



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:03 PM UTC

PDB ID : 9J1U / pdb_00009j1u
Title : Structural basis of the bifunctionality of *M. salinexigens* ZYF650T glucosyl-glycerol phosphorylase in glucosylglycerol catabolism
Authors : Lu, D.; Ma, H.L.
Deposited on : 2024-08-05
Resolution : 2.72 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

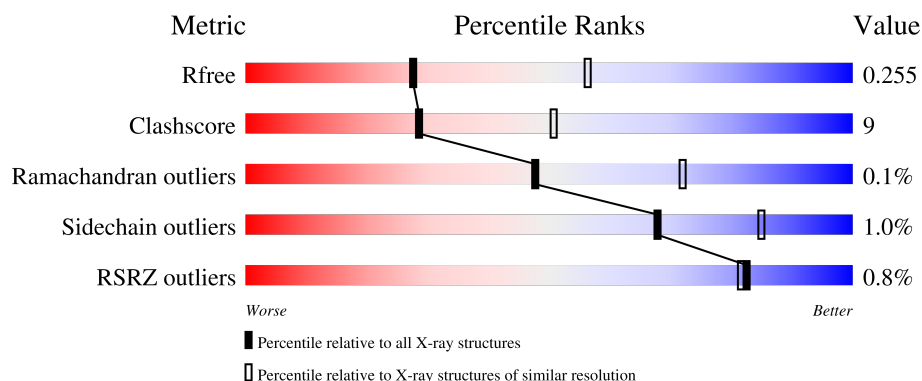
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	480	80% 18% .
1	B	480	78% 21%
1	C	480	81% 18% .
1	D	480	79% 21%
1	E	480	79% 21%

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Mol	Chain	Length	Quality of chain
1	F	480	% 79% 20% .

2 Entry composition [i](#)

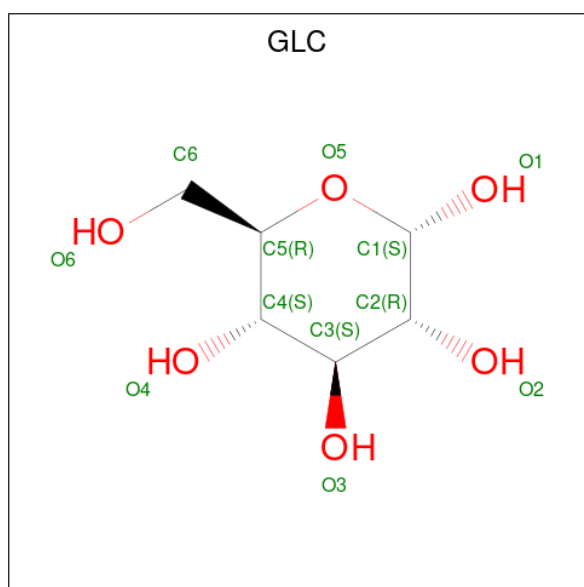
There are 6 unique types of molecules in this entry. The entry contains 23371 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sucrose phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	479	Total	C	N	O	S	0	0	0
			3855	2457	645	731	22			
1	B	479	Total	C	N	O	S	0	0	0
			3855	2457	645	731	22			
1	C	479	Total	C	N	O	S	0	0	0
			3855	2457	645	731	22			
1	D	479	Total	C	N	O	S	0	0	0
			3855	2457	645	731	22			
1	E	479	Total	C	N	O	S	0	0	0
			3855	2457	645	731	22			
1	A	479	Total	C	N	O	S	0	0	0
			3855	2457	645	731	22			

- Molecule 2 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

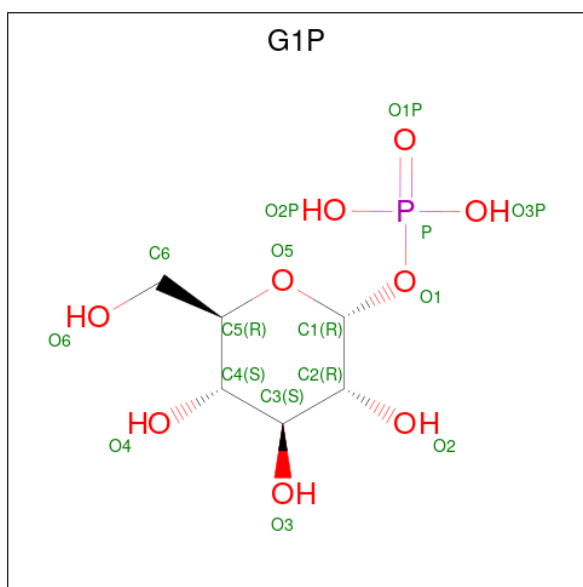


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0

- Molecule 5 is 1-O-phosphono-alpha-D-glucopyranose (CCD ID: G1P) (formula: C₆H₁₃O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O P 16 6 9 1	0	0
5	A	1	Total C O P 16 6 9 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	33	Total O 33 33	0	0
6	B	29	Total O 29 29	0	0
6	C	15	Total O 15 15	0	0
6	D	26	Total O 26 26	0	0

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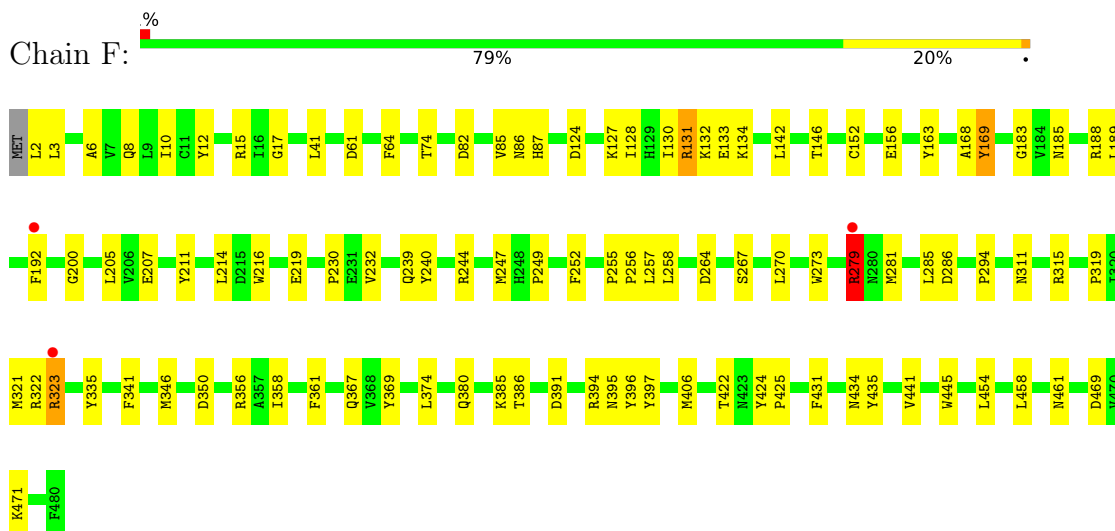
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	12	Total	O	0	0
			12	12		
6	A	19	Total	O	0	0
			19	19		

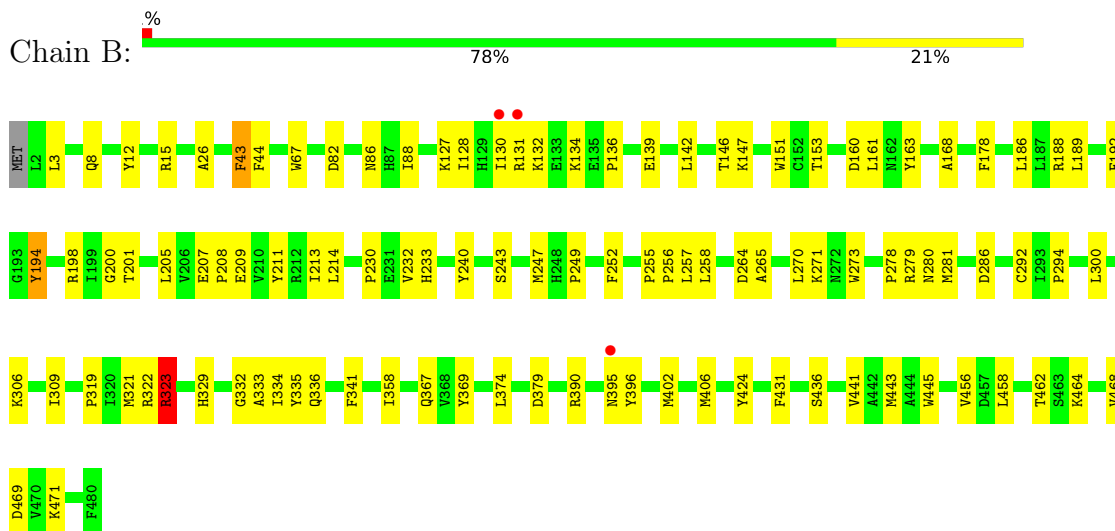
3 Residue-property plots

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.

