



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:41 AM UTC

PDB ID : 5WSA / pdb_00005wsa
Title : Pyruvate kinase (PYK) from Mycobacterium tuberculosis in complex with Oxalate and allosteric activator Glucose 6-Phosphate
Authors : Zhong, W.; Cai, Q.; El Sahili, A.; Lescar, J.; Dedon, P.C.
Deposited on : 2016-12-06
Resolution : 2.85 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

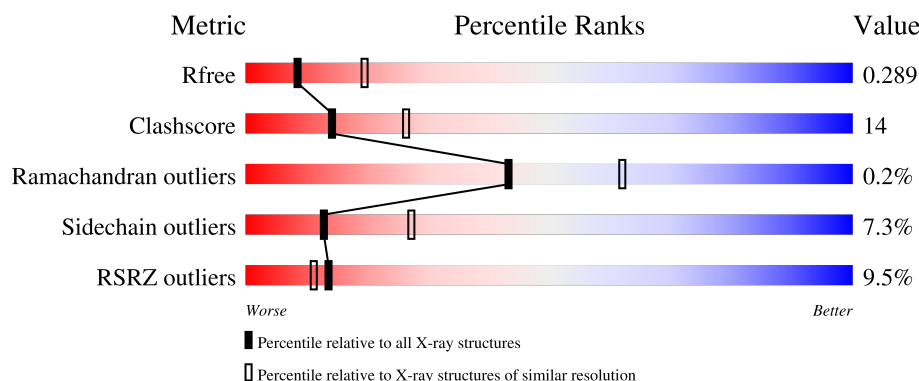
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	475	5% 73% 23% ..
1	B	475	7% 72% 24% ..
1	C	475	14% 69% 28% ..
1	D	475	12% 69% 28% ..

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
4	OXL	A	503	-	X	-	-
4	OXL	B	503	-	X	-	-
4	OXL	C	503	-	X	-	-
4	OXL	D	503	-	X	-	-
5	PO4	A	504	-	-	X	-
5	PO4	B	504	-	-	X	-
5	PO4	C	504	-	-	X	-
5	PO4	D	504	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14456 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.

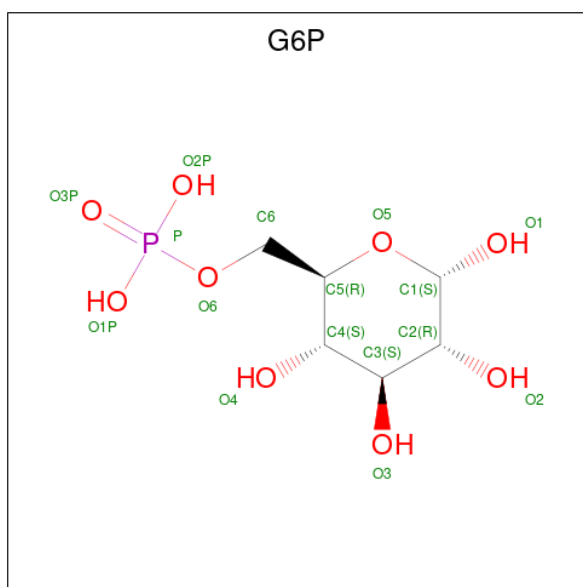
- Molecule 1 is a protein called Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3543	2206	640	679	18			
1	B	471	Total	C	N	O	S	0	0	0
			3543	2206	640	679	18			
1	C	471	Total	C	N	O	S	0	0	0
			3543	2206	640	679	18			
1	D	471	Total	C	N	O	S	0	0	0
			3543	2206	640	679	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P9WKE5
A	-1	GLY	-	expression tag	UNP P9WKE5
A	0	HIS	-	expression tag	UNP P9WKE5
B	-2	GLY	-	expression tag	UNP P9WKE5
B	-1	GLY	-	expression tag	UNP P9WKE5
B	0	HIS	-	expression tag	UNP P9WKE5
C	-2	GLY	-	expression tag	UNP P9WKE5
C	-1	GLY	-	expression tag	UNP P9WKE5
C	0	HIS	-	expression tag	UNP P9WKE5
D	-2	GLY	-	expression tag	UNP P9WKE5
D	-1	GLY	-	expression tag	UNP P9WKE5
D	0	HIS	-	expression tag	UNP P9WKE5

- Molecule 2 is 6-O-phosphono-alpha-D-glucopyranose (CCD ID: G6P) (formula: C₆H₁₃O₉P).

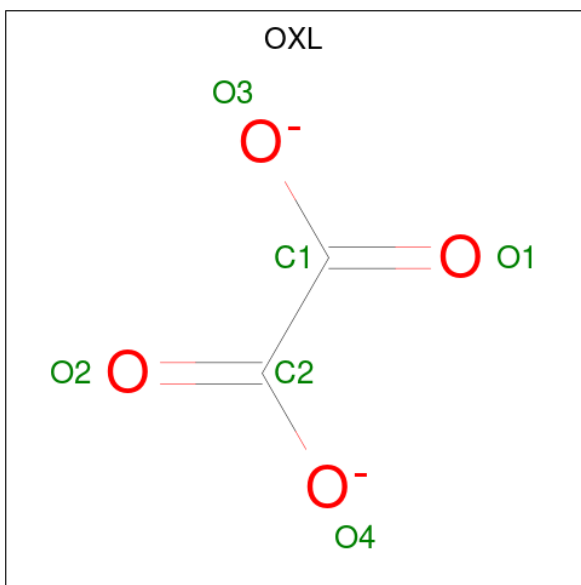


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	C	1	Total	C	O	P	0	0
			16	6	9	1		
2	D	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

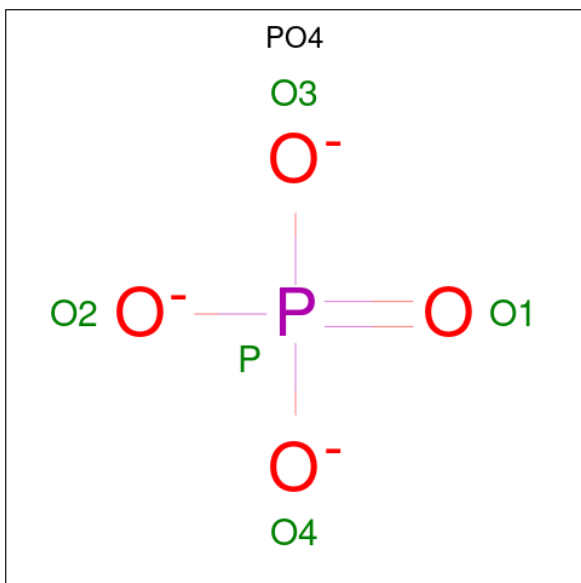
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is OXALATE ION (CCD ID: OXL) (formula: C₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	2	4		
4	B	1	Total	C	O	0	0
			6	2	4		
4	C	1	Total	C	O	0	0
			6	2	4		
4	D	1	Total	C	O	0	0
			6	2	4		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

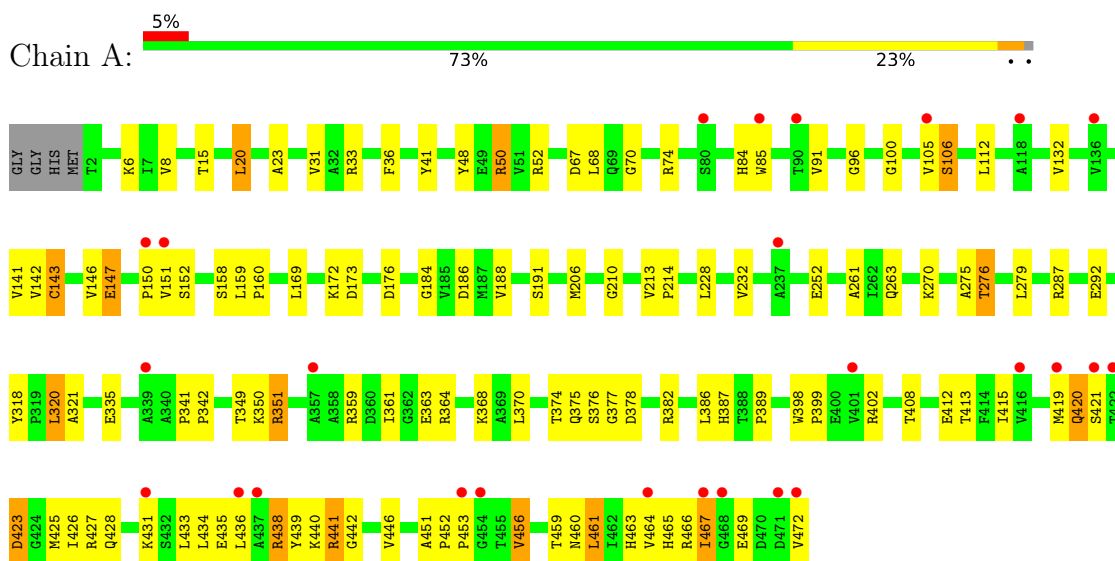
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	46	Total O 46 46	0	0
6	B	43	Total O 43 43	0	0
6	C	49	Total O 49 49	0	0
6	D	34	Total O 34 34	0	0

