



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:42 AM UTC

PDB ID : 7Y4I / pdb_00007y4i
Title : Crystal structure of SPINDLY in complex with GDP
Authors : Xu, S.T.; Wan, L.H.
Deposited on : 2022-06-14
Resolution : 2.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

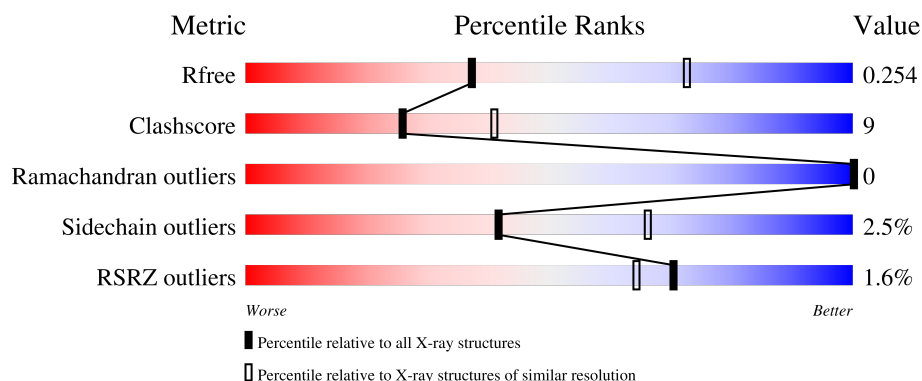
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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

Mol	Chain	Length	Quality of chain
1	A	914	70% 20% 10%
1	B	914	2% 68% 20% 11%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12812 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.

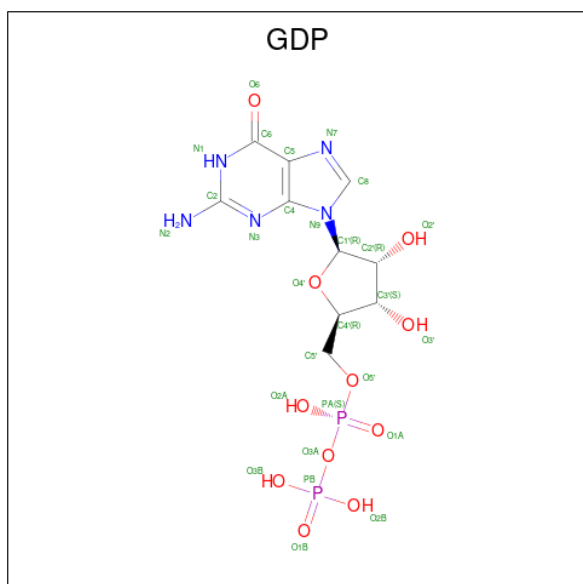
- Molecule 1 is a protein called Probable UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase SPINDLY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	0	0	0
			6419	4083	1076	1211	49			
1	B	815	Total	C	N	O	S	0	0	0
			6360	4048	1064	1199	49			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	645	SER	CYS	engineered mutation	UNP Q96301
B	645	SER	CYS	engineered mutation	UNP Q96301

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

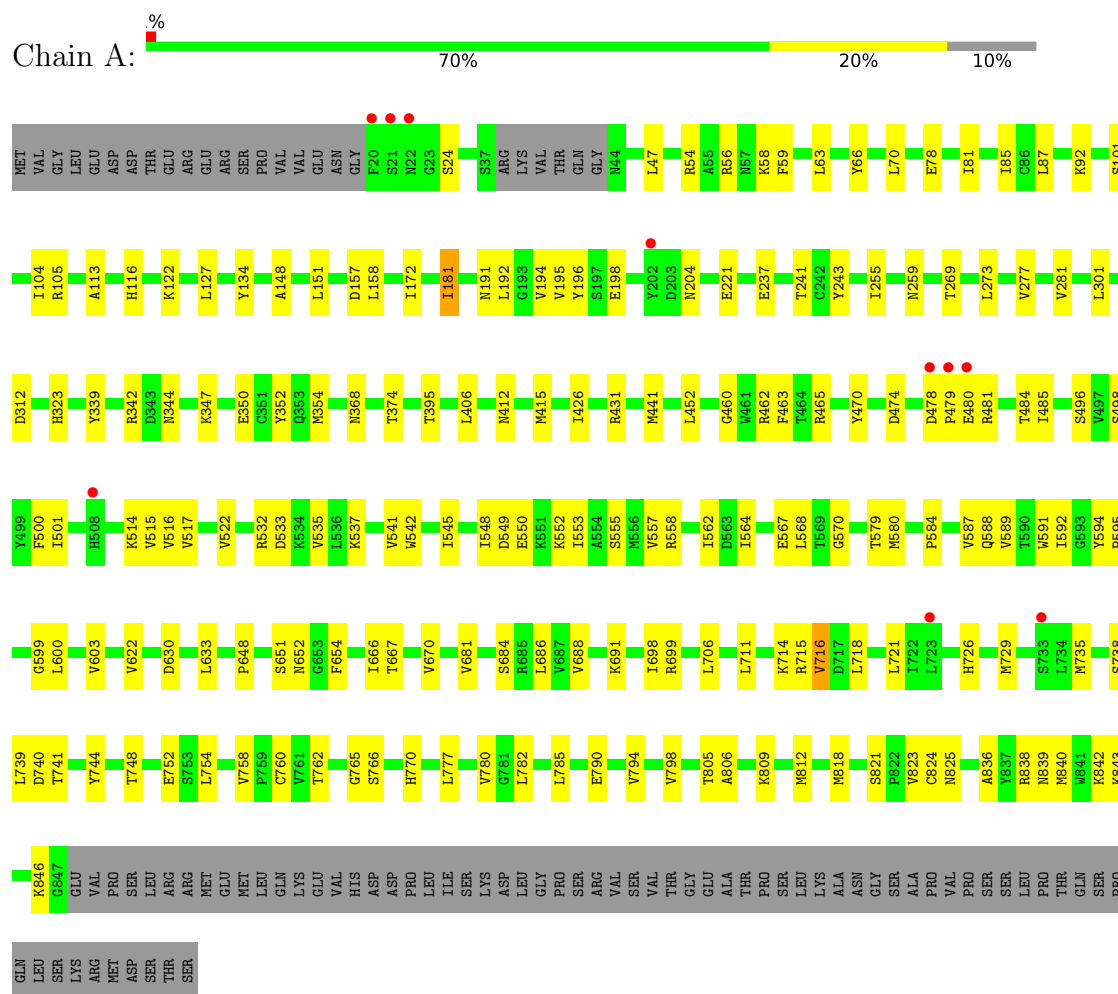
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	2	Total	O	0	0
			2	2		

