	1022[B]	ALB	O4-C4	2.17	1.27	1.23
7	A	1022[A]	ALB	C6-N1	2.03	1.50	1.45
7	A	1022[B]	ALB	C6-N1	2.03	1.50	1.45

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1022[A]	ALB	C30-S-C31	18.92	115.53	94.38
7	A	1022[B]	ALB	C30-S-C31	17.93	114.42	94.38
7	A	1022[B]	ALB	C36-N8-C32	-15.62	90.13	117.33
7	A	1022[A]	ALB	C29-C30-S	-15.49	87.73	106.07
7	A	1022[B]	ALB	C29-C30-S	-12.77	90.94	106.07
3	A	1004	FTT	O2-C1-C2	-11.59	91.64	125.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1022[A]	ALB	O11-C24-N7	-11.31	102.71	122.96
3	A	1002	FTT	O2-C1-C2	-10.96	93.49	125.38
7	A	1022[B]	ALB	O11-C24-N7	-10.16	104.78	122.96
7	A	1022[A]	ALB	C36-N8-C32	-10.13	99.69	117.33
7	A	1022[B]	ALB	O11-C24-C22	-9.80	99.95	120.48
7	A	1022[A]	ALB	C33-N9-C32	-9.14	114.33	121.80
7	A	1022[B]	ALB	C33-C35-C34	8.13	127.99	118.75
7	A	1022[A]	ALB	C33-C35-C34	7.78	127.60	118.75
7	A	1022[A]	ALB	O9-C21-C6	-7.46	104.86	120.48
7	A	1022[B]	ALB	O9-C21-C6	-7.46	104.86	120.48
7	A	1022[A]	ALB	O4-C4-C8	-7.42	104.66	120.28
7	A	1022[B]	ALB	O4-C4-C8	-7.42	104.66	120.28
7	A	1022[A]	ALB	S-C30-N9	-7.14	104.63	112.68
7	A	1022[A]	ALB	C11-C8-C4	6.40	123.84	110.76
7	A	1022[B]	ALB	C11-C8-C4	6.40	123.84	110.76
7	A	1022[A]	ALB	C30-N9-C32	6.28	124.27	117.43
7	A	1022[B]	ALB	O12-C26-O13	-6.23	109.94	124.08
7	A	1022[A]	ALB	O12-C26-O13	-6.22	109.97	124.08
7	A	1022[A]	ALB	O16-C37-N11	-6.01	111.95	125.36
7	A	1022[A]	ALB	O9-C21-N6	-5.33	113.42	122.96
7	A	1022[B]	ALB	O9-C21-N6	-5.33	113.42	122.96
7	A	1022[B]	ALB	C26-C25-N7	-5.03	99.12	110.17
7	A	1022[A]	ALB	C21-C6-N1	4.88	124.30	111.11
7	A	1022[B]	ALB	C21-C6-N1	4.88	124.30	111.11
