



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:10 PM GMT

PDB ID : 4KQ1
Title : Crystal structure of yeast glycogen synthase in complex with uridine-5'-mono
phosphate
Authors : Chikwana, V.M.; Hurley, T.D.
Deposited on : 2013-05-14
Resolution : 2.66 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

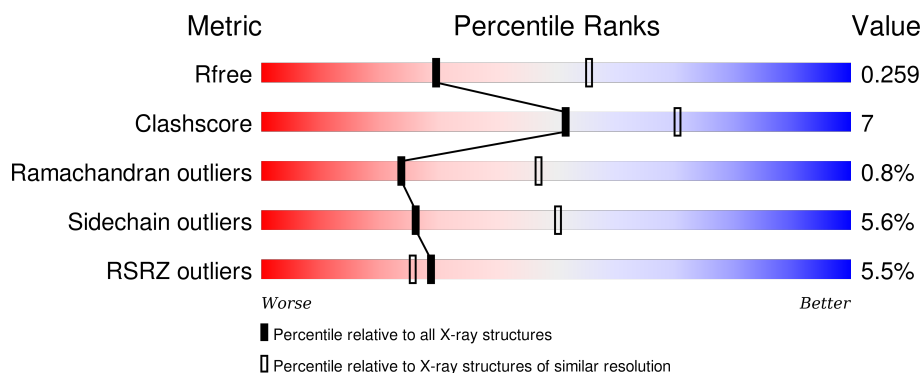
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	724	<div> <div>5%</div> <div>71% 16% • 12%</div> </div>
1	B	724	<div> <div>3%</div> <div>70% 17% • 12%</div> </div>
1	C	724	<div> <div>5%</div> <div>70% 16% • 12%</div> </div>
1	D	724	<div> <div>7%</div> <div>69% 18% • 12%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	C	803	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20739 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 Gsy2p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			5145	3286	896	944	19			
1	B	638	Total	C	N	O	S	0	0	0
			5145	3286	896	944	19			
1	C	638	Total	C	N	O	S	0	0	0
			5145	3286	896	944	19			
1	D	636	Total	C	N	O	S	0	0	0
			5128	3274	894	941	19			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	INITIATING METHIONINE	UNP E7NKU1
A	-17	GLY	-	EXPRESSION TAG	UNP E7NKU1
A	-16	SER	-	EXPRESSION TAG	UNP E7NKU1
A	-15	SER	-	EXPRESSION TAG	UNP E7NKU1
A	-14	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-13	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-12	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-11	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-10	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-9	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-8	SER	-	EXPRESSION TAG	UNP E7NKU1
A	-7	SER	-	EXPRESSION TAG	UNP E7NKU1
A	-6	GLY	-	EXPRESSION TAG	UNP E7NKU1
A	-5	LEU	-	EXPRESSION TAG	UNP E7NKU1
A	-4	VAL	-	EXPRESSION TAG	UNP E7NKU1
A	-3	PRO	-	EXPRESSION TAG	UNP E7NKU1
A	-2	ARG	-	EXPRESSION TAG	UNP E7NKU1
A	-1	GLY	-	EXPRESSION TAG	UNP E7NKU1
A	0	SER	-	EXPRESSION TAG	UNP E7NKU1
A	589	ALA	ARG	ENGINEERED MUTATION	UNP E7NKU1
A	592	ALA	ARG	ENGINEERED MUTATION	UNP E7NKU1

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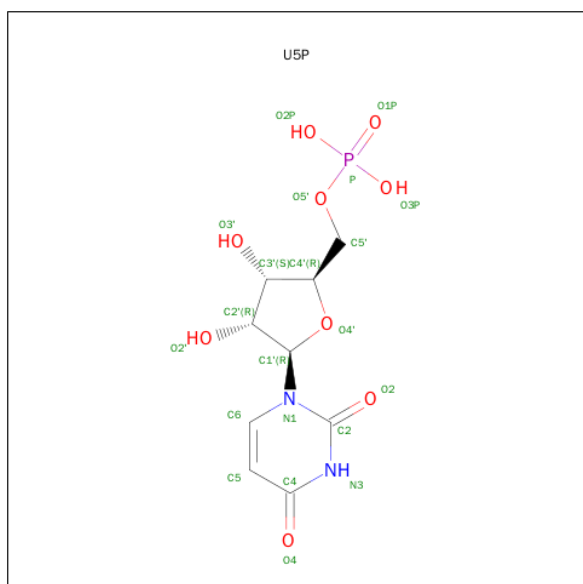
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	INITIATING METHIONINE	UNP E7NKU1
B	-17	GLY	-	EXPRESSION TAG	UNP E7NKU1
B	-16	SER	-	EXPRESSION TAG	UNP E7NKU1
B	-15	SER	-	EXPRESSION TAG	UNP E7NKU1
B	-14	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-13	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-12	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-11	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-10	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-9	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-8	SER	-	EXPRESSION TAG	UNP E7NKU1
B	-7	SER	-	EXPRESSION TAG	UNP E7NKU1
B	-6	GLY	-	EXPRESSION TAG	UNP E7NKU1
B	-5	LEU	-	EXPRESSION TAG	UNP E7NKU1
B	-4	VAL	-	EXPRESSION TAG	UNP E7NKU1
B	-3	PRO	-	EXPRESSION TAG	UNP E7NKU1
B	-2	ARG	-	EXPRESSION TAG	UNP E7NKU1
B	-1	GLY	-	EXPRESSION TAG	UNP E7NKU1
B	0	SER	-	EXPRESSION TAG	UNP E7NKU1
B	589	ALA	ARG	ENGINEERED MUTATION	UNP E7NKU1
B	592	ALA	ARG	ENGINEERED MUTATION	UNP E7NKU1
C	-18	MET	-	INITIATING METHIONINE	UNP E7NKU1
C	-17	GLY	-	EXPRESSION TAG	UNP E7NKU1
C	-16	SER	-	EXPRESSION TAG	UNP E7NKU1
C	-15	SER	-	EXPRESSION TAG	UNP E7NKU1
C	-14	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-13	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-12	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-11	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-10	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-9	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-8	SER	-	EXPRESSION TAG	UNP E7NKU1
C	-7	SER	-	EXPRESSION TAG	UNP E7NKU1
C	-6	GLY	-	EXPRESSION TAG	UNP E7NKU1
C	-5	LEU	-	EXPRESSION TAG	UNP E7NKU1
C	-4	VAL	-	EXPRESSION TAG	UNP E7NKU1
C	-3	PRO	-	EXPRESSION TAG	UNP E7NKU1
C	-2	ARG	-	EXPRESSION TAG	UNP E7NKU1
C	-1	GLY	-	EXPRESSION TAG	UNP E7NKU1
C	0	SER	-	EXPRESSION TAG	UNP E7NKU1
C	589	ALA	ARG	ENGINEERED MUTATION	UNP E7NKU1
C	592	ALA	ARG	ENGINEERED MUTATION	UNP E7NKU1