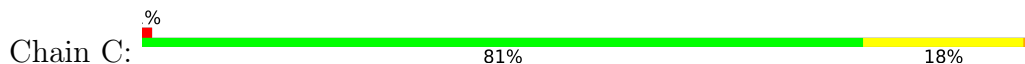
- Molecule 1: Sucrose phosphorylase

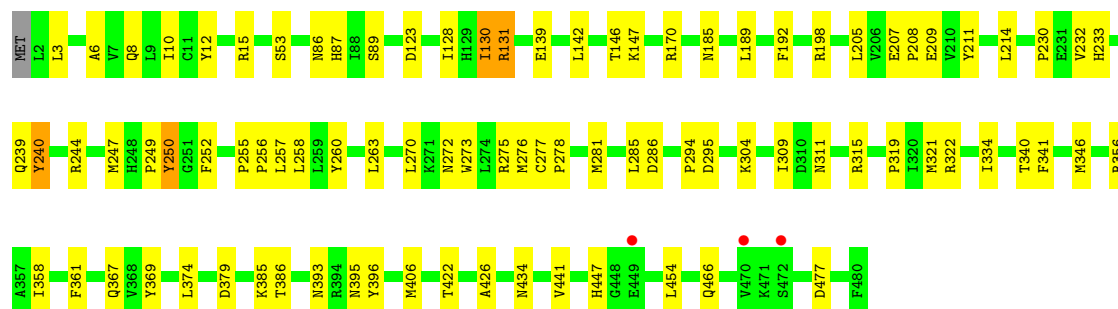


- Molecule 1: Sucrose phosphorylase

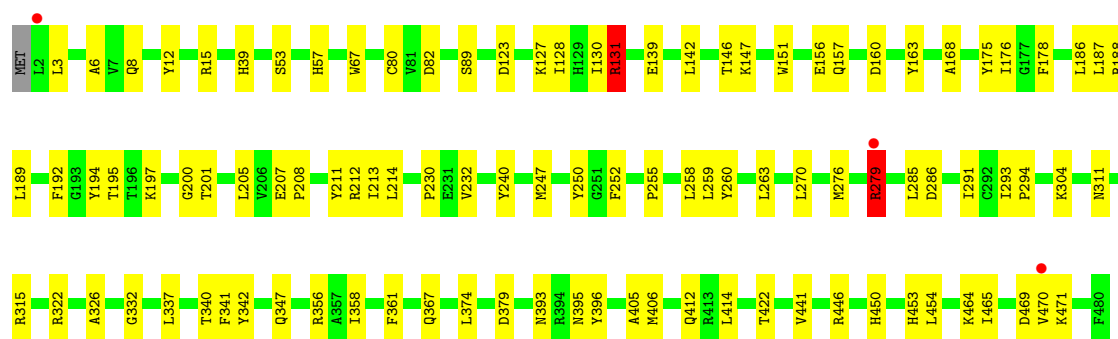
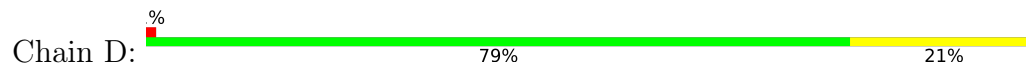


- Molecule 1: Sucrose phosphorylase

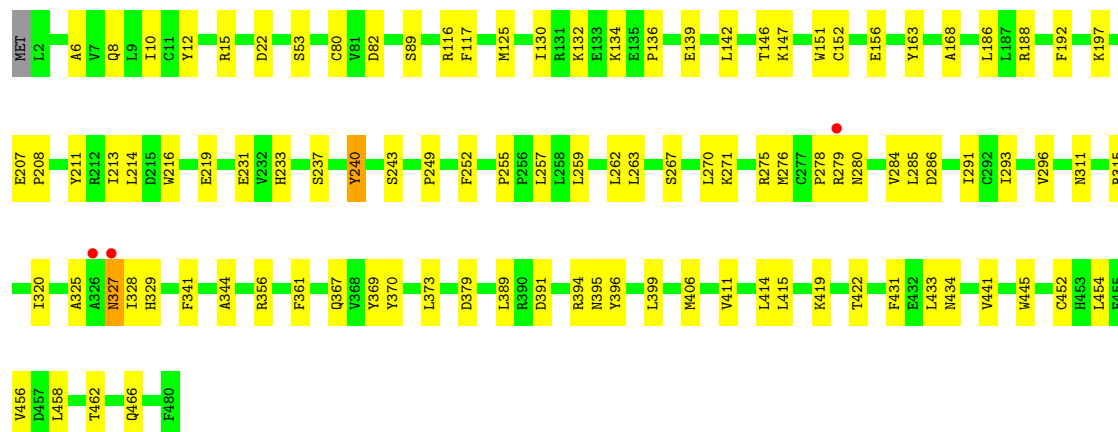
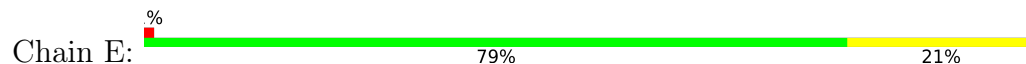




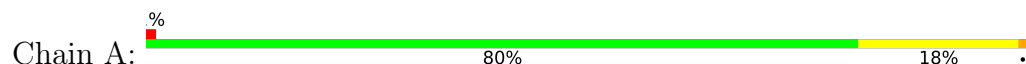
• Molecule 1: Sucrose phosphorylase

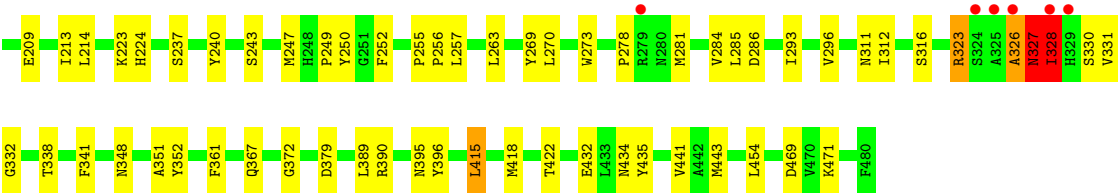


• Molecule 1: Sucrose phosphorylase



• Molecule 1: Sucrose phosphorylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.83Å 178.50Å 180.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.04 – 2.72 21.04 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.3 (21.04-2.72) 99.1 (21.04-2.72)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.72Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.214 , 0.254 0.216 , 0.255	Depositor DCC
R_{free} test set	4624 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23371	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1952e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: G1P, NA, GOL, GLC

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	0.31	0/3952	0.55	3/5369 (0.1%)
1	B	0.32	0/3952	0.59	1/5369 (0.0%)
1	C	0.26	0/3952	0.54	4/5369 (0.1%)
1	D	0.29	0/3952	0.53	1/5369 (0.0%)
1	E	0.28	0/3952	0.55	0/5369
1	F	0.32	0/3952	0.64	6/5369 (0.1%)
All	All	0.30	0/23712	0.57	15/32214 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	LEU	CA-CB-CG	7.02	140.87	116.30
1	A	223	LYS	CA-CB-CG	6.92	127.95	114.10
1	F	323	ARG	CB-CG-CD	-6.65	96.00	111.30
1	C	131	ARG	CB-CG-CD	6.59	126.45	111.30
1	F	279	ARG	CD-NE-CZ	-6.39	115.46	124.40
1	A	326	ALA	N-CA-C	-6.20	105.40	114.39
1	B	323	ARG	N-CA-C	6.04	118.75	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	130	ILE	CA-C-N	-5.70	113.53	122.65
1	C	130	ILE	C-N-CA	-5.70	113.53	122.65
1	F	279	ARG	CG-CD-NE	5.34	123.76	112.00
1	F	131	ARG	CA-C-N	-5.31	113.55	123.05
1	F	131	ARG	C-N-CA	-5.31	113.55	123.05
1	C	170	ARG	CG-CD-NE	-5.11	100.77	112.00
1	D	131	ARG	CD-NE-CZ	5.10	131.55	124.40
1	F	132	LYS	CB-CG-CD	-5.10	99.58	111.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	ARG	Sidechain
1	B	323	ARG	Sidechain
1	D	279	ARG	Sidechain

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	3855	0	3706	63	0
1	B	3855	0	3706	77	0
1	C	3855	0	3706	63	0
1	D	3855	0	3706	67	0
1	E	3855	0	3706	66	0
1	F	3855	0	3706	83	0
2	B	12	0	12	1	0
2	F	12	0	12	0	0
3	B	24	0	32	3	0
3	D	12	0	16	2	0
3	E	6	0	8	0	0
3	F	6	0	8	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	A	16	0	11	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	16	0	11	0	0
6	A	19	0	0	3	0
6	B	29	0	0	3	0
6	C	15	0	0	0	0
6	D	26	0	0	6	0
6	E	12	0	0	0	0
6	F	33	0	0	6	0
All	All	23371	0	22346	400	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 9.

