Full wwPDB X-ray Structure Validation Report (i)

Dec 5, 2023 – 09:25 am GMT

PDB ID	:	1QJQ
Title	:	FERRIC HYDROXAMATE RECEPTOR FROM ESCHERICHIA COLI (FHUA)
Authors	:	Ferguson, A.D.; Braun, V.; Fiedler, H.-P.; Coulton, J.W.; Diederichs, K.; Welte, W.
Deposited on	:	1999-06-29
Resolution	:	2.95 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 (i) 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 (i)) were used in the production of this report:

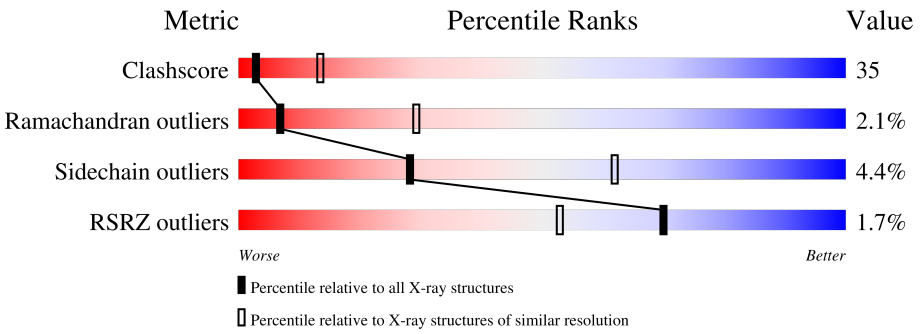
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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% 46% 47% . .
2	B	11	45% 55%

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	-	-	-
2	GLC	B	8	X	-	-	X
3	FTT	A	1006	X	-	-	-
5	PO4	A	1014	-	-	X	-
7	PFC	A	1022	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6218 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.

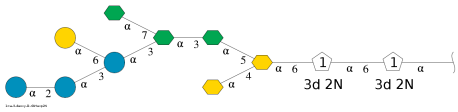
- Molecule 1 is a protein called FERRIC HYDROXAMATE RECEPTOR.

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:

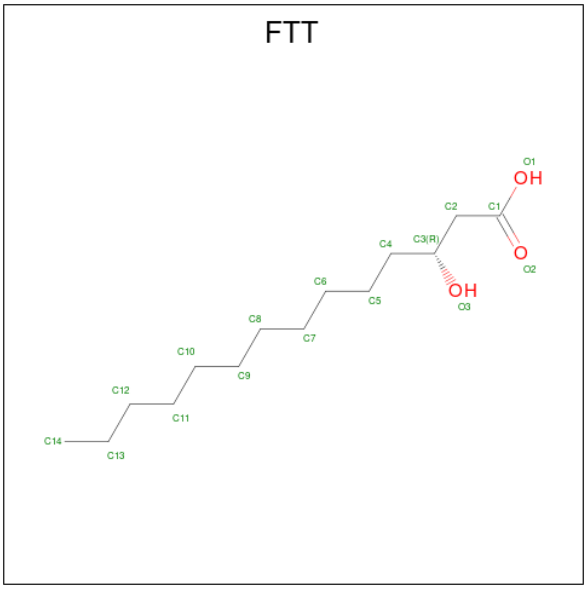
Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	insertion	UNP P06971
A	407	SER	-	insertion	UNP P06971
A	408	HIS	-	insertion	UNP P06971
A	409	HIS	-	insertion	UNP P06971
A	410	HIS	-	insertion	UNP P06971
A	411	HIS	-	insertion	UNP P06971
A	412	HIS	-	insertion	UNP P06971
A	413	HIS	-	insertion	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-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-glucoyranose-(1-6)-2-amino-2,3-dideoxy-alpha-D-glucoyranose.



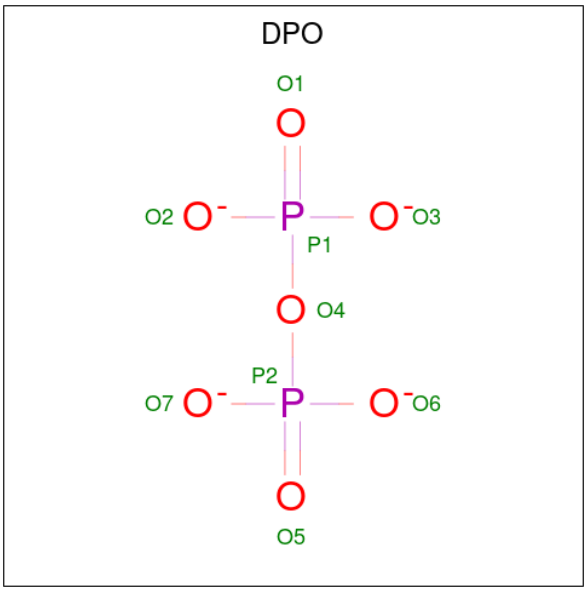
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	11	134	73	2	59	0	0	0

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



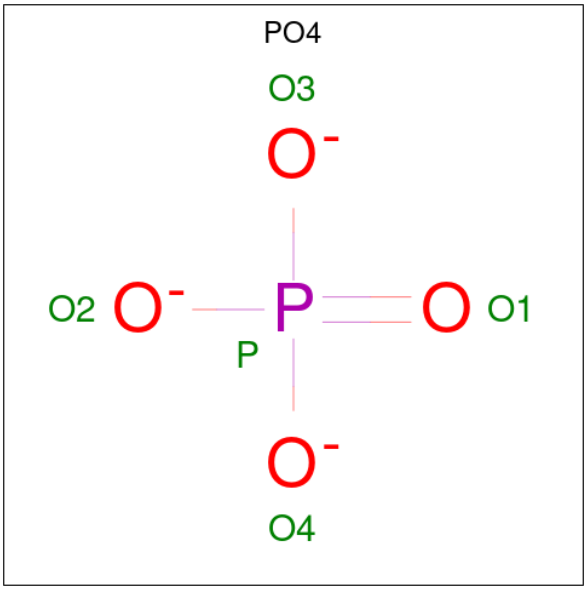
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			16	14	2			
3	A	1	Total	C	O		0	0
			8	5	3			
3	A	1	Total	C	O		0	0
			16	14	2			
3	A	1	Total	C	O		0	0
			13	12	1			
3	A	1	Total	C	O		0	0
			17	14	3			
3	A	1	Total	C	O		0	0
			15	14	1			

- Molecule 4 is DIPHOSPHATE (three-letter code: DPO) (formula: O_7P_2).



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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

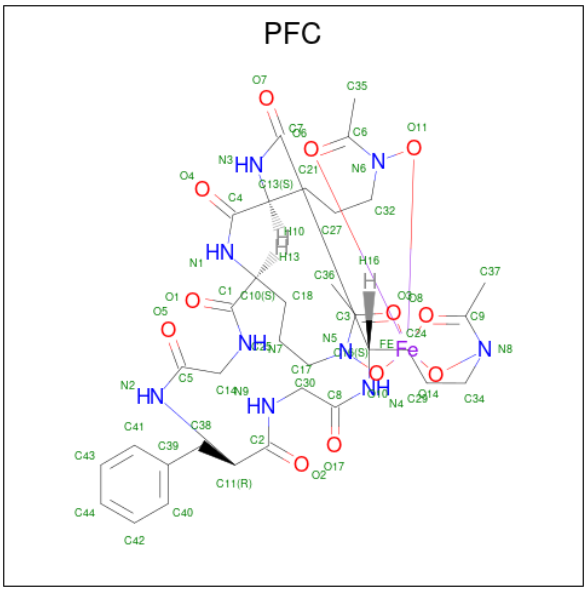


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 4 3 1	0	0
5	A	1	Total O P 4 3 1	0	0

- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 7 is PHENYLFERRICROCIN-IRON (three-letter code: PFC) (formula: $C_{34}H_{48}FeN_9O_{12}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
7	A	1	56	34	1	9	12	0	0

- Molecule 8 is water.