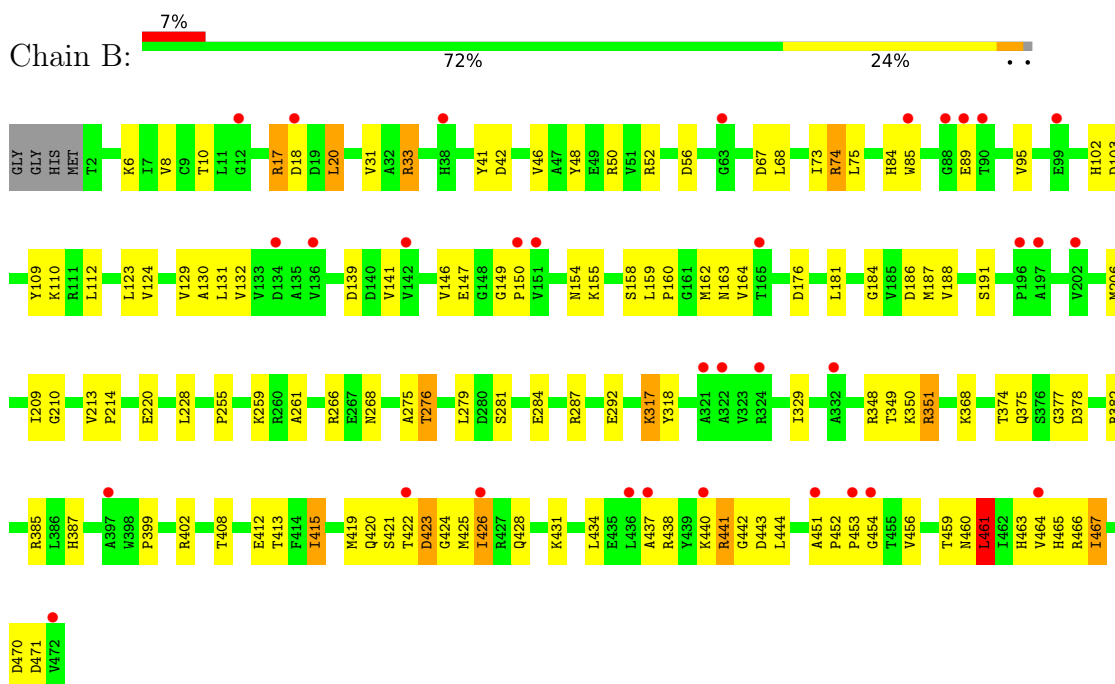
3 Residue-property plots

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

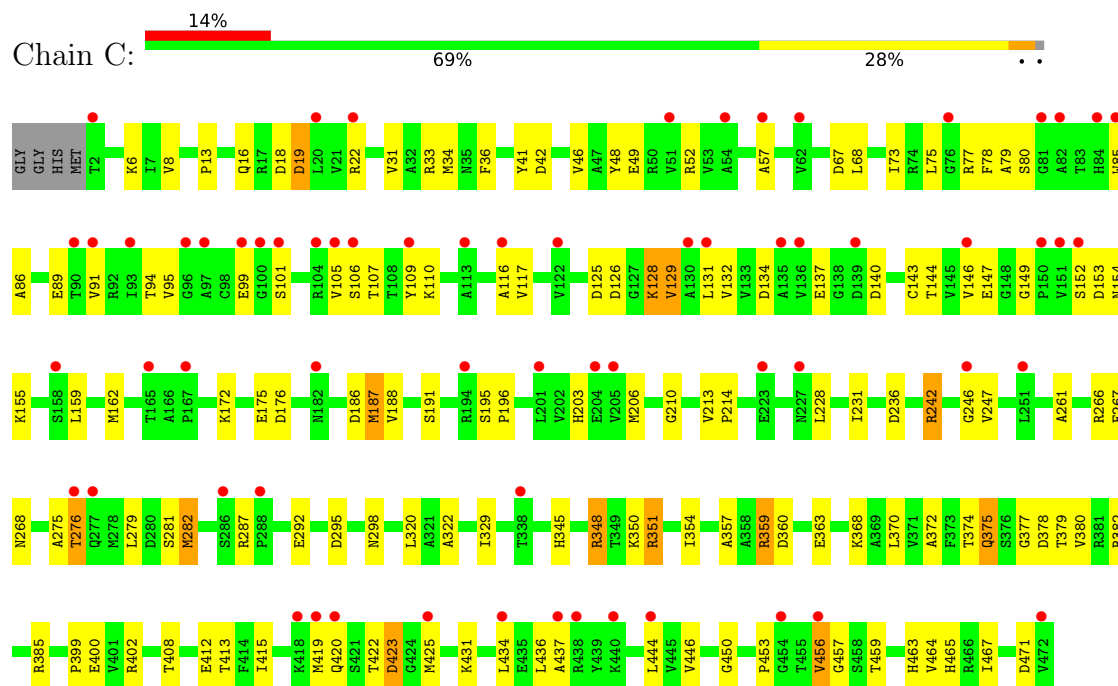
• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	125.42Å 125.42Å 144.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.71 – 2.85 62.71 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.71-2.85) 100.0 (62.71-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.151 , 0.195 (Not available) , 0.289	Depositor DCC
R_{free} test set	3001 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.830	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.467 for -h,-k,l 0.467 for h,-h-k,-l 0.478 for -k,-h,-l	Xtriage
Reported twinning fraction	0.278 for H, K, L 0.277 for -K, -H, -L 0.218 for K, H, -L 0.227 for -h,-k,l	Depositor
Outliers	0 of 59195 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	14456	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: G6P, PO4, MG, OXL

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	1.05	3/3593 (0.1%)	0.93	3/4881 (0.1%)
1	B	1.05	1/3593 (0.0%)	0.93	2/4881 (0.0%)
1	C	1.00	0/3593	0.91	0/4881
1	D	1.00	1/3593 (0.0%)	0.91	1/4881 (0.0%)
All	All	1.02	5/14372 (0.0%)	0.92	6/19524 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	386	LEU	C-O	-5.59	1.16	1.24
1	A	263	GLN	C-O	-5.55	1.17	1.24
1	A	387	HIS	CA-C	-5.38	1.48	1.53
1	B	387	HIS	CA-C	-5.26	1.48	1.53
1	D	157	ILE	C-O	-5.22	1.18	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	426	ILE	CB-CA-C	-5.60	104.49	112.22
1	A	398	TRP	CA-C-N	5.45	125.12	119.56
1	A	398	TRP	C-N-CA	5.45	125.12	119.56
1	A	438	ARG	N-CA-C	5.37	119.32	112.34
1	B	437	ALA	N-CA-C	-5.31	105.39	111.07
1	B	461	LEU	N-CA-C	5.23	117.19	108.99

There are no chirality outliers.

There are no planarity outliers.

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	3543	0	3608	88	0
1	B	3543	0	3608	109	1
1	C	3543	0	3607	115	1
1	D	3543	0	3608	115	1
2	A	16	0	11	1	0
2	B	16	0	11	2	0
2	C	16	0	11	4	0
2	D	16	0	11	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	C	6	0	0	1	0
4	D	6	0	0	0	0
5	A	5	0	0	2	0
5	B	5	0	0	2	0
5	C	5	0	0	2	0
5	D	5	0	0	2	0
6	A	46	0	0	3	0
6	B	43	0	0	4	0
6	C	49	0	0	5	0
6	D	34	0	0	4	1
All	All	14456	0	14475	407	2

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 14.