All (400) 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:269:TYR:OH	6:A:601:HOH:O	1.90	0.86
1:C:385:LYS:HD3	1:C:386:THR:HG23	1.58	0.85
1:D:250:TYR:OH	6:D:601:HOH:O	1.93	0.83
1:B:294:PRO:HG3	1:B:322:ARG:HH21	1.46	0.79
1:F:380:GLN:NE2	6:F:601:HOH:O	2.15	0.78
1:B:214:LEU:HB3	1:B:247:MET:HE1	1.66	0.77
1:C:128:ILE:HG22	1:C:130:ILE:HG12	1.67	0.76
1:F:133:GLU:HG2	1:F:323:ARG:HG3	1.68	0.74
1:F:128:ILE:HG22	1:F:130:ILE:HG12	1.69	0.74
1:F:131:ARG:NH1	6:F:604:HOH:O	2.19	0.74
1:B:322:ARG:HD2	1:B:332:GLY:O	1.87	0.74
1:E:379:ASP:HB2	1:E:395:ASN:OD1	1.87	0.73
1:D:128:ILE:HG22	1:D:130:ILE:HG12	1.72	0.72
1:F:458:LEU:O	6:D:602:HOH:O	2.08	0.72
3:D:501:GOL:O3	6:D:602:HOH:O	2.01	0.71
1:A:131:ARG:NH2	5:A:501:G1P:O3P	2.26	0.69
1:A:214:LEU:HG	1:A:247:MET:HE1	1.74	0.69
1:C:286:ASP:HB3	1:C:341:PHE:HB2	1.74	0.69
1:F:374:LEU:HD21	1:F:406:MET:HE2	1.75	0.68
1:B:130:ILE:HG13	1:B:136:PRO:HB3	1.74	0.68
1:D:342:TYR:CE2	1:D:347:GLN:HG3	2.28	0.68
1:E:286:ASP:HB3	1:E:341:PHE:HB2	1.74	0.68
1:C:239:GLN:NE2	1:C:250:TYR:O	2.28	0.67
1:D:8:GLN:HB2	1:D:367:GLN:HG2	1.77	0.66
1:A:198:ARG:NH1	1:A:209:GLU:OE2	2.29	0.66
1:B:128:ILE:HG22	1:B:130:ILE:HG12	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASP:HB3	1:A:341:PHE:HB2	1.79	0.65
1:A:142:LEU:HD12	1:A:146:THR:HB	1.79	0.65
1:A:182:LYS:NZ	6:A:604:HOH:O	2.28	0.65
1:B:3:LEU:HD11	1:B:186:LEU:HD13	1.79	0.64
1:E:262:LEU:HD23	1:E:458:LEU:HD22	1.78	0.64
1:A:134:LYS:NZ	1:A:156:GLU:OE2	2.31	0.64
1:D:212:ARG:NH2	1:A:432:GLU:OE1	2.30	0.64
1:A:249:PRO:HG2	1:A:281:MET:HB3	1.80	0.63
1:D:294:PRO:HG3	1:D:322:ARG:NH2	2.13	0.63
1:A:132:LYS:HG2	1:A:133:GLU:H	1.62	0.63
1:D:6:ALA:HB1	1:D:422:THR:HG23	1.80	0.63
1:C:273:TRP:CH2	1:C:281:MET:HE1	2.34	0.63
1:B:309:ILE:HD13	1:B:334:ILE:HD13	1.80	0.62
1:F:257:LEU:HD21	1:F:270:LEU:HA	1.81	0.62
1:F:219:GLU:OE1	6:F:603:HOH:O	2.16	0.61
1:D:286:ASP:HB3	1:D:341:PHE:HB2	1.82	0.61
1:D:142:LEU:HD12	1:D:146:THR:HB	1.82	0.61
1:E:8:GLN:HB2	1:E:367:GLN:HG2	1.82	0.61
1:B:294:PRO:HG3	1:B:322:ARG:NH2	2.14	0.61
1:B:249:PRO:HG2	1:B:281:MET:HB3	1.83	0.60
1:F:252:PHE:O	1:F:255:PRO:HD2	2.01	0.60
1:D:15:ARG:HG2	1:D:396:TYR:CE1	2.37	0.60
1:F:17:GLY:O	6:F:602:HOH:O	2.16	0.60
1:C:142:LEU:HD12	1:C:146:THR:HB	1.83	0.60
1:A:12:TYR:CD2	1:A:15:ARG:HD2	2.37	0.59
1:F:273:TRP:CH2	1:F:281:MET:HE1	2.37	0.59
1:A:240:TYR:CE1	1:A:278:PRO:HD3	2.37	0.59
1:B:270:LEU:HD23	1:B:441:VAL:HG21	1.85	0.59
1:D:3:LEU:HD11	1:D:186:LEU:HD13	1.84	0.58
1:F:15:ARG:NH1	1:F:396:TYR:HE1	2.01	0.58
1:B:43:PHE:HE1	1:B:44:PHE:CE1	2.22	0.58
1:F:239:GLN:HE21	1:F:249:PRO:HB2	1.69	0.58
1:F:142:LEU:HD12	1:F:146:THR:HB	1.86	0.58
1:F:6:ALA:HB1	1:F:422:THR:HG23	1.85	0.58
1:B:390:ARG:HH12	2:B:502:GLC:H3	1.68	0.58
1:F:322:ARG:NH1	6:F:605:HOH:O	2.21	0.57
1:F:15:ARG:HG2	1:F:396:TYR:CD1	2.39	0.57
1:D:139:GLU:OE2	1:D:147:LYS:HD3	2.04	0.57
1:D:176:ILE:HG23	1:D:187:LEU:HD11	1.86	0.57
1:F:335:TYR:OH	3:F:502:GOL:H2	2.03	0.57
1:C:239:GLN:HE22	1:C:250:TYR:H	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:LYS:NZ	1:D:200:GLY:O	2.37	0.57
1:B:264:ASP:O	6:B:601:HOH:O	2.18	0.56
1:C:249:PRO:HG2	1:C:281:MET:HB3	1.87	0.56
1:F:192:PHE:CZ	1:F:232:VAL:HB	2.40	0.56
1:D:276:MET:HE3	1:A:240:TYR:CE2	2.40	0.56
1:E:152:CYS:SG	1:E:156:GLU:HA	2.46	0.56
1:F:315:ARG:NH2	1:F:346:MET:HG3	2.20	0.56
1:A:390:ARG:HH12	5:A:501:G1P:H3	1.69	0.56
1:E:116:ARG:HH21	1:E:117:PHE:HZ	1.53	0.56
1:E:139:GLU:OE2	1:E:147:LYS:HD3	2.05	0.56
1:E:12:TYR:CD2	1:E:15:ARG:HD2	2.40	0.56
1:A:361:PHE:CE2	1:A:454:LEU:HB2	2.41	0.56
1:F:15:ARG:CZ	1:F:396:TYR:HE1	2.18	0.55
1:B:192:PHE:CD2	1:B:214:LEU:HD11	2.42	0.55
1:B:130:ILE:HG22	1:B:132:LYS:HG2	1.88	0.55
1:B:43:PHE:HD1	1:B:43:PHE:H	1.55	0.55
1:C:15:ARG:HG2	1:C:396:TYR:CE1	2.42	0.54
1:C:275:ARG:NE	1:E:207:GLU:OE2	2.31	0.54
1:E:130:ILE:HD12	1:E:136:PRO:HD3	1.89	0.54
1:A:284:VAL:HG12	1:A:367:GLN:HB2	1.90	0.54
1:F:279:ARG:NH2	1:B:279:ARG:CZ	2.71	0.54
1:B:233:HIS:CD2	3:B:503:GOL:H31	2.43	0.54
1:C:8:GLN:HB2	1:C:367:GLN:HG2	1.88	0.54
1:F:205:LEU:HD11	1:F:232:VAL:HG21	1.90	0.54
1:E:415:LEU:HD21	1:E:419:LYS:HE3	1.89	0.54
1:E:284:VAL:HG12	1:E:367:GLN:HB2	1.90	0.54
1:B:207:GLU:HG2	1:B:211:TYR:CE2	2.43	0.54
1:D:379:ASP:HB2	1:D:395:ASN:OD1	2.08	0.53
1:F:315:ARG:HH21	1:F:346:MET:HG3	1.73	0.53
1:B:8:GLN:HB2	1:B:367:GLN:HG2	1.91	0.53
1:C:3:LEU:HD21	1:C:185:ASN:HB3	1.91	0.53
1:A:252:PHE:O	1:A:255:PRO:HD2	2.09	0.53
1:A:273:TRP:CH2	1:A:281:MET:HE1	2.44	0.53
1:C:379:ASP:HB2	1:C:395:ASN:OD1	2.09	0.52
1:C:270:LEU:HD23	1:C:441:VAL:HG21	1.90	0.52
1:C:294:PRO:HG3	1:C:322:ARG:NH1	2.22	0.52
1:D:163:TYR:CE1	1:D:168:ALA:HB1	2.44	0.52
1:D:189:LEU:HB2	1:D:230:PRO:HA	1.90	0.52
1:D:259:LEU:HD11	1:D:291:ILE:HD13	1.91	0.52
1:A:15:ARG:HG2	1:A:396:TYR:CE1	2.44	0.52
1:F:385:LYS:HG3	1:F:386:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ASP:HB2	1:A:395:ASN:OD1	2.10	0.52
1:C:198:ARG:NH1	1:C:209:GLU:OE2	2.42	0.52
1:B:86:ASN:ND2	1:B:194:TYR:HB2	2.24	0.52
1:D:205:LEU:HD11	1:D:232:VAL:HG21	1.90	0.52
1:A:134:LYS:O	1:A:134:LYS:HG3	2.02	0.52
1:F:214:LEU:HG	1:F:247:MET:HE1	1.93	0.51
1:A:243:SER:HB2	1:A:249:PRO:HG3	1.92	0.51
1:D:252:PHE:O	1:D:255:PRO:HD2	2.11	0.51
1:E:142:LEU:HD12	1:E:146:THR:HB	1.92	0.51
1:A:82:ASP:OD1	1:A:188:ARG:HD3	2.10	0.51
1:A:178:PHE:O	1:A:181:SER:OG	2.27	0.51
1:B:431:PHE:HB2	1:B:445:TRP:CH2	2.45	0.51
1:C:12:TYR:CD2	1:C:15:ARG:HD2	2.45	0.51
1:F:431:PHE:HB2	1:F:445:TRP:CH2	2.46	0.51
1:D:347:GLN:HG2	3:D:502:GOL:H2	1.92	0.51
1:E:82:ASP:OD1	1:E:188:ARG:HD3	2.11	0.51
1:B:142:LEU:HD12	1:B:146:THR:HB	1.92	0.51
1:D:258:LEU:HD12	1:D:285:LEU:HD21	1.92	0.51
1:C:240:TYR:HD1	1:C:240:TYR:N	2.09	0.51
1:E:15:ARG:NH1	1:E:396:TYR:HE1	2.08	0.51
1:A:285:LEU:HD22	1:A:341:PHE:CZ	2.46	0.50
1:F:82:ASP:OD1	1:F:188:ARG:HD3	2.11	0.50
1:D:12:TYR:CD2	1:D:15:ARG:HD2	2.46	0.50
1:D:67:TRP:CZ2	1:D:178:PHE:HE2	2.30	0.50
1:F:189:LEU:HD12	1:F:230:PRO:HG3	1.93	0.50
1:B:15:ARG:NH1	1:B:396:TYR:HE1	2.10	0.50
1:B:379:ASP:HB2	1:B:395:ASN:OD1	2.12	0.50
1:A:263:LEU:HD13	1:A:311:ASN:ND2	2.26	0.50
1:F:244:ARG:NH1	1:B:279:ARG:HH21	2.10	0.50
1:F:396:TYR:O	1:F:397:TYR:HD1	1.94	0.50
1:E:361:PHE:CE2	1:E:454:LEU:HB2	2.47	0.50
