



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:22 AM UTC

PDB ID : 8BUG / pdb\_00008bug  
Title : Structure of DDB1 bound to HQ461-engaged CDK12-cyclin K  
Authors : Kozicka, Z.; Kempf, G.; Focht, V.; Thoma, N.H.  
Deposited on : 2022-11-30  
Resolution : 3.53 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](mailto: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

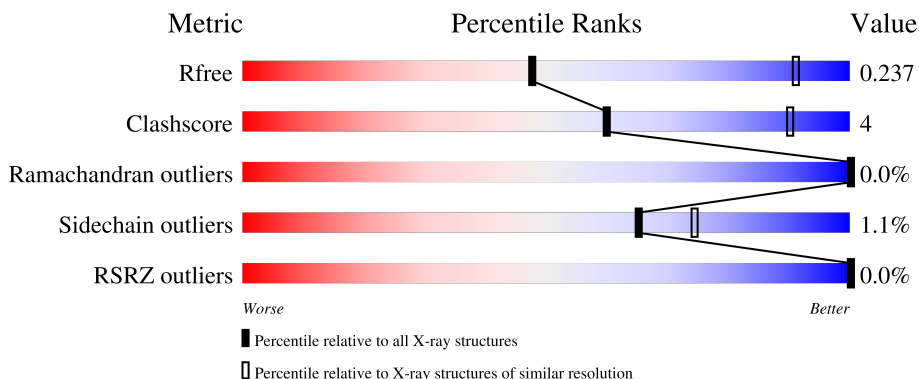
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.53 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	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)

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  $\geq 3$ , 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	840	88% (green), 11% (yellow), 1% (orange), 0% (red), 0% (grey)
1	D	840	87% (green), 11% (yellow), 1% (orange), 0% (red), 0% (grey)
1	G	840	86% (green), 12% (yellow), 1% (orange), 0% (red), 0% (grey)
2	B	344	75% (green), 19% (yellow), 5% (orange), 0% (red), 0% (grey)
2	E	344	79% (green), 15% (yellow), 6% (orange), 0% (red), 0% (grey)

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	H	344	 78% 16% • 6%
3	C	271	 89% • 8%
3	F	271	 89% • 8%
3	I	271	 87% 5% 8%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 67369 atoms, of which 33595 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	826	12938	4105	6451	1094	1252	36	6451	0	0
1	D	827	12958	4111	6463	1095	1253	36	6463	0	0
1	G	826	12941	4106	6455	1093	1251	36	6455	0	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
A	700	GLY	-	linker	UNP Q16531
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531
A	705	GLY	-	linker	UNP Q16531
A	706	GLU	-	linker	UNP Q16531
A	707	ILE	-	linker	UNP Q16531
A	708	GLN	-	linker	UNP Q16531
D	-3	GLY	-	expression tag	UNP Q16531
D	-2	GLY	-	expression tag	UNP Q16531
D	-1	GLY	-	expression tag	UNP Q16531
D	0	ARG	-	expression tag	UNP Q16531
D	700	GLY	-	linker	UNP Q16531
D	701	ASN	-	linker	UNP Q16531
D	702	GLY	-	linker	UNP Q16531
D	703	ASN	-	linker	UNP Q16531
D	704	SER	-	linker	UNP Q16531
D	705	GLY	-	linker	UNP Q16531

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	706	GLU	-	linker	UNP Q16531
D	707	ILE	-	linker	UNP Q16531
D	708	GLN	-	linker	UNP Q16531
G	-3	GLY	-	expression tag	UNP Q16531
G	-2	GLY	-	expression tag	UNP Q16531
G	-1	GLY	-	expression tag	UNP Q16531
G	0	ARG	-	expression tag	UNP Q16531
G	700	GLY	-	linker	UNP Q16531
G	701	ASN	-	linker	UNP Q16531
G	702	GLY	-	linker	UNP Q16531
G	703	ASN	-	linker	UNP Q16531
G	704	SER	-	linker	UNP Q16531
G	705	GLY	-	linker	UNP Q16531
G	706	GLU	-	linker	UNP Q16531
G	707	ILE	-	linker	UNP Q16531
G	708	GLN	-	linker	UNP Q16531

- Molecule 2 is a protein called Cyclin-dependent kinase 12.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P	S			
2	B	327	Total	C	H	N	O	P	S	2676	0	0
			5341	1706	2676	451	490	1	17			
2	E	325	Total	C	H	N	O	P	S	2674	0	0
			5309	1695	2663	447	486	1	17			
2	H	325	Total	C	H	N	O	P	S	2671	0	0
			5309	1695	2663	447	486	1	17			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	709	GLY	-	expression tag	UNP Q9NYV4
B	710	GLY	-	expression tag	UNP Q9NYV4
B	711	GLY	-	expression tag	UNP Q9NYV4
B	965	ARG	LYS	engineered mutation	UNP Q9NYV4
B	1052	GLN	-	expression tag	UNP Q9NYV4
E	709	GLY	-	expression tag	UNP Q9NYV4
E	710	GLY	-	expression tag	UNP Q9NYV4
E	711	GLY	-	expression tag	UNP Q9NYV4
E	965	ARG	LYS	engineered mutation	UNP Q9NYV4
E	1052	GLN	-	expression tag	UNP Q9NYV4
H	709	GLY	-	expression tag	UNP Q9NYV4
H	710	GLY	-	expression tag	UNP Q9NYV4

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	711	GLY	-	expression tag	UNP Q9NYV4
H	965	ARG	LYS	engineered mutation	UNP Q9NYV4
H	1052	GLN	-	expression tag	UNP Q9NYV4

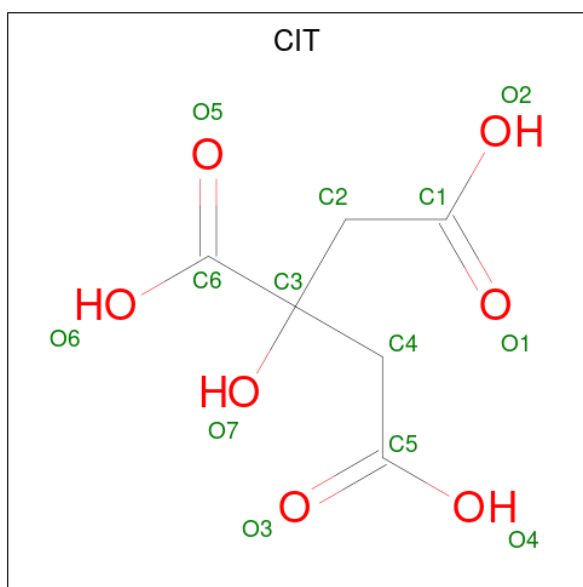
- Molecule 3 is a protein called Cyclin-K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	C	248	Total	C	H	N	O	S	2048	0	0
			4111	1341	2048	346	363	13			
3	F	248	Total	C	H	N	O	S	2048	0	0
			4111	1341	2048	346	363	13			
3	I	248	Total	C	H	N	O	S	2048	0	0
			4111	1341	2048	346	363	13			

There are 12 discrepancies between the modelled and reference sequences:

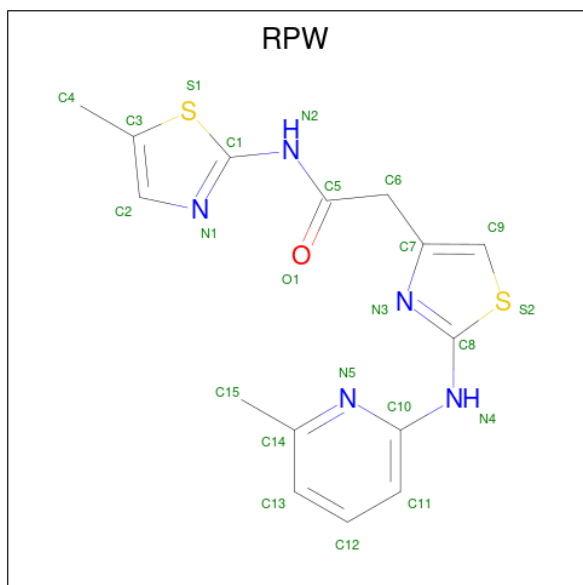
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP O75909
C	-2	GLY	-	expression tag	UNP O75909
C	-1	GLY	-	expression tag	UNP O75909
C	0	ARG	-	expression tag	UNP O75909
F	-3	GLY	-	expression tag	UNP O75909
F	-2	GLY	-	expression tag	UNP O75909
F	-1	GLY	-	expression tag	UNP O75909
F	0	ARG	-	expression tag	UNP O75909
I	-3	GLY	-	expression tag	UNP O75909
I	-2	GLY	-	expression tag	UNP O75909
I	-1	GLY	-	expression tag	UNP O75909
I	0	ARG	-	expression tag	UNP O75909

