



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 5, 2017 – 03:01 PM EDT

PDB ID : 5SUK
Title : G6P bound activated state of yeast glycogen synthase 2
Authors : Baskaran, S.; Mahalingan, K.K.; Hurley, T.D.
Deposited on : 2016-08-03
Resolution : 2.88 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

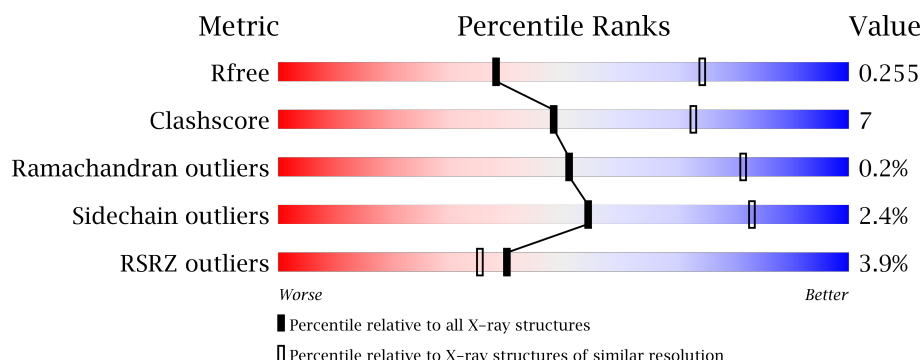
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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}	100719	2135 (2.90-2.86)
Clashscore	112137	2400 (2.90-2.86)
Ramachandran outliers	110173	2346 (2.90-2.86)
Sidechain outliers	110143	2349 (2.90-2.86)
RSRZ outliers	101464	2149 (2.90-2.86)

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

Mol	Chain	Length	Quality of chain
1	A	725	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>12%</div> </div> </div>
1	B	725	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>12%</div> </div> </div>
1	C	725	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>12%</div> <div>12%</div> </div> </div>
1	D	725	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>14%</div> <div>17%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	G6P	A	902	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19585 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 Glycogen [starch] synthase isoform 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			5020	3207	869	925	19			
1	B	637	Total	C	N	O	S	0	0	0
			5018	3198	877	925	18			
1	C	639	Total	C	N	O	S	0	0	0
			4869	3095	847	909	18			
1	D	604	Total	C	N	O	S	0	0	0
			4582	2921	797	847	17			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P27472
A	-18	GLY	-	expression tag	UNP P27472
A	-17	SER	-	expression tag	UNP P27472
A	-16	SER	-	expression tag	UNP P27472
A	-15	HIS	-	expression tag	UNP P27472
A	-14	HIS	-	expression tag	UNP P27472
A	-13	HIS	-	expression tag	UNP P27472
A	-12	HIS	-	expression tag	UNP P27472
A	-11	HIS	-	expression tag	UNP P27472
A	-10	HIS	-	expression tag	UNP P27472
A	-9	SER	-	expression tag	UNP P27472
A	-8	SER	-	expression tag	UNP P27472
A	-7	GLY	-	expression tag	UNP P27472
A	-6	LEU	-	expression tag	UNP P27472
A	-5	VAL	-	expression tag	UNP P27472
A	-4	PRO	-	expression tag	UNP P27472
A	-3	ARG	-	expression tag	UNP P27472
A	-2	GLY	-	expression tag	UNP P27472
A	-1	SER	-	expression tag	UNP P27472
A	0	HIS	-	expression tag	UNP P27472
A	535	SER	ALA	conflict	UNP P27472

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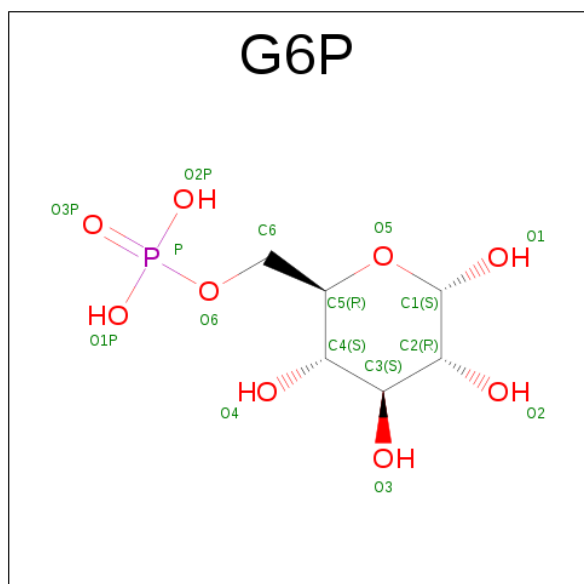
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P27472
B	-18	GLY	-	expression tag	UNP P27472
B	-17	SER	-	expression tag	UNP P27472
B	-16	SER	-	expression tag	UNP P27472
B	-15	HIS	-	expression tag	UNP P27472
B	-14	HIS	-	expression tag	UNP P27472
B	-13	HIS	-	expression tag	UNP P27472
B	-12	HIS	-	expression tag	UNP P27472
B	-11	HIS	-	expression tag	UNP P27472
B	-10	HIS	-	expression tag	UNP P27472
B	-9	SER	-	expression tag	UNP P27472
B	-8	SER	-	expression tag	UNP P27472
B	-7	GLY	-	expression tag	UNP P27472
B	-6	LEU	-	expression tag	UNP P27472
B	-5	VAL	-	expression tag	UNP P27472
B	-4	PRO	-	expression tag	UNP P27472
B	-3	ARG	-	expression tag	UNP P27472
B	-2	GLY	-	expression tag	UNP P27472
B	-1	SER	-	expression tag	UNP P27472
B	0	HIS	-	expression tag	UNP P27472
B	535	SER	ALA	conflict	UNP P27472
C	-19	MET	-	initiating methionine	UNP P27472
C	-18	GLY	-	expression tag	UNP P27472
C	-17	SER	-	expression tag	UNP P27472
C	-16	SER	-	expression tag	UNP P27472
C	-15	HIS	-	expression tag	UNP P27472
C	-14	HIS	-	expression tag	UNP P27472
C	-13	HIS	-	expression tag	UNP P27472
C	-12	HIS	-	expression tag	UNP P27472
C	-11	HIS	-	expression tag	UNP P27472
C	-10	HIS	-	expression tag	UNP P27472
C	-9	SER	-	expression tag	UNP P27472
C	-8	SER	-	expression tag	UNP P27472
C	-7	GLY	-	expression tag	UNP P27472
C	-6	LEU	-	expression tag	UNP P27472
C	-5	VAL	-	expression tag	UNP P27472
C	-4	PRO	-	expression tag	UNP P27472
C	-3	ARG	-	expression tag	UNP P27472
C	-2	GLY	-	expression tag	UNP P27472
C	-1	SER	-	expression tag	UNP P27472
C	0	HIS	-	expression tag	UNP P27472
C	535	SER	ALA	conflict	UNP P27472

