



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:51 AM GMT

PDB ID : 3NB0
Title : Glucose-6-Phosphate activated form of Yeast Glycogen Synthase
Authors : Baskaran, S.; Hurley, T.D.
Deposited on : 2010-06-02
Resolution : 2.41 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

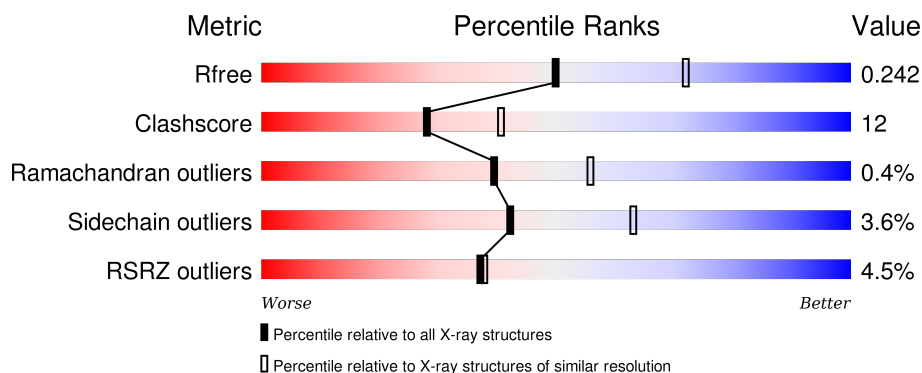
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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>72%</div> <div>15%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	725	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>22%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	725	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>21%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	725	<div> <div>6%</div> <div> <div></div> <div>60%</div> <div>26%</div> <div>•</div> <div>12%</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 criteria:

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21392 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	4	0
			5169	3302	899	949	19			
1	B	645	Total	C	N	O	S	0	3	0
			5213	3332	911	951	19			
1	C	646	Total	C	N	O	S	0	2	0
			5213	3331	910	953	19			
1	D	636	Total	C	N	O	S	0	1	0
			5135	3279	896	941	19			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	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	SEE REMARK 999	UNP P27472

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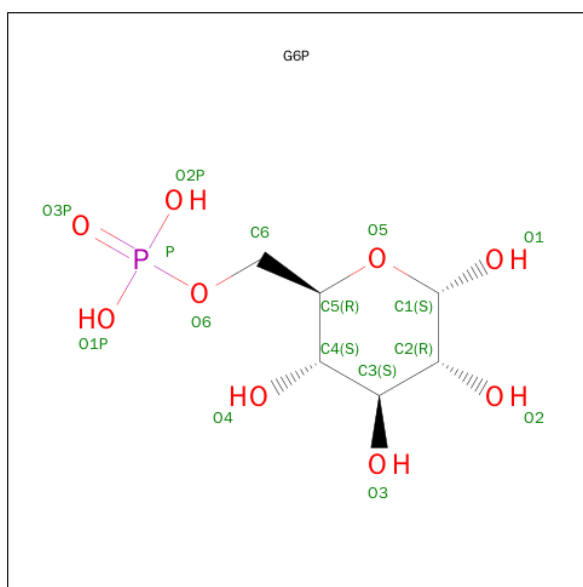
Chain	Residue	Modelled	Actual	Comment	Reference
A	589	ALA	ARG	ENGINEERED MUTATION	UNP P27472
A	592	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	-19	MET	-	EXPRESSION TAG	UNP P27472
B	-18	GLY	-	EXPRESSION TAG	UNP P27472
B	-17	SER	-	EXPRESSION TAG	UNP P27472
B	-16	SER	-	EXPRESSION TAG	UNP P27472
B	-15	HIS	-	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	SEE REMARK 999	UNP P27472
B	589	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	592	ALA	ARG	ENGINEERED MUTATION	UNP P27472
C	-19	MET	-	EXPRESSION TAG	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

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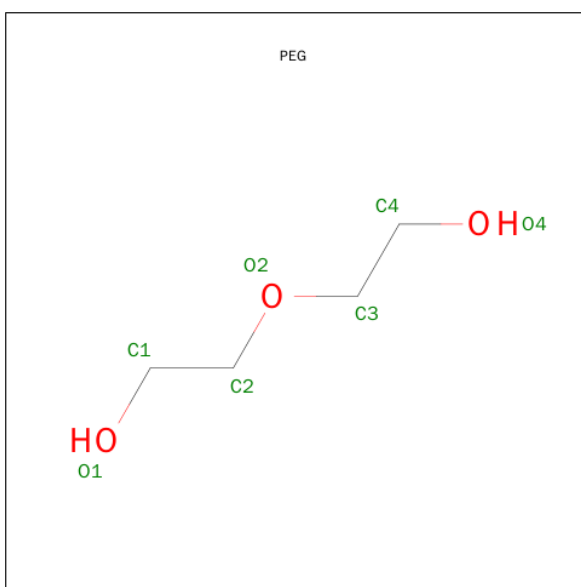
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	EXPRESSION TAG	UNP P27472
C	-1	SER	-	EXPRESSION TAG	UNP P27472
C	0	HIS	-	EXPRESSION TAG	UNP P27472
C	535	SER	ALA	SEE REMARK 999	UNP P27472
C	589	ALA	ARG	ENGINEERED MUTATION	UNP P27472
C	592	ALA	ARG	ENGINEERED MUTATION	UNP P27472
D	-19	MET	-	EXPRESSION TAG	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	SEE REMARK 999	UNP P27472
D	589	ALA	ARG	ENGINEERED MUTATION	UNP P27472
D	592	ALA	ARG	ENGINEERED MUTATION	UNP P27472

- Molecule 2 is SUGAR (ALPHA-D-GLUCOSE-6-PHOSPHATE) (three-letter code: G6P) (formula: C₆H₁₃O₉P).



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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	176	Total	O	0	0
			176	176		
4	B	127	Total	O	0	0
			127	127		
4	C	102	Total	O	0	0
			102	102		
4	D	119	Total	O	0	0
			119	119		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

- [illegible]

- Chain B:
-
- | | | |
|------|------|------|
| L30 | L208 | L335 |
| Q81 | N211 | K348 |
| T82 | K349 | K348 |
| M83 | C212 | T350 |
| | L213 | E214 |
| R86 | E214 | P358 |
| | S215 | F364 |
| G93 | V216 | A368 |
| L96 | E220 | Q372 |
| D107 | E229 | V375 |
| V111 | T246 | R376 |
| R112 | F253 | A377 |
| G113 | E254 | L378 |
| | | K391 |
| W118 | E257 | H396 |
| K119 | L258 | Y400 |
| | | T407 |
| L122 | N269 | E408 |
| W123 | V273 | E415 |
| S124 | | L416 |
| L125 | F279 | L417 |
| V126 | K289 | K418 |
| G127 | | D295 |
| I128 | K292 | F296 |
| P129 | I293 | S420 |
| S130 | N294 | D421 |
| A18 | D295 | K422 |
| M19 | S420 | V423 |
| | D297 | L430 |
| A32 | K298 | A431 |
| P33 | G299 | L432 |
| K40 | | R433 |
| L45 | H302 | R434 |
| L46 | G303 | P440 |
| G47 | C304 | P441 |
| P48 | | M447 |
| | F307 | D450 |
| K51 | D308 | I455 |
| Y54 | D310 | K458 |
| | N311 | L459 |
| D59 | T312 | R460 |
| L60 | R320 | Q461 |
| L61 | Y321 | V462 |
| D62 | E322 | K463 |
| W63 | Y323 | L464 |
| | | |
| B67 | | |
| E72 | K326 | |
| M73 | D329 | |
| R74 | D330 | |
| P75 | F331 | |
| | | |
| | | |