All (407) 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:D:77:ARG:HA	1:D:153:ASP:OD1	1.33	1.22
1:A:441:ARG:HA	1:A:467:ILE:CG2	1.79	1.12
1:D:77:ARG:CA	1:D:153:ASP:OD1	1.96	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:GLN:HG2	1:A:456:VAL:HG23	1.28	1.10
1:B:375:GLN:HG2	1:B:456:VAL:HG12	1.32	1.06
1:D:78:PHE:N	1:D:153:ASP:OD1	1.90	1.05
1:B:284:GLU:OE2	1:B:317:LYS:NZ	1.90	1.03
1:C:281:SER:HB3	1:C:292:GLU:OE1	1.59	1.03
1:A:441:ARG:HA	1:A:467:ILE:HG22	1.04	1.01
1:C:107:THR:O	1:C:110:LYS:NZ	1.94	1.01
1:C:375:GLN:HG2	1:C:456:VAL:HG12	1.46	0.98
1:A:441:ARG:CA	1:A:467:ILE:HG22	1.95	0.96
1:B:441:ARG:HA	1:B:467:ILE:HG22	1.48	0.92
1:B:351:ARG:HG2	1:B:351:ARG:HH11	1.32	0.92
1:D:399:PRO:HA	1:D:415:ILE:HD12	1.52	0.91
1:A:41:TYR:OH	1:A:176:ASP:OD1	1.91	0.89
1:D:281:SER:HB3	1:D:292:GLU:OE1	1.73	0.88
1:D:130:ALA:HB3	1:D:147:GLU:HG3	1.53	0.88
1:C:99:GLU:OE2	6:C:601:HOH:O	1.92	0.87
1:C:375:GLN:CG	1:C:456:VAL:HG12	2.04	0.87
1:B:281:SER:HB3	1:B:292:GLU:OE1	1.73	0.87
1:B:41:TYR:OH	1:B:176:ASP:OD1	1.93	0.87
1:C:41:TYR:OH	1:C:176:ASP:OD1	1.93	0.86
1:B:33:ARG:HG2	1:B:33:ARG:HH11	1.39	0.86
1:C:399:PRO:HA	1:C:415:ILE:HD12	1.56	0.86
1:B:350:LYS:HD3	1:B:459:THR:O	1.76	0.85
1:B:375:GLN:HG2	1:B:456:VAL:CG1	2.07	0.85
1:A:431:LYS:O	1:A:435:GLU:HG3	1.76	0.84
1:D:77:ARG:C	1:D:153:ASP:OD1	2.20	0.84
1:D:442:GLY:O	1:D:466:ARG:HG3	1.78	0.83
1:B:375:GLN:CG	1:B:456:VAL:HG12	2.10	0.81
1:D:90:THR:HG23	6:D:623:HOH:O	1.81	0.80
1:B:130:ALA:HB3	1:B:147:GLU:HG3	1.63	0.79
1:C:268:ASN:O	2:C:501:G6P:O1	1.99	0.79
1:A:186:ASP:O	1:A:214:PRO:HD2	1.84	0.78
1:D:345:HIS:NE2	2:D:501:G6P:O1P	2.13	0.78
1:A:147:GLU:OE2	1:B:287:ARG:NH2	2.17	0.78
1:B:186:ASP:O	1:B:214:PRO:HD2	1.85	0.77
1:A:351:ARG:NH1	5:A:504:PO4:O2	2.18	0.76
1:B:351:ARG:HG2	1:B:351:ARG:NH1	1.99	0.76
1:A:375:GLN:HG2	1:A:456:VAL:CG2	2.13	0.76
1:A:33:ARG:NH2	1:A:67:ASP:OD2	2.19	0.75
1:D:235:PHE:O	1:D:270:LYS:NZ	2.20	0.75
1:C:131:LEU:HD23	1:C:143:CYS:HB2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:THR:OG1	1:B:33:ARG:NH1	2.21	0.74
4:C:503:OXL:O4	6:C:602:HOH:O	2.04	0.74
1:B:17:ARG:O	1:B:50:ARG:NH1	2.17	0.73
1:C:19:ASP:HA	6:C:611:HOH:O	1.88	0.73
1:D:99:GLU:OE2	6:D:602:HOH:O	2.06	0.73
1:D:77:ARG:HA	1:D:153:ASP:CG	2.14	0.72
1:B:89:GLU:OE1	1:B:102:HIS:NE2	2.22	0.72
1:B:95:VAL:HG22	1:B:139:ASP:HB2	1.71	0.72
1:B:351:ARG:HH11	1:B:351:ARG:CG	2.01	0.72
1:A:420:GLN:OE1	6:A:601:HOH:O	2.08	0.71
1:C:75:LEU:O	1:C:154:ASN:HA	1.90	0.71
1:A:402:ARG:HG3	1:A:413:THR:HB	1.73	0.70
1:C:125:ASP:HB3	1:C:128:LYS:HB2	1.70	0.70
1:D:14:ALA:O	1:D:20:LEU:CD2	2.40	0.70
1:C:132:VAL:HG23	1:C:146:VAL:HG21	1.72	0.70
1:B:423:ASP:OD1	1:B:423:ASP:N	2.22	0.69
1:C:279:LEU:HD13	1:C:282:MET:CE	2.23	0.69
1:D:15:THR:HA	1:D:20:LEU:HD23	1.75	0.68
1:C:282:MET:HE3	1:C:322:ALA:HA	1.75	0.68
1:D:375:GLN:HG2	1:D:456:VAL:HG12	1.74	0.68
1:B:463:HIS:CD2	1:B:465:HIS:HB2	2.29	0.68
1:D:42:ASP:O	1:D:46:VAL:HG23	1.95	0.67
1:D:402:ARG:HG3	1:D:413:THR:HB	1.77	0.66
1:D:331:CYS:O	1:D:335:GLU:HG3	1.95	0.66
1:C:129:VAL:CG1	1:C:147:GLU:O	2.43	0.66
1:B:350:LYS:HA	1:D:365:LEU:HD21	1.77	0.66
1:C:86:ALA:O	1:C:89:GLU:HG3	1.94	0.66
1:D:281:SER:HB3	1:D:292:GLU:CD	2.21	0.65
1:C:402:ARG:HB2	1:C:415:ILE:HD11	1.77	0.65
1:D:442:GLY:O	1:D:466:ARG:CG	2.44	0.65
1:C:375:GLN:HG2	1:C:456:VAL:CG1	2.24	0.65
1:C:279:LEU:HD13	1:C:282:MET:HE2	1.78	0.65
1:B:421:SER:OG	1:B:424:GLY:HA3	1.97	0.64
1:A:375:GLN:HB3	1:A:456:VAL:HG22	1.79	0.64
1:C:423:ASP:N	1:C:423:ASP:OD1	2.22	0.64
1:C:425:MET:CE	1:C:453:PRO:HB3	2.26	0.64
1:A:438:ARG:HD3	6:A:643:HOH:O	1.96	0.64
1:C:129:VAL:HG13	1:C:147:GLU:O	1.98	0.64
1:C:33:ARG:NH2	1:C:67:ASP:OD2	2.30	0.64
1:A:6:LYS:NZ	1:A:408:THR:O	2.30	0.64
1:D:375:GLN:HG2	1:D:456:VAL:CG1	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:382:ARG:HH12	2:D:501:G6P:H62	1.62	0.63
1:B:402:ARG:HG3	1:B:413:THR:HB	1.81	0.63
1:B:463:HIS:CE1	1:B:471:ASP:O	2.51	0.63
1:C:281:SER:HB3	1:C:292:GLU:CD	2.23	0.63
1:A:361:ILE:HD11	1:C:357:ALA:CB	2.29	0.63
1:C:402:ARG:HG3	1:C:413:THR:HB	1.81	0.63
1:D:77:ARG:HG2	1:D:153:ASP:OD2	1.98	0.62
1:D:68:LEU:O	1:D:191:SER:OG	2.15	0.62
1:B:399:PRO:HA	1:B:415:ILE:HD13	1.81	0.62
1:D:402:ARG:HB2	1:D:415:ILE:HD11	1.82	0.62
1:C:6:LYS:NZ	1:C:408:THR:O	2.32	0.61
1:D:268:ASN:O	2:D:501:G6P:O1	2.09	0.61
1:D:279:LEU:HD13	1:D:282:MET:CE	2.31	0.61
1:A:85:TRP:CE3	1:A:151:VAL:HG11	2.36	0.61
1:D:14:ALA:O	1:D:20:LEU:HD23	2.00	0.61
1:A:374:THR:HG21	1:A:377:GLY:HA2	1.82	0.61
1:A:399:PRO:HA	1:A:415:ILE:HD13	1.83	0.61
1:C:68:LEU:O	1:C:191:SER:OG	2.15	0.61
1:B:255:PRO:O	1:B:259:LYS:HG3	2.01	0.61
1:B:6:LYS:NZ	1:B:408:THR:O	2.33	0.61
1:A:287:ARG:O	6:A:603:HOH:O	2.16	0.60
1:C:457:GLY:N	5:C:504:PO4:O3	2.34	0.60
1:D:425:MET:CE	1:D:453:PRO:HB3	2.31	0.60
1:C:242:ARG:HD3	1:C:275:ALA:O	2.02	0.60
1:C:463:HIS:HD2	1:C:465:HIS:HB2	1.66	0.60
1:D:6:LYS:NZ	1:D:408:THR:O	2.33	0.60
1:A:375:GLN:CG	1:A:456:VAL:HG23	2.19	0.60
1:B:255:PRO:HA	6:B:624:HOH:O	2.01	0.60
1:C:213:VAL:HB	1:C:214:PRO:HD2	1.82	0.60
1:B:268:ASN:O	2:B:501:G6P:O1	2.20	0.59
1:B:441:ARG:HA	1:B:467:ILE:CG2	2.30	0.59
1:A:132:VAL:O	1:A:143:CYS:HB3	2.02	0.59
1:B:20:LEU:HD13	1:B:20:LEU:O	2.03	0.59
1:B:351:ARG:NH1	5:B:504:PO4:O4	2.36	0.59
1:B:213:VAL:HB	1:B:214:PRO:HD2	1.84	0.58
1:D:132:VAL:HG23	1:D:146:VAL:HG21	1.85	0.58
1:B:471:ASP:HB2	1:D:460:ASN:ND2	2.18	0.58
1:A:464:VAL:HG21	1:C:354:ILE:HD11	1.86	0.58
1:A:461:LEU:C	1:A:461:LEU:HD12	2.29	0.58
1:C:422:THR:HA	1:C:425:MET:HG3	1.85	0.58
1:B:442:GLY:O	1:B:466:ARG:HD2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:ASN:ND2	1:D:471:ASP:HB2	2.18	0.57
1:C:242:ARG:HH22	1:C:295:ASP:CG	2.10	0.57
1:D:463:HIS:CD2	1:D:465:HIS:HB2	2.39	0.57
1:B:470:ASP:OD1	1:B:470:ASP:O	2.22	0.57
1:C:134:ASP:OD2	1:C:144:THR:OG1	2.19	0.57
1:D:33:ARG:NH2	1:D:67:ASP:OD2	2.35	0.56
1:A:440:LYS:O	1:A:467:ILE:HG21	2.06	0.56
1:C:94:THR:HB	1:C:140:ASP:OD1	2.06	0.56
1:C:85:TRP:CZ2	1:C:91:VAL:HG11	2.40	0.56
1:B:68:LEU:O	1:B:191:SER:OG	2.15	0.56
1:A:68:LEU:O	1:A:191:SER:OG	2.16	0.56
1:C:374:THR:HG21	1:C:377:GLY:HA2	1.89	0.55
1:A:96:GLY:O	1:A:106:SER:OG	2.22	0.55
1:B:33:ARG:HG2	1:B:33:ARG:NH1	2.10	0.55
1:B:213:VAL:HB	1:B:214:PRO:CD	2.37	0.55
1:D:33:ARG:NE	1:D:67:ASP:OD2	2.37	0.55
1:D:172:LYS:NZ	1:D:176:ASP:OD2	2.37	0.55
1:B:89:GLU:OE1	1:B:102:HIS:CE1	2.60	0.54
1:B:158:SER:O	1:B:160:PRO:HD3	2.07	0.54
1:D:187:MET:SD	1:D:407:MET:HE2	2.47	0.54
1:C:408:THR:HG23	6:C:604:HOH:O	2.08	0.54
1:D:31:VAL:HG21	1:D:407:MET:HB3	1.88	0.54
1:D:382:ARG:HH12	2:D:501:G6P:H1	1.73	0.54
1:A:433:LEU:O	1:A:439:TYR:HB2	2.08	0.54
1:A:23:ALA:HB1	1:A:320:LEU:HD21	1.90	0.54
1:C:77:ARG:HG3	1:C:153:ASP:OD2	2.08	0.54
1:A:213:VAL:HB	1:A:214:PRO:HD2	1.88	0.54
1:A:461:LEU:HD12	1:A:461:LEU:O	2.08	0.53
1:A:213:VAL:HB	1:A:214:PRO:CD	2.38	0.53
1:C:13:PRO:HA	1:C:16:GLN:HG3	1.90	0.53
1:C:385:ARG:NH2	2:C:501:G6P:O2P	2.39	0.53
1:D:77:ARG:NH1	1:D:79:ALA:HA	2.23	0.53
1:D:279:LEU:HD13	1:D:282:MET:HE3	1.90	0.53
1:D:279:LEU:HD23	1:D:292:GLU:HB3	1.90	0.53
1:A:364:ARG:HG2	1:C:348:ARG:HH11	1.72	0.53
1:C:77:ARG:HG2	1:C:78:PHE:N	2.23	0.53
1:B:374:THR:HG21	1:B:377:GLY:HA2	1.91	0.53
1:D:463:HIS:HD2	1:D:465:HIS:HB2	1.73	0.53
1:C:129:VAL:HG12	1:C:147:GLU:O	2.09	0.53
1:C:463:HIS:CD2	1:C:465:HIS:HB2	2.44	0.53
1:A:23:ALA:CB	1:A:320:LEU:HD21	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ARG:HB2	1:A:469:GLU:HG3	1.91	0.53
1:C:186:ASP:O	1:C:214:PRO:HD2	2.08	0.53
1:C:206:MET:HE2	1:C:213:VAL:HG22	1.89	0.53
1:C:213:VAL:HB	1:C:214:PRO:CD	2.38	0.52
1:B:440:LYS:O	1:B:467:ILE:HG21	2.09	0.52
1:B:451:ALA:HB3	1:D:471:ASP:O	2.10	0.52
1:C:279:LEU:HD23	1:C:292:GLU:HB3	1.92	0.52
1:D:374:THR:HG21	1:D:377:GLY:HA2	1.91	0.52
1:D:213:VAL:HB	1:D:214:PRO:CD	2.39	0.52
1:C:147:GLU:HG2	1:D:286:SER:CB	2.40	0.52
1:A:279:LEU:HD23	1:A:292:GLU:HB3	1.92	0.52
1:D:41:TYR:OH	1:D:176:ASP:OD1	2.19	0.52
1:A:423:ASP:HB3	1:A:427:ARG:NH1	2.25	0.52
1:B:318:TYR:C	6:B:603:HOH:O	2.53	0.52
1:C:33:ARG:NE	1:C:67:ASP:OD2	2.40	0.51
1:A:112:LEU:HG	1:A:141:VAL:HG21	1.92	0.51
1:D:77:ARG:CG	1:D:153:ASP:OD2	2.58	0.51
1:A:361:ILE:HD11	1:C:357:ALA:HB3	1.91	0.51
1:A:425:MET:CE	1:A:453:PRO:HB3	2.40	0.51
1:C:77:ARG:NH1	1:C:79:ALA:HA	2.25	0.51
1:B:279:LEU:HD23	1:B:292:GLU:HB3	1.93	0.51
1:C:85:TRP:CH2	1:C:91:VAL:HG11	2.46	0.51
1:A:50:ARG:CG	1:A:50:ARG:HH21	2.24	0.51
1:B:461:LEU:HD12	1:B:461:LEU:C	2.36	0.51
1:B:460:ASN:HD21	1:D:471:ASP:HB2	1.74	0.51
1:B:461:LEU:HD12	1:B:461:LEU:O	2.09	0.51
1:A:463:HIS:ND1	1:A:465:HIS:HB2	2.26	0.51
1:A:399:PRO:CA	1:A:415:ILE:HD13	2.41	0.50
1:C:385:ARG:NH1	2:C:501:G6P:O2P	2.42	0.50
1:B:75:LEU:O	1:B:154:ASN:HA	2.10	0.50
1:D:374:THR:OG1	5:D:504:PO4:O3	2.26	0.50
1:B:421:SER:O	1:B:425:MET:HG3	2.11	0.50
1:D:350:LYS:HE3	1:D:459:THR:O	2.11	0.50
1:A:463:HIS:CE1	1:A:465:HIS:HB2	2.47	0.50
1:D:186:ASP:O	1:D:214:PRO:HD2	2.12	0.50
1:C:444:LEU:HD11	1:C:464:VAL:CG1	2.41	0.49
1:D:213:VAL:HB	1:D:214:PRO:HD2	1.94	0.49