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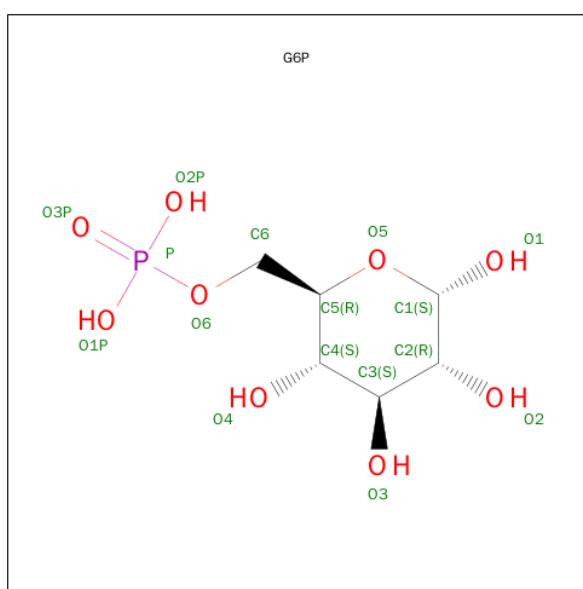
Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	MET	-	INITIATING METHIONINE	UNP E7NKU1
D	-17	GLY	-	EXPRESSION TAG	UNP E7NKU1
D	-16	SER	-	EXPRESSION TAG	UNP E7NKU1
D	-15	SER	-	EXPRESSION TAG	UNP E7NKU1
D	-14	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-13	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-12	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-11	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-10	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-9	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-8	SER	-	EXPRESSION TAG	UNP E7NKU1
D	-7	SER	-	EXPRESSION TAG	UNP E7NKU1
D	-6	GLY	-	EXPRESSION TAG	UNP E7NKU1
D	-5	LEU	-	EXPRESSION TAG	UNP E7NKU1
D	-4	VAL	-	EXPRESSION TAG	UNP E7NKU1
D	-3	PRO	-	EXPRESSION TAG	UNP E7NKU1
D	-2	ARG	-	EXPRESSION TAG	UNP E7NKU1
D	-1	GLY	-	EXPRESSION TAG	UNP E7NKU1
D	0	SER	-	EXPRESSION TAG	UNP E7NKU1
D	589	ALA	ARG	ENGINEERED MUTATION	UNP E7NKU1
D	592	ALA	ARG	ENGINEERED MUTATION	UNP E7NKU1

- Molecule 2 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U5P) (formula: $C_9H_{13}N_2O_9P$).



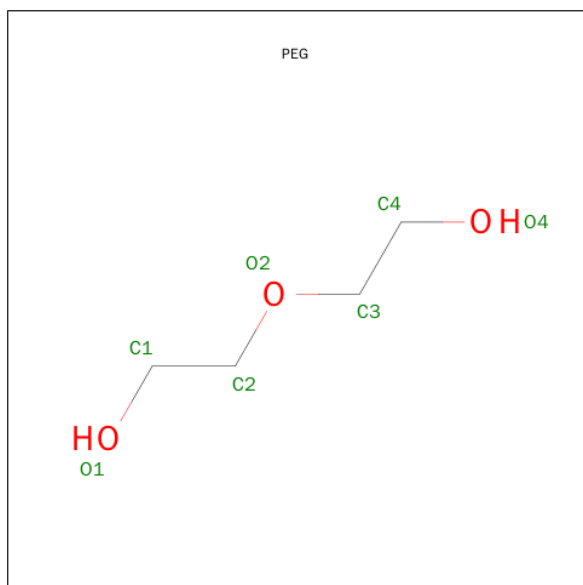
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	B	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	C	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	D	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

- Molecule 3 is SUGAR (ALPHA-D-GLUCOSE-6-PHOSPHATE) (three-letter code: G6P) (formula: C₆H₁₃O₉P).

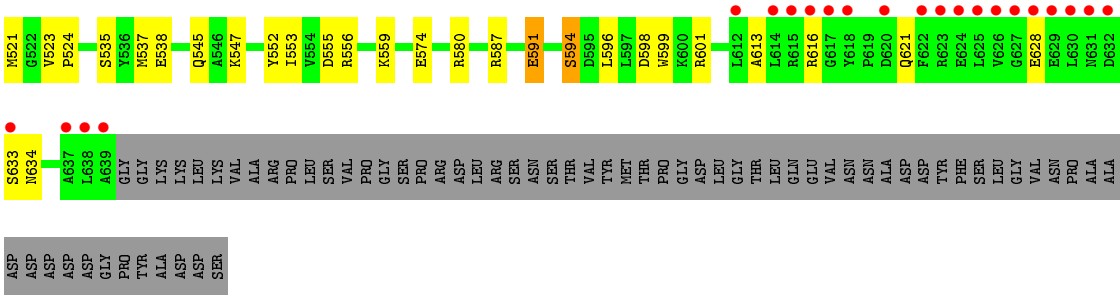


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	C	1	Total	C	O	P	0	0
			16	6	9	1		
3	D	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	193.09Å 204.37Å 206.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.46 – 2.66 48.41 – 2.66	Depositor EDS
% Data completeness (in resolution range)	95.0 (48.46-2.66) 95.0 (48.41-2.66)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.208 , 0.260 0.207 , 0.259	Depositor DCC
R_{free} test set	5560 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.2	EDS
Estimated twinning fraction	0.003 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 111216 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20739	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 2.76% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, PEG, U5P

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	0.41	0/5270	0.60	0/7141
1	B	0.49	0/5270	0.66	0/7141
1	C	0.42	0/5270	0.61	0/7141
1	D	0.44	0/5251	0.61	1/7114 (0.0%)
All	All	0.44	0/21061	0.62	1/28537 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	488	LEU	CA-CB-CG	6.86	131.07	115.30

