



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:30 PM UTC

PDB ID : 1HOX / pdb_00001hox
Title : CRYSTAL STRUCTURE OF RABBIT PHOSPHOGLUCOSE ISOMERASE
COMPLEXED WITH FRUCTOSE-6-PHOSPHATE
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Deposited on : 2000-12-11
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

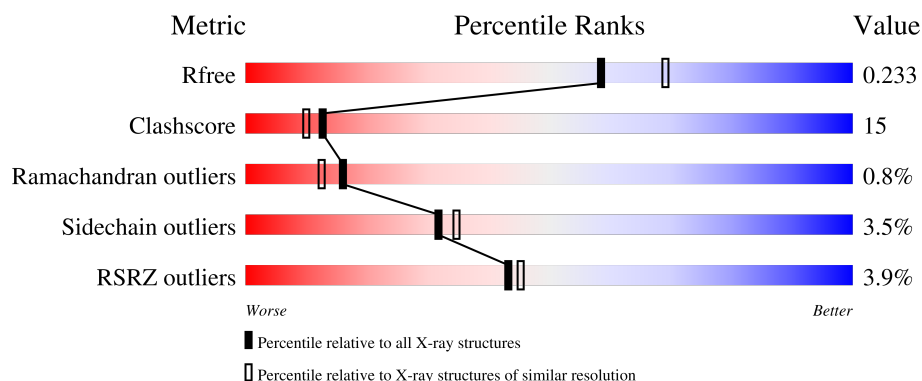
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	558	3% 71% 24% 5% •
1	B	558	4% 72% 25% • •

2 Entry composition [i](#)

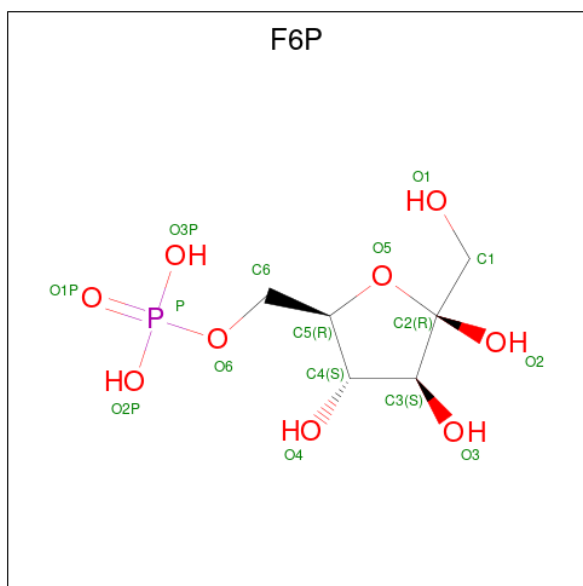
There are 3 unique types of molecules in this entry. The entry contains 9690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHOGLUCOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4395	2805	765	806	19			
1	B	555	Total	C	N	O	S	0	0	0
			4395	2805	765	806	19			

- Molecule 2 is 6-O-phosphono-beta-D-fructofuranose (CCD ID: F6P) (formula: $C_6H_{13}O_9P$).



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		

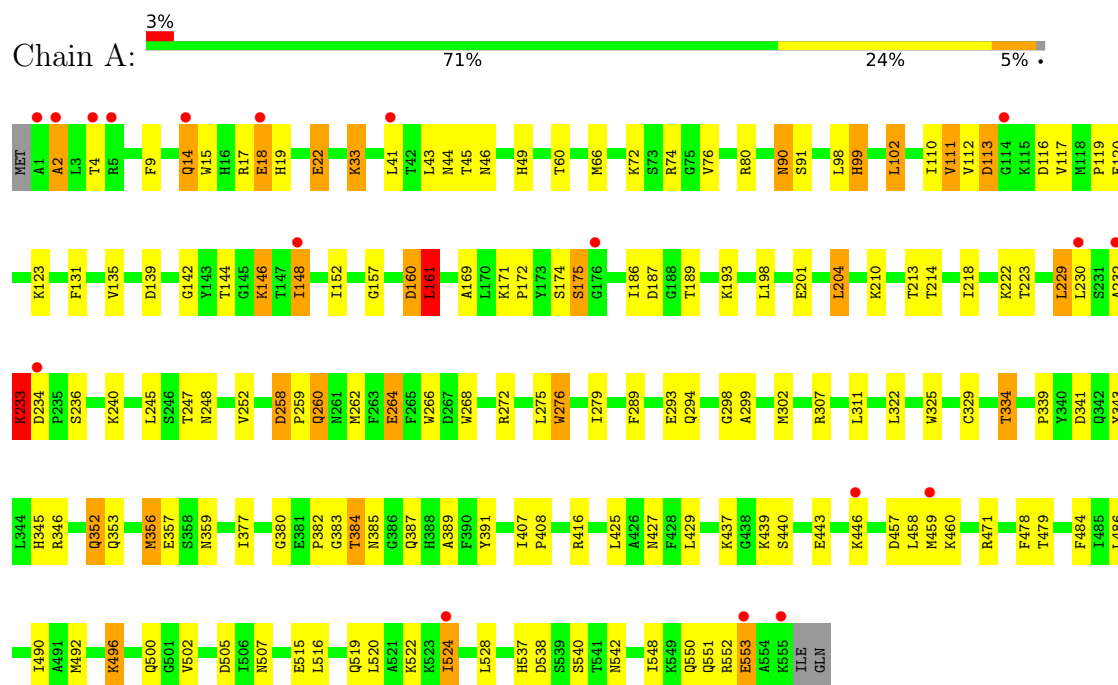
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	424	Total 424	O 424	0	0
3	B	444	Total 444	O 444	0	0