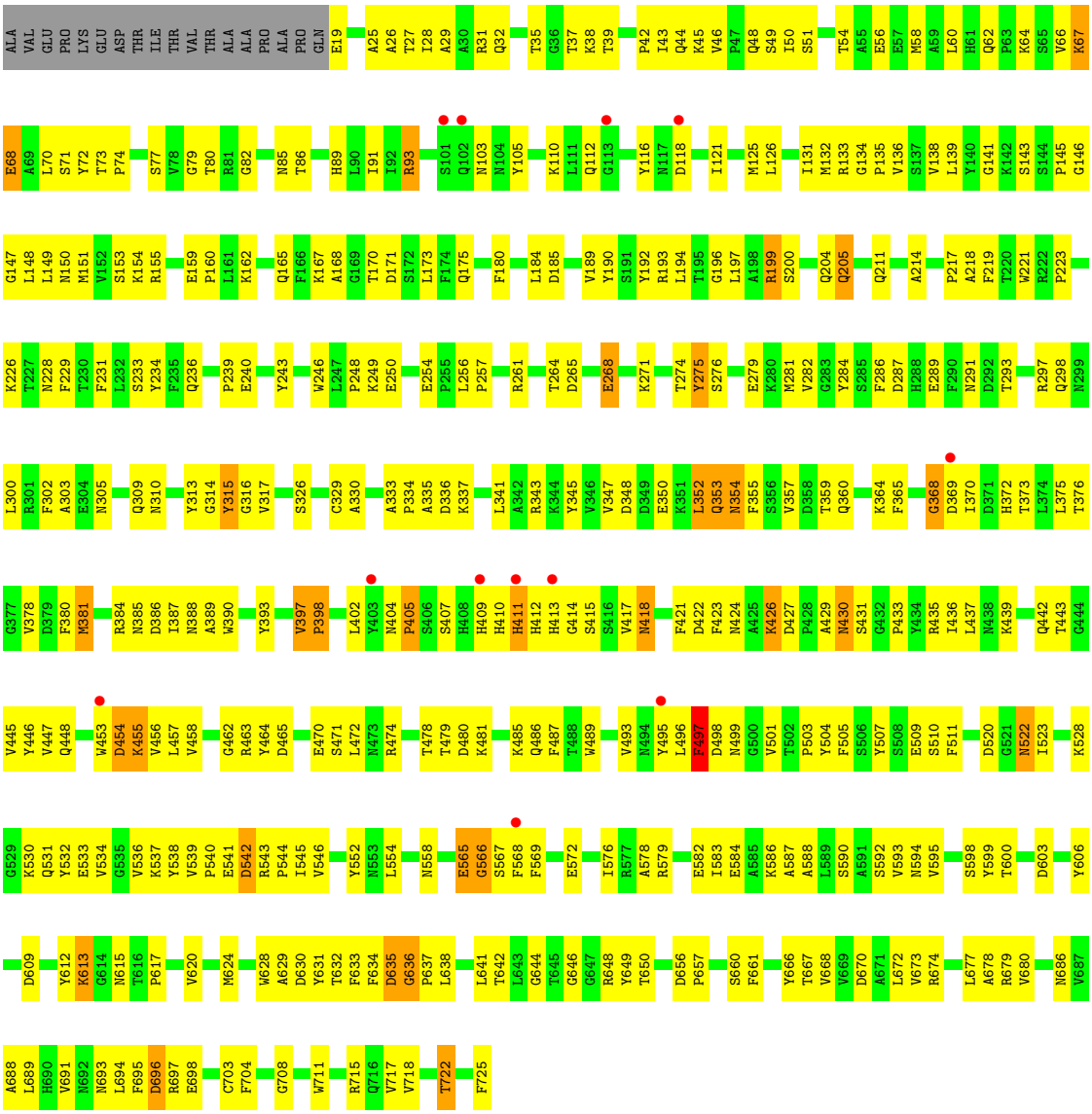
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	395	395	395	0	0

3 Residue-property plots (i)

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

• Molecule 1: FERRIC HYDROXAMATE RECEPTOR

Chain A:



• Molecule 2: alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-[alpha-D-galactopyranos

e-(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-glucoyranose-(1-6)-2-amino-2,3-dideoxy-alpha-D-glucoyranose

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	172.10Å 172.10Å 87.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.95 41.34 – 2.89	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-2.95) 92.2 (41.34-2.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 2.90Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.225 , 0.278 0.226 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	63.7	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 54.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.020 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6218	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FTT, NI, GLC, KDO, GLA, GMH, PFC, PO4, GCN, 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	0.40	0/5663	0.65	0/7696

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5523	0	5223	380	0
2	B	134	0	104	7	0
3	A	85	0	128	15	0
4	A	16	0	0	1	0
5	A	8	0	0	2	0
6	A	1	0	0	0	0
7	A	56	0	48	2	0
8	A	395	0	0	66	0
All	All	6218	0	5503	397	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 35.