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP P27472
D	-18	GLY	-	expression tag	UNP P27472
D	-17	SER	-	expression tag	UNP P27472
D	-16	SER	-	expression tag	UNP P27472
D	-15	HIS	-	expression tag	UNP P27472
D	-14	HIS	-	expression tag	UNP P27472
D	-13	HIS	-	expression tag	UNP P27472
D	-12	HIS	-	expression tag	UNP P27472
D	-11	HIS	-	expression tag	UNP P27472
D	-10	HIS	-	expression tag	UNP P27472
D	-9	SER	-	expression tag	UNP P27472
D	-8	SER	-	expression tag	UNP P27472
D	-7	GLY	-	expression tag	UNP P27472
D	-6	LEU	-	expression tag	UNP P27472
D	-5	VAL	-	expression tag	UNP P27472
D	-4	PRO	-	expression tag	UNP P27472
D	-3	ARG	-	expression tag	UNP P27472
D	-2	GLY	-	expression tag	UNP P27472
D	-1	SER	-	expression tag	UNP P27472
D	0	HIS	-	expression tag	UNP P27472
D	535	SER	ALA	conflict	UNP P27472

- Molecule 2 is ALPHA-D-GLUCOSE-6-PHOSPHATE (three-letter code: G6P) (formula: $C_6H_{13}O_9P$).



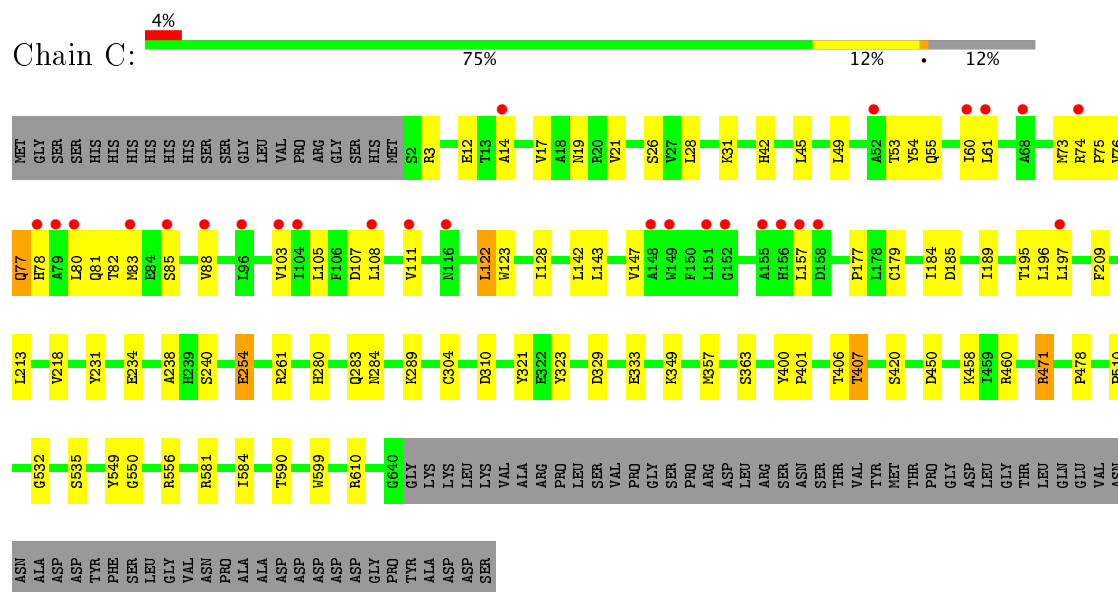
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 16	C 6	O 9	P 1	0	0
2	A	1	Total 16	C 6	O 9	P 1	0	0
2	B	1	Total 16	C 6	O 9	P 1	0	0
2	B	1	Total 16	C 6	O 9	P 1	0	0
2	C	1	Total 16	C 6	O 9	P 1	0	0
2	D	1	Total 16	C 6	O 9	P 1	0	0

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

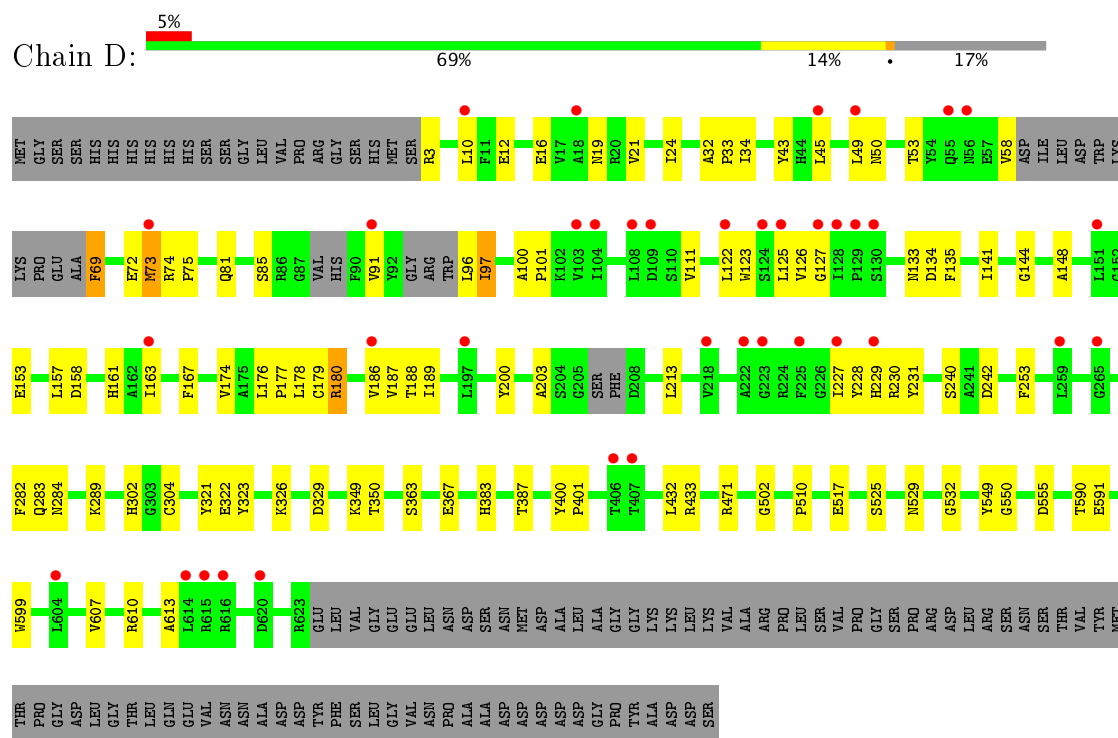
- [illegible]