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	5145	0	5054	70	0
1	B	5145	0	5054	63	0
1	C	5145	0	5054	72	0
1	D	5128	0	5039	78	0
2	A	21	0	11	0	0
2	B	21	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	21	0	11	0	0
2	D	21	0	11	0	0
3	A	16	0	11	2	0
3	B	16	0	11	0	0
3	C	16	0	11	2	0
3	D	16	0	11	2	0
4	B	14	0	20	1	0
4	C	7	0	10	0	0
4	D	7	0	10	1	0
All	All	20739	0	20329	278	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 (278) 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:180:ARG:HH11	1:A:180:ARG:HG3	1.29	0.97
1:C:579:THR:H	1:C:582:GLN:HE21	1.10	0.95
1:D:482:ASN:HD22	1:D:484:ASN:H	1.21	0.89
1:A:280:HIS:CE1	1:D:283:GLN:HG2	2.12	0.84
1:B:450:ASP:OD1	1:B:460:ARG:NH2	2.12	0.83
1:A:283:GLN:HG2	1:D:280:HIS:CE1	2.18	0.79
1:B:3:ARG:NH2	1:B:158:ASP:O	2.17	0.78
1:D:507:TYR:HB2	1:D:556:ARG:NH2	1.98	0.78
1:C:579:THR:H	1:C:582:GLN:NE2	1.81	0.77
1:D:513:TYR:H	1:D:513:TYR:HD1	1.30	0.77
1:B:128:ILE:HG12	1:B:232:CYS:HB3	1.66	0.76
1:D:3:ARG:NH2	1:D:158:ASP:O	2.21	0.74
1:B:445:HIS:ND1	1:B:478:PRO:HD2	2.03	0.74
1:C:458:LYS:O	1:C:462:VAL:HG22	1.89	0.73
1:C:484:ASN:HD22	1:C:484:ASN:N	1.89	0.70
1:D:128:ILE:HG12	1:D:232:CYS:HB3	1.73	0.70
1:D:591:GLU:O	1:D:594:SER:HB3	1.92	0.70
1:C:296:PHE:HE1	1:C:487:ILE:HD12	1.56	0.70
1:A:492:TYR:O	1:A:496:VAL:HG23	1.91	0.69
1:D:144:GLY:HA3	1:D:174:VAL:HB	1.75	0.68
1:D:31:LYS:NZ	1:D:35:THR:HG21	2.09	0.68
1:D:513:TYR:CD1	1:D:513:TYR:N	2.60	0.67
1:A:379:GLU:HG2	4:B:1004:PEG:H41	1.75	0.67
1:B:8:HIS:HA	1:B:161:HIS:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:MET:HG3	1:C:565:VAL:HG22	1.77	0.66
1:B:339:ASN:O	1:B:343:LYS:HG3	1.96	0.66
1:D:74:ARG:N	1:D:75:PRO:HD2	2.10	0.66
1:D:493:ASP:HB2	1:D:521:MET:HE1	1.80	0.64
1:C:634:ASN:ND2	1:C:637:ALA:H	1.96	0.64
1:A:283:GLN:HG3	3:A:802:G6P:O1	1.97	0.64
1:A:92:TYR:OH	1:A:102:LYS:HD3	1.97	0.64
1:D:493:ASP:HB2	1:D:521:MET:CE	2.28	0.63
1:D:399:ARG:HG3	1:D:399:ARG:HH11	1.62	0.63
1:A:355:ILE:HD11	1:A:474:MET:HE2	1.81	0.63
1:B:471:ARG:HH11	1:B:471:ARG:HG2	1.63	0.62
1:C:296:PHE:CE1	1:C:487:ILE:HD12	2.34	0.62
1:D:389:ILE:HG23	1:D:416:LEU:HB3	1.83	0.60
1:B:419:SER:O	1:B:423:VAL:HG23	2.03	0.59
1:A:283:GLN:HG2	1:D:280:HIS:HE1	1.67	0.58
1:C:174:VAL:O	1:C:177:PRO:HD2	2.04	0.57
1:D:59:ASP:HB3	1:D:94:ARG:HB2	1.86	0.57
1:A:323:TYR:OH	1:A:458:LYS:HG3	2.04	0.57
1:C:634:ASN:HD22	1:C:634:ASN:C	2.07	0.57
1:C:331:PHE:CZ	1:C:335:LEU:HD11	2.39	0.57
1:B:634:ASN:HB2	1:B:637:ALA:H	1.69	0.57
1:A:634:ASN:HB3	1:A:637:ALA:H	1.70	0.57
1:A:450:ASP:OD2	1:A:460:ARG:NH2	2.38	0.57
1:D:399:ARG:HD3	1:D:403:ASN:HD22	1.69	0.57
1:A:61:LEU:HB2	1:A:93:GLY:HA2	1.87	0.56
1:A:348:LYS:HA	1:A:348:LYS:HE3	1.84	0.56
1:A:327:GLY:HA3	1:A:505:PRO:O	2.04	0.56
1:D:547:LYS:HE3	1:D:574:GLU:OE2	2.05	0.56
1:D:350:THR:OG1	1:D:471:ARG:NH1	2.38	0.56
1:B:95:TRP:HB3	1:B:101:PRO:HD2	1.88	0.56
1:C:445:HIS:ND1	1:C:478:PRO:HD2	2.21	0.56
1:D:214:GLU:HG3	1:D:257:HIS:CD2	2.41	0.55
1:B:463:GLN:HG2	1:B:465:PHE:CE2	2.42	0.55
1:C:163:ILE:HB	1:C:186:VAL:HG12	1.86	0.55
1:D:176:LEU:HD22	1:D:241:ALA:HB2	1.88	0.55
1:B:214:GLU:HG2	1:B:257:HIS:CD2	2.41	0.55
1:C:350:THR:OG1	1:C:471:ARG:NH1	2.40	0.54
1:C:150:PHE:O	1:C:154:VAL:HG23	2.08	0.54
1:A:513:TYR:N	1:A:513:TYR:CD2	2.74	0.54