All (397) 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:649:TYR:HA	8:A:2340:HOH:O	1.45	1.17
1:A:66:VAL:HG21	1:A:151:MET:HE3	1.34	1.07
1:A:455:LYS:N	1:A:455:LYS:HE2	1.80	0.96
1:A:248:PRO:HB3	8:A:2217:HOH:O	1.67	0.94
1:A:219:PHE:HA	8:A:2135:HOH:O	1.67	0.93
1:A:28:ILE:HD12	1:A:28:ILE:H	1.32	0.92
1:A:274:THR:HG22	1:A:310:ASN:HB2	1.49	0.92
1:A:136:VAL:HG21	1:A:148:LEU:HD12	1.51	0.91
1:A:667:THR:HA	8:A:2340:HOH:O	1.72	0.87
3:A:1003:FTT:H41	8:A:2377:HOH:O	1.74	0.87
1:A:134:GLY:CA	1:A:146:GLY:HA2	2.05	0.87
1:A:691:VAL:HG22	1:A:717:VAL:HG22	1.57	0.87
1:A:121:ILE:HB	1:A:151:MET:CE	2.06	0.86
1:A:455:LYS:HE2	1:A:455:LYS:H	1.38	0.85
1:A:165:GLN:HE21	1:A:722:THR:HB	1.42	0.83
1:A:668:VAL:HG13	1:A:693:ASN:HA	1.58	0.82
1:A:281:MET:HB3	1:A:303:ALA:HB2	1.60	0.81
1:A:93:ARG:HD3	1:A:133:ARG:HG2	1.60	0.81
1:A:378:VAL:HG12	1:A:445:VAL:HG12	1.62	0.81
1:A:121:ILE:HB	1:A:151:MET:HE1	1.61	0.81
1:A:544:PRO:HG2	1:A:588:ALA:HB3	1.61	0.81
1:A:446:TYR:HB3	1:A:463:ARG:HB2	1.64	0.78
1:A:205:GLN:HG3	1:A:243:TYR:CG	2.19	0.78
1:A:677:LEU:HD13	1:A:686:ASN:HA	1.66	0.78
1:A:217:PRO:HD2	1:A:233:SER:OG	1.85	0.77
1:A:656:ASP:OD2	1:A:660:SER:HB3	1.84	0.77
1:A:648:ARG:NH1	1:A:670:ASP:OD2	2.19	0.76
1:A:531:GLN:HB2	1:A:554:LEU:HD13	1.68	0.75
1:A:125:MET:HG3	1:A:234:TYR:HE1	1.51	0.75
1:A:175:GLN:HG3	1:A:199:ARG:HB2	1.68	0.75
1:A:497:PHE:HB2	1:A:501:VAL:O	1.87	0.75
1:A:71:SER:HB3	1:A:648:ARG:HD2	1.69	0.73
1:A:64:LYS:HD2	1:A:85:ASN:ND2	2.04	0.73
1:A:167:LYS:HB2	1:A:175:GLN:HB3	1.71	0.73
1:A:221:TRP:CE2	1:A:223:PRO:HG3	2.25	0.72
1:A:384:ARG:HD2	8:A:2376:HOH:O	1.90	0.71
1:A:148:LEU:C	1:A:148:LEU:HD23	2.11	0.71
1:A:199:ARG:HD2	8:A:2139:HOH:O	1.89	0.71
1:A:264:THR:HA	1:A:711:TRP:CD1	2.26	0.71
1:A:541:GLU:HB3	8:A:2309:HOH:O	1.92	0.70
1:A:162:LYS:HA	1:A:180:PHE:HD1	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:GLU:HB3	8:A:2363:HOH:O	1.93	0.68
1:A:693:ASN:O	1:A:715:ARG:HB2	1.93	0.68
1:A:633:PHE:HA	8:A:2336:HOH:O	1.94	0.68
1:A:390:TRP:CH2	1:A:433:PRO:HG3	2.29	0.68
1:A:51:SER:OG	1:A:133:ARG:NH2	2.27	0.67
1:A:148:LEU:HD23	1:A:149:LEU:N	2.10	0.67
1:A:211:GLN:HG2	8:A:2146:HOH:O	1.92	0.67
1:A:600:THR:HB	1:A:624:MET:HB2	1.77	0.67
1:A:27:THR:HB	8:A:2007:HOH:O	1.94	0.67
1:A:126:LEU:HD11	1:A:151:MET:HE3	1.77	0.67
1:A:594:ASN:HB2	1:A:630:ASP:OD1	1.94	0.67
1:A:642:THR:HB	1:A:674:ARG:HB3	1.76	0.67
1:A:219:PHE:CD1	8:A:2135:HOH:O	2.47	0.66
1:A:71:SER:HB3	1:A:648:ARG:CD	2.25	0.66
1:A:315:TYR:HB3	8:A:2215:HOH:O	1.96	0.66
1:A:657:PRO:HB3	8:A:2329:HOH:O	1.96	0.66
1:A:134:GLY:HA2	1:A:146:GLY:HA2	1.78	0.66
1:A:162:LYS:HA	1:A:180:PHE:CD1	2.31	0.66
1:A:228:ASN:HB3	1:A:287:ASP:OD1	1.96	0.65
1:A:633:PHE:HB2	1:A:638:LEU:O	1.97	0.65
1:A:64:LYS:HG3	1:A:199:ARG:NH2	2.12	0.65
1:A:219:PHE:HD1	8:A:2135:HOH:O	1.79	0.64
1:A:300:LEU:CG	1:A:357:VAL:HG12	2.27	0.64
1:A:613:LYS:C	1:A:615:ASN:H	2.00	0.64
1:A:54:THR:HB	8:A:2022:HOH:O	1.96	0.64
1:A:67:LYS:HE3	8:A:2050:HOH:O	1.96	0.64
1:A:390:TRP:CZ3	1:A:433:PRO:HG3	2.32	0.64
1:A:397:VAL:HG23	1:A:398:PRO:HD2	1.79	0.64
2:B:5:GMH:O6	2:B:10:GMH:H5	1.97	0.64
1:A:80:THR:HG21	1:A:89:HIS:CE1	2.32	0.64
1:A:121:ILE:HB	1:A:151:MET:HE2	1.80	0.64
1:A:200:SER:HA	8:A:2146:HOH:O	1.97	0.63
1:A:211:GLN:HA	8:A:2146:HOH:O	1.99	0.63
1:A:279:GLU:HA	1:A:305:ASN:OD1	1.99	0.62
1:A:540:PRO:HG3	1:A:545:ILE:CG1	2.29	0.62
1:A:132:MET:HE2	1:A:136:VAL:HG12	1.82	0.62
1:A:590:SER:HB3	1:A:593:VAL:HB	1.82	0.62
1:A:154:LYS:HD3	1:A:193:ARG:NH2	2.15	0.62
1:A:457:LEU:HD22	8:A:2274:HOH:O	2.00	0.61
1:A:503:PRO:HA	1:A:536:VAL:HG12	1.82	0.61
1:A:134:GLY:C	1:A:146:GLY:HA2	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ASN:HD22	1:A:355:PHE:N	1.98	0.61
1:A:35:THR:CG2	1:A:150:ASN:HD22	2.13	0.61
1:A:126:LEU:HD11	1:A:151:MET:CE	2.30	0.61
1:A:609:ASP:HB3	1:A:612:TYR:O	2.00	0.61
2:B:3:KDO:H7	2:B:4:GMH:C1	2.31	0.61
1:A:192:TYR:HA	8:A:2135:HOH:O	2.00	0.61
1:A:470:GLU:HG3	1:A:481:LYS:HG2	1.82	0.60
1:A:715:ARG:HH11	1:A:715:ARG:HG2	1.66	0.60
1:A:409:HIS:O	1:A:414:GLY:HA2	2.02	0.60
3:A:1002:FTT:H143	3:A:1005:FTT:H91	1.83	0.60
1:A:592:SER:HB2	1:A:632:THR:O	2.02	0.60
3:A:1006:FTT:H52	3:A:1007:FTT:C1	2.32	0.60
1:A:240:GLU:HA	1:A:275:TYR:O	2.01	0.59
1:A:27:THR:HG23	8:A:2025:HOH:O	2.02	0.59
1:A:35:THR:HG22	1:A:150:ASN:HD22	1.65	0.59
1:A:116:TYR:OH	7:A:1022:PFC:H302	2.01	0.59
1:A:583:ILE:HG12	1:A:599:TYR:HB3	1.83	0.59
1:A:45:LYS:HE2	1:A:496:LEU:HD22	1.84	0.59
1:A:265:ASP:HB3	8:A:2368:HOH:O	2.02	0.59
1:A:135:PRO:HB3	1:A:509:GLU:C	2.23	0.59
1:A:44:GLN:HB3	1:A:539:VAL:HG21	1.85	0.58
1:A:617:PRO:O	1:A:620:VAL:HG12	2.04	0.58
1:A:49:SER:O	1:A:50:ILE:HD12	2.04	0.58
1:A:249:LYS:HG2	1:A:250:GLU:OE1	2.04	0.58
1:A:105:TYR:CE2	1:A:110:LYS:HB2	2.38	0.58
1:A:281:MET:HB3	1:A:303:ALA:CB	2.33	0.58
1:A:370:ILE:HG22	1:A:372:HIS:CD2	2.39	0.58
1:A:352:LEU:C	1:A:352:LEU:HD12	2.24	0.58
1:A:365:PHE:HE1	1:A:372:HIS:HD1	1.52	0.57
1:A:49:SER:C	1:A:50:ILE:HD12	2.25	0.57
1:A:678:ALA:HB2	8:A:2358:HOH:O	2.05	0.57
1:A:28:ILE:H	1:A:28:ILE:CD1	2.08	0.57
1:A:291:ASN:OD1	1:A:293:THR:HG22	2.05	0.57
3:A:1002:FTT:C10	3:A:1005:FTT:H71	2.35	0.57
1:A:44:GLN:HB3	1:A:539:VAL:CG2	2.35	0.57
1:A:205:GLN:HG3	1:A:243:TYR:CB	2.35	0.57
1:A:628:TRP:CH2	1:A:630:ASP:HB3	2.40	0.57
1:A:673:VAL:HG23	1:A:673:VAL:O	2.04	0.57
1:A:249:LYS:HE2	1:A:254:GLU:OE1	2.05	0.57
1:A:545:ILE:HG22	1:A:587:ALA:HB1	1.86	0.57
1:A:66:VAL:HG21	1:A:151:MET:CE	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:THR:HG22	1:A:447:VAL:HG22	1.85	0.56
1:A:246:TRP:HZ3	1:A:315:TYR:CE1	2.24	0.56
1:A:343:ARG:O	1:A:397:VAL:HG13	2.05	0.56
1:A:79:GLY:HA2	8:A:2044:HOH:O	2.05	0.56
1:A:300:LEU:HD12	1:A:357:VAL:CG1	2.35	0.56
1:A:497:PHE:HD2	1:A:499:ASN:OD1	1.89	0.56
1:A:694:LEU:O	1:A:715:ARG:HD3	2.06	0.56
1:A:695:PHE:O	1:A:696:ASP:C	2.45	0.56