- Chain B:
-
- Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.15). The x-axis shows positions 1 to 300. A green bar at the top indicates a 76% overall conservation, with 12% yellow and 12% grey. A 3% scale bar is shown at the top left. Red dots above the bars indicate specific mutations.
- | Position | Amino Acid | Information Content (bits) |
|----------|------------|----------------------------|
| 1 | GLY | 0.02 |
| 2 | THR | 0.02 |
| 3 | LEU | 0.02 |
| 4 | GLN | 0.02 |
| 5 | GLU | 0.02 |
| 6 | VAL | 0.02 |
| 7 | ASN | 0.02 |
| 8 | ASN | 0.02 |
| 9 | ALA | 0.02 |
| 10 | ASP | 0.02 |
| 11 | ASP | 0.02 |
| 12 | THR | 0.02 |
| 13 | PHE | 0.02 |
| 14 | SER | 0.02 |
| 15 | LEU | 0.02 |
| 16 | GLY | 0.02 |
| 17 | VAL | 0.02 |
| 18 | ASN | 0.02 |
| 19 | PRO | 0.02 |
| 20 | ALA | 0.02 |
| 21 | ALA | 0.02 |
| 22 | ASP | 0.02 |
| 23 | ASP | 0.02 |
| 24 | ASP | 0.02 |
| 25 | ASP | 0.02 |
| 26 | ASP | 0.02 |
| 27 | GLY | 0.02 |
| 28 | GLY | 0.02 |
| 29 | LYS | 0.02 |
| 30 | LYS | 0.02 |
| 31 | LYS | 0.02 |
| 32 | VAL | 0.02 |
| 33 | ALA | 0.02 |
| 34 | ARG | 0.02 |
| 35 | PRO | 0.02 |
| 36 | LEU | 0.02 |
| 37 | SER | 0.02 |
| 38 | VAL | 0.02 |
| 39 | PRO | 0.02 |
| 40 | GLY | 0.02 |
| 41 | SER | 0.02 |
| 42 | PRO | 0.02 |
| 43 | ARG | 0.02 |
| 44 | ASP | 0.02 |
| 45 | LEU | 0.02 |
| 46 | ARG | 0.02 |
| 47 | SER | 0.02 |
| 48 | ASN | 0.02 |
| 49 | SER | 0.02 |
| 50 | THR | 0.02 |
| 51 | VAL | 0.02 |
| 52 | TTR | 0.02 |
| 53 | MET | 0.02 |
| 54 | THR | 0.02 |
| 55 | PRO | 0.02 |
| 56 | GLY | 0.02 |
| 57 | ASP | 0.02 |
| 58 | LEU | 0.02 |
| 59 | THR | 0.02 |
| 60 | GLY | 0.02 |
| 61 | THR | 0.02 |
| 62 | GLY | 0.02 |
| 63 | ASP | 0.02 |
| 64 | LEU | 0.02 |
| 65 | THR | 0.02 |
| 66 | GLY | 0.02 |
| 67 | ASP | 0.02 |
| 68 | LEU | 0.02 |
| 69 | THR | 0.02 |
| 70 | GLY | 0.02 |
| 71 | THR | 0.02 |
| 72 | GLY | 0.02 |
| 73 | THR | 0.02 |
| 74 | GLY | 0.02 |
| 75 | THR | 0.02 |
| 76 | GLY | 0.02 |
| 77 | THR | 0.02 |
| 78 | GLY | 0.02 |
| 79 | THR | 0.02 |
| 80 | GLY | 0.02 |
| 81 | THR | 0.02 |
| 82 | GLY | 0.02 |
| 83 | THR | 0.02 |
| 84 | GLY | 0.02 |
| 85 | THR | 0.02 |
| 86 | GLY | 0.02 |
| 87 | THR | 0.02 |
| 88 | GLY | 0.02 |
| 89 | THR | 0.02 |
| 90 | GLY | 0.02 |
| 91 | THR | 0.02 |
| 92 | GLY | 0.02 |
| 93 | THR | 0.02 |
| 94 | GLY | 0.02 |
| 95 | THR | 0.02 |
| 96 | GLY | 0.02 |
| 97 | THR | 0.02 |
| 98 | GLY | 0.02 |
| 99 | THR | 0.02 |
| 100 | GLY | 0.02 |
| 101 | THR | 0.02 |
| 102 | GLY | 0.02 |
| 103 | THR | 0.02 |
| 104 | GLY | 0.02 |
| 105 | THR | 0.02 |
| 106 | GLY | 0.02 |
| 107 | THR | 0.02 |
| 108 | GLY | 0.02 |
| 109 | THR | 0.02 |
| 110 | GLY | 0.02 |
| 111 | THR | 0.02 |
| 112 | GLY | 0.02 |
| 113 | THR | 0.02 |
| 114 | GLY | 0.02 |
| 115 | THR | 0.02 |
| 116 | GLY | 0.02 |
| 117 | THR | 0.02 |
| 118 | GLY | 0.02 |
| 119 | THR | 0.02 |
| 120 | GLY | 0.02 |
| 121 | THR | 0.02 |
| 122 | GLY | 0.02 |
| 123 | THR | 0.02 |
| 124 | GLY | 0.02 |
| 125 | THR | 0.02 |
| 126 | GLY | 0.02 |
| 127 | THR | 0.02 |
| 128 | GLY | 0.02 |
| 129 | THR | 0.02 |
| 130 | GLY | 0.02 |
| 131 | THR | 0.02 |
| 132 | GLY | 0.02 |
| 133 | THR | 0.02 |
| 134 | GLY | 0.02 |
| 135 | THR | 0.02 |
| 136 | GLY | 0.02 |
| 137 | THR | 0.02 |
| 138 | GLY | 0.02 |
| 139 | THR | 0.02 |
| 140 | GLY | 0.02 |
| 141 | THR | 0.02 |
| 142 | GLY | 0.02 |
| 143 | THR | 0.02 |
| 144 | GLY | 0.02 |
| 145 | THR | |

• Molecule 1: Glycogen [starch] synthase isoform 2



• Molecule 1: Glycogen [starch] synthase isoform 2



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	191.98Å 204.56Å 205.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.09 – 2.88 45.80 – 2.88	Depositor EDS
% Data completeness (in resolution range)	98.0 (145.09-2.88) 98.0 (45.80-2.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.219 , 0.260 0.217 , 0.255	Depositor DCC
R_{free} test set	4461 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.0	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	0.94	EDS
Total number of atoms	19585	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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

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	0.42	0/5140	0.60	0/6983
1	B	0.39	0/5136	0.60	0/6977
1	C	0.39	0/4975	0.59	0/6776
1	D	0.41	0/4677	0.61	0/6363
All	All	0.40	0/19928	0.60	0/27099

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5020	0	4846	54	0
1	B	5018	0	4844	50	0
1	C	4869	0	4619	73	0
1	D	4582	0	4371	87	0
2	A	32	0	22	2	0
2	B	32	0	22	3	0
2	C	16	0	11	0	0
2	D	16	0	11	1	0
All	All	19585	0	18746	263	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 7.