1:D:155:LYS:HE3	1:D:156:GLY:H	1.78	0.49
1:D:279:LEU:HD22	1:D:282:MET:HE2	1.94	0.49
1:D:158:SER:O	1:D:160:PRO:HD3	2.12	0.49
1:D:209:ILE:O	1:D:209:ILE:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:LEU:HG	1:B:141:VAL:HG21	1.94	0.49
1:C:95:VAL:HG13	1:C:110:LYS:HD2	1.95	0.49
1:A:442:GLY:N	1:A:467:ILE:O	2.26	0.49
1:B:374:THR:OG1	1:B:377:GLY:N	2.42	0.49
1:C:350:LYS:HE3	1:C:459:THR:O	2.11	0.49
1:D:206:MET:O	1:D:210:GLY:N	2.45	0.49
1:A:84:HIS:HA	1:A:150:PRO:HA	1.95	0.49
1:A:85:TRP:CZ2	1:A:91:VAL:HG11	2.48	0.49
1:C:116:ALA:HA	1:C:162:MET:HE2	1.94	0.49
1:D:442:GLY:C	1:D:466:ARG:HG3	2.37	0.49
1:D:382:ARG:NH1	2:D:501:G6P:H62	2.27	0.49
1:B:444:LEU:HD11	1:B:464:VAL:CG1	2.43	0.49
1:B:463:HIS:HD2	1:B:465:HIS:HB2	1.74	0.49
1:C:126:ASP:HA	1:C:247:VAL:HG11	1.94	0.49
1:C:203:HIS:O	1:C:206:MET:HB2	2.12	0.49
1:D:228:LEU:HD21	1:D:261:ALA:HA	1.95	0.48
1:B:281:SER:HB3	1:B:292:GLU:CD	2.37	0.48
1:D:163:ASN:OD1	1:D:163:ASN:N	2.46	0.48
1:B:73:ILE:HG23	1:B:109:TYR:HB2	1.95	0.48
1:B:48:TYR:C	1:B:48:TYR:CD2	2.91	0.48
1:B:350:LYS:CD	1:B:459:THR:O	2.55	0.48
1:C:228:LEU:HD21	1:C:261:ALA:HA	1.95	0.48
1:A:48:TYR:C	1:A:48:TYR:CD2	2.91	0.48
1:C:41:TYR:CZ	1:C:176:ASP:OD1	2.67	0.48
1:D:92:ARG:NH2	1:D:137:GLU:OE1	2.47	0.48
1:A:349:THR:OG1	2:A:501:G6P:O1P	2.22	0.47
1:B:85:TRP:O	1:B:149:GLY:N	2.43	0.47
1:C:359:ARG:NH1	1:C:360:ASP:OD1	2.47	0.47
1:D:48:TYR:CD2	1:D:48:TYR:C	2.92	0.47
1:B:109:TYR:HE2	1:B:162:MET:HE1	1.79	0.47
1:D:376:SER:OG	5:D:504:PO4:O4	2.31	0.47
1:A:399:PRO:HB3	1:A:415:ILE:HD13	1.96	0.47
1:A:36:PHE:O	1:A:172:LYS:NZ	2.48	0.47
1:C:126:ASP:HB3	1:D:290:ARG:HH22	1.80	0.47
1:C:242:ARG:NH2	1:C:295:ASP:OD1	2.47	0.47
1:B:209:ILE:O	1:B:209:ILE:HG22	2.14	0.47
1:C:41:TYR:CE1	1:C:176:ASP:OD1	2.68	0.47
1:C:48:TYR:CD2	1:C:48:TYR:C	2.93	0.47
1:D:85:TRP:CZ2	1:D:91:VAL:HG11	2.49	0.47
1:B:95:VAL:CG2	1:B:139:ASP:HB2	2.44	0.47
1:B:421:SER:OG	1:B:424:GLY:CA	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:VAL:O	1:D:211:ARG:NH1	2.47	0.46
1:A:70:GLY:HA2	1:A:173:ASP:OD2	2.15	0.46
1:B:124:VAL:HB	1:B:129:VAL:HB	1.97	0.46
1:B:109:TYR:CZ	1:B:164:VAL:HG13	2.51	0.46
1:C:85:TRP:O	1:C:149:GLY:N	2.47	0.46
1:C:214:PRO:HA	1:C:236:ASP:OD2	2.15	0.46
1:A:206:MET:O	1:A:210:GLY:N	2.48	0.46
1:A:363:GLU:OE2	1:A:389:PRO:HD2	2.15	0.46
1:A:376:SER:OG	5:A:504:PO4:O4	2.30	0.46
1:D:267:GLU:OE2	1:D:345:HIS:ND1	2.49	0.46
1:B:132:VAL:HG23	1:B:146:VAL:HG21	1.96	0.46
1:D:425:MET:HE1	1:D:453:PRO:HB3	1.96	0.46
1:D:75:LEU:O	1:D:154:ASN:HA	2.16	0.46
1:C:375:GLN:CD	1:C:456:VAL:HG12	2.41	0.46
1:D:73:ILE:HG23	1:D:109:TYR:HB2	1.98	0.46
1:A:399:PRO:HA	1:A:415:ILE:CD1	2.45	0.46
1:B:74:ARG:HG2	1:B:154:ASN:O	2.16	0.46
1:C:206:MET:O	1:C:210:GLY:N	2.48	0.46
1:D:85:TRP:CH2	1:D:91:VAL:HG11	2.51	0.46
1:D:431:LYS:O	1:D:435:GLU:HG3	2.16	0.45
1:A:146:VAL:HG12	1:A:146:VAL:O	2.15	0.45
1:B:206:MET:O	1:B:210:GLY:N	2.48	0.45
1:B:375:GLN:HE22	1:B:454:GLY:C	2.23	0.45
1:C:172:LYS:NZ	1:C:176:ASP:OD2	2.42	0.45
1:A:452:PRO:HA	1:A:453:PRO:HD3	1.87	0.45
1:D:399:PRO:HA	1:D:415:ILE:CD1	2.34	0.45
1:B:52:ARG:NH1	1:B:184:GLY:O	2.49	0.45
1:C:399:PRO:HA	1:C:415:ILE:CD1	2.37	0.45
1:D:266:ARG:O	1:D:385:ARG:HD2	2.17	0.45
1:D:282:MET:HE1	1:D:325:THR:HB	1.99	0.45
1:D:434:LEU:HD23	1:D:434:LEU:HA	1.83	0.45
1:A:423:ASP:HB3	1:A:427:ARG:CZ	2.47	0.45
1:B:228:LEU:HD21	1:B:261:ALA:HA	1.98	0.45
1:C:34:MET:HE3	1:C:36:PHE:CE1	2.52	0.45
1:C:152:SER:OG	1:C:155:LYS:HE2	2.17	0.45
1:B:463:HIS:HE1	1:B:471:ASP:O	1.98	0.45
1:A:169:LEU:HD23	1:A:173:ASP:HB3	1.99	0.45
1:A:375:GLN:HB3	1:A:456:VAL:CG2	2.47	0.45
1:C:48:TYR:O	1:C:52:ARG:HG2	2.17	0.45
1:D:208:ARG:NE	6:D:601:HOH:O	2.06	0.45
1:C:382:ARG:HH12	2:C:501:G6P:H1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ILE:HG22	1:A:467:ILE:O	2.17	0.44
1:C:434:LEU:HD23	1:C:434:LEU:HA	1.82	0.44
1:D:359:ARG:NH1	1:D:360:ASP:OD1	2.50	0.44
1:A:350:LYS:HE3	1:A:459:THR:O	2.18	0.44
1:B:442:GLY:O	1:B:466:ARG:CD	2.65	0.44
1:C:351:ARG:HG2	1:C:379:THR:OG1	2.17	0.44
1:D:85:TRP:O	1:D:148:GLY:HA2	2.18	0.44
1:A:426:ILE:CD1	1:A:472:VAL:HG13	2.48	0.44
1:D:85:TRP:O	1:D:149:GLY:N	2.51	0.44
1:A:252:GLU:HB2	1:B:329:ILE:HA	2.00	0.44
1:A:318:TYR:HB3	1:A:321:ALA:HB3	1.99	0.44
1:B:349:THR:OG1	2:B:501:G6P:O3P	2.22	0.44
1:B:443:ASP:O	1:B:466:ARG:HA	2.17	0.44
1:C:266:ARG:O	1:C:385:ARG:HD2	2.18	0.44
1:C:379:THR:OG1	5:C:504:PO4:O1	2.19	0.44
1:B:146:VAL:HG12	1:B:146:VAL:O	2.18	0.44
1:D:426:ILE:HG21	1:D:472:VAL:HG21	1.99	0.44
1:B:8:VAL:HG22	1:B:31:VAL:HB	2.00	0.44
1:B:17:ARG:H	1:B:17:ARG:HG2	1.61	0.44
1:C:128:LYS:HD2	1:C:128:LYS:HA	1.57	0.44
1:A:351:ARG:H	1:A:351:ARG:HG2	1.50	0.43
1:A:378:ASP:O	1:A:382:ARG:HG3	2.18	0.43
1:B:471:ASP:HB2	1:D:460:ASN:HD22	1.83	0.43
1:D:378:ASP:O	1:D:382:ARG:HG3	2.18	0.43
1:A:399:PRO:CB	1:A:415:ILE:HD13	2.48	0.43
1:C:186:ASP:HB2	1:C:187:MET:HE3	1.99	0.43
1:D:421:SER:O	1:D:425:MET:HG3	2.18	0.43
1:A:52:ARG:NH2	1:A:184:GLY:O	2.51	0.43
1:B:375:GLN:CB	1:B:456:VAL:HG12	2.48	0.43
1:C:73:ILE:HG23	1:C:109:TYR:HB2	2.01	0.43
1:C:450:GLY:HA3	1:C:459:THR:HA	2.01	0.43
1:A:460:ASN:ND2	1:C:471:ASP:HB2	2.33	0.43
1:B:440:LYS:O	1:B:467:ILE:CG2	2.66	0.43
1:C:363:GLU:OE2	6:C:603:HOH:O	2.21	0.43
1:C:425:MET:HE3	1:C:453:PRO:CG	2.47	0.43
1:B:109:TYR:CE1	1:B:164:VAL:HG13	2.54	0.43
1:C:195:SER:OG	1:C:196:PRO:HD2	2.19	0.43
1:D:214:PRO:HA	1:D:236:ASP:OD2	2.19	0.43
1:D:249:LEU:HD21	6:D:630:HOH:O	2.17	0.43
1:B:206:MET:HE2	1:B:213:VAL:HG22	2.00	0.43
1:B:378:ASP:O	1:B:382:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:VAL:HG22	1:D:31:VAL:HB	2.01	0.43
1:B:220:GLU:OE2	6:B:601:HOH:O	2.21	0.43
1:C:42:ASP:O	1:C:46:VAL:HG23	2.19	0.43
1:D:131:LEU:HD23	1:D:143:CYS:HB2	2.00	0.43
1:A:158:SER:O	1:A:160:PRO:HD3	2.19	0.43
1:B:452:PRO:HA	1:B:453:PRO:HD3	1.94	0.43
1:C:267:GLU:OE2	1:C:345:HIS:ND1	2.52	0.43
1:A:426:ILE:HD13	1:A:472:VAL:HG13	2.00	0.42
1:C:425:MET:HE1	1:C:453:PRO:HB3	2.01	0.42
1:D:72:LYS:HE3	1:D:156:GLY:HA3	1.99	0.42
1:D:77:ARG:HG2	1:D:153:ASP:CG	2.44	0.42
1:D:124:VAL:HB	1:D:129:VAL:HB	2.01	0.42
1:D:130:ALA:C	1:D:131:LEU:HD12	2.44	0.42
1:C:131:LEU:CD2	1:C:143:CYS:HB2	2.46	0.42
1:B:20:LEU:HA	1:B:20:LEU:HD22	1.74	0.42
1:D:141:VAL:HG12	1:D:143:CYS:SG	2.60	0.42
1:A:206:MET:HE2	1:A:213:VAL:HG22	2.00	0.42
1:A:421:SER:O	1:A:425:MET:HG3	2.19	0.42
1:B:422:THR:O	1:B:426:ILE:HD12	2.20	0.42
1:D:423:ASP:OD1	1:D:472:VAL:HG12	2.19	0.42
1:B:434:LEU:HD23	1:B:434:LEU:HA	1.92	0.42
1:C:372:ALA:HB3	1:C:380:VAL:HG22	2.02	0.42
1:D:281:SER:HB3	1:D:292:GLU:OE2	2.20	0.42
1:B:275:ALA:O	1:B:276:THR:HB	2.19	0.42
1:B:181:LEU:HD11	1:B:206:MET:HG2	2.02	0.42
1:B:266:ARG:O	1:B:385:ARG:HD2	2.19	0.42
1:D:263:GLN:O	1:D:267:GLU:HG2	2.20	0.42
1:A:159:LEU:HD13	1:A:159:LEU:HA	1.89	0.42
1:A:370:LEU:HD23	1:A:446:VAL:HB	2.02	0.42
1:B:162:MET:HE2	1:B:164:VAL:HG22	2.01	0.42
1:B:375:GLN:HB3	1:B:456:VAL:HG12	2.01	0.42
1:A:232:VAL:O	1:A:270:LYS:HE3	2.19	0.41
1:A:15:THR:HA	1:A:20:LEU:HD12	2.02	0.41
1:B:42:ASP:O	1:B:46:VAL:HG23	2.20	0.41
1:C:22:ARG:NH1	1:C:57:ALA:CB	2.84	0.41
1:C:246:GLY:HA3	1:D:290:ARG:HE	1.85	0.41
1:D:22:ARG:NH1	1:D:57:ALA:CB	2.83	0.41
1:D:139:ASP:OD1	1:D:139:ASP:N	2.53	0.41
1:D:162:MET:HE2	1:D:164:VAL:CG2	2.50	0.41
1:D:181:LEU:HD11	1:D:206:MET:HG2	2.02	0.41
1:B:423:ASP:HB3	6:B:633:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:LEU:N	1:C:436:LEU:HD12	2.35	0.41
1:A:451:ALA:HB3	1:C:471:ASP:O	2.19	0.41
1:B:84:HIS:HA	1:B:150:PRO:HA	2.03	0.41
1:D:375:GLN:HB3	1:D:456:VAL:HG12	2.03	0.41
1:C:175:GLU:O	1:C:175:GLU:HG2	2.21	0.41
1:C:242:ARG:CD	1:C:275:ALA:O	2.69	0.41
1:D:175:GLU:O	1:D:175:GLU:HG2	2.20	0.41
1:C:329:ILE:HA	1:D:252:GLU:HB2	2.02	0.41
1:C:436:LEU:O	1:C:437:ALA:C	2.63	0.41
1:A:50:ARG:CG	1:A:50:ARG:NH2	2.81	0.41
1:A:100:GLY:HA3	1:A:105:VAL:HG23	2.02	0.41
1:B:464:VAL:HG21	1:D:354:ILE:HD11	2.03	0.41
1:B:465:HIS:ND1	1:B:471:ASP:OD1	2.53	0.41
1:C:8:VAL:HG22	1:C:31:VAL:HB	2.03	0.41
1:C:275:ALA:O	1:C:276:THR:HB	2.19	0.41
1:C:378:ASP:O	1:C:382:ARG:HG3	2.21	0.41
1:C:298:ASN:CG	1:D:298:ASN:CG	2.89	0.41
1:B:33:ARG:NE	1:B:67:ASP:OD2	2.40	0.40
1:B:461:LEU:C	1:B:461:LEU:CD1	2.93	0.40
1:C:287:ARG:HH12	1:D:123:LEU:HD12	1.86	0.40
1:D:372:ALA:HB3	1:D:380:VAL:HG22	2.03	0.40
1:A:341:PRO:HA	1:A:342:PRO:HD3	1.98	0.40
1:C:75:LEU:HD22	1:C:105:VAL:HG11	2.03	0.40
1:C:351:ARG:CD	1:C:457:GLY:HA2	2.52	0.40
1:C:370:LEU:HD23	1:C:446:VAL:HB	2.02	0.40
1:A:275:ALA:O	1:A:276:THR:HB	2.21	0.40
1:B:33:ARG:NH1	1:B:33:ARG:CG	2.78	0.40
1:A:228:LEU:HD21	1:A:261:ALA:HA	2.02	0.40
1:B:375:GLN:NE2	1:B:454:GLY:C	2.79	0.40
1:B:456:VAL:HA	5:B:504:PO4:O1	2.22	0.40
1:C:375:GLN:OE1	1:C:456:VAL:CG1	2.69	0.40
1:A:8:VAL:HG22	1:A:31:VAL:HB	2.04	0.40
1:A:434:LEU:HD23	1:A:434:LEU:HA	1.94	0.40
1:B:20:LEU:HD13	1:B:20:LEU:C	2.47	0.40
1:D:206:MET:HE2	1:D:213:VAL:HG22	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:GLU:OE1	6:D:602:HOH:O[2_655]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ASP:OD2	1:D:134:ASP:OD1[3_564]	2.16	0.04