7	A	1022[B]	ALB	C24-C22-N6	4.84	124.21	111.11
7	A	1022[A]	ALB	C24-C22-N6	-4.61	98.65	111.11
7	A	1022[B]	ALB	C30-N9-C32	4.37	122.19	117.43
7	A	1022[A]	ALB	O2-C2-N1	-4.35	115.18	122.96
7	A	1022[B]	ALB	O2-C2-N1	-4.35	115.18	122.96
7	A	1022[A]	ALB	C35-C34-N11	4.01	132.80	128.32
3	A	1003	FTT	O1-C1-O2	-3.97	113.11	123.33
7	A	1022[A]	ALB	C11-C8-N12	3.67	119.68	110.12
7	A	1022[B]	ALB	C11-C8-N12	3.67	119.68	110.12
7	A	1022[A]	ALB	O17-C29-C30	-3.56	104.55	111.61
7	A	1022[A]	ALB	O15-C32-N8	-3.44	116.58	121.33
7	A	1022[A]	ALB	C29-C28-C31	3.28	109.55	106.34
7	A	1022[B]	ALB	C33-N9-C32	-3.24	119.15	121.80
7	A	1022[A]	ALB	O2-C2-C7	-3.19	113.80	120.48
7	A	1022[B]	ALB	O2-C2-C7	-3.19	113.80	120.48
3	A	1006	FTT	O1-C1-O2	-3.17	115.17	123.33
7	A	1022[A]	ALB	N10-C37-N11	3.08	122.66	112.52
7	A	1022[A]	ALB	C7-N2-C4	3.04	128.18	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1022[B]	ALB	C7-N2-C4	3.04	128.18	121.65
7	A	1022[B]	ALB	O17-C29-C30	-2.74	106.18	111.61
7	A	1022[A]	ALB	O15-C32-N9	-2.68	116.80	122.78
4	A	1013	DPO	O6-P2-O4	2.63	113.41	104.64
7	A	1022[B]	ALB	O16-C37-N11	-2.63	119.50	125.36
7	A	1022[A]	ALB	C10-C7-C2	-2.60	103.75	110.11
7	A	1022[B]	ALB	C10-C7-C2	-2.60	103.75	110.11
7	A	1022[B]	ALB	C29-C28-C31	2.59	108.87	106.34
3	A	1004	FTT	O3-C3-C2	2.48	116.04	109.45
3	A	1004	FTT	C4-C3-C2	-2.39	105.35	113.05
7	A	1022[A]	ALB	C8-C4-N2	2.33	119.37	116.21
7	A	1022[B]	ALB	C8-C4-N2	2.33	119.37	116.21
7	A	1022[B]	ALB	C30-N9-C33	-2.26	118.66	121.18
7	A	1022[A]	ALB	C26-C25-N7	2.24	115.09	110.17
7	A	1022[A]	ALB	O6-N3-C1	-2.07	113.35	116.68
7	A	1022[B]	ALB	O6-N3-C1	-2.07	113.35	116.68
3	A	1003	FTT	C4-C3-C2	-2.04	107.78	111.64

