



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 09:58 PM GMT

PDB ID : 3R2W
Title : Crystal Structure of UDP-glucose Pyrophosphorylase of Homo Sapiens
Authors : Zheng, X.; Yu, Q.
Deposited on : 2011-03-14
Resolution : 3.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

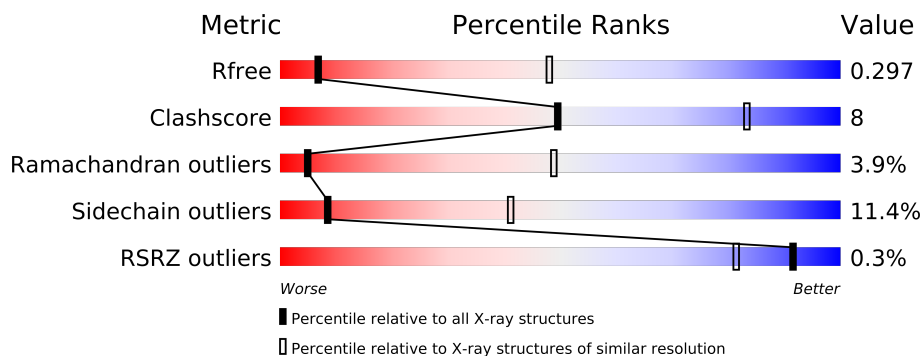
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.60 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}	66092	1020 (3.86-3.34)
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	528	
1	B	528	
1	C	528	
1	D	528	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13938 atoms, of which 0 are hydrogen and 0 are deuterium.

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 UTP--glucose-1-phosphateuridylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3539	2253	604	672	10			
1	B	467	Total	C	N	O	S	0	0	0
			3534	2251	605	667	11			
1	C	450	Total	C	N	O	S	0	0	0
			3299	2088	557	646	8			
1	D	468	Total	C	N	O	S	0	0	0
			3566	2275	608	672	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	EXPRESSION TAG	UNP Q16851
A	-29	GLY	-	EXPRESSION TAG	UNP Q16851
A	-28	SER	-	EXPRESSION TAG	UNP Q16851
A	-27	SER	-	EXPRESSION TAG	UNP Q16851
A	-26	HIS	-	EXPRESSION TAG	UNP Q16851
A	-25	HIS	-	EXPRESSION TAG	UNP Q16851
A	-24	HIS	-	EXPRESSION TAG	UNP Q16851
A	-23	HIS	-	EXPRESSION TAG	UNP Q16851
A	-22	HIS	-	EXPRESSION TAG	UNP Q16851
A	-21	HIS	-	EXPRESSION TAG	UNP Q16851
A	-20	SER	-	EXPRESSION TAG	UNP Q16851
A	-19	SER	-	EXPRESSION TAG	UNP Q16851
A	-18	GLY	-	EXPRESSION TAG	UNP Q16851
A	-17	LEU	-	EXPRESSION TAG	UNP Q16851
A	-16	VAL	-	EXPRESSION TAG	UNP Q16851
A	-15	PRO	-	EXPRESSION TAG	UNP Q16851
A	-14	ARG	-	EXPRESSION TAG	UNP Q16851
A	-13	GLY	-	EXPRESSION TAG	UNP Q16851
A	-12	SER	-	EXPRESSION TAG	UNP Q16851
A	-11	HIS	-	EXPRESSION TAG	UNP Q16851
B	-30	MET	-	EXPRESSION TAG	UNP Q16851