ALA	S653	D539	T387	T246
ASP	M634	L540	S368	
ASP	M635	I541	I389	F253
ASP	D636	E542	R399	H257
ASP	A637	T543	Y400	
ASP	L638	M544	P401	K260
GLY	A639	K547	H402	
PRO	GLY	D548	M403	P268
TYR	GLY	Y549	L416	V273
ALA	LYS		L417	I274
ASP	LEU	Y552		
ASP	LYS	I553	R428	Q277
SER	VAL			A278
	ALA	V565	L432	F279
	ARG	E566	R433	H280
	PRO		R434	
	LEU	V569	P435	Q283
	SER		E436	N284
	VAL	R581		
	PRO		P440	K289
	GLY	Q586	P441	
	SER	R587		
	PRO		K292	
	ARG	T590	D450	K296
	ASP	E591		
	LEU		L454	F301
	ARG	L596	I455	H302
	SER	L597	L456	G303
	ASN	D598		C304
	SER		R460	
	THR	V602	S469	L309
	VAL	G603	D470	D310
	TYR	L604	R471	
	MET	E605		Y321
	THR	V606	F480	K324
	PRO	V607	L481	
	GLY		M482	
	ASP	R610	A483	M330
	LEU	Q611	N484	
	GLY	L612	N485	E333
	THR	A613	P486	
	LEU	L614	L487	R337
	GLN	R615	L488	
	GLU		G489	K343
	VAL	Y618	L490	
	ASN	P619		K349
	ASN	D620	E494	
	ALA	Q621		P358
	ASP	F622		
	ASP	R623	P610	F364
	TYR	E624		T365
	PHE	L625	T514	V366
	SER	V626	P515	
	LEU	G627	I526	K370
	GLY	E628		G371
	VAL	E629		Q372
	ASN	L630	G532	A373
	PRO	M631		
	ALA	D632	E538	

S653

M634

M635

D636

A637

L638

A639

GLY

GLY

LYS

LYS

LEU

LYS

VAL

ALA

ARG

PRO

LEU

SER

VAL

PRO

GLY

SER

PRO

ARG

ASP

LEU

ARG

SER

ASN

SER

THR

VAL

TYR

MET

THR

THR

PRO

GLY

ASP

LEU

GLY

THR

LEU

GLN

GLU

VAL

ASN

ASN

ALA

ASP

ASP

TYR

PHE

SER

LEU

GLY

VAL

ASN

PRO

ALA

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	192.74Å 206.98Å 205.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.23 – 2.41 46.23 – 2.41	Depositor EDS
% Data completeness (in resolution range)	93.6 (46.23-2.41) 99.1 (46.23-2.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.211 , 0.242 0.214 , 0.242	Depositor DCC
R_{free} test set	7893 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.4	EDS
Estimated twinning fraction	0.006 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 157071 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21392	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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

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	0.26	0/5307	0.43	0/7191
1	B	0.26	0/5349	0.42	0/7246
1	C	0.25	0/5345	0.41	0/7239
1	D	0.25	0/5262	0.41	0/7129
All	All	0.25	0/21263	0.42	0/28805

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	5169	0	5079	78	0
1	B	5213	0	5136	123	0
1	C	5213	0	5139	122	0
1	D	5135	0	5046	161	0
2	A	32	0	20	1	0
2	B	32	0	20	2	0
2	C	16	0	10	2	0
2	D	16	0	10	3	0
3	A	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	21	0	30	2	0
3	C	7	0	10	0	0
3	D	7	0	10	0	0
4	A	176	0	0	4	0
4	B	127	0	0	5	0
4	C	102	0	0	7	0
4	D	119	0	0	9	0
All	All	21392	0	20520	482	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 12.