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	396/475 (83%)	380 (96%)	15 (4%)	1 (0%)	36	54
1	B	469/475 (99%)	457 (97%)	11 (2%)	1 (0%)	43	62
1	C	469/475 (99%)	457 (97%)	11 (2%)	1 (0%)	43	62
1	D	469/475 (99%)	456 (97%)	12 (3%)	1 (0%)	43	62
All	All	1803/1900 (95%)	1750 (97%)	49 (3%)	4 (0%)	43	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	THR
1	B	276	THR
1	C	276	THR
1	D	276	THR

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	379/381 (100%)	355 (94%)	24 (6%)	16	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	379/381 (100%)	349 (92%)	30 (8%)	11	24
1	C	379/381 (100%)	350 (92%)	29 (8%)	12	25
1	D	379/381 (100%)	351 (93%)	28 (7%)	13	26
All	All	1516/1524 (100%)	1405 (93%)	111 (7%)	13	27

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	50	ARG
1	A	74	ARG
1	A	106	SER
1	A	142	VAL
1	A	143	CYS
1	A	147	GLU
1	A	152	SER
1	A	188	VAL
1	A	320	LEU
1	A	335	GLU
1	A	351	ARG
1	A	359	ARG
1	A	368	LYS
1	A	412	GLU
1	A	419	MET
1	A	420	GLN
1	A	423	ASP
1	A	428	GLN
1	A	436	LEU
1	A	441	ARG
1	A	456	VAL
1	A	461	LEU
1	A	467	ILE
1	B	17	ARG
1	B	18	ASP
1	B	20	LEU
1	B	33	ARG
1	B	74	ARG
1	B	103	ASP
1	B	110	LYS
1	B	123	LEU
1	B	131	LEU

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Mol	Chain	Res	Type
1	B	155	LYS
1	B	159	LEU
1	B	163	ASN
1	B	187	MET
1	B	188	VAL
1	B	317	LYS
1	B	348	ARG
1	B	351	ARG
1	B	368	LYS
1	B	412	GLU
1	B	415	ILE
1	B	419	MET
1	B	420	GLN
1	B	423	ASP
1	B	426	ILE
1	B	428	GLN
1	B	431	LYS
1	B	438	ARG
1	B	441	ARG
1	B	461	LEU
1	B	467	ILE
1	C	18	ASP
1	C	19	ASP
1	C	80	SER
1	C	101	SER
1	C	106	SER
1	C	117	VAL
1	C	128	LYS
1	C	129	VAL
1	C	137	GLU
1	C	159	LEU
1	C	187	MET
1	C	188	VAL
1	C	231	ILE
1	C	242	ARG
1	C	282	MET
1	C	320	LEU
1	C	348	ARG
1	C	351	ARG
1	C	359	ARG
1	C	368	LYS
1	C	375	GLN