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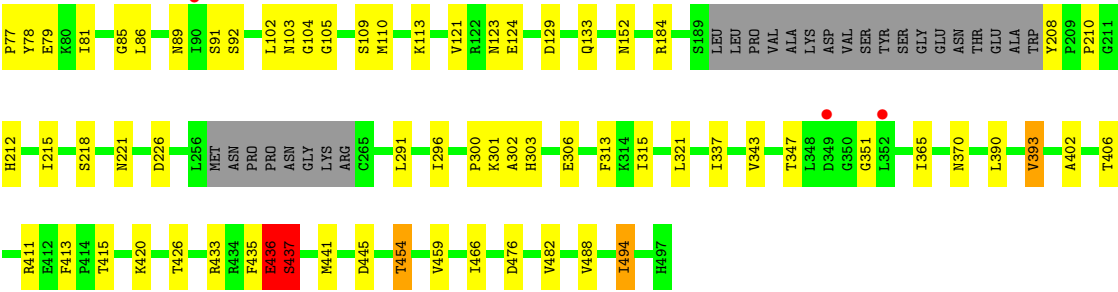
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-29	GLY	-	EXPRESSION TAG	UNP Q16851
B	-28	SER	-	EXPRESSION TAG	UNP Q16851
B	-27	SER	-	EXPRESSION TAG	UNP Q16851
B	-26	HIS	-	EXPRESSION TAG	UNP Q16851
B	-25	HIS	-	EXPRESSION TAG	UNP Q16851
B	-24	HIS	-	EXPRESSION TAG	UNP Q16851
B	-23	HIS	-	EXPRESSION TAG	UNP Q16851
B	-22	HIS	-	EXPRESSION TAG	UNP Q16851
B	-21	HIS	-	EXPRESSION TAG	UNP Q16851
B	-20	SER	-	EXPRESSION TAG	UNP Q16851
B	-19	SER	-	EXPRESSION TAG	UNP Q16851
B	-18	GLY	-	EXPRESSION TAG	UNP Q16851
B	-17	LEU	-	EXPRESSION TAG	UNP Q16851
B	-16	VAL	-	EXPRESSION TAG	UNP Q16851
B	-15	PRO	-	EXPRESSION TAG	UNP Q16851
B	-14	ARG	-	EXPRESSION TAG	UNP Q16851
B	-13	GLY	-	EXPRESSION TAG	UNP Q16851
B	-12	SER	-	EXPRESSION TAG	UNP Q16851
B	-11	HIS	-	EXPRESSION TAG	UNP Q16851
C	-30	MET	-	EXPRESSION TAG	UNP Q16851
C	-29	GLY	-	EXPRESSION TAG	UNP Q16851
C	-28	SER	-	EXPRESSION TAG	UNP Q16851
C	-27	SER	-	EXPRESSION TAG	UNP Q16851
C	-26	HIS	-	EXPRESSION TAG	UNP Q16851
C	-25	HIS	-	EXPRESSION TAG	UNP Q16851
C	-24	HIS	-	EXPRESSION TAG	UNP Q16851
C	-23	HIS	-	EXPRESSION TAG	UNP Q16851
C	-22	HIS	-	EXPRESSION TAG	UNP Q16851
C	-21	HIS	-	EXPRESSION TAG	UNP Q16851
C	-20	SER	-	EXPRESSION TAG	UNP Q16851
C	-19	SER	-	EXPRESSION TAG	UNP Q16851
C	-18	GLY	-	EXPRESSION TAG	UNP Q16851
C	-17	LEU	-	EXPRESSION TAG	UNP Q16851
C	-16	VAL	-	EXPRESSION TAG	UNP Q16851
C	-15	PRO	-	EXPRESSION TAG	UNP Q16851
C	-14	ARG	-	EXPRESSION TAG	UNP Q16851
C	-13	GLY	-	EXPRESSION TAG	UNP Q16851
C	-12	SER	-	EXPRESSION TAG	UNP Q16851
C	-11	HIS	-	EXPRESSION TAG	UNP Q16851
D	-30	MET	-	EXPRESSION TAG	UNP Q16851
D	-29	GLY	-	EXPRESSION TAG	UNP Q16851
D	-28	SER	-	EXPRESSION TAG	UNP Q16851

