



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:28 AM UTC

PDB ID : 1QFG / pdb_00001qfg
Title : E. COLI FERRIC HYDROXAMATE RECEPTOR (FHUA)
Authors : Ferguson, A.D.; Welte, W.; Hofmann, E.; Lindner, B.; Holst, O.; Coulton, J.W.; Diederichs, K.
Deposited on : 1999-04-10
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

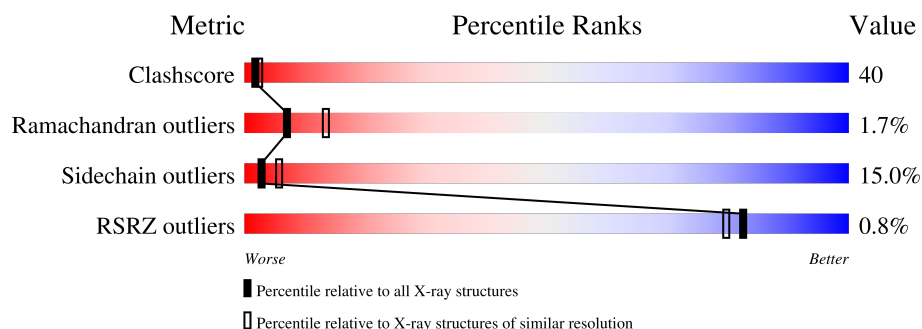
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	% 37% 44% 15% ..
2	B	9	11% 56% 33%

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
10	GOL	A	1103	-	X	-	-
10	GOL	A	1104	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	GOL	A	1105	-	-	X	-
10	GOL	A	1106	-	X	-	-
10	GOL	A	1107	-	X	X	-
10	GOL	A	1108	-	X	-	-
5	FTT	A	1013	-	-	X	-
7	MYR	A	1014	-	-	X	-
9	DPO	A	2000	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 6077 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.

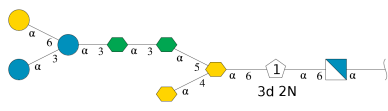
- Molecule 1 is a protein called PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	707	5524	3475	944	1091	14	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-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.

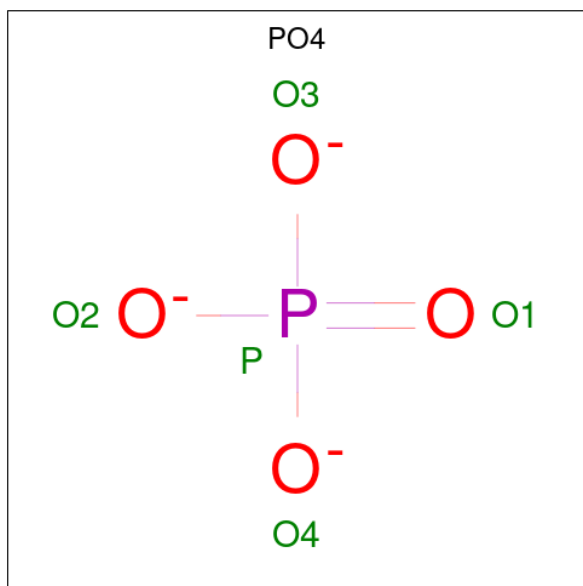


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	9	110	60	2	48	0	0	0

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

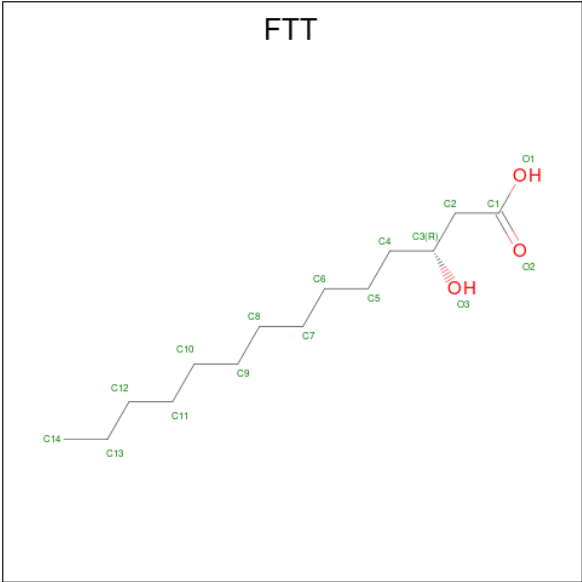
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



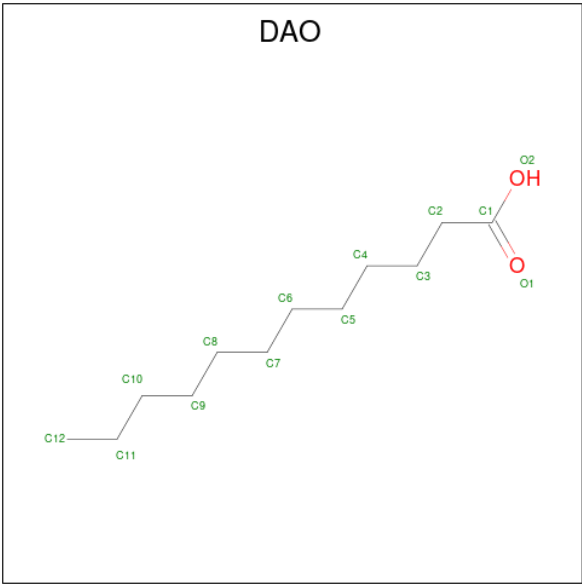
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 4 3 1	0	0
4	A	1	Total O P 4 3 1	0	0

- Molecule 5 is 3-HYDROXY-TETRADECANOIC ACID (CCD ID: FTT) (formula: C₁₄H₂₈O₃).



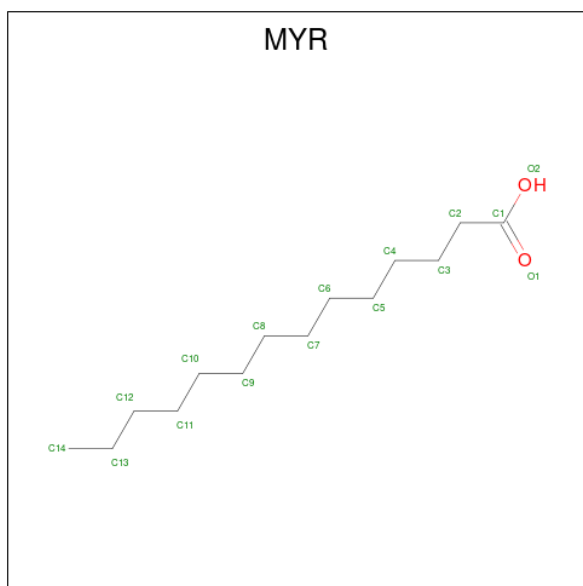
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	14	2		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			16	14	2		
5	A	1	Total	C	O	0	0
			17	14	3		

- Molecule 6 is LAURIC ACID (CCD ID: DAO) (formula: C₁₂H₂₄O₂).



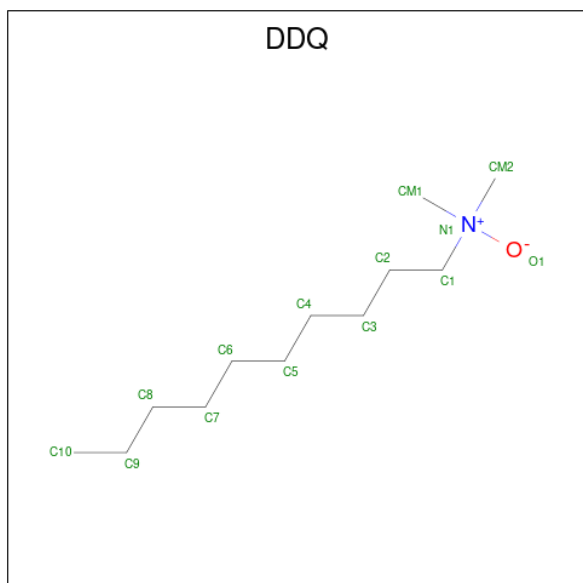
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	12	1		

- Molecule 7 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



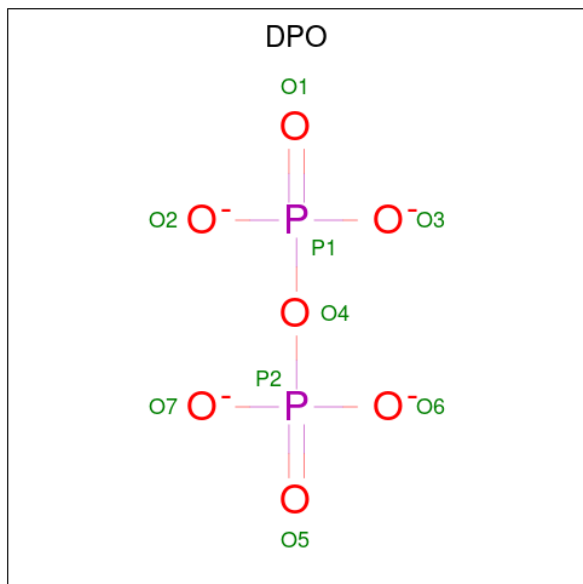
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			15	14	1		

- Molecule 8 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (CCD ID: DDQ) (formula: $C_{12}H_{27}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	12	1	1		
8	A	1	Total	C	N	O	0	0
			14	12	1	1		
8	A	1	Total	C	N	O	0	0
			14	12	1	1		

- Molecule 9 is DIPHOSPHATE (CCD ID: DPO) (formula: O_7P_2).



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

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		

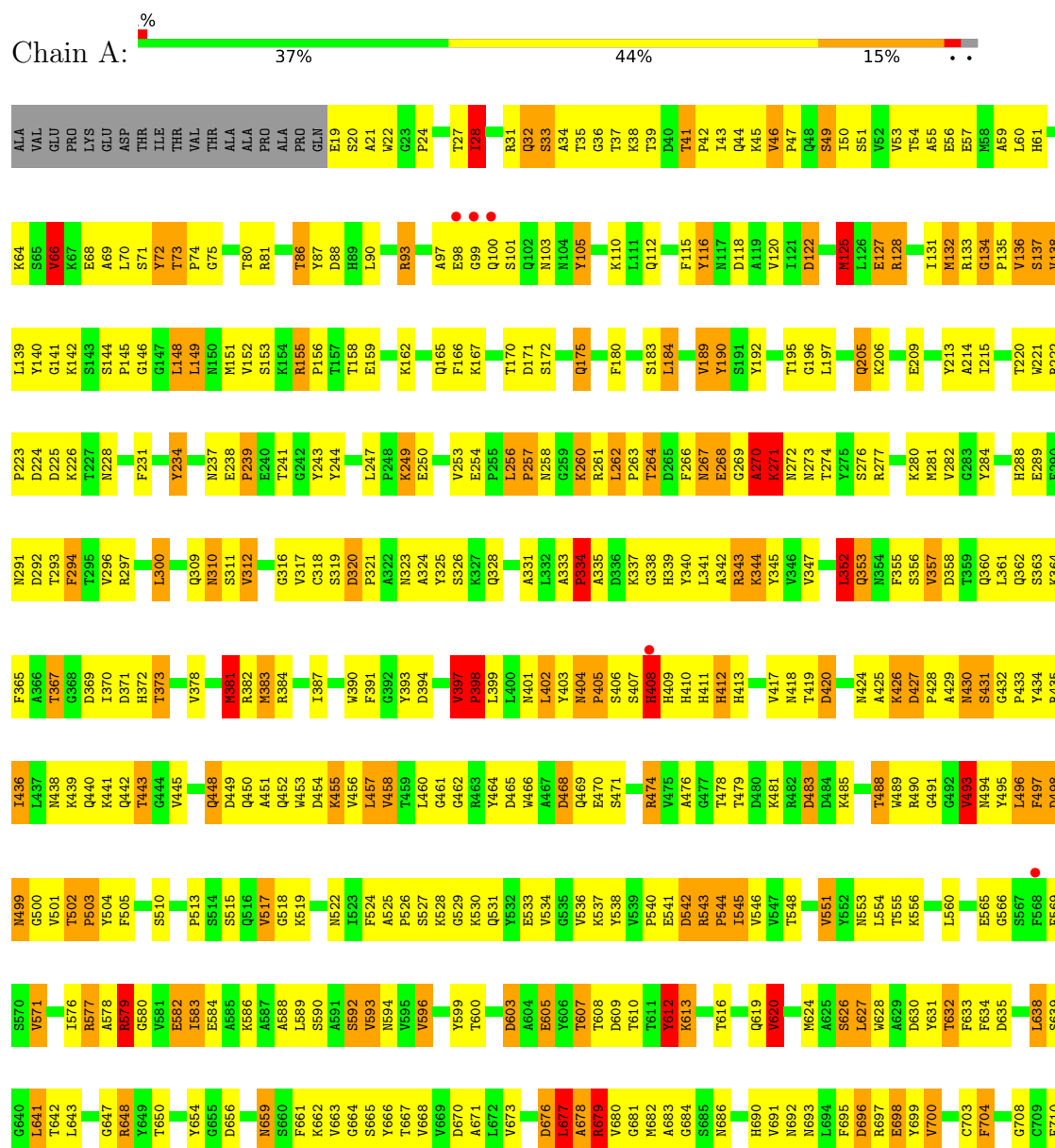
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	244	Total	O	0	0
			244	244		