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	Total 18	C 6	H 5	O 7	5	0
4	C	1	Total 18	C 6	H 5	O 7	5	0
4	D	1	Total 18	C 6	H 5	O 7	5	0
4	F	1	Total 18	C 6	H 5	O 7	5	0
4	H	1	Total 18	C 6	H 5	O 7	5	0
4	H	1	Total 18	C 6	H 5	O 7	5	0
4	I	1	Total 18	C 6	H 5	O 7	5	0

- Molecule 5 is 2-[2-[(6-methylpyridin-2-yl)amino]-1,3-thiazol-4-yl]-{N}-(5-methyl-1,3-thiazol-2-yl)ethanamide (CCD ID: RPW) (formula: C<sub>15</sub>H<sub>15</sub>N<sub>5</sub>OS<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

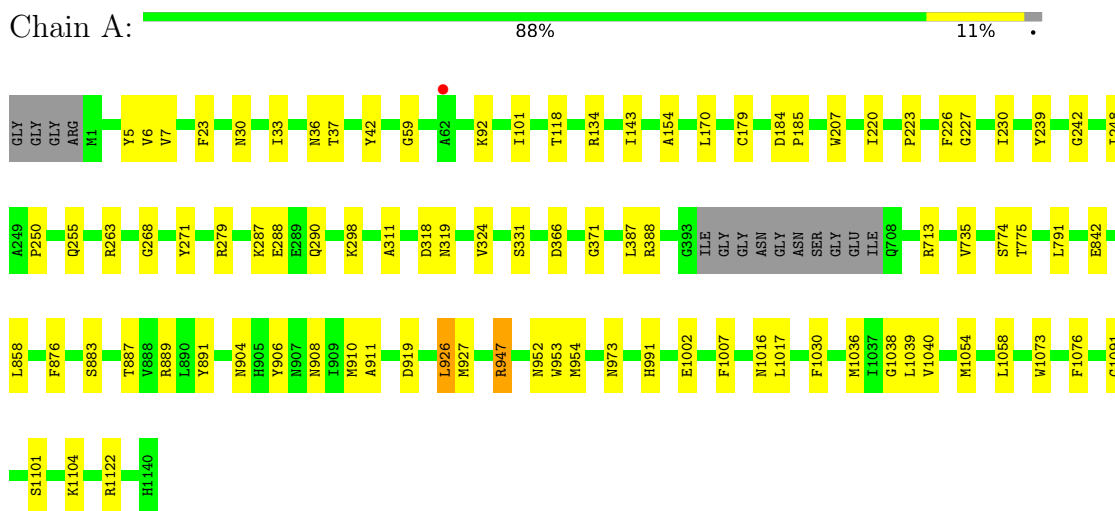


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
5	B	1	Total	C	H	N	O	S	15	0
			38	15	15	5	1	2		
5	D	1	Total	C	H	N	O	S	15	0
			38	15	15	5	1	2		
5	G	1	Total	C	H	N	O	S	15	0
			38	15	15	5	1	2		

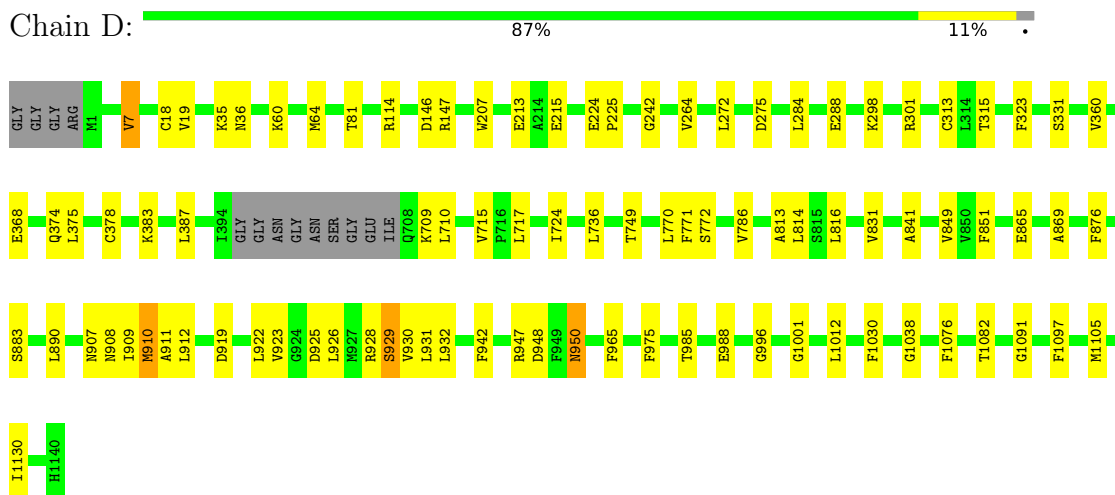
### 3 Residue-property plots [i](#)

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.

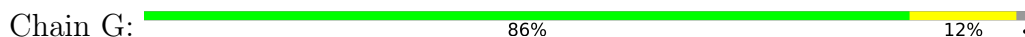
- Molecule 1: DNA damage-binding protein 1

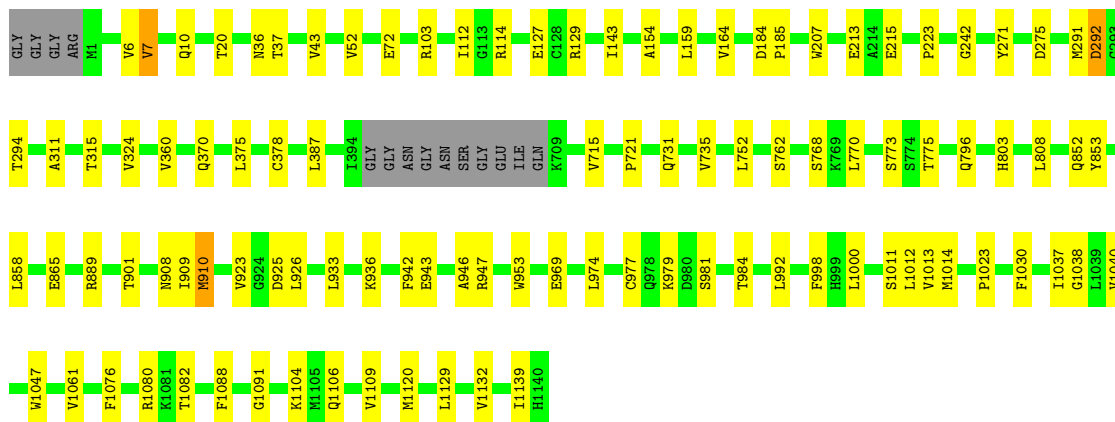


- Molecule 1: DNA damage-binding protein 1



- Molecule 1: DNA damage-binding protein 1

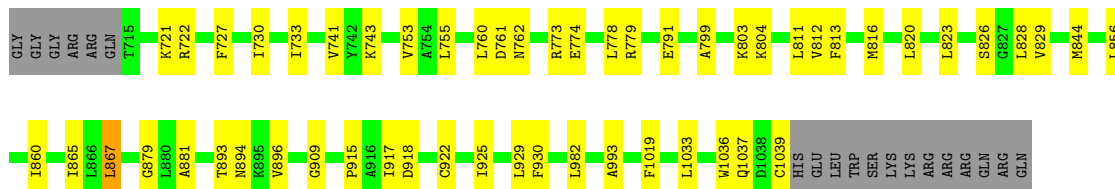
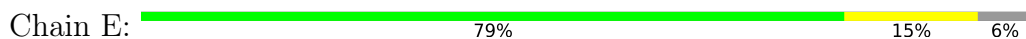