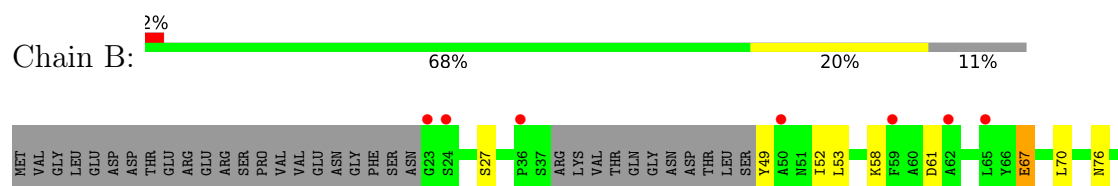
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Probable UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase SPINDLY



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ASN	C824	L706	D604	P479	L236	A79
GLY	N825	E707	Y605	E480	E237	K83
SER	G826	L711	R606	R481	M238	C86
ALA			I607		A239	L87
PRO			T608	F493	I240	
VAL	F829	R715			T241	
PRO		V716	L611	S496		Q90
SER	L833	D717	A612	Y497	M260	
SER		L718	D613	S498	Y284	N94
LEU	A836	L719	P614	Y499		
PRO	Y837	P720		F500	N300	C99
THR	R838	L721	T617	I501		F100
GLN	N839	I722	K618		D312	I104
SER	M840	L723	Q619	P504	H323	K122
PRO	W841		K620	L505		E129
GLN		Y732	Q621	T506	R342	E132
LEU	K846	S733	R627	H507	E350	K136
SER	G847	L734	L628	H508	C351	L151
LYS	E848	M735	P629	Y510	Y352	A152
ARG	VAL	D738			Q353	I153
PRO	PRO	I737	C634	Y518	M354	D157
SER	SER	S738		S519		K163
ASP	LEU		E640		I358	I172
SER	ARG	Y744		F531	N368	Q173
THR	ARG	T747	T647		V372	K174
SER	MET	T748	P648	V535		K175
	GLU					Y176
LEU	MET	S753	S651	K538		E177
GLN	LEU					A178
LYS	LYS	V758	T656	I545		L179
GLU	GLU		F657			I181
VAL	VAL	S766	G658			Y185
HIS	HIS	A769	N662	I548		Y189
ASP	ASP		L663	D549	M379	
PRO	ASP	S775	A664	E550	T395	L192
LEU	PRO			K551	M412	Y196
LEU	LEU	V780	K689	M556	I413	
ILE	ILE	G781		V557	T414	N204
SER	SER	L782	V673	R558	M415	A205
LYS	LYS				I426	L206
ASP	ASP	V794	L678	I562		K211
LEU	LEU	Q795			D450	
GLY	GLY	L796	S684	Y566	E454	Y230
PRO	PRO	S797	R685		G460	
SER	SER	V798	L686	T569		N204
ARG	ARG		V687	G570		A205
VAL	VAL	D799				L206
SER	SER	L800	P692	R583		K211
VAL	VAL					
THR	THR	K809			P468	
GLY	GLY		D696	V587	Q469	
ALA	ALA	M812		Q588	Y470	N204
THR	THR	S813	R699	V589		L206
PRO	PRO	L814	Q700		W473	
THR	THR		R701	Y594	D474	K211
SER	SER	L817	F702	P595	M475	
LEU	LEU	M818	L703		L476	Y230
LYS	LYS		T704	G599	K477	
ALA	ALA	S821	T705		D478	D235

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.73Å 130.68Å 141.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.34 – 2.85 35.34 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.34-2.85) 99.6 (35.34-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.213 , 0.270 (Not available) , 0.254	Depositor DCC
R_{free} test set	2930 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 78.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12812	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8287e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.15	0/6562	0.33	0/8905
1	B	0.14	0/6502	0.33	0/8824
All	All	0.15	0/13064	0.33	0/17729

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

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	6419	0	6336	120	0
1	B	6360	0	6278	130	0
2	A	28	0	12	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
All	All	12812	0	12626	241	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 9.