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: PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR)





- Molecule 2: alpha-D-glucopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-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: 11% 56% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	171.55Å 171.55Å 87.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.30 – 2.50 42.30 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.30-2.50) 99.4 (42.30-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.45Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.271 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6077	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: GLA, PA1, GCN, DAO, FTT, DDQ, GOL, PO4, KDO, DPO, GMH, GLC, NI, MYR

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	1.48	38/5664 (0.7%)	1.68	127/7696 (1.7%)

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	7

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	397	VAL	CA-CB	11.25	1.68	1.54
1	A	488	THR	CA-CB	8.66	1.68	1.53
1	A	125	MET	SD-CE	-7.97	1.59	1.79
1	A	33	SER	C-O	-7.60	1.15	1.23
1	A	189	VAL	CA-CB	7.37	1.63	1.54
1	A	166	PHE	CA-C	-7.30	1.43	1.52
1	A	151	MET	SD-CE	-6.91	1.62	1.79
1	A	53	VAL	CA-C	-6.67	1.44	1.52
1	A	27	THR	CA-CB	6.60	1.64	1.53
1	A	381	MET	SD-CE	-6.41	1.63	1.79
1	A	277	ARG	CZ-NH1	6.41	1.41	1.32
1	A	41	THR	C-O	-6.29	1.15	1.24
1	A	488	THR	C-O	6.00	1.31	1.23
1	A	270	ALA	CA-CB	-5.99	1.43	1.53
1	A	698	GLU	CG-CD	5.96	1.67	1.52
1	A	66	VAL	CB-CG2	-5.93	1.32	1.52
1	A	383	MET	SD-CE	5.92	1.94	1.79
1	A	439	LYS	CA-C	-5.91	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	ASP	C-O	-5.85	1.16	1.24
1	A	387	ILE	CA-CB	5.84	1.61	1.54
1	A	145	PRO	CA-CB	-5.78	1.45	1.53
1	A	263	PRO	CA-C	5.77	1.59	1.52
1	A	471	SER	CA-C	5.67	1.59	1.52
1	A	267	ASN	N-CA	-5.62	1.39	1.46
1	A	718	VAL	CA-CB	5.62	1.63	1.54
1	A	88	ASP	N-CA	-5.47	1.38	1.46
1	A	105	TYR	CA-C	5.45	1.60	1.52
1	A	671	ALA	CA-CB	-5.43	1.44	1.53
1	A	626	SER	C-O	5.41	1.30	1.23
1	A	90	LEU	N-CA	-5.39	1.39	1.46
1	A	237	ASN	CA-C	5.39	1.58	1.52
1	A	152	VAL	CA-CB	5.37	1.61	1.54
1	A	483	ASP	C-O	-5.37	1.17	1.24
1	A	152	VAL	C-O	-5.13	1.18	1.24
1	A	175	GLN	CA-C	-5.07	1.46	1.52
1	A	120	VAL	CA-CB	5.04	1.63	1.54
1	A	149	LEU	CA-C	-5.02	1.46	1.52
1	A	663	VAL	CA-CB	-5.00	1.48	1.54

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	VAL	CA-C-N	17.39	141.58	119.84
1	A	46	VAL	C-N-CA	17.39	141.58	119.84
1	A	238	GLU	CA-C-N	13.12	132.62	118.97
1	A	238	GLU	C-N-CA	13.12	132.62	118.97
1	A	427	ASP	CA-C-N	9.69	129.32	119.82
1	A	427	ASP	C-N-CA	9.69	129.32	119.82
1	A	271	LYS	N-CA-C	-9.65	100.71	114.12
1	A	189	VAL	N-CA-C	-8.71	100.39	112.50
1	A	620	VAL	CA-C-N	8.35	128.28	119.85
1	A	620	VAL	C-N-CA	8.35	128.28	119.85
1	A	664	GLY	N-CA-C	8.32	124.30	112.82
1	A	565	GLU	N-CA-C	8.18	121.81	112.57
1	A	145	PRO	N-CA-C	-8.16	99.18	111.41
1	A	408	HIS	N-CA-C	-8.12	102.40	111.82
1	A	43	ILE	N-CA-C	8.05	123.31	112.04
1	A	566	GLY	N-CA-C	7.92	126.71	115.30
1	A	488	THR	N-CA-C	-7.80	96.43	108.76
1	A	394	ASP	CA-C-N	-7.78	106.67	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ASP	C-N-CA	-7.78	106.67	121.54
1	A	450	GLN	N-CA-C	-7.62	96.09	108.52
1	A	710	PHE	N-CA-C	7.40	120.48	108.34
1	A	226	LYS	N-CA-C	-7.17	102.82	112.94
1	A	73	THR	CA-C-N	-7.17	113.28	120.31
1	A	73	THR	C-N-CA	-7.17	113.28	120.31
1	A	225	ASP	N-CA-C	7.15	120.94	112.93
1	A	21	ALA	N-CA-C	7.06	123.02	111.37
1	A	59	ALA	N-CA-C	-6.94	103.80	111.36
1	A	125	MET	CG-SD-CE	-6.90	85.71	100.90
1	A	605	GLU	N-CA-C	6.89	120.89	108.69
1	A	527	SER	N-CA-C	-6.89	99.47	110.14
1	A	294	PHE	N-CA-C	6.87	120.04	108.02
1	A	352	LEU	N-CA-C	6.83	120.28	109.50
1	A	39	THR	N-CA-C	-6.82	98.73	109.50
1	A	86	THR	N-CA-C	6.81	120.47	111.75
1	A	648	ARG	NE-CZ-NH1	-6.79	114.71	121.50
1	A	525	ALA	CA-C-N	6.72	127.11	119.92
1	A	525	ALA	C-N-CA	6.72	127.11	119.92
1	A	700	VAL	N-CA-C	-6.70	98.09	107.80
1	A	425	ALA	CA-C-N	-6.67	112.90	122.77
1	A	425	ALA	C-N-CA	-6.67	112.90	122.77
1	A	704	PHE	N-CA-C	-6.60	105.26	113.38
1	A	497	PHE	CB-CA-C	-6.50	99.36	110.22
1	A	249	LYS	N-CA-C	-6.45	105.27	113.01
1	A	110	LYS	N-CA-C	6.45	119.63	109.96
1	A	412	HIS	CA-C-N	-6.43	112.44	122.67
1	A	412	HIS	C-N-CA	-6.43	112.44	122.67
1	A	496	LEU	N-CA-C	6.42	119.19	108.20
1	A	479	THR	N-CA-C	6.39	118.88	108.26
1	A	518	GLY	N-CA-C	6.38	122.46	112.31
1	A	145	PRO	O-C-N	-6.37	115.23	123.00
1	A	612	TYR	N-CA-C	6.34	123.21	113.19
1	A	262	LEU	CA-C-N	-6.31	113.45	120.14
1	A	262	LEU	C-N-CA	-6.31	113.45	120.14
1	A	145	PRO	CA-C-N	-6.30	109.06	121.41
1	A	145	PRO	C-N-CA	-6.30	109.06	121.41
1	A	499	ASN	N-CA-C	-6.29	105.46	113.01
1	A	593	VAL	N-CA-C	6.27	116.90	107.75
1	A	254	GLU	CA-C-N	-6.26	114.17	120.31
1	A	254	GLU	C-N-CA	-6.26	114.17	120.31
1	A	394	ASP	N-CA-C	6.14	121.51	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571	VAL	N-CA-C	-6.12	98.95	108.44
1	A	71	SER	N-CA-C	6.09	120.26	112.34
1	A	579	ARG	N-CA-C	-6.09	99.78	109.59
1	A	320	ASP	CA-C-N	6.08	127.43	119.84
1	A	320	ASP	C-N-CA	6.08	127.43	119.84
1	A	97	ALA	N-CA-C	6.07	118.53	110.53
1	A	239	PRO	N-CA-C	-6.04	104.84	113.47
1	A	515	SER	N-CA-C	-6.00	105.69	114.39
1	A	127	GLU	N-CA-C	-5.97	106.13	113.41
1	A	137	SER	N-CA-C	-5.97	104.90	111.82
1	A	465	ASP	N-CA-C	5.96	119.12	109.40
1	A	590	SER	N-CA-C	-5.96	98.59	108.07
1	A	256	LEU	CA-C-N	-5.96	112.53	119.32
1	A	256	LEU	C-N-CA	-5.96	112.53	119.32
1	A	300	LEU	N-CA-C	5.92	118.41	109.23
1	A	443	THR	N-CA-C	-5.92	98.76	108.76
1	A	691	VAL	CB-CA-C	-5.89	102.47	110.42
1	A	503	PRO	N-CA-C	-5.86	101.22	112.01
1	A	391	PHE	N-CA-C	5.85	118.43	108.90
1	A	74	PRO	N-CA-C	5.84	120.44	111.57
1	A	28	ILE	N-CA-C	5.79	116.57	110.72
1	A	352	LEU	CA-CB-CG	5.78	136.52	116.30
1	A	310	ASN	N-CA-C	-5.61	98.04	108.02
1	A	122	ASP	CA-C-N	-5.59	113.86	119.56
1	A	122	ASP	C-N-CA	-5.59	113.86	119.56
1	A	253	VAL	CB-CA-C	-5.52	104.68	112.14
1	A	582	GLU	CA-C-N	-5.49	115.31	122.94
1	A	582	GLU	C-N-CA	-5.49	115.31	122.94
1	A	373	THR	N-CA-C	-5.47	98.45	108.02
1	A	577	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	A	344	LYS	CA-C-N	-5.44	112.50	121.80
1	A	344	LYS	C-N-CA	-5.44	112.50	121.80
1	A	66	VAL	CB-CA-C	-5.44	103.73	112.16
1	A	458	VAL	CA-C-N	-5.43	115.50	123.00
1	A	458	VAL	C-N-CA	-5.43	115.50	123.00
1	A	616	THR	CA-C-N	-5.43	114.37	119.85
1	A	616	THR	C-N-CA	-5.43	114.37	119.85
1	A	64	LYS	N-CA-C	-5.41	105.38	111.28
1	A	342	ALA	N-CA-C	-5.41	101.66	110.20
1	A	261	ARG	N-CA-C	5.38	117.86	109.52
1	A	270	ALA	CA-C-N	-5.33	113.86	122.23
1	A	270	ALA	C-N-CA	-5.33	113.86	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ASN	N-CA-C	-5.31	102.00	109.96
1	A	659	ASN	N-CA-C	-5.31	104.57	111.74
1	A	347	VAL	N-CA-C	-5.26	100.55	108.12
1	A	593	VAL	CB-CA-C	-5.21	103.37	110.77
1	A	292	ASP	N-CA-C	5.21	119.39	113.19
1	A	325	TYR	N-CA-C	5.18	119.24	113.02
1	A	296	VAL	CA-C-N	-5.18	114.34	122.73
1	A	296	VAL	C-N-CA	-5.18	114.34	122.73
1	A	260	LYS	N-CA-C	5.17	118.38	110.36
1	A	358	ASP	N-CA-C	-5.17	100.02	108.76
1	A	103	ASN	N-CA-C	-5.15	101.27	108.54
1	A	190	TYR	N-CA-C	5.12	116.74	108.34
1	A	44	GLN	N-CA-C	-5.12	106.54	112.89
1	A	311	SER	N-CA-C	5.10	117.71	108.69
1	A	638	LEU	N-CA-C	-5.10	103.96	111.81
1	A	723	PHE	N-CA-C	5.08	117.25	109.07
1	A	471	SER	N-CA-C	5.08	116.69	108.41
1	A	555	THR	N-CA-C	5.07	117.32	108.76
1	A	419	THR	CA-C-O	-5.06	115.71	121.68
1	A	493	VAL	CB-CA-C	-5.05	102.72	110.50
1	A	61	HIS	N-CA-C	5.04	117.67	111.82
1	A	37	THR	CB-CA-C	-5.03	101.70	109.80
1	A	134	GLY	CA-C-N	5.03	124.93	119.85
1	A	134	GLY	C-N-CA	5.03	124.93	119.85
1	A	155	ARG	CA-CB-CG	5.00	124.10	114.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	TYR	Sidechain
1	A	213	TYR	Sidechain
1	A	234	TYR	Sidechain
1	A	599	TYR	Sidechain
1	A	612	TYR	Sidechain
1	A	699	TYR	Sidechain
1	A	72	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	5524	0	5223	424	0
2	B	110	0	84	3	0
3	A	1	0	0	0	0
4	A	8	0	0	0	0
5	A	56	0	83	18	0
6	A	13	0	23	3	0
7	A	15	0	27	9	0
8	A	42	0	81	5	0
9	A	16	0	0	5	0
10	A	48	0	39	18	0
11	A	244	0	0	40	0
All	All	6077	0	5560	457	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 40.