All (482) 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:482:ASN:HD22	1:D:484:ASN:H	1.01	0.97
1:C:180:ARG:HG3	1:C:180:ARG:HH11	1.27	0.96
1:C:283:GLN:HG2	1:D:280:HIS:CE1	2.07	0.90
1:C:399:ARG:HD3	1:C:403:ASN:HD22	1.40	0.86
1:C:280:HIS:CE1	1:D:283:GLN:HG2	2.12	0.85
1:C:59:ASP:HB2	1:C:96:LEU:HD21	1.61	0.83
1:B:312:THR:HG22	1:B:350:THR:HB	1.59	0.83
1:C:542:GLU:HB3	1:C:545:GLN:HG3	1.61	0.82
1:D:540:LEU:HB3	1:D:541:ILE:HD12	1.62	0.81
1:D:482:ASN:ND2	1:D:484:ASN:H	1.76	0.81
1:C:372[A]:GLN:NE2	1:C:376:ARG:HH21	1.79	0.80
1:A:60:ILE:HD12	1:A:60:ILE:H	1.48	0.79
1:B:391:LYS:HD3	3:B:1001:PEG:H41	1.65	0.79
1:D:343:LYS:HD3	1:D:469:SER:O	1.83	0.78
1:D:440:PRO:HG3	4:D:763:HOH:O	1.83	0.78
1:C:519:THR:HG23	4:C:805:HOH:O	1.84	0.77
1:B:634:ASN:ND2	1:B:637:ALA:H	1.81	0.76
1:D:110:SER:O	1:D:111:VAL:HG23	1.86	0.76
1:B:626:VAL:HG11	1:B:630:LEU:HD11	1.68	0.75
1:D:292:LYS:HD2	1:D:490:LEU:HD21	1.68	0.75
1:A:187:VAL:CG1	1:A:613:ALA:HB1	2.17	0.74
1:D:213:LEU:HD21	1:D:253:PHE:CE2	2.25	0.72
1:B:86:ARG:HG2	1:B:149:TRP:HZ2	1.54	0.72
1:D:213:LEU:HD21	1:D:253:PHE:HE2	1.53	0.72
1:B:579:THR:H	1:B:582:GLN:NE2	1.87	0.71
1:D:302:HIS:HD2	1:D:432:LEU:O	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:ILE:HG21	1:B:474:MET:HG2	1.71	0.71
1:B:307:PHE:HD1	1:B:312:THR:HG21	1.55	0.71
1:C:180:ARG:NH1	1:C:180:ARG:HG3	2.05	0.71
1:D:283:GLN:NE2	1:D:587:ARG:HH21	1.88	0.70
1:D:192:THR:HG22	1:D:246:THR:HG22	1.71	0.70
1:D:615:ARG:HD3	1:D:622:PHE:CD1	2.26	0.70
1:D:214:GLU:HA	1:D:257:HIS:HD2	1.57	0.70
1:B:86:ARG:HG2	1:B:149:TRP:CZ2	2.28	0.69
1:C:236:ALA:O	1:C:240:SER:HB2	1.93	0.69
1:B:63:TRP:HZ3	1:B:81:GLN:HG3	1.58	0.68
1:B:493:ASP:O	1:B:497:ARG:HG3	1.93	0.68
1:C:450:ASP:OD1	1:C:460:ARG:NH2	2.26	0.68
1:B:579:THR:H	1:B:582:GLN:HE21	1.39	0.68
1:D:32:ALA:HB3	1:D:33:PRO:HD3	1.77	0.67
1:B:364:PHE:CD1	1:B:487:ILE:HD12	2.29	0.67
1:A:296:PHE:HA	1:A:372[B]:GLN:HE22	1.59	0.67
1:A:542:GLU:OE1	1:A:545:GLN:HB2	1.95	0.67
1:D:31:LYS:NZ	1:D:35:THR:HG21	2.10	0.66
1:B:304:CYS:SG	1:B:434:ARG:HD3	2.35	0.66
1:A:187:VAL:HG11	1:A:613:ALA:HB1	1.76	0.66
2:B:902:G6P:H1	4:B:823:HOH:O	1.96	0.66
1:B:126:VAL:HG22	1:B:181:LYS:HZ2	1.59	0.66
1:D:101:PRO:HD2	4:D:784:HOH:O	1.96	0.65
1:D:100:ALA:HA	4:D:784:HOH:O	1.96	0.65
1:A:213:LEU:HA	1:A:216:VAL:HG13	1.78	0.65
1:D:209:PHE:O	1:D:213:LEU:HB3	1.96	0.65
1:B:458:LYS:HD3	1:B:458:LYS:O	1.96	0.65
1:A:339:ASN:O	1:A:343:LYS:HG3	1.97	0.65
1:B:307:PHE:CD1	1:B:312:THR:HG21	2.32	0.65
1:B:458:LYS:HE2	1:B:461:GLN:OE1	1.96	0.65
1:A:8:HIS:HA	1:A:161:HIS:HB3	1.76	0.65
1:D:514:THR:HB	1:D:515:PRO:HD3	1.79	0.64
1:C:634:ASN:HB2	1:C:637:ALA:H	1.62	0.64
1:B:634:ASN:C	1:B:634:ASN:HD22	2.02	0.63
1:D:183:ARG:HG3	1:D:183:ARG:O	1.97	0.63
1:B:119:LYS:HE3	1:B:130:SER:O	1.98	0.63
1:A:254:GLU:HB3	4:A:878:HOH:O	1.98	0.63
1:B:126:VAL:HG22	1:B:181:LYS:NZ	2.13	0.63
1:D:612:LEU:HD22	1:D:635:MET:HG2	1.81	0.63
1:B:133:ASN:H	1:B:133:ASN:ND2	1.96	0.63
1:D:399:ARG:HD3	1:D:403:ASN:HD22	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ASP:O	1:B:312:THR:HG23	1.98	0.62
1:D:128:ILE:HG12	1:D:232:CYS:HB3	1.80	0.62
1:B:513:TYR:O	1:B:517:GLU:HG2	2.00	0.61
1:B:273:VAL:HG13	1:B:520:VAL:HG13	1.83	0.61
1:D:180:ARG:HE	1:D:180:ARG:HA	1.65	0.61
1:B:246:THR:HB	4:B:793:HOH:O	1.99	0.61
1:B:213:LEU:O	1:B:216:VAL:HG13	2.00	0.60
1:D:606:TYR:O	1:D:610:ARG:HG3	2.01	0.60
1:C:199:ARG:HG3	1:C:508:TYR:CE2	2.35	0.60
1:A:128:ILE:HG12	1:A:232:CYS:HB3	1.83	0.60
1:C:284:ASN:HD21	1:D:284:ASN:HD21	1.47	0.60
1:D:227:ILE:HG22	1:D:227:ILE:O	2.00	0.60
1:C:458:LYS:HE2	1:C:461:GLN:OE1	2.00	0.60
1:D:482:ASN:HD22	1:D:484:ASN:N	1.86	0.60
1:D:289:LYS:HE3	1:D:494:GLU:HG2	1.83	0.60
1:D:296:PHE:HE1	1:D:487:ILE:HD12	1.67	0.60
1:B:295:ASP:CG	1:B:376:ARG:HH22	2.06	0.60
1:C:458:LYS:O	1:C:458:LYS:HD3	2.02	0.59
1:A:32:ALA:HB3	1:A:33:PRO:HD3	1.84	0.59
1:C:209:PHE:O	1:C:213:LEU:HB3	2.02	0.59
1:D:66:PRO:HA	1:D:74:ARG:HH12	1.67	0.59
1:B:174:VAL:O	1:B:177:PRO:HD2	2.03	0.59
1:B:450:ASP:OD1	1:B:460:ARG:NH2	2.36	0.59
1:C:493:ASP:O	1:C:497:ARG:HG3	2.02	0.59
1:B:295:ASP:OD1	1:B:376:ARG:NH2	2.35	0.59
1:C:299:GLY:HA2	1:C:375:VAL:HG21	1.85	0.59
1:C:372[A]:GLN:HE21	1:C:376:ARG:HH21	1.46	0.59
1:D:129:PRO:HG2	1:D:229:HIS:HB3	1.84	0.59
1:A:78:HIS:HB3	1:A:157:LEU:HD23	1.85	0.59
1:B:323:TYR:CZ	1:B:329:ASP:HB3	2.38	0.59
1:D:137:THR:HG21	1:D:229:HIS:HD2	1.67	0.59
1:A:83:MET:HG2	1:A:88:VAL:HG11	1.85	0.58
1:A:187:VAL:HG12	1:A:613:ALA:HB1	1.85	0.58
1:C:197:LEU:HD23	1:C:227:ILE:HD11	1.85	0.58
1:D:97:ILE:HG12	4:D:784:HOH:O	2.03	0.58
1:D:109:ASP:HA	1:D:112:ARG:NH1	2.18	0.58
1:B:396:HIS:HD2	1:B:415:GLU:OE2	1.87	0.58
1:B:430:LEU:HD12	1:B:433:ARG:HD3	1.84	0.58
1:D:586:GLN:O	1:D:590:THR:HG22	2.04	0.57
1:B:111:VAL:CG1	1:B:118:TRP:CH2	2.87	0.57
1:D:144:GLY:HA3	1:D:174:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:VAL:HG12	1:C:111:VAL:O	2.04	0.57
1:C:485:ASN:CG	4:C:706:HOH:O	2.43	0.57
1:A:146:THR:O	1:A:149:TRP:HB3	2.05	0.57
1:C:213:LEU:HA	1:C:216:VAL:HG13	1.85	0.57
1:D:79:ALA:O	1:D:83:MET:HG2	2.05	0.57
1:A:624:GLU:C	1:A:626:VAL:H	2.08	0.57
1:D:31:LYS:HZ2	1:D:35:THR:HG21	1.69	0.57
1:C:31:LYS:O	1:C:35:THR:HG23	2.05	0.57
1:A:32:ALA:HB1	1:A:101:PRO:HG3	1.87	0.57
1:C:399:ARG:CD	1:C:403:ASN:HD22	2.17	0.56
1:B:331:PHE:CZ	1:B:335:LEU:HD11	2.41	0.56
1:B:299:GLY:HA2	1:B:375:VAL:HG21	1.86	0.56