1:F:2:LEU:N	6:F:609:HOH:O	2.44	0.50
1:F:12:TYR:CD2	1:F:15:ARG:HD2	2.47	0.50
1:A:8:GLN:HB2	1:A:367:GLN:HG2	1.94	0.50
1:A:163:TYR:HD2	1:A:213:ILE:HD13	1.76	0.50
1:B:273:TRP:CH2	1:B:281:MET:HE1	2.47	0.49
1:A:152:CYS:SG	1:A:156:GLU:HA	2.52	0.49
1:F:8:GLN:HB2	1:F:367:GLN:HG2	1.93	0.49
1:B:15:ARG:HG2	1:B:396:TYR:CE1	2.48	0.49
1:D:214:LEU:HG	1:D:247:MET:HE1	1.94	0.49
1:C:207:GLU:OE2	1:E:275:ARG:NE	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:169:TYR:HB3	1:F:216:TRP:CH2	2.47	0.49
1:B:252:PHE:O	1:B:255:PRO:HD2	2.12	0.49
3:B:503:GOL:O1	6:B:602:HOH:O	2.19	0.49
1:C:205:LEU:HD11	1:C:232:VAL:HG21	1.93	0.49
1:C:239:GLN:HE22	1:C:250:TYR:N	2.11	0.49
1:C:309:ILE:HD13	1:C:334:ILE:HD12	1.95	0.49
1:D:189:LEU:HD12	1:D:230:PRO:HG3	1.95	0.49
1:F:85:VAL:O	1:F:163:TYR:OH	2.23	0.49
1:E:151:TRP:CD1	1:E:197:LYS:HE2	2.48	0.49
1:E:325:ALA:C	1:E:327:ASN:H	2.20	0.49
1:D:82:ASP:OD1	1:D:188:ARG:HD3	2.13	0.48
1:D:374:LEU:HD22	1:D:405:ALA:HB3	1.94	0.48
1:E:315:ARG:HH22	1:E:344:ALA:C	2.21	0.48
1:F:469:ASP:OD1	1:F:471:LYS:HG2	2.14	0.48
1:F:169:TYR:HD1	1:F:169:TYR:N	2.12	0.48
1:E:356:ARG:HG3	1:E:414:LEU:HD13	1.94	0.48
1:E:456:VAL:HA	1:E:462:THR:O	2.14	0.48
1:F:124:ASP:OD1	1:F:200:GLY:HA2	2.13	0.48
1:B:194:TYR:CD1	1:B:194:TYR:N	2.82	0.48
1:C:426:ALA:HA	1:C:447:HIS:HB3	1.95	0.48
1:D:123:ASP:O	1:D:127:LYS:HG3	2.13	0.48
1:E:10:ILE:HB	1:E:369:TYR:HA	1.94	0.48
1:A:270:LEU:HD23	1:A:441:VAL:HG21	1.94	0.48
1:D:276:MET:HB2	1:A:240:TYR:CD2	2.49	0.48
1:E:243:SER:HB2	1:E:249:PRO:HG3	1.94	0.48
1:F:214:LEU:HG	1:F:247:MET:SD	2.54	0.48
1:B:15:ARG:CZ	1:B:396:TYR:HE1	2.26	0.48
1:D:263:LEU:HD13	1:D:311:ASN:ND2	2.27	0.48
1:A:326:ALA:O	1:A:327:ASN:C	2.56	0.48
1:A:348:ASN:HB3	1:A:351:ALA:HB3	1.96	0.48
1:F:270:LEU:HD23	1:F:441:VAL:HG21	1.95	0.48
1:F:169:TYR:N	1:F:169:TYR:CD1	2.81	0.48
1:C:240:TYR:N	1:C:240:TYR:CD1	2.81	0.48
1:E:125:MET:HE3	1:E:325:ALA:HB1	1.96	0.48
1:F:395:ASN:HB3	1:F:397:TYR:CE1	2.49	0.47
1:F:286:ASP:OD1	1:F:286:ASP:N	2.46	0.47
1:B:139:GLU:OE2	1:B:147:LYS:HD3	2.14	0.47
1:B:192:PHE:CE1	1:B:232:VAL:HB	2.49	0.47
1:D:270:LEU:HD23	1:D:441:VAL:HG21	1.97	0.47
1:E:431:PHE:HB2	1:E:445:TRP:CH2	2.50	0.47
1:F:279:ARG:HD3	1:F:279:ARG:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:PHE:CE1	1:C:232:VAL:HB	2.50	0.47
1:D:163:TYR:HE1	1:D:168:ALA:HB1	1.79	0.47
1:E:370:TYR:O	1:E:373:LEU:HB3	2.14	0.47
1:A:177:GLY:HA2	1:A:224:HIS:CD2	2.50	0.47
1:A:257:LEU:HD21	1:A:270:LEU:HA	1.96	0.47
1:E:249:PRO:HD2	1:E:280:ASN:O	2.15	0.47
1:F:294:PRO:HG3	1:F:322:ARG:NH2	2.30	0.47
1:B:265:ALA:HA	1:B:458:LEU:HB3	1.97	0.47
1:D:469:ASP:OD1	1:D:471:LYS:HG2	2.15	0.47
1:A:330:SER:O	1:A:332:GLY:N	2.47	0.47
1:E:6:ALA:HB1	1:E:422:THR:HG23	1.96	0.47
1:C:86:ASN:HB3	1:C:87:HIS:ND1	2.29	0.46
1:D:260:TYR:CZ	1:D:304:LYS:HD2	2.50	0.46
1:E:15:ARG:HG2	1:E:396:TYR:CE1	2.49	0.46
1:B:15:ARG:HG2	1:B:396:TYR:CD1	2.50	0.46
1:A:469:ASP:OD1	1:A:471:LYS:HG2	2.14	0.46
1:B:322:ARG:HG2	1:B:333:ALA:O	2.16	0.46
1:C:6:ALA:HB1	1:C:422:THR:HG23	1.97	0.46
1:D:201:THR:HA	1:A:435:TYR:CE2	2.51	0.46
1:E:188:ARG:NH2	1:E:231:GLU:HG3	2.30	0.46
1:D:192:PHE:CE1	1:D:232:VAL:HB	2.50	0.46
1:F:189:LEU:HB2	1:F:230:PRO:HA	1.98	0.46
1:C:10:ILE:HB	1:C:369:TYR:HA	1.97	0.46
1:E:233:HIS:CE1	1:E:252:PHE:CE2	3.04	0.46
1:D:89:SER:HA	1:D:157:GLN:O	2.16	0.46
1:D:260:TYR:OH	1:D:304:LYS:HD2	2.15	0.46
1:D:163:TYR:HD2	1:D:213:ILE:HD13	1.80	0.46
1:C:139:GLU:OE2	1:C:147:LYS:HD3	2.16	0.46
1:E:163:TYR:CE1	1:E:168:ALA:HB1	2.50	0.46
1:F:249:PRO:HG2	1:F:281:MET:HB3	1.98	0.46
1:F:258:LEU:HD21	1:F:358:ILE:HG21	1.97	0.46
1:B:319:PRO:HG2	1:B:321:MET:CE	2.46	0.45
1:C:214:LEU:HG	1:C:247:MET:SD	2.56	0.45
1:E:267:SER:O	1:E:271:LYS:HG3	2.16	0.45
1:B:207:GLU:HG2	1:B:211:TYR:HE2	1.81	0.45
1:D:131:ARG:HG2	1:D:322:ARG:HA	1.97	0.45
1:A:327:ASN:O	1:A:328:ILE:C	2.58	0.45
1:A:7:VAL:HG11	1:A:418:MET:HE3	1.97	0.45
1:F:207:GLU:HG2	1:F:211:TYR:CE2	2.52	0.45
1:B:198:ARG:NH1	1:B:209:GLU:OE2	2.49	0.45
1:C:263:LEU:HD13	1:C:311:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:TYR:CD2	1:D:195:THR:HB	2.52	0.45
1:D:258:LEU:HD21	1:D:358:ILE:HG21	1.99	0.45
1:A:180:THR:OG1	1:A:224:HIS:HB3	2.15	0.45
1:F:350:ASP:HB3	1:F:461:ASN:O	2.17	0.45
1:B:88:ILE:HG12	1:B:161:LEU:HD21	1.99	0.45
1:E:285:LEU:HD13	1:E:341:PHE:CE2	2.50	0.45
1:B:194:TYR:N	1:B:194:TYR:HD1	2.14	0.45
1:C:53:SER:O	1:C:89:SER:HB2	2.16	0.45
1:C:257:LEU:HD21	1:C:270:LEU:HA	1.98	0.45
1:C:319:PRO:HG2	1:C:321:MET:HE2	1.98	0.45
1:D:322:ARG:HD2	1:D:332:GLY:O	2.15	0.45
1:A:441:VAL:HG12	1:A:443:MET:HG3	1.99	0.45
1:A:256:PRO:HG2	1:A:296:VAL:HB	1.98	0.45
1:B:243:SER:HB2	1:B:249:PRO:HG3	1.99	0.45
1:C:189:LEU:HB2	1:C:230:PRO:HA	1.98	0.45
1:D:53:SER:O	1:D:89:SER:HB2	2.17	0.45
1:F:74:THR:HG21	1:F:183:GLY:HA3	1.99	0.45
1:C:10:ILE:HD11	1:C:367:GLN:OE1	2.17	0.45
1:C:272:ASN:O	1:C:276:MET:HG2	2.17	0.45
1:D:151:TRP:HD1	1:D:160:ASP:OD2	2.00	0.44
1:D:263:LEU:HD22	1:D:311:ASN:HD21	1.82	0.44
1:E:207:GLU:HG2	1:E:211:TYR:CE2	2.52	0.44
1:A:137:PHE:HB2	1:A:149:ARG:HH21	1.82	0.44
1:F:15:ARG:HG2	1:F:396:TYR:CE1	2.53	0.44
1:F:255:PRO:HG3	1:F:285:LEU:HA	1.99	0.44
1:B:271:LYS:HD3	1:B:436:SER:OG	2.17	0.44
1:C:361:PHE:CE2	1:C:454:LEU:HB2	2.52	0.44
1:E:391:ASP:HA	1:E:394:ARG:HB2	1.99	0.44
1:B:189:LEU:HB2	1:B:230:PRO:HA	1.99	0.44
1:D:276:MET:HB3	1:A:237:SER:HA	1.99	0.44
1:E:259:LEU:HD11	1:E:291:ILE:HD13	1.99	0.44
1:A:131:ARG:HH22	5:A:501:G1P:P	2.40	0.44
1:A:352:TYR:OH	1:A:372:GLY:O	2.34	0.44
1:B:12:TYR:CD2	1:B:15:ARG:HD2	2.52	0.44
1:B:286:ASP:HB3	1:B:341:PHE:HB2	1.98	0.44
1:B:335:TYR:OH	3:B:503:GOL:H32	2.17	0.44
1:B:441:VAL:HG12	1:B:443:MET:HG3	2.00	0.44
1:B:456:VAL:HA	1:B:462:THR:O	2.18	0.44
1:A:338:THR:HG21	1:A:389:LEU:HG	1.98	0.44
1:C:340:THR:HG22	1:C:393:ASN:HA	1.99	0.44
1:D:57:HIS:HB2	1:D:175:TYR:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:385:LYS:O	1:F:386:THR:OG1	2.28	0.44
1:C:240:TYR:CE1	1:C:278:PRO:HD3	2.52	0.44
1:D:356:ARG:HG3	1:D:414:LEU:HD13	1.99	0.44
1:F:134:LYS:HB3	1:F:134:LYS:HE2	1.74	0.44
1:F:163:TYR:CE1	1:F:168:ALA:HB1	2.52	0.44
1:D:340:THR:HG22	1:D:393:ASN:HA	2.00	0.44
1:A:293:ILE:O	1:A:296:VAL:HG12	2.18	0.44