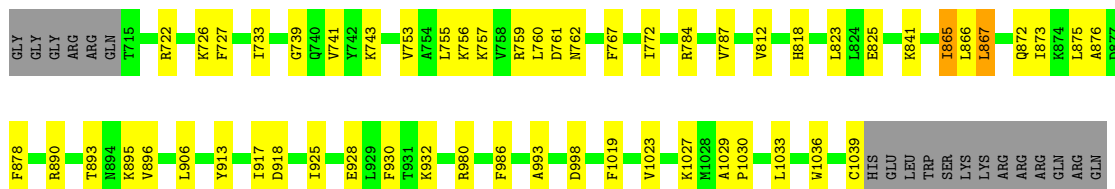
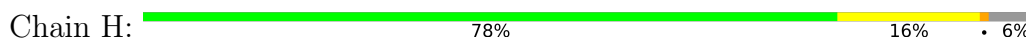
• Molecule 2: Cyclin-dependent kinase 12



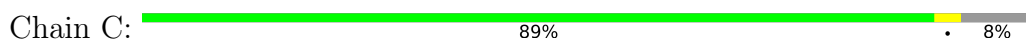
• Molecule 2: Cyclin-dependent kinase 12

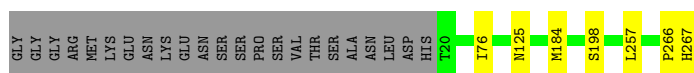


• Molecule 2: Cyclin-dependent kinase 12



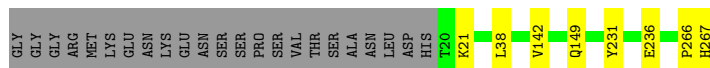
• Molecule 3: Cyclin-K





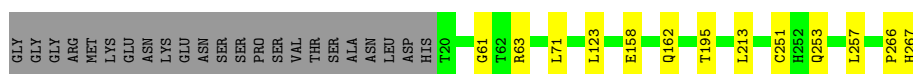
- Molecule 3: Cyclin-K

Chain F: 89% 8%



- Molecule 3: Cyclin-K

Chain I: 87% 5% 8%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	249.65Å 249.65Å 216.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.09 – 3.53 60.09 – 3.53	Depositor EDS
% Data completeness (in resolution range)	82.4 (60.09-3.53) 82.6 (60.09-3.53)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 3.49Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.188 , 0.231 0.201 , 0.237	Depositor DCC
$R_{free}$ test set	3955 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	146.3	Xtrriage
Anisotropy	0.010	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 144.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.067 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	67369	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	178.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: RPW, TPO, CIT

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	0.20	0/6604	0.47	0/8931
1	D	0.19	0/6612	0.44	0/8942
1	G	0.23	1/6603 (0.0%)	0.46	0/8930
2	B	0.20	0/2713	0.47	0/3657
2	E	0.21	0/2693	0.46	0/3630
2	H	0.27	1/2693 (0.0%)	0.50	1/3630 (0.0%)
3	C	0.15	0/2120	0.37	0/2868
3	F	0.16	0/2120	0.40	0/2868
3	I	0.14	0/2120	0.37	0/2868
All	All	0.20	2/34278 (0.0%)	0.45	1/46324 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1030	PRO	CA-C	8.37	1.57	1.52
1	G	292	ASP	CB-CG	-7.78	1.32	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1030	PRO	O-C-N	8.58	125.18	121.15

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	6487	6451	6451	57	2
1	D	6495	6463	6464	52	1
1	G	6486	6455	6454	64	2
2	B	2665	2676	2676	39	0
2	E	2646	2663	2663	37	0
2	H	2646	2663	2663	34	1
3	C	2063	2048	2048	5	0
3	F	2063	2048	2048	6	0
3	I	2063	2048	2048	8	0
4	A	13	5	5	0	0
4	C	13	5	5	0	0
4	D	13	5	5	0	0
4	F	13	5	5	0	0
4	H	26	10	10	0	0
4	I	13	5	5	0	0
5	B	23	15	0	0	0
5	D	23	15	0	2	0
5	G	23	15	0	1	0
All	All	33774	33595	33550	289	3

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 4.