All (457) 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)
10:A:1109:GOL:O1	10:A:1109:GOL:C1	1.64	1.44
10:A:1103:GOL:C1	10:A:1103:GOL:O1	1.65	1.44
10:A:1105:GOL:C1	10:A:1105:GOL:O1	1.66	1.43
10:A:1104:GOL:O1	10:A:1104:GOL:C1	1.65	1.42
10:A:1107:GOL:O1	10:A:1107:GOL:C1	1.65	1.41
10:A:1110:GOL:O1	10:A:1110:GOL:C1	1.68	1.40
1:A:648:ARG:HD2	11:A:2145:HOH:O	1.51	1.09
1:A:643:LEU:HD23	1:A:673:VAL:HG12	1.41	1.03
1:A:586:LYS:HG2	1:A:596:VAL:CG2	1.88	1.03
1:A:628:TRP:CH2	1:A:630:ASP:HB3	1.94	1.02
1:A:367:THR:HG22	1:A:370:ILE:HB	1.41	1.02
1:A:328:GLN:HB3	1:A:399:LEU:HD11	1.41	1.01
1:A:715:ARG:HH11	1:A:715:ARG:HG2	1.29	0.96
1:A:70:LEU:HD13	1:A:131:ILE:HD11	1.48	0.96
1:A:19:GLU:HG2	1:A:634:PHE:CZ	2.01	0.95
1:A:370:ILE:HG22	1:A:372:HIS:NE2	1.84	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:THR:OG1	1:A:57:GLU:HG3	1.68	0.92
1:A:722:THR:HG21	11:A:2114:HOH:O	1.68	0.92
1:A:274:THR:HG22	1:A:310:ASN:HB2	1.52	0.92
1:A:430:ASN:C	1:A:430:ASN:HD22	1.78	0.90
1:A:586:LYS:HG2	1:A:596:VAL:HG22	1.54	0.89
1:A:260:LYS:HB2	1:A:406:SER:OG	1.73	0.88
1:A:32:GLN:O	1:A:128:ARG:NH2	2.07	0.87
1:A:390:TRP:NE1	1:A:431:SER:OG	2.06	0.87
1:A:353:GLN:HG3	11:A:2030:HOH:O	1.75	0.87
1:A:93:ARG:HD2	1:A:582:GLU:OE2	1.75	0.86
1:A:300:LEU:HD12	1:A:357:VAL:HG13	1.56	0.85
1:A:42:PRO:HG3	10:A:1105:GOL:H12	1.58	0.84
1:A:241:THR:HG22	11:A:2016:HOH:O	1.78	0.84
1:A:500:GLY:O	1:A:538:TYR:HD1	1.59	0.83
1:A:381:MET:HE2	1:A:382:ARG:N	1.94	0.82
1:A:589:LEU:HB2	1:A:593:VAL:HG12	1.62	0.81
1:A:381:MET:HG2	11:A:2097:HOH:O	1.79	0.80
1:A:538:TYR:CE2	1:A:545:ILE:HD11	2.16	0.80
1:A:162:LYS:HA	1:A:180:PHE:HD1	1.45	0.80
5:A:1013:FTT:H122	7:A:1014:MYR:H92	1.63	0.80
1:A:540:PRO:HG3	1:A:545:ILE:CD1	2.11	0.79
1:A:370:ILE:HG12	1:A:453:TRP:HB2	1.65	0.78
1:A:577:ARG:HD2	1:A:579:ARG:HG2	1.64	0.78
1:A:678:ALA:HA	1:A:683:ALA:HA	1.65	0.77
1:A:132:MET:HG2	1:A:136:VAL:HG11	1.66	0.77
1:A:494:ASN:ND2	1:A:504:TYR:HB3	1.99	0.77
1:A:99:GLY:O	1:A:100:GLN:HB2	1.84	0.77
1:A:522:ASN:ND2	11:A:2085:HOH:O	2.18	0.76
1:A:540:PRO:HG3	1:A:545:ILE:HD11	1.68	0.76
1:A:86:THR:HG23	1:A:241:THR:HG21	1.68	0.76
1:A:365:PHE:HE1	1:A:372:HIS:HD1	1.34	0.75
1:A:390:TRP:CZ3	1:A:433:PRO:HG3	2.21	0.75
1:A:282:VAL:HG21	5:A:1013:FTT:H81	1.67	0.75
1:A:352:LEU:HB2	1:A:384:ARG:O	1.85	0.75
1:A:435:ARG:NH1	1:A:474:ARG:HD3	2.02	0.75
1:A:488:THR:HG23	11:A:2124:HOH:O	1.86	0.74
5:A:1013:FTT:H41	7:A:1014:MYR:H22	1.69	0.74
1:A:70:LEU:HD22	1:A:131:ILE:HG13	1.70	0.74
1:A:162:LYS:HA	1:A:180:PHE:CD1	2.22	0.73
1:A:390:TRP:CZ2	1:A:426:LYS:HB2	2.24	0.73
1:A:540:PRO:CG	1:A:545:ILE:HG12	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ASN:OD1	1:A:403:TYR:HB2	1.89	0.73
1:A:271:LYS:HG2	1:A:420:ASP:OD1	1.87	0.72
1:A:457:LEU:HD12	1:A:458:VAL:N	2.05	0.72
1:A:594:ASN:HB2	1:A:630:ASP:OD1	1.89	0.72
1:A:269:GLY:HA2	1:A:312:VAL:HG12	1.69	0.72
1:A:613:LYS:HD2	11:A:2066:HOH:O	1.89	0.72
1:A:51:SER:OG	1:A:133:ARG:NH2	2.23	0.72
1:A:451:ALA:HB3	1:A:458:VAL:HG12	1.71	0.72
1:A:497:PHE:HB3	1:A:499:ASN:OD1	1.90	0.72
5:A:1009:FTT:H101	6:A:1012:DAO:H62	1.72	0.72
1:A:586:LYS:HG2	1:A:596:VAL:HG23	1.72	0.71
1:A:676:ASP:O	1:A:678:ALA:N	2.25	0.70
1:A:367:THR:O	1:A:367:THR:CG2	2.40	0.70
1:A:474:ARG:HH11	1:A:474:ARG:HG2	1.55	0.70
5:A:1013:FTT:C4	7:A:1014:MYR:H22	2.22	0.69
1:A:650:THR:HB	1:A:666:TYR:CE1	2.27	0.69
1:A:159:GLU:OE1	1:A:159:GLU:N	2.18	0.69
1:A:633:PHE:HB3	1:A:638:LEU:O	1.92	0.69
1:A:28:ILE:HA	1:A:31:ARG:HG3	1.73	0.69
1:A:222:ARG:HH11	1:A:222:ARG:HG3	1.58	0.69
1:A:540:PRO:HG3	1:A:545:ILE:HG12	1.75	0.68
1:A:628:TRP:CZ2	11:A:2012:HOH:O	2.46	0.68
1:A:435:ARG:HH12	1:A:474:ARG:HD3	1.58	0.68
1:A:19:GLU:HG2	1:A:634:PHE:CE2	2.28	0.68
5:A:1013:FTT:H143	7:A:1014:MYR:H112	1.76	0.68
1:A:316:GLY:O	1:A:341:LEU:HD12	1.94	0.68
1:A:343:ARG:O	1:A:397:VAL:HG13	1.93	0.68
1:A:384:ARG:HG2	11:A:2234:HOH:O	1.93	0.68
1:A:370:ILE:CG2	1:A:372:HIS:NE2	2.58	0.67
1:A:148:LEU:C	1:A:148:LEU:HD23	2.20	0.67
1:A:189:VAL:HG23	1:A:223:PRO:HA	1.76	0.67
1:A:60:LEU:HD21	1:A:628:TRP:HH2	1.57	0.67
1:A:38:LYS:HG3	1:A:139:LEU:HD22	1.76	0.67
1:A:540:PRO:HG3	1:A:545:ILE:CG1	2.24	0.67
1:A:353:GLN:CG	11:A:2030:HOH:O	2.38	0.67
1:A:496:LEU:HD13	1:A:502:THR:HG23	1.76	0.67
1:A:381:MET:HE2	1:A:382:ARG:CA	2.26	0.66
1:A:367:THR:HG22	1:A:367:THR:O	1.94	0.66
1:A:496:LEU:HD13	1:A:502:THR:CG2	2.25	0.66
1:A:633:PHE:HD2	1:A:641:LEU:HD23	1.59	0.66
1:A:24:PRO:O	1:A:28:ILE:HG12	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLY:N	11:A:2164:HOH:O	2.04	0.66
9:A:2004:DPO:O3	11:A:2022:HOH:O	2.14	0.66
1:A:205:GLN:HG3	1:A:243:TYR:HB2	1.78	0.66
1:A:205:GLN:HG3	1:A:243:TYR:CB	2.26	0.66
1:A:99:GLY:O	1:A:100:GLN:CB	2.43	0.65
1:A:222:ARG:HG3	1:A:222:ARG:NH1	2.09	0.65
1:A:686:ASN:ND2	11:A:2010:HOH:O	2.28	0.65
1:A:715:ARG:HG2	1:A:715:ARG:NH1	2.04	0.64
1:A:46:VAL:O	1:A:537:LYS:NZ	2.29	0.64
1:A:370:ILE:HG22	1:A:372:HIS:CD2	2.33	0.64
1:A:500:GLY:O	1:A:538:TYR:CD1	2.46	0.64
1:A:264:THR:HA	1:A:711:TRP:CD1	2.32	0.64
1:A:378:VAL:HG12	1:A:445:VAL:HG12	1.79	0.63
1:A:28:ILE:O	1:A:31:ARG:HG3	1.98	0.63
1:A:643:LEU:CD2	1:A:673:VAL:HG12	2.21	0.63
1:A:189:VAL:HG23	1:A:222:ARG:O	1.98	0.63
1:A:192:TYR:CD1	1:A:192:TYR:C	2.77	0.62
1:A:205:GLN:HG3	1:A:243:TYR:CG	2.34	0.62
1:A:60:LEU:HD21	1:A:628:TRP:CH2	2.34	0.62
1:A:430:ASN:C	1:A:430:ASN:ND2	2.51	0.62
1:A:132:MET:CG	1:A:136:VAL:HG11	2.30	0.62
1:A:648:ARG:HG3	1:A:648:ARG:HH11	1.65	0.62
1:A:328:GLN:CB	1:A:399:LEU:HD11	2.23	0.61
1:A:628:TRP:NE1	11:A:2012:HOH:O	2.32	0.61
1:A:632:THR:HG23	1:A:642:THR:OG1	2.01	0.61
1:A:241:THR:CG2	11:A:2016:HOH:O	2.44	0.61
10:A:1103:GOL:C1	10:A:1103:GOL:HO1	2.08	0.61
1:A:142:LYS:HG2	1:A:442:GLN:OE1	2.00	0.61
1:A:294:PHE:HE1	1:A:363:SER:HG	1.49	0.61
10:A:1109:GOL:C1	10:A:1109:GOL:HO1	2.08	0.60
1:A:155:ARG:HH11	1:A:155:ARG:HG3	1.65	0.60
1:A:541:GLU:CD	1:A:541:GLU:O	2.44	0.60
1:A:679:ARG:NH1	1:A:679:ARG:HB3	2.16	0.60
1:A:125:MET:HE2	1:A:234:TYR:HE1	1.65	0.60
1:A:171:ASP:O	1:A:172:SER:HB2	2.02	0.60
1:A:189:VAL:CG2	1:A:223:PRO:HA	2.32	0.60
10:A:1107:GOL:C1	10:A:1107:GOL:HO1	2.09	0.60
1:A:256:LEU:HD11	1:A:402:LEU:HB3	1.82	0.60
1:A:579:ARG:NH1	1:A:603:ASP:OD2	2.34	0.59
1:A:165:GLN:HG3	1:A:722:THR:HB	1.84	0.59
1:A:589:LEU:HB2	1:A:593:VAL:CG1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:TYR:HE2	1:A:633:PHE:CE1	2.20	0.59
1:A:33:SER:OG	1:A:34:ALA:N	2.35	0.59
1:A:293:THR:O	1:A:363:SER:HA	2.02	0.59
1:A:317:VAL:HA	1:A:340:TYR:O	2.03	0.59
1:A:22:TRP:HD1	11:A:2102:HOH:O	1.86	0.58
1:A:607:THR:HG22	1:A:608:THR:N	2.18	0.58
1:A:612:TYR:O	1:A:613:LYS:C	2.45	0.58
1:A:93:ARG:HH11	1:A:582:GLU:CD	2.11	0.58
1:A:441:LYS:HZ1	9:A:2000:DPO:P2	2.27	0.58
1:A:538:TYR:CZ	1:A:545:ILE:HD11	2.39	0.58