1:D:3:ARG:H	1:D:621:GLN:HE22	1.56	0.54
1:A:357:MET:O	1:A:478:PRO:HA	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:VAL:HG11	1:B:613:ALA:O	2.08	0.54
1:C:536:TYR:OH	1:C:601:ARG:NH1	2.41	0.53
1:A:517:GLU:O	1:A:521:MET:HG2	2.08	0.53
1:B:490:LEU:HD13	1:B:495:PHE:HA	1.89	0.53
1:C:549:TYR:HB3	1:C:593:LEU:HD11	1.89	0.53
1:B:295:ASP:CG	1:B:376:ARG:HH22	2.12	0.53
1:B:488:LEU:O	1:B:490:LEU:N	2.36	0.53
1:B:59:ASP:HB3	1:B:94:ARG:HB2	1.90	0.53
1:D:164:VAL:HA	1:D:187:VAL:HG23	1.90	0.53
1:B:17:VAL:HG21	1:B:47:GLY:HA3	1.90	0.53
1:C:177:PRO:HA	1:C:240:SER:OG	2.09	0.53
1:B:187:VAL:HG21	1:B:614:LEU:HD23	1.90	0.53
1:C:598:ASP:OD2	1:C:600:LYS:HB2	2.09	0.53
1:A:374:GLU:HB3	1:A:432:LEU:HD23	1.90	0.53
1:B:337:ARG:NH1	1:B:566:GLU:OE2	2.41	0.53
1:A:195:THR:OG1	1:A:254:GLU:OE1	2.16	0.52
1:A:180:ARG:CG	1:A:180:ARG:HH11	2.12	0.52
1:C:17:VAL:HG12	1:C:18:ALA:N	2.24	0.52
1:D:482:ASN:ND2	1:D:484:ASN:H	1.99	0.52
1:C:312:THR:HG22	1:C:350:THR:HB	1.92	0.52
1:A:521:MET:HA	1:A:521:MET:HE2	1.90	0.52
1:D:331:PHE:CZ	1:D:335:LEU:HD11	2.44	0.52
1:A:328:ALA:O	1:A:332:ILE:HG13	2.10	0.52
1:D:217:ASP:O	1:D:221:GLU:HG2	2.09	0.52
1:D:282:PHE:CE2	1:D:591:GLU:HG3	2.45	0.52
1:D:485:ASN:OD1	1:D:487:ILE:HG13	2.10	0.51
1:A:180:ARG:NH1	1:A:180:ARG:HG3	2.08	0.51
1:A:510:PRO:O	1:A:532:GLY:HA3	2.10	0.51
1:D:283:GLN:HG3	3:D:802:G6P:O1	2.11	0.51
1:A:355:ILE:HD11	1:A:474:MET:CE	2.41	0.51
1:D:273:VAL:HG13	1:D:520:VAL:HG13	1.93	0.51
1:D:213:LEU:HD21	1:D:253:PHE:HE2	1.75	0.51
1:A:520:VAL:HG12	1:A:521:MET:HE3	1.93	0.51
1:C:283:GLN:O	3:C:802:G6P:H1	2.11	0.51
1:D:616:ARG:HH21	1:D:633:SER:HA	1.76	0.51
1:C:510:PRO:O	1:C:532:GLY:HA3	2.11	0.50
1:D:391:LYS:HG2	4:D:803:PEG:H42	1.93	0.50
1:B:82:THR:O	1:B:85:SER:HB2	2.12	0.50
1:D:74:ARG:NH1	1:D:77:GLN:OE1	2.44	0.50
1:D:227:ILE:HG22	1:D:227:ILE:O	2.11	0.50
1:D:197:LEU:HD12	1:D:258:LEU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:THR:HG21	1:B:229:HIS:HD2	1.77	0.49
1:B:410:PRO:HG2	1:B:416:LEU:HD21	1.94	0.49
1:A:319:GLY:HA3	1:A:326:LYS:HE3	1.93	0.49
1:C:30:SER:O	1:C:33:PRO:HD2	2.13	0.49
1:C:217:ASP:HB3	1:C:220:HIS:HB2	1.95	0.49
1:B:606:TYR:HB3	1:B:610:ARG:NH1	2.27	0.49
1:B:540:LEU:C	1:B:541:ILE:HG13	2.33	0.49
1:D:61:LEU:HB2	1:D:93:GLY:HA2	1.95	0.48
1:C:252:ALA:HB2	1:C:266:ILE:HD11	1.95	0.48
1:B:580:ARG:O	1:B:584:ILE:HG13	2.14	0.48
1:B:189:ILE:HD11	1:B:610:ARG:HA	1.95	0.48
1:A:526:ILE:HA	1:A:552:TYR:HB2	1.95	0.48
1:D:320:ARG:NH1	1:D:322:GLU:OE1	2.47	0.48
1:C:484:ASN:ND2	1:C:484:ASN:N	2.58	0.48
1:C:382:VAL:O	1:C:386:THR:HG23	2.13	0.48
1:A:175:ALA:HA	1:A:178:LEU:HD12	1.94	0.48
1:D:596:LEU:HA	1:D:601:ARG:HD3	1.94	0.48
1:B:153:GLU:O	1:B:157:LEU:HG	2.13	0.48
1:C:308:ASP:O	1:C:312:THR:HG23	2.13	0.48
1:C:583:ARG:NH1	3:C:802:G6P:O1P	2.47	0.48
1:B:352:VAL:CG1	1:B:475:ILE:HD12	2.43	0.48
1:D:137:THR:HG21	1:D:229:HIS:HD2	1.79	0.48
1:B:55:GLN:HE21	1:B:55:GLN:HA	1.79	0.48
1:A:269:ASN:HB2	1:A:511:TRP:CD1	2.49	0.48
1:D:213:LEU:HD21	1:D:253:PHE:CE2	2.48	0.48
1:D:538:GLU:HB3	1:D:553:ILE:HD13	1.96	0.48
1:C:503:VAL:HG11	1:C:572:MET:HE3	1.95	0.48
1:A:513:TYR:H	1:A:513:TYR:HD2	1.59	0.48
1:D:322:GLU:HB3	1:D:325:ASN:HB2	1.95	0.48
1:C:618:TYR:HB3	1:C:621:GLN:HG3	1.95	0.47