All (263) 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:167:PHE:CD2	1:D:176:LEU:HD21	1.87	1.09
1:C:83:MET:C	1:C:88:VAL:HG22	1.73	1.09
1:C:83:MET:CA	1:C:88:VAL:HG22	1.92	0.98
1:D:176:LEU:HD11	1:D:188:THR:OG1	1.67	0.95
1:D:134:ASP:OD2	1:D:229:HIS:NE2	2.04	0.90
1:D:227:ILE:O	1:D:229:HIS:N	2.08	0.87
1:C:280:HIS:CE1	1:D:283:GLN:HG2	2.13	0.84
1:C:82:THR:HG22	1:C:83:MET:H	1.41	0.83
1:C:122:LEU:HD12	1:C:128:ILE:HB	1.64	0.79
1:C:83:MET:CB	1:C:88:VAL:CG2	2.62	0.77
1:A:7:ASN:ND2	1:A:72:GLU:OE2	2.17	0.77
1:D:148:ALA:HB1	1:D:178:LEU:HD11	1.67	0.77
1:C:83:MET:CA	1:C:88:VAL:CG2	2.63	0.76
2:B:902:G6P:O4	2:B:902:G6P:O1P	2.00	0.75
1:C:83:MET:O	1:C:88:VAL:HG22	1.86	0.75
1:D:163:ILE:HB	1:D:186:VAL:HG22	1.68	0.75
1:D:167:PHE:CG	1:D:176:LEU:HD21	2.23	0.73
1:C:196:LEU:HD12	1:C:234:GLU:OE2	1.89	0.72
1:D:549:TYR:O	1:D:590:THR:HG22	1.89	0.72
1:D:176:LEU:CD1	1:D:188:THR:OG1	2.38	0.72
1:A:153:GLU:O	1:A:157:LEU:HD13	1.91	0.70
1:C:143:LEU:O	1:C:147:VAL:HG23	1.91	0.70
1:D:187:VAL:HG11	1:D:613:ALA:HB1	1.73	0.69
1:D:167:PHE:CD2	1:D:176:LEU:CD2	2.71	0.69
1:A:3:ARG:NH2	1:A:158:ASP:O	2.24	0.69
1:B:123:TRP:O	1:B:127:GLY:HA2	1.91	0.69
1:B:450:ASP:OD1	1:B:460:ARG:NH2	2.25	0.69
1:C:53:THR:O	1:C:55:GLN:N	2.24	0.69
1:A:549:TYR:O	1:A:590:THR:HG22	1.95	0.67
1:D:178:LEU:HD12	1:D:179:CYS:N	2.09	0.67
1:C:49:LEU:HD23	1:C:107:ASP:CB	2.25	0.66
1:A:5:LEU:O	1:A:8:HIS:HB3	1.95	0.66
1:B:74:ARG:NH1	1:B:77:GLN:OE1	2.29	0.66
1:D:302:HIS:HD2	1:D:432:LEU:O	1.79	0.65
1:C:179:CYS:HA	1:C:184:ILE:HD12	1.78	0.65
1:D:187:VAL:CG1	1:D:613:ALA:HB1	2.27	0.65
1:A:415:GLU:O	1:A:418:LYS:NZ	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:HIS:NE2	1:B:72:GLU:OE2	2.30	0.65
1:C:83:MET:O	1:C:88:VAL:N	2.27	0.65
1:A:71:ASP:HA	1:A:74:ARG:HG2	1.79	0.65
1:C:218:VAL:HG11	1:C:231:TYR:CZ	2.32	0.65
1:B:19:ASN:OD1	1:B:21:VAL:HG23	1.98	0.64
1:C:42:HIS:HA	1:C:73:MET:CE	2.28	0.64
1:C:284:ASN:HD21	1:D:284:ASN:HD21	1.45	0.64
1:C:122:LEU:CD1	1:C:128:ILE:HB	2.27	0.63
1:C:42:HIS:HA	1:C:73:MET:HE1	1.79	0.63
1:C:49:LEU:HB3	1:C:107:ASP:HA	1.81	0.63
1:C:77:GLN:HA	1:C:80:LEU:HB2	1.79	0.63
1:A:71:ASP:HA	1:A:74:ARG:CG	2.29	0.63
1:C:197:LEU:HD11	1:C:218:VAL:HG13	1.81	0.63
1:D:167:PHE:CG	1:D:176:LEU:CD2	2.82	0.63
1:C:12:GLU:HB3	1:C:45:LEU:HD23	1.79	0.62
1:C:83:MET:HA	1:C:88:VAL:HG22	1.81	0.62
1:C:510:PRO:O	1:C:532:GLY:HA3	2.00	0.62
1:C:77:GLN:O	1:C:81:GLN:N	2.32	0.62
1:C:45:LEU:HB2	1:C:103:VAL:HG22	1.82	0.61
1:D:227:ILE:HG23	1:D:230:ARG:CB	2.32	0.60
1:B:549:TYR:O	1:B:590:THR:HG22	2.01	0.59
1:D:188:THR:CG2	1:D:242:ASP:H	2.14	0.59
1:C:78:HIS:CB	1:C:157:LEU:HD13	2.33	0.59
1:D:97:ILE:H	1:D:97:ILE:HD13	1.67	0.59
1:D:148:ALA:CB	1:D:178:LEU:HD11	2.33	0.59
1:C:218:VAL:HG11	1:C:231:TYR:OH	2.03	0.58
1:A:187:VAL:HG12	1:A:613:ALA:HB1	1.83	0.58
1:C:450:ASP:OD1	1:C:460:ARG:NH2	2.36	0.58
1:A:12:GLU:HB3	1:A:45:LEU:HD23	1.85	0.58
1:C:78:HIS:CB	1:C:157:LEU:CD1	2.82	0.58
1:C:195:THR:OG1	1:C:254:GLU:OE1	2.19	0.58
1:B:18:ALA:HB2	1:B:105:LEU:CD2	2.34	0.57
1:D:176:LEU:N	1:D:177:PRO:HD2	2.19	0.57
1:C:550:GLY:HA3	1:C:590:THR:CG2	2.34	0.57
1:C:108:LEU:O	1:C:111:VAL:N	2.32	0.57
1:D:188:THR:HG23	1:D:242:ASP:H	1.70	0.57
1:A:158:ASP:OD2	1:A:161:HIS:ND1	2.30	0.56
1:C:73:MET:C	1:C:75:PRO:HD2	2.26	0.56
1:D:177:PRO:HA	1:D:240:SER:OG	2.05	0.55
1:A:187:VAL:CG1	1:A:613:ALA:HB1	2.36	0.55
1:B:353:ALA:HB3	1:B:474:MET:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:HD12	1:C:234:GLU:CD	2.26	0.55
1:C:82:THR:HA	1:C:85:SER:HB3	1.87	0.55
1:A:3:ARG:NH1	1:A:185:ASP:OD2	2.40	0.55
1:A:5:LEU:HD23	1:A:5:LEU:N	2.22	0.55
1:D:510:PRO:O	1:D:532:GLY:HA3	2.07	0.55
1:D:74:ARG:N	1:D:75:PRO:HD2	2.21	0.54
1:D:3:ARG:NH2	1:D:158:ASP:O	2.40	0.54
1:A:213:LEU:HD21	1:A:254:GLU:HA	1.89	0.54
1:D:227:ILE:HG22	1:D:231:TYR:H	1.73	0.54
1:B:213:LEU:HD21	1:B:254:GLU:HA	1.90	0.54
1:D:12:GLU:HB3	1:D:45:LEU:HD23	1.90	0.54
1:B:12:GLU:HB3	1:B:45:LEU:HD23	1.89	0.54
1:C:82:THR:HG22	1:C:83:MET:N	2.15	0.53