1:A:579:ARG:HG3	1:A:603:ASP:OD2	2.04	0.58
1:A:73:THR:HG22	11:A:2024:HOH:O	2.02	0.58
1:A:260:LYS:NZ	11:A:2165:HOH:O	2.35	0.58
1:A:442:GLN:HA	1:A:466:TRP:O	2.04	0.58
1:A:722:THR:CG2	11:A:2010:HOH:O	2.51	0.57
1:A:679:ARG:CB	1:A:679:ARG:HH11	2.17	0.57
1:A:593:VAL:HG23	1:A:631:TYR:CD1	2.40	0.57
1:A:448:GLN:HG2	1:A:449:ASP:N	2.18	0.57
1:A:167:LYS:HG3	1:A:720:THR:HG23	1.87	0.57
1:A:19:GLU:CG	1:A:634:PHE:CE2	2.88	0.57
1:A:381:MET:HE2	1:A:381:MET:C	2.29	0.57
1:A:650:THR:HB	1:A:666:TYR:CD1	2.38	0.57
1:A:458:VAL:O	1:A:458:VAL:CG1	2.52	0.56
1:A:260:LYS:CB	1:A:406:SER:OG	2.48	0.56
1:A:300:LEU:HB2	1:A:357:VAL:HG13	1.86	0.56
1:A:49:SER:HB2	11:A:2008:HOH:O	2.04	0.56
1:A:654:TYR:CE2	1:A:662:LYS:HD2	2.41	0.56
1:A:430:ASN:ND2	1:A:431:SER:HB3	2.20	0.56
1:A:593:VAL:HG12	1:A:593:VAL:O	2.05	0.56
1:A:441:LYS:NZ	9:A:2000:DPO:O5	2.37	0.56
1:A:628:TRP:HZ2	11:A:2012:HOH:O	1.87	0.56
1:A:38:LYS:HD3	1:A:360:GLN:HE22	1.70	0.55
1:A:153:SER:O	1:A:155:ARG:HD3	2.05	0.55
1:A:355:PHE:CZ	1:A:357:VAL:HG22	2.41	0.55
1:A:503:PRO:HA	1:A:536:VAL:HG12	1.88	0.55
1:A:670:ASP:OD1	1:A:692:ASN:HA	2.07	0.55
10:A:1104:GOL:C1	10:A:1104:GOL:HO1	2.08	0.55
1:A:681:GLY:O	1:A:683:ALA:N	2.40	0.55
1:A:256:LEU:O	1:A:257:PRO:C	2.48	0.55
1:A:531:GLN:HB2	1:A:554:LEU:HD13	1.89	0.54
1:A:548:THR:HG22	1:A:584:GLU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:THR:CB	1:A:666:TYR:CE1	2.89	0.54
1:A:390:TRP:HE1	1:A:431:SER:HG	1.50	0.54
1:A:693:ASN:O	1:A:715:ARG:HB2	2.08	0.54
1:A:41:THR:CG2	1:A:46:VAL:HG23	2.38	0.53
1:A:24:PRO:HG3	1:A:588:ALA:HB2	1.91	0.53
1:A:676:ASP:O	1:A:677:LEU:C	2.51	0.53
1:A:593:VAL:CG2	1:A:631:TYR:HD1	2.22	0.53
1:A:93:ARG:NH2	1:A:533:GLU:OE1	2.22	0.53
1:A:137:SER:OG	1:A:510:SER:HA	2.09	0.53
2:B:3:KDO:H7	2:B:4:GMH:C1	2.38	0.53
1:A:449:ASP:OD2	1:A:451:ALA:HB2	2.08	0.53
1:A:679:ARG:NH1	1:A:679:ARG:CB	2.72	0.53
1:A:247:LEU:HD21	1:A:268:GLU:HG3	1.91	0.53
1:A:495:TYR:O	1:A:503:PRO:HD2	2.07	0.53
1:A:458:VAL:O	1:A:458:VAL:HG13	2.08	0.53
1:A:381:MET:HE2	1:A:382:ARG:C	2.33	0.53
1:A:381:MET:CE	1:A:382:ARG:C	2.82	0.53
1:A:402:LEU:O	1:A:406:SER:HB2	2.09	0.53
1:A:470:GLU:HG3	1:A:481:LYS:HG2	1.91	0.53
1:A:142:LYS:NZ	1:A:440:GLN:OE1	2.43	0.52
1:A:318:CYS:HB2	1:A:337:LYS:O	2.09	0.52
1:A:677:LEU:O	1:A:678:ALA:C	2.53	0.52
1:A:159:GLU:H	1:A:159:GLU:CD	2.12	0.52
1:A:639:SER:HB3	1:A:679:ARG:HE	1.72	0.52
1:A:404:ASN:HB3	1:A:405:PRO:HD3	1.90	0.52
1:A:668:VAL:HG13	1:A:693:ASN:HA	1.90	0.52
1:A:648:ARG:HH11	1:A:648:ARG:CG	2.22	0.52
1:A:288:HIS:C	1:A:288:HIS:CD2	2.88	0.52
1:A:457:LEU:HD12	1:A:457:LEU:C	2.34	0.52
1:A:542:ASP:OD2	1:A:543:ARG:HG3	2.10	0.52
1:A:224:ASP:C	1:A:224:ASP:OD1	2.52	0.51
1:A:390:TRP:CE3	1:A:426:LYS:NZ	2.79	0.51
1:A:35:THR:O	1:A:140:TYR:OH	2.19	0.51
1:A:50:ILE:HB	1:A:132:MET:CE	2.41	0.51
1:A:135:PRO:HA	11:A:2040:HOH:O	2.10	0.51
10:A:1105:GOL:C1	10:A:1105:GOL:HO1	2.09	0.51
10:A:1110:GOL:C1	10:A:1110:GOL:HO1	2.11	0.51
1:A:132:MET:SD	1:A:136:VAL:HG11	2.50	0.51
1:A:367:THR:HG22	1:A:370:ILE:CB	2.30	0.51
1:A:184:LEU:HD23	1:A:184:LEU:N	2.24	0.51
1:A:577:ARG:CG	1:A:578:ALA:N	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:VAL:HG22	1:A:620:VAL:O	2.09	0.51
1:A:80:THR:CG2	1:A:619:GLN:NE2	2.74	0.51
1:A:586:LYS:HE3	11:A:2069:HOH:O	2.10	0.51
1:A:137:SER:O	1:A:138:VAL:C	2.51	0.51
1:A:284:TYR:CE2	1:A:300:LEU:HD22	2.45	0.51
1:A:148:LEU:HD23	1:A:149:LEU:N	2.26	0.51
1:A:538:TYR:CE2	1:A:545:ILE:CD1	2.89	0.51
1:A:125:MET:HE2	1:A:234:TYR:CE1	2.45	0.50
5:A:1013:FTT:H91	7:A:1014:MYR:H81	1.93	0.50
1:A:722:THR:HG23	11:A:2010:HOH:O	2.12	0.50
1:A:115:PHE:H	10:A:1110:GOL:C3	2.25	0.50
1:A:135:PRO:HB3	1:A:510:SER:HB3	1.94	0.50
1:A:258:ASN:C	1:A:258:ASN:OD1	2.54	0.50
1:A:381:MET:HE1	1:A:383:MET:HB2	1.93	0.50
1:A:469:GLN:HG2	11:A:2051:HOH:O	2.12	0.50
1:A:628:TRP:CE2	11:A:2012:HOH:O	2.62	0.50
1:A:367:THR:HB	1:A:372:HIS:CE1	2.47	0.50
1:A:684:GLY:O	1:A:724:ARG:HG3	2.11	0.50
1:A:320:ASP:OD1	1:A:321:PRO:HD2	2.11	0.50
9:A:2000:DPO:O6	2:B:1:PA1:O1	2.29	0.50
1:A:73:THR:CG2	11:A:2024:HOH:O	2.60	0.50
1:A:50:ILE:HD12	1:A:132:MET:HE3	1.94	0.49
1:A:68:GLU:OE1	1:A:68:GLU:N	2.35	0.49
1:A:133:ARG:NH1	11:A:2056:HOH:O	2.45	0.49
1:A:228:ASN:OD1	1:A:228:ASN:C	2.55	0.49
1:A:519:LYS:HG3	1:A:569:PHE:CD2	2.47	0.49
1:A:648:ARG:HG3	1:A:648:ARG:NH1	2.27	0.49
1:A:22:TRP:CD1	11:A:2102:HOH:O	2.64	0.49
1:A:260:LYS:HB2	1:A:406:SER:HG	1.73	0.49
1:A:435:ARG:HH12	1:A:474:ARG:HB3	1.78	0.49
1:A:365:PHE:CE1	1:A:372:HIS:ND1	2.77	0.49
1:A:577:ARG:HG2	1:A:578:ALA:N	2.21	0.49
1:A:633:PHE:CB	1:A:638:LEU:O	2.58	0.49
5:A:1009:FTT:C10	6:A:1012:DAO:H62	2.41	0.49
1:A:93:ARG:NH1	1:A:582:GLU:OE1	2.46	0.49
1:A:148:LEU:C	1:A:148:LEU:CD2	2.86	0.49
1:A:50:ILE:HD12	1:A:132:MET:CE	2.43	0.49
1:A:31:ARG:NH2	1:A:540:PRO:O	2.45	0.49
1:A:45:LYS:HD3	1:A:457:LEU:CD2	2.43	0.49
1:A:86:THR:HG22	1:A:87:TYR:CE2	2.48	0.49
1:A:60:LEU:O	1:A:690:HIS:HE1	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:HIS:CD2	1:A:413:HIS:NE2	2.81	0.49
1:A:28:ILE:HG22	1:A:31:ARG:NH1	2.28	0.48
1:A:138:VAL:HG23	1:A:489:TRP:HA	1.94	0.48
1:A:264:THR:CG2	1:A:698:GLU:HG2	2.43	0.48
1:A:365:PHE:HE1	1:A:372:HIS:ND1	2.06	0.48
1:A:493:VAL:HG23	1:A:505:PHE:CZ	2.48	0.48
1:A:704:PHE:CE2	1:A:708:GLY:HA3	2.48	0.48
1:A:427:ASP:CG	1:A:429:ALA:HB3	2.38	0.48
1:A:505:PHE:CD1	1:A:505:PHE:C	2.90	0.48
1:A:538:TYR:CD1	1:A:540:PRO:HD3	2.48	0.48
1:A:344:LYS:O	1:A:345:TYR:HB3	2.13	0.48
1:A:697:ARG:NH2	11:A:2070:HOH:O	2.46	0.48
1:A:70:LEU:HD22	1:A:131:ILE:CG1	2.43	0.48
1:A:297:ARG:NH2	1:A:362:GLN:OE1	2.41	0.48
1:A:650:THR:HG1	1:A:666:TYR:HE1	1.57	0.48
9:A:2000:DPO:O6	2:B:1:PA1:N2	2.43	0.48
1:A:205:GLN:H	1:A:205:GLN:HG2	1.31	0.48
1:A:541:GLU:O	1:A:541:GLU:OE2	2.31	0.48
1:A:679:ARG:HH11	1:A:679:ARG:HB2	1.79	0.48
1:A:424:ASN:O	1:A:426:LYS:HG2	2.14	0.48
1:A:141:GLY:O	1:A:142:LYS:C	2.57	0.48
1:A:220:THR:HG22	1:A:221:TRP:N	2.26	0.48
1:A:409:HIS:O	1:A:413:HIS:N	2.36	0.48
1:A:412:HIS:CD2	1:A:413:HIS:CD2	3.02	0.48
1:A:494:ASN:ND2	1:A:504:TYR:CB	2.73	0.47
1:A:72:TYR:CE2	1:A:628:TRP:HB2	2.50	0.47
1:A:596:VAL:HG12	1:A:628:TRP:HB3	1.96	0.47
1:A:627:LEU:HG	1:A:628:TRP:N	2.29	0.47
1:A:215:ILE:HG23	1:A:215:ILE:O	2.14	0.47
1:A:548:THR:HG23	11:A:2111:HOH:O	2.15	0.47
1:A:343:ARG:C	1:A:397:VAL:HG13	2.40	0.47
1:A:19:GLU:CG	1:A:634:PHE:CZ	2.86	0.47
1:A:271:LYS:HB2	1:A:417:VAL:CG2	2.45	0.47
1:A:345:TYR:CD1	1:A:345:TYR:C	2.92	0.47
1:A:288:HIS:HD2	1:A:289:GLU:N	2.12	0.47
1:A:544:PRO:HG2	1:A:588:ALA:HB3	1.97	0.47
1:A:42:PRO:CG	10:A:1105:GOL:H12	2.38	0.47
1:A:300:LEU:HD12	1:A:357:VAL:CG1	2.37	0.47
1:A:397:VAL:O	1:A:398:PRO:O	2.33	0.47
1:A:46:VAL:HA	1:A:47:PRO:HD2	1.27	0.46
1:A:183:SER:C	1:A:184:LEU:HD23	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ARG:NH1	1:A:474:ARG:CB	2.77	0.46