1:E:192:PHE:CD2	1:E:214:LEU:HD13	2.53	0.44
1:B:240:TYR:CD1	1:B:278:PRO:HB3	2.53	0.43
1:D:446:ARG:NH1	6:D:604:HOH:O	2.33	0.43
1:E:263:LEU:HD13	1:E:311:ASN:ND2	2.33	0.43
1:B:205:LEU:HD11	1:B:232:VAL:HG21	2.00	0.43
1:F:285:LEU:HD12	1:F:356:ARG:HD3	2.01	0.43
1:F:374:LEU:HD13	1:F:397:TYR:CD2	2.53	0.43
1:B:292:CYS:SG	1:B:294:PRO:HD2	2.58	0.43
1:C:12:TYR:CG	1:C:15:ARG:HD2	2.53	0.43
1:A:192:PHE:CE2	1:A:214:LEU:HD13	2.53	0.43
1:F:396:TYR:C	1:F:397:TYR:HD1	2.26	0.43
1:C:207:GLU:HG2	1:C:211:TYR:CE2	2.52	0.43
1:C:466:GLN:HG2	1:C:477:ASP:OD1	2.19	0.43
1:F:152:CYS:SG	1:F:156:GLU:HA	2.59	0.43
1:F:311:ASN:C	1:F:315:ARG:HH11	2.27	0.43
1:B:335:TYR:CD2	1:B:336:GLN:HG3	2.52	0.43
1:B:374:LEU:HD21	1:B:406:MET:HE2	1.99	0.43
1:C:258:LEU:HD12	1:C:285:LEU:HD21	2.01	0.43
1:C:273:TRP:O	1:C:277:CYS:N	2.51	0.43
1:D:406:MET:O	1:D:412:GLN:NE2	2.44	0.43
1:E:15:ARG:HG2	1:E:396:TYR:CD1	2.53	0.43
1:E:270:LEU:HD23	1:E:441:VAL:HG21	1.99	0.43
1:F:435:TYR:CE2	1:B:201:THR:HA	2.54	0.43
1:C:207:GLU:HB3	1:E:433:LEU:O	2.18	0.43
1:C:208:PRO:HD3	1:E:434:ASN:OD1	2.19	0.43
1:E:252:PHE:O	1:E:255:PRO:HD2	2.19	0.43
1:F:286:ASP:HB3	1:F:341:PHE:HB2	2.01	0.43
1:C:374:LEU:HD21	1:C:406:MET:HE2	2.01	0.43
1:A:312:ILE:HG22	1:A:316:SER:HB3	2.01	0.43
1:F:10:ILE:HD11	1:F:367:GLN:HB3	2.01	0.43
1:B:67:TRP:CZ2	1:B:178:PHE:HE2	2.37	0.43
1:B:258:LEU:HD21	1:B:358:ILE:HG21	2.01	0.43
1:C:260:TYR:OH	1:C:304:LYS:HD2	2.19	0.43
1:C:385:LYS:O	1:C:386:THR:OG1	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:ASN:OD1	1:E:327:ASN:O	2.37	0.43
1:E:80:CYS:HA	1:E:186:LEU:O	2.19	0.42
1:B:469:ASP:OD1	1:B:471:LYS:HG2	2.19	0.42
1:C:244:ARG:HH12	1:E:276:MET:C	2.27	0.42
1:C:250:TYR:CD2	1:C:252:PHE:CZ	3.08	0.42
1:D:291:ILE:HB	1:D:337:LEU:HB2	2.00	0.42
1:A:10:ILE:HD11	1:A:367:GLN:OE1	2.19	0.42
1:D:214:LEU:HG	1:D:247:MET:SD	2.59	0.42
1:D:279:ARG:HB2	6:D:625:HOH:O	2.19	0.42
1:F:61:ASP:HB3	1:F:64:PHE:CD2	2.54	0.42
1:F:267:SER:HB2	1:F:441:VAL:HG22	2.01	0.42
1:B:424:TYR:OH	1:B:468:VAL:O	2.31	0.42
1:C:233:HIS:ND1	1:C:295:ASP:OD2	2.33	0.42
1:E:328:ILE:HG13	1:E:329:HIS:ND1	2.35	0.42
1:A:96:ARG:NH1	6:A:607:HOH:O	2.51	0.42
1:F:255:PRO:HB2	1:F:256:PRO:HD3	2.01	0.42
1:E:132:LYS:HE3	1:E:134:LYS:HG2	2.02	0.42
1:F:86:ASN:HB3	1:F:87:HIS:ND1	2.34	0.42
1:F:395:ASN:HB3	1:F:397:TYR:HE1	1.85	0.42
1:B:127:LYS:NZ	1:B:200:GLY:O	2.52	0.42
1:B:163:TYR:CE1	1:B:168:ALA:HB1	2.55	0.42
1:E:257:LEU:HD21	1:E:270:LEU:HA	2.02	0.42
1:F:244:ARG:CZ	1:B:279:ARG:HH21	2.33	0.42
1:B:240:TYR:CE1	1:B:278:PRO:HD3	2.55	0.42
1:C:285:LEU:HD12	1:C:356:ARG:HD3	2.01	0.42
1:F:434:ASN:OD1	1:B:208:PRO:HD3	2.20	0.42
1:F:361:PHE:CE2	1:F:454:LEU:HB2	2.55	0.41
1:B:280:ASN:N	6:B:604:HOH:O	2.34	0.41
1:D:156:GLU:HG2	6:D:614:HOH:O	2.20	0.41
1:E:130:ILE:HD11	1:E:325:ALA:HB2	2.01	0.41
1:A:240:TYR:HE1	1:A:278:PRO:HD3	1.81	0.41
1:F:267:SER:HB2	1:F:441:VAL:CG2	2.49	0.41
1:C:130:ILE:HA	1:C:130:ILE:HD13	1.81	0.41
1:E:240:TYR:CE1	1:E:278:PRO:HD3	2.55	0.41
1:A:6:ALA:HB1	1:A:422:THR:HG23	2.02	0.41
1:B:163:TYR:HD2	1:B:213:ILE:HD13	1.85	0.41
1:B:257:LEU:HD12	1:B:300:LEU:HD13	2.01	0.41
1:A:45:PRO:O	1:A:54:PRO:HA	2.20	0.41
1:C:434:ASN:OD1	1:E:208:PRO:HD3	2.20	0.41
1:E:406:MET:HA	1:E:411:VAL:HG11	2.02	0.41
1:F:3:LEU:HD21	1:F:185:ASN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:TRP:HD1	1:B:160:ASP:OD2	2.04	0.41
1:C:276:MET:HB3	1:E:237:SER:HA	2.03	0.41
1:D:208:PRO:HD3	1:A:434:ASN:OD1	2.20	0.41
1:E:163:TYR:HD2	1:E:213:ILE:HD13	1.86	0.41
1:A:285:LEU:HD13	1:A:341:PHE:CE2	2.55	0.41
1:F:41:LEU:HA	1:F:41:LEU:HD23	1.89	0.41
1:F:131:ARG:O	1:F:131:ARG:HG3	2.19	0.41
1:C:258:LEU:HD21	1:C:358:ILE:HG21	2.01	0.41
1:D:361:PHE:CE2	1:D:454:LEU:HB2	2.56	0.41
1:E:22:ASP:HB3	1:E:399:LEU:HD21	2.03	0.41
1:A:53:SER:O	1:A:89:SER:HB2	2.20	0.41
1:A:151:TRP:HD1	1:A:160:ASP:OD2	2.03	0.41
1:B:26:ALA:HB1	1:B:402:MET:SD	2.60	0.41
1:B:132:LYS:C	1:B:134:LYS:H	2.28	0.41
1:B:198:ARG:HH11	1:B:198:ARG:HD3	1.76	0.41
1:D:194:TYR:O	1:D:197:LYS:NZ	2.49	0.41
1:E:53:SER:O	1:E:89:SER:HB2	2.20	0.41
1:F:127:LYS:NZ	1:C:123:ASP:OD2	2.53	0.41
1:F:391:ASP:HA	1:F:394:ARG:HB2	2.03	0.41
1:B:153:THR:HG21	1:B:194:TYR:CD2	2.56	0.41
1:B:255:PRO:HB2	1:B:256:PRO:HD3	2.03	0.41
1:B:286:ASP:CG	1:B:369:TYR:HB3	2.46	0.41
1:C:255:PRO:HB2	1:C:256:PRO:HD3	2.01	0.41
1:C:315:ARG:CD	1:C:346:MET:HG2	2.51	0.41
1:D:207:GLU:HG2	1:D:211:TYR:CE2	2.56	0.41
1:E:452:CYS:HA	1:E:466:GLN:O	2.20	0.41
1:A:137:PHE:HE1	1:A:151:TRP:CZ3	2.38	0.41
1:E:216:TRP:O	1:E:219:GLU:HB3	2.21	0.41
1:D:293:ILE:HD13	1:D:293:ILE:HA	1.82	0.40
1:F:319:PRO:HG2	1:F:321:MET:CE	2.51	0.40
1:B:82:ASP:OD1	1:B:188:ARG:HD3	2.22	0.40
1:D:453:HIS:O	1:D:465:ILE:HA	2.22	0.40
1:A:250:TYR:CD2	1:A:252:PHE:CZ	3.09	0.40
1:F:264:ASP:HB2	1:D:326:ALA:HB3	2.04	0.40
1:B:240:TYR:CD1	1:B:240:TYR:N	2.89	0.40
1:D:39:HIS:HA	1:D:80:CYS:HB3	2.01	0.40
1:D:450:HIS:NE2	1:D:470:VAL:HG11	2.36	0.40
1:E:320:ILE:HD13	1:E:389:LEU:HD23	2.03	0.40
1:F:286:ASP:CG	1:F:369:TYR:HB3	2.46	0.40
1:F:424:TYR:HA	1:F:425:PRO:HD3	1.87	0.40
1:B:306:LYS:NZ	1:B:329:HIS:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:LEU:HG	1:C:247:MET:HE1	2.03	0.40
1:C:276:MET:HE3	1:E:240:TYR:CE2	2.57	0.40
1:E:15:ARG:CZ	1:E:396:TYR:HE1	2.35	0.40
1:E:207:GLU:HG2	1:E:211:TYR:HE2	1.86	0.40
1:E:293:ILE:O	1:E:296:VAL:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	477/480 (99%)	460 (96%)	14 (3%)	3 (1%)	21	42
1	B	477/480 (99%)	463 (97%)	14 (3%)	0	100	100
1	C	477/480 (99%)	462 (97%)	15 (3%)	0	100	100
1	D	477/480 (99%)	466 (98%)	11 (2%)	0	100	100
1	E	477/480 (99%)	463 (97%)	14 (3%)	0	100	100
1	F	477/480 (99%)	464 (97%)	13 (3%)	0	100	100
All	All	2862/2880 (99%)	2778 (97%)	81 (3%)	3 (0%)	48	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ASN
1	A	331	VAL
1	A	328	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	420/421 (100%)	414 (99%)	6 (1%)	59	80
1	B	420/421 (100%)	415 (99%)	5 (1%)	63	82
1	C	420/421 (100%)	417 (99%)	3 (1%)	76	89
1	D	420/421 (100%)	415 (99%)	5 (1%)	63	82
1	E	420/421 (100%)	417 (99%)	3 (1%)	76	89
1	F	420/421 (100%)	417 (99%)	3 (1%)	76	89
All	All	2520/2526 (100%)	2495 (99%)	25 (1%)	68	85