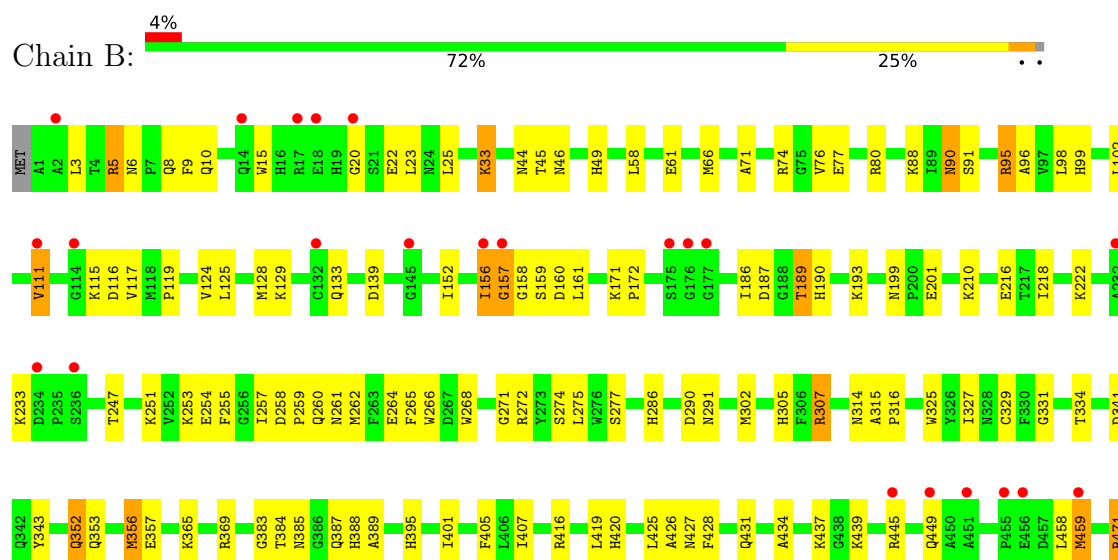
3 Residue-property plots

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: PHOSPHOGLUCOSE ISOMERASE



• Molecule 1: PHOSPHOGLUCOSE ISOMERASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	82.44Å 119.43Å 272.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.1 (30.00-2.10) 93.1 (30.00-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.95 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.248 0.194 , 0.233	Depositor DCC
R_{free} test set	7810 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9690	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F6P

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	0.46	2/4504 (0.0%)	0.94	19/6101 (0.3%)
1	B	0.45	1/4504 (0.0%)	0.95	16/6101 (0.3%)
All	All	0.46	3/9008 (0.0%)	0.94	35/12202 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	TRP	NE1-CE2	-5.39	1.31	1.37
1	A	266	TRP	NE1-CE2	-5.33	1.31	1.37
1	B	266	TRP	NE1-CE2	-5.30	1.31	1.37

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	471	ARG	CA-C-N	8.13	128.13	119.76
1	B	471	ARG	C-N-CA	8.13	128.13	119.76
1	B	91	SER	N-CA-C	7.36	119.31	111.28
1	A	352	GLN	N-CA-C	-7.02	103.71	111.36
1	A	91	SER	N-CA-C	6.92	118.48	111.07
1	B	538	ASP	N-CA-C	-6.45	102.48	110.41
1	A	437	LYS	N-CA-C	6.35	118.28	111.36
1	A	264	GLU	N-CA-C	6.01	119.74	110.42
1	B	437	LYS	N-CA-C	6.01	117.91	111.36
1	B	274	SER	N-CA-C	5.93	120.68	113.38
1	B	383	GLY	O-C-N	-5.84	117.51	123.35
1	A	258	ASP	CA-C-N	5.83	125.30	119.24
1	A	258	ASP	C-N-CA	5.83	125.30	119.24
1	A	496	LYS	N-CA-C	-5.71	105.06	111.28
1	B	356	MET	N-CA-C	5.63	117.42	111.28
1	B	515	GLU	N-CA-C	5.57	117.03	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	VAL	N-CA-C	5.56	116.31	108.36
1	A	334	THR	N-CA-C	5.51	118.23	109.81
1	B	385	ASN	O-C-N	5.46	127.69	122.07
1	B	352	GLN	N-CA-C	-5.44	105.43	111.36
1	A	99	HIS	N-CA-C	-5.42	105.93	112.54
1	A	380	GLY	N-CA-C	5.36	117.34	110.96
1	A	383	GLY	CA-C-N	5.33	131.30	121.70
1	A	383	GLY	C-N-CA	5.33	131.30	121.70
1	A	359	ASN	N-CA-C	5.26	119.39	112.92
1	B	307	ARG	N-CA-C	5.25	118.15	111.69
1	B	401	ILE	N-CA-C	5.24	113.33	108.15
1	A	322	LEU	N-CA-C	-5.23	105.58	111.28
1	A	356	MET	N-CA-C	5.16	116.91	111.28
1	B	99	HIS	N-CA-C	-5.11	106.56	112.89
1	A	247	THR	N-CA-C	-5.09	107.10	113.72
1	B	334	THR	N-CA-C	5.08	117.58	109.81
1	B	3	LEU	N-CA-C	5.04	117.17	111.02
1	A	384	THR	CA-C-N	5.02	128.35	120.82
1	A	384	THR	C-N-CA	5.02	128.35	120.82

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	4395	0	4352	148	0
1	B	4395	0	4352	133	0
2	A	16	0	11	2	0
2	B	16	0	11	3	0
3	A	424	0	0	20	0
3	B	444	0	0	11	0
All	All	9690	0	8726	267	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 15.