1:A:134:GLY:C	11:A:2164:HOH:O	2.58	0.46
1:A:267:ASN:O	1:A:418:ASN:ND2	2.49	0.46
1:A:427:ASP:HA	1:A:428:PRO:HD3	1.61	0.46
1:A:631:TYR:HE2	1:A:633:PHE:CD1	2.33	0.46
1:A:220:THR:CG2	1:A:221:TRP:N	2.77	0.46
1:A:36:GLY:HA2	1:A:132:MET:SD	2.56	0.46
1:A:189:VAL:HG23	1:A:223:PRO:CA	2.46	0.45
1:A:435:ARG:C	1:A:436:ILE:HG12	2.40	0.45
1:A:528:LYS:O	1:A:556:LYS:HA	2.15	0.45
1:A:538:TYR:CE1	1:A:540:PRO:HD3	2.51	0.45
1:A:650:THR:O	1:A:665:SER:HA	2.16	0.45
1:A:41:THR:HG21	1:A:46:VAL:HG23	1.98	0.45
1:A:328:GLN:HE21	1:A:328:GLN:HB2	1.59	0.45
1:A:628:TRP:CZ3	1:A:630:ASP:HB3	2.48	0.45
1:A:677:LEU:HD12	1:A:677:LEU:HA	1.58	0.45
1:A:586:LYS:CG	1:A:596:VAL:HG23	2.42	0.45
1:A:633:PHE:O	1:A:639:SER:HA	2.16	0.45
1:A:294:PHE:HE1	1:A:363:SER:OG	1.98	0.45
1:A:390:TRP:CH2	1:A:433:PRO:HG3	2.52	0.45
1:A:648:ARG:CG	1:A:648:ARG:NH1	2.78	0.45
1:A:239:PRO:O	1:A:276:SER:HB3	2.17	0.45
5:A:1013:FTT:C5	7:A:1014:MYR:H22	2.46	0.45
1:A:656:ASP:OD1	1:A:659:ASN:N	2.49	0.45
1:A:155:ARG:HG3	1:A:155:ARG:NH1	2.32	0.45
1:A:28:ILE:HA	1:A:31:ARG:CG	2.44	0.45
1:A:404:ASN:HB2	11:A:2037:HOH:O	2.17	0.44
1:A:551:VAL:HA	1:A:580:GLY:O	2.17	0.44
1:A:300:LEU:CD1	1:A:357:VAL:HG13	2.39	0.44
1:A:430:ASN:HD22	1:A:431:SER:HB3	1.83	0.44
1:A:495:TYR:O	1:A:503:PRO:CD	2.65	0.44
5:A:1009:FTT:H122	8:A:1100:DDQ:H92	1.99	0.44
1:A:75:GLY:HA2	1:A:600:THR:HG21	1.98	0.44
1:A:372:HIS:HB3	1:A:449:ASP:OD1	2.17	0.44
1:A:693:ASN:O	1:A:715:ARG:HD3	2.17	0.44
1:A:700:VAL:HG23	1:A:711:TRP:CZ3	2.53	0.44
1:A:55:ALA:HB2	1:A:127:GLU:O	2.18	0.44
1:A:137:SER:CB	1:A:510:SER:HA	2.48	0.44
1:A:249:LYS:HD2	1:A:661:PHE:CE2	2.52	0.44
1:A:524:PHE:CD2	1:A:560:LEU:HD11	2.53	0.44
1:A:583:ILE:HD11	11:A:2174:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:THR:HG23	1:A:619:GLN:NE2	2.32	0.44
1:A:462:GLY:HA2	1:A:489:TRP:HA	1.99	0.44
1:A:626:SER:HA	1:A:647:GLY:O	2.17	0.44
1:A:264:THR:HG21	1:A:698:GLU:HG2	2.00	0.44
1:A:639:SER:O	1:A:679:ARG:CD	2.66	0.44
1:A:352:LEU:HD13	1:A:383:MET:HG2	2.00	0.44
1:A:424:ASN:O	1:A:426:LYS:N	2.51	0.44
1:A:468:ASP:HB3	1:A:483:ASP:OD1	2.18	0.43
1:A:189:VAL:HG23	1:A:222:ARG:C	2.43	0.43
1:A:695:PHE:O	1:A:696:ASP:C	2.61	0.43
1:A:105:TYR:CD1	1:A:148:LEU:HG	2.54	0.43
5:A:1009:FTT:H72	8:A:1100:DDQ:H51	2.00	0.43
1:A:125:MET:HE3	1:A:125:MET:HB3	1.34	0.43
1:A:258:ASN:HB3	1:A:403:TYR:CE1	2.54	0.43
1:A:319:SER:HB3	1:A:338:GLY:N	2.33	0.43
1:A:410:HIS:C	1:A:412:HIS:N	2.73	0.43
1:A:452:GLN:HA	1:A:456:VAL:O	2.18	0.43
1:A:703:CYS:HA	1:A:708:GLY:O	2.17	0.43
1:A:162:LYS:HB3	1:A:725:PHE:HB2	2.00	0.43
1:A:264:THR:HA	1:A:711:TRP:CG	2.54	0.43
1:A:430:ASN:HD22	1:A:431:SER:N	2.15	0.43
1:A:75:GLY:N	11:A:2068:HOH:O	2.51	0.43
1:A:427:ASP:C	1:A:429:ALA:H	2.27	0.43
1:A:494:ASN:HD22	1:A:504:TYR:HB3	1.78	0.43
1:A:517:VAL:HA	1:A:522:ASN:O	2.18	0.43
1:A:41:THR:HG22	1:A:46:VAL:HG23	2.01	0.43
1:A:56:GLU:CD	1:A:56:GLU:H	2.27	0.43
1:A:407:SER:O	1:A:411:HIS:HD2	2.01	0.43
1:A:434:TYR:CZ	1:A:436:ILE:HG13	2.53	0.43
10:A:1107:GOL:O1	10:A:1107:GOL:C2	2.52	0.43
1:A:196:GLY:HA2	1:A:214:ALA:O	2.19	0.43
5:A:1013:FTT:C9	7:A:1014:MYR:H81	2.48	0.43
8:A:1100:DDQ:H21	8:A:1100:DDQ:HM13	1.59	0.43
1:A:293:THR:OG1	1:A:364:LYS:O	2.28	0.42
1:A:577:ARG:O	1:A:605:GLU:N	2.36	0.42
1:A:382:ARG:NH1	5:A:1011:FTT:H21	2.34	0.42
1:A:438:ASN:HB3	11:A:2088:HOH:O	2.19	0.42
1:A:339:HIS:CD2	1:A:339:HIS:O	2.72	0.42
1:A:586:LYS:HE2	11:A:2122:HOH:O	2.18	0.42
1:A:24:PRO:HD2	11:A:2154:HOH:O	2.18	0.42
1:A:676:ASP:C	1:A:678:ALA:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ALA:HB1	1:A:272:ASN:OD1	2.19	0.42
1:A:476:ALA:O	1:A:478:THR:HG23	2.19	0.42
1:A:589:LEU:HD23	1:A:589:LEU:HA	1.69	0.42
1:A:609:ASP:O	1:A:610:THR:C	2.63	0.42
1:A:22:TRP:CD1	1:A:60:LEU:HD22	2.55	0.42
5:A:1009:FTT:H51	8:A:1100:DDQ:H31	2.02	0.42
1:A:66:VAL:O	1:A:69:ALA:HB3	2.20	0.42
1:A:81:ARG:O	1:A:81:ARG:HG3	2.20	0.42
1:A:42:PRO:HG2	1:A:45:LYS:HG3	2.01	0.42
1:A:231:PHE:CE1	5:A:1013:FTT:H131	2.55	0.42
1:A:262:LEU:HD22	1:A:266:PHE:CD2	2.55	0.42
1:A:291:ASN:C	1:A:291:ASN:OD1	2.62	0.42
1:A:317:VAL:HG12	1:A:340:TYR:O	2.19	0.42
1:A:680:VAL:HG12	1:A:680:VAL:O	2.19	0.42
1:A:122:ASP:CG	1:A:197:LEU:HD21	2.45	0.42
1:A:274:THR:O	1:A:309:GLN:HA	2.20	0.42
1:A:371:ASP:C	1:A:372:HIS:CD2	2.97	0.42
1:A:529:GLY:O	1:A:530:LYS:HD3	2.20	0.42
1:A:244:TYR:OH	10:A:1107:GOL:H31	2.20	0.41
1:A:461:GLY:O	1:A:489:TRP:HB2	2.20	0.41
5:A:1013:FTT:H52	7:A:1014:MYR:H22	2.02	0.41
1:A:28:ILE:CA	1:A:31:ARG:HG3	2.46	0.41
1:A:247:LEU:CD2	1:A:268:GLU:HG3	2.49	0.41
1:A:454:ASP:C	1:A:455:LYS:HE2	2.44	0.41
1:A:496:LEU:HD13	1:A:502:THR:HG21	2.02	0.41
1:A:577:ARG:HH11	1:A:577:ARG:HD3	1.51	0.41
1:A:51:SER:OG	1:A:73:THR:HG23	2.21	0.41
1:A:257:PRO:HD2	1:A:339:HIS:HB3	2.02	0.41
1:A:397:VAL:HG23	1:A:398:PRO:HD2	2.03	0.41
1:A:435:ARG:NH1	1:A:474:ARG:HB3	2.35	0.41
1:A:86:THR:CG2	1:A:241:THR:HG21	2.45	0.41
1:A:167:LYS:HB2	1:A:175:GLN:HB3	2.03	0.41
1:A:249:LYS:HG2	1:A:250:GLU:OE1	2.21	0.41
1:A:195:THR:O	1:A:215:ILE:HD12	2.21	0.41
1:A:673:VAL:O	1:A:673:VAL:HG23	2.20	0.41
1:A:373:THR:O	1:A:449:ASP:HA	2.21	0.41
1:A:408:HIS:O	1:A:409:HIS:C	2.59	0.41
1:A:531:GLN:HA	1:A:553:ASN:O	2.21	0.41
1:A:586:LYS:CG	1:A:596:VAL:CG2	2.78	0.41
5:A:1009:FTT:H82	6:A:1012:DAO:H42	2.03	0.41
1:A:22:TRP:NE1	1:A:630:ASP:OD2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ALA:O	1:A:334:PRO:C	2.63	0.41
1:A:371:ASP:O	1:A:451:ALA:HA	2.20	0.41
1:A:678:ALA:O	1:A:680:VAL:N	2.52	0.41
1:A:137:SER:HB2	1:A:510:SER:HA	2.03	0.41
1:A:189:VAL:HG13	1:A:190:TYR:CD2	2.56	0.41
1:A:356:SER:HB3	11:A:2074:HOH:O	2.20	0.41
1:A:628:TRP:HH2	1:A:630:ASP:HB3	1.70	0.41
1:A:648:ARG:O	1:A:667:THR:HA	2.21	0.41
5:A:1013:FTT:H91	7:A:1014:MYR:C8	2.51	0.41
1:A:256:LEU:HA	1:A:256:LEU:HD23	1.54	0.40
1:A:323:ASN:O	1:A:324:ALA:C	2.64	0.40
1:A:333:ALA:O	1:A:335:ALA:N	2.54	0.40
1:A:365:PHE:CD1	1:A:365:PHE:C	2.98	0.40
1:A:390:TRP:NE1	1:A:426:LYS:HB3	2.36	0.40
1:A:381:MET:HE1	1:A:383:MET:N	2.36	0.40
1:A:408:HIS:ND1	1:A:408:HIS:C	2.79	0.40
1:A:464:TYR:CE2	1:A:466:TRP:CZ2	3.09	0.40
1:A:592:SER:O	1:A:632:THR:N	2.39	0.40
1:A:639:SER:HB3	1:A:679:ARG:NE	2.34	0.40
1:A:393:TYR:OH	1:A:432:GLY:HA3	2.21	0.40
1:A:490:ARG:HG2	1:A:491:GLY:N	2.35	0.40
1:A:28:ILE:C	1:A:31:ARG:HG3	2.46	0.40
1:A:98:GLU:HG3	1:A:513:PRO:O	2.21	0.40
1:A:116:TYR:OH	10:A:1108:GOL:H12	2.21	0.40
1:A:364:LYS:HA	1:A:372:HIS:O	2.22	0.40
1:A:407:SER:OG	1:A:409:HIS:HB3	2.21	0.40
1:A:319:SER:HB3	1:A:337:LYS:C	2.46	0.40
1:A:435:ARG:HH12	1:A:474:ARG:CB	2.34	0.40
1:A:443:THR:OG1	8:A:1100:DDQ:HM11	2.21	0.40
1:A:493:VAL:HG23	1:A:505:PHE:CE2	2.56	0.40
1:A:498:ASP:OD1	1:A:498:ASP:N	2.53	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%)	639 (91%)	54 (8%)	12 (2%)	7	13