1:A:435:ARG:O	1:A:436:ILE:HD13	2.06	0.55
1:A:693:ASN:HB2	8:A:2365:HOH:O	2.05	0.55
1:A:462:GLY:HA2	1:A:489:TRP:HA	1.88	0.55
1:A:192:TYR:CA	8:A:2135:HOH:O	2.55	0.55
1:A:185:ASP:CG	1:A:189:VAL:HG12	2.27	0.55
1:A:234:TYR:HB3	1:A:281:MET:HG3	1.88	0.55
1:A:486:GLN:OE1	1:A:528:LYS:HE2	2.07	0.55
1:A:268:GLU:OE1	1:A:314:GLY:N	2.39	0.55
1:A:493:VAL:HB	1:A:505:PHE:CE2	2.42	0.55
1:A:350:GLU:HG2	1:A:387:ILE:HA	1.88	0.54
1:A:472:LEU:HD12	1:A:478:THR:O	2.08	0.54
1:A:62:GLN:OE1	1:A:167:LYS:NZ	2.39	0.54
1:A:317:VAL:N	8:A:2217:HOH:O	2.40	0.54
1:A:165:GLN:NE2	1:A:722:THR:HB	2.17	0.54
1:A:352:LEU:HB2	1:A:384:ARG:O	2.08	0.54
1:A:520:ASP:OD2	1:A:522:ASN:HB2	2.08	0.54
4:A:1015:DPO:O6	2:B:4:GMH:H6	2.08	0.54
1:A:297:ARG:HH11	1:A:360:GLN:HE21	1.56	0.54
3:A:1002:FTT:H102	3:A:1005:FTT:H71	1.90	0.54
1:A:704:PHE:CE2	1:A:708:GLY:HA3	2.44	0.53
1:A:93:ARG:HD2	1:A:582:GLU:OE2	2.08	0.53
1:A:390:TRP:CZ2	1:A:426:LYS:HB2	2.43	0.53
1:A:504:TYR:CE2	1:A:537:LYS:HE3	2.43	0.53
1:A:38:LYS:HE3	1:A:139:LEU:O	2.08	0.53
1:A:214:ALA:HB1	8:A:2166:HOH:O	2.07	0.53
1:A:567:SER:O	1:A:568:PHE:HB2	2.07	0.53
1:A:72:TYR:CE2	1:A:628:TRP:HB2	2.43	0.53
1:A:427:ASP:C	1:A:429:ALA:H	2.12	0.53
1:A:595:VAL:HG12	1:A:629:ALA:HB2	1.90	0.53
1:A:38:LYS:HG3	1:A:139:LEU:HD22	1.90	0.53
1:A:67:LYS:HZ2	1:A:67:LYS:CB	2.22	0.53
1:A:300:LEU:HG	1:A:357:VAL:HG12	1.90	0.53
1:A:509:GLU:HB3	8:A:2305:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:VAL:HG13	1:A:190:TYR:CD2	2.44	0.53
1:A:143:SER:HB2	8:A:2092:HOH:O	2.08	0.53
1:A:404:ASN:HB3	1:A:405:PRO:HD3	1.90	0.52
1:A:261:ARG:O	1:A:410:HIS:HE1	1.92	0.52
1:A:544:PRO:CG	1:A:588:ALA:HB3	2.38	0.52
3:A:1002:FTT:C14	3:A:1005:FTT:H91	2.40	0.52
1:A:28:ILE:HG13	1:A:56:GLU:OE1	2.09	0.52
1:A:126:LEU:HD22	1:A:151:MET:HB3	1.91	0.52
1:A:341:LEU:HB2	1:A:402:LEU:HD21	1.91	0.52
1:A:592:SER:HB3	1:A:634:PHE:HE1	1.74	0.52
1:A:433:PRO:HD2	8:A:2264:HOH:O	2.10	0.52
1:A:505:PHE:HB2	1:A:534:VAL:HG12	1.92	0.52
1:A:353:GLN:HG3	8:A:2376:HOH:O	2.09	0.51
1:A:703:CYS:HA	1:A:708:GLY:O	2.10	0.51
1:A:45:LYS:HB3	1:A:457:LEU:CD2	2.40	0.51
1:A:496:LEU:HD21	8:A:2011:HOH:O	2.10	0.51
1:A:58:MET:C	1:A:60:LEU:H	2.14	0.51
1:A:300:LEU:C	1:A:300:LEU:HD23	2.31	0.51
1:A:347:VAL:O	1:A:389:ALA:HB1	2.10	0.51
1:A:45:LYS:HD3	8:A:2274:HOH:O	2.11	0.51
1:A:192:TYR:CB	8:A:2135:HOH:O	2.58	0.51
1:A:538:TYR:CD2	1:A:540:PRO:HD3	2.45	0.51
1:A:628:TRP:CD1	1:A:646:GLY:HA3	2.45	0.51
1:A:205:GLN:HG3	1:A:243:TYR:HB2	1.93	0.51
1:A:133:ARG:HD2	1:A:582:GLU:OE1	2.11	0.51
1:A:148:LEU:C	1:A:148:LEU:CD2	2.79	0.51
1:A:297:ARG:HH11	1:A:360:GLN:NE2	2.09	0.51
1:A:300:LEU:CB	1:A:357:VAL:HG12	2.40	0.51
1:A:231:PHE:CD1	3:A:1004:FTT:H143	2.46	0.50
1:A:300:LEU:HD12	1:A:357:VAL:HG11	1.92	0.50
1:A:316:GLY:C	8:A:2217:HOH:O	2.50	0.50
1:A:390:TRP:HE1	1:A:431:SER:HB2	1.75	0.50
1:A:542:ASP:OD2	1:A:543:ARG:HG3	2.11	0.50
1:A:313:TYR:HA	8:A:2211:HOH:O	2.11	0.50
1:A:422:ASP:O	1:A:423:PHE:HB2	2.11	0.50
1:A:370:ILE:HG22	1:A:372:HIS:NE2	2.27	0.50
1:A:25:ALA:O	1:A:26:ALA:HB3	2.12	0.50
1:A:39:THR:HG23	1:A:375:LEU:HD22	1.93	0.50
1:A:650:THR:HB	1:A:666:TYR:CE1	2.47	0.50
1:A:60:LEU:HD21	1:A:628:TRP:CZ3	2.47	0.50
1:A:159:GLU:HA	8:A:2109:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:O	1:A:43:ILE:HG12	2.12	0.50
1:A:422:ASP:O	1:A:424:ASN:N	2.40	0.50
1:A:540:PRO:HD2	1:A:545:ILE:O	2.12	0.49
1:A:45:LYS:HE2	1:A:496:LEU:CD2	2.42	0.49
1:A:86:THR:HA	8:A:2047:HOH:O	2.12	0.49
1:A:364:LYS:HG2	8:A:2231:HOH:O	2.12	0.49
1:A:386:ASP:OD2	1:A:437:LEU:HD13	2.13	0.49
1:A:628:TRP:HD1	1:A:646:GLY:HA3	1.78	0.49
1:A:93:ARG:HG3	1:A:552:TYR:OH	2.13	0.49
1:A:333:ALA:O	1:A:335:ALA:N	2.46	0.49
1:A:424:ASN:HA	8:A:2258:HOH:O	2.12	0.49
1:A:637:PRO:HA	8:A:2359:HOH:O	2.13	0.49
1:A:693:ASN:HD22	1:A:715:ARG:N	2.11	0.49
1:A:67:LYS:CE	8:A:2050:HOH:O	2.57	0.49
1:A:540:PRO:HG3	1:A:545:ILE:HG13	1.95	0.49
1:A:93:ARG:HG3	1:A:552:TYR:CZ	2.47	0.49
1:A:402:LEU:O	1:A:405:PRO:HD2	2.13	0.49
1:A:455:LYS:N	1:A:455:LYS:CE	2.66	0.49
1:A:134:GLY:N	1:A:146:GLY:HA2	2.27	0.49
1:A:387:ILE:O	1:A:435:ARG:HA	2.12	0.49
1:A:422:ASP:C	1:A:424:ASN:H	2.17	0.49
1:A:680:VAL:HG12	1:A:680:VAL:O	2.12	0.48
1:A:330:ALA:HA	1:A:337:LYS:NZ	2.28	0.48
1:A:165:GLN:NE2	8:A:2115:HOH:O	2.46	0.48
1:A:693:ASN:HB3	1:A:715:ARG:HA	1.95	0.48
1:A:19:GLU:HG2	8:A:2087:HOH:O	2.14	0.48
1:A:82:GLY:HA2	8:A:2044:HOH:O	2.12	0.48
1:A:192:TYR:HB3	8:A:2135:HOH:O	2.13	0.48
1:A:29:ALA:HB1	1:A:546:VAL:HG23	1.94	0.48
1:A:454:ASP:C	1:A:456:VAL:H	2.16	0.48
1:A:600:THR:HG23	8:A:2036:HOH:O	2.14	0.48
1:A:674:ARG:HG3	1:A:688:ALA:HB2	1.96	0.48
1:A:167:LYS:HD2	1:A:175:GLN:CD	2.33	0.48
1:A:264:THR:HA	1:A:711:TRP:CG	2.49	0.48
1:A:393:TYR:HB3	8:A:2247:HOH:O	2.12	0.47
1:A:412:HIS:CD2	1:A:412:HIS:H	2.32	0.47
1:A:93:ARG:NH2	1:A:533:GLU:OE1	2.27	0.47
1:A:153:SER:HB3	8:A:2106:HOH:O	2.14	0.47
1:A:337:LYS:HD3	8:A:2222:HOH:O	2.13	0.47
1:A:384:ARG:NH2	2:B:11:KDO:O1B	2.47	0.47
1:A:410:HIS:O	1:A:411:HIS:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:TYR:HE2	1:A:633:PHE:CE1	2.32	0.47
1:A:381:MET:HG3	1:A:442:GLN:HB3	1.94	0.47
1:A:594:ASN:O	1:A:629:ALA:HA	2.15	0.47
1:A:480:ASP:HB3	1:A:523:ILE:HD11	1.96	0.47
1:A:204:GLN:HB2	8:A:2141:HOH:O	2.14	0.47
1:A:430:ASN:C	1:A:430:ASN:HD22	2.16	0.47
1:A:184:LEU:HD12	1:A:190:TYR:HB3	1.97	0.46
1:A:218:ALA:HA	1:A:231:PHE:O	2.14	0.46
1:A:567:SER:O	1:A:569:PHE:N	2.41	0.46
1:A:155:ARG:O	1:A:193:ARG:HD2	2.15	0.46
1:A:486:GLN:HG2	1:A:511:PHE:CG	2.51	0.46
1:A:505:PHE:HA	1:A:534:VAL:HA	1.96	0.46
3:A:1004:FTT:H42	3:A:1006:FTT:H22	1.97	0.46
1:A:185:ASP:OD2	1:A:189:VAL:HG12	2.15	0.46
1:A:298:GLN:HG3	1:A:359:THR:OG1	2.16	0.46
1:A:309:GLN:HG2	1:A:348:ASP:HB3	1.97	0.46
1:A:465:ASP:O	1:A:485:LYS:HA	2.16	0.46
1:A:495:TYR:HD1	1:A:497:PHE:HD1	1.63	0.46
1:A:644:GLY:O	1:A:672:LEU:N	2.49	0.46
8:A:2389:HOH:O	2:B:9:GLA:H3	2.15	0.46