1:A:335:LEU:HB3	1:A:472:VAL:HG11	1.96	0.47
1:B:192:THR:HG22	1:B:246:THR:HG22	1.95	0.47
1:C:323:TYR:OH	1:C:458:LYS:HG3	2.14	0.47
1:D:183:ARG:HG3	1:D:183:ARG:O	2.14	0.47
1:C:144:GLY:HA3	1:C:174:VAL:HB	1.96	0.47
1:C:102:LYS:HG2	1:C:102:LYS:H	1.54	0.47
1:B:479:GLU:OE1	1:B:479:GLU:HA	2.15	0.47
1:B:330:MET:HG2	1:B:565:VAL:HG22	1.96	0.47
1:B:485:ASN:OD1	1:B:488:LEU:N	2.42	0.47
1:D:283:GLN:NE2	1:D:587:ARG:HH21	2.12	0.47
1:A:576:VAL:O	1:A:576:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:526:ILE:HG12	1:C:552:TYR:HB2	1.97	0.47
1:A:634:ASN:HB2	1:A:637:ALA:CB	2.45	0.46
1:B:61:LEU:HB2	1:B:93:GLY:HA2	1.96	0.46
1:A:312:THR:HG22	1:A:313:LEU:N	2.30	0.46
1:D:399:ARG:HG3	1:D:399:ARG:NH1	2.27	0.46
1:A:30:SER:O	1:A:33:PRO:HD2	2.16	0.46
1:A:410:PRO:HG2	1:A:416:LEU:HD21	1.98	0.46
1:A:29:LYS:HG3	1:A:97:ILE:HD13	1.98	0.46
1:C:458:LYS:O	1:C:458:LYS:HD3	2.15	0.46
1:C:214:GLU:HG3	1:C:257:HIS:CD2	2.49	0.46
1:D:189:ILE:HG23	1:D:243:VAL:HB	1.97	0.46
1:B:542:GLU:OE1	1:B:545:GLN:HG3	2.16	0.46
1:C:443:VAL:HG22	1:C:445:HIS:H	1.81	0.46
1:A:269:ASN:HB2	1:A:511:TRP:NE1	2.30	0.46
1:A:447:MET:HG3	1:A:456:LEU:HD11	1.97	0.46
1:C:318:ALA:HA	1:C:356:VAL:O	2.16	0.46
1:C:175:ALA:HA	1:C:178:LEU:HD12	1.97	0.46
1:D:366:VAL:O	1:D:370:LYS:HB2	2.16	0.46
1:D:163:ILE:HB	1:D:186:VAL:HG12	1.99	0.45
1:A:144:GLY:HA3	1:A:174:VAL:HB	1.98	0.45
1:A:333:GLU:O	1:A:337:ARG:HG3	2.15	0.45
1:B:326:LYS:HD2	1:B:326:LYS:HA	1.69	0.45
1:A:108:LEU:HD22	1:A:142:LEU:HB3	1.99	0.45
1:B:174:VAL:O	1:B:177:PRO:HD2	2.15	0.45
1:A:371:GLY:O	1:A:375:VAL:HG23	2.16	0.45
1:D:141:ILE:HA	1:D:174:VAL:HG11	1.99	0.45
1:D:31:LYS:HZ2	1:D:35:THR:HG21	1.82	0.45
1:A:323:TYR:CE2	1:A:329:ASP:HB3	2.51	0.45
1:D:547:LYS:HG2	1:D:552:TYR:CD2	2.51	0.45
1:C:440:PRO:HA	1:C:441:PRO:HD3	1.77	0.45
1:C:227:ILE:HG22	1:C:227:ILE:O	2.17	0.45
1:B:176:LEU:HD22	1:B:241:ALA:HB2	1.99	0.45
1:D:301:PHE:CD2	1:D:440:PRO:HG2	2.52	0.45
1:C:128:ILE:HG12	1:C:232:CYS:HB3	1.98	0.45
1:B:74:ARG:N	1:B:75:PRO:CD	2.80	0.44
1:B:490:LEU:HD22	1:B:494:GLU:HB3	1.99	0.44
1:B:55:GLN:NE2	1:B:55:GLN:HA	2.32	0.44
1:A:555:ASP:HB3	1:A:559:LYS:HD2	1.99	0.44
1:B:3:ARG:H	1:B:621:GLN:HE22	1.66	0.44
1:D:282:PHE:CD2	1:D:591:GLU:HG3	2.53	0.44
1:A:19:ASN:OD1	1:A:21:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:ASN:CB	1:A:637:ALA:H	2.31	0.44
1:A:214:GLU:HG3	1:A:257:HIS:CD2	2.53	0.44
1:B:17:VAL:CG2	1:B:47:GLY:HA3	2.47	0.44
1:B:184:ILE:HG22	1:B:186:VAL:HG23	2.00	0.44
1:C:199:ARG:HH22	1:C:320:ARG:HH22	1.63	0.44
1:A:278:ALA:HB1	1:A:280:HIS:CE1	2.53	0.44
1:B:214:GLU:HG2	1:B:257:HIS:NE2	2.33	0.44
1:A:213:LEU:CD1	1:A:257:HIS:HB2	2.48	0.44
1:C:593:LEU:O	1:C:594:SER:C	2.56	0.44
1:D:514:THR:HB	1:D:515:PRO:CD	2.48	0.44
1:C:41:ASP:OD1	1:C:41:ASP:N	2.50	0.44
1:B:357:MET:O	1:B:478:PRO:HA	2.18	0.43
1:D:103:VAL:HG12	1:D:105:LEU:HG	1.99	0.43
1:A:213:LEU:C	1:A:215:SER:H	2.21	0.43
1:B:299:GLY:O	1:B:302:HIS:HD2	2.00	0.43
1:C:323:TYR:CE2	1:C:329:ASP:HB3	2.53	0.43
1:C:47:GLY:O	1:C:105:LEU:HA	2.19	0.43
1:B:382:VAL:O	1:B:386:THR:HG23	2.18	0.43
1:B:114:TYR:N	1:B:114:TYR:CD1	2.87	0.43
1:D:221:GLU:OE2	1:D:224:ARG:NH1	2.52	0.43
1:B:38:GLN:OE1	1:B:39:TYR:CE1	2.72	0.43
1:B:144:GLY:HA3	1:B:174:VAL:HB	2.00	0.43
1:A:392:ARG:HD2	1:A:415:GLU:O	2.18	0.43