1:C:122:LEU:HD11	1:C:128:ILE:HD12	1.91	0.53
1:A:434:ARG:NH1	1:A:438:GLN:OE1	2.42	0.52
1:D:96:LEU:N	1:D:100:ALA:HA	2.24	0.52
1:C:83:MET:CB	1:C:88:VAL:HG21	2.39	0.52
1:C:80:LEU:O	1:C:82:THR:O	2.27	0.52
1:A:199:ARG:NH2	2:A:902:G6P:O3P	2.33	0.52
1:C:14:ALA:O	1:C:17:VAL:HG23	2.09	0.52
1:B:323:TYR:OH	1:B:458:LYS:HG2	2.10	0.52
1:B:115:SER:HB3	1:B:142:LEU:HD21	1.92	0.52
1:D:123:TRP:O	1:D:127:GLY:HA2	2.10	0.51
1:D:73:MET:HA	1:D:73:MET:CE	2.39	0.51
1:B:308:ASP:O	1:B:312:THR:HG23	2.10	0.51
1:D:133:ASN:O	1:D:135:PHE:N	2.44	0.51
1:D:383:HIS:O	1:D:387:THR:HG23	2.11	0.51
1:A:189:ILE:HD11	1:A:610:ARG:HA	1.93	0.51
1:C:60:ILE:HG22	1:C:61:LEU:N	2.26	0.51
1:C:76:VAL:O	1:C:77:GLN:CB	2.58	0.51
1:A:74:ARG:N	1:A:75:PRO:CD	2.74	0.50
1:D:227:ILE:HG22	1:D:231:TYR:N	2.27	0.50
1:C:323:TYR:CZ	1:C:329:ASP:HB3	2.46	0.50
1:D:34:ILE:HD13	1:D:599:TRP:HB3	1.94	0.50
1:B:126:VAL:HG12	1:B:128:ILE:HG13	1.93	0.50
1:A:188:THR:O	1:A:242:ASP:HB2	2.12	0.50
1:C:82:THR:O	1:C:83:MET:CB	2.60	0.50
1:B:45:LEU:HB2	1:B:103:VAL:HG12	1.94	0.50
1:B:333:GLU:OE1	1:B:458:LYS:NZ	2.45	0.49
1:B:369:LEU:HA	1:B:487:ILE:HD11	1.94	0.49
1:D:49:LEU:HD11	1:D:91:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:HIS:HE1	1:B:407:THR:O	1.94	0.49
1:C:83:MET:HA	1:C:88:VAL:CG2	2.40	0.49
1:C:218:VAL:CG1	1:C:231:TYR:CZ	2.95	0.49
1:C:406:THR:O	1:C:407:THR:OG1	2.15	0.49
1:B:63:TRP:O	1:B:77:GLN:NE2	2.44	0.49
1:C:213:LEU:HD21	1:C:254:GLU:HA	1.94	0.49
1:D:10:LEU:HD13	1:D:610:ARG:HD3	1.94	0.49
1:D:72:GLU:O	1:D:161:HIS:HE1	1.95	0.49
1:D:550:GLY:HA3	1:D:590:THR:CG2	2.43	0.49
1:A:450:ASP:OD1	1:A:460:ARG:NH2	2.44	0.48
1:C:549:TYR:O	1:C:590:THR:HG22	2.12	0.48
1:D:97:ILE:HD13	1:D:97:ILE:N	2.28	0.48
1:B:60:ILE:C	1:B:61:LEU:HD12	2.33	0.48
1:C:189:ILE:HD11	1:C:610:ARG:HA	1.95	0.48
1:C:83:MET:C	1:C:88:VAL:CG2	2.64	0.48
1:B:307:PHE:HD1	1:B:312:THR:HG21	1.78	0.48
1:A:510:PRO:O	1:A:532:GLY:HA3	2.14	0.48
1:B:18:ALA:HB2	1:B:105:LEU:HD22	1.96	0.48
1:A:34:ILE:CD1	1:A:600:LYS:HA	2.44	0.47
1:B:493:ASP:O	1:B:497:ARG:HG3	2.14	0.47
1:D:187:VAL:HG11	1:D:613:ALA:O	2.15	0.47
1:B:200:TYR:CD1	1:B:227:ILE:HD11	2.49	0.47
1:D:322:GLU:HB2	1:D:326:LYS:HG2	1.96	0.47
1:D:49:LEU:CD1	1:D:91:VAL:HG21	2.45	0.47
1:B:146:THR:O	1:B:149:TRP:HB3	2.15	0.47
1:B:396:HIS:HD2	1:B:415:GLU:OE2	1.97	0.47
1:D:49:LEU:CD1	1:D:91:VAL:CG2	2.92	0.47
1:A:153:GLU:HA	1:A:153:GLU:OE1	2.14	0.47
1:D:126:VAL:O	1:D:126:VAL:HG12	2.15	0.47
1:D:97:ILE:HD13	1:D:101:PRO:HD2	1.95	0.47
1:C:123:TRP:C	1:C:123:TRP:CD1	2.88	0.47
1:C:49:LEU:HB3	1:C:107:ASP:CA	2.45	0.47
1:A:295:ASP:CG	1:A:376:ARG:HH22	2.19	0.47
1:D:189:ILE:HD11	1:D:610:ARG:HA	1.96	0.47
1:D:43:TYR:OH	1:D:45:LEU:HD21	2.15	0.47
1:B:463:GLN:HA	1:B:465:PHE:CE2	2.50	0.47
1:B:74:ARG:N	1:B:75:PRO:CD	2.78	0.47
1:C:14:ALA:CB	1:C:28:LEU:HD11	2.45	0.47
1:C:19:ASN:OD1	1:C:21:VAL:HG23	2.15	0.47
1:D:187:VAL:HG12	1:D:188:THR:N	2.31	0.46
1:A:349:LYS:O	1:A:471:ARG:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ALA:O	1:B:17:VAL:HG23	2.16	0.46
1:A:3:ARG:NH2	1:A:155:ALA:O	2.42	0.46
1:B:3:ARG:NH1	1:B:185:ASP:OD2	2.49	0.46
1:B:550:GLY:HA3	1:B:590:THR:CG2	2.45	0.46
1:D:49:LEU:HD12	1:D:91:VAL:CG2	2.45	0.46
1:A:169:GLU:HA	1:A:169:GLU:OE2	2.16	0.46
1:A:249:GLN:HG2	1:A:266:ILE:HD11	1.98	0.46
1:C:238:ALA:O	1:C:261:ARG:NH1	2.47	0.46
1:D:81:GLN:O	1:D:85:SER:N	2.44	0.46
1:B:335:LEU:HD13	1:B:474:MET:CE	2.46	0.46
1:D:187:VAL:HG11	1:D:613:ALA:C	2.36	0.46
1:A:502:GLY:O	1:A:525:SER:HA	2.15	0.46
1:B:189:ILE:HD11	1:B:610:ARG:HA	1.97	0.46
1:B:295:ASP:CG	1:B:376:ARG:HH22	2.19	0.46
1:B:331:PHE:CZ	1:B:335:LEU:HD11	2.50	0.46
1:C:357:MET:O	1:C:478:PRO:HA	2.16	0.46
1:C:60:ILE:CG2	1:C:61:LEU:N	2.79	0.46
1:C:283:GLN:NE2	1:C:584:ILE:HG23	2.31	0.45
1:A:400:TYR:CD1	1:A:401:PRO:HA	2.51	0.45
1:D:200:TYR:O	1:D:203:ALA:HB2	2.16	0.45
1:D:73:MET:HE2	1:D:73:MET:HA	1.98	0.45
1:A:59:ASP:HB2	1:A:96:LEU:HD21	1.97	0.45
1:C:31:LYS:HD3	1:C:599:TRP:CH2	2.51	0.45