1:A:578:ALA:HA	1:A:603:ASP:O	2.15	0.46
1:A:74:PRO:HG3	1:A:584:GLU:HB2	1.97	0.46
1:A:326:SER:HB3	1:A:329:CYS:HB2	1.96	0.46
1:A:436:ILE:HG22	1:A:437:LEU:N	2.31	0.46
1:A:474:ARG:HH11	1:A:474:ARG:HG2	1.80	0.46
1:A:628:TRP:CZ3	1:A:630:ASP:OD1	2.69	0.46
1:A:345:TYR:CD1	1:A:345:TYR:C	2.89	0.46
1:A:368:GLY:O	1:A:369:ASP:HB2	2.15	0.46
1:A:583:ILE:O	1:A:598:SER:HA	2.16	0.46
1:A:427:ASP:C	1:A:429:ALA:N	2.69	0.46
1:A:199:ARG:HG3	1:A:199:ARG:HH11	1.81	0.45
1:A:631:TYR:O	1:A:642:THR:HA	2.17	0.45
1:A:673:VAL:CG2	1:A:689:LEU:HB3	2.46	0.45
1:A:352:LEU:HB3	1:A:385:ASN:OD1	2.16	0.45
1:A:635:ASP:O	1:A:636:GLY:O	2.34	0.45
1:A:80:THR:HG21	1:A:89:HIS:ND1	2.30	0.45
1:A:390:TRP:HE1	1:A:431:SER:CB	2.28	0.45
1:A:446:TYR:CB	1:A:463:ARG:HB2	2.41	0.45
1:A:678:ALA:C	1:A:680:VAL:H	2.20	0.45
1:A:80:THR:OG1	1:A:91:ILE:HG13	2.16	0.45
1:A:167:LYS:HD2	1:A:175:GLN:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLN:HB2	8:A:2166:HOH:O	2.17	0.45
1:A:522:ASN:HD22	1:A:522:ASN:HA	1.58	0.45
1:A:725:PHE:CD1	1:A:725:PHE:N	2.85	0.45
1:A:412:HIS:CD2	1:A:412:HIS:N	2.83	0.45
1:A:586:LYS:HA	1:A:595:VAL:O	2.16	0.45
5:A:1014:PO4:O3	2:B:2:GCN:C6	2.64	0.45
1:A:576:ILE:HD11	1:A:606:TYR:CE1	2.52	0.45
1:A:126:LEU:CD2	1:A:151:MET:HB3	2.47	0.45
1:A:42:PRO:CG	1:A:45:LYS:HD2	2.48	0.45
1:A:246:TRP:CZ3	1:A:315:TYR:CE1	3.04	0.45
1:A:390:TRP:CE2	1:A:426:LYS:HB2	2.52	0.45
1:A:390:TRP:CE2	1:A:426:LYS:CB	3.00	0.45
1:A:592:SER:O	1:A:631:TYR:HA	2.16	0.45
1:A:302:PHE:CE2	3:A:1006:FTT:H3	2.53	0.44
1:A:486:GLN:HG2	1:A:511:PHE:CB	2.48	0.44
1:A:583:ILE:O	1:A:583:ILE:HG13	2.15	0.44
1:A:93:ARG:HH11	1:A:133:ARG:HD2	1.82	0.44
1:A:390:TRP:NE1	1:A:431:SER:HB2	2.32	0.44
1:A:82:GLY:CA	8:A:2044:HOH:O	2.64	0.44
1:A:507:TYR:HD1	1:A:532:TYR:CE1	2.35	0.44
1:A:612:TYR:O	1:A:613:LYS:HB2	2.18	0.44
1:A:28:ILE:HD12	8:A:2025:HOH:O	2.18	0.44
1:A:407:SER:HA	8:A:2250:HOH:O	2.17	0.44
1:A:397:VAL:HB	1:A:421:PHE:CE1	2.52	0.44
1:A:595:VAL:HG12	1:A:629:ALA:CB	2.47	0.44
1:A:234:TYR:HB3	1:A:281:MET:CG	2.48	0.43
1:A:370:ILE:HG12	1:A:453:TRP:CD1	2.52	0.43
1:A:470:GLU:HG3	1:A:481:LYS:CG	2.47	0.43
1:A:636:GLY:HA3	1:A:637:PRO:HD2	1.90	0.43
1:A:384:ARG:NH1	1:A:439:LYS:HE2	2.33	0.43
1:A:418:ASN:HB3	8:A:2256:HOH:O	2.18	0.43
1:A:507:TYR:OH	1:A:530:LYS:HD2	2.18	0.43
1:A:565:GLU:O	1:A:566:GLY:O	2.35	0.43
1:A:695:PHE:O	1:A:697:ARG:N	2.50	0.43
1:A:722:THR:HG21	8:A:2115:HOH:O	2.17	0.43
1:A:471:SER:O	1:A:479:THR:HA	2.18	0.43
1:A:558:ASN:OD1	1:A:572:GLU:HB2	2.18	0.43
1:A:633:PHE:HD2	1:A:641:LEU:HB3	1.82	0.43
1:A:284:TYR:HD2	3:A:1004:FTT:H131	1.84	0.43
1:A:365:PHE:HE1	1:A:372:HIS:ND1	2.15	0.43
1:A:612:TYR:CZ	1:A:657:PRO:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:TYR:CE2	1:A:633:PHE:CE1	3.06	0.43
1:A:413:HIS:HD2	8:A:2252:HOH:O	2.01	0.43
1:A:427:ASP:O	1:A:429:ALA:N	2.52	0.43
1:A:430:ASN:HD22	1:A:431:SER:N	2.17	0.43
1:A:135:PRO:HB3	1:A:510:SER:HB3	2.01	0.43
1:A:196:GLY:HA2	1:A:214:ALA:O	2.19	0.43
1:A:44:GLN:HG2	1:A:45:LYS:N	2.34	0.42
1:A:197:LEU:C	1:A:197:LEU:HD12	2.40	0.42
1:A:80:THR:HB	8:A:2055:HOH:O	2.18	0.42
1:A:93:ARG:NH1	1:A:582:GLU:OE1	2.52	0.42
1:A:300:LEU:HB2	1:A:357:VAL:HG12	2.00	0.42
1:A:64:LYS:HG3	1:A:199:ARG:HH22	1.82	0.42
1:A:134:GLY:O	1:A:136:VAL:HG13	2.20	0.42
1:A:264:THR:HG21	1:A:698:GLU:HG2	2.00	0.42
1:A:495:TYR:HD1	1:A:497:PHE:CD1	2.38	0.42
1:A:103:ASN:ND2	1:A:147:GLY:O	2.52	0.42
1:A:229:PHE:HB2	1:A:286:PHE:HD1	1.84	0.42
1:A:357:VAL:O	1:A:357:VAL:HG23	2.20	0.42
1:A:364:LYS:CD	1:A:373:THR:HG23	2.49	0.42
3:A:1002:FTT:C10	3:A:1005:FTT:H51	2.50	0.42
1:A:282:VAL:HG11	3:A:1007:FTT:H72	2.02	0.42
1:A:300:LEU:HD12	1:A:357:VAL:HG12	2.00	0.42
1:A:661:PHE:CD1	1:A:661:PHE:N	2.87	0.42
1:A:28:ILE:HD12	1:A:28:ILE:N	2.16	0.42
1:A:138:VAL:HG23	1:A:462:GLY:HA2	2.01	0.42
1:A:173:LEU:HD23	1:A:718:VAL:HG22	2.02	0.42
1:A:46:VAL:HG12	1:A:48:GLN:H	1.85	0.42
1:A:199:ARG:HG3	1:A:199:ARG:NH1	2.35	0.42
1:A:465:ASP:N	1:A:486:GLN:O	2.48	0.42
7:A:1022:PFC:O11	7:A:1022:PFC:N3	2.46	0.42
1:A:155:ARG:O	1:A:193:ARG:CD	2.68	0.42
1:A:194:LEU:HD12	1:A:194:LEU:HA	1.88	0.42
1:A:271:LYS:HG3	1:A:417:VAL:HG21	2.02	0.42
1:A:410:HIS:HB3	1:A:411:HIS:H	1.71	0.42
1:A:160:PRO:HG3	8:A:2126:HOH:O	2.20	0.42
1:A:226:LYS:HB3	1:A:289:GLU:HB3	2.01	0.42
1:A:388:ASN:HD22	1:A:435:ARG:HG2	1.84	0.42
1:A:628:TRP:HZ3	1:A:630:ASP:OD1	2.02	0.42
1:A:715:ARG:HG2	1:A:715:ARG:NH1	2.33	0.42
1:A:633:PHE:CE2	1:A:641:LEU:HD23	2.55	0.41
1:A:458:VAL:HG13	1:A:458:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1002:FTT:O2	3:A:1005:FTT:H22	2.21	0.41
1:A:131:ILE:HD13	1:A:149:LEU:HA	2.02	0.41
1:A:145:PRO:HD2	8:A:2057:HOH:O	2.19	0.41
1:A:590:SER:HB3	1:A:593:VAL:CB	2.50	0.41
1:A:497:PHE:HB3	1:A:498:ASP:H	1.61	0.41
1:A:673:VAL:HG22	1:A:689:LEU:HB3	2.02	0.41
1:A:184:LEU:HB2	1:A:190:TYR:HB2	2.01	0.41
1:A:256:LEU:O	1:A:257:PRO:C	2.59	0.41
1:A:613:LYS:C	1:A:615:ASN:N	2.67	0.41
1:A:422:ASP:C	1:A:424:ASN:N	2.74	0.41
1:A:62:GLN:HB3	1:A:167:LYS:HZ1	1.86	0.41
1:A:170:THR:HG22	1:A:171:ASP:N	2.36	0.41
1:A:446:TYR:HB3	1:A:463:ARG:CB	2.44	0.41
1:A:507:TYR:CD1	1:A:532:TYR:CE1	3.09	0.41
1:A:32:GLN:HB2	8:A:2087:HOH:O	2.21	0.41
1:A:68:GLU:C	1:A:70:LEU:H	2.24	0.41
1:A:141:GLY:HA3	1:A:442:GLN:HE22	1.86	0.41
3:A:1002:FTT:H101	3:A:1005:FTT:H51	2.02	0.41
1:A:579:ARG:HH11	1:A:579:ARG:HG3	1.86	0.40
5:A:1014:PO4:O3	2:B:2:GCN:H61	2.21	0.40
1:A:67:LYS:HZ2	1:A:67:LYS:HB3	1.86	0.40
1:A:138:VAL:HG13	1:A:139:LEU:HG	2.02	0.40
1:A:168:ALA:HA	1:A:173:LEU:O	2.22	0.40
1:A:37:THR:HB	1:A:448:GLN:HE22	1.86	0.40
1:A:217:PRO:CB	3:A:1007:FTT:H143	2.51	0.40
1:A:239:PRO:O	1:A:276:SER:HB3	2.22	0.40
1:A:380:PHE:HD1	1:A:443:THR:OG1	2.05	0.40
1:A:464:TYR:HD1	1:A:487:PHE:HB2	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	705/725 (97%)	618 (88%)	72 (10%)	15 (2%)	7 29