All (267) 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:33:LYS:HE3	1:A:33:LYS:H	1.08	1.09
1:B:157:GLY:HA3	2:B:1002:F6P:H5	1.36	1.06
1:A:146:LYS:HE2	1:A:146:LYS:H	1.21	1.02
1:A:146:LYS:H	1:A:146:LYS:CE	1.74	0.99
1:A:33:LYS:HE3	1:A:33:LYS:N	1.82	0.93
1:A:262:MET:HE2	1:A:264:GLU:HB3	1.51	0.93
1:A:387:GLN:HE22	1:A:427:ASN:HB3	1.36	0.89
1:B:305:HIS:HE1	1:B:315:ALA:H	1.23	0.86
1:A:14:GLN:HE21	1:A:14:GLN:HA	1.43	0.83
1:B:90:ASN:ND2	1:B:507:ASN:HD21	1.77	0.82
1:A:537:HIS:H	1:A:542:ASN:HD21	1.25	0.82
1:A:144:THR:H	1:A:146:LYS:HZ1	1.25	0.81
1:A:144:THR:OG1	1:A:146:LYS:HD3	1.82	0.80
1:B:156:ILE:HG23	1:B:157:GLY:H	1.47	0.80
1:A:144:THR:H	1:A:146:LYS:NZ	1.79	0.80
1:A:160:ASP:O	1:A:161:LEU:HB2	1.81	0.77
1:B:124:VAL:HG12	1:B:128:MET:HE2	1.65	0.77
1:A:519:GLN:HE22	1:B:439:LYS:NZ	1.83	0.75
1:A:352:GLN:O	1:A:356:MET:HB2	1.86	0.74
1:B:384:THR:O	1:B:387:GLN:HB2	1.87	0.74
1:B:156:ILE:HG23	1:B:157:GLY:N	2.05	0.70
1:A:14:GLN:HA	1:A:14:GLN:NE2	2.06	0.70
1:B:6:ASN:HD21	1:B:8:GLN:HB2	1.57	0.69
1:B:387:GLN:HE22	1:B:427:ASN:HB3	1.58	0.69
1:B:125:LEU:HA	1:B:128:MET:HE3	1.75	0.69
1:B:25:LEU:HD21	1:B:58:LEU:HD12	1.74	0.69
1:A:384:THR:O	1:A:387:GLN:HB2	1.93	0.68
1:A:14:GLN:HE21	1:A:14:GLN:CA	2.03	0.68
2:A:1001:F6P:O1	1:B:388:HIS:HA	1.93	0.68
1:B:33:LYS:HE3	1:B:33:LYS:HA	1.76	0.68
1:A:440:SER:OG	1:A:443:GLU:HG3	1.94	0.67
1:B:74:ARG:HA	1:B:74:ARG:HH11	1.61	0.66
1:B:262:MET:HE2	1:B:264:GLU:HB3	1.77	0.66
1:B:171:LYS:HD3	1:B:286:HIS:HE1	1.61	0.66
1:A:439:LYS:NZ	1:B:519:GLN:HE22	1.94	0.65
1:B:445:ARG:O	1:B:449:GLN:HG3	1.98	0.64
1:B:189:THR:HG21	3:B:1004:HOH:O	1.98	0.64
1:B:537:HIS:H	1:B:542:ASN:HD21	1.44	0.64
1:A:44:ASN:ND2	1:A:46:ASN:H	1.97	0.63
1:B:218:ILE:HG22	1:B:222:LYS:HE3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:HIS:HD2	3:B:1090:HOH:O	1.81	0.63
1:A:123:LYS:HD2	3:A:1398:HOH:O	1.99	0.63
1:A:232:ALA:O	1:A:234:ASP:N	2.29	0.63
1:B:352:GLN:O	1:B:356:MET:HB2	1.99	0.62
1:B:58:LEU:HD13	1:B:472:PRO:HB3	1.81	0.62
1:B:77:GLU:HG3	3:B:1336:HOH:O	1.99	0.62
1:A:218:ILE:HG22	1:A:222:LYS:HE2	1.82	0.61
1:A:294:GLN:HG2	3:A:1139:HOH:O	1.99	0.61
1:B:129:LYS:O	1:B:133:GLN:HG3	2.01	0.61
1:A:213:THR:O	1:A:214:THR:C	2.43	0.61
1:B:6:ASN:ND2	1:B:8:GLN:H	1.98	0.61
1:A:233:LYS:NZ	1:A:233:LYS:HB3	2.16	0.61
1:A:175:SER:HB3	3:A:1132:HOH:O	2.00	0.61
1:B:157:GLY:CA	2:B:1002:F6P:H5	2.23	0.60
1:A:45:THR:O	1:A:46:ASN:HB2	2.01	0.60
1:A:160:ASP:O	1:A:161:LEU:CB	2.50	0.60
3:A:1019:HOH:O	1:B:49:HIS:HD2	1.85	0.60
1:B:44:ASN:ND2	1:B:46:ASN:H	2.00	0.60
1:B:258:ASP:CG	1:B:260:GLN:HG2	2.27	0.60
1:A:232:ALA:C	1:A:233:LYS:HG2	2.27	0.60
1:A:341:ASP:OD2	1:A:343:TYR:HB2	2.01	0.60
1:A:439:LYS:HZ3	1:B:519:GLN:HE22	1.49	0.60
1:B:95:ARG:HD2	3:B:1397:HOH:O	2.01	0.60
1:B:407:ILE:HD13	1:B:425:LEU:HD23	1.83	0.59
1:A:515:GLU:O	1:A:519:GLN:HG3	2.02	0.59
1:B:305:HIS:CE1	1:B:315:ALA:H	2.13	0.59
1:A:90:ASN:ND2	1:A:507:ASN:HD21	2.01	0.59
1:A:98:LEU:HB2	1:A:268:TRP:CE3	2.37	0.59
1:B:33:LYS:HE2	3:B:1060:HOH:O	2.02	0.59
1:A:457:ASP:O	1:A:460:LYS:HG2	2.02	0.58
1:A:189:THR:O	1:A:193:LYS:HG2	2.04	0.58
1:A:240:LYS:HE2	3:A:1169:HOH:O	2.03	0.58
1:A:33:LYS:H	1:A:33:LYS:CE	1.99	0.57
1:B:445:ARG:HG2	1:B:445:ARG:HH11	1.67	0.57
1:A:174:SER:O	1:A:175:SER:C	2.46	0.57
1:B:45:THR:O	1:B:46:ASN:HB2	2.04	0.57
1:B:158:GLY:HA3	1:B:271:GLY:O	2.03	0.57
1:B:156:ILE:O	1:B:160:ASP:HB3	2.04	0.57
1:A:112:VAL:O	1:A:113:ASP:C	2.47	0.57
1:B:253:LYS:O	1:B:253:LYS:HD3	2.04	0.57
1:B:458:LEU:HD23	1:B:458:LEU:C	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LYS:CD	1:A:201:GLU:HB3	2.34	0.56
1:A:519:GLN:HE22	1:B:439:LYS:HZ1	1.51	0.56
1:A:232:ALA:O	1:A:233:LYS:HG2	2.06	0.56
1:B:156:ILE:CG2	1:B:157:GLY:H	2.18	0.56
1:B:90:ASN:C	1:B:90:ASN:HD22	2.13	0.56
1:B:111:VAL:HG23	1:B:115:LYS:N	2.21	0.56
1:B:157:GLY:C	1:B:159:SER:H	2.13	0.55
1:A:113:ASP:O	1:A:113:ASP:OD1	2.25	0.55
1:A:135:VAL:HG13	1:A:148:ILE:HG12	1.88	0.55
1:A:116:ASP:O	1:A:119:PRO:HD2	2.07	0.55