All (289) 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:910:MET:HE3	1:D:926:LEU:HD22	1.56	0.86
1:A:926:LEU:HD21	2:B:828:LEU:HD11	1.57	0.85
1:A:926:LEU:HD21	2:B:828:LEU:CD1	2.14	0.76
1:A:926:LEU:HD23	1:A:927:MET:HB3	1.71	0.72
2:E:799:ALA:HB1	2:E:804:LYS:HB2	1.80	0.64
1:G:946:ALA:HB1	1:G:992:LEU:HG	1.79	0.63
1:A:926:LEU:HD23	1:A:926:LEU:C	2.23	0.63
2:B:828:LEU:HD22	2:B:1034:PRO:HB3	1.80	0.63
1:G:114:ARG:HD3	2:H:930:PHE:O	1.99	0.62
2:H:1027:LYS:HE2	2:H:1029:ALA:HB2	1.81	0.62
1:G:773:SER:O	1:G:775:THR:N	2.31	0.62
1:D:912:LEU:HD11	1:D:926:LEU:HD13	1.81	0.62
2:B:956:CYS:SG	2:B:959:VAL:HG22	2.41	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:947:ARG:HD3	5:D:1202:RPW:C15	2.31	0.60
1:A:926:LEU:O	1:A:953:TRP:HA	2.01	0.60
1:G:7:VAL:HG13	1:G:1091:GLY:HA3	1.84	0.60
2:H:787:VAL:HB	2:H:875:LEU:O	2.02	0.59
2:E:820:LEU:HD21	2:E:929:LEU:HD21	1.84	0.59
2:E:755:LEU:HD22	2:E:812:VAL:HG22	1.84	0.59
1:G:7:VAL:HG21	1:G:1139:ILE:HD11	1.85	0.59
1:G:770:LEU:HD21	1:G:865:GLU:HB2	1.85	0.59
1:D:368:GLU:OE1	1:D:374:GLN:NE2	2.36	0.59
2:B:821:MET:HE3	2:B:863:SER:HB3	1.83	0.59
1:A:366:ASP:OD2	1:A:371:GLY:N	2.35	0.58
1:G:1047:TRP:HZ3	1:G:1132:VAL:HG13	1.67	0.58
2:B:963:VAL:HA	2:B:966:LEU:HD12	1.84	0.58
2:H:865:ILE:HD11	2:H:925:ILE:HD13	1.86	0.58
1:G:43:VAL:HG23	1:G:52:VAL:HG21	1.85	0.58
1:G:773:SER:C	1:G:775:THR:H	2.11	0.58
1:G:72:GLU:OE2	1:G:103:ARG:NH2	2.37	0.58
1:G:852:GLN:O	1:G:858:LEU:HA	2.04	0.57
2:H:841:LYS:HD2	2:H:1023:VAL:HB	1.87	0.57
2:E:823:LEU:CD1	2:E:867:LEU:HD23	2.35	0.57
1:G:1109:VAL:HG12	1:G:1129:LEU:HD12	1.85	0.57
1:D:770:LEU:HD13	1:D:865:GLU:HB2	1.86	0.56
2:H:733:ILE:CG2	2:H:743:LYS:HB2	2.35	0.56
1:G:974:LEU:HD11	1:G:1000:LEU:HD22	1.88	0.56
3:I:63:ARG:HE	3:I:123:LEU:HD21	1.71	0.56
1:D:7:VAL:HG13	1:D:1091:GLY:HA3	1.88	0.55
1:G:947:ARG:HD3	5:G:1201:RPW:C15	2.37	0.55
3:F:231:TYR:OH	3:F:236:GLU:OE1	2.17	0.55
2:B:865:ILE:HD12	2:B:875:LEU:HD12	1.87	0.55
1:A:904:ASN:HB3	1:A:906:TYR:CE1	2.41	0.55
2:E:823:LEU:O	2:E:829:VAL:HG22	2.06	0.55
2:B:951:LEU:HD21	2:B:986:PHE:HE2	1.71	0.55
2:E:755:LEU:CD2	2:E:812:VAL:HG22	2.37	0.55
2:H:823:LEU:CD1	2:H:867:LEU:HD23	2.36	0.55
1:A:1002:GLU:HG3	1:A:1036:MET:HE3	1.89	0.54
1:D:907:ASN:HB2	2:E:730:ILE:HG22	1.89	0.54
2:E:894:ASN:HD21	2:E:909:GLY:HA2	1.73	0.54
2:B:819:ASP:O	2:B:823:LEU:HD12	2.08	0.54
2:E:865:ILE:CD1	2:E:925:ILE:HD13	2.38	0.54
1:A:775:THR:HG22	1:A:775:THR:O	2.07	0.54
1:D:883:SER:HB2	1:D:911:ALA:HB3	1.88	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:977:CYS:HB3	1:G:992:LEU:HD22	1.90	0.53
1:A:36:ASN:O	1:A:37:THR:OG1	2.20	0.53
1:G:768:SER:HB3	1:G:808:LEU:HD11	1.89	0.53
2:H:784:ARG:HH21	2:H:872:GLN:HG3	1.72	0.53
2:E:823:LEU:HB3	2:E:829:VAL:HG11	1.91	0.53
2:E:760:LEU:HD12	2:E:760:LEU:N	2.23	0.52
1:A:926:LEU:HD23	1:A:927:MET:CB	2.38	0.52
2:H:818:HIS:HB3	2:H:823:LEU:HD21	1.91	0.52
2:H:760:LEU:HD12	2:H:760:LEU:N	2.25	0.52
1:D:909:ILE:HD12	1:D:928:ARG:HG2	1.90	0.52
1:G:858:LEU:HD12	1:G:858:LEU:O	2.09	0.52
3:F:38:LEU:O	1:G:752:LEU:HA	2.09	0.52
1:G:1047:TRP:CZ3	1:G:1132:VAL:HG13	2.43	0.52
1:D:207:TRP:HB3	1:D:242:GLY:HA2	1.92	0.52
1:G:1023:PRO:HB3	1:G:1047:TRP:CE2	2.45	0.52
2:H:895:LYS:H	2:H:906:LEU:HD22	1.75	0.52
1:A:311:ALA:HB2	1:A:324:VAL:HG13	1.92	0.51
2:E:823:LEU:HD13	2:E:867:LEU:HD23	1.92	0.51
1:D:213:GLU:HG2	1:D:215:GLU:H	1.75	0.51
1:G:112:ILE:HD13	2:H:986:PHE:CE2	2.46	0.51
1:D:908:ASN:ND2	1:D:923:VAL:HG11	2.26	0.51
2:H:928:GLU:O	2:H:932:LYS:N	2.43	0.51
2:E:803:LYS:HG3	3:F:142:VAL:HG21	1.93	0.51
1:A:953:TRP:HD1	1:A:954:MET:N	2.09	0.51
1:D:816:LEU:HD13	1:D:831:VAL:HG22	1.93	0.51
2:E:856:LEU:HD11	2:E:915:PRO:HG3	1.93	0.51
1:A:387:LEU:HD11	1:A:735:VAL:HG21	1.92	0.50
2:E:727:PHE:CE1	2:E:753:VAL:HG21	2.46	0.50
1:A:7:VAL:HG12	1:A:1091:GLY:HA3	1.93	0.50
1:A:207:TRP:HB3	1:A:242:GLY:HA2	1.94	0.50
1:D:19:VAL:HG22	1:D:64:MET:HE3	1.93	0.50
2:H:755:LEU:HD22	2:H:812:VAL:HG22	1.93	0.50
1:A:887:THR:HG23	1:A:906:TYR:CE1	2.47	0.50
1:D:60:LYS:O	1:D:81:THR:HA	2.12	0.50
2:E:733:ILE:CG2	2:E:743:LYS:HB2	2.42	0.49
1:G:378:CYS:HB3	1:G:721:PRO:HB2	1.94	0.49
2:H:741:VAL:HG22	2:H:756:LYS:HE3	1.94	0.49
1:G:1061:VAL:HG11	1:G:1104:LYS:HB3	1.95	0.49
2:H:865:ILE:CD1	2:H:925:ILE:HD13	2.42	0.49
2:B:954:SER:OG	2:B:978:TYR:N	2.43	0.49
3:C:184:MET:HE2	3:C:267:HIS:HA	1.95	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:929:SER:HB3	1:D:948:ASP:HB3	1.94	0.49
1:A:926:LEU:HD23	1:A:927:MET:N	2.27	0.48
1:D:1105:MET:SD	1:D:1130:ILE:HD11	2.53	0.48
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.48	0.48
2:B:820:LEU:HD12	2:B:824:LEU:HG	1.95	0.48
1:A:170:LEU:HD11	1:A:179:CYS:HB2	1.95	0.48
2:E:844:MET:HE1	2:E:922:CYS:SG	2.54	0.48
2:B:895:LYS:H	2:B:906:LEU:HD22	1.78	0.48
1:G:311:ALA:HB2	1:G:324:VAL:HG13	1.96	0.48
2:B:856:LEU:HD21	2:B:915:PRO:HG3	1.96	0.48
2:B:910:GLU:O	2:B:911:GLU:HB2	2.14	0.47
1:D:922:LEU:HD11	1:D:930:VAL:HB	1.95	0.47
2:E:733:ILE:HD11	2:E:741:VAL:HG12	1.94	0.47
1:G:292:ASP:OD2	1:G:294:THR:HG23	2.13	0.47
2:E:826:SER:HB2	2:E:828:LEU:HD12	1.95	0.47
1:G:36:ASN:O	1:G:37:THR:OG1	2.21	0.47
2:B:896:VAL:HG23	2:B:906:LEU:HD11	1.95	0.47
1:A:953:TRP:HD1	1:A:954:MET:H	1.60	0.47
1:A:926:LEU:CD2	1:A:927:MET:HB3	2.42	0.47
1:D:264:VAL:CG2	1:D:272:LEU:HG	2.45	0.47
2:E:823:LEU:HB3	2:E:829:VAL:CG1	2.45	0.47
1:G:207:TRP:HB3	1:G:242:GLY:HA2	1.96	0.47
1:D:146:ASP:OD1	1:D:147:ARG:N	2.48	0.47
1:G:375:LEU:HB2	1:G:1012:LEU:HD21	1.95	0.47
1:A:5:TYR:CE2	1:A:7:VAL:HG13	2.50	0.47
2:B:732:ILE:HG23	2:B:732:ILE:O	2.14	0.47
1:D:387:LEU:HG	1:D:717:LEU:HD11	1.97	0.47
2:E:811:LEU:HB2	2:E:813:PHE:HE1	1.80	0.47
2:H:727:PHE:CE1	2:H:753:VAL:HG21	2.49	0.47
2:B:1010:THR:O	2:B:1014:THR:HG23	2.15	0.46
1:A:248:ILE:HG12	1:A:250:PRO:HD3	1.97	0.46
1:D:224:GLU:N	1:D:225:PRO:HD2	2.30	0.46
2:E:865:ILE:HD12	2:E:925:ILE:HD13	1.96	0.46
1:G:387:LEU:HD11	1:G:735:VAL:HG21	1.97	0.46
1:G:908:ASN:ND2	1:G:923:VAL:HG11	2.29	0.46
2:H:865:ILE:HD11	2:H:925:ILE:CD1	2.45	0.46
1:D:1097:PHE:O	1:D:1105:MET:HE2	2.15	0.46
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.46	0.46
2:B:865:ILE:HD13	2:B:865:ILE:N	2.31	0.46
1:D:985:THR:HB	1:D:988:GLU:HG2	1.98	0.46
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.50	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:917:ILE:HG13	2:H:918:ASP:N	2.31	0.46
1:D:925:ASP:OD1	1:D:926:LEU:N	2.46	0.46
1:G:43:VAL:HG23	1:G:52:VAL:CG2	2.46	0.46
1:D:36:ASN:ND2	1:D:1001:GLY:O	2.49	0.46
1:D:912:LEU:HD11	1:D:926:LEU:CD1	2.45	0.46
2:B:917:ILE:HG13	2:B:918:ASP:N	2.31	0.45
1:D:709:LYS:HG2	1:D:710:LEU:N	2.31	0.45
1:D:736:LEU:HD13	1:D:813:ALA:HB1	1.97	0.45