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	411	HIS
1	A	636	GLY
1	A	368	GLY
1	A	418	ASN
1	A	454	ASP
1	A	497	PHE
1	A	566	GLY
1	A	613	LYS
1	A	696	ASP
1	A	334	PRO
1	A	415	SER
1	A	679	ARG
1	A	635	ASP
1	A	405	PRO
1	A	398	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	587/601 (98%)	561 (96%)	26 (4%)	28 62

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LYS
1	A	68	GLU
1	A	73	THR
1	A	77	SER
1	A	93	ARG
1	A	112	GLN

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Mol	Chain	Res	Type
1	A	118	ASP
1	A	199	ARG
1	A	205	GLN
1	A	268	GLU
1	A	275	TYR
1	A	315	TYR
1	A	336	ASP
1	A	352	LEU
1	A	353	GLN
1	A	354	ASN
1	A	381	MET
1	A	397	VAL
1	A	426	LYS
1	A	430	ASN
1	A	455	LYS
1	A	497	PHE
1	A	522	ASN
1	A	542	ASP
1	A	565	GLU
1	A	722	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	112	GLN
1	A	165	GLN
1	A	202	ASN
1	A	205	GLN
1	A	310	ASN
1	A	328	GLN
1	A	354	ASN
1	A	360	GLN
1	A	388	ASN
1	A	404	ASN
1	A	410	HIS
1	A	412	HIS
1	A	430	ASN
1	A	438	ASN
1	A	522	ASN
1	A	594	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	GCN	B	1	3,2	11,11,11	1.03	1 (9%)	14,15,15	2.44	4 (28%)
2	GMH	B	10	2	13,13,14	0.80	0	17,18,20	1.64	3 (17%)
2	KDO	B	11	2	15,15,16	0.89	0	19,21,24	0.97	1 (5%)
2	GCN	B	2	3,2	10,10,11	1.38	1 (10%)	13,13,15	4.41	9 (69%)
2	KDO	B	3	2	15,15,16	0.88	0	19,21,24	1.12	1 (5%)
2	GMH	B	4	4,2	13,13,14	0.77	0	17,18,20	0.75	0
2	GMH	B	5	2,5	13,13,14	0.96	1 (7%)	17,18,20	1.22	3 (17%)
2	GLC	B	6	2	11,11,12	1.08	1 (9%)	15,15,17	1.61	3 (20%)
2	GLC	B	7	2	11,11,12	1.06	1 (9%)	15,15,17	1.81	3 (20%)
2	GLC	B	8	2	11,11,12	1.44	2 (18%)	15,15,17	0.96	1 (6%)
2	GLA	B	9	2	11,11,12	0.69	0	15,15,17	0.98	1 (6%)

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	GCN	B	1	3,2	-	0/2/18/18	0/1/1/1
2	GMH	B	10	2	1/1/5/6	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KDO	B	11	2	-	3/10/26/30	0/1/1/1
2	GCN	B	2	3,2	1/1/3/4	1/2/15/18	0/1/1/1
2	KDO	B	3	2	-	5/10/26/30	0/1/1/1
2	GMH	B	4	4,2	-	0/6/23/26	0/1/1/1
2	GMH	B	5	2,5	1/1/5/6	4/6/23/26	1/1/1/1
2	GLC	B	6	2	-	0/2/19/22	0/1/1/1
2	GLC	B	7	2	-	2/2/19/22	0/1/1/1
2	GLC	B	8	2	1/1/4/5	0/2/19/22	0/1/1/1
2	GLA	B	9	2	-	2/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	GLC	C2-C3	3.19	1.57	1.52
2	B	8	GLC	C1-C2	2.56	1.58	1.52
2	B	7	GLC	C4-C3	2.48	1.58	1.52
2	B	2	GCN	O5-C5	2.41	1.48	1.43
2	B	1	GCN	C3-C4	-2.34	1.48	1.52
2	B	5	GMH	O5-C5	2.23	1.46	1.43
2	B	6	GLC	O5-C5	2.02	1.47	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	GCN	C3-C2-C1	12.09	119.64	109.82
2	B	1	GCN	C6-C5-C4	-7.72	102.77	113.54
2	B	2	GCN	C3-C4-C5	4.85	117.06	110.77
2	B	2	GCN	C6-C5-C4	-4.60	107.12	113.54
2	B	7	GLC	C1-C2-C3	-4.43	104.22	109.67
2	B	2	GCN	O5-C1-C2	-4.41	104.75	111.47
2	B	10	GMH	C1-O5-C5	3.89	117.86	111.48
2	B	6	GLC	C6-C5-C4	-3.53	104.73	113.00
2	B	10	GMH	O5-C1-C2	3.52	116.21	110.77
2	B	2	GCN	C4-C3-C2	-3.51	108.28	112.39
2	B	7	GLC	C6-C5-C4	3.47	121.12	113.00
2	B	10	GMH	C1-C2-C3	3.43	113.88	109.67
2	B	6	GLC	C1-O5-C5	3.34	116.71	112.19
2	B	2	GCN	C1-C2-N2	3.02	117.86	111.60
2	B	5	GMH	C6-C5-C4	-2.93	109.16	114.03
2	B	5	GMH	C7-C6-C5	2.82	117.88	112.17
2	B	2	GCN	C1-O5-C5	2.72	115.87	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	5	GMH	C1-O5-C5	2.69	115.88	111.48
2	B	8	GLC	C1-C2-C3	-2.67	106.39	109.67
2	B	6	GLC	O3-C3-C2	2.54	114.85	109.99
2	B	9	GLA	C1-O5-C5	2.49	115.56	112.19
2	B	1	GCN	C1-C2-N2	2.47	115.01	110.49
2	B	2	GCN	O5-C5-C6	2.46	111.06	107.20
2	B	1	GCN	C3-C2-N2	-2.16	103.16	110.84
2	B	2	GCN	O5-C5-C4	2.16	113.27	109.64
2	B	7	GLC	C3-C4-C5	-2.15	106.41	110.24
2	B	3	KDO	C7-C6-C5	-2.13	110.51	114.03
2	B	1	GCN	O5-C5-C4	2.09	112.94	110.06
2	B	11	KDO	O1B-C1-C2	2.03	118.82	113.03

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2	GCN	C1
2	B	5	GMH	C6
2	B	8	GLC	C1
2	B	10	GMH	C6

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	KDO	C5-C6-C7-O7
2	B	3	KDO	O6-C6-C7-O7
2	B	5	GMH	C4-C5-C6-C7
2	B	5	GMH	C4-C5-C6-O6
2	B	5	GMH	O5-C5-C6-C7
2	B	5	GMH	O5-C5-C6-O6
2	B	11	KDO	O7-C7-C8-O8
2	B	9	GLA	O5-C5-C6-O6
2	B	11	KDO	C6-C7-C8-O8
2	B	7	GLC	O5-C5-C6-O6
2	B	9	GLA	C4-C5-C6-O6
2	B	7	GLC	C4-C5-C6-O6
2	B	3	KDO	O6-C6-C7-C8
2	B	2	GCN	O5-C5-C6-O6
2	B	11	KDO	O1A-C1-C2-O6
2	B	3	KDO	O1A-C1-C2-C3
2	B	3	KDO	C5-C6-C7-C8

All (1) ring outliers are listed below:

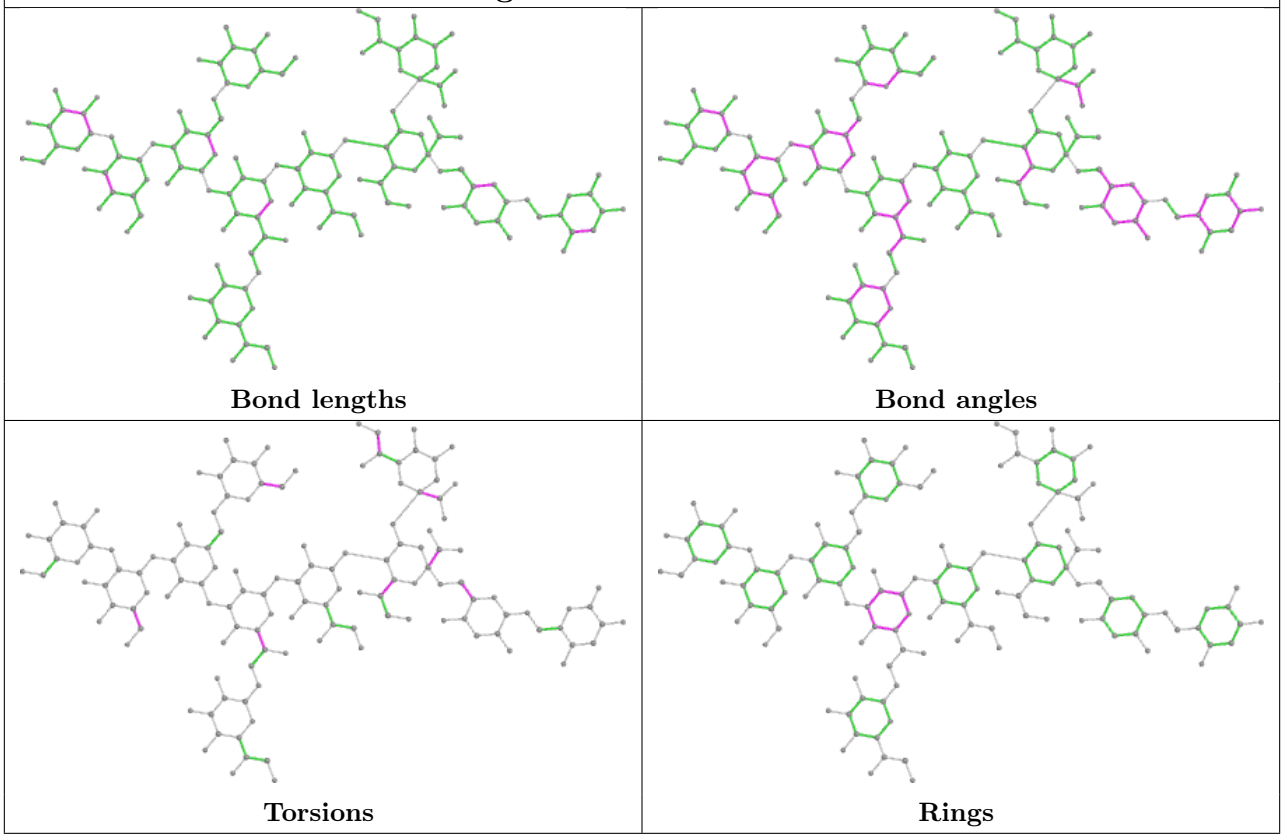
Mol	Chain	Res	Type	Atoms
2	B	5	GMH	C1-C2-C3-C4-C5-O5

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	GCN	2	0
2	B	4	GMH	2	0
2	B	9	GLA	1	0
2	B	5	GMH	1	0
2	B	10	GMH	1	0
2	B	11	KDO	1	0
2	B	3	KDO	1	0

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

Oligosaccharide Chain B



5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	PFC	A	1022	-	62,62,62	0.66	0	71,95,95	0.86	2 (2%)
3	FTT	A	1004	3,2	15,15,16	0.97	1 (6%)	15,15,17	1.85	3 (20%)
3	FTT	A	1002	2	15,15,16	0.43	0	15,15,17	0.78	1 (6%)
3	FTT	A	1006	3,2	16,16,16	1.08	1 (6%)	17,17,17	0.95	1 (5%)
5	PO4	A	1016	6,2	0,3,4	-	-	0,3,6	-	-
3	FTT	A	1005	3	12,12,16	0.43	0	11,11,17	0.64	0
3	FTT	A	1007	3	14,14,16	0.33	0	13,13,17	0.76	0
4	DPO	A	1013	-	3,7,8	1.38	0	6,10,13	0.81	0
4	DPO	A	1015	2	3,7,8	1.14	0	6,10,13	0.87	0
5	PO4	A	1014	-	0,3,4	-	-	0,3,6	-	-
3	FTT	A	1003	2	7,7,16	1.88	1 (14%)	8,8,17	1.34	1 (12%)

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	PFC	A	1022	-	3/3/17/23	12/64/118/118	0/5/7/7
3	FTT	A	1004	3,2	-	3/14/14/15	-
3	FTT	A	1002	2	-	1/14/14/15	-
3	FTT	A	1006	3,2	1/1/2/2	1/15/15/15	-
3	FTT	A	1005	3	-	1/9/10/15	-
3	FTT	A	1007	3	-	0/11/12/15	-
4	DPO	A	1013	-	-	0/2/5/6	-
4	DPO	A	1015	2	-	0/2/5/6	-
3	FTT	A	1003	2	-	3/6/6/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	FTT	O1-C1	4.23	1.45	1.30
3	A	1006	FTT	O1-C1	4.10	1.44	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1004	FTT	C10-C9	3.14	1.69	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1004	FTT	C12-C11-C10	5.52	142.43	114.42
3	A	1003	FTT	O1-C1-O2	-2.87	116.15	123.30
3	A	1004	FTT	O2-C1-C2	-2.84	117.15	125.43
3	A	1006	FTT	O1-C1-O2	-2.76	116.43	123.30
3	A	1004	FTT	C11-C10-C9	2.63	127.78	114.42
7	A	1022	PFC	O17-C8-N4	-2.59	118.58	122.95
7	A	1022	PFC	C17-C8-N4	2.37	121.76	116.10
3	A	1002	FTT	O2-C1-C2	-2.34	118.60	125.43

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1006	FTT	C3
7	A	1022	PFC	N5
7	A	1022	PFC	N6
7	A	1022	PFC	N8

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	FTT	C1-C2-C3-C4
3	A	1003	FTT	C1-C2-C3-C4
3	A	1003	FTT	C2-C3-C4-C5
7	A	1022	PFC	C24-C16-C7-N3
7	A	1022	PFC	C24-C16-C7-O7
7	A	1022	PFC	C38-C11-C2-O2
7	A	1022	PFC	C38-C11-C2-N9
3	A	1004	FTT	O3-C3-C4-C5
3	A	1004	FTT	C9-C10-C11-C12
7	A	1022	PFC	C11-C38-C39-C41
7	A	1022	PFC	C11-C38-C39-C40
3	A	1006	FTT	C11-C10-C9-C8
3	A	1004	FTT	C2-C3-C4-C5
7	A	1022	PFC	N4-C16-C24-C29
3	A	1005	FTT	C1-C2-C3-C4
7	A	1022	PFC	C2-C11-N2-C5
7	A	1022	PFC	C7-C16-C24-C29

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Mol	Chain	Res	Type	Atoms
3	A	1003	FTT	O3-C3-C4-C5
7	A	1022	PFC	C24-C29-C34-N8
7	A	1022	PFC	O1-C1-C10-C18
7	A	1022	PFC	C5-C14-N7-C1

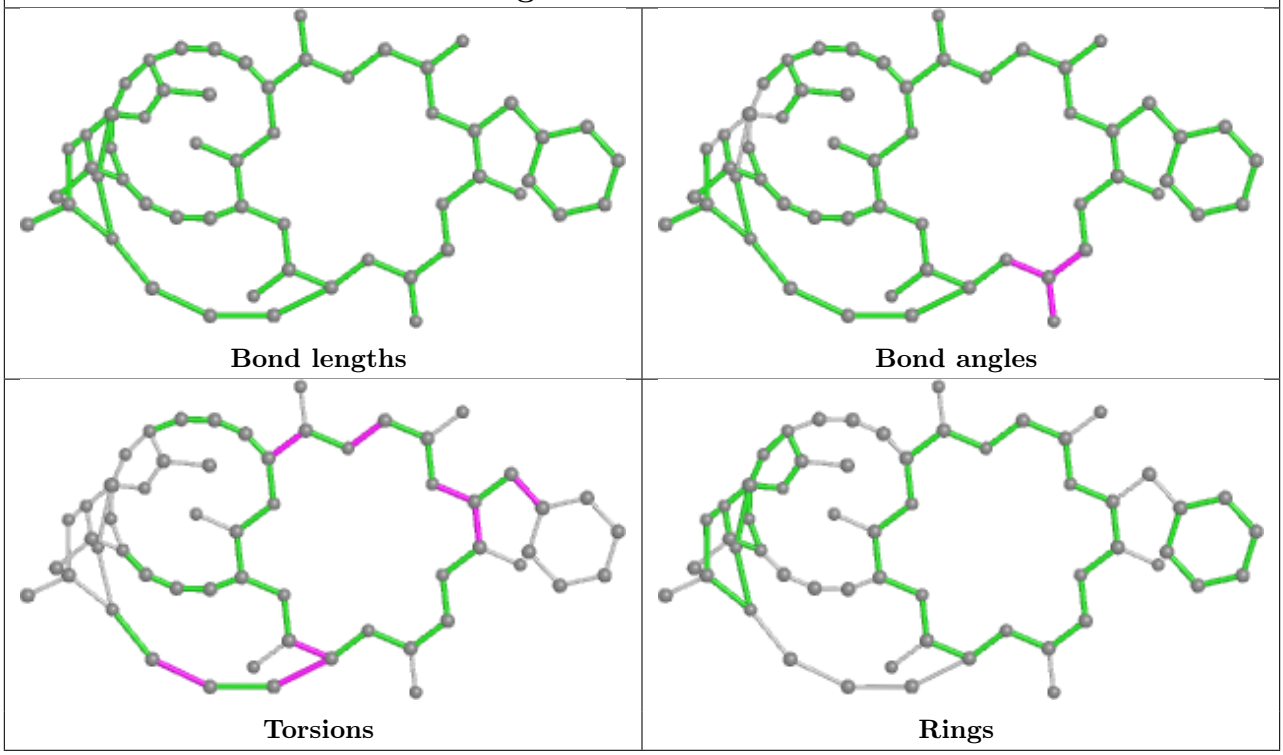
There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1022	PFC	2	0
3	A	1004	FTT	3	0
3	A	1002	FTT	7	0
3	A	1006	FTT	3	0
3	A	1005	FTT	7	0
3	A	1007	FTT	3	0
4	A	1015	DPO	1	0
5	A	1014	PO4	2	0
3	A	1003	FTT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PFC A 1022