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Mol	Chain	Res	Type
1	C	400	GLU
1	C	412	GLU
1	C	419	MET
1	C	420	GLN
1	C	423	ASP
1	C	431	LYS
1	C	456	VAL
1	C	467	ILE
1	D	45	LYS
1	D	72	LYS
1	D	95	VAL
1	D	106	SER
1	D	117	VAL
1	D	123	LEU
1	D	142	VAL
1	D	155	LYS
1	D	163	ASN
1	D	188	VAL
1	D	201	LEU
1	D	231	ILE
1	D	348	ARG
1	D	351	ARG
1	D	359	ARG
1	D	375	GLN
1	D	412	GLU
1	D	415	ILE
1	D	419	MET
1	D	420	GLN
1	D	426	ILE
1	D	433	LEU
1	D	436	LEU
1	D	445	VAL
1	D	461	LEU
1	D	466	ARG
1	D	467	ILE
1	D	471	ASP

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	404	GLN
1	A	420	GLN

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Mol	Chain	Res	Type
1	B	203	HIS
1	B	336	ASN
1	B	404	GLN
1	B	428	GLN
1	B	463	HIS
1	C	268	ASN
1	C	336	ASN
1	C	387	HIS
1	C	404	GLN
1	C	463	HIS
1	D	203	HIS
1	D	285	ASN
1	D	336	ASN
1	D	404	GLN
1	D	463	HIS

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 16 ligands modelled in this entry, 4 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
5	PO4	B	504	-	4,4,4	0.87	0	6,6,6	0.61	0
4	OXL	D	503	3	5,5,5	2.24	2 (40%)	6,6,6	2.25	2 (33%)
2	G6P	D	501	-	16,16,16	0.55	0	23,24,24	0.91	0
5	PO4	A	504	-	4,4,4	0.80	0	6,6,6	0.90	0
4	OXL	B	503	3	5,5,5	2.32	2 (40%)	6,6,6	2.47	3 (50%)
2	G6P	B	501	-	16,16,16	0.53	0	23,24,24	1.33	2 (8%)
4	OXL	A	503	3	5,5,5	2.61	2 (40%)	6,6,6	2.38	3 (50%)
5	PO4	C	504	-	4,4,4	0.88	0	6,6,6	0.96	0
2	G6P	C	501	-	16,16,16	0.69	0	23,24,24	1.03	1 (4%)
2	G6P	A	501	-	16,16,16	0.72	0	23,24,24	0.77	0
4	OXL	C	503	3	5,5,5	2.15	3 (60%)	6,6,6	2.48	3 (50%)
5	PO4	D	504	-	4,4,4	1.26	0	6,6,6	0.51	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
4	OXL	D	503	3	-	2/4/4/4	-
2	G6P	D	501	-	-	5/6/26/26	0/1/1/1
4	OXL	B	503	3	-	4/4/4/4	-
2	G6P	B	501	-	-	0/6/26/26	0/1/1/1
4	OXL	A	503	3	-	4/4/4/4	-
2	G6P	C	501	-	-	2/6/26/26	0/1/1/1
2	G6P	A	501	-	-	0/6/26/26	0/1/1/1
4	OXL	C	503	3	-	4/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	OXL	C2-C1	-5.05	1.45	1.54
4	B	503	OXL	C2-C1	-4.15	1.47	1.54
4	D	503	OXL	C2-C1	-3.75	1.48	1.54
4	C	503	OXL	C2-C1	-2.79	1.49	1.54
4	C	503	OXL	O4-C2	-2.56	1.23	1.30
4	B	503	OXL	O3-C1	-2.49	1.23	1.30
4	C	503	OXL	O1-C1	2.37	1.28	1.22
4	A	503	OXL	O3-C1	-2.31	1.24	1.30
4	D	503	OXL	O4-C2	-2.29	1.24	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	OXL	O4-C2-C1	4.16	120.91	112.83
2	B	501	G6P	O5-C1-C2	4.10	117.50	110.30
4	C	503	OXL	O4-C2-C1	4.07	120.72	112.83
4	A	503	OXL	O4-C2-C1	4.04	120.66	112.83
4	D	503	OXL	O4-C2-C1	3.68	119.96	112.83
4	C	503	OXL	O3-C1-C2	3.43	119.47	112.83
4	D	503	OXL	O3-C1-C2	3.29	119.21	112.83
4	B	503	OXL	O3-C1-C2	3.22	119.07	112.83
4	A	503	OXL	O2-C2-C1	-2.92	114.55	120.63
4	A	503	OXL	O3-C1-C2	2.83	118.31	112.83
4	B	503	OXL	O2-C2-C1	-2.60	115.21	120.63
2	C	501	G6P	O5-C5-C6	2.60	111.85	106.69
2	B	501	G6P	C1-O5-C5	2.57	118.62	113.65
4	C	503	OXL	O4-C2-O2	-2.38	118.22	123.90

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	G6P	C4-C5-C6-O6
2	C	501	G6P	O5-C5-C6-O6
2	D	501	G6P	C4-C5-C6-O6
2	D	501	G6P	O5-C5-C6-O6
2	D	501	G6P	C6-O6-P-O1P
2	D	501	G6P	C6-O6-P-O2P
4	B	503	OXL	O1-C1-C2-O2
4	B	503	OXL	O1-C1-C2-O4
4	B	503	OXL	O3-C1-C2-O2
4	B	503	OXL	O3-C1-C2-O4
4	C	503	OXL	O1-C1-C2-O4
4	C	503	OXL	O3-C1-C2-O2
4	C	503	OXL	O1-C1-C2-O2
4	C	503	OXL	O3-C1-C2-O4
4	A	503	OXL	O1-C1-C2-O2
2	D	501	G6P	C6-O6-P-O3P
4	A	503	OXL	O3-C1-C2-O4
4	A	503	OXL	O3-C1-C2-O2
4	A	503	OXL	O1-C1-C2-O4
4	D	503	OXL	O3-C1-C2-O4
4	D	503	OXL	O1-C1-C2-O2

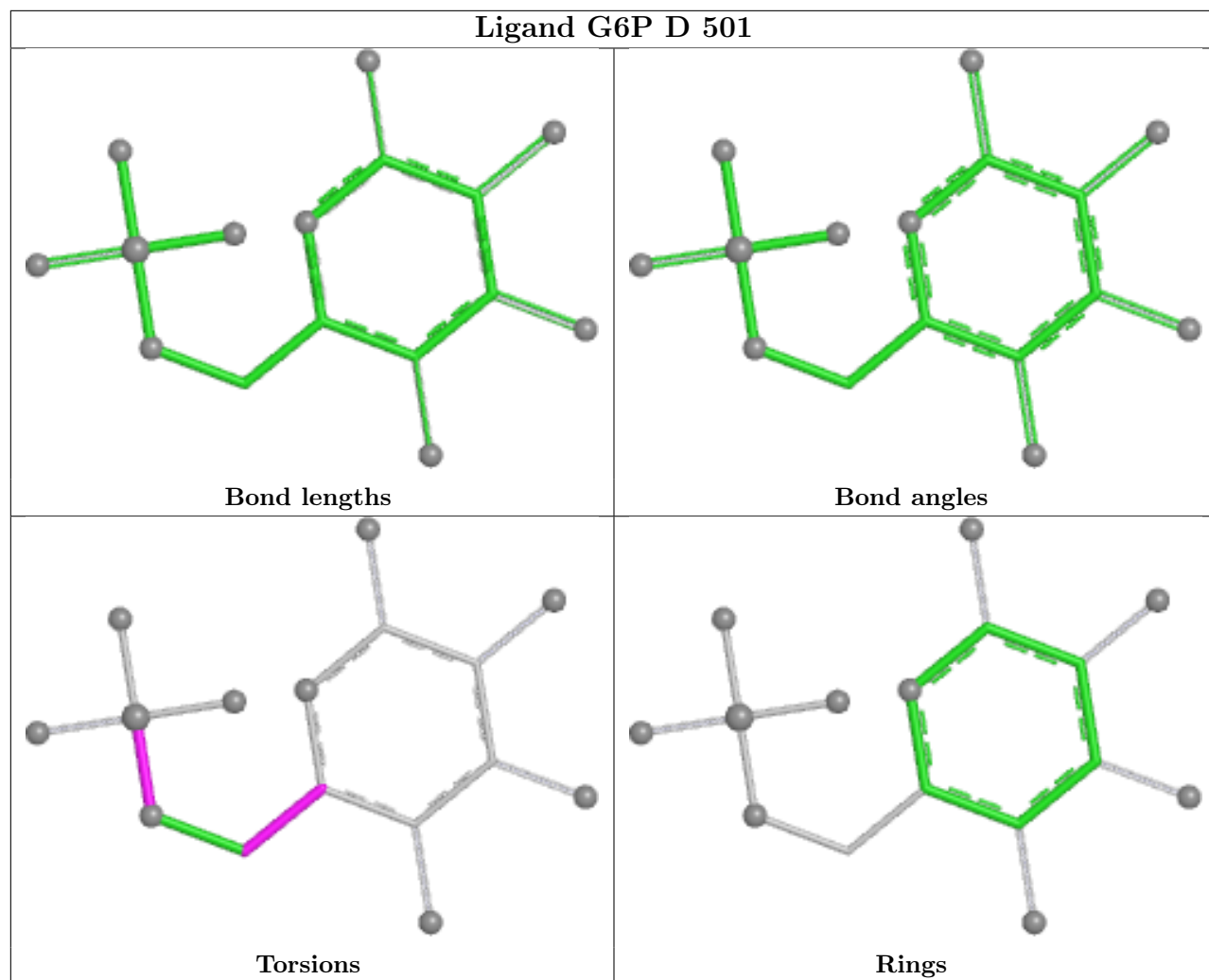
There are no ring outliers.