2:E:774:GLU:HG2	2:E:778:LEU:HD12	1.98	0.45
1:A:1054:MET:HE2	1:A:1058:LEU:HD11	1.98	0.45
1:G:370:GLN:HG2	1:G:1014:MET:HE1	1.98	0.45
1:G:908:ASN:HD21	1:G:923:VAL:HG11	1.80	0.45
2:H:739:GLY:HA3	2:H:757:LYS:O	2.17	0.45
2:H:890:ARG:HD3	2:H:890:ARG:HA	1.70	0.45
2:E:773:ARG:HD2	2:E:879:GLY:O	2.17	0.45
1:G:275:ASP:C	1:G:275:ASP:OD1	2.59	0.45
1:G:946:ALA:CB	1:G:992:LEU:HG	2.47	0.45
1:G:159:LEU:HD21	1:G:164:VAL:HG21	1.99	0.45
1:G:984:THR:O	1:G:984:THR:HG22	2.16	0.45
2:H:767:PHE:HD2	2:H:772:ILE:HG13	1.80	0.45
1:A:6:VAL:HG22	1:A:1040:VAL:HG22	1.99	0.45
1:D:114:ARG:HD3	2:E:930:PHE:O	2.16	0.45
2:E:733:ILE:HD11	2:E:741:VAL:CG1	2.46	0.45
1:G:10:GLN:HB3	1:G:1037:ILE:HB	1.99	0.45
1:G:387:LEU:HB2	1:G:715:VAL:HB	1.98	0.45
2:B:791:GLU:HG3	2:B:812:VAL:HG21	1.98	0.44
2:B:839:PHE:HA	2:B:873:ILE:HD13	1.99	0.44
2:E:844:MET:HE2	2:E:844:MET:HA	1.99	0.44
1:G:213:GLU:HG2	1:G:215:GLU:H	1.81	0.44
1:G:936:LYS:HE3	1:G:943:GLU:OE1	2.16	0.44
1:G:291:MET:HE3	1:G:291:MET:HB2	1.90	0.44
2:B:773:ARG:HD3	2:B:881:ALA:O	2.18	0.44
1:G:909:ILE:HB	1:G:925:ASP:OD2	2.17	0.44
1:G:910:MET:CE	1:G:926:LEU:HD22	2.47	0.44
1:A:220:ILE:HB	1:A:230:ILE:HB	2.00	0.44
2:H:761:ASP:OD1	2:H:762:ASN:N	2.51	0.44
1:A:842:GLU:OE2	1:A:910:MET:HE2	2.17	0.44
1:D:932:LEU:HD22	1:D:965:PHE:CZ	2.53	0.44
1:A:255:GLN:HB2	1:A:279:ARG:HH22	1.83	0.44
2:B:910:GLU:HG3	2:B:912:ARG:H	1.82	0.44
1:G:1011:SER:OG	1:G:1013:VAL:HG22	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:866:LEU:HD21	2:H:876:ALA:CB	2.48	0.44
1:D:950:ASN:OD1	1:D:950:ASN:N	2.51	0.44
2:E:721:LYS:HE3	3:F:149:GLN:O	2.18	0.44
1:G:853:TYR:HA	1:G:858:LEU:HA	2.00	0.44
1:A:118:THR:OG1	1:A:134:ARG:NH2	2.33	0.43
1:A:953:TRP:CD1	1:A:954:MET:N	2.86	0.43
1:A:973:ASN:HB3	1:A:1076:PHE:CE2	2.52	0.43
1:D:814:LEU:CD1	1:D:869:ALA:HB1	2.48	0.43
1:A:288:GLU:HB2	1:A:298:LYS:HB2	2.00	0.43
1:A:774:SER:O	1:A:775:THR:HB	2.18	0.43
2:H:866:LEU:HD21	2:H:876:ALA:HB2	1.99	0.43
1:A:947:ARG:HH11	1:A:947:ARG:CG	2.32	0.43
1:G:184:ASP:HB2	1:G:185:PRO:CD	2.48	0.43
1:G:910:MET:HE3	1:G:926:LEU:HD22	2.01	0.43
1:D:890:LEU:HB2	1:D:942:PHE:HZ	1.83	0.43
1:G:953:TRP:O	1:G:969:GLU:HA	2.19	0.43
3:I:195:THR:HG21	3:I:257:LEU:HD11	2.01	0.43
2:B:751:GLU:OE1	2:B:790:LYS:NZ	2.51	0.43
1:D:18:CYS:SG	1:D:313:CYS:SG	3.13	0.43
1:D:35:LYS:O	1:D:36:ASN:C	2.61	0.43
1:D:378:CYS:SG	1:D:724:ILE:HB	2.59	0.43
1:A:223:PRO:HD3	1:A:271:TYR:OH	2.19	0.43
1:A:388:ARG:HA	1:A:713:ARG:O	2.19	0.43
2:H:757:LYS:HE3	2:H:759:ARG:HG2	2.00	0.43
3:I:195:THR:CG2	3:I:257:LEU:HD11	2.49	0.43
1:A:263:ARG:HB2	1:A:271:TYR:CE2	2.54	0.43
1:G:762:SER:O	1:G:803:HIS:HA	2.18	0.43
1:A:227:GLY:O	1:A:239:TYR:OH	2.34	0.43
2:B:859:ASP:O	2:B:864:ASN:ND2	2.51	0.43
1:G:933:LEU:HD22	1:G:942:PHE:HB3	2.00	0.43
1:A:876:PHE:CZ	1:A:919:ASP:HA	2.54	0.43
1:A:92:LYS:HD2	1:A:101:ILE:HD11	2.00	0.42
1:D:1030:PHE:CZ	1:D:1038:GLY:HA3	2.54	0.42
3:I:253:GLN:O	3:I:257:LEU:HG	2.19	0.42
1:A:1016:ASN:O	1:A:1017:LEU:HB2	2.20	0.42
2:B:828:LEU:HD13	2:B:1034:PRO:HG3	2.02	0.42
2:B:844:MET:HE1	2:B:922:CYS:HB3	2.01	0.42
2:E:722:ARG:NH1	2:E:791:GLU:OE2	2.52	0.42
2:H:993:ALA:HB2	2:H:1019:PHE:CE1	2.54	0.42
3:I:266:PRO:O	3:I:267:HIS:C	2.61	0.42
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.55	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:771:PHE:O	1:D:772:SER:C	2.62	0.42
3:I:61:GLY:HA3	3:I:71:LEU:CD2	2.49	0.42
3:I:213:LEU:HB2	3:I:251:CYS:SG	2.60	0.42
1:A:991:HIS:HB2	2:B:735:GLU:OE2	2.19	0.42
2:E:917:ILE:HG13	2:E:918:ASP:N	2.35	0.42
1:G:20:THR:HG23	1:G:315:THR:OG1	2.19	0.42
2:H:755:LEU:CD2	2:H:812:VAL:HG22	2.49	0.42
1:A:1039:LEU:C	1:A:1039:LEU:HD23	2.44	0.42
2:B:821:MET:CE	2:B:863:SER:HB3	2.50	0.42
2:B:849:TYR:O	2:B:853:LYS:HG2	2.20	0.42
1:D:849:VAL:HG11	1:D:851:PHE:CZ	2.55	0.42
1:G:731:GLN:OE1	1:G:796:GLN:NE2	2.52	0.42
1:A:223:PRO:HD2	1:A:268:GLY:HA3	2.01	0.42
1:D:841:ALA:HA	2:E:1037:GLN:HE22	1.85	0.42
1:A:226:PHE:CE2	1:A:287:LYS:HG2	2.54	0.42
1:A:1101:SER:OG	1:A:1104:LYS:HG2	2.19	0.42
2:B:841:LYS:HD2	2:B:1023:VAL:HB	2.02	0.42
1:A:23:PHE:N	1:A:30:ASN:OD1	2.53	0.42
2:B:1035:HIS:ND1	2:B:1037:GLN:HB2	2.35	0.42
1:D:1076:PHE:O	1:D:1082:THR:HA	2.20	0.42
1:G:998:PHE:HB2	1:G:1088:PHE:CG	2.55	0.42
1:G:1080:ARG:HD3	2:H:825:GLU:HA	2.01	0.42
1:D:288:GLU:HB2	1:D:298:LYS:HB2	2.02	0.42
2:E:993:ALA:HB2	2:E:1019:PHE:CE1	2.55	0.42
1:G:143:ILE:HG12	1:G:154:ALA:HB2	2.02	0.42
1:A:1007:PHE:CD1	1:A:1030:PHE:HB3	2.55	0.41
2:H:722:ARG:HE	2:H:726:LYS:HG3	1.85	0.41
3:I:158:GLU:OE1	3:I:162:GLN:NE2	2.50	0.41
1:A:883:SER:HB2	1:A:911:ALA:HB3	2.02	0.41
2:B:842:GLN:HG2	2:B:1025:LEU:HD11	2.02	0.41
1:D:375:LEU:HB2	1:D:1012:LEU:HD21	2.01	0.41
1:G:1030:PHE:CZ	1:G:1038:GLY:HA3	2.54	0.41
1:D:387:LEU:HB2	1:D:715:VAL:HB	2.02	0.41
5:D:1202:RPW:C6	2:E:816:MET:O	2.69	0.41
2:E:779:ARG:HB3	3:F:21:LYS:HE2	2.02	0.41
2:B:823:LEU:CD1	2:B:867:LEU:HD21	2.51	0.41
2:H:867:LEU:HB2	2:H:873:ILE:CD1	2.50	0.41
2:B:856:LEU:HD11	2:B:884:TYR:HB2	2.03	0.41
3:C:76:ILE:CD1	3:C:198:SER:HB3	2.51	0.41
2:E:773:ARG:HD3	2:E:881:ALA:O	2.20	0.41
1:G:979:LYS:O	1:G:981:SER:N	2.44	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:HD12	1:A:42:TYR:CE1	2.56	0.41
2:B:897:ILE:HD12	2:B:903:PRO:HD3	2.03	0.41
3:C:266:PRO:O	3:C:267:HIS:C	2.64	0.41
1:D:315:THR:CG2	1:D:323:PHE:HB3	2.51	0.41
3:C:184:MET:CE	3:C:267:HIS:HA	2.51	0.41
2:E:982:LEU:C	2:E:982:LEU:HD23	2.46	0.41
1:G:1106:GLN:HA	1:G:1109:VAL:HG22	2.03	0.41
2:H:980:ARG:NH2	2:H:998:ASP:OD1	2.50	0.41
1:A:318:ASP:OD1	1:A:319:ASN:N	2.54	0.41
1:D:749:THR:HG21	1:D:786:VAL:HG11	2.02	0.41
1:D:931:LEU:HD22	1:D:947:ARG:HH21	1.86	0.41
1:G:6:VAL:HG22	1:G:1040:VAL:HG22	2.03	0.41
2:B:773:ARG:HD2	2:B:879:GLY:O	2.20	0.41
3:F:266:PRO:O	3:F:267:HIS:C	2.63	0.41
2:H:876:ALA:O	2:H:878:PHE:HD1	2.03	0.41
2:H:906:LEU:HD21	2:H:913:TYR:CD1	2.56	0.41
3:C:125:ASN:OD1	3:C:125:ASN:C	2.63	0.40
1:A:791:LEU:HD23	1:A:858:LEU:HD21	2.03	0.40
1:D:275:ASP:OD1	1:D:275:ASP:C	2.65	0.40
1:D:284:LEU:HB2	1:D:301:ARG:HB3	2.03	0.40
1:D:975:PHE:HA	1:D:996:GLY:O	2.22	0.40
2:E:761:ASP:OD1	2:E:762:ASN:N	2.54	0.40
1:G:127:GLU:HB2	1:G:129:ARG:HG3	2.02	0.40
1:G:223:PRO:HD3	1:G:271:TYR:OH	2.21	0.40
2:B:865:ILE:CD1	2:B:875:LEU:HD12	2.49	0.40
1:D:876:PHE:CZ	1:D:919:ASP:HA	2.56	0.40
1:A:143:ILE:HG12	1:A:154:ALA:HB2	2.04	0.40
2:B:724:VAL:O	2:B:724:VAL:HG22	2.22	0.40
1:G:889:ARG:HD3	1:G:901:THR:HG23	2.02	0.40
1:G:1076:PHE:O	1:G:1082:THR:HA	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1122:ARG:NH1	1:G:292:ASP:O[2_565]	1.86	0.34
1:D:368:GLU:O	2:H:890:ARG:NH2[4_565]	1.99	0.21
1:A:1122:ARG:HH12	1:G:292:ASP:O[2_565]	1.53	0.07