1:B:126:VAL:O	1:B:126:VAL:HG12	2.16	0.45
1:D:19:ASN:OD1	1:D:21:VAL:HG23	2.16	0.45
1:D:141:ILE:HA	1:D:174:VAL:HG11	1.97	0.45
1:D:187:VAL:HG11	1:D:613:ALA:CB	2.44	0.45
1:C:108:LEU:HD13	1:C:142:LEU:HB2	1.98	0.45
1:D:134:ASP:OD2	1:D:229:HIS:CD2	2.69	0.45
1:B:200:TYR:CE1	1:B:227:ILE:HD11	2.52	0.45
1:A:396:HIS:CE1	1:A:405:LEU:HD22	2.52	0.44
1:A:550:GLY:HA3	1:A:590:THR:CG2	2.48	0.44
1:B:323:TYR:CZ	1:B:329:ASP:HB3	2.52	0.44
1:D:283:GLN:HG3	2:D:901:G6P:O1	2.18	0.44
1:A:157:LEU:N	1:A:157:LEU:HD12	2.32	0.44
1:A:190:PHE:CE2	1:A:192:THR:HG23	2.52	0.44
1:A:514:THR:OG1	2:A:902:G6P:H1	2.17	0.44
1:C:550:GLY:HA3	1:C:590:THR:HG22	1.99	0.44
1:D:350:THR:OG1	1:D:471:ARG:NH1	2.50	0.44
1:C:196:LEU:CD1	1:C:234:GLU:CD	2.86	0.44
1:D:213:LEU:HD23	1:D:253:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:PHE:N	1:D:69:PHE:CD2	2.86	0.44
1:C:177:PRO:HA	1:C:240:SER:OG	2.18	0.44
1:A:72:GLU:OE2	1:A:161:HIS:NE2	2.51	0.44
1:A:400:TYR:HA	1:A:405:LEU:HD12	1.99	0.44
1:C:209:PHE:O	1:C:213:LEU:HB2	2.18	0.43
1:D:227:ILE:CG2	1:D:230:ARG:CB	2.96	0.43
1:B:111:VAL:HG11	1:B:118:TRP:CH2	2.53	0.43
1:C:74:ARG:N	1:C:75:PRO:HD2	2.33	0.43
1:D:111:VAL:O	1:D:111:VAL:HG22	2.18	0.43
1:D:163:ILE:HG22	1:D:186:VAL:HG13	2.00	0.43
1:A:249:GLN:OE1	1:A:266:ILE:HD11	2.19	0.43
1:A:320:ARG:NH1	1:A:322:GLU:OE1	2.52	0.43
1:A:63:TRP:O	1:A:69:PHE:HE2	2.01	0.43
1:D:529:ASN:ND2	1:D:555:ASP:OD2	2.52	0.43
1:A:364:PHE:CE2	1:A:486:PRO:HD2	2.53	0.42
1:D:122:LEU:HA	1:D:125:LEU:HB2	2.01	0.42
1:A:34:ILE:HD11	1:A:600:LYS:HA	2.02	0.42
1:B:126:VAL:HG11	1:B:128:ILE:HD12	2.02	0.42
1:A:548:ASP:O	1:A:589:ARG:NH1	2.52	0.42
1:B:290:LYS:NZ	2:B:901:G6P:O1P	2.43	0.42
1:A:228:TYR:CE2	1:A:232:CYS:SG	3.12	0.42
1:B:78:HIS:HB2	1:B:157:LEU:HD13	2.01	0.42
1:C:333:GLU:OE1	1:C:458:LYS:NZ	2.52	0.42
1:D:122:LEU:CD1	1:D:141:ILE:HG12	2.50	0.42
1:A:323:TYR:CZ	1:A:329:ASP:HB3	2.54	0.42
1:A:323:TYR:OH	1:A:458:LYS:HG2	2.20	0.42
1:B:238:ALA:O	1:B:261:ARG:NH1	2.53	0.42
1:D:180:ARG:HD3	1:D:180:ARG:HA	1.83	0.42
1:D:200:TYR:CE2	1:D:227:ILE:HD11	2.55	0.42
1:D:50:ASN:ND2	1:D:53:THR:OG1	2.53	0.42
1:B:213:LEU:HD23	1:B:253:PHE:CE2	2.55	0.41
1:D:163:ILE:HG22	1:D:186:VAL:CG1	2.49	0.41
1:A:191:THR:HA	1:A:245:THR:O	2.19	0.41
1:D:32:ALA:HB3	1:D:33:PRO:HD3	2.02	0.41
1:D:302:HIS:HE1	1:D:367:GLU:OE2	2.02	0.41
1:A:295:ASP:OD1	1:A:376:ARG:NH2	2.53	0.41
1:D:323:TYR:CZ	1:D:329:ASP:HB3	2.55	0.41
1:B:128:ILE:HG12	1:B:232:CYS:HB3	2.03	0.41
1:D:174:VAL:O	1:D:177:PRO:HG2	2.21	0.41
1:C:323:TYR:OH	1:C:458:LYS:HG2	2.21	0.41
1:C:400:TYR:CD1	1:C:401:PRO:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LYS:NZ	1:A:138:ASN:OD1	2.53	0.41
1:D:144:GLY:HA3	1:D:174:VAL:HB	2.02	0.41
1:D:16:GLU:HG3	1:D:24:ILE:HB	2.03	0.41
1:D:400:TYR:CD1	1:D:401:PRO:HA	2.56	0.41
1:D:58:VAL:O	1:D:58:VAL:HG12	2.20	0.41
1:B:188:THR:O	1:B:242:ASP:HB2	2.21	0.41
1:B:369:LEU:HD23	1:B:487:ILE:HD11	2.03	0.41
1:D:349:LYS:O	1:D:471:ARG:HD3	2.21	0.41
1:A:213:LEU:HD23	1:A:253:PHE:CE1	2.56	0.41
1:D:282:PHE:CD1	1:D:591:GLU:OE1	2.73	0.41
1:A:366:VAL:O	1:A:370:LYS:HB2	2.21	0.41
1:B:199:ARG:HH22	2:B:902:G6P:P	2.44	0.41
1:B:17:VAL:HG21	1:B:46:ILE:O	2.21	0.40
1:B:59:ASP:HB2	1:B:96:LEU:HD21	2.03	0.40
1:D:97:ILE:CD1	1:D:101:PRO:HD2	2.51	0.40
1:D:502:GLY:O	1:D:525:SER:HA	2.21	0.40
1:D:607:VAL:HA	1:D:610:ARG:NH1	2.36	0.40
1:C:349:LYS:O	1:C:471:ARG:HG3	2.21	0.40
1:A:286:HIS:ND1	1:A:497:ARG:O	2.54	0.40
1:D:153:GLU:O	1:D:157:LEU:HG	2.21	0.40
1:C:3:ARG:NH1	1:C:185:ASP:OD2	2.53	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	636/725 (88%)	607 (95%)	29 (5%)	0	100	100
1	B	635/725 (88%)	612 (96%)	22 (4%)	1 (0%)	51	81
1	C	637/725 (88%)	605 (95%)	29 (5%)	3 (0%)	32	66
1	D	594/725 (82%)	570 (96%)	22 (4%)	2 (0%)	44	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2502/2900 (86%)	2394 (96%)	102 (4%)	6 (0%)	51 81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	54	TYR
1	D	228	TYR
1	D	363	SER
1	B	169	GLU
1	C	407	THR
1	C	77	GLN