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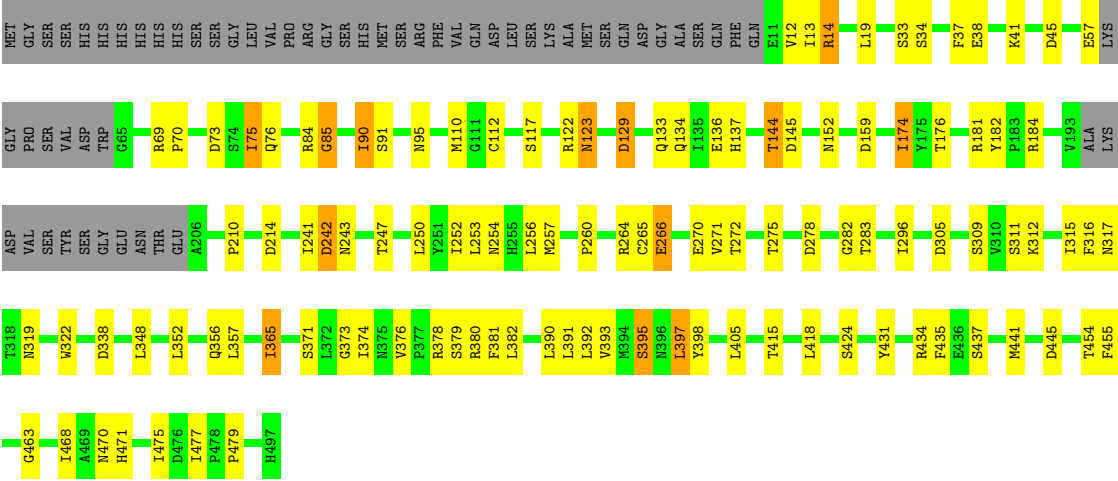
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-27	SER	-	EXPRESSION TAG	UNP Q16851
D	-26	HIS	-	EXPRESSION TAG	UNP Q16851
D	-25	HIS	-	EXPRESSION TAG	UNP Q16851
D	-24	HIS	-	EXPRESSION TAG	UNP Q16851
D	-23	HIS	-	EXPRESSION TAG	UNP Q16851
D	-22	HIS	-	EXPRESSION TAG	UNP Q16851
D	-21	HIS	-	EXPRESSION TAG	UNP Q16851
D	-20	SER	-	EXPRESSION TAG	UNP Q16851
D	-19	SER	-	EXPRESSION TAG	UNP Q16851
D	-18	GLY	-	EXPRESSION TAG	UNP Q16851
D	-17	LEU	-	EXPRESSION TAG	UNP Q16851
D	-16	VAL	-	EXPRESSION TAG	UNP Q16851
D	-15	PRO	-	EXPRESSION TAG	UNP Q16851
D	-14	ARG	-	EXPRESSION TAG	UNP Q16851
D	-13	GLY	-	EXPRESSION TAG	UNP Q16851
D	-12	SER	-	EXPRESSION TAG	UNP Q16851
D	-11	HIS	-	EXPRESSION TAG	UNP Q16851