1:B:323:TYR:CE1	1:B:329:ASP:HB3	2.41	0.56
1:B:59:ASP:HB2	1:B:96:LEU:HD21	1.86	0.56
1:D:213:LEU:O	1:D:216:VAL:HG22	2.06	0.56
1:C:109:ASP:HA	1:C:112:ARG:NH1	2.21	0.56
1:B:634:ASN:HD21	1:B:637:ALA:H	1.49	0.55
1:D:540:LEU:HD21	1:D:596:LEU:HD13	1.88	0.55
1:B:455:ILE:O	1:B:459:ILE:HG12	2.06	0.55
1:D:301:PHE:HA	4:D:763:HOH:O	2.06	0.55
1:C:586:GLN:O	1:C:590:THR:HG23	2.06	0.55
1:D:221:GLU:HA	1:D:224:ARG:HB3	1.87	0.55
1:D:31:LYS:O	1:D:34:ILE:HG22	2.07	0.55
1:B:144:GLY:HA3	1:B:174:VAL:HB	1.89	0.55
1:A:485:ASN:HB3	4:A:722:HOH:O	2.07	0.55
1:A:295[A]:ASP:CG	1:A:376:ARG:HH22	2.09	0.55
1:A:626:VAL:HG12	1:A:627:GLY:N	2.22	0.55
1:A:458:LYS:HD3	1:A:458:LYS:O	2.07	0.55
1:D:283:GLN:HE21	1:D:587:ARG:HH21	1.52	0.54
1:B:514:THR:HB	1:B:515:PRO:HD3	1.89	0.54
1:D:208:ASP:OD1	1:D:209:PHE:N	2.40	0.54
1:A:144:GLY:HA3	1:A:174:VAL:HB	1.89	0.54
1:C:192:THR:HG22	1:C:246:THR:HG22	1.89	0.54
1:C:323:TYR:CZ	1:C:329:ASP:HB3	2.42	0.54
1:A:3:ARG:NH2	1:A:158:ASP:O	2.41	0.54
1:D:623:ARG:HA	1:D:628:GLU:O	2.08	0.54
1:D:547:LYS:HG2	1:D:552:TYR:CD1	2.43	0.54
1:D:31:LYS:O	1:D:35:THR:HG23	2.07	0.53
1:C:137:THR:O	1:C:141:ILE:HG13	2.08	0.53
1:C:578:LYS:NZ	1:C:586:GLN:NE2	2.56	0.53
1:B:199:ARG:HB3	1:B:508:TYR:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:ASN:O	1:C:54:TYR:HB3	2.08	0.53
1:D:59:ASP:HB2	1:D:96:LEU:HD21	1.91	0.53
1:C:487:ILE:HG12	4:C:706:HOH:O	2.08	0.53
1:C:510:PRO:O	1:C:532:GLY:HA3	2.08	0.53
1:D:510:PRO:O	1:D:532:GLY:HA3	2.09	0.53
1:D:615:ARG:HG3	1:D:632:ASP:OD2	2.08	0.53
1:D:222:ALA:HB1	1:D:228:TYR:HA	1.91	0.53
1:C:382:VAL:O	1:C:386:THR:HG23	2.09	0.53
1:C:485:ASN:ND2	4:C:706:HOH:O	2.41	0.53
1:C:372[A]:GLN:NE2	1:C:376:ARG:NH2	2.55	0.53
1:B:536:TYR:O	1:B:540:LEU:HD23	2.09	0.53
1:C:146:THR:O	1:C:149:TRP:HB3	2.09	0.52
1:A:199:ARG:HH22	2:A:902:G6P:P	2.33	0.52
1:B:176:LEU:HB2	1:B:177:PRO:HD3	1.91	0.52
1:C:180:ARG:CG	1:C:180:ARG:HH11	2.08	0.52
1:C:399:ARG:HD3	1:C:403:ASN:ND2	2.18	0.52
1:A:45:LEU:HB2	1:A:103:VAL:HG12	1.91	0.52
1:C:48:PRO:HG3	1:C:143:LEU:HD22	1.92	0.52
1:B:378:LEU:HD22	1:B:432:LEU:HD11	1.91	0.52
2:B:902:G6P:O4	2:B:902:G6P:O3P	2.12	0.52
1:C:507:TYR:HB2	1:C:556:ARG:NH2	2.23	0.52
1:B:396:HIS:HE1	1:B:407:THR:O	1.93	0.52
1:D:217:ASP:O	1:D:221:GLU:HG2	2.09	0.52
1:D:164:VAL:HA	1:D:187:VAL:HG23	1.92	0.52
1:D:137:THR:O	1:D:141:ILE:HG13	2.10	0.51
1:B:565:VAL:O	1:B:569:VAL:HG23	2.09	0.51
1:D:621:GLN:O	1:D:625:LEU:HB2	2.10	0.51
1:C:176:LEU:HB2	1:C:177:PRO:HD3	1.92	0.51
1:C:288:LEU:HD23	1:C:289:LYS:HD3	1.92	0.51
1:B:122:LEU:HD11	1:B:128:ILE:HD12	1.91	0.51
1:C:610:ARG:HD2	4:C:729:HOH:O	2.10	0.51
1:C:596:LEU:CD1	1:C:646:VAL:HG21	2.40	0.51
1:B:463:GLN:HA	1:B:465:PHE:CE2	2.46	0.51
1:A:291[A]:GLU:OE1	1:A:291[A]:GLU:HA	2.11	0.51
1:C:449:ASP:OD2	1:C:452:ASN:HB2	2.11	0.51
1:D:482:ASN:ND2	1:D:484:ASN:HB2	2.26	0.50
1:D:549:TYR:O	1:D:590:THR:HB	2.11	0.50
1:A:83:MET:HE1	1:A:153:GLU:HG3	1.91	0.50
1:B:493:ASP:HB2	1:B:521:MET:CE	2.41	0.50
1:C:357:MET:O	1:C:478:PRO:HA	2.10	0.50
1:D:180:ARG:NE	1:D:180:ARG:HA	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:PRO:O	1:D:181:LYS:HG2	2.11	0.50
1:D:485:ASN:HB3	4:D:710:HOH:O	2.11	0.50
1:C:366:VAL:O	1:C:370:LYS:HB2	2.12	0.50
1:C:333:GLU:OE2	1:C:337:ARG:HD2	2.11	0.50
1:A:392:ARG:CZ	1:A:418:LYS:HG2	2.42	0.50
1:D:214:GLU:HA	1:D:257:HIS:CD2	2.44	0.50
1:A:266:ILE:HG22	1:A:268:PRO:HD3	1.94	0.50
1:A:70:SER:O	1:A:74:ARG:HG2	2.12	0.50
1:C:283:GLN:HG3	2:C:901:G6P:O1	2.12	0.50
1:D:487:ILE:HG13	1:D:488:LEU:N	2.26	0.50
1:D:109:ASP:HA	1:D:112:ARG:HH12	1.74	0.50
1:D:450:ASP:OD1	1:D:456:LEU:HD13	2.12	0.50
1:D:434:ARG:NH1	4:D:763:HOH:O	2.44	0.49
1:C:79:ALA:O	1:C:83:MET:HG2	2.12	0.49
1:C:19:ASN:N	1:C:19:ASN:HD22	2.10	0.49
1:B:542:GLU:CD	1:B:544:ASN:H	2.15	0.49
1:A:153:GLU:O	1:A:157:LEU:HD13	2.11	0.49
1:B:417:LEU:HD23	1:B:421:ASP:HB2	1.94	0.49
1:B:158:ASP:OD2	1:B:161:HIS:HD2	1.96	0.49
1:D:72:GLU:O	1:D:161:HIS:HE1	1.96	0.49
1:C:578:LYS:HZ1	1:C:586:GLN:NE2	2.11	0.49
1:A:298:ARG:NH2	4:A:760:HOH:O	2.46	0.49
1:C:526:ILE:HG12	1:C:552:TYR:HB2	1.95	0.49
1:D:587:ARG:HA	1:D:590:THR:HG23	1.94	0.49
1:A:25:TYR:CE1	1:A:95:TRP:HZ2	2.31	0.49
1:C:302:HIS:O	1:C:434:ARG:HD2	2.12	0.49
1:A:264:ASP:O	1:A:635:MET:HG3	2.13	0.48
1:B:349:LYS:O	1:B:471:ARG:CG	2.61	0.48
1:B:293:ILE:O	1:B:297:VAL:HG23	2.13	0.48
1:C:323:TYR:CE1	1:C:329:ASP:HB3	2.48	0.48
1:C:514:THR:HB	1:C:515:PRO:HD3	1.96	0.48
1:A:35:THR:HG21	1:A:43:TYR:CE1	2.48	0.48
1:C:493:ASP:HB2	1:C:521:MET:CE	2.44	0.48
1:A:458:LYS:HD3	1:A:458:LYS:C	2.33	0.48
1:D:296:PHE:CE1	1:D:487:ILE:HD12	2.49	0.48
1:A:78:HIS:CB	1:A:157:LEU:HD23	2.43	0.48
1:A:164:VAL:HG11	1:A:610:ARG:HG2	1.95	0.48
1:B:419:SER:O	1:B:423:VAL:HG23	2.14	0.48
1:B:447:MET:HB2	1:B:450:ASP:HB2	1.95	0.48
1:A:305:PHE:HZ	1:A:309:LEU:HG	1.79	0.48
1:C:80:LEU:HD22	1:C:90:PHE:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:LEU:HD13	1:B:474:MET:HE3	1.96	0.48
1:C:17:VAL:HG21	1:C:46:ILE:O	2.14	0.47
1:D:17:VAL:HG21	1:D:46:ILE:O	2.14	0.47
1:B:273:VAL:HG13	1:B:520:VAL:CG1	2.44	0.47
1:D:526:ILE:HG12	1:D:552:TYR:HB2	1.96	0.47
1:B:163:ILE:HB	1:B:186:VAL:HG12	1.96	0.47
1:B:54:TYR:CE1	1:B:60:ILE:HD11	2.50	0.47
1:B:302:HIS:O	1:B:434:ARG:HD2	2.13	0.47
1:C:399:ARG:HH11	1:C:403:ASN:ND2	2.12	0.47
1:D:74:ARG:N	1:D:75:PRO:HD2	2.29	0.47
1:B:517:GLU:O	1:B:521:MET:HG2	2.13	0.47