9 monomers are involved in 21 short contacts:

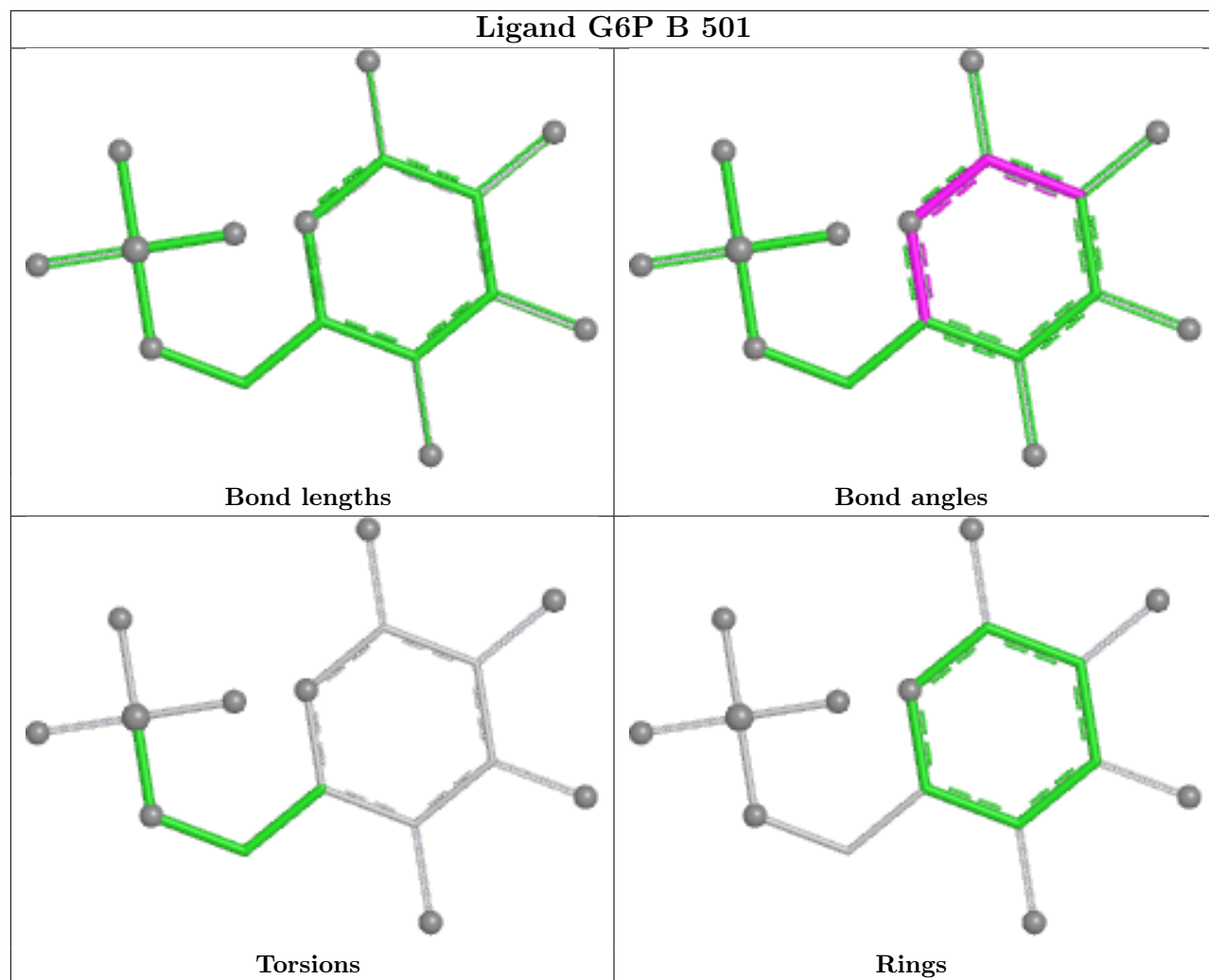
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	504	PO4	2	0
2	D	501	G6P	5	0
5	A	504	PO4	2	0
2	B	501	G6P	2	0
5	C	504	PO4	2	0
2	C	501	G6P	4	0
2	A	501	G6P	1	0
4	C	503	OXL	1	0
5	D	504	PO4	2	0

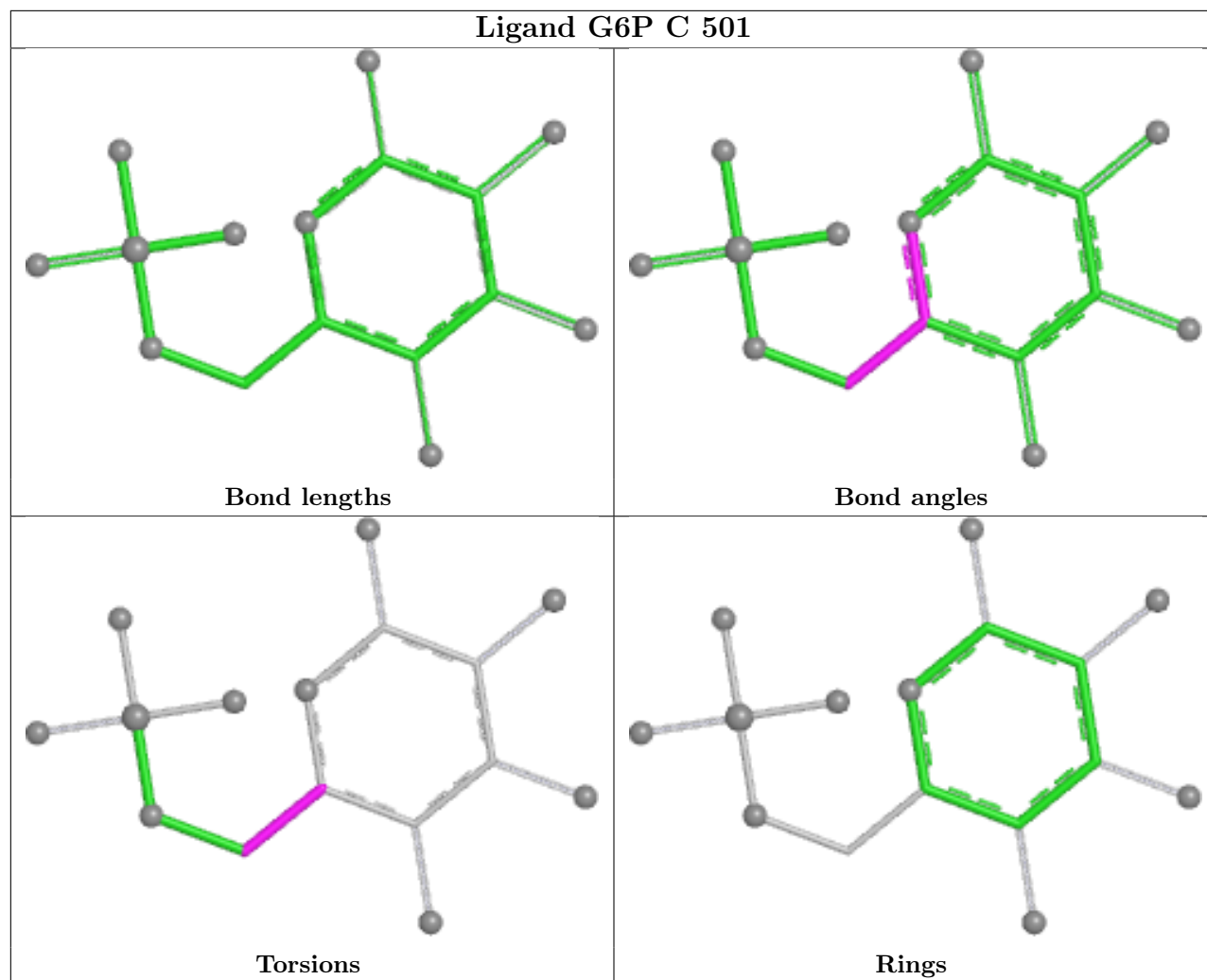
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand G6P D 501



Ligand G6P B 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	471/475 (99%)	0.91	26 (5%)	30	23	25, 40, 57, 77	0
1	B	471/475 (99%)	0.92	33 (7%)	22	16	26, 40, 57, 75	0
1	C	471/475 (99%)	1.16	65 (13%)	6	5	27, 44, 63, 83	0
1	D	471/475 (99%)	1.14	55 (11%)	9	7	26, 44, 66, 96	0
All	All	1884/1900 (99%)	1.03	179 (9%)	14	11	25, 42, 62, 96	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	338	THR	5.8
1	D	338	THR	5.7
1	D	99	GLU	4.4
1	C	106	SER	4.0
1	D	456	VAL	3.9
1	D	82	ALA	3.8
1	D	106	SER	3.8
1	B	151	VAL	3.7
1	D	116	ALA	3.7
1	D	100	GLY	3.6
1	B	422	THR	3.6
1	D	80	SER	3.6
1	C	113	ALA	3.5
1	B	472	VAL	3.5
1	C	105	VAL	3.4
1	A	437	ALA	3.4
1	D	101	SER	3.3
1	D	81	GLY	3.3
1	C	99	GLU	3.3
1	D	76	GLY	3.2
1	D	107	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	85	TRP	3.2
1	A	422	THR	3.2
1	B	88	GLY	3.1
1	D	139	ASP	3.1
1	C	472	VAL	3.1
1	C	116	ALA	3.1
1	D	113	ALA	3.1
1	B	454	GLY	3.1
1	C	81	GLY	3.0
1	D	79	ALA	3.0
1	C	136	VAL	3.0
1	C	96	GLY	2.9
1	D	137	GLU	2.9
1	C	437	ALA	2.9
1	C	204	GLU	2.8
1	C	150	PRO	2.8
1	B	134	ASP	2.8
1	C	152	SER	2.8
1	C	456	VAL	2.8
1	C	130	ALA	2.8
1	C	51	VAL	2.7
1	C	109	TYR	2.7
1	C	101	SER	2.7
1	D	147	GLU	2.7
1	D	131	LEU	2.7
1	D	155	LYS	2.7
1	B	63	GLY	2.7
1	D	104	ARG	2.7
1	D	161	GLY	2.7
1	A	416	VAL	2.7
1	D	105	VAL	2.7
1	C	419	MET	2.7
1	B	436	LEU	2.7
1	C	131	LEU	2.7
1	C	194	ARG	2.6
1	B	197	ALA	2.6
1	B	451	ALA	2.6
1	B	196	PRO	2.6
1	D	246	GLY	2.6
1	C	139	ASP	2.6
1	B	38	HIS	2.6
1	D	138	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	434	LEU	2.6
1	A	339	ALA	2.6
1	A	421	SER	2.5
1	A	472	VAL	2.5
1	A	118	ALA	2.5
1	D	22	ARG	2.5
1	C	286	SER	2.5
1	B	150	PRO	2.5
1	D	93	ILE	2.5
1	A	454	GLY	2.5
1	B	89	GLU	2.5
1	C	93	ILE	2.4
1	C	167	PRO	2.4
1	D	136	VAL	2.4
1	B	321	ALA	2.4
1	D	130	ALA	2.4
1	B	90	THR	2.4
1	D	396	THR	2.4
1	A	150	PRO	2.4
1	A	467	ILE	2.4
1	D	78	PHE	2.4
1	D	85	TRP	2.4
1	C	62	VAL	2.4
1	B	440	LYS	2.4
1	C	97	ALA	2.4
1	D	437	ALA	2.4
1	C	100	GLY	2.4
1	C	205	VAL	2.4
1	B	332	ALA	2.4
1	A	401	VAL	2.3
1	A	431	LYS	2.3
1	B	324	ARG	2.3
1	B	18	ASP	2.3
1	C	82	ALA	2.3
1	C	201	LEU	2.3
1	C	251	LEU	2.3
1	A	136	VAL	2.3
1	D	472	VAL	2.3
1	D	129	VAL	2.3
1	A	436	LEU	2.3
1	C	158	SER	2.3
1	C	104	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	77	ARG	2.3
1	A	237	ALA	2.3
1	C	85	TRP	2.3
1	C	90	THR	2.3
1	D	109	TYR	2.3
1	B	202	VAL	2.3
1	D	167	PRO	2.3
1	C	76	GLY	2.3
1	D	166	ALA	2.2
1	D	20	LEU	2.2
1	C	420	GLN	2.2
1	C	165	THR	2.2
1	A	105	VAL	2.2
1	D	158	SER	2.2
1	A	419	MET	2.2
1	C	135	ALA	2.2
1	C	223	GLU	2.2
1	D	427	ARG	2.2
1	C	2	THR	2.2
1	B	12	GLY	2.2
1	B	99	GLU	2.2
1	D	97	ALA	2.2
1	B	136	VAL	2.2
1	D	51	VAL	2.2
1	A	90	THR	2.2
1	C	454	GLY	2.2
1	D	430	ASP	2.2
1	D	245	LEU	2.2
1	A	357	ALA	2.2
1	B	397	ALA	2.2
1	C	54	ALA	2.2
1	A	80	SER	2.1
1	D	47	ALA	2.1
1	C	438	ARG	2.1
1	A	453	PRO	2.1
1	C	91	VAL	2.1
1	C	122	VAL	2.1
1	C	288	PRO	2.1
1	D	150	PRO	2.1
1	D	416	VAL	2.1
1	A	468	GLY	2.1
1	C	246	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	437	ALA	2.1
1	A	151	VAL	2.1
1	C	146	VAL	2.1
1	B	453	PRO	2.1
1	C	418	LYS	2.1
1	D	227	ASN	2.1
1	B	426	ILE	2.1
1	D	403	SER	2.1
1	C	440	LYS	2.1
1	C	182	ASN	2.1
1	C	20	LEU	2.1
1	D	436	LEU	2.1
1	A	471	ASP	2.1
1	B	165	THR	2.1
1	D	92	ARG	2.1
1	A	85	TRP	2.1
1	B	322	ALA	2.1
1	C	22	ARG	2.0
1	C	276	THR	2.0
1	D	283	ILE	2.0
1	D	423	ASP	2.0
1	C	84	HIS	2.0
1	C	151	VAL	2.0
1	C	277	GLN	2.0
1	C	444	LEU	2.0
1	C	227	ASN	2.0
1	C	57	ALA	2.0
1	C	425	MET	2.0
1	A	464	VAL	2.0
1	B	142	VAL	2.0
1	B	464	VAL	2.0
1	D	62	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