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	ALA
1	A	420	ASP
1	A	677	LEU
1	A	679	ARG
1	A	682	MET
1	A	264	THR
1	A	331	ALA
1	A	398	PRO
1	A	676	ASP
1	A	696	ASP
1	A	678	ALA
1	A	334	PRO

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%)	499 (85%)	88 (15%)	3	6

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	28	ILE
1	A	32	GLN
1	A	49	SER
1	A	66	VAL
1	A	93	ARG
1	A	101	SER

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Mol	Chain	Res	Type
1	A	112	GLN
1	A	118	ASP
1	A	125	MET
1	A	128	ARG
1	A	132	MET
1	A	136	VAL
1	A	138	VAL
1	A	144	SER
1	A	148	LEU
1	A	156	PRO
1	A	158	THR
1	A	170	THR
1	A	184	LEU
1	A	205	GLN
1	A	206	LYS
1	A	209	GLU
1	A	257	PRO
1	A	268	GLU
1	A	271	LYS
1	A	280	LYS
1	A	281	MET
1	A	312	VAL
1	A	326	SER
1	A	334	PRO
1	A	343	ARG
1	A	352	LEU
1	A	353	GLN
1	A	357	VAL
1	A	361	LEU
1	A	367	THR
1	A	369	ASP
1	A	381	MET
1	A	397	VAL
1	A	398	PRO
1	A	402	LEU
1	A	404	ASN
1	A	405	PRO
1	A	408	HIS
1	A	426	LYS
1	A	430	ASN
1	A	431	SER
1	A	436	ILE

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Mol	Chain	Res	Type
1	A	448	GLN
1	A	455	LYS
1	A	457	LEU
1	A	460	LEU
1	A	468	ASP
1	A	474	ARG
1	A	485	LYS
1	A	493	VAL
1	A	498	ASP
1	A	501	VAL
1	A	502	THR
1	A	517	VAL
1	A	526	PRO
1	A	534	VAL
1	A	542	ASP
1	A	543	ARG
1	A	544	PRO
1	A	545	ILE
1	A	546	VAL
1	A	551	VAL
1	A	571	VAL
1	A	576	ILE
1	A	579	ARG
1	A	583	ILE
1	A	592	SER
1	A	596	VAL
1	A	603	ASP
1	A	607	THR
1	A	613	LYS
1	A	620	VAL
1	A	624	MET
1	A	627	LEU
1	A	632	THR
1	A	635	ASP
1	A	641	LEU
1	A	677	LEU
1	A	679	ARG
1	A	715	ARG
1	A	722	THR

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

Mol	Chain	Res	Type
1	A	44	GLN
1	A	112	GLN
1	A	165	GLN
1	A	205	GLN
1	A	211	GLN
1	A	237	ASN
1	A	278	ASN
1	A	288	HIS
1	A	310	ASN
1	A	328	GLN
1	A	353	GLN
1	A	388	ASN
1	A	404	ASN
1	A	410	HIS
1	A	412	HIS
1	A	418	ASN
1	A	430	ASN
1	A	438	ASN
1	A	448	GLN
1	A	486	GLN
1	A	494	ASN
1	A	522	ASN
1	A	619	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 ⓘ

9 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	2,9,5	11,11,12	0.90	0	15,15,17	1.83	4 (26%)
2	GCN	B	2	2,5	10,10,11	1.50	3 (30%)	13,13,15	3.57	5 (38%)
2	KDO	B	3	2	15,15,16	1.37	1 (6%)	17,21,24	1.42	2 (11%)
2	GMH	B	4	2	13,13,14	1.42	1 (7%)	16,18,20	1.16	1 (6%)
2	GMH	B	5	2	13,13,14	2.67	7 (53%)	16,18,20	1.56	3 (18%)
2	GLC	B	6	2	11,11,12	0.68	0	15,15,17	1.35	3 (20%)
2	GLC	B	7	2	11,11,12	1.42	2 (18%)	15,15,17	0.95	1 (6%)
2	GLA	B	8	2	11,11,12	0.84	0	15,15,17	0.63	0
2	KDO	B	9	2	15,15,16	1.22	3 (20%)	17,21,24	1.56	5 (29%)

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	2,9,5	-	2/2/18/22	0/1/1/1
2	GCN	B	2	2,5	-	0/2/15/18	0/1/1/1
2	KDO	B	3	2	-	0/10/26/30	0/1/1/1
2	GMH	B	4	2	-	0/6/23/26	0/1/1/1
2	GMH	B	5	2	-	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	-	2/2/19/22	0/1/1/1
2	GLA	B	8	2	-	0/2/19/22	0/1/1/1
2	KDO	B	9	2	-	2/10/26/30	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	GMH	C2-C3	4.86	1.59	1.52
2	B	5	GMH	O5-C5	3.99	1.48	1.43
2	B	4	GMH	C2-C3	3.91	1.58	1.52
2	B	5	GMH	O4-C4	3.75	1.52	1.43
2	B	5	GMH	C7-C6	3.30	1.60	1.52
2	B	5	GMH	C4-C5	3.21	1.61	1.52
2	B	2	GCN	C4-C5	-2.99	1.46	1.52
2	B	3	KDO	C2-C1	-2.91	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	GLC	C4-C5	2.74	1.58	1.53
2	B	5	GMH	C4-C3	2.63	1.59	1.52
2	B	7	GLC	C1-C2	2.51	1.58	1.52
2	B	2	GCN	C3-C2	2.39	1.58	1.53
2	B	2	GCN	O5-C1	-2.34	1.39	1.43
2	B	9	KDO	C4-C5	-2.23	1.49	1.52
2	B	9	KDO	C3-C2	2.14	1.55	1.52
2	B	5	GMH	C1-C2	-2.13	1.47	1.52
2	B	9	KDO	O1A-C1	2.08	1.28	1.22