1:B:72:GLU:OE2	1:B:161:HIS:HE1	1.98	0.47
1:B:54:TYR:HE1	1:B:60:ILE:HD11	1.78	0.47
1:D:163:ILE:HB	1:D:186:VAL:HG12	1.97	0.47
1:A:628:GLU:HG2	1:A:629:GLU:N	2.30	0.47
1:C:126:VAL:HG21	1:C:177:PRO:HB3	1.97	0.47
1:B:133:ASN:N	1:B:133:ASN:ND2	2.62	0.46
1:A:634:ASN:HB2	1:A:637:ALA:H	1.80	0.46
1:B:507:TYR:HB2	1:B:556:ARG:NH2	2.30	0.46
1:A:322:GLU:HB2	1:A:326:LYS:HG2	1.97	0.46
1:B:493:ASP:HB2	1:B:521:MET:HE1	1.97	0.46
1:B:17:VAL:HG12	1:B:18:ALA:N	2.29	0.46
1:D:19:ASN:HD22	1:D:19:ASN:N	2.11	0.46
1:D:12:GLU:OE2	1:D:168:HIS:HE1	1.98	0.46
1:B:129:PRO:HB2	1:B:229:HIS:HB3	1.98	0.46
1:B:408:GLU:HG2	4:B:799:HOH:O	2.15	0.46
1:D:615:ARG:NH1	1:D:619:PRO:HB3	2.30	0.46
1:D:436:GLU:OE1	1:D:436:GLU:HA	2.15	0.46
1:D:631:ASN:HB3	1:D:637:ALA:HB1	1.97	0.46
1:B:125:LEU:O	1:B:181:LYS:NZ	2.49	0.46
1:C:213:LEU:HD11	1:C:257:HIS:HB2	1.98	0.46
1:D:168:HIS:HD2	1:D:193:HIS:NE2	2.14	0.46
1:B:458:LYS:HD3	1:B:458:LYS:C	2.34	0.46
1:A:8:HIS:HB2	1:A:162:ALA:O	2.15	0.46
1:B:111:VAL:CG1	1:B:118:TRP:HH2	2.28	0.46
1:A:119:LYS:HE3	1:A:130:SER:OG	2.16	0.46
1:C:32:ALA:HB3	1:C:33:PRO:HD3	1.98	0.46
1:C:5:LEU:HD22	1:C:614:LEU:HD22	1.97	0.46
1:C:283:GLN:HG3	2:C:901:G6P:C1	2.46	0.46
1:D:74:ARG:N	1:D:75:PRO:CD	2.79	0.46
1:B:349:LYS:HG2	1:B:576:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:O	1:C:200:TYR:HD2	1.99	0.46
1:A:99:GLY:O	1:A:100:ALA:C	2.54	0.46
1:D:304:CYS:SG	1:D:434:ARG:HD3	2.56	0.46
1:D:615:ARG:HD3	1:D:622:PHE:HD1	1.77	0.46
1:A:199:ARG:HD2	4:A:871:HOH:O	2.16	0.46
1:B:269:ASN:HB2	1:B:511:TRP:CD1	2.50	0.46
1:C:207:PHE:CE2	1:C:209:PHE:HA	2.51	0.45
1:C:25:TYR:CE1	1:C:95:TRP:HZ2	2.34	0.45
1:D:279:PHE:CE1	1:D:591:GLU:OE1	2.69	0.45
1:B:111:VAL:HG12	1:B:111:VAL:O	2.16	0.45
1:C:337:ARG:HH21	1:C:566:GLU:HG2	1.81	0.45
1:D:450:ASP:OD1	1:D:460:ARG:NH2	2.49	0.45
1:D:54:TYR:HE1	1:D:60:ILE:HD11	1.82	0.45
1:A:285:LEU:O	1:A:289:LYS:HG2	2.17	0.45
1:B:391:LYS:HZ2	3:B:1001:PEG:H22	1.80	0.45
1:D:490:LEU:HD22	1:D:494:GLU:HB3	1.97	0.45
1:A:74:ARG:N	1:A:75:PRO:CD	2.79	0.45
1:D:218:VAL:HG23	1:D:219:ASP:N	2.32	0.45
1:B:634:ASN:ND2	1:B:634:ASN:C	2.70	0.45
1:B:400:TYR:CD1	1:B:408:GLU:HA	2.51	0.45
1:B:206:SER:O	1:B:207:PHE:HB3	2.16	0.45
1:B:459:ILE:H	1:B:459:ILE:HG12	1.49	0.45
1:D:137:THR:HG21	1:D:229:HIS:CD2	2.49	0.45
1:C:458:LYS:C	1:C:458:LYS:HD3	2.36	0.45
1:C:71:ASP:O	1:C:74:ARG:HG2	2.17	0.45
1:A:174:VAL:O	1:A:177:PRO:HG2	2.17	0.45
1:D:177:PRO:HA	1:D:240:SER:OG	2.16	0.45
1:D:485:ASN:HA	1:D:486:PRO:HD3	1.76	0.45
1:B:51:LYS:HE3	1:B:107:ASP:OD1	2.16	0.45
1:C:565:VAL:O	1:C:569:VAL:HG23	2.16	0.45
1:D:366:VAL:O	1:D:370:LYS:HB2	2.17	0.45
1:C:108:LEU:HB3	1:C:142:LEU:HD13	1.99	0.45
1:B:254:GLU:HG3	1:B:258:LEU:HD12	1.98	0.45
1:D:634:ASN:HB3	1:D:636:ASP:H	1.80	0.45
1:D:542:GLU:CD	1:D:544:ASN:H	2.20	0.45
1:A:268:PRO:HB2	1:A:602:MET:CE	2.47	0.44
1:D:273:VAL:HB	1:D:598:ASP:OD1	2.17	0.44
1:A:382:VAL:O	1:A:386:THR:HG23	2.17	0.44
1:C:372[A]:GLN:HE22	1:C:376:ARG:HE	1.66	0.44
1:D:31:LYS:HZ3	1:D:35:THR:HG21	1.82	0.44
1:A:213:LEU:HD12	1:A:213:LEU:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:GLY:O	1:B:515:PRO:HD2	2.17	0.44
1:A:94:ARG:HD2	1:A:100:ALA:HB1	1.99	0.44
1:D:428:ARG:HA	1:D:428:ARG:HD2	1.58	0.44
1:C:542:GLU:OE1	1:C:545:GLN:CG	2.65	0.44
1:A:612:LEU:CD2	1:A:635:MET:HG2	2.48	0.44
1:D:581:ARG:HG3	4:D:724:HOH:O	2.15	0.44
1:A:534:GLY:O	1:A:538:GLU:HB2	2.17	0.44
1:C:249:GLN:NE2	1:C:249:GLN:HA	2.32	0.44
1:C:305:PHE:HZ	1:C:309:LEU:HG	1.81	0.44
1:A:510:PRO:O	1:A:532:GLY:HA3	2.18	0.44
1:B:547:LYS:HG2	1:B:552:TYR:CE1	2.53	0.44
1:A:113:GLY:C	1:A:115:SER:H	2.20	0.44
1:B:111:VAL:HG11	1:B:118:TRP:HH2	1.82	0.44
1:C:129:PRO:O	1:C:229:HIS:HB2	2.18	0.44
1:C:271:LEU:HD13	1:C:520:VAL:HG21	1.99	0.44
1:B:74:ARG:N	1:B:75:PRO:CD	2.80	0.44
1:B:368:ALA:HB1	1:B:487:ILE:HD13	1.98	0.44
1:C:100:ALA:N	1:C:101:PRO:HD3	2.33	0.44
1:B:32:ALA:HB3	1:B:33:PRO:HD3	1.99	0.44
1:B:16:GLU:OE2	1:B:16:GLU:N	2.51	0.44
1:C:126:VAL:HG12	1:C:126:VAL:O	2.18	0.44
1:B:323:TYR:OH	1:B:458:LYS:CG	2.66	0.44
1:D:128:ILE:HA	1:D:129:PRO:HD2	1.91	0.44
1:D:19:ASN:ND2	1:D:19:ASN:N	2.66	0.44
1:C:222:ALA:HB1	1:C:228:TYR:HA	1.99	0.44
1:D:274:ILE:O	1:D:274:ILE:HG23	2.17	0.44
1:D:192:THR:CG2	1:D:246:THR:HG22	2.45	0.44
1:D:63:TRP:CZ3	1:D:80:LEU:HB3	2.53	0.44
1:D:90:PHE:HB3	1:D:106:PHE:HD1	1.82	0.44
1:C:92:TYR:OH	1:C:102:LYS:HD3	2.17	0.44
1:B:208:ASP:CG	1:B:211:ASN:HB2	2.38	0.44
1:B:119:LYS:HE3	1:B:130:SER:HB2	1.99	0.44
1:D:75:PRO:HG2	1:D:158:ASP:OD2	2.18	0.44
1:A:213:LEU:HA	1:A:216:VAL:CG1	2.47	0.43
1:A:83:MET:CE	1:A:153:GLU:HG3	2.48	0.43
1:B:349:LYS:O	1:B:471:ARG:HG3	2.18	0.43
1:B:79:ALA:O	1:B:83:MET:HB2	2.18	0.43
1:A:95:TRP:HB3	1:A:101:PRO:HD2	1.99	0.43
1:B:12:GLU:HB3	1:B:45:LEU:HD23	2.00	0.43
1:D:565:VAL:O	1:D:569:VAL:HG23	2.18	0.43
1:C:618:TYR:N	1:C:619:PRO:HD3	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:TYR:HB3	1:B:593:LEU:HD11	1.99	0.43
1:D:349:LYS:O	1:D:471:ARG:CD	2.66	0.43
1:C:378:LEU:O	1:C:382:VAL:HG23	2.18	0.43
1:D:19:ASN:ND2	1:D:19:ASN:H	2.16	0.43
1:A:180:ARG:HD2	1:A:240:SER:O	2.18	0.43
1:D:94:ARG:HB2	1:D:94:ARG:HE	1.64	0.43
1:D:471:ARG:HA	1:D:471:ARG:NE	2.33	0.43
1:D:620:ASP:O	1:D:624:GLU:HG2	2.18	0.43
1:C:9:LEU:HD13	1:C:161:HIS:CG	2.53	0.43
1:C:509:GLU:OE2	1:C:531:SER:HB2	2.19	0.43
1:C:40:LYS:HB3	1:C:41:ASP:H	1.50	0.43