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1006	FTT	C3
7	A	1022[A]	ALB	C22
7	A	1022[A]	ALB	N3
7	A	1022[A]	ALB	N5
7	A	1022[A]	ALB	N4
7	A	1022[A]	ALB	C8
7	A	1022[B]	ALB	C22
7	A	1022[B]	ALB	N3
7	A	1022[B]	ALB	N5
7	A	1022[B]	ALB	C25
7	A	1022[B]	ALB	N4
7	A	1022[B]	ALB	C8
7	A	1022[B]	ALB	C27

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1022[A]	ALB	N2-C4-C8-C11
7	A	1022[A]	ALB	O4-C4-C8-C11
7	A	1022[A]	ALB	C8-C4-N2-C7
7	A	1022[A]	ALB	C14-C11-C8-N12

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Mol	Chain	Res	Type	Atoms
7	A	1022[A]	ALB	C12-C15-N3-C1
7	A	1022[A]	ALB	C12-C15-N3-O6
7	A	1022[A]	ALB	C6-C21-N6-C22
7	A	1022[A]	ALB	C26-C25-C27-C31
7	A	1022[A]	ALB	C26-C25-C27-O14
7	A	1022[A]	ALB	N7-C25-C27-C31
7	A	1022[A]	ALB	N7-C25-C27-O14
7	A	1022[A]	ALB	C25-C27-C31-C28
7	A	1022[A]	ALB	O14-C27-C31-C28
7	A	1022[A]	ALB	O14-C27-C31-S
7	A	1022[A]	ALB	S-C30-N9-C33
7	A	1022[A]	ALB	C35-C34-N11-C37
7	A	1022[A]	ALB	N8-C34-N11-C37
7	A	1022[B]	ALB	N2-C4-C8-C11
7	A	1022[B]	ALB	O4-C4-C8-C11
7	A	1022[B]	ALB	C8-C4-N2-C7
7	A	1022[B]	ALB	C14-C11-C8-N12
7	A	1022[B]	ALB	C12-C15-N3-C1
7	A	1022[B]	ALB	C12-C15-N3-O6
7	A	1022[B]	ALB	C6-C21-N6-C22
7	A	1022[B]	ALB	C22-C24-N7-C25
7	A	1022[B]	ALB	C26-C25-C27-C31
7	A	1022[B]	ALB	C26-C25-C27-O14
7	A	1022[B]	ALB	N7-C25-C27-C31
7	A	1022[B]	ALB	N7-C25-C27-O14
7	A	1022[B]	ALB	C27-C25-N7-C24
7	A	1022[B]	ALB	C25-C27-C31-C28
7	A	1022[B]	ALB	O14-C27-C31-C28
7	A	1022[B]	ALB	S-C30-N9-C32
7	A	1022[B]	ALB	S-C30-N9-C33
7	A	1022[B]	ALB	C35-C34-N11-C37
7	A	1022[B]	ALB	N8-C34-N11-C37
7	A	1022[A]	ALB	C7-C2-N1-C6
7	A	1022[A]	ALB	C22-C24-N7-C25
7	A	1022[B]	ALB	C7-C2-N1-C6
7	A	1022[A]	ALB	N6-C22-C23-O10
7	A	1022[B]	ALB	N6-C22-C23-O10
7	A	1022[A]	ALB	O4-C4-N2-C7
7	A	1022[B]	ALB	O4-C4-N2-C7
7	A	1022[A]	ALB	C23-C22-C24-N7
7	A	1022[A]	ALB	O9-C21-C6-C9
7	A	1022[B]	ALB	O9-C21-C6-C9

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Mol	Chain	Res	Type	Atoms
7	A	1022[A]	ALB	C23-C22-N6-C21
7	A	1022[B]	ALB	C23-C22-N6-C21
7	A	1022[A]	ALB	C27-C25-C26-O13
7	A	1022[A]	ALB	N7-C25-C26-O12
7	A	1022[A]	ALB	O4-C4-C8-N12
7	A	1022[B]	ALB	O4-C4-C8-N12
7	A	1022[A]	ALB	C7-C10-C13-C16
7	A	1022[B]	ALB	C7-C10-C13-C16
7	A	1022[A]	ALB	O9-C21-C6-N1
7	A	1022[B]	ALB	O9-C21-C6-N1
7	A	1022[A]	ALB	O2-C2-C7-N2
7	A	1022[B]	ALB	O2-C2-C7-N2
3	A	1006	FTT	C4-C5-C6-C7
7	A	1022[B]	ALB	C27-C25-C26-O12
7	A	1022[A]	ALB	C24-C22-C23-O10
7	A	1022[A]	ALB	N6-C22-C24-O11
7	A	1022[B]	ALB	N6-C22-C24-N7
7	A	1022[A]	ALB	S-C30-N9-C32
3	A	1007	FTT	C4-C5-C6-C7
3	A	1002	FTT	C3-C4-C5-C6
7	A	1022[A]	ALB	O2-C2-C7-C10
7	A	1022[B]	ALB	O2-C2-C7-C10
7	A	1022[A]	ALB	C24-C22-N6-C21
7	A	1022[A]	ALB	N1-C6-C9-C12
7	A	1022[B]	ALB	N1-C6-C9-C12
7	A	1022[A]	ALB	C27-C25-C26-O12
3	A	1004	FTT	O2-C1-C2-C3
3	A	1003	FTT	C1-C2-C3-C4
7	A	1022[A]	ALB	C23-C22-C24-O11
7	A	1022[A]	ALB	C15-C12-C9-C6
7	A	1022[B]	ALB	C15-C12-C9-C6
3	A	1002	FTT	O2-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 25 short contacts:

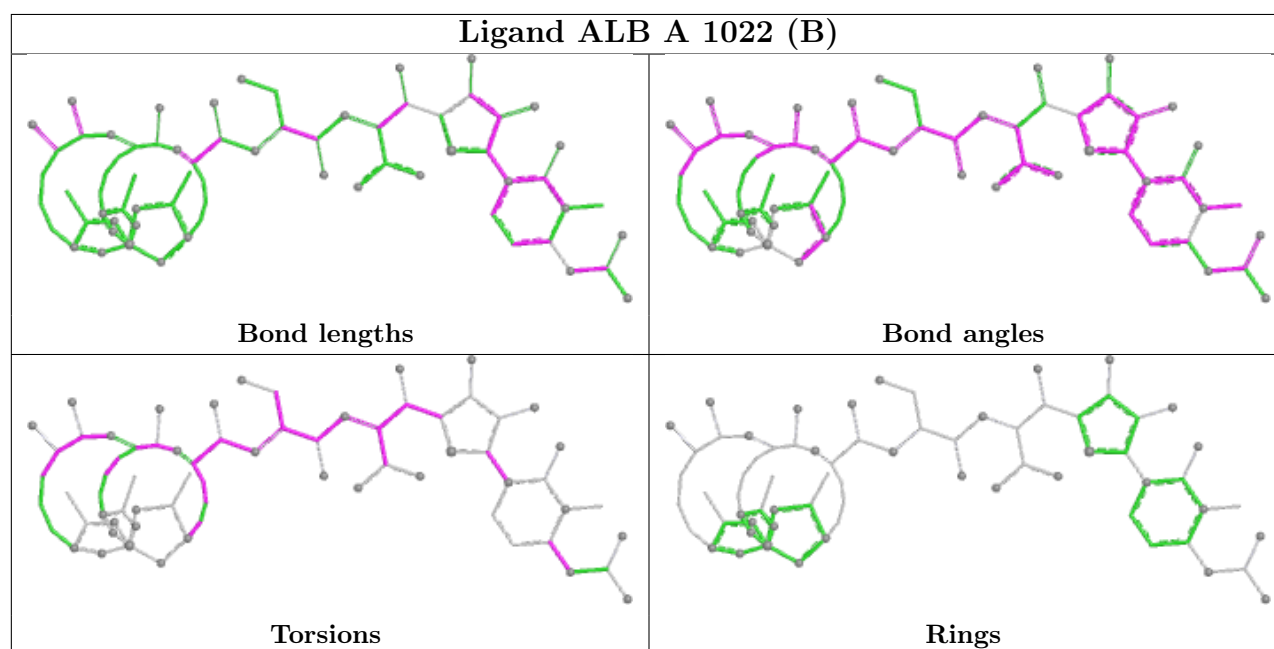
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1022[B]	ALB	8	0
3	A	1007	FTT	2	0
3	A	1005	FTT	1	0
3	A	1006	FTT	6	0
3	A	1004	FTT	4	0