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	524/625 (84%)	512 (98%)	12 (2%)	56 84
1	B	524/625 (84%)	510 (97%)	14 (3%)	50 81
1	C	494/625 (79%)	480 (97%)	14 (3%)	49 80
1	D	463/625 (74%)	454 (98%)	9 (2%)	62 87
All	All	2005/2500 (80%)	1956 (98%)	49 (2%)	54 83

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	81	GLN
1	A	85	SER
1	A	254	GLU
1	A	289	LYS
1	A	304	CYS
1	A	310	ASP
1	A	321	TYR
1	A	376	ARG

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Mol	Chain	Res	Type
1	A	388	SER
1	A	408	GLU
1	A	556	ARG
1	B	34	ILE
1	B	35	THR
1	B	64	LYS
1	B	204	SER
1	B	224	ARG
1	B	254	GLU
1	B	304	CYS
1	B	310	ASP
1	B	321	TYR
1	B	363	SER
1	B	376	ARG
1	B	408	GLU
1	B	467	SER
1	B	471	ARG
1	C	26	SER
1	C	105	LEU
1	C	122	LEU
1	C	254	GLU
1	C	289	LYS
1	C	304	CYS
1	C	310	ASP
1	C	321	TYR
1	C	363	SER
1	C	420	SER
1	C	471	ARG
1	C	535	SER
1	C	556	ARG
1	C	581	ARG
1	D	69	PHE
1	D	73	MET
1	D	97	ILE
1	D	180	ARG
1	D	289	LYS
1	D	304	CYS
1	D	321	TYR
1	D	433	ARG
1	D	517	GLU

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

Mol	Chain	Res	Type
1	A	50	ASN
1	A	283	GLN
1	A	484	ASN
1	B	6	GLN
1	B	161	HIS
1	B	396	HIS
1	B	452	ASN
1	B	582	GLN
1	B	585	ASN
1	C	283	GLN
1	C	284	ASN
1	C	403	ASN
1	D	50	ASN
1	D	161	HIS
1	D	168	HIS
1	D	211	ASN
1	D	302	HIS
1	D	403	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	G6P	A	901	-	16,16,16	0.51	0	24,24,24	0.98	1 (4%)
2	G6P	A	902	-	16,16,16	0.54	0	24,24,24	1.16	3 (12%)
2	G6P	B	901	-	16,16,16	0.51	0	24,24,24	0.85	0
2	G6P	B	902	-	16,16,16	0.65	0	24,24,24	1.75	8 (33%)
2	G6P	C	901	-	16,16,16	0.54	0	24,24,24	0.93	2 (8%)
2	G6P	D	901	-	16,16,16	0.66	0	24,24,24	1.30	2 (8%)