1:B:440:PRO:HA	1:B:441:PRO:HD3	1.85	0.43
1:A:65:LYS:HA	1:A:66:PRO:HD3	1.83	0.43
1:A:526:ILE:HG12	1:A:552:TYR:HB2	2.01	0.43
1:C:428:ARG:HD3	1:C:428:ARG:HA	1.75	0.43
1:C:580:ARG:HB3	1:D:277:GLN:NE2	2.34	0.43
1:D:302:HIS:CD2	1:D:432:LEU:O	2.63	0.43
1:C:199:ARG:HG3	1:C:508:TYR:HE2	1.80	0.43
1:D:54:TYR:CE1	1:D:60:ILE:HD11	2.54	0.43
1:D:337:ARG:HH21	1:D:566:GLU:HG2	1.83	0.43
1:D:12:GLU:HB3	1:D:45:LEU:HD23	2.01	0.42
1:D:604:LEU:O	1:D:607:VAL:HB	2.19	0.42
1:D:78:HIS:HB2	1:D:157:LEU:HD13	2.00	0.42
1:A:86:ARG:HH11	1:A:86:ARG:HA	1.84	0.42
1:C:601:ARG:HH21	1:C:644:LEU:HD23	1.83	0.42
1:C:59:ASP:HB2	1:C:96:LEU:CD2	2.40	0.42
1:B:517:GLU:H	1:B:517:GLU:HG2	1.72	0.42
1:B:542:GLU:OE1	1:B:544:ASN:HB2	2.19	0.42
1:D:19:ASN:HB3	1:D:50:ASN:HD22	1.83	0.42
1:D:400:TYR:CD1	1:D:401:PRO:HA	2.54	0.42
1:A:214:GLU:HG2	1:A:257:HIS:NE2	2.34	0.42
1:B:534:GLY:O	1:B:538:GLU:HB2	2.19	0.42
1:D:111:VAL:HG13	1:D:118:TRP:CH2	2.54	0.42
1:C:634:ASN:HB2	1:C:637:ALA:CB	2.49	0.42
1:C:14:ALA:O	1:C:17:VAL:HG23	2.19	0.42
1:D:47:GLY:O	1:D:105:LEU:HA	2.19	0.42
1:D:358:PRO:HG2	1:D:480:PHE:CZ	2.54	0.42
1:C:326:LYS:HE3	4:C:804:HOH:O	2.20	0.42
1:D:176:LEU:HD22	1:D:241:ALA:HB2	2.01	0.42
1:D:302:HIS:O	1:D:434:ARG:HD2	2.20	0.42
1:B:17:VAL:HG21	1:B:46:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:THR:HG22	1:A:246:THR:HG22	2.01	0.42
1:D:321:TYR:CZ	1:D:455:ILE:HG12	2.55	0.42
1:C:292:LYS:HD3	1:C:490:LEU:HD21	2.00	0.42
1:A:62:ASP:OD2	1:A:65:LYS:HG3	2.18	0.42
1:D:309:LEU:HA	1:D:309:LEU:HD23	1.90	0.42
1:A:34:ILE:HD13	1:A:599:TRP:HB3	2.02	0.42
1:D:292:LYS:HD2	1:D:490:LEU:CD2	2.43	0.42
1:D:5:LEU:HD13	1:D:622:PHE:HD2	1.84	0.42
1:C:493:ASP:HB2	1:C:521:MET:HE1	2.02	0.42
1:A:326:LYS:HA	1:A:326:LYS:HD3	1.82	0.42
1:C:626:VAL:HG11	1:C:630:LEU:HD11	2.01	0.42
1:D:283:GLN:HG3	2:D:901:G6P:C1	2.49	0.42
1:C:482:ASN:OD1	1:C:484:ASN:HB2	2.18	0.42
1:C:545:GLN:HE21	1:C:647:ALA:HA	1.85	0.42
1:B:474:MET:HB2	1:B:474:MET:HE3	1.78	0.42
1:D:13:THR:HB	1:D:167:PHE:CD1	2.55	0.42
1:A:419:SER:O	1:A:423:VAL:HG23	2.19	0.42
1:B:125:LEU:HD11	4:B:738:HOH:O	2.19	0.42
1:D:364:PHE:CE2	1:D:486:PRO:HD2	2.55	0.42
1:C:542:GLU:OE1	1:C:542:GLU:C	2.58	0.42
1:B:323:TYR:OH	1:B:458:LYS:HG2	2.20	0.42
1:D:90:PHE:HB3	1:D:106:PHE:CD1	2.54	0.42
1:C:634:ASN:CB	1:C:637:ALA:H	2.30	0.41
1:C:590:THR:HB	4:C:805:HOH:O	2.20	0.41
1:C:357:MET:HA	1:C:358:PRO:HD3	1.92	0.41
1:C:95:TRP:HB3	1:C:101:PRO:HD2	2.02	0.41
1:A:396:HIS:CE1	1:A:405:LEU:HD22	2.55	0.41
1:C:14:ALA:HB3	1:C:28:LEU:HD11	2.03	0.41
1:B:326:LYS:HD3	1:B:326:LYS:HA	1.86	0.41
1:D:456:LEU:O	1:D:460:ARG:HG3	2.21	0.41
1:D:349:LYS:O	1:D:471:ARG:HD2	2.20	0.41
1:B:372:GLN:HE21	1:B:372:GLN:HB3	1.69	0.41
1:D:283:GLN:HG3	2:D:901:G6P:H1	2.03	0.41
1:D:29:LYS:HG3	1:D:97:ILE:HD12	2.01	0.41
1:B:561:PRO:O	1:B:565:VAL:HG23	2.20	0.41
1:C:617:GLY:C	1:C:619:PRO:HD3	2.40	0.41
1:D:268:PRO:HB2	1:D:602:MET:CE	2.51	0.41
1:B:48:PRO:HG3	1:B:143:LEU:HD22	2.03	0.41
1:B:292:LYS:HD2	1:B:490:LEU:HD21	2.02	0.41
1:B:9:LEU:HD13	1:B:161:HIS:CG	2.55	0.41
1:C:434:ARG:HB2	1:C:435:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:512:GLY:C	1:C:515:PRO:HD2	2.40	0.41
1:A:11:PHE:HD1	1:A:46:ILE:HD11	1.85	0.41
1:C:471:ARG:CZ	1:C:471:ARG:HA	2.50	0.41
1:D:11:PHE:CD1	1:D:44:HIS:HB2	2.56	0.41
1:D:283:GLN:HG3	2:D:901:G6P:O1	2.20	0.41
1:C:177:PRO:HA	1:C:240:SER:OG	2.21	0.41
1:C:74:ARG:HB2	1:C:75:PRO:HD3	2.02	0.41
1:D:321:TYR:OH	1:D:455:ILE:HG12	2.21	0.41
1:D:283:GLN:NE2	1:D:587:ARG:NH2	2.65	0.41
1:B:326:LYS:NZ	1:B:509:GLU:HG3	2.35	0.41
1:D:538:GLU:HB3	1:D:553:ILE:HD12	2.02	0.41
1:D:371:GLY:HA3	4:D:739:HOH:O	2.21	0.41
1:A:621:GLN:O	1:A:625:LEU:HD13	2.21	0.41
1:B:497:ARG:NH2	4:B:777:HOH:O	2.54	0.41
1:C:282:PHE:HB2	1:C:497:ARG:HH21	1.84	0.41
1:D:17:VAL:O	1:D:17:VAL:CG1	2.69	0.41
1:A:19:ASN:ND2	1:A:19:ASN:O	2.54	0.41
1:D:125:LEU:HA	1:D:125:LEU:HD23	1.83	0.41
1:D:389:ILE:HG23	1:D:416:LEU:HB3	2.03	0.41
1:D:214:GLU:HG3	1:D:257:HIS:CD2	2.56	0.40
1:D:218:VAL:CG1	1:D:260:LYS:HE2	2.50	0.40
1:D:333:GLU:OE2	1:D:337:ARG:HD2	2.21	0.40
1:A:17:VAL:HG22	1:A:47:GLY:HA3	2.03	0.40
1:B:61:LEU:HG	1:B:93:GLY:HA2	2.04	0.40
1:A:56:ASN:N	1:A:56:ASN:OD1	2.53	0.40
1:B:196:LEU:O	1:B:200:TYR:HD2	2.04	0.40
1:C:542:GLU:OE1	1:C:544:ASN:N	2.54	0.40
1:D:615:ARG:HD2	1:D:615:ARG:O	2.21	0.40
1:D:227:ILE:O	1:D:227:ILE:CG2	2.68	0.40
1:C:111:VAL:CG1	1:C:118:TRP:CH2	3.04	0.40
1:D:189:ILE:HD11	1:D:610:ARG:HA	2.03	0.40
1:C:197:LEU:HB2	1:C:258:LEU:HD13	2.02	0.40
1:A:624:GLU:C	1:A:626:VAL:N	2.73	0.40
1:D:274:ILE:CG2	1:D:274:ILE:O	2.70	0.40
1:B:358:PRO:HG2	1:B:480:PHE:CZ	2.57	0.40
1:C:188:THR:O	1:C:242:ASP:HB2	2.21	0.40
1:B:214:GLU:HA	1:B:257[B]:HIS:CE1	2.56	0.40
1:B:455:ILE:HG22	1:B:459:ILE:HD11	2.02	0.40
1:A:214:GLU:HG2	1:A:257:HIS:CD2	2.56	0.40
1:D:454:LEU:HA	1:D:454:LEU:HD23	1.84	0.40
1:C:60:ILE:H	1:C:60:ILE:HG13	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:PRO:HA	1:D:441:PRO:HD3	1.96	0.40
1:B:213:LEU:HD21	1:B:254:GLU:HA	2.03	0.40
1:D:372:GLN:HG3	1:D:373:ALA:N	2.35	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	640/725 (88%)	606 (95%)	32 (5%)	2 (0%)	46	63
1	B	646/725 (89%)	622 (96%)	22 (3%)	2 (0%)	46	63
1	C	646/725 (89%)	618 (96%)	25 (4%)	3 (0%)	34	48
1	D	633/725 (87%)	597 (94%)	32 (5%)	4 (1%)	30	43
All	All	2565/2900 (88%)	2443 (95%)	111 (4%)	11 (0%)	39	56