1:A:522:LYS:HE2	3:A:1290:HOH:O	2.07	0.55
1:B:537:HIS:HB2	1:B:542:ASN:ND2	2.22	0.55
1:B:6:ASN:HD22	1:B:9:PHE:H	1.55	0.55
1:A:41:LEU:HD12	1:A:41:LEU:O	2.07	0.54
1:B:15:TRP:CG	1:B:66:MET:HE1	2.41	0.54
1:B:255:PHE:HD2	1:B:257:ILE:HG13	1.72	0.54
1:B:369:ARG:HG2	1:B:369:ARG:HH11	1.72	0.54
1:B:459:MET:HE3	3:B:1296:HOH:O	2.06	0.54
1:A:275:LEU:C	1:A:275:LEU:HD12	2.31	0.54
1:B:272:ARG:HH12	1:B:511:GLN:HE21	1.56	0.54
1:A:146:LYS:CE	1:A:146:LYS:N	2.57	0.54
1:A:223:THR:OG1	1:B:420:HIS:HE1	1.90	0.54
1:A:524:ILE:HD11	1:B:426:ALA:HA	1.89	0.54
1:B:6:ASN:O	1:B:10:GLN:HG3	2.08	0.54
1:A:516:LEU:HA	1:A:519:GLN:HE21	1.72	0.54
1:A:524:ILE:HD12	1:A:528:LEU:HG	1.90	0.54
1:A:152:ILE:HD12	1:A:152:ILE:N	2.23	0.54
1:B:33:LYS:HG3	3:B:1060:HOH:O	2.07	0.54
1:A:260:GLN:HA	1:A:260:GLN:HE21	1.73	0.53
1:A:384:THR:O	1:A:387:GLN:N	2.41	0.53
1:B:218:ILE:CG2	1:B:222:LYS:HE3	2.39	0.53
1:B:6:ASN:ND2	1:B:8:GLN:HB2	2.22	0.53
1:A:223:THR:OG1	1:B:416:ARG:NH1	2.41	0.53
1:B:251:LYS:HE2	1:B:251:LYS:HA	1.89	0.53
1:A:233:LYS:HB3	1:A:233:LYS:HZ2	1.74	0.52
1:A:258:ASP:OD2	1:A:258:ASP:N	2.38	0.52
1:A:458:LEU:C	1:A:458:LEU:HD23	2.35	0.52
1:A:80:ARG:HD2	1:A:307:ARG:HA	1.91	0.52
1:A:289:PHE:O	1:A:293:GLU:HG3	2.09	0.52
1:A:146:LYS:HE2	1:A:146:LYS:N	2.05	0.52
1:A:548:ILE:HD13	1:B:425:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:THR:HG22	3:B:1209:HOH:O	2.10	0.51
1:A:74:ARG:NH2	1:A:505:ASP:HB2	2.26	0.51
1:B:549:LYS:HG2	1:B:552:ARG:NH2	2.26	0.51
1:A:294:GLN:HG3	1:A:484:PHE:HB2	1.93	0.51
1:A:387:GLN:HA	1:A:391:TYR:CG	2.46	0.51
1:B:253:LYS:HD3	1:B:253:LYS:C	2.36	0.51
1:A:519:GLN:HE22	1:B:439:LYS:HZ3	1.59	0.50
1:A:248:ASN:O	1:A:252:VAL:HG23	2.11	0.50
1:B:5:ARG:HG2	3:B:1349:HOH:O	2.11	0.50
1:B:305:HIS:HE1	1:B:315:ALA:N	2.01	0.50
1:A:74:ARG:HH21	1:A:505:ASP:HB2	1.76	0.50
1:B:125:LEU:HD23	1:B:128:MET:HE3	1.92	0.50
1:A:15:TRP:CG	1:A:66:MET:HE1	2.46	0.50
1:A:41:LEU:HD13	1:A:43:LEU:HD21	1.92	0.50
1:A:446:LYS:HD3	3:A:1287:HOH:O	2.12	0.50
1:B:189:THR:O	1:B:193:LYS:HG2	2.12	0.50
1:A:161:LEU:HD23	1:A:353:GLN:HE21	1.76	0.50
1:B:275:LEU:HD12	1:B:275:LEU:C	2.36	0.50
1:A:131:PHE:HZ	1:A:204:LEU:HD11	1.77	0.49
1:A:446:LYS:HG2	3:A:1332:HOH:O	2.10	0.49
1:A:144:THR:HG1	1:A:146:LYS:HD3	1.77	0.49
1:A:2:ALA:HB2	3:A:1190:HOH:O	2.12	0.49
1:A:41:LEU:HD12	1:A:41:LEU:C	2.36	0.49
1:A:325:TRP:O	1:A:329:CYS:HB2	2.13	0.49
1:B:139:ASP:C	1:B:139:ASP:OD2	2.55	0.49
1:B:395:HIS:HE1	1:B:431:GLN:OE1	1.95	0.49
1:A:148:ILE:HD12	1:A:148:ILE:C	2.38	0.49
1:B:157:GLY:C	1:B:159:SER:N	2.71	0.49
1:A:245:LEU:HD13	1:A:279:ILE:HA	1.94	0.49
1:A:552:ARG:HD2	3:A:1198:HOH:O	2.13	0.49
1:A:139:ASP:OD2	1:A:139:ASP:C	2.55	0.48
1:B:88:LYS:HA	1:B:96:ALA:HA	1.95	0.48
1:A:171:LYS:N	1:A:172:PRO:CD	2.76	0.48
1:A:142:GLY:C	1:A:146:LYS:HZ1	2.21	0.48
1:A:429:LEU:HD13	1:B:545:ILE:HG12	1.96	0.48
1:B:405:PHE:HB3	1:B:428:PHE:CE1	2.48	0.48
1:B:258:ASP:OD2	1:B:259:PRO:HD2	2.14	0.48
1:A:157:GLY:O	1:A:160:ASP:O	2.32	0.48
1:A:232:ALA:C	1:A:234:ASP:H	2.19	0.48
1:A:407:ILE:HD13	1:A:425:LEU:HD23	1.95	0.48
1:A:520:LEU:HD12	1:B:434:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:GLN:O	1:A:553:GLU:OE2	2.32	0.48
1:B:6:ASN:ND2	1:B:8:GLN:N	2.62	0.48
1:B:258:ASP:OD2	1:B:260:GLN:HG2	2.14	0.48
1:A:230:LEU:HD23	1:A:230:LEU:C	2.39	0.47
1:A:259:PRO:HG2	3:A:1248:HOH:O	2.13	0.47
1:B:152:ILE:N	1:B:152:ILE:HD12	2.29	0.47
1:A:334:THR:HG22	1:A:377:ILE:HB	1.96	0.47
1:B:471:ARG:HG3	1:B:471:ARG:HH11	1.80	0.47
1:B:125:LEU:HD23	1:B:128:MET:CE	2.44	0.47
1:B:341:ASP:OD2	1:B:343:TYR:HB2	2.13	0.47
1:A:18:GLU:OE1	1:A:19:HIS:NE2	2.48	0.47
1:B:156:ILE:CG2	1:B:157:GLY:N	2.73	0.47
1:B:302:MET:HE3	1:B:492:MET:HB2	1.96	0.47
1:B:116:ASP:OD2	1:B:119:PRO:HD3	2.15	0.47
1:B:445:ARG:HG2	1:B:445:ARG:NH1	2.30	0.47
1:A:146:LYS:HD2	1:A:201:GLU:HB3	1.97	0.46
1:B:272:ARG:HH12	1:B:511:GLN:NE2	2.12	0.46
1:B:459:MET:HE2	1:B:459:MET:O	2.15	0.46
1:A:186:ILE:O	1:A:187:ASP:C	2.58	0.46
1:A:385:ASN:CG	3:A:1284:HOH:O	2.59	0.46