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	169	TYR
1	F	240	TYR
1	F	279	ARG
1	B	43	PHE
1	B	131	ARG
1	B	194	TYR
1	B	323	ARG
1	B	464	LYS
1	C	131	ARG
1	C	240	TYR
1	C	250	TYR
1	D	131	ARG
1	D	240	TYR
1	D	279	ARG
1	D	315	ARG
1	D	464	LYS
1	E	240	TYR
1	E	279	ARG
1	E	327	ASN
1	A	134	LYS
1	A	149	ARG
1	A	323	ARG

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Mol	Chain	Res	Type
1	A	327	ASN
1	A	328	ILE
1	A	415	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	239	GLN
1	F	459	ASN
1	B	113	HIS
1	B	129	HIS
1	B	459	ASN
1	C	239	GLN
1	C	329	HIS
1	D	129	HIS
1	D	280	ASN
1	D	311	ASN
1	D	329	HIS
1	D	434	ASN
1	D	453	HIS
1	D	461	ASN
1	A	158	GLN
1	A	329	HIS
1	A	453	HIS
1	A	459	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	501	-	5,5,5	0.98	0	5,5,5	0.89	0
3	GOL	B	504	-	5,5,5	1.14	0	5,5,5	0.89	0
5	G1P	E	501	-	15,16,16	1.53	3 (20%)	24,24,24	1.46	4 (16%)
2	GLC	B	502	-	12,12,12	0.36	0	17,17,17	0.55	0
3	GOL	D	502	-	5,5,5	1.08	0	5,5,5	0.97	0
3	GOL	B	505	-	5,5,5	1.09	0	5,5,5	0.92	0
3	GOL	D	501	-	5,5,5	0.09	0	5,5,5	0.35	0
3	GOL	B	503	-	5,5,5	1.11	0	5,5,5	1.04	0
2	GLC	F	501	-	12,12,12	0.12	0	17,17,17	0.43	0
3	GOL	E	502	-	5,5,5	0.94	0	5,5,5	0.99	0
3	GOL	F	502	-	5,5,5	1.12	0	5,5,5	0.98	0
5	G1P	A	501	-	15,16,16	1.50	3 (20%)	24,24,24	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	501	-	-	2/4/4/4	-
3	GOL	B	504	-	-	0/4/4/4	-
5	G1P	E	501	-	-	3/7/27/27	0/1/1/1
2	GLC	B	502	-	-	1/2/22/22	0/1/1/1
3	GOL	D	502	-	-	0/4/4/4	-
3	GOL	B	505	-	-	0/4/4/4	-
3	GOL	D	501	-	-	4/4/4/4	-
3	GOL	B	503	-	-	3/4/4/4	-
2	GLC	F	501	-	-	0/2/22/22	0/1/1/1
3	GOL	E	502	-	-	4/4/4/4	-
3	GOL	F	502	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	G1P	A	501	-	-	4/7/27/27	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	501	G1P	P-O1	3.84	1.66	1.59
5	A	501	G1P	P-O1	3.24	1.65	1.59
5	A	501	G1P	O5-C1	2.61	1.48	1.41
5	E	501	G1P	O5-C5	2.30	1.50	1.44
5	A	501	G1P	O5-C5	2.28	1.50	1.44
5	E	501	G1P	O5-C1	2.16	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	501	G1P	O5-C5-C4	3.74	116.44	109.70
5	E	501	G1P	C3-C4-C5	3.35	116.31	110.23
5	E	501	G1P	O5-C1-O1	-2.35	108.30	111.36
5	E	501	G1P	O5-C1-C2	-2.26	105.73	110.37