All (241) 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:B:549:ASP:H	1:B:552:LYS:HE3	1.43	0.83
1:A:545:ILE:HA	1:A:548:ILE:HD12	1.64	0.78
1:B:678:LEU:HD11	1:B:686:LEU:HB2	1.69	0.75
1:A:479:PRO:O	1:A:838:ARG:NH1	2.20	0.74
1:A:780:VAL:HG12	1:A:782:LEU:HD23	1.70	0.74
1:A:478:ASP:HB2	1:A:481:ARG:HB2	1.70	0.73
1:B:548:ILE:HG23	1:B:552:LYS:HD2	1.72	0.70
1:B:583:ARG:NH2	1:B:604:ASP:OD1	2.24	0.70
1:B:501:ILE:HD12	1:B:504:PRO:HG2	1.73	0.70
1:A:148:ALA:HA	1:A:181:ILE:HD11	1.73	0.69
1:A:686:LEU:HB3	1:A:716:VAL:HG12	1.74	0.69
1:A:570:GLY:HA3	1:A:594:TYR:HB2	1.75	0.69
1:B:468:PRO:HD2	1:B:551:LYS:HE2	1.75	0.69
1:B:500:PHE:HE2	1:B:748:THR:HG22	1.57	0.69
1:B:481:ARG:NH2	1:B:841:TRP:CH2	2.62	0.68
1:B:566:VAL:HG22	1:B:589:VAL:HB	1.75	0.67
1:A:395:THR:HA	1:A:426:ILE:HD13	1.75	0.67
1:A:812:MET:SD	1:A:812:MET:N	2.67	0.67
1:A:535:VAL:HG11	1:A:542:TRP:HE3	1.60	0.66
1:A:58:LYS:HE3	1:B:717:ASP:OD1	1.95	0.66
1:B:496:SER:HB3	1:B:748:THR:HG21	1.77	0.66
1:B:230:TYR:CD1	1:B:238:MET:HB3	2.31	0.66
1:A:58:LYS:NZ	1:B:716:VAL:O	2.29	0.65
1:B:611:LEU:HD23	1:B:775:SER:HA	1.79	0.65
1:A:350:GLU:HG2	1:A:354:MET:HE3	1.79	0.65
1:B:312:ASP:OD1	1:B:342:ARG:NH2	2.28	0.65
1:B:628:LEU:HG	1:B:629:PRO:HD2	1.79	0.64
1:A:312:ASP:OD1	1:A:342:ARG:NH2	2.30	0.64
1:B:583:ARG:HA	1:B:588:GLN:NE2	2.11	0.64
1:B:640:GLU:OE2	1:B:640:GLU:N	2.31	0.64
1:B:506:THR:O	1:B:538:LYS:NZ	2.31	0.64
1:A:485:ILE:HD13	1:A:564:ILE:HB	1.80	0.63
1:B:518:TYR:HB3	1:B:545:ILE:HD13	1.80	0.63
1:B:498:SER:HA	1:B:501:ILE:HG22	1.81	0.63
1:B:656:THR:HG22	1:B:685:ARG:HB2	1.80	0.62
1:B:196:TYR:CD2	1:B:204:ASN:HB3	2.35	0.62
1:B:557:VAL:HG13	1:B:562:ILE:HB	1.81	0.62
1:B:76:ASN:ND2	1:B:79:ALA:H	1.98	0.62
1:A:56:ARG:NH1	1:B:717:ASP:OD2	2.33	0.61
1:A:567:GLU:OE2	1:A:570:GLY:N	2.28	0.61
1:B:53:LEU:HB3	1:B:58:LYS:HB2	1.83	0.61
1:A:47:LEU:HD21	1:A:78:GLU:HG2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:ILE:O	1:A:557:VAL:HG23	2.02	0.60
1:B:570:GLY:HA3	1:B:594:TYR:HB2	1.84	0.60
1:A:237:GLU:OE1	1:A:237:GLU:N	2.25	0.60
1:A:441:MET:HE3	1:A:452:LEU:HD13	1.83	0.60
1:B:605:TYR:CE2	1:B:840:MET:HG2	2.36	0.59
1:B:687:VAL:HG23	1:B:717:ASP:HB2	1.85	0.59
1:B:818:MET:HA	1:B:821:SER:HB3	1.84	0.59
1:B:240:ILE:HG23	1:B:260:MET:HE1	1.84	0.58
1:A:706:LEU:HD13	1:A:716:VAL:HG11	1.86	0.58
1:B:476:LEU:HB3	1:B:481:ARG:NH1	2.18	0.58
1:B:549:ASP:OD1	1:B:550:GLU:N	2.37	0.57
1:A:323:HIS:HE1	1:B:323:HIS:NE2	2.02	0.57
1:B:606:ARG:HH21	1:B:621:GLN:HE22	1.53	0.57
1:B:812:MET:SD	1:B:812:MET:N	2.78	0.57
1:A:58:LYS:CE	1:B:717:ASP:OD1	2.52	0.56
1:A:681:VAL:HG23	1:A:798:VAL:HG12	1.88	0.56
1:B:846:LYS:C	1:B:846:LYS:HD3	2.31	0.56
1:A:836:ALA:O	1:A:840:MET:HG3	2.06	0.56
1:B:352:TYR:CZ	1:B:368:ASN:HB3	2.40	0.56