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	625	LEU
1	B	17	VAL
1	B	643	LYS
1	C	543	THR
1	D	111	VAL
1	C	363	SER
1	D	40	LYS
1	D	194	ALA
1	C	17	VAL
1	D	115	SER
1	A	627	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	555/623 (89%)	538 (97%)	17 (3%)	47	69
1	B	558/623 (90%)	533 (96%)	25 (4%)	34	52
1	C	558/623 (90%)	538 (96%)	20 (4%)	42	63
1	D	550/623 (88%)	530 (96%)	20 (4%)	42	63
All	All	2221/2492 (89%)	2139 (96%)	82 (4%)	42	62

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	19	ASN
1	A	56	ASN
1	A	83	MET
1	A	110	SER
1	A	124	SER
1	A	180	ARG
1	A	283	GLN
1	A	310	ASP
1	A	321	TYR
1	A	372[A]	GLN
1	A	372[B]	GLN
1	A	376	ARG
1	A	458	LYS
1	A	556	ARG
1	A	568	LEU
1	A	590	THR
1	B	19	ASN
1	B	40	LYS
1	B	133	ASN
1	B	199	ARG
1	B	216	VAL
1	B	220	HIS
1	B	289	LYS

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Mol	Chain	Res	Type
1	B	310	ASP
1	B	320	ARG
1	B	321	TYR
1	B	348	LYS
1	B	372	GLN
1	B	376	ARG
1	B	408	GLU
1	B	420	SER
1	B	458	LYS
1	B	459	ILE
1	B	471	ARG
1	B	484	ASN
1	B	518	CYS
1	B	539	ASP
1	B	590	THR
1	B	614	LEU
1	B	634	ASN
1	B	645	LYS
1	C	19	ASN
1	C	180	ARG
1	C	181	LYS
1	C	213	LEU
1	C	240	SER
1	C	310	ASP
1	C	321	TYR
1	C	372[A]	GLN
1	C	372[B]	GLN
1	C	376	ARG
1	C	458	LYS
1	C	471	ARG
1	C	475	ILE
1	C	505	PRO
1	C	531	SER
1	C	543	THR
1	C	545	GLN
1	C	568	LEU
1	C	590	THR
1	C	645	LYS
1	D	6	GLN
1	D	19	ASN
1	D	41	ASP
1	D	42	HIS