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	GOL	C1-C2-C3-O3
3	D	501	GOL	C1-C2-C3-O3
3	E	502	GOL	O1-C1-C2-C3
5	E	501	G1P	O5-C1-O1-P
5	A	501	G1P	O5-C1-O1-P
5	A	501	G1P	O5-C5-C6-O6
5	A	501	G1P	C4-C5-C6-O6
3	E	502	GOL	O1-C1-C2-O2
5	A	501	G1P	C2-C1-O1-P
5	E	501	G1P	C4-C5-C6-O6
3	B	501	GOL	O1-C1-C2-C3
3	D	501	GOL	O1-C1-C2-C3
3	E	502	GOL	C1-C2-C3-O3
3	B	501	GOL	O1-C1-C2-O2
3	B	503	GOL	O2-C2-C3-O3
3	D	501	GOL	O2-C2-C3-O3
5	E	501	G1P	O5-C5-C6-O6

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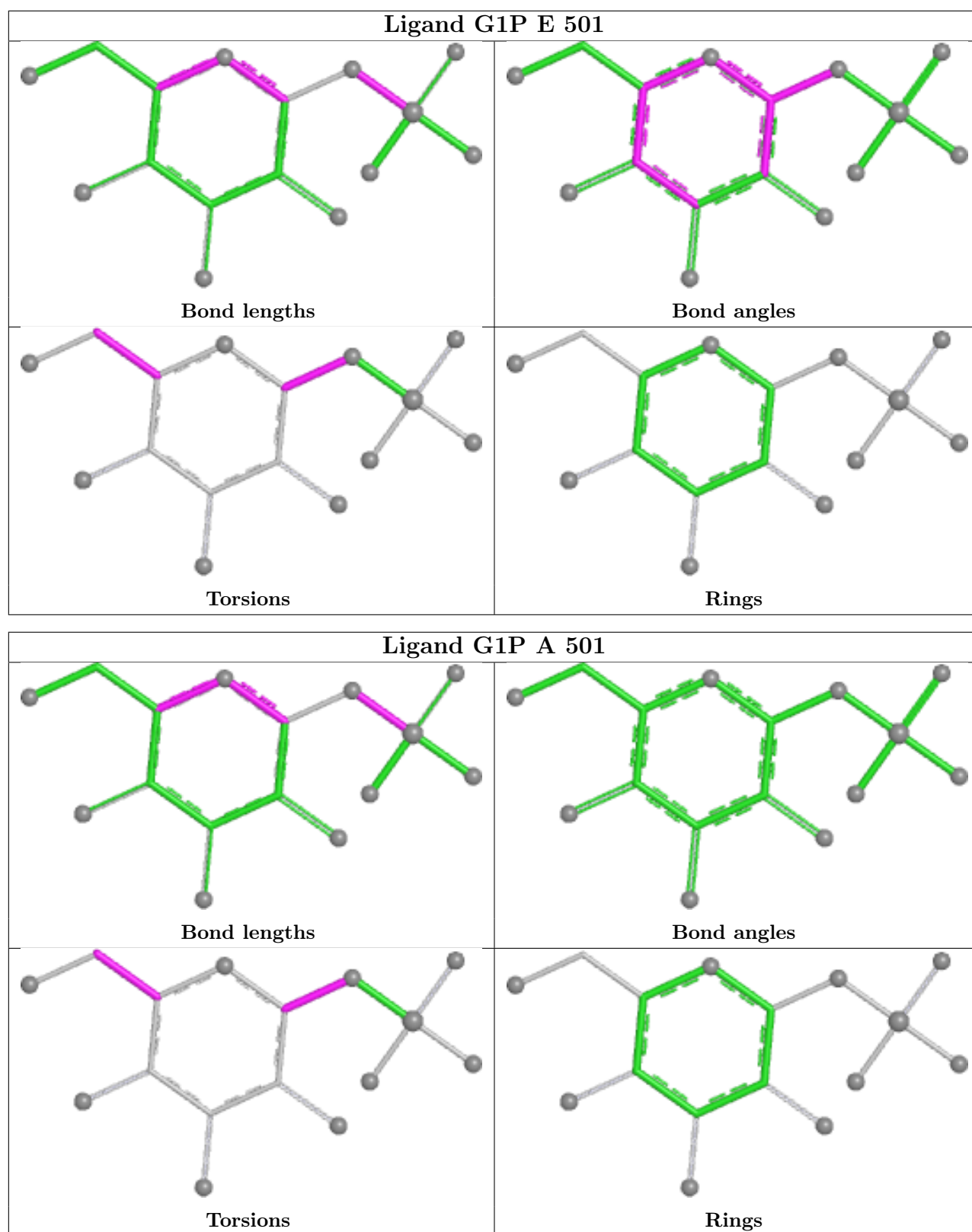
Mol	Chain	Res	Type	Atoms
2	B	502	GLC	O5-C5-C6-O6
3	D	501	GOL	O1-C1-C2-O2
3	F	502	GOL	O1-C1-C2-O2
3	E	502	GOL	O2-C2-C3-O3
3	B	503	GOL	O1-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	GLC	1	0
3	D	502	GOL	1	0
3	D	501	GOL	1	0
3	B	503	GOL	3	0
3	F	502	GOL	1	0
5	A	501	G1P	3	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	479/480 (99%)	-0.16	7 (1%)	72 70	51, 90, 128, 195	0
1	B	479/480 (99%)	-0.44	3 (0%)	85 85	40, 62, 93, 119	0
1	C	479/480 (99%)	-0.23	3 (0%)	85 85	58, 87, 116, 150	0
1	D	479/480 (99%)	-0.34	3 (0%)	85 85	48, 73, 100, 141	0
1	E	479/480 (99%)	-0.27	3 (0%)	85 85	46, 77, 113, 130	0
1	F	479/480 (99%)	-0.42	3 (0%)	85 85	35, 62, 98, 123	0
All	All	2874/2880 (99%)	-0.31	22 (0%)	82 81	35, 75, 114, 195	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	325	ALA	5.3
1	B	130	ILE	4.6
1	A	329	HIS	3.6
1	C	470	VAL	3.6
1	A	326	ALA	3.1
1	E	279	ARG	2.8
1	D	2	LEU	2.7
1	C	472	SER	2.7
1	A	279	ARG	2.6
1	B	131	ARG	2.6
1	E	327	ASN	2.5
1	A	328	ILE	2.5
1	D	470	VAL	2.5
1	F	279	ARG	2.5
1	A	324	SER	2.4
1	F	323	ARG	2.4
1	A	98	PHE	2.3
1	F	192	PHE	2.2
1	C	449	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	279	ARG	2.0
1	E	326	ALA	2.0
1	B	395	ASN	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](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