1:A:588:GLN:HB2	1:A:603:VAL:HA	1.88	0.56
1:A:151:LEU:HD23	1:A:181:ILE:HD12	1.88	0.56
1:B:545:ILE:HA	1:B:548:ILE:HD12	1.87	0.56
1:A:58:LYS:NZ	1:B:717:ASP:OD1	2.39	0.56
1:A:754:LEU:C	1:A:818:MET:HE1	2.31	0.56
1:A:431:ARG:HH21	1:A:463:PHE:HZ	1.53	0.56
1:B:237:GLU:H	1:B:237:GLU:CD	2.14	0.56
1:A:843:LYS:O	1:A:843:LYS:HD3	2.06	0.56
1:A:535:VAL:HG11	1:A:542:TRP:CE3	2.41	0.55
1:B:617:THR:HG22	1:B:619:GLN:H	1.71	0.55
1:B:238:MET:HA	1:B:241:THR:HG22	1.89	0.55
1:A:66:TYR:O	1:A:70:LEU:HD12	2.06	0.54
1:B:658:GLY:HA3	1:B:735:MET:HE2	1.89	0.54
1:A:474:ASP:OD2	1:A:474:ASP:N	2.35	0.54
1:A:821:SER:HB2	1:A:823:VAL:HG22	1.88	0.54
1:A:691:LYS:HD2	1:A:721:LEU:HD12	1.90	0.54
1:A:782:LEU:HB3	1:A:785:LEU:CD1	2.37	0.54
1:B:129:GLU:OE1	1:B:129:GLU:N	2.31	0.54
1:B:611:LEU:HB3	1:B:775:SER:HB2	1.90	0.54
1:B:493:PHE:HD1	1:B:493:PHE:H	1.56	0.54
1:B:678:LEU:HD12	1:B:711:LEU:HD21	1.89	0.53
1:A:806:ALA:HA	1:A:809:LYS:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:PRO:HG3	1:A:744:TYR:CZ	2.43	0.53
1:B:83:LYS:HG2	1:B:87:LEU:HD13	1.90	0.53
1:B:175:TYR:O	1:B:179:LEU:HD12	2.09	0.53
1:B:839:ASN:C	1:B:839:ASN:HD22	2.17	0.53
1:A:85:ILE:HD11	1:A:116:HIS:NE2	2.24	0.52
1:A:533:ASP:O	1:A:537:LYS:HG3	2.10	0.52
1:B:94:ASN:OD1	1:B:94:ASN:N	2.43	0.52
1:A:760:CYS:O	1:A:777:LEU:HD11	2.09	0.52
1:B:780:VAL:HG13	1:B:818:MET:HB3	1.91	0.52
1:B:595:PRO:HG3	1:B:744:TYR:CZ	2.44	0.52
1:B:395:THR:HA	1:B:426:ILE:HD13	1.93	0.51
1:B:413:ILE:HD11	1:B:664:ALA:HB1	1.91	0.51
1:A:729:MET:HE1	1:A:752:GLU:HG2	1.92	0.51
1:A:699:ARG:HG2	1:A:718:LEU:HD12	1.92	0.51
1:B:701:ARG:O	1:B:705:THR:HG23	2.11	0.51
1:B:706:LEU:HD22	1:B:711:LEU:HD23	1.93	0.51
1:A:56:ARG:HH21	1:B:734:LEU:HD23	1.76	0.50
1:A:127:LEU:HB3	1:A:158:LEU:HD11	1.93	0.50
1:B:132:GLU:O	1:B:136:LYS:HG2	2.10	0.50
1:B:552:LYS:O	1:B:556:MET:HG3	2.10	0.50
1:B:735:MET:HG2	1:B:758:VAL:HG11	1.93	0.50
1:B:628:LEU:HD11	1:B:833:LEU:HA	1.94	0.50
1:A:549:ASP:OD1	1:A:550:GLU:N	2.44	0.50
1:B:49:TYR:O	1:B:53:LEU:HD12	2.11	0.50
1:B:613:ASP:O	1:B:627:ARG:NH1	2.45	0.50
1:B:237:GLU:OE2	1:B:237:GLU:N	2.33	0.50
1:B:450:ASP:O	1:B:454:GLU:HG3	2.12	0.49
1:B:737:ILE:HG12	1:B:800:LEU:HD22	1.95	0.49
1:A:412:ASN:ND2	1:A:415:MET:HG3	2.27	0.49
1:B:83:LYS:HZ3	1:B:99:CYS:HB3	1.76	0.49
1:B:67:GLU:HA	1:B:70:LEU:HD12	1.94	0.49
1:A:462:ARG:HG2	1:A:465:ARG:HH12	1.77	0.49
1:A:374:THR:HG23	1:A:406:LEU:HD23	1.93	0.49
1:A:735:MET:HE3	1:A:758:VAL:HG11	1.95	0.49
1:A:517:VAL:HG11	1:A:542:TRP:CZ3	2.47	0.49
1:B:412:ASN:OD1	1:B:415:MET:HE3	2.13	0.49
1:B:230:TYR:HD1	1:B:238:MET:HB3	1.75	0.48
1:A:762:THR:HG23	1:A:777:LEU:HD12	1.95	0.48
1:A:194:VAL:O	1:A:198:GLU:HG2	2.13	0.48
1:A:480:GLU:N	1:A:480:GLU:OE1	2.47	0.48