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Mol	Chain	Res	Type
1	D	95	TRP
1	D	122	LEU
1	D	133	ASN
1	D	213	LEU
1	D	310	ASP
1	D	321	TYR
1	D	324	LYS
1	D	330	MET
1	D	372	GLN
1	D	387	THR
1	D	417	LEU
1	D	471	ARG
1	D	482	ASN
1	D	540	LEU
1	D	590	THR
1	D	636	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	283	GLN
1	A	403	ASN
1	A	484	ASN
1	B	7	ASN
1	B	133	ASN
1	B	161	HIS
1	B	396	HIS
1	B	484	ASN
1	B	582	GLN
1	B	621	GLN
1	B	634	ASN
1	C	19	ASN
1	C	81	GLN
1	C	249	GLN
1	C	257	HIS
1	C	284	ASN
1	C	403	ASN
1	C	477	HIS
1	C	545	GLN
1	C	586	GLN
1	D	19	ASN

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Mol	Chain	Res	Type
1	D	50	ASN
1	D	161	HIS
1	D	168	HIS
1	D	211	ASN
1	D	249	GLN
1	D	257	HIS
1	D	283	GLN
1	D	302	HIS
1	D	403	ASN
1	D	482	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	PEG	A	1001	-	6,6,6	0.61	0	5,5,5	0.41	0
2	G6P	A	901	-	16,16,16	0.92	1 (6%)	23,24,24	1.45	4 (17%)
2	G6P	A	902	-	16,16,16	0.91	1 (6%)	23,24,24	1.42	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	B	1001	-	6,6,6	0.55	0	5,5,5	0.46	0
3	PEG	B	1002	-	6,6,6	0.57	0	5,5,5	0.47	0
3	PEG	B	706	-	6,6,6	0.61	0	5,5,5	0.47	0
2	G6P	B	901	-	16,16,16	0.90	1 (6%)	23,24,24	1.39	3 (13%)
2	G6P	B	902	-	16,16,16	0.90	0	23,24,24	1.97	6 (26%)
3	PEG	C	1001	-	6,6,6	0.61	0	5,5,5	0.41	0
2	G6P	C	901	-	16,16,16	0.87	1 (6%)	23,24,24	1.48	4 (17%)
3	PEG	D	1002	-	6,6,6	0.63	0	5,5,5	0.48	0
2	G6P	D	901	-	16,16,16	0.87	0	23,24,24	1.37	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	1001	-	-	0/4/4/4	0/0/0/0
2	G6P	A	901	-	-	0/6/26/26	0/1/1/1
2	G6P	A	902	-	-	0/6/26/26	0/1/1/1
3	PEG	B	1001	-	-	0/4/4/4	0/0/0/0
3	PEG	B	1002	-	-	0/4/4/4	0/0/0/0
3	PEG	B	706	-	-	0/4/4/4	0/0/0/0
2	G6P	B	901	-	-	0/6/26/26	0/1/1/1
2	G6P	B	902	-	-	0/6/26/26	0/1/1/1
3	PEG	C	1001	-	-	0/4/4/4	0/0/0/0
2	G6P	C	901	-	-	0/6/26/26	0/1/1/1
3	PEG	D	1002	-	-	0/4/4/4	0/0/0/0
2	G6P	D	901	-	-	0/6/26/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	G6P	P-O2P	-2.10	1.47	1.54
2	C	901	G6P	P-O2P	-2.09	1.47	1.54
2	A	901	G6P	P-O2P	-2.07	1.47	1.54
2	A	902	G6P	P-O2P	-2.05	1.47	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	G6P	C4-C3-C2	-4.85	101.74	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	G6P	O5-C5-C4	-3.99	102.19	109.68
2	A	901	G6P	C4-C3-C2	-3.41	104.42	110.79
2	C	901	G6P	C4-C3-C2	-3.14	104.94	110.79
2	B	901	G6P	C4-C3-C2	-2.84	105.50	110.79
2	D	901	G6P	C4-C3-C2	-2.74	105.68	110.79
2	A	901	G6P	O2-C2-C1	-2.59	104.11	109.82
2	A	902	G6P	O2-C2-C1	-2.50	104.31	109.82
2	A	902	G6P	C1-O5-C5	-2.35	109.12	113.47
2	A	902	G6P	C4-C3-C2	-2.32	106.47	110.79
2	C	901	G6P	O6-P-O3P	-2.31	101.25	107.14
2	C	901	G6P	O2-C2-C1	-2.31	104.73	109.82
2	B	901	G6P	O2-C2-C1	-2.22	104.94	109.82
2	A	902	G6P	O6-P-O3P	-2.20	101.55	107.14
2	B	902	G6P	C3-C4-C5	-2.08	106.57	110.20
2	A	901	G6P	O6-P-O3P	-2.07	101.88	107.14
2	D	901	G6P	O5-C5-C6	-2.00	102.51	106.61
2	D	901	G6P	O1P-P-O3P	2.11	117.36	110.58
2	B	902	G6P	O6-C6-C5	2.13	116.97	109.12
2	B	901	G6P	O1P-P-O3P	2.16	117.55	110.58
2	A	901	G6P	O1P-P-O3P	2.38	118.25	110.58
2	B	902	G6P	O1P-P-O3P	2.41	118.34	110.58
2	A	902	G6P	O1P-P-O3P	2.42	118.36	110.58
2	C	901	G6P	O1P-P-O3P	2.73	119.36	110.58
2	B	902	G6P	O5-C1-C2	3.03	114.64	109.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	G6P	1	0
3	B	1001	PEG	2	0
2	B	902	G6P	2	0
2	C	901	G6P	2	0
2	D	901	G6P	3	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	638/725 (88%)	0.23	16 (2%) 61 60	25, 49, 89, 101	0
1	B	645/725 (88%)	0.11	28 (4%) 39 40	33, 50, 83, 96	0
1	C	646/725 (89%)	0.21	25 (3%) 43 44	36, 53, 87, 101	0
1	D	636/725 (87%)	0.35	47 (7%) 17 17	28, 61, 103, 114	0
All	All	2565/2900 (88%)	0.22	116 (4%) 37 38	25, 52, 95, 114	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	630	LEU	8.3
1	D	627	GLY	7.4
1	D	622	PHE	6.5
1	D	126	VAL	6.2
1	B	644	LEU	6.2
1	D	623	ARG	6.1
1	D	626	VAL	5.8
1	B	646	VAL	5.7
1	D	638	LEU	5.6
1	B	645	LYS	5.4
1	D	629	GLU	5.4
1	D	125	LEU	5.3
1	B	128	ILE	5.2
1	D	625	LEU	5.1
1	D	122	LEU	5.1
1	D	133	ASN	5.0
1	B	125	LEU	4.9
1	A	623	ARG	4.3
1	C	645	LYS	4.2
1	D	639	ALA	4.1
1	D	128	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	205	GLY	4.0
1	D	637	ALA	3.9
1	D	628	GLU	3.9
1	D	129	PRO	3.8
1	D	624	GLU	3.8
1	A	90	PHE	3.7
1	C	68	ALA	3.6
1	D	631	ASN	3.6
1	B	543	THR	3.5
1	A	624	GLU	3.5
1	C	62	ASP	3.5
1	D	119	LYS	3.4
1	B	641	GLY	3.4
1	C	647	ALA	3.3
1	D	227	ILE	3.3
1	D	618	TYR	3.3
1	B	127	GLY	3.3
1	A	5	LEU	3.3
1	B	642	LYS	3.2
1	C	59	ASP	3.2
1	D	633	SER	3.2
1	D	636	ASP	3.2
1	D	632	ASP	3.2
1	A	61	LEU	3.1
1	C	133	ASN	3.1
1	A	630	LEU	3.1
1	D	2	SER	3.1
1	D	115	SER	3.1
1	B	130	SER	3.0
1	B	643	LYS	3.0
1	D	132	GLU	3.0
1	B	123	TRP	3.0
1	B	544	ASN	3.0
1	B	126	VAL	2.9
1	A	94	ARG	2.9
1	A	63	TRP	2.9
1	D	635	MET	2.8
1	D	124	SER	2.8
1	B	279	PHE	2.8
1	A	2	SER	2.8
1	C	76	VAL	2.8
1	B	541	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	6	GLN	2.7
1	D	60	ILE	2.7
1	C	279	PHE	2.7
1	B	132	GLU	2.7
1	A	67	GLU	2.7
1	C	207	PHE	2.7
1	A	132	GLU	2.7
1	C	641	GLY	2.7
1	D	197	LEU	2.6
1	D	615	ARG	2.6
1	D	85	SER	2.6
1	D	91	VAL	2.6
1	C	213	LEU	2.6
1	D	135	PHE	2.6
1	B	253	PHE	2.5
1	B	206	SER	2.5
1	D	223	GLY	2.5
1	C	111	VAL	2.5
1	C	644	LEU	2.5
1	C	89	HIS	2.4
1	C	83	MET	2.4
1	B	62	ASP	2.4
1	D	619	PRO	2.4
1	D	5	LEU	2.4
1	C	204	SER	2.4
1	B	181	LYS	2.4
1	B	545	GLN	2.4
1	C	135	PHE	2.3
1	A	637	ALA	2.3
1	C	63	TRP	2.3
1	D	123	TRP	2.3
1	D	620	ASP	2.3
1	B	124	SER	2.3
1	B	113	GLY	2.2
1	A	631	ASN	2.2
1	C	88	VAL	2.2
1	C	543	THR	2.2
1	C	64	LYS	2.2
1	D	614	LEU	2.2
1	A	636	ASP	2.2
1	B	131	PRO	2.2
1	D	213	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	67	GLU	2.1
1	C	67	GLU	2.1
1	D	118	TRP	2.1
1	A	71	ASP	2.1
1	D	621	GLN	2.0
1	A	76	VAL	2.0
1	D	130	SER	2.0
1	B	623	ARG	2.0
1	C	65	LYS	2.0
1	B	129	PRO	2.0
1	C	61	LEU	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 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(Å ²)	Q<0.9
2	G6P	A	902	16/16	0.92	0.21	2.06	46,52,58,60	16
2	G6P	A	901	16/16	0.99	0.18	1.54	30,35,38,40	0
3	PEG	D	1002	7/7	0.86	0.15	1.52	47,50,55,58	0
2	G6P	C	901	16/16	0.99	0.16	0.22	39,42,43,44	0
2	G6P	D	901	16/16	0.99	0.14	0.14	32,34,36,38	0
3	PEG	A	1001	7/7	0.85	0.16	-0.47	49,50,54,56	0
2	G6P	B	902	16/16	0.93	0.15	-0.54	51,54,56,60	0
2	G6P	B	901	16/16	0.99	0.13	-0.77	35,38,42,42	0
3	PEG	B	1001	7/7	0.87	0.13	-0.79	42,44,46,50	0
3	PEG	C	1001	7/7	0.90	0.12	-1.43	43,45,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PEG	B	706	7/7	0.93	0.11	-2.11	43,46,48,49	0
3	PEG	B	1002	7/7	0.81	0.29	-	60,61,65,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.