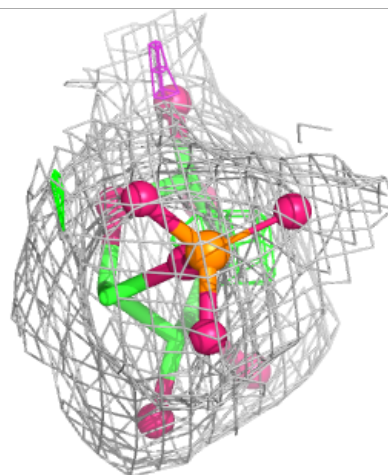
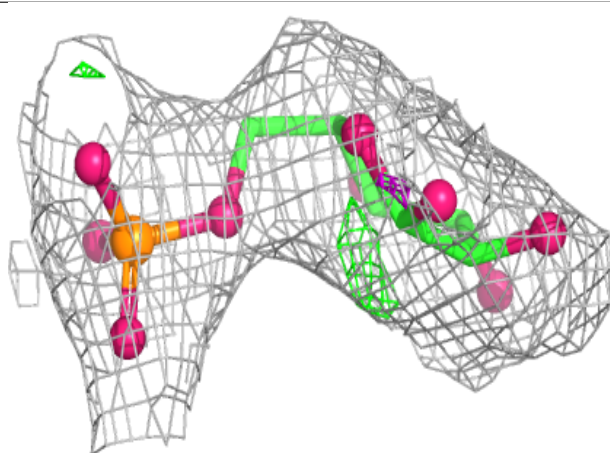
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	OXL	B	503	6/6	0.73	0.14	17,19,24,26	0
4	OXL	A	503	6/6	0.77	0.13	24,26,28,28	0
4	OXL	C	503	6/6	0.80	0.16	21,33,44,47	0
4	OXL	D	503	6/6	0.84	0.15	15,24,38,46	0
2	G6P	B	501	16/16	0.88	0.13	22,31,34,35	0
5	PO4	A	504	5/5	0.90	0.12	29,33,40,42	0
5	PO4	C	504	5/5	0.90	0.12	33,33,37,39	0
2	G6P	A	501	16/16	0.91	0.12	24,36,41,44	0
5	PO4	B	504	5/5	0.91	0.10	40,41,43,44	0
3	MG	B	502	1/1	0.91	0.08	25,25,25,25	0
3	MG	A	502	1/1	0.92	0.05	27,27,27,27	0
5	PO4	D	504	5/5	0.92	0.11	30,31,34,39	0
2	G6P	D	501	16/16	0.93	0.10	20,37,41,45	0
3	MG	D	502	1/1	0.95	0.05	33,33,33,33	0
2	G6P	C	501	16/16	0.96	0.07	24,29,31,41	0
3	MG	C	502	1/1	0.99	0.04	24,24,24,24	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.

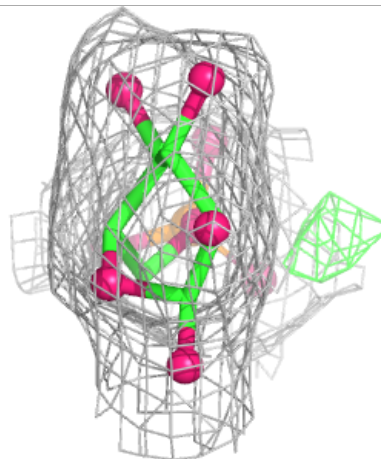
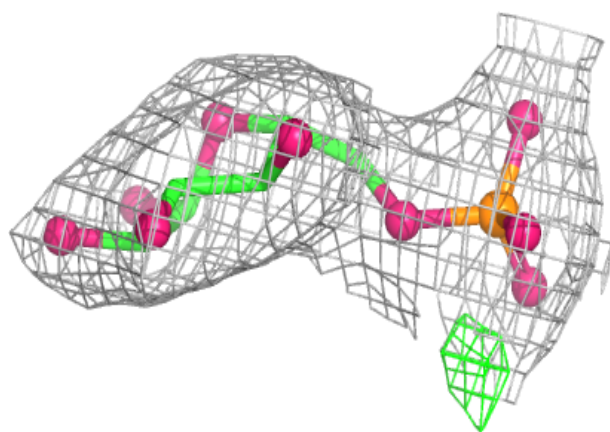
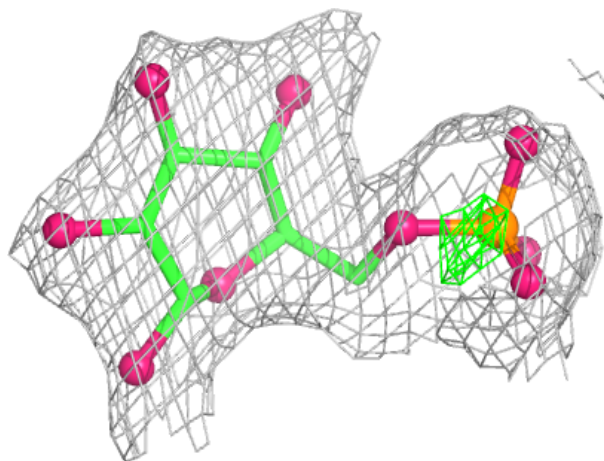
Electron density around G6P B 501:

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



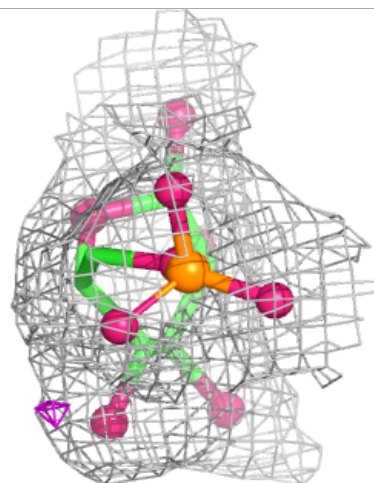
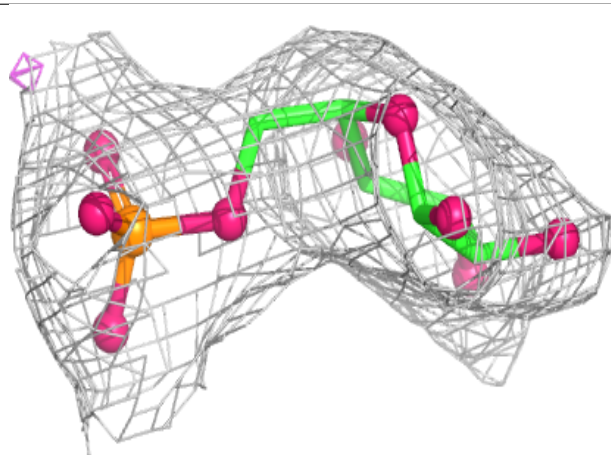
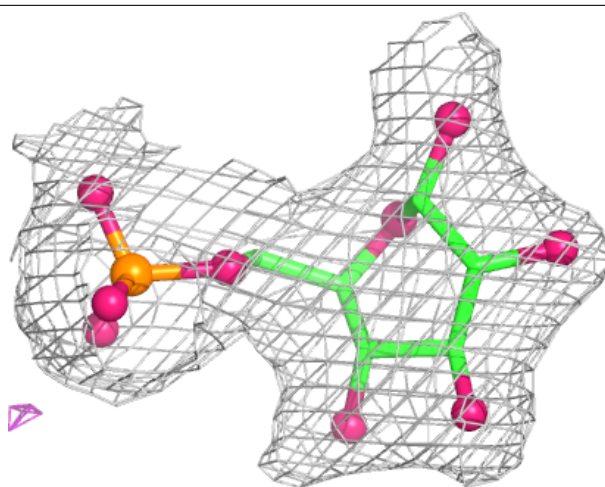
Electron density around G6P D 501:

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



Electron density around G6P C 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.