1:D:48:PRO:HG3	1:D:143:LEU:HD22	2.01	0.43
1:A:31:LYS:HB3	1:A:31:LYS:HE3	1.90	0.43
1:A:264:ASP:CG	1:A:616:ARG:HH12	2.22	0.43
1:B:435:PRO:HD2	1:B:438:GLN:NE2	2.34	0.43
1:D:428:ARG:HD3	1:D:428:ARG:HA	1.71	0.43
1:D:445:HIS:ND1	1:D:478:PRO:HD2	2.34	0.43
1:A:521:MET:HA	1:A:521:MET:CE	2.49	0.43
1:A:14:ALA:O	1:A:17:VAL:HG23	2.19	0.43
1:D:493:ASP:HB2	1:D:521:MET:HE3	2.00	0.42
1:D:14:ALA:HB2	1:D:168:HIS:HB2	2.01	0.42
1:C:474:MET:HB2	1:C:474:MET:HE3	1.91	0.42
1:C:95:TRP:HB3	1:C:101:PRO:HD2	2.00	0.42
1:B:593:LEU:O	1:B:594:SER:C	2.56	0.42
1:D:520:VAL:HA	1:D:594:SER:HB2	2.01	0.42
1:A:322:GLU:O	1:A:326:LYS:HB2	2.18	0.42
1:C:12:GLU:HG3	1:C:166:HIS:HB3	2.01	0.42
1:A:634:ASN:HB2	1:A:637:ALA:HB3	2.01	0.42
1:C:538:GLU:HB2	1:C:553:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ALA:HB2	3:A:802:G6P:H2	2.00	0.42
1:B:522:GLY:HA2	1:B:590:THR:HG22	2.01	0.42
1:C:176:LEU:HB2	1:C:177:PRO:HD3	2.00	0.42
1:C:349:LYS:O	1:C:471:ARG:HG3	2.20	0.42
1:A:16:GLU:HB3	1:A:25:TYR:HB2	2.02	0.42
1:D:598:ASP:OD1	1:D:599:TRP:N	2.52	0.42
1:B:110:SER:O	1:B:111:VAL:HG13	2.20	0.42
1:C:378:LEU:HD22	1:C:432:LEU:HD11	2.01	0.42
1:C:575:PHE:O	1:C:578:LYS:HB2	2.20	0.42
1:D:477:HIS:O	1:D:479:GLU:N	2.46	0.42
1:D:349:LYS:O	1:D:471:ARG:HD3	2.19	0.42
1:C:334:ALA:HB2	1:C:568:LEU:HD23	2.02	0.42
1:A:117:GLU:HG3	1:A:117:GLU:H	1.66	0.42
1:A:95:TRP:HB3	1:A:101:PRO:HD2	2.02	0.42
1:A:323:TYR:CZ	1:A:329:ASP:HB3	2.55	0.41
1:D:301:PHE:O	1:D:302:HIS:C	2.57	0.41
1:A:458:LYS:O	1:A:462:VAL:HG22	2.21	0.41
1:B:39:TYR:CB	1:B:43:TYR:HB2	2.51	0.41
1:A:366:VAL:O	1:A:370:LYS:HB2	2.21	0.41
1:C:513:TYR:O	1:C:517:GLU:HG2	2.21	0.41
1:D:523:VAL:HA	1:D:524:PRO:HD2	1.89	0.41
1:C:181:LYS:C	1:C:183:ARG:H	2.23	0.41
1:B:357:MET:HA	1:B:358:PRO:HD3	1.83	0.41
1:C:330:MET:HE1	1:C:564:SER:HB3	2.03	0.41
1:C:621:GLN:HB3	1:C:621:GLN:HE21	1.70	0.41
1:B:399:ARG:HB3	1:B:399:ARG:HH11	1.85	0.41
1:B:248:SER:HA	1:B:266:ILE:HG23	2.03	0.41
1:D:580:ARG:HE	3:D:802:G6P:H62	1.86	0.41
1:B:319:GLY:O	1:B:357:MET:HG2	2.20	0.41
1:C:323:TYR:CZ	1:C:329:ASP:HB3	2.56	0.41
1:D:12:GLU:HB3	1:D:45:LEU:HD23	2.02	0.41
1:B:268:PRO:HB2	1:B:602:MET:CE	2.49	0.41
1:C:540:LEU:HA	1:C:540:LEU:HD13	1.83	0.41
1:B:80:LEU:HD22	1:B:90:PHE:CE2	2.56	0.41
1:C:11:PHE:HA	1:C:44:HIS:O	2.21	0.41
1:C:458:LYS:HE3	1:C:461:GLN:OE1	2.21	0.40
1:C:503:VAL:HG11	1:C:572:MET:CE	2.51	0.40
1:D:504:PHE:CE1	1:D:514:THR:HG22	2.56	0.40
1:A:542:GLU:O	1:A:545:GLN:HB2	2.21	0.40
1:D:296:PHE:CB	1:D:488:LEU:HD13	2.51	0.40
1:D:555:ASP:HB3	1:D:559:LYS:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:LYS:HA	1:C:66:PRO:HD3	1.90	0.40
1:A:431:ALA:HB2	1:C:484:ASN:OD1	2.21	0.40
1:C:386:THR:HG21	1:D:390:GLY:CA	2.51	0.40
1:C:210:TYR:CZ	1:C:530:VAL:HB	2.57	0.40
1:C:313:LEU:HA	1:C:500:HIS:ND1	2.36	0.40
1:D:187:VAL:HG11	1:D:613:ALA:O	2.22	0.40
1:A:322:GLU:HB3	1:A:325:ASN:HB2	2.04	0.40
1:D:388:SER:HB3	1:D:392:ARG:NH2	2.37	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	636/724 (88%)	588 (92%)	42 (7%)	6 (1%)	21	44
1	B	636/724 (88%)	585 (92%)	42 (7%)	9 (1%)	14	31
1	C	636/724 (88%)	597 (94%)	37 (6%)	2 (0%)	46	72
1	D	632/724 (87%)	592 (94%)	36 (6%)	4 (1%)	30	54
All	All	2540/2896 (88%)	2362 (93%)	157 (6%)	21 (1%)	24	47