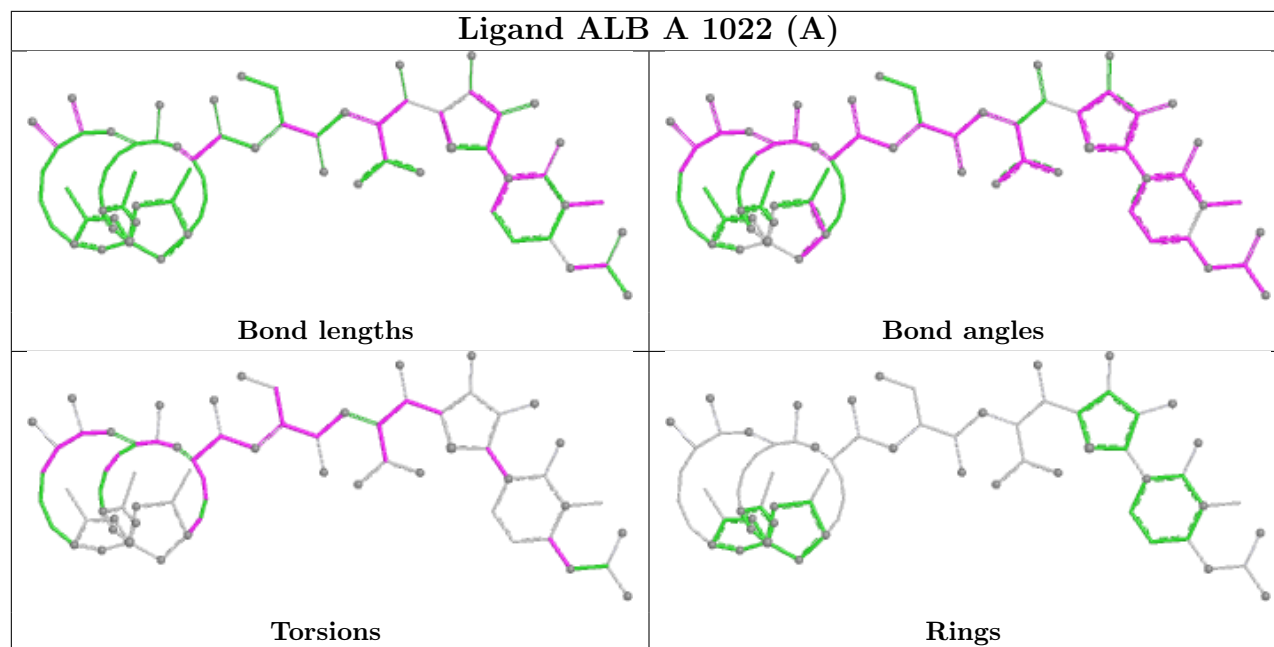
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	FTT	1	0
5	A	1014	PO4	2	0
7	A	1022[A]	ALB	6	0
4	A	1015	DPO	1	0

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 than 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.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	707/725 (97%)	-0.21	0 100 100	44, 80, 113, 117	0

There are no RSRZ outliers to report.