● Molecule 1: UTP--glucose-1-phosphateuridylyltransferase

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.44Å 140.44Å 311.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.60 20.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-3.60) 94.0 (20.00-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 3.62Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.247 , 0.304 0.250 , 0.297	Depositor DCC
R_{free} test set	1983 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	113.6	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 54.8	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 39283 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13938	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.61	2/3602 (0.1%)	0.72	1/4894 (0.0%)
1	B	0.58	0/3596	0.79	1/4889 (0.0%)
1	C	0.51	0/3353	0.66	0/4578
1	D	0.67	0/3630	0.83	3/4936 (0.1%)
All	All	0.60	2/14181 (0.0%)	0.75	5/19297 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	SER	CB-OG	10.91	1.56	1.42
1	A	379	SER	CB-OG	7.32	1.51	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	382	LEU	CA-CB-CG	5.99	129.08	115.30
1	D	33	SER	N-CA-C	-5.80	95.35	111.00
1	A	444	LEU	CA-CB-CG	5.35	127.60	115.30
1	B	86	LEU	CA-CB-CG	5.28	127.45	115.30
1	D	33	SER	C-N-CA	5.09	134.43	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	91	SER	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3539	0	116	20	0
1	B	3534	0	89	42	0
1	C	3299	0	132	18	0
1	D	3566	0	192	33	0
All	All	13938	0	529	110	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (110) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:129:ASP:O	1:D:133:GLN:CG	2.34	0.73
1:B:265:CYS:CA	1:B:266:GLU:CB	2.67	0.72
1:B:75:ILE:HA	1:B:373:GLY:O	1.90	0.71
1:D:90:ILE:N	1:D:91:SER:CA	2.54	0.70
1:B:441:MET:O	1:B:443:GLU:N	2.25	0.70
1:B:497:HIS:O	1:C:420:LYS:NZ	2.27	0.67
1:A:179:GLN:NE2	1:A:211:GLY:O	2.27	0.66
1:D:75:ILE:HA	1:D:373:GLY:O	1.97	0.64
1:C:494:ILE:CG2	1:C:494:ILE:O	2.47	0.62
1:C:303:HIS:ND1	1:C:306:GLU:OE1	2.34	0.61
1:C:218:SER:HA	1:C:221:ASN:CB	2.31	0.60
1:B:257:MET:O	1:B:258:ASN:C	2.39	0.60
1:A:309:SER:CA	1:A:310:VAL:C	2.70	0.60
1:D:424:SER:OG	1:D:434:ARG:NH2	2.35	0.59
1:A:264:ARG:NE	1:A:370:ASN:O	2.37	0.58
1:B:129:ASP:O	1:B:133:GLN:CG	2.52	0.58
1:A:441:MET:O	1:A:443:GLU:N	2.36	0.57
1:B:126:THR:OG1	1:B:127:PHE:N	2.38	0.56
1:B:84:ARG:N	1:B:85:GLY:CA	2.69	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:91:SER:N	1:C:92:SER:CA	2.69	0.56
1:B:10:GLN:HA	1:B:13:ILE:HD12	1.88	0.56
1:C:454:THR:CG2	1:C:476:ASP:OD1	2.55	0.55
1:B:264:ARG:O	1:B:265:CYS:CB	2.55	0.55
1:B:267:PHE:CE2	1:B:365:ILE:CG1	2.89	0.55
1:B:71:PRO:HG2	1:B:74:SER:OG	2.07	0.54
1:B:490:GLY:O	1:B:491:ASN:CB	2.56	0.54
1:A:90:ILE:N	1:A:91:SER:CA	2.71	0.53
1:B:278:ASP:OD2	1:B:378:ARG:NH2	2.42	0.53
1:B:435:PHE:CE1	1:B:455:PHE:CD2	2.97	0.52
1:C:77:PRO:C	1:C:79:GLU:N	2.63	0.51
1:D:317:ASN:OD1	1:D:319:ASN:N	2.43	0.51
1:B:313:PHE:O	1:B:315:ILE:N	2.43	0.51
1:C:436:GLU:O	1:C:437:SER:CB	2.59	0.51
1:B:90:ILE:N	1:B:91:SER:CA	2.74	0.50
1:A:215:ILE:HG23	1:A:216:TYR:N	2.26	0.50
1:B:51:PHE:O	1:B:54:PHE:N	2.44	0.50
1:B:313:PHE:CD2	1:B:313:PHE:N	2.78	0.50
1:D:13:ILE:HD12	1:D:14:ARG:HG3	1.95	0.49
1:D:73:ASP:O	1:D:76:GLN:NE2	2.46	0.49