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	VAL
1	C	17	VAL
1	D	111	VAL
1	B	115	SER
1	B	304	CYS
1	B	483	ALA
1	A	169	GLU

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Mol	Chain	Res	Type
1	A	183	ARG
1	D	40	LYS
1	B	48	PRO
1	D	304	CYS
1	B	194	ALA
1	D	169	GLU
1	A	112	ARG
1	A	194	ALA
1	B	111	VAL
1	C	489	GLY
1	A	561	PRO
1	B	489	GLY
1	B	626	VAL
1	A	512	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	551/622 (89%)	523 (95%)	28 (5%)	29	55
1	B	551/622 (89%)	523 (95%)	28 (5%)	29	55
1	C	551/622 (89%)	517 (94%)	34 (6%)	23	45
1	D	549/622 (88%)	516 (94%)	33 (6%)	24	47
All	All	2202/2488 (88%)	2079 (94%)	123 (6%)	26	50

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	40	LYS
1	A	61	LEU
1	A	111	VAL
1	A	117	GLU
1	A	180	ARG
1	A	181	LYS

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Mol	Chain	Res	Type
1	A	272	ASN
1	A	295	ASP
1	A	304	CYS
1	A	310	ASP
1	A	321	TYR
1	A	348	LYS
1	A	363	SER
1	A	376	ARG
1	A	398	ILE
1	A	406	THR
1	A	461	GLN
1	A	485	ASN
1	A	513	TYR
1	A	539	ASP
1	A	541	ILE
1	A	556	ARG
1	A	568	LEU
1	A	591	GLU
1	A	595	ASP
1	A	601	ARG
1	A	622	PHE
1	B	16	GLU
1	B	17	VAL
1	B	40	LYS
1	B	42	HIS
1	B	56	ASN
1	B	71	ASP
1	B	83	MET
1	B	111	VAL
1	B	114	TYR
1	B	124	SER
1	B	180	ARG
1	B	187	VAL
1	B	199	ARG
1	B	254	GLU
1	B	288	LEU
1	B	310	ASP
1	B	321	TYR
1	B	324	LYS
1	B	363	SER
1	B	376	ARG
1	B	399	ARG

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Mol	Chain	Res	Type
1	B	458	LYS
1	B	518	CYS
1	B	543	THR
1	B	556	ARG
1	B	564	SER
1	B	568	LEU
1	B	581	ARG
1	C	2	SER
1	C	35	THR
1	C	40	LYS
1	C	45	LEU
1	C	56	ASN
1	C	102	LYS
1	C	103	VAL
1	C	108	LEU
1	C	156	HIS
1	C	220	HIS
1	C	242	ASP
1	C	250	ILE
1	C	320	ARG
1	C	321	TYR
1	C	326	LYS
1	C	348	LYS
1	C	370	LYS
1	C	376	ARG
1	C	398	ILE
1	C	417	LEU
1	C	424	MET
1	C	458	LYS
1	C	467	SER
1	C	471	ARG
1	C	484	ASN
1	C	513	TYR
1	C	520	VAL
1	C	539	ASP
1	C	540	LEU
1	C	556	ARG
1	C	594	SER
1	C	614	LEU
1	C	621	GLN
1	C	634	ASN
1	D	6	GLN

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Mol	Chain	Res	Type
1	D	12	GLU
1	D	15	THR
1	D	19	ASN
1	D	35	THR
1	D	60	ILE
1	D	67	GLU
1	D	74	ARG
1	D	81	GLN
1	D	125	LEU
1	D	132	GLU
1	D	212	CYS
1	D	213	LEU
1	D	240	SER
1	D	289	LYS
1	D	304	CYS
1	D	321	TYR
1	D	330	MET
1	D	348	LYS
1	D	363	SER
1	D	376	ARG
1	D	379	GLU
1	D	467	SER
1	D	482	ASN
1	D	513	TYR
1	D	518	CYS
1	D	535	SER
1	D	537	MET
1	D	545	GLN
1	D	591	GLU
1	D	594	SER
1	D	628	GLU
1	D	634	ASN

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

Mol	Chain	Res	Type
1	B	55	GLN
1	B	116	ASN
1	B	484	ASN
1	B	621	GLN
1	C	161	HIS
1	C	582	GLN

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Mol	Chain	Res	Type
1	C	585	ASN
1	C	621	GLN
1	C	634	ASN
1	D	19	ASN
1	D	50	ASN
1	D	211	ASN
1	D	229	HIS
1	D	280	HIS
1	D	283	GLN
1	D	403	ASN
1	D	482	ASN
1	D	621	GLN

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](#)