3:A:1091:HOH:O	1:B:537:HIS:HE1	1.98	0.46
1:B:516:LEU:HA	1:B:519:GLN:HE21	1.81	0.46
1:B:449:GLN:HG2	1:B:458:LEU:CD1	2.45	0.46
1:B:74:ARG:HA	1:B:74:ARG:NH1	2.29	0.46
1:B:210:LYS:HA	1:B:265:PHE:CZ	2.51	0.46
1:A:446:LYS:HE3	3:A:1291:HOH:O	2.16	0.46
1:B:71:ALA:O	1:B:76:VAL:HG23	2.15	0.46
1:A:99:HIS:HA	1:A:102:LEU:HD22	1.97	0.46
1:A:459:MET:HE3	1:A:459:MET:O	2.16	0.46
1:A:460:LYS:HE3	3:A:1347:HOH:O	2.16	0.46
1:B:365:LYS:HG3	1:B:505:ASP:O	2.15	0.46
1:A:357:GLU:HB2	1:B:389:ALA:O	2.16	0.46
1:A:144:THR:OG1	1:A:146:LYS:CD	2.61	0.46
1:A:169:ALA:HA	1:A:343:TYR:HB3	1.98	0.46
1:B:187:ASP:OD2	1:B:189:THR:HG23	2.16	0.45
1:B:90:ASN:HD22	1:B:507:ASN:HD21	1.60	0.45
1:B:553:GLU:O	1:B:554:ALA:C	2.59	0.45
1:A:234:ASP:OD2	1:A:236:SER:OG	2.33	0.45
1:B:247:THR:HG22	1:B:265:PHE:O	2.17	0.45
1:A:19:HIS:O	1:A:22:GLU:HB2	2.16	0.45
1:A:146:LYS:HD3	1:A:201:GLU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:HIS:O	1:B:193:LYS:HG2	2.16	0.45
1:A:60:THR:HG22	3:A:1294:HOH:O	2.17	0.45
1:B:98:LEU:HB2	1:B:268:TRP:CE3	2.51	0.45
1:B:258:ASP:OD1	1:B:260:GLN:HG2	2.16	0.45
1:A:229:LEU:HD12	1:A:229:LEU:HA	1.84	0.44
1:A:161:LEU:HD12	1:A:161:LEU:HA	1.91	0.44
1:B:186:ILE:HB	1:B:216:GLU:HG3	2.00	0.44
1:A:272:ARG:HG2	3:A:1092:HOH:O	2.18	0.44
1:A:389:ALA:O	1:B:353:GLN:HA	2.18	0.44
1:A:294:GLN:HG2	3:A:1186:HOH:O	2.17	0.44
1:A:551:GLN:NE2	1:B:479:THR:OG1	2.51	0.44
1:B:61:GLU:HG2	3:B:1258:HOH:O	2.17	0.44
1:A:382:PRO:O	1:A:385:ASN:HB2	2.17	0.44
1:B:258:ASP:HB3	1:B:261:ASN:ND2	2.33	0.43
1:A:14:GLN:HE22	1:A:17:ARG:HD2	1.84	0.43
1:A:74:ARG:HH11	1:A:74:ARG:HA	1.83	0.43
1:B:325:TRP:O	1:B:329:CYS:HB2	2.18	0.43
1:A:102:LEU:HD23	1:A:276:TRP:HB2	1.99	0.43
1:A:76:VAL:HA	1:A:502:VAL:HG11	2.01	0.43
1:A:146:LYS:H	1:A:146:LYS:HE3	1.71	0.43
1:B:272:ARG:NH1	1:B:357:GLU:HG2	2.32	0.43
1:B:49:HIS:H	1:B:479:THR:HG1	1.67	0.43
1:A:117:VAL:O	1:A:120:GLU:HG2	2.19	0.43
1:A:72:LYS:HE2	1:A:311:LEU:HD12	2.01	0.42
1:A:210:LYS:N	2:A:1001:F6P:O1P	2.37	0.42
1:A:440:SER:HG	1:A:443:GLU:HG3	1.82	0.42
1:A:346:ARG:HD3	3:A:1187:HOH:O	2.18	0.42
1:B:471:ARG:HA	1:B:472:PRO:HD2	1.85	0.42
1:A:302:MET:HE3	1:A:492:MET:HB2	2.01	0.42
1:A:537:HIS:N	1:A:542:ASN:HD21	2.05	0.42
1:B:314:ASN:OD1	1:B:316:PRO:HG2	2.19	0.42
1:A:49:HIS:H	1:A:479:THR:HG1	1.68	0.42
1:A:339:PRO:O	1:A:382:PRO:HA	2.20	0.42
1:A:345:HIS:HA	1:A:382:PRO:HG3	2.01	0.42
1:B:327:ILE:O	1:B:331:GLY:HA2	2.19	0.42
1:A:4:THR:HA	1:A:9:PHE:CD2	2.55	0.41
1:A:90:ASN:HD22	1:A:507:ASN:HD21	1.65	0.41
1:B:171:LYS:NZ	1:B:286:HIS:CE1	2.88	0.41
1:A:152:ILE:HD11	1:A:198:LEU:HD13	2.02	0.41
1:B:22:GLU:N	1:B:22:GLU:CD	2.79	0.41
1:A:298:GLY:HA3	1:A:484:PHE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:LEU:O	1:A:490:ILE:HG13	2.20	0.41
1:B:495:HIS:O	1:B:499:VAL:HG23	2.20	0.41
1:A:110:ILE:O	1:A:117:VAL:HG22	2.20	0.41
1:A:276:TRP:CZ3	1:A:299:ALA:HB2	2.56	0.41
1:A:90:ASN:HD22	1:A:90:ASN:C	2.28	0.41
1:A:408:PRO:HA	1:A:478:PHE:O	2.20	0.41
1:B:80:ARG:HD2	1:B:307:ARG:HA	2.02	0.41
1:B:102:LEU:HD13	1:B:277:SER:HB3	2.02	0.41
1:B:157:GLY:HA3	2:B:1002:F6P:C5	2.27	0.41
1:A:496:LYS:O	1:A:500:GLN:HG3	2.20	0.41
1:A:356:MET:HE3	1:A:377:ILE:HA	2.03	0.41
1:A:538:ASP:OD1	1:A:540:SER:HB3	2.20	0.41
1:B:5:ARG:HE	1:B:5:ARG:HA	1.86	0.41
1:B:171:LYS:HE3	3:B:1384:HOH:O	2.20	0.41
1:B:199:ASN:OD1	1:B:201:GLU:HB2	2.22	0.40
1:B:171:LYS:N	1:B:172:PRO:CD	2.84	0.40
1:A:471:ARG:HG3	3:A:1125:HOH:O	2.20	0.40
1:B:291:ASN:HD22	1:B:291:ASN:HA	1.67	0.40
1:A:384:THR:O	1:A:387:GLN:CB	2.66	0.40
1:B:186:ILE:HB	1:B:216:GLU:CG	2.50	0.40
1:B:511:GLN:O	1:B:511:GLN:HG2	2.21	0.40
1:B:44:ASN:C	1:B:44:ASN:HD22	2.29	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	553/558 (99%)	518 (94%)	30 (5%)	5 (1%)	14	10
1	B	553/558 (99%)	523 (95%)	26 (5%)	4 (1%)	18	15
All	All	1106/1116 (99%)	1041 (94%)	56 (5%)	9 (1%)	16	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	ASP
1	A	161	LEU
1	A	233	LYS
1	B	157	GLY
1	A	175	SER
1	B	554	ALA
1	A	2	ALA
1	B	233	LYS
1	B	20	GLY