1:C:435:PHE:O	1:C:436:GLU:C	2.51	0.48
1:B:273:ASN:CA	1:B:314:LYS:O	2.61	0.48
1:B:337:ILE:CD1	1:B:337:ILE:N	2.76	0.48
1:D:122:ARG:O	1:D:123:ASN:CB	2.62	0.48
1:B:413:PHE:N	1:B:413:PHE:CD2	2.81	0.48
1:D:392:LEU:O	1:D:395:SER:OG	2.32	0.47
1:A:185:ILE:O	1:A:355:ILE:N	2.47	0.47
1:C:103:ASN:O	1:C:105:GLY:N	2.48	0.47
1:A:33:SER:O	1:A:35:HIS:N	2.48	0.47
1:B:317:ASN:OD1	1:B:318:THR:N	2.48	0.47
1:A:267:PHE:CD2	1:A:267:PHE:C	2.89	0.46
1:D:470:ASN:O	1:D:471:HIS:C	2.53	0.46
1:D:435:PHE:CE1	1:D:455:PHE:CD2	3.05	0.45
1:D:182:TYR:CE2	1:D:210:PRO:HG3	2.51	0.45
1:C:347:THR:OG1	1:C:351:GLY:O	2.35	0.45
1:D:283:THR:OG1	1:D:315:ILE:O	2.34	0.45
1:C:482:VAL:N	1:D:479:PRO:O	2.50	0.45
1:B:129:ASP:OD1	1:B:167:TYR:OH	2.34	0.45
1:C:129:ASP:O	1:C:133:GLN:CG	2.65	0.45
1:B:123:ASN:N	1:B:124:GLU:CA	2.80	0.44
1:A:123:ASN:N	1:A:124:GLU:CA	2.80	0.44
1:B:332:GLN:C	1:B:334:GLN:N	2.72	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:282:GLY:O	1:D:317:ASN:N	2.52	0.43
1:B:312:LYS:O	1:B:314:LYS:N	2.51	0.43
1:D:184:ARG:NE	1:D:356:GLN:OE1	2.51	0.43
1:A:309:SER:OG	1:A:311:SER:OG	2.36	0.43
1:A:491:ASN:O	1:B:491:ASN:N	2.52	0.43
1:D:397:LEU:CD2	1:D:398:TYR:CE2	3.01	0.43
1:D:144:THR:OG1	1:D:145:ASP:N	2.51	0.43
1:C:413:PHE:O	1:C:415:THR:N	2.52	0.43
1:B:184:ARG:CD	1:B:184:ARG:N	2.82	0.43
1:C:212:HIS:H	1:C:212:HIS:CD2	2.35	0.43
1:A:126:THR:CG2	1:A:129:ASP:OD2	2.67	0.42
1:D:398:TYR:CD2	1:D:398:TYR:N	2.86	0.42
1:A:256:LEU:O	1:A:258:ASN:N	2.53	0.42
1:B:378:ARG:O	1:B:380:ARG:N	2.52	0.42
1:B:478:PRO:O	1:B:479:PRO:C	2.58	0.42
1:A:91:SER:CA	1:A:92:SER:CB	2.97	0.42
1:A:184:ARG:NH1	1:A:356:GLN:NE2	2.68	0.42
1:B:271:VAL:O	1:B:376:VAL:N	2.53	0.42
1:D:210:PRO:HG2	1:D:214:ASP:HB2	2.01	0.42
1:D:253:LEU:O	1:D:256:LEU:N	2.53	0.42
1:B:324:SER:O	1:B:327:ALA:N	2.53	0.41
1:B:378:ARG:C	1:B:380:ARG:N	2.73	0.41
1:B:212:HIS:O	1:B:214:ASP:N	2.52	0.41
1:B:157:ASP:O	1:B:158:GLU:C	2.57	0.41
1:B:266:GLU:OE2	1:B:330:ARG:NH2	2.52	0.41
1:A:362:GLY:O	1:A:364:ALA:N	2.52	0.41
1:D:134:GLN:O	1:D:137:HIS:N	2.54	0.41
1:B:317:ASN:OD1	1:B:319:ASN:N	2.53	0.41
1:A:310:VAL:O	1:A:312:LYS:N	2.54	0.41
1:C:390:LEU:O	1:C:393:VAL:N	2.54	0.41
1:D:265:CYS:CA	1:D:266:GLU:CB	2.99	0.41
1:D:390:LEU:O	1:D:391:LEU:C	2.59	0.41
1:D:69:ARG:HA	1:D:70:PRO:HD3	1.93	0.41
1:D:270:GLU:OE1	1:D:380:ARG:NH2	2.54	0.41
1:B:107:GLY:O	1:B:112:CYS:N	2.54	0.41
1:A:278:ASP:OD2	1:A:316:PHE:CE2	2.74	0.41
1:D:37:PHE:O	1:D:41:LYS:N	2.54	0.41
1:C:184:ARG:CA	1:C:208:TYR:HE2	2.34	0.41
1:C:300:PRO:O	1:C:302:ALA:N	2.54	0.40
1:D:84:ARG:N	1:D:85:GLY:CA	2.83	0.40
1:D:242:ASP:OD1	1:D:242:ASP:N	2.54	0.40
1:B:365:ILE:O	1:B:366:LYS:C	2.60	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:445:ASP:N	1:D:463:GLY:O	2.55	0.40
1:D:378:ARG:O	1:D:381:PHE:N	2.54	0.40
1:D:174:ILE:CG2	1:D:174:ILE:O	2.69	0.40
1:D:134:GLN:C	1:D:136:GLU:N	2.75	0.40
1:B:255:HIS:O	1:B:255:HIS:CD2	2.75	0.40
1:B:94:LEU:C	1:B:96:LYS:N	2.74	0.40
1:A:392:LEU:O	1:A:395:SER:OG	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	459/528 (87%)	376 (82%)	64 (14%)	19 (4%)	4	47
1	B	461/528 (87%)	377 (82%)	58 (13%)	26 (6%)	3	37
1	C	442/528 (84%)	363 (82%)	65 (15%)	14 (3%)	6	55
1	D	462/528 (88%)	384 (83%)	65 (14%)	13 (3%)	8	59
All	All	1824/2112 (86%)	1500 (82%)	252 (14%)	72 (4%)	5	49