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	GCN	C1-O5-C5	8.23	123.21	112.19
2	B	2	GCN	C3-C2-C1	6.87	115.42	109.87
2	B	1	PA1	C4-C3-C2	-4.95	102.52	112.65
2	B	2	GCN	C3-C4-C5	-4.47	105.06	110.76
2	B	3	KDO	C3-C4-C5	-3.99	104.92	110.67
2	B	5	GMH	C1-O5-C5	3.95	117.96	111.48
2	B	2	GCN	O5-C1-C2	3.43	116.63	111.28
2	B	6	GLC	C1-O5-C5	3.16	116.42	112.19
2	B	2	GCN	O5-C5-C4	3.11	114.82	109.66
2	B	9	KDO	O1A-C1-C2	-2.86	116.67	122.85
2	B	1	PA1	O1-C1-C2	2.76	114.65	108.96
2	B	9	KDO	C3-C4-C5	-2.70	106.78	110.67
2	B	9	KDO	O5-C5-C4	-2.69	104.57	110.05
2	B	4	GMH	C1-C2-C3	2.53	113.32	109.64
2	B	1	PA1	C1-O5-C5	2.51	118.51	113.65
2	B	3	KDO	O6-C6-C7	2.30	111.08	106.60
2	B	6	GLC	C6-C5-C4	-2.27	107.44	113.02
2	B	5	GMH	O7-C7-C6	2.19	115.76	111.16
2	B	7	GLC	O2-C2-C1	2.18	114.20	109.22
2	B	5	GMH	C3-C4-C5	-2.17	104.77	109.68
2	B	6	GLC	C1-C2-C3	2.16	112.78	109.64
2	B	9	KDO	O1B-C1-C2	2.09	118.13	112.71
2	B	9	KDO	O6-C6-C5	2.06	110.85	107.94
2	B	1	PA1	O5-C1-C2	2.00	111.84	109.51

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	9	KDO	C6-C7-C8-O8
2	B	9	KDO	O7-C7-C8-O8
2	B	7	GLC	O5-C5-C6-O6
2	B	1	PA1	C4-C5-C6-O6
2	B	7	GLC	C4-C5-C6-O6
2	B	1	PA1	O5-C5-C6-O6
2	B	6	GLC	O5-C5-C6-O6
2	B	6	GLC	C4-C5-C6-O6

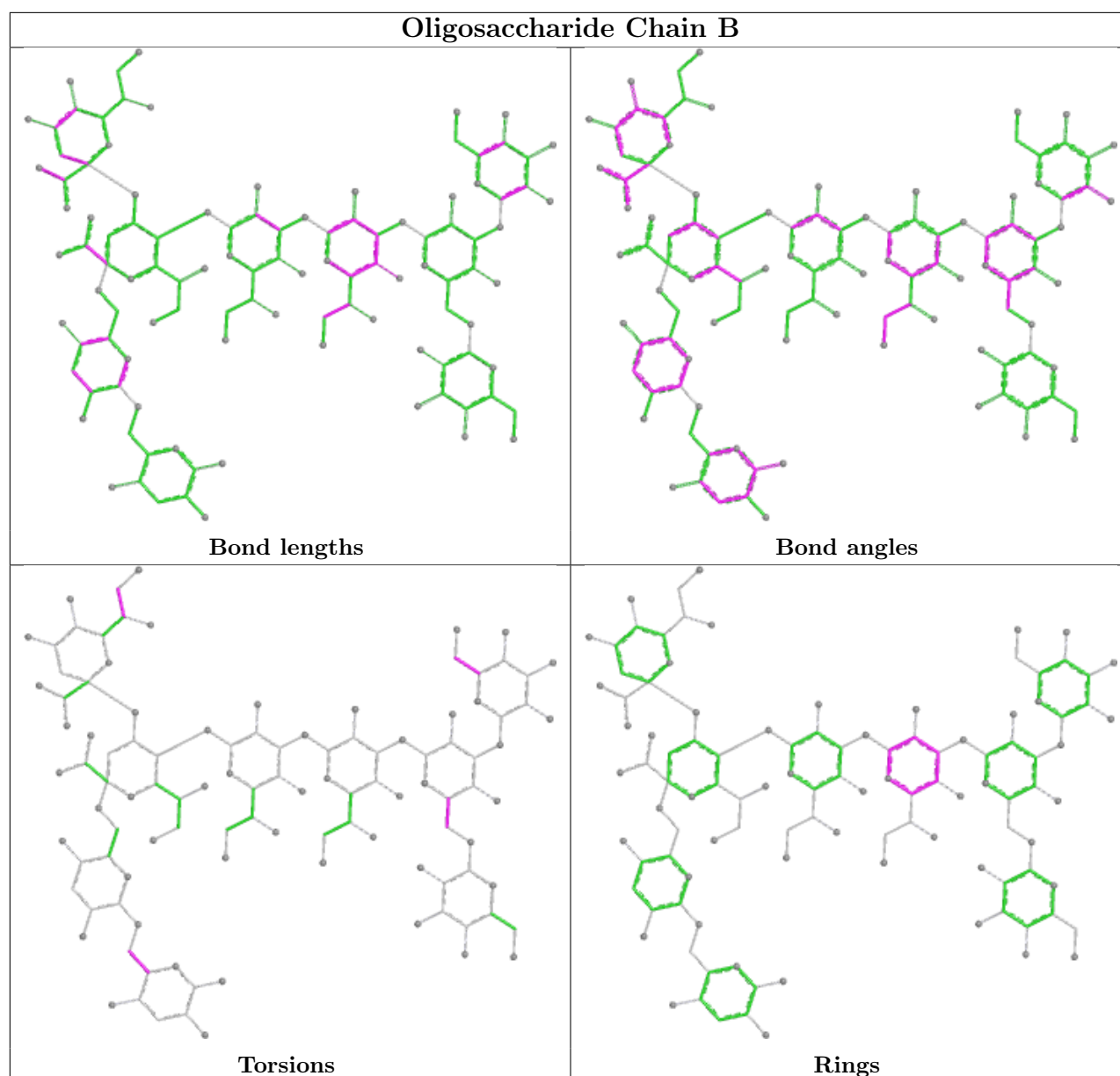
All (1) ring outliers are listed below:

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

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	KDO	1	0
2	B	1	PA1	2	0
2	B	4	GMH	1	0

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



5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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
5	FTT	A	1009	2	14,15,16	0.49	0	15,15,17	1.13	1 (6%)
7	MYR	A	1014	5	14,14,15	1.04	1 (7%)	13,13,15	0.79	1 (7%)
4	PO4	A	2001	-	0,3,4	-	-	0,3,6	-	-
5	FTT	A	1010	2	6,6,16	1.56	1 (16%)	6,7,17	1.07	1 (16%)
10	GOL	A	1108	-	5,5,5	4.46	5 (100%)	5,5,5	0.54	0
5	FTT	A	1011	6,2	14,15,16	0.68	0	15,15,17	1.31	3 (20%)
10	GOL	A	1105	-	5,5,5	4.43	3 (60%)	5,5,5	0.58	0
4	PO4	A	2005	3	0,3,4	-	-	0,3,6	-	-
9	DPO	A	2004	-	4,7,8	3.70	3 (75%)	5,10,13	2.35	3 (60%)
10	GOL	A	1103	-	5,5,5	4.64	5 (100%)	5,5,5	0.31	0
10	GOL	A	1107	-	5,5,5	4.35	4 (80%)	5,5,5	0.75	0
5	FTT	A	1013	7,2	16,16,16	1.15	2 (12%)	16,17,17	1.94	4 (25%)
8	DDQ	A	1102	-	11,13,13	1.01	1 (9%)	12,15,15	1.20	1 (8%)
6	DAO	A	1012	5	12,12,13	1.27	1 (8%)	11,11,13	0.81	0
9	DPO	A	2000	2	3,7,8	1.70	1 (33%)	6,10,13	0.93	0
8	DDQ	A	1100	-	11,13,13	0.99	1 (9%)	12,15,15	0.57	0
10	GOL	A	1109	-	5,5,5	4.89	5 (100%)	5,5,5	0.31	0
10	GOL	A	1104	-	5,5,5	4.61	5 (100%)	5,5,5	0.23	0
8	DDQ	A	1101	-	11,13,13	0.84	0	12,15,15	0.90	0
10	GOL	A	1110	-	5,5,5	4.48	3 (60%)	5,5,5	0.77	0
10	GOL	A	1106	-	5,5,5	4.74	5 (100%)	5,5,5	0.38	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
5	FTT	A	1009	2	-	3/14/14/15	-
7	MYR	A	1014	5	-	5/12/12/13	-
5	FTT	A	1010	2	-	2/4/4/15	-
10	GOL	A	1108	-	-	4/4/4/4	-
5	FTT	A	1011	6,2	-	1/14/14/15	-
10	GOL	A	1105	-	-	2/4/4/4	-
9	DPO	A	2004	-	-	0/2/5/6	-
10	GOL	A	1103	-	-	2/4/4/4	-
10	GOL	A	1107	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FTT	A	1013	7,2	-	4/15/15/15	-
8	DDQ	A	1102	-	-	4/11/11/11	-
6	DAO	A	1012	5	-	2/10/10/11	-
9	DPO	A	2000	2	-	1/2/5/6	-
8	DDQ	A	1100	-	-	4/11/11/11	-
10	GOL	A	1109	-	-	0/4/4/4	-
10	GOL	A	1104	-	-	3/4/4/4	-
8	DDQ	A	1101	-	-	0/11/11/11	-
10	GOL	A	1110	-	-	2/4/4/4	-
10	GOL	A	1106	-	-	2/4/4/4	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1106	GOL	C3-C2	-7.88	1.21	1.51
10	A	1109	GOL	C3-C2	-7.58	1.22	1.51
10	A	1104	GOL	C3-C2	-7.34	1.23	1.51
10	A	1103	GOL	C3-C2	-7.26	1.24	1.51
10	A	1105	GOL	C3-C2	-6.96	1.25	1.51
10	A	1108	GOL	C3-C2	-6.81	1.25	1.51
10	A	1110	GOL	C3-C2	-6.49	1.27	1.51
10	A	1107	GOL	C3-C2	-6.24	1.28	1.51
9	A	2004	DPO	P1-O4	-6.19	1.45	1.63
10	A	1110	GOL	O1-C1	6.16	1.68	1.42
10	A	1105	GOL	O1-C1	5.70	1.66	1.42
10	A	1107	GOL	O1-C1	5.56	1.65	1.42
10	A	1104	GOL	O1-C1	5.41	1.65	1.42
10	A	1103	GOL	O1-C1	5.37	1.65	1.42
10	A	1109	GOL	O1-C1	5.22	1.64	1.42
10	A	1106	GOL	O1-C1	4.86	1.62	1.42
10	A	1108	GOL	O1-C1	4.63	1.61	1.42
10	A	1108	GOL	O3-C3	4.58	1.61	1.42
10	A	1107	GOL	O3-C3	4.22	1.60	1.42
10	A	1110	GOL	O3-C3	4.14	1.59	1.42
6	A	1012	DAO	O2-C1	-3.98	1.21	1.42
10	A	1109	GOL	O3-C3	3.81	1.58	1.42
10	A	1103	GOL	O3-C3	3.76	1.58	1.42
5	A	1010	FTT	O1-C1	3.57	1.42	1.30
10	A	1105	GOL	O3-C3	3.56	1.57	1.42
10	A	1106	GOL	O3-C3	3.54	1.57	1.42
10	A	1109	GOL	O2-C2	-3.52	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1104	GOL	O3-C3	3.35	1.56	1.42
7	A	1014	MYR	O2-C1	-3.03	1.26	1.42
10	A	1106	GOL	C1-C2	-2.93	1.40	1.51
10	A	1109	GOL	C1-C2	-2.85	1.40	1.51
8	A	1102	DDQ	C1-N1	2.79	1.54	1.51
9	A	2004	DPO	P2-O5	2.78	1.59	1.50
8	A	1100	DDQ	C1-N1	2.75	1.54	1.51
9	A	2004	DPO	P2-O7	2.68	1.64	1.54
10	A	1103	GOL	C1-C2	-2.63	1.41	1.51
10	A	1104	GOL	C1-C2	-2.46	1.42	1.51
10	A	1107	GOL	C1-C2	-2.45	1.42	1.51
10	A	1104	GOL	O2-C2	-2.41	1.36	1.43
10	A	1108	GOL	C1-C2	-2.40	1.42	1.51
10	A	1106	GOL	O2-C2	-2.32	1.36	1.43
9	A	2000	DPO	P2-O6	-2.27	1.46	1.54
10	A	1103	GOL	O2-C2	-2.23	1.36	1.43
10	A	1108	GOL	O2-C2	-2.23	1.36	1.43
5	A	1013	FTT	C4-C3	2.18	1.58	1.52
5	A	1013	FTT	C2-C3	-2.01	1.46	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1013	FTT	O3-C3-C4	5.10	122.95	109.35
5	A	1013	FTT	C5-C4-C3	3.87	125.36	114.68
9	A	2004	DPO	O6-P2-O4	3.82	117.40	104.64
8	A	1102	DDQ	CM2-N1-C1	3.20	116.97	110.23
5	A	1011	FTT	O2-C1-C2	-3.09	116.37	125.38
5	A	1013	FTT	C4-C3-C2	-2.84	103.33	112.88
9	A	2004	DPO	O6-P2-O5	-2.80	99.91	110.83
5	A	1009	FTT	C4-C3-C2	-2.45	105.14	113.05
5	A	1011	FTT	O3-C3-C2	2.43	115.92	109.45
5	A	1013	FTT	O3-C3-C2	-2.43	103.34	109.64
9	A	2004	DPO	O7-P2-O5	2.17	119.30	110.83
5	A	1010	FTT	C4-C3-C2	2.14	115.69	111.64
7	A	1014	MYR	O2-C1-C2	2.05	124.47	111.44
5	A	1011	FTT	C4-C3-C2	-2.03	106.51	113.05