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	475/479 (99%)	457 (96%)	18 (4%)	29	32
1	B	475/479 (99%)	460 (97%)	15 (3%)	34	38
All	All	950/958 (99%)	917 (96%)	33 (4%)	32	35

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	18	GLU
1	A	22	GLU
1	A	33	LYS
1	A	90	ASN
1	A	102	LEU
1	A	111	VAL
1	A	146	LYS
1	A	148	ILE
1	A	160	ASP
1	A	161	LEU
1	A	204	LEU
1	A	229	LEU
1	A	233	LYS

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Mol	Chain	Res	Type
1	A	260	GLN
1	A	416	ARG
1	A	524	ILE
1	A	553	GLU
1	B	5	ARG
1	B	23	LEU
1	B	33	LYS
1	B	90	ASN
1	B	95	ARG
1	B	111	VAL
1	B	117	VAL
1	B	156	ILE
1	B	161	LEU
1	B	189	THR
1	B	254	GLU
1	B	290	ASP
1	B	419	LEU
1	B	459	MET
1	B	511	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	14	GLN
1	A	37	ASN
1	A	44	ASN
1	A	46	ASN
1	A	57	ASN
1	A	85	ASN
1	A	90	ASN
1	A	104	ASN
1	A	133	GLN
1	A	153	ASN
1	A	260	GLN
1	A	352	GLN
1	A	353	GLN
1	A	387	GLN
1	A	412	GLN
1	A	449	GLN
1	A	474	ASN
1	A	519	GLN

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Mol	Chain	Res	Type
1	A	542	ASN
1	A	550	GLN
1	A	551	GLN
1	B	6	ASN
1	B	10	GLN
1	B	13	GLN
1	B	44	ASN
1	B	46	ASN
1	B	49	HIS
1	B	57	ASN
1	B	90	ASN
1	B	153	ASN
1	B	215	GLN
1	B	286	HIS
1	B	291	ASN
1	B	294	GLN
1	B	305	HIS
1	B	353	GLN
1	B	359	ASN
1	B	387	GLN
1	B	395	HIS
1	B	410	GLN
1	B	420	HIS
1	B	449	GLN
1	B	511	GLN
1	B	519	GLN
1	B	542	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