1:B:189:TYR:CZ	1:B:211:LYS:HG2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:VAL:O	1:A:281:VAL:HG23	2.12	0.48
1:B:90:GLN:N	1:B:90:GLN:OE1	2.47	0.48
1:B:173:GLN:O	1:B:177:GLU:HG3	2.14	0.48
1:A:667:THR:HG23	1:A:670:VAL:H	1.77	0.48
1:B:782:LEU:HD11	1:B:814:LEU:HD21	1.94	0.48
1:A:122:LYS:NZ	1:A:157:ASP:OD2	2.40	0.48
1:A:352:TYR:CZ	1:A:368:ASN:HB3	2.49	0.48
1:A:579:THR:O	1:A:584:PRO:HD3	2.14	0.48
1:A:56:ARG:NH2	1:B:734:LEU:HD23	2.29	0.47
1:A:101:SER:HA	1:A:104:ILE:HG13	1.96	0.47
1:A:500:PHE:CD2	1:A:633:LEU:HB3	2.47	0.47
1:B:350:GLU:O	1:B:354:MET:HG3	2.14	0.47
1:B:479:PRO:HA	1:B:841:TRP:CD1	2.49	0.47
1:B:658:GLY:O	1:B:738:SER:HA	2.15	0.47
1:A:484:THR:OG1	1:A:562:ILE:HA	2.14	0.47
1:B:510:TYR:CE2	1:B:538:LYS:HB2	2.50	0.47
1:A:191:ASN:O	1:A:195:VAL:HG23	2.15	0.47
1:B:510:TYR:CD2	1:B:538:LYS:HB2	2.49	0.47
1:A:221:GLU:OE1	1:A:221:GLU:N	2.37	0.46
1:A:134:TYR:HB3	1:A:151:LEU:HB2	1.96	0.46
1:A:344:ASN:C	1:A:344:ASN:HD22	2.22	0.46
1:B:500:PHE:CE2	1:B:748:THR:HG22	2.43	0.46
1:B:836:ALA:O	1:B:840:MET:HG3	2.16	0.46
1:A:568:LEU:HD22	1:A:592:ILE:HD12	1.98	0.46
1:B:189:TYR:CE2	1:B:211:LYS:HG2	2.51	0.46
1:B:684:SER:N	1:B:715:ARG:HH21	2.13	0.46
1:A:56:ARG:HG3	1:A:56:ARG:HH11	1.81	0.46
1:A:243:TYR:CZ	1:A:259:ASN:HB3	2.50	0.46
1:A:735:MET:HE2	1:A:735:MET:HB3	1.72	0.46
1:B:460:GLY:HA3	1:B:599:GLY:O	2.16	0.46
1:B:696:ASP:CG	1:B:699:ARG:HE	2.24	0.46
1:B:122:LYS:NZ	1:B:157:ASP:OD2	2.37	0.46
1:A:564:ILE:HG12	1:A:587:VAL:HB	1.97	0.45
1:A:805:THR:O	1:A:809:LYS:HG3	2.17	0.45
1:A:782:LEU:HB3	1:A:785:LEU:HD12	1.98	0.45
1:B:837:TYR:O	1:B:840:MET:HB2	2.16	0.45
1:A:470:TYR:CE2	1:A:558:ARG:HD2	2.52	0.45
1:A:501:ILE:O	1:A:501:ILE:HG13	2.17	0.45
1:A:339:TYR:CD2	1:A:347:LYS:HG2	2.51	0.45
1:A:842:LYS:O	1:A:846:LYS:HG3	2.17	0.45
1:B:507:HIS:ND1	1:B:826:GLY:HA3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:MET:HE3	1:B:692:PRO:HB3	1.99	0.45
1:A:498:SER:HA	1:A:501:ILE:HG22	1.99	0.44
1:B:605:TYR:CD2	1:B:840:MET:HG2	2.52	0.44
1:B:476:LEU:HB3	1:B:481:ARG:HH11	1.83	0.44
1:B:818:MET:O	1:B:824:CYS:HB2	2.17	0.44
1:A:56:ARG:NH1	1:A:56:ARG:HG3	2.32	0.44
1:B:235:ASP:OD1	1:B:238:MET:HB2	2.18	0.44
1:B:608:THR:HG21	1:B:613:ASP:HB2	1.99	0.44
1:A:196:TYR:CD2	1:A:204:ASN:HB3	2.52	0.44
1:B:470:TYR:CD2	1:B:558:ARG:HD2	2.53	0.44
1:B:151:LEU:HD23	1:B:181:ILE:HG21	2.00	0.44
1:B:700:GLN:O	1:B:704:THR:HG23	2.18	0.44
1:B:76:ASN:HD22	1:B:79:ALA:H	1.62	0.44
1:B:737:ILE:HG12	1:B:800:LEU:CD2	2.48	0.44
1:A:654:PHE:HZ	1:B:52:ILE:HG21	1.83	0.43
1:B:172:ILE:HG23	1:B:192:LEU:HD21	2.00	0.43
1:B:628:LEU:HD21	1:B:833:LEU:HB2	2.01	0.43
1:B:648:PRO:HG3	1:B:733:SER:O	2.17	0.43
1:B:669:LYS:O	1:B:673:VAL:HG23	2.18	0.43
1:A:721:LEU:HD23	1:A:721:LEU:HA	1.83	0.43
1:A:818:MET:HA	1:A:821:SER:OG	2.19	0.43