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

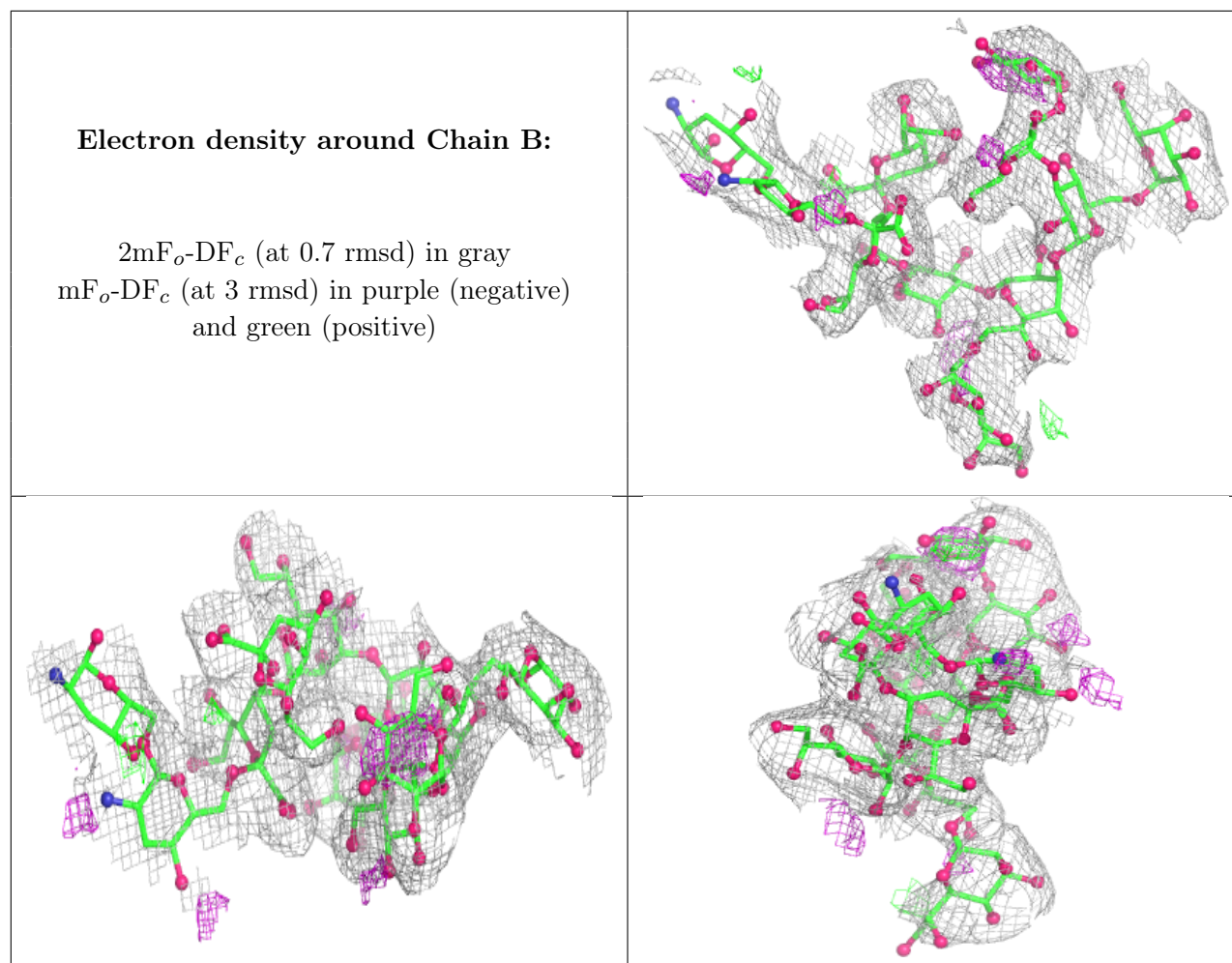
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	B	8	11/12	0.56	0.16	116,116,117,118	0
2	GMH	B	10	13/14	0.75	0.15	115,116,117,118	0
2	GLC	B	7	11/12	0.80	0.10	111,114,116,117	0
2	GLA	B	9	11/12	0.82	0.10	110,112,113,113	0
2	GMH	B	5	13/14	0.88	0.08	89,98,111,116	0
2	GLC	B	6	11/12	0.89	0.08	93,101,110,113	0
2	KDO	B	11	15/16	0.90	0.07	80,84,88,90	0
2	GMH	B	4	13/14	0.94	0.07	72,78,83,87	0
2	PA1	B	1	11/12	0.94	0.06	53,64,78,81	0
2	KDO	B	3	15/16	0.95	0.07	67,74,78,84	0
2	GCN	B	2	10/11	0.97	0.05	46,54,63,71	0

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



6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FTT	A	1003	7/17	0.82	0.15	88,103,108,109	0
3	FTT	A	1002	16/17	0.88	0.17	80,91,96,96	0
5	PO4	A	1016	4/5	0.88	0.09	112,113,114,114	0
5	PO4	A	1014	4/5	0.91	0.11	76,77,78,84	0
4	DPO	A	1015	8/9	0.91	0.09	86,89,93,94	4
3	FTT	A	1006	17/17	0.92	0.14	67,91,100,100	0
3	FTT	A	1005	13/17	0.92	0.16	77,80,89,90	0
3	FTT	A	1007	15/17	0.93	0.16	79,99,107,110	0
3	FTT	A	1004	16/17	0.93	0.13	70,73,77,78	0
4	DPO	A	1013	8/9	0.94	0.08	84,86,90,92	4