2 ligands 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	F6P	B	1002	-	15,16,16	0.97	0	16,25,25	1.60	5 (31%)
2	F6P	A	1001	-	15,16,16	1.05	1 (6%)	16,25,25	1.13	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	F6P	B	1002	-	-	8/9/28/28	0/1/1/1
2	F6P	A	1001	-	-	7/9/28/28	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	F6P	O2-C2	2.10	1.44	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	F6P	O3-C3-C4	3.44	125.40	113.25
2	B	1002	F6P	O4-C4-C5	2.40	117.98	111.08
2	B	1002	F6P	O1-C1-C2	-2.38	106.40	111.67
2	B	1002	F6P	O2P-P-O6	2.20	112.39	106.67
2	B	1002	F6P	O2-C2-O5	2.19	113.54	109.33
2	A	1001	F6P	O4-C4-C5	2.11	117.13	111.08

There are no chirality outliers.

All (15) torsion outliers are listed below:

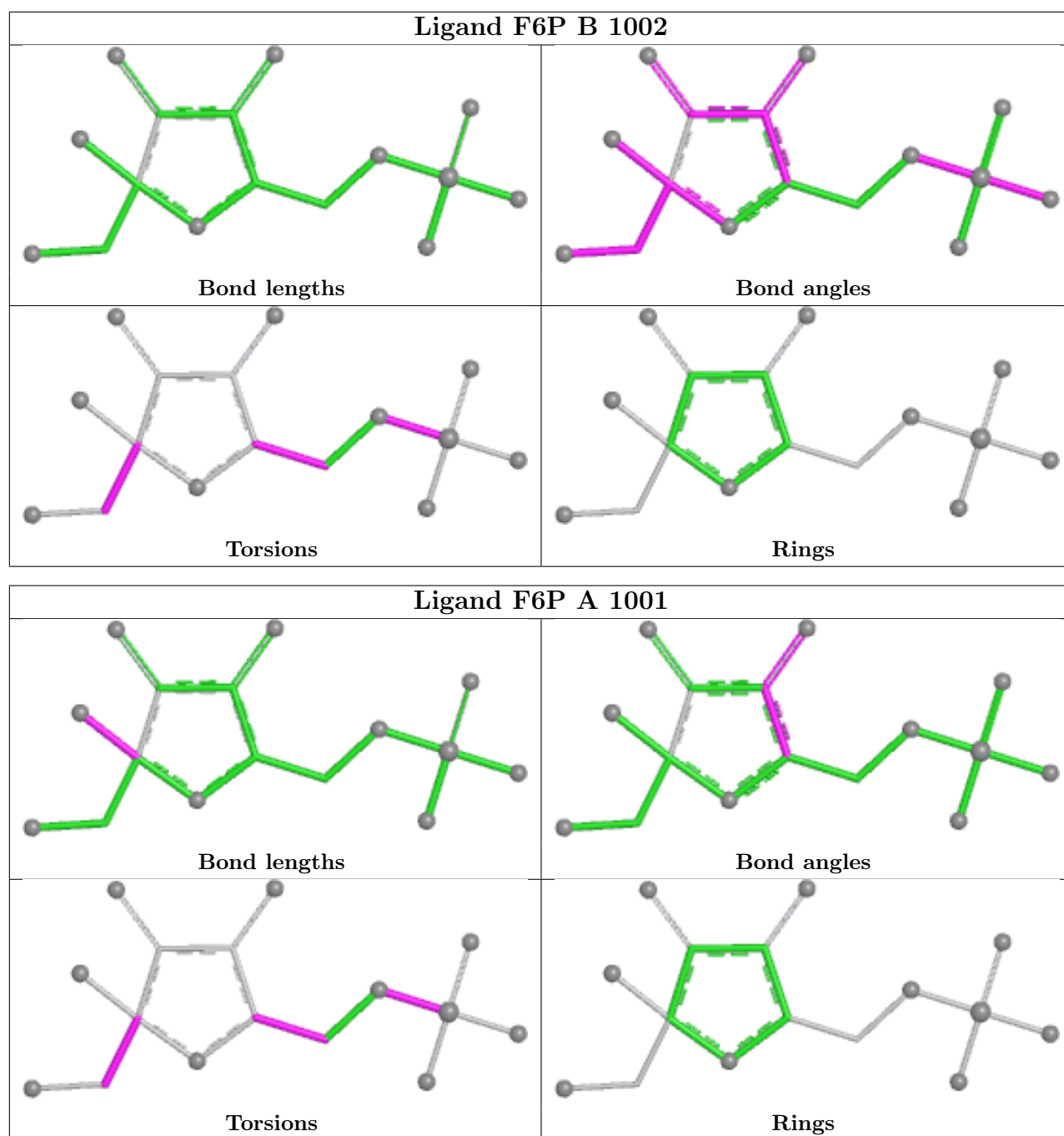
Mol	Chain	Res	Type	Atoms
2	A	1001	F6P	O1-C1-C2-O2
2	A	1001	F6P	C6-O6-P-O1P
2	A	1001	F6P	C6-O6-P-O2P
2	A	1001	F6P	C6-O6-P-O3P
2	B	1002	F6P	O1-C1-C2-O2
2	B	1002	F6P	O1-C1-C2-O5
2	B	1002	F6P	C6-O6-P-O1P
2	A	1001	F6P	O5-C5-C6-O6
2	B	1002	F6P	O5-C5-C6-O6
2	B	1002	F6P	C4-C5-C6-O6
2	A	1001	F6P	O1-C1-C2-O5
2	A	1001	F6P	C4-C5-C6-O6
2	B	1002	F6P	O1-C1-C2-C3
2	B	1002	F6P	C6-O6-P-O2P
2	B	1002	F6P	C6-O6-P-O3P

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	F6P	3	0
2	A	1001	F6P	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.