1:A:87:LEU:HD22	1:A:92:LYS:HD2	2.01	0.43
1:A:591:TRP:CD2	1:A:592:ILE:HG13	2.54	0.43
1:A:172:ILE:HG23	1:A:192:LEU:HD21	2.00	0.43
1:B:100:PHE:O	1:B:104:ILE:HG23	2.19	0.43
1:A:726:HIS:CD2	1:A:726:HIS:C	2.96	0.43
1:A:54:ARG:HG3	1:A:59:PHE:HE1	1.83	0.43
1:A:790:GLU:O	1:A:794:VAL:HG12	2.18	0.43
1:A:81:ILE:HD11	1:A:113:ALA:HB2	2.00	0.43
1:B:809:LYS:HA	1:B:809:LYS:HD2	1.65	0.43
1:A:104:ILE:HD12	1:A:105:ARG:N	2.34	0.43
1:B:177:GLU:O	1:B:181:ILE:HG12	2.18	0.43
1:B:474:ASP:OD2	1:B:474:ASP:C	2.61	0.42
1:B:614:PRO:O	1:B:617:THR:OG1	2.28	0.42
1:A:648:PRO:HB2	1:A:652:ASN:ND2	2.34	0.42
1:A:684:SER:H	1:A:715:ARG:NH2	2.17	0.42
1:A:599:GLY:HA2	1:A:622:VAL:HG21	2.01	0.42
1:B:732:TYR:CE2	1:B:753:SER:HA	2.55	0.42
1:A:532:ARG:HG3	1:A:542:TRP:CG	2.55	0.42
1:A:549:ASP:HB3	1:A:552:LYS:HG2	2.01	0.42
1:A:839:ASN:O	1:A:842:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:PRO:HB2	1:B:769:ALA:HB2	2.02	0.42
1:B:372:VAL:O	1:B:376:GLN:HG3	2.20	0.42
1:B:703:LEU:O	1:B:707:GLU:HG3	2.20	0.42
1:A:496:SER:HB3	1:A:748:THR:HG21	2.01	0.42
1:A:570:GLY:HA3	1:A:594:TYR:CB	2.44	0.42
1:A:765:GLY:HA3	1:A:770:HIS:CG	2.55	0.42
1:A:516:VAL:HG22	1:A:541:VAL:CG2	2.50	0.42
1:B:794:VAL:O	1:B:798:VAL:HG12	2.20	0.41
1:B:829:PHE:HE2	1:B:833:LEU:HD22	1.84	0.41
1:A:589:VAL:CG2	1:A:840:MET:HE1	2.50	0.41
1:B:470:TYR:CE2	1:B:558:ARG:HD2	2.55	0.41
1:A:714:LYS:HB3	1:A:714:LYS:HE2	1.80	0.41
1:B:354:MET:O	1:B:358:ILE:HD12	2.20	0.41
1:B:172:ILE:HD13	1:B:196:TYR:HE1	1.84	0.41
1:A:591:TRP:CG	1:A:592:ILE:HG13	2.55	0.41
1:A:818:MET:HB3	1:A:818:MET:HE2	1.70	0.41
1:A:54:ARG:HD2	1:A:85:ILE:HG21	2.03	0.41
1:A:460:GLY:HA2	1:A:600:LEU:HD23	2.03	0.41
1:A:580:MET:HE3	1:A:580:MET:HB3	1.86	0.41
1:A:738:SER:O	1:A:760:CYS:HA	2.21	0.41
1:A:269:THR:O	1:A:273:LEU:HG	2.20	0.41
1:A:484:THR:HA	1:A:514:LYS:O	2.20	0.41
1:B:719:LEU:HA	1:B:720:PRO:HD3	1.94	0.41
1:B:813:SER:O	1:B:817:LEU:HB2	2.21	0.41
1:A:237:GLU:O	1:A:241:THR:HG23	2.21	0.41
1:A:740:ASP:OD2	1:A:741:THR:N	2.54	0.41
1:B:153:ILE:HG12	1:B:185:TYR:CE1	2.56	0.41
1:B:473:TRP:HA	1:B:558:ARG:NH2	2.36	0.41
1:B:531:PHE:O	1:B:535:VAL:HG23	2.21	0.41
1:A:281:VAL:HG13	1:A:301:LEU:HD23	2.03	0.40
1:A:823:VAL:HG23	1:A:824:CYS:SG	2.61	0.40
1:A:412:ASN:CG	1:A:415:MET:HG3	2.46	0.40
1:A:738:SER:C	1:A:739:LEU:HD23	2.46	0.40
1:B:206:LEU:HD21	1:B:230:TYR:CE2	2.56	0.40
1:B:284:TYR:CZ	1:B:300:ASN:HB3	2.56	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	818/914 (90%)	813 (99%)	5 (1%)	0	100	100
1	B	811/914 (89%)	807 (100%)	4 (0%)	0	100	100
All	All	1629/1828 (89%)	1620 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	691/774 (89%)	675 (98%)	16 (2%)	44	68
1	B	683/774 (88%)	664 (97%)	19 (3%)	38	62
All	All	1374/1548 (89%)	1339 (98%)	35 (2%)	42	66