## 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	822/840 (98%)	797 (97%)	25 (3%)	0	100	100
1	D	823/840 (98%)	800 (97%)	23 (3%)	0	100	100
1	G	822/840 (98%)	802 (98%)	20 (2%)	0	100	100
2	B	324/344 (94%)	315 (97%)	8 (2%)	1 (0%)	36	66
2	E	322/344 (94%)	314 (98%)	8 (2%)	0	100	100
2	H	322/344 (94%)	315 (98%)	7 (2%)	0	100	100
3	C	246/271 (91%)	242 (98%)	4 (2%)	0	100	100
3	F	246/271 (91%)	242 (98%)	4 (2%)	0	100	100
3	I	246/271 (91%)	243 (99%)	3 (1%)	0	100	100
All	All	4173/4365 (96%)	4070 (98%)	102 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1029	ALA

### 5.3.2 Protein sidechains [i](#)

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	721/728 (99%)	715 (99%)	6 (1%)	73	77
1	D	722/728 (99%)	715 (99%)	7 (1%)	68	75
1	G	721/728 (99%)	717 (99%)	4 (1%)	78	80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	294/308 (96%)	282 (96%)	12 (4%)	27	53
2	E	292/308 (95%)	286 (98%)	6 (2%)	47	66
2	H	292/308 (95%)	286 (98%)	6 (2%)	47	66
3	C	223/242 (92%)	222 (100%)	1 (0%)	84	81
3	F	223/242 (92%)	223 (100%)	0	100	100
3	I	223/242 (92%)	223 (100%)	0	100	100
All	All	3711/3834 (97%)	3669 (99%)	42 (1%)	65	74

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	GLN
1	A	331	SER
1	A	908	ASN
1	A	926	LEU
1	A	947	ARG
1	A	952	ASN
2	B	740	GLN
2	B	760	LEU
2	B	820	LEU
2	B	821	MET
2	B	896	VAL
2	B	905	GLU
2	B	991	SER
2	B	1025	LEU
2	B	1033	LEU
2	B	1036	TRP
2	B	1039	CYS
2	B	1040	HIS
3	C	257	LEU
1	D	7	VAL
1	D	331	SER
1	D	360	VAL
1	D	383	LYS
1	D	910	MET
1	D	929	SER
1	D	950	ASN
2	E	860	ILE
2	E	867	LEU
2	E	896	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	1033	LEU
2	E	1036	TRP
2	E	1039	CYS
1	G	7	VAL
1	G	360	VAL
1	G	910	MET
1	G	1120	MET
2	H	865	ILE
2	H	867	LEU
2	H	896	VAL
2	H	1033	LEU
2	H	1036	TRP
2	H	1039	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	105	HIS
1	A	711	HIS
1	A	778	HIS
1	A	790	ASN
1	A	852	GLN
1	A	877	ASN
1	A	1034	ASN
1	A	1113	GLN
2	B	797	GLN
3	C	149	GLN
3	C	267	HIS
1	D	4	ASN
1	D	374	GLN
1	D	790	ASN
1	D	826	ASN
1	D	852	GLN
1	D	907	ASN
1	D	978	GLN
1	D	1016	ASN
2	E	977	GLN
3	F	37	GLN
3	F	179	GLN
1	G	105	HIS
1	G	778	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	790	ASN
1	G	796	GLN
1	G	797	HIS
1	G	907	ASN
1	G	990	GLN
1	G	1034	ASN
2	H	740	GLN
2	H	977	GLN
3	I	37	GLN
3	I	156	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TPO	B	893	2	8,10,11	1.24	0	10,14,16	1.45	2 (20%)
2	TPO	H	893	2	8,10,11	1.19	0	10,14,16	1.39	2 (20%)
2	TPO	E	893	2	8,10,11	1.76	1 (12%)	10,14,16	1.28	2 (20%)