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	257	MET
1	A	263	LYS
1	B	265	CYS
1	B	266	GLU
1	B	313	PHE
1	B	491	ASN
1	C	121	VAL
1	C	437	SER
1	D	34	SER
1	D	371	SER

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Mol	Chain	Res	Type
1	A	84	ARG
1	A	346	LYS
1	A	363	ALA
1	A	370	ASN
1	A	379	SER
1	B	143	ASN
1	B	314	LYS
1	B	379	SER
1	B	442	LEU
1	C	78	TYR
1	C	301	LYS
1	C	343	VAL
1	C	370	ASN
1	C	436	GLU
1	D	38	GLU
1	D	254	ASN
1	D	264	ARG
1	D	266	GLU
1	D	365	ILE
1	A	210	PRO
1	A	246	ALA
1	A	261	ASN
1	A	267	PHE
1	A	442	LEU
1	B	92	SER
1	B	95	ASN
1	B	261	ASN
1	B	333	GLU
1	B	371	SER
1	B	415	THR
1	B	437	SER
1	C	113	LYS
1	C	411	ARG
1	D	309	SER
1	A	122	ARG
1	A	258	ASN
1	A	412	GLU
1	B	34	SER
1	B	165	GLN
1	B	224	LEU
1	B	392	LEU
1	D	85	GLY

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Mol	Chain	Res	Type
1	A	209	PRO
1	B	38	GLU
1	B	117	SER
1	B	213	GLY
1	C	210	PRO
1	C	402	ALA
1	D	117	SER
1	D	123	ASN
1	D	129	ASP
1	D	379	SER
1	B	209	PRO
1	C	104	GLY
1	B	121	VAL
1	B	258	ASN
1	A	163	ILE
1	B	289	GLY
1	C	85	GLY
1	C	215	ILE
1	A	422	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	381/470 (81%)	345 (91%)	36 (9%)	13	53
1	B	380/470 (81%)	331 (87%)	49 (13%)	6	34
1	C	341/470 (73%)	310 (91%)	31 (9%)	14	55
1	D	385/470 (82%)	331 (86%)	54 (14%)	5	30
All	All	1487/1880 (79%)	1317 (89%)	170 (11%)	8	41

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	31	THR
1	A	67	ILE

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Mol	Chain	Res	Type
1	A	80	LYS
1	A	81	ILE
1	A	118	LEU
1	A	145	ASP
1	A	148	LEU
1	A	152	ASN
1	A	189	SER
1	A	236	ILE
1	A	240	ASN
1	A	253	LEU
1	A	267	PHE
1	A	271	VAL
1	A	275	THR
1	A	283	THR
1	A	296	ILE
1	A	312	LYS
1	A	321	LEU
1	A	343	VAL
1	A	352	LEU
1	A	367	SER
1	A	372	LEU
1	A	379	SER
1	A	382	LEU
1	A	395	SER
1	A	399	SER
1	A	405	LEU
1	A	408	SER
1	A	424	SER
1	A	444	LEU
1	A	453	VAL
1	A	464	THR
1	A	476	ASP
1	A	477	ILE
1	B	30	THR
1	B	31	THR
1	B	40	THR
1	B	73	ASP
1	B	86	LEU
1	B	91	SER
1	B	92	SER
1	B	112	CYS
1	B	156	THR