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	G6P	A	901	-	-	0/6/26/26	0/1/1/1
2	G6P	A	902	-	-	0/6/26/26	0/1/1/1
2	G6P	B	901	-	-	0/6/26/26	0/1/1/1
2	G6P	B	902	-	-	0/6/26/26	0/1/1/1
2	G6P	C	901	-	-	0/6/26/26	0/1/1/1
2	G6P	D	901	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	G6P	O2P-P-O6	-4.03	96.00	106.73
2	B	902	G6P	C3-C4-C5	-3.23	104.52	110.22
2	B	902	G6P	C4-C3-C2	-3.14	105.30	110.84
2	B	902	G6P	O5-C5-C4	-2.38	105.28	109.66
2	B	902	G6P	O1P-P-O6	-2.20	100.88	106.73
2	A	902	G6P	C6-C5-C4	-2.14	107.43	112.00
2	C	901	G6P	O3-C3-C2	-2.10	105.80	110.36
2	A	902	G6P	C4-C3-C2	-2.00	107.31	110.84
2	C	901	G6P	O2P-P-O1P	2.08	116.02	107.61
2	B	902	G6P	O5-C1-C2	2.49	114.16	110.04
2	B	902	G6P	O3-C3-C4	2.51	115.81	110.36
2	A	902	G6P	O5-C5-C6	2.52	111.66	106.64
2	B	902	G6P	O4-C4-C3	2.57	115.94	110.36
2	D	901	G6P	O2P-P-O1P	2.64	118.25	107.61
2	A	901	G6P	C1-O5-C5	2.84	118.52	113.39
2	B	902	G6P	O5-C5-C6	3.49	113.60	106.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	G6P	2	0
2	B	901	G6P	1	0
2	B	902	G6P	2	0
2	D	901	G6P	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	638/725 (88%)	0.11	11 (1%) 70 69	32, 67, 119, 145	4 (0%)
1	B	637/725 (87%)	0.18	23 (3%) 43 38	44, 75, 119, 137	3 (0%)
1	C	639/725 (88%)	0.29	27 (4%) 37 32	47, 81, 135, 160	2 (0%)
1	D	604/725 (83%)	0.31	38 (6%) 21 16	37, 80, 146, 168	1 (0%)
All	All	2518/2900 (86%)	0.22	99 (3%) 40 35	32, 77, 133, 168	10 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	61	LEU	6.2
1	C	111	VAL	5.6
1	D	108	LEU	5.3
1	C	79	ALA	4.9
1	C	85	SER	4.9
1	C	96	LEU	4.3
1	B	129	PRO	4.2
1	B	124	SER	4.2
1	D	122	LEU	4.1
1	C	157	LEU	3.9
1	D	265	GLY	3.9
1	D	129	PRO	3.8
1	C	68	ALA	3.8
1	C	116	ASN	3.8
1	B	126	VAL	3.7
1	D	45	LEU	3.7
1	A	637	ALA	3.6
1	C	149	TRP	3.5
1	C	108	LEU	3.5
1	D	49	LEU	3.4
1	C	83	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	197	LEU	3.3
1	B	93	GLY	3.3
1	C	88	VAL	3.3
1	D	128	ILE	3.3
1	B	76	VAL	3.2
1	A	61	LEU	3.2
1	A	67	GLU	3.2
1	C	78	HIS	3.2
1	C	80	LEU	3.2
1	A	71	ASP	3.1
1	D	259	LEU	3.1
1	B	91	VAL	3.1
1	C	152	GLY	3.1
1	C	103	VAL	3.0
1	D	91	VAL	3.0
1	D	103	VAL	3.0
1	D	615	ARG	3.0
1	A	407	THR	3.0
1	B	206	SER	3.0
1	D	616	ARG	2.9
1	B	127	GLY	2.9
1	C	74	ARG	2.8
1	C	148	ALA	2.8
1	B	68	ALA	2.8
1	B	122	LEU	2.8
1	A	78	HIS	2.8
1	B	131	PRO	2.8
1	D	130	SER	2.7
1	C	104	ILE	2.7
1	C	60	ILE	2.7
1	A	406	THR	2.7
1	B	596	LEU	2.7
1	D	407	THR	2.7
1	D	218	VAL	2.6
1	D	104	ILE	2.6
1	B	66	PRO	2.6
1	B	63	TRP	2.6
1	D	614	LEU	2.6
1	D	225	PHE	2.5
1	D	227	ILE	2.4
1	A	417	LEU	2.4
1	B	62	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	10	LEU	2.4
1	C	52	ALA	2.4
1	D	604	LEU	2.4
1	D	109	ASP	2.3
1	D	18	ALA	2.3
1	C	197	LEU	2.3
1	A	636	ASP	2.3
1	A	68	ALA	2.3
1	B	116	ASN	2.3
1	D	229	HIS	2.3
1	B	96	LEU	2.3
1	D	163	ILE	2.3
1	C	156	HIS	2.3
1	B	125	LEU	2.2
1	D	151	LEU	2.2
1	D	73	MET	2.2
1	C	14	ALA	2.2
1	D	406	THR	2.2
1	B	544	ASN	2.2
1	D	56	ASN	2.2
1	B	18	ALA	2.1
1	D	620	ASP	2.1
1	A	416	LEU	2.1
1	B	61	LEU	2.1
1	D	186	VAL	2.1
1	B	419	SER	2.1
1	D	124	SER	2.1
1	C	151	LEU	2.1
1	D	55	GLN	2.1
1	D	222	ALA	2.1
1	D	127	GLY	2.1
1	D	223	GLY	2.1
1	C	158	ASP	2.0
1	C	155	ALA	2.0
1	B	626	VAL	2.0
1	D	125	LEU	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 [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	G6P	A	902	16/16	0.90	0.32	6.19	54,63,66,68	16
2	G6P	B	902	16/16	0.92	0.23	0.56	76,85,94,94	0
2	G6P	A	901	16/16	0.98	0.18	-0.17	42,49,54,54	0
2	G6P	C	901	16/16	0.98	0.17	-0.76	46,61,69,70	0
2	G6P	B	901	16/16	0.98	0.15	-0.85	50,60,64,66	0
2	G6P	D	901	16/16	0.98	0.14	-1.28	41,45,49,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.