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	63	LEU
1	A	181	ILE
1	A	255	ILE
1	A	515	VAL
1	A	522	VAL
1	A	555	SER
1	A	630	ASP

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Mol	Chain	Res	Type
1	A	651	SER
1	A	666	ILE
1	A	688	VAL
1	A	698	ILE
1	A	711	LEU
1	A	716	VAL
1	A	766	SER
1	A	825	ASN
1	B	27	SER
1	B	61	ASP
1	B	67	GLU
1	B	90	GLN
1	B	163	LYS
1	B	206	LEU
1	B	478	ASP
1	B	508	HIS
1	B	519	SER
1	B	569	THR
1	B	587	VAL
1	B	611	LEU
1	B	647	THR
1	B	651	SER
1	B	662	ASN
1	B	723	LEU
1	B	747	THR
1	B	766	SER
1	B	797	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	279	GLN
1	A	323	HIS
1	A	325	ASN
1	A	327	HIS
1	A	344	ASN
1	A	401	ASN
1	A	445	ASN
1	A	726	HIS
1	A	728	HIS
1	A	730	GLN

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Mol	Chain	Res	Type
1	B	76	ASN
1	B	167	ASN
1	B	173	GLN
1	B	279	GLN
1	B	445	ASN
1	B	467	HIS
1	B	588	GLN
1	B	652	ASN
1	B	768	HIS
1	B	839	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	GDP	A	1901	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)