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%)	-0.29	12 (1%) 70 53	37, 68, 106, 121	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	HIS	5.1
1	A	411	HIS	4.6
1	A	495	TYR	3.3
1	A	403	TYR	3.0
1	A	118	ASP	2.3
1	A	101	SER	2.2
1	A	568	PHE	2.2
1	A	409	HIS	2.2
1	A	102	GLN	2.1
1	A	369	ASP	2.1
1	A	453	TRP	2.0
1	A	113	GLY	2.0

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

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

6.3 Carbohydrates (i)

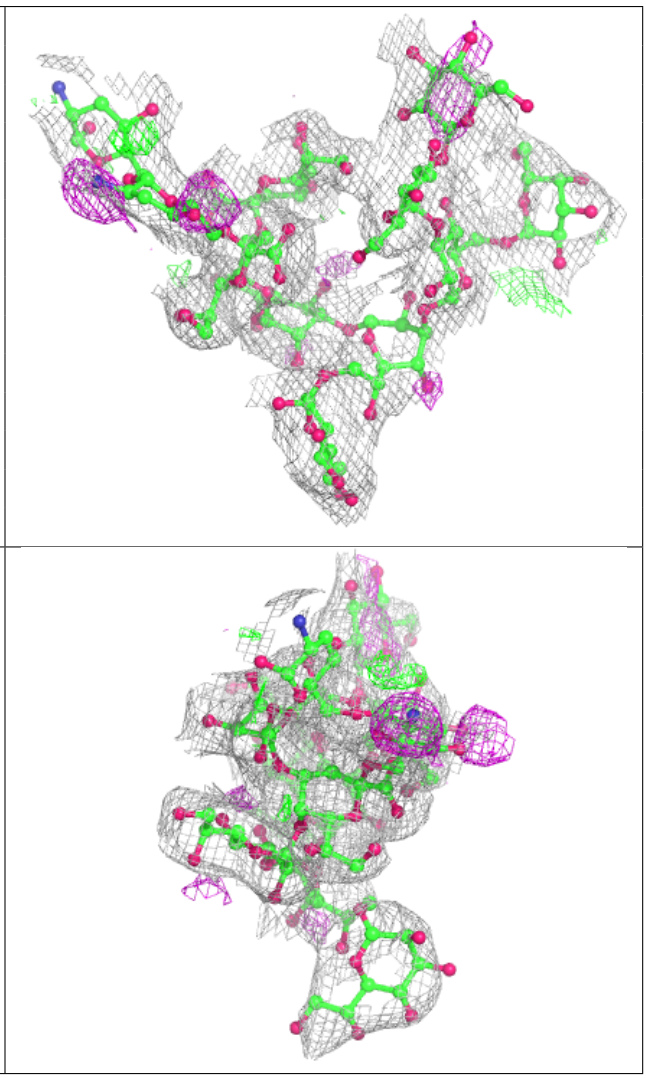
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	B	8	11/12	0.60	0.52	116,120,120,120	0
2	GLA	B	9	11/12	0.77	0.27	120,120,120,120	0
2	GMH	B	10	13/14	0.81	0.22	115,119,120,120	0
2	GLC	B	6	11/12	0.82	0.19	108,112,119,120	0
2	GLC	B	7	11/12	0.86	0.36	120,120,120,120	0
2	GMH	B	5	13/14	0.88	0.12	93,104,117,118	0
2	GCN	B	2	10/11	0.89	0.13	35,49,58,61	0
2	KDO	B	11	15/16	0.90	0.18	84,88,91,93	0
2	GCN	B	1	11/11	0.95	0.11	51,63,74,80	0
2	GMH	B	4	13/14	0.96	0.12	71,76,84,85	0
2	KDO	B	3	15/16	0.97	0.09	64,67,75,78	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.

Electron density around Chain B:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands (i)

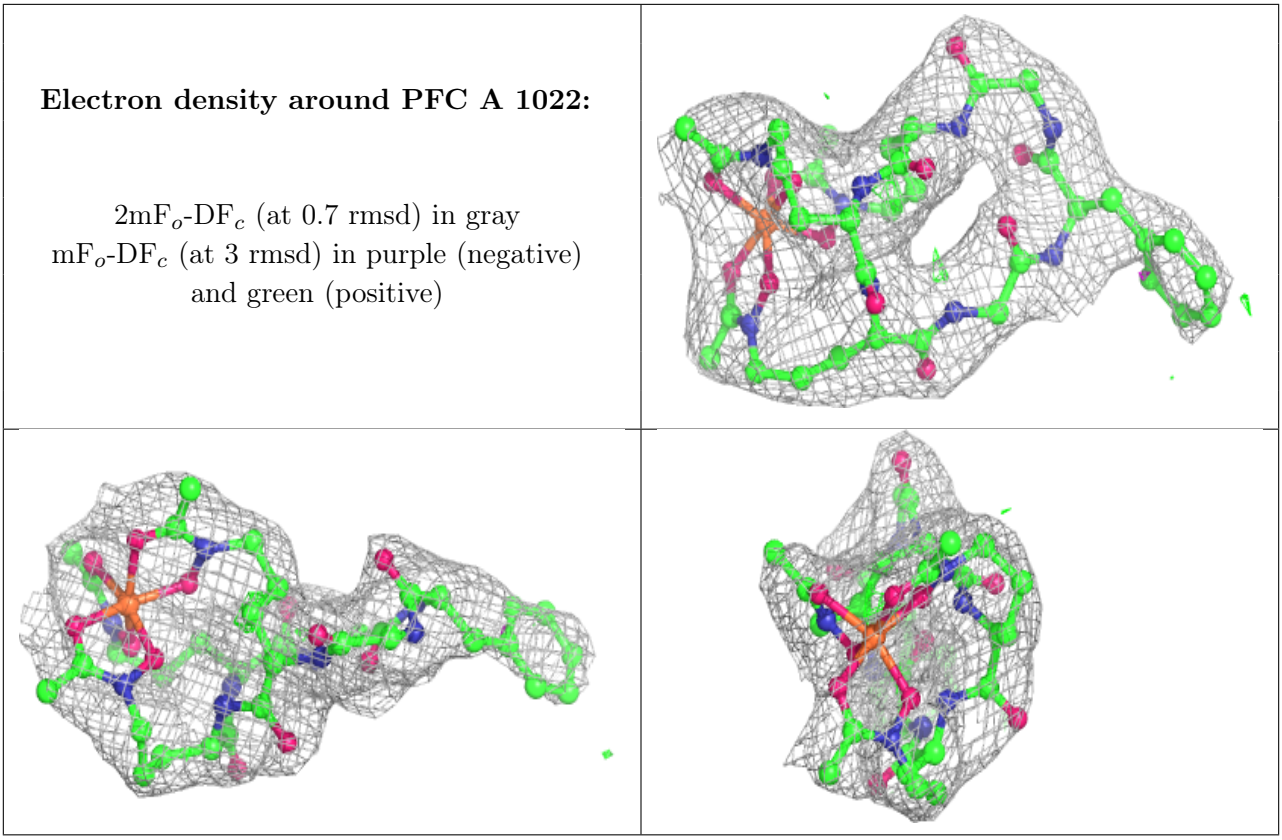
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PO4	A	1016	4/5	0.86	0.09	116,117,120,120	0
3	FTT	A	1007	15/17	0.89	0.69	76,91,104,107	0
3	FTT	A	1002	16/17	0.89	0.33	63,68,77,81	0
3	FTT	A	1003	8/17	0.90	0.19	81,89,91,97	0
6	NI	A	1021	1/1	0.90	0.07	120,120,120,120	0
3	FTT	A	1006	17/17	0.92	0.25	67,77,82,82	0
3	FTT	A	1005	13/17	0.92	0.37	58,65,69,69	0
3	FTT	A	1004	16/17	0.93	0.27	46,60,65,66	0
4	DPO	A	1015	8/9	0.94	0.11	84,99,111,113	0
5	PO4	A	1014	4/5	0.94	0.14	70,71,72,73	0
7	PFC	A	1022	56/56	0.96	0.22	43,57,96,99	0
4	DPO	A	1013	8/9	0.97	0.12	64,71,81,82	4

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 PFC A 1022:

$2mF_o$-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.