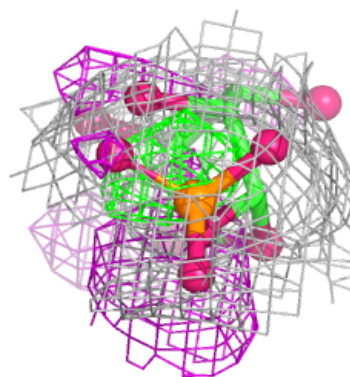
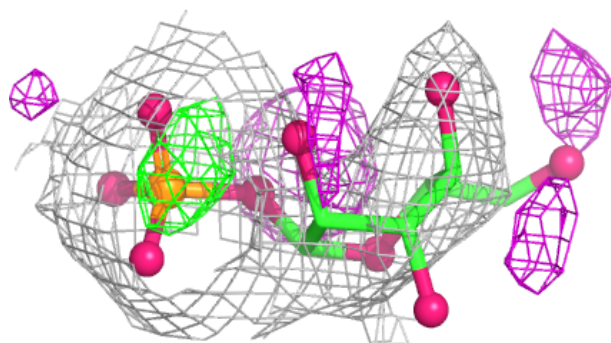
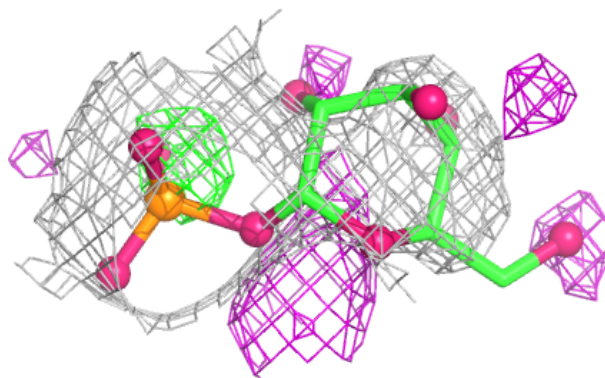
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	502	12/12	0.61	0.22	142,143,144,146	0
3	GOL	D	501	6/6	0.62	0.28	20,20,20,20	0
3	GOL	D	502	6/6	0.63	0.15	104,105,106,107	0
2	GLC	F	501	12/12	0.68	0.16	120,121,123,125	0
3	GOL	B	503	6/6	0.69	0.15	68,73,77,83	0
3	GOL	F	502	6/6	0.76	0.12	62,69,70,70	0
3	GOL	B	505	6/6	0.79	0.18	102,104,104,104	0
3	GOL	E	502	6/6	0.79	0.12	77,79,79,80	0
5	G1P	A	501	16/16	0.83	0.17	128,149,153,155	0
5	G1P	E	501	16/16	0.84	0.16	94,122,126,131	0
3	GOL	B	504	6/6	0.85	0.14	77,79,81,81	0
4	NA	A	502	1/1	0.89	0.12	43,43,43,43	0
3	GOL	B	501	6/6	0.92	0.12	56,58,59,59	0
4	NA	E	503	1/1	0.94	0.15	36,36,36,36	0
4	NA	B	506	1/1	0.97	0.13	38,38,38,38	0

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

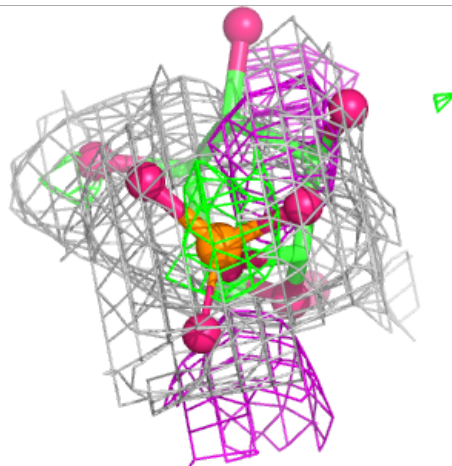
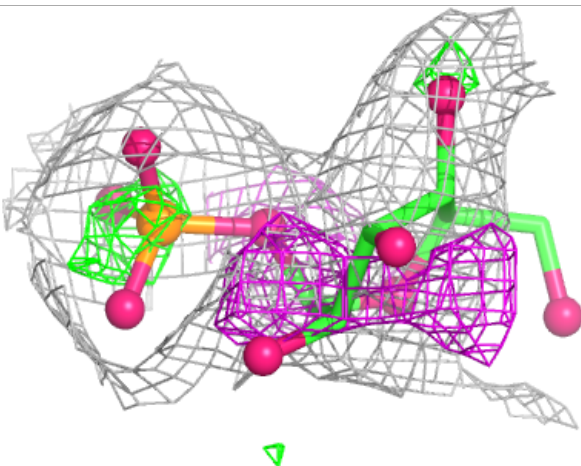
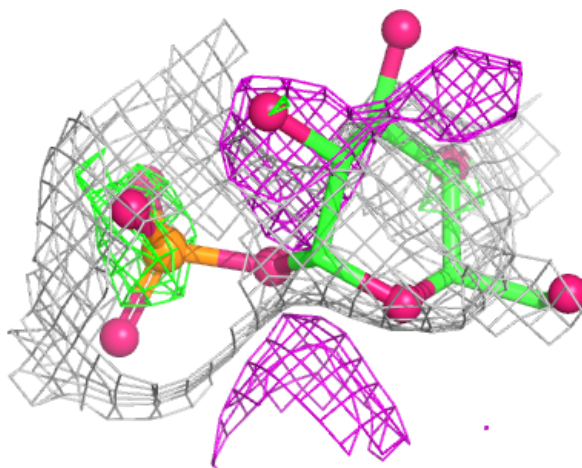
Electron density around G1P A 501:

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



Electron density around G1P E 501:

$2mF_o-DF_c$ (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.