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1009	FTT	C1-C2-C3-O3
5	A	1010	FTT	C1-C2-C3-C4
5	A	1010	FTT	C1-C2-C3-O3
5	A	1013	FTT	C1-C2-C3-C4
5	A	1013	FTT	C1-C2-C3-O3
8	A	1102	DDQ	C2-C1-N1-O1
8	A	1102	DDQ	C2-C1-N1-CM1
8	A	1102	DDQ	C2-C1-N1-CM2
8	A	1102	DDQ	N1-C1-C2-C3
10	A	1103	GOL	O1-C1-C2-C3
10	A	1104	GOL	O1-C1-C2-C3
10	A	1105	GOL	O1-C1-C2-C3
10	A	1107	GOL	O1-C1-C2-C3
10	A	1108	GOL	C1-C2-C3-O3
10	A	1108	GOL	O2-C2-C3-O3
10	A	1110	GOL	O1-C1-C2-C3
10	A	1103	GOL	O1-C1-C2-O2
7	A	1014	MYR	C7-C8-C9-C10
10	A	1106	GOL	C1-C2-C3-O3
10	A	1107	GOL	C1-C2-C3-O3
10	A	1108	GOL	O1-C1-C2-C3
10	A	1104	GOL	O1-C1-C2-O2
10	A	1105	GOL	O1-C1-C2-O2
10	A	1107	GOL	O1-C1-C2-O2
10	A	1110	GOL	O1-C1-C2-O2
7	A	1014	MYR	O2-C1-C2-C3
6	A	1012	DAO	C1-C2-C3-C4
7	A	1014	MYR	C2-C3-C4-C5
5	A	1013	FTT	C11-C10-C9-C8
5	A	1013	FTT	C7-C8-C9-C10
5	A	1009	FTT	C11-C12-C13-C14
7	A	1014	MYR	C10-C11-C12-C13
10	A	1106	GOL	O2-C2-C3-O3
7	A	1014	MYR	C1-C2-C3-C4
8	A	1100	DDQ	C4-C5-C6-C7
10	A	1108	GOL	O1-C1-C2-O2
5	A	1009	FTT	C1-C2-C3-C4
5	A	1011	FTT	O2-C1-C2-C3
10	A	1107	GOL	O2-C2-C3-O3
10	A	1104	GOL	C1-C2-C3-O3
8	A	1100	DDQ	N1-C1-C2-C3
6	A	1012	DAO	O2-C1-C2-C3
9	A	2000	DPO	P1-O4-P2-O6

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Mol	Chain	Res	Type	Atoms
8	A	1100	DDQ	C2-C1-N1-CM1
8	A	1100	DDQ	C3-C4-C5-C6

There are no ring outliers.

15 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1009	FTT	6	0
7	A	1014	MYR	9	0
10	A	1108	GOL	1	0
5	A	1011	FTT	1	0
10	A	1105	GOL	4	0
9	A	2004	DPO	1	0
10	A	1103	GOL	2	0
10	A	1107	GOL	4	0
5	A	1013	FTT	11	0
6	A	1012	DAO	3	0
9	A	2000	DPO	4	0
8	A	1100	DDQ	5	0
10	A	1109	GOL	2	0
10	A	1104	GOL	2	0
10	A	1110	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	0.25	6 (0%) 82 80	34, 63, 94, 119	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	GLN	3.9
1	A	99	GLY	3.3
1	A	568	PHE	3.2
1	A	98	GLU	2.6
1	A	725	PHE	2.3
1	A	408	HIS	2.2

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.

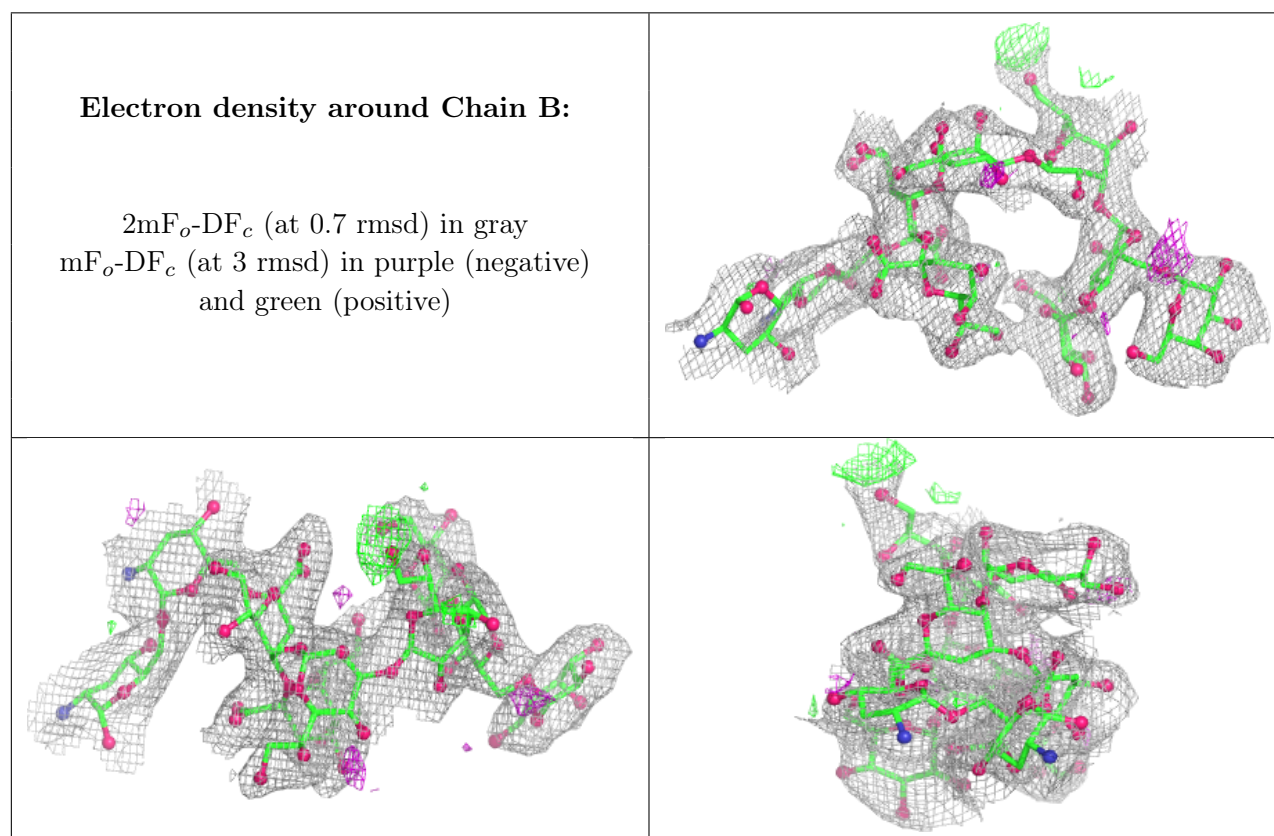
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	B	7	11/12	0.67	0.13	93,104,107,109	0
2	GLA	B	8	11/12	0.80	0.10	92,97,102,103	0
2	GMH	B	5	13/14	0.84	0.14	51,70,96,97	0
2	KDO	B	9	15/16	0.89	0.10	64,73,81,83	0
2	GLC	B	6	11/12	0.90	0.12	76,86,96,98	0
2	KDO	B	3	15/16	0.95	0.08	49,58,64,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PA1	B	1	11/12	0.95	0.07	48,57,65,67	0
2	GMH	B	4	13/14	0.96	0.08	52,56,68,75	0
2	GCN	B	2	10/11	0.97	0.06	35,45,53,54	0

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	DDQ	A	1102	14/14	0.75	0.23	53,86,138,138	0
4	PO4	A	2005	4/5	0.77	0.14	68,69,83,88	0
10	GOL	A	1105	6/6	0.79	0.15	91,100,103,104	0
10	GOL	A	1110	6/6	0.79	0.35	74,100,107,111	0
8	DDQ	A	1101	14/14	0.82	0.20	62,82,104,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FTT	A	1010	7/17	0.84	0.15	67,78,91,97	0
5	FTT	A	1009	16/17	0.86	0.13	61,67,82,88	0
8	DDQ	A	1100	14/14	0.86	0.19	76,84,94,97	0
5	FTT	A	1013	17/17	0.87	0.15	59,75,84,85	0
7	MYR	A	1014	15/16	0.88	0.15	70,75,81,82	0
10	GOL	A	1107	6/6	0.88	0.24	74,79,82,88	0
10	GOL	A	1103	6/6	0.88	0.13	81,83,83,83	0
10	GOL	A	1106	6/6	0.90	0.16	86,100,102,104	0
6	DAO	A	1012	13/14	0.92	0.10	57,60,69,75	0
10	GOL	A	1104	6/6	0.92	0.11	78,81,86,97	0
10	GOL	A	1108	6/6	0.92	0.17	46,77,91,99	0
10	GOL	A	1109	6/6	0.92	0.25	88,94,95,98	0
9	DPO	A	2004	8/9	0.92	0.09	64,82,91,92	0
9	DPO	A	2000	8/9	0.94	0.09	56,69,75,82	4
5	FTT	A	1011	16/17	0.95	0.08	41,55,60,62	0
3	NI	A	1030	1/1	0.96	0.05	95,95,95,95	0
4	PO4	A	2001	4/5	0.97	0.09	54,68,68,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.