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	GDP	A	1901	-	-	3/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1901	GDP	C5-C4	3.15	1.47	1.38
2	A	1901	GDP	C6-N1	-2.37	1.34	1.38
2	A	1901	GDP	C5-N7	-2.04	1.35	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1901	GDP	C5-C4-N3	-5.96	118.90	128.39
2	A	1901	GDP	C2-N3-C4	4.95	120.82	112.30
2	A	1901	GDP	N9-C4-N3	4.49	134.94	125.95
2	A	1901	GDP	C6-C5-N7	3.24	136.18	130.29
2	A	1901	GDP	C4-C5-N7	-2.46	106.78	110.67
2	A	1901	GDP	C3'-C2'-C1'	2.39	105.98	101.46
2	A	1901	GDP	O6-C6-C5	-2.18	120.78	126.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

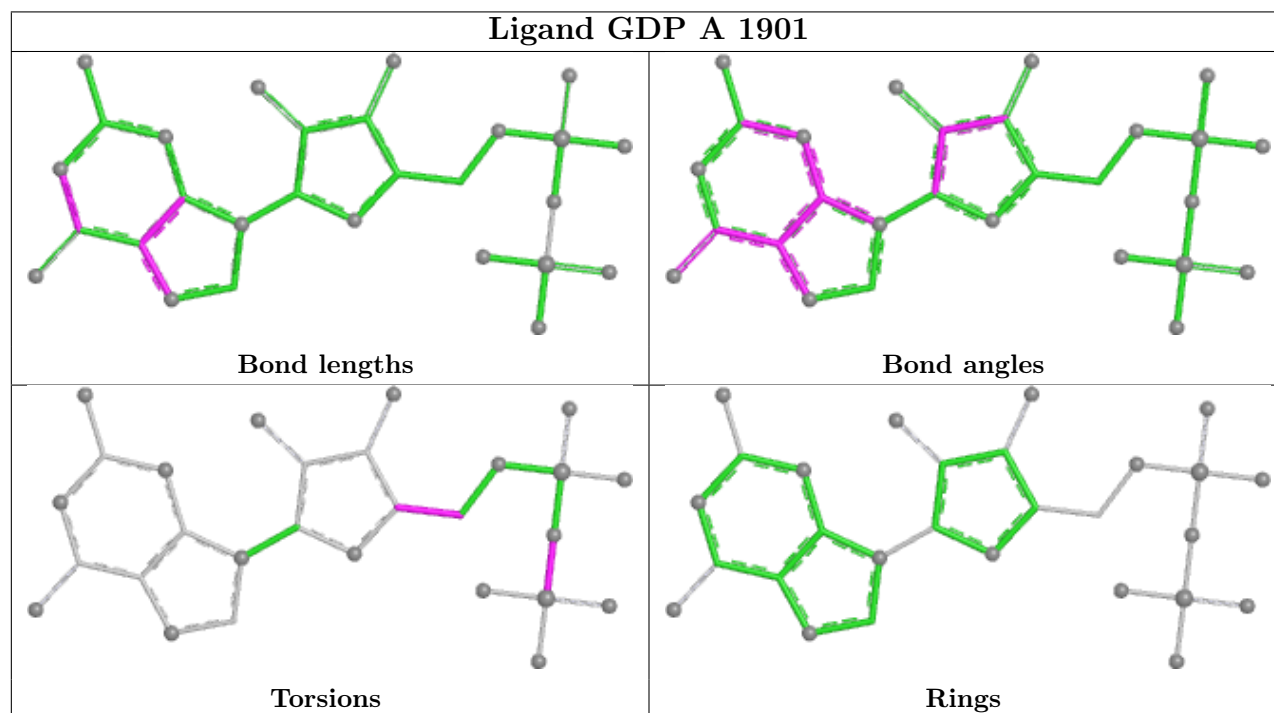
Mol	Chain	Res	Type	Atoms
2	A	1901	GDP	PA-O3A-PB-O2B
2	A	1901	GDP	C3'-C4'-C5'-O5'
2	A	1901	GDP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	822/914 (89%)	-0.02	10 (1%) 76 71	40, 84, 133, 168	0
1	B	815/914 (89%)	-0.11	16 (1%) 65 57	37, 83, 134, 178	0
All	All	1637/1828 (89%)	-0.06	26 (1%) 70 64	37, 84, 134, 178	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	SER	4.9
1	A	478	ASP	4.4
1	A	20	PHE	3.5
1	A	480	GLU	3.3
1	A	508	HIS	2.9
1	A	202	TYR	2.9
1	B	841	TRP	2.8
1	A	479	PRO	2.8
1	B	634	CYS	2.8
1	B	100	PHE	2.7
1	B	59	PHE	2.6
1	B	479	PRO	2.5
1	B	65	LEU	2.5
1	B	36	PRO	2.4
1	B	722	ILE	2.4
1	B	23	GLY	2.3
1	A	723	LEU	2.3
1	B	24	SER	2.3
1	B	62	ALA	2.3
1	B	796	LEU	2.1
1	A	733	SER	2.1
1	A	22	ASN	2.1
1	B	86	CYS	2.1
1	B	723	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	50	ALA	2.1
1	B	720	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

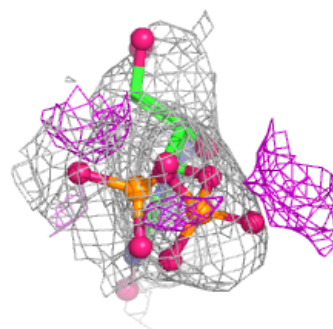
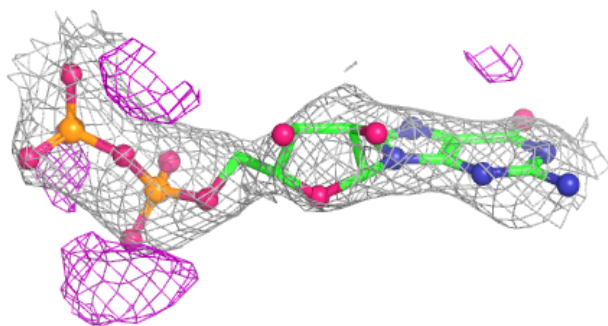
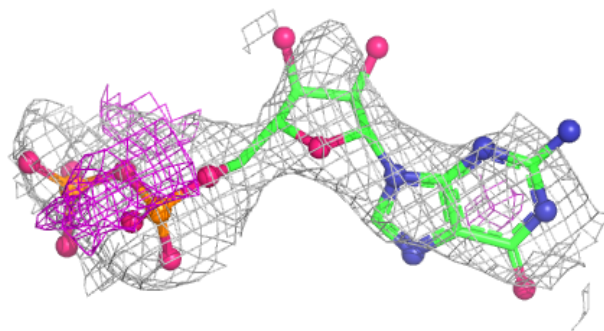
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GDP	A	1901	28/28	0.71	0.13	161,168,183,190	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GDP A 1901:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.