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	555/558 (99%)	0.12	18 (3%)	50 53	20, 32, 51, 65	0
1	B	555/558 (99%)	0.13	25 (4%)	38 40	22, 32, 53, 68	0
All	All	1110/1116 (99%)	0.13	43 (3%)	43 45	20, 32, 52, 68	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	157	GLY	4.7
1	A	2	ALA	4.3
1	B	176	GLY	4.1
1	A	1	ALA	3.8
1	A	459	MET	3.6
1	B	156	ILE	3.6
1	B	20	GLY	3.4
1	A	5	ARG	3.2
1	B	236	SER	3.1
1	B	17	ARG	2.9
1	A	114	GLY	2.9
1	B	175	SER	2.8
1	A	230	LEU	2.8
1	A	446	LYS	2.7
1	A	14	GLN	2.5
1	B	449	GLN	2.5
1	B	459	MET	2.5
1	A	524	ILE	2.5
1	A	553	GLU	2.5
1	B	111	VAL	2.4
1	B	2	ALA	2.4
1	B	18	GLU	2.4
1	B	14	GLN	2.4
1	B	553	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	232	ALA	2.3
1	A	41	LEU	2.3
1	B	445	ARG	2.3
1	B	132	CYS	2.3
1	B	145	GLY	2.3
1	B	234	ASP	2.3
1	B	555	LYS	2.3
1	A	234	ASP	2.2
1	A	232	ALA	2.2
1	B	451	ALA	2.2
1	B	456	GLU	2.2
1	A	148	ILE	2.2
1	A	18	GLU	2.2
1	A	555	LYS	2.2
1	B	177	GLY	2.1
1	A	4	THR	2.1
1	B	455	PRO	2.1
1	A	176	GLY	2.0
1	B	114	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](#)

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.

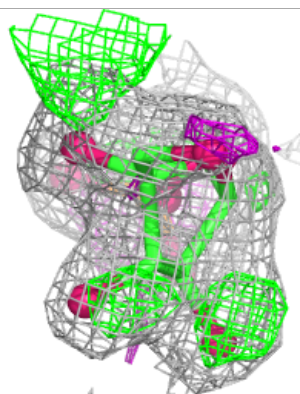
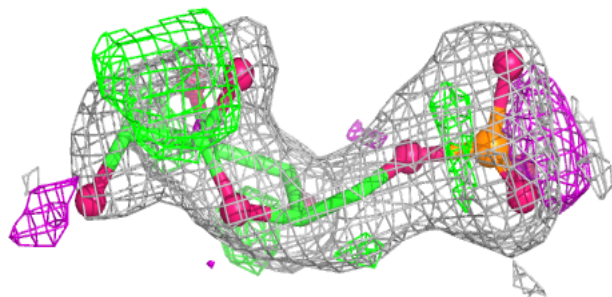
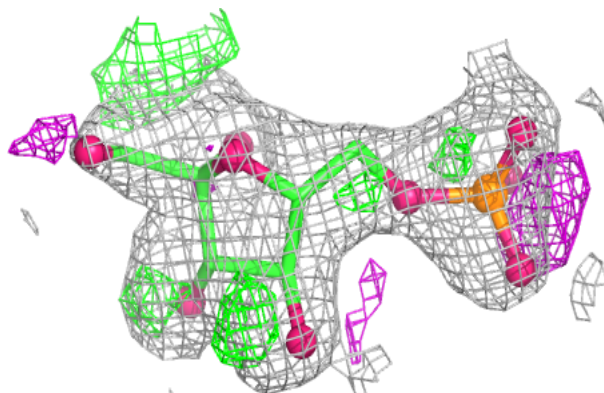
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	F6P	A	1001	16/16	0.89	0.15	32,37,42,45	0
2	F6P	B	1002	16/16	0.92	0.12	31,39,45,48	0

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.

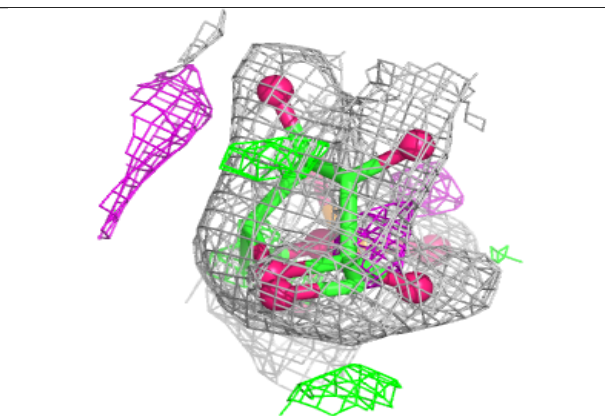
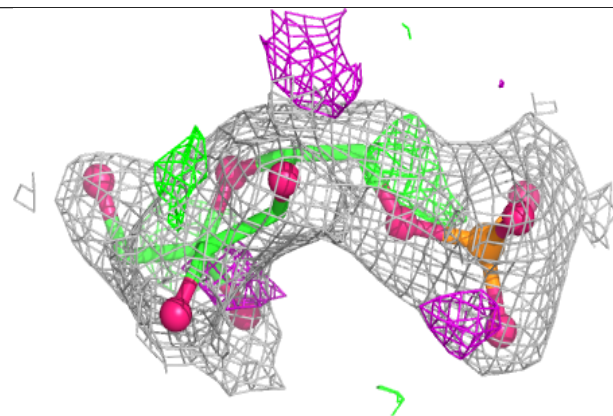
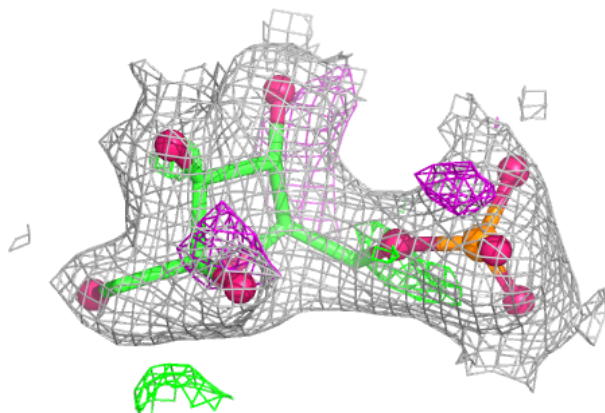
Electron density around F6P A 1001:

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



Electron density around F6P B 1002:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.