12 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	U5P	A	801	-	16,22,22	0.70	0	21,33,33	1.84	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	G6P	A	802	-	16,16,16	0.46	0	23,24,24	1.19	2 (8%)
4	PEG	B	1001	-	6,6,6	0.41	0	5,5,5	0.50	0
2	U5P	B	1002	-	16,22,22	0.73	0	21,33,33	1.76	2 (9%)
3	G6P	B	1003	-	16,16,16	0.63	0	23,24,24	1.55	3 (13%)
4	PEG	B	1004	-	6,6,6	0.53	0	5,5,5	0.15	0
2	U5P	C	801	-	16,22,22	0.86	1 (6%)	21,33,33	1.64	3 (14%)
3	G6P	C	802	-	16,16,16	0.47	0	23,24,24	0.95	1 (4%)
4	PEG	C	803	-	6,6,6	0.50	0	5,5,5	0.21	0
2	U5P	D	801	-	16,22,22	0.71	0	21,33,33	1.81	2 (9%)
3	G6P	D	802	-	16,16,16	0.54	0	23,24,24	1.40	2 (8%)
4	PEG	D	803	-	6,6,6	0.46	0	5,5,5	0.35	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
2	U5P	A	801	-	-	0/6/26/26	0/2/2/2
3	G6P	A	802	-	-	0/6/26/26	0/1/1/1
4	PEG	B	1001	-	-	0/4/4/4	0/0/0/0
2	U5P	B	1002	-	-	0/6/26/26	0/2/2/2
3	G6P	B	1003	-	-	0/6/26/26	0/1/1/1
4	PEG	B	1004	-	-	0/4/4/4	0/0/0/0
2	U5P	C	801	-	-	0/6/26/26	0/2/2/2
3	G6P	C	802	-	-	0/6/26/26	0/1/1/1
4	PEG	C	803	-	-	0/4/4/4	0/0/0/0
2	U5P	D	801	-	-	0/6/26/26	0/2/2/2
3	G6P	D	802	-	-	0/6/26/26	0/1/1/1
4	PEG	D	803	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	U5P	O4'-C1'	2.46	1.44	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	802	G6P	O6-P-O3P	-2.93	99.69	107.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	G6P	C3-C4-C5	-2.71	105.47	110.20
3	B	1003	G6P	O2-C2-C1	-2.30	104.76	109.82
2	C	801	U5P	O3P-P-O2P	2.04	115.16	107.38
3	C	802	G6P	O2P-P-O1P	2.18	115.68	107.38
2	D	801	U5P	O3P-P-O2P	2.27	116.04	107.38
2	C	801	U5P	O4'-C1'-N1	2.28	112.89	108.08
2	B	1002	U5P	O3P-P-O2P	2.28	116.08	107.38
2	A	801	U5P	O2P-P-O1P	2.34	118.10	110.58
3	A	802	G6P	O2P-P-O1P	2.44	116.67	107.38
3	B	1003	G6P	O2P-P-O3P	2.90	119.91	110.58
3	D	802	G6P	C1-O5-C5	3.37	119.70	113.47
3	B	1003	G6P	C1-O5-C5	4.84	122.43	113.47
2	C	801	U5P	C4-N3-C2	5.78	119.87	114.14
2	A	801	U5P	C4-N3-C2	6.20	120.28	114.14
2	B	1002	U5P	C4-N3-C2	6.25	120.33	114.14
2	D	801	U5P	C4-N3-C2	6.46	120.54	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	G6P	2	0
4	B	1004	PEG	1	0
3	C	802	G6P	2	0
3	D	802	G6P	2	0
4	D	803	PEG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	638/724 (88%)	0.25	36 (5%)	28 25	39, 76, 136, 163	0
1	B	638/724 (88%)	0.11	22 (3%)	49 47	24, 65, 126, 170	0
1	C	638/724 (88%)	0.21	34 (5%)	30 27	30, 74, 122, 182	0
1	D	636/724 (87%)	0.34	49 (7%)	16 14	32, 81, 152, 185	0
All	All	2550/2896 (88%)	0.23	141 (5%)	29 26	24, 73, 139, 185	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	638	LEU	9.8
1	D	630	LEU	9.0
1	D	639	ALA	6.9
1	D	622	PHE	6.9
1	D	627	GLY	6.7
1	D	629	GLU	6.1
1	C	128	ILE	5.7
1	D	628	GLU	5.3
1	D	2	SER	5.1
1	A	66	PRO	5.0
1	A	62	ASP	4.8
1	D	620	ASP	4.7
1	D	67	GLU	4.7
1	A	92	TYR	4.7
1	B	630	LEU	4.7
1	C	83	MET	4.6
1	C	91	VAL	4.6
1	C	127	GLY	4.6
1	D	637	ALA	4.5
1	A	104	ILE	4.4
1	C	133	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	625	LEU	4.3
1	A	69	PHE	4.3
1	D	631	ASN	4.2
1	D	624	GLU	4.2
1	D	633	SER	4.1
1	A	78	HIS	4.0
1	A	64	LYS	4.0
1	D	626	VAL	3.9
1	A	61	LEU	3.9
1	B	637	ALA	3.7
1	A	63	TRP	3.7
1	D	623	ARG	3.7
1	C	125	LEU	3.6
1	D	128	ILE	3.6
1	C	135	PHE	3.5
1	A	76	VAL	3.5
1	B	623	ARG	3.5
1	D	126	VAL	3.5
1	A	91	VAL	3.4
1	C	131	PRO	3.4
1	B	631	ASN	3.3
1	A	77	GLN	3.3
1	A	67	GLU	3.3
1	B	636	ASP	3.3
1	C	142	LEU	3.2
1	D	618	TYR	3.2
1	B	624	GLU	3.2
1	C	108	LEU	3.2
1	A	90	PHE	3.2
1	A	157	LEU	3.2
1	D	45	LEU	3.1
1	D	127	GLY	3.1
1	B	632	ASP	3.0
1	B	629	GLU	3.0
1	B	67	GLU	3.0
1	A	88	VAL	3.0
1	C	126	VAL	3.0
1	A	507	TYR	2.9
1	B	628	GLU	2.9
1	A	81	GLN	2.9
1	C	227	ILE	2.9
1	A	59	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	68	ALA	2.8
1	A	108	LEU	2.8
1	D	66	PRO	2.7
1	D	122	LEU	2.7
1	C	88	VAL	2.7
1	A	80	LEU	2.7
1	D	96	LEU	2.7
1	B	71	ASP	2.7
1	C	123	TRP	2.7
1	A	106	PHE	2.7
1	D	68	ALA	2.7
1	D	123	TRP	2.7
1	C	197	LEU	2.6
1	D	223	GLY	2.6
1	D	6	GLN	2.6
1	C	129	PRO	2.6
1	D	615	ARG	2.6
1	C	122	LEU	2.6
1	D	185	ASP	2.6
1	D	129	PRO	2.6
1	D	93	GLY	2.6
1	D	125	LEU	2.5
1	A	65	LYS	2.5
1	B	106	PHE	2.5
1	D	614	LEU	2.5
1	C	229	HIS	2.5
1	B	108	LEU	2.4
1	A	214	GLU	2.4
1	D	132	GLU	2.4
1	C	63	TRP	2.4
1	A	79	ALA	2.4
1	D	85	SER	2.4
1	D	133	ASN	2.4
1	A	49	LEU	2.4
1	C	111	VAL	2.4
1	C	149	TRP	2.4
1	B	2	SER	2.4
1	A	11	PHE	2.3
1	B	61	LEU	2.3
1	B	163	ILE	2.3
1	C	141	ILE	2.3
1	C	67	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	60	ILE	2.3
1	A	93	GLY	2.3
1	B	90	PHE	2.3
1	B	633	SER	2.3
1	A	89	HIS	2.3
1	C	436	GLU	2.3
1	C	87	GLY	2.3
1	D	616	ARG	2.3
1	D	617	GLY	2.3
1	C	626	VAL	2.3
1	C	132	GLU	2.3
1	D	61	LEU	2.2
1	C	113	GLY	2.2
1	C	124	SER	2.2
1	B	5	LEU	2.2
1	C	114	TYR	2.1
1	B	78	HIS	2.1
1	B	596	LEU	2.1
1	C	82	THR	2.1
1	D	64	LYS	2.1
1	D	62	ASP	2.1
1	A	87	GLY	2.1
1	D	406	THR	2.1
1	A	107	ASP	2.1
1	A	156	HIS	2.1
1	D	59	ASP	2.1
1	C	119	LYS	2.1
1	D	612	LEU	2.1
1	C	106	PHE	2.1
1	B	150	PHE	2.0
1	C	545	GLN	2.0
1	A	82	THR	2.0
1	D	17	VAL	2.0
1	D	632	ASP	2.0
1	A	74	ARG	2.0
1	D	219	ASP	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
4	PEG	C	803	7/7	0.94	0.24	3.10	66,67,78,78	0
4	PEG	D	803	7/7	0.89	0.22	1.86	85,88,95,96	0
4	PEG	B	1004	7/7	0.88	0.23	1.53	83,87,92,92	0
3	G6P	B	1003	16/16	0.98	0.18	0.35	37,43,48,49	0
2	U5P	C	801	21/21	0.95	0.20	-0.01	63,68,91,98	0
4	PEG	B	1001	7/7	0.95	0.17	-0.24	68,69,72,81	0
3	G6P	A	802	16/16	0.98	0.16	-0.30	54,59,62,63	0
3	G6P	C	802	16/16	0.98	0.17	-0.39	51,54,56,61	0
2	U5P	A	801	21/21	0.96	0.18	-0.39	65,71,91,93	0
3	G6P	D	802	16/16	0.98	0.15	-0.75	39,46,50,51	0
2	U5P	B	1002	21/21	0.94	0.15	-1.31	66,80,86,87	0
2	U5P	D	801	21/21	0.94	0.13	-1.79	66,80,99,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.