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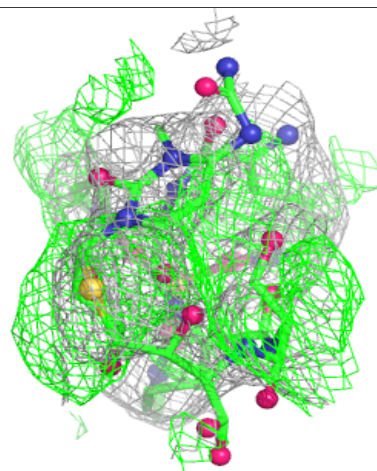
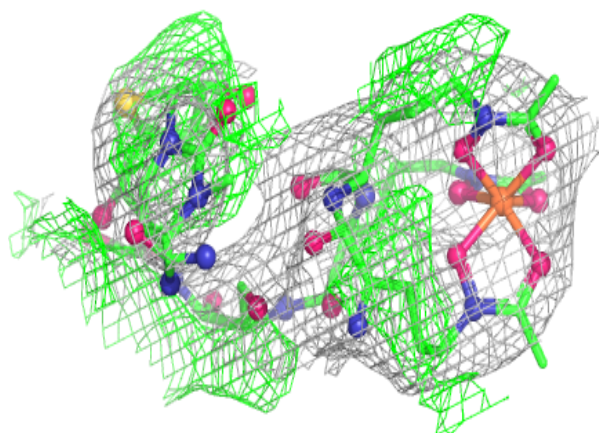
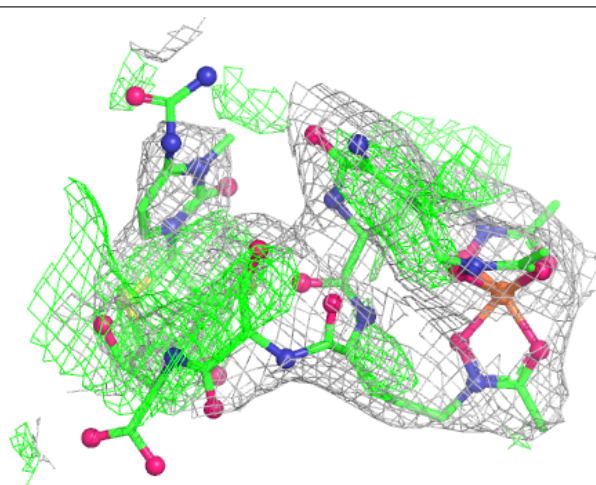
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NI	A	1021	1/1	0.94	0.09	119,119,119,119	0
7	ALB	A	1022[A]	69/69	0.95	0.20	69,88,114,120	28
7	ALB	A	1022[B]	69/69	0.95	0.20	69,87,115,120	28

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.

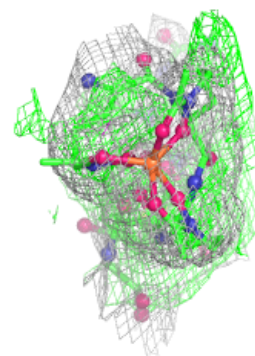
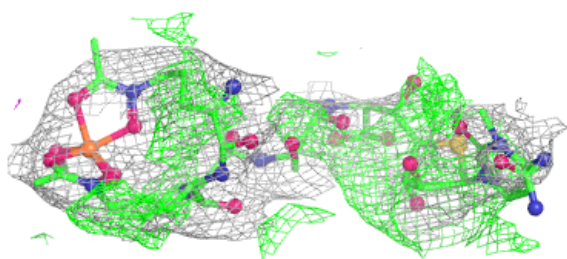
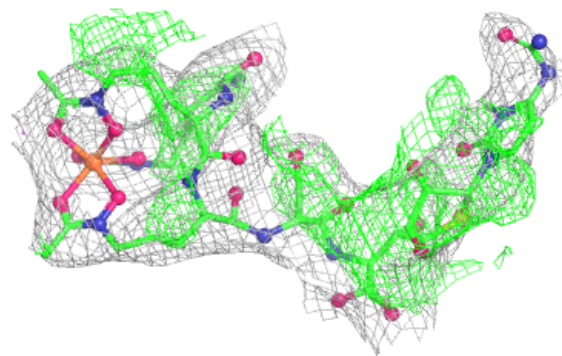
Electron density around ALB A 1022 (A):

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 ALB A 1022 (B):

$2mF_o-DF_c$ (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.