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Mol	Chain	Res	Type
1	B	163	ILE
1	B	168	ASN
1	B	174	ILE
1	B	180	SER
1	B	184	ARG
1	B	185	ILE
1	B	214	ASP
1	B	236	ILE
1	B	239	SER
1	B	247	THR
1	B	265	CYS
1	B	272	THR
1	B	278	ASP
1	B	296	ILE
1	B	301	LYS
1	B	305	ASP
1	B	311	SER
1	B	313	PHE
1	B	316	PHE
1	B	324	SER
1	B	337	ILE
1	B	340	GLU
1	B	349	ASP
1	B	361	VAL
1	B	366	LYS
1	B	371	SER
1	B	374	ILE
1	B	376	VAL
1	B	378	ARG
1	B	390	LEU
1	B	395	SER
1	B	397	LEU
1	B	400	LEU
1	B	405	LEU
1	B	424	SER
1	B	429	GLN
1	B	462	LYS
1	B	473	ASP
1	B	477	ILE
1	B	491	ASN
1	C	66	LYS
1	C	81	ILE

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Mol	Chain	Res	Type
1	C	86	LEU
1	C	89	ASN
1	C	102	LEU
1	C	109	SER
1	C	110	MET
1	C	123	ASN
1	C	124	GLU
1	C	152	ASN
1	C	226	ASP
1	C	291	LEU
1	C	296	ILE
1	C	313	PHE
1	C	315	ILE
1	C	321	LEU
1	C	337	ILE
1	C	365	ILE
1	C	393	VAL
1	C	406	THR
1	C	426	THR
1	C	433	ARG
1	C	436	GLU
1	C	437	SER
1	C	441	MET
1	C	445	ASP
1	C	454	THR
1	C	459	VAL
1	C	466	ILE
1	C	488	VAL
1	C	494	ILE
1	D	12	VAL
1	D	14	ARG
1	D	19	LEU
1	D	45	ASP
1	D	57	GLU
1	D	75	ILE
1	D	90	ILE
1	D	95	ASN
1	D	110	MET
1	D	112	CYS
1	D	144	THR
1	D	152	ASN
1	D	159	ASP

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Mol	Chain	Res	Type
1	D	174	ILE
1	D	176	THR
1	D	181	ARG
1	D	241	ILE
1	D	242	ASP
1	D	243	ASN
1	D	247	THR
1	D	250	LEU
1	D	252	ILE
1	D	257	MET
1	D	260	PRO
1	D	271	VAL
1	D	272	THR
1	D	275	THR
1	D	278	ASP
1	D	296	ILE
1	D	305	ASP
1	D	311	SER
1	D	312	LYS
1	D	316	PHE
1	D	322	TRP
1	D	338	ASP
1	D	348	LEU
1	D	352	LEU
1	D	357	LEU
1	D	365	ILE
1	D	374	ILE
1	D	376	VAL
1	D	393	VAL
1	D	395	SER
1	D	397	LEU
1	D	405	LEU
1	D	415	THR
1	D	418	LEU
1	D	431	TYR
1	D	437	SER
1	D	441	MET
1	D	454	THR
1	D	468	ILE
1	D	475	ILE
1	D	477	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	212	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

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	465/528 (88%)	-0.10	2 (0%) 90 76	80, 145, 200, 335	0
1	B	467/528 (88%)	-0.20	0 100 100	72, 130, 184, 231	0
1	C	450/528 (85%)	0.02	4 (0%) 81 57	85, 190, 241, 272	0
1	D	468/528 (88%)	-0.24	0 100 100	58, 114, 164, 227	0
All	All	1850/2112 (87%)	-0.13	6 (0%) 91 81	58, 135, 218, 335	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	55	LEU	2.8
1	A	208	TYR	2.7
1	C	349	ASP	2.1
1	A	209	PRO	2.1
1	C	90	ILE	2.1
1	C	352	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.