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	TPO	B	893	2	-	6/9/11/13	-
2	TPO	H	893	2	-	6/9/11/13	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	E	893	2	-	6/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	893	TPO	P-O1P	3.61	1.61	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	893	TPO	P-OG1-CB	-3.33	114.28	123.33
2	H	893	TPO	P-OG1-CB	-3.05	115.05	123.33
2	E	893	TPO	P-OG1-CB	-2.60	116.26	123.33
2	H	893	TPO	CG2-CB-CA	-2.06	109.24	113.26
2	B	893	TPO	CG2-CB-CA	-2.04	109.30	113.26
2	E	893	TPO	CG2-CB-CA	-2.01	109.35	113.26

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	893	TPO	N-CA-CB-OG1
2	B	893	TPO	C-CA-CB-CG2
2	E	893	TPO	N-CA-CB-CG2
2	E	893	TPO	N-CA-CB-OG1
2	E	893	TPO	C-CA-CB-CG2
2	H	893	TPO	N-CA-CB-OG1
2	H	893	TPO	C-CA-CB-CG2
2	B	893	TPO	CG2-CB-OG1-P
2	E	893	TPO	CG2-CB-OG1-P
2	H	893	TPO	CG2-CB-OG1-P
2	H	893	TPO	N-CA-CB-CG2
2	B	893	TPO	CB-OG1-P-O3P
2	E	893	TPO	CB-OG1-P-O3P
2	H	893	TPO	CB-OG1-P-O3P
2	B	893	TPO	CB-OG1-P-O1P
2	E	893	TPO	O-C-CA-CB
2	H	893	TPO	CB-OG1-P-O1P
2	B	893	TPO	N-CA-CB-CG2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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
4	CIT	F	301	-	12,12,12	1.10	0	17,17,17	1.58	2 (11%)
5	RPW	G	1201	-	25,25,25	0.44	0	34,34,34	1.28	2 (5%)
4	CIT	H	1101	-	12,12,12	1.11	0	17,17,17	1.42	2 (11%)
5	RPW	D	1202	-	25,25,25	0.46	0	34,34,34	1.30	2 (5%)
4	CIT	D	1201	-	12,12,12	1.09	0	17,17,17	1.48	2 (11%)
4	CIT	C	301	-	12,12,12	1.18	0	17,17,17	1.99	5 (29%)
4	CIT	A	1201	-	12,12,12	1.11	0	17,17,17	1.44	1 (5%)
4	CIT	H	1102	-	12,12,12	1.14	0	17,17,17	1.34	1 (5%)
4	CIT	I	301	-	12,12,12	1.12	0	17,17,17	1.85	4 (23%)
5	RPW	B	1101	-	25,25,25	0.41	0	34,34,34	1.39	3 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	F	301	-	-	0/16/16/16	-
5	RPW	G	1201	-	-	6/12/12/12	0/3/3/3
4	CIT	H	1101	-	-	7/16/16/16	-
5	RPW	D	1202	-	-	6/12/12/12	0/3/3/3

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	D	1201	-	-	0/16/16/16	-
4	CIT	C	301	-	-	10/16/16/16	-
4	CIT	A	1201	-	-	0/16/16/16	-
4	CIT	H	1102	-	-	3/16/16/16	-
4	CIT	I	301	-	-	2/16/16/16	-
5	RPW	B	1101	-	-	6/12/12/12	0/3/3/3

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1101	RPW	C10-N4-C8	-5.43	119.92	126.67
5	D	1202	RPW	C10-N4-C8	-5.07	120.36	126.67
5	G	1201	RPW	C10-N4-C8	-4.72	120.79	126.67
4	I	301	CIT	O6-C6-C3	4.22	121.23	113.14
4	D	1201	CIT	O6-C6-C3	3.89	120.60	113.14
4	C	301	CIT	O6-C6-C3	3.83	120.49	113.14
4	A	1201	CIT	O6-C6-C3	3.76	120.35	113.14
4	F	301	CIT	O6-C6-C3	3.56	119.97	113.14
4	H	1101	CIT	O6-C6-C3	3.49	119.83	113.14
4	H	1102	CIT	O6-C6-C3	3.46	119.78	113.14
4	C	301	CIT	C4-C3-C2	2.88	116.71	109.31
4	C	301	CIT	O7-C3-C6	-2.88	104.87	108.96
5	B	1101	RPW	C5-C6-C7	2.75	119.62	112.68
4	I	301	CIT	O7-C3-C6	-2.71	105.12	108.96
4	C	301	CIT	O2-C1-C2	2.66	122.78	114.35
4	C	301	CIT	O7-C3-C2	-2.60	103.46	109.38
5	D	1202	RPW	C5-C6-C7	2.54	119.07	112.68
5	G	1201	RPW	C5-C6-C7	2.52	119.02	112.68
4	I	301	CIT	O7-C3-C2	-2.34	104.04	109.38
4	H	1101	CIT	O4-C5-C4	2.20	121.32	114.35
4	I	301	CIT	O4-C5-C4	2.20	121.31	114.35
4	F	301	CIT	O4-C5-C4	2.14	121.14	114.35
4	D	1201	CIT	O4-C5-C4	2.07	120.90	114.35
5	B	1101	RPW	N4-C10-N5	2.06	118.32	113.33

There are no chirality outliers.

All (40) torsion outliers are listed below:

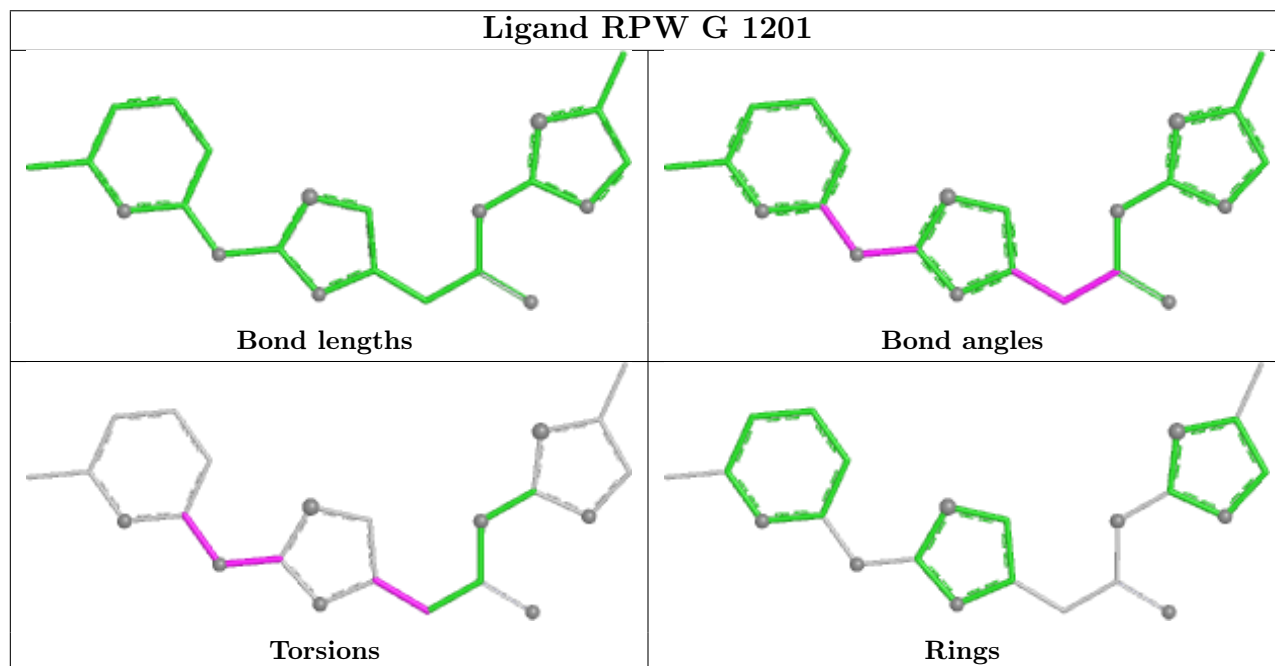
Mol	Chain	Res	Type	Atoms
4	C	301	CIT	C1-C2-C3-O7
4	C	301	CIT	C1-C2-C3-C4
4	C	301	CIT	O7-C3-C6-O5
4	C	301	CIT	O7-C3-C6-O6
4	C	301	CIT	C4-C3-C6-O5
4	C	301	CIT	C4-C3-C6-O6
4	H	1102	CIT	C2-C3-C4-C5
4	H	1102	CIT	C6-C3-C4-C5
5	B	1101	RPW	N3-C8-N4-C10
5	B	1101	RPW	C5-C6-C7-N3
5	B	1101	RPW	C5-C6-C7-C9
5	D	1202	RPW	N3-C8-N4-C10
5	D	1202	RPW	S2-C8-N4-C10
5	D	1202	RPW	C5-C6-C7-N3
5	D	1202	RPW	C5-C6-C7-C9
5	G	1201	RPW	N3-C8-N4-C10
5	G	1201	RPW	S2-C8-N4-C10
5	G	1201	RPW	C5-C6-C7-N3
5	G	1201	RPW	C5-C6-C7-C9
5	B	1101	RPW	S2-C8-N4-C10
4	H	1101	CIT	C3-C4-C5-O4
4	H	1101	CIT	C3-C4-C5-O3
4	C	301	CIT	C1-C2-C3-C6
4	H	1102	CIT	O7-C3-C4-C5
5	D	1202	RPW	N5-C10-N4-C8
5	G	1201	RPW	N5-C10-N4-C8
5	B	1101	RPW	N5-C10-N4-C8
4	C	301	CIT	O7-C3-C4-C5
4	H	1101	CIT	C2-C3-C6-O6
5	B	1101	RPW	C11-C10-N4-C8
5	D	1202	RPW	C11-C10-N4-C8
5	G	1201	RPW	C11-C10-N4-C8
4	H	1101	CIT	C4-C3-C6-O6
4	I	301	CIT	C2-C3-C6-O5
4	I	301	CIT	C2-C3-C6-O6
4	H	1101	CIT	O7-C3-C6-O5
4	H	1101	CIT	O7-C3-C6-O6
4	H	1101	CIT	C2-C3-C6-O5
4	C	301	CIT	O1-C1-C2-C3
4	C	301	CIT	O2-C1-C2-C3

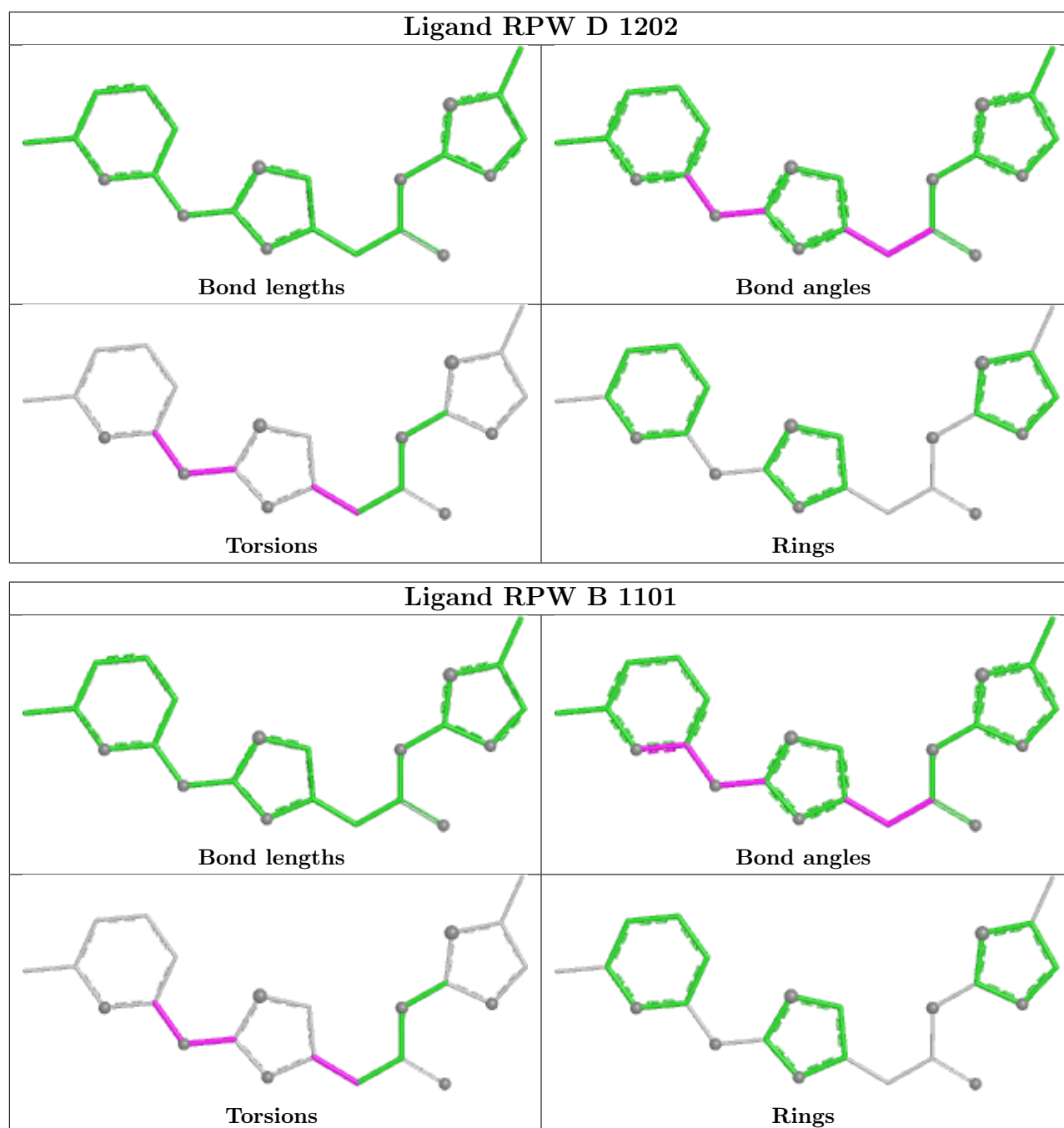
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1201	RPW	1	0
5	D	1202	RPW	2	0

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	826/840 (98%)	-0.72	1 (0%) 92   85	48, 81, 136, 219	0
1	D	827/840 (98%)	-0.75	0 100   100	43, 77, 128, 194	0
1	G	826/840 (98%)	-0.70	0 100   100	50, 87, 144, 246	0
2	B	326/344 (94%)	-0.62	0 100   100	54, 89, 139, 218	0
2	E	323/344 (93%)	-0.59	0 100   100	48, 82, 133, 190	0
2	H	323/344 (93%)	-0.51	0 100   100	41, 73, 124, 225	0
3	C	248/271 (91%)	-0.80	0 100   100	50, 78, 121, 153	0
3	F	248/271 (91%)	-0.75	0 100   100	44, 67, 110, 147	0
3	I	248/271 (91%)	-0.79	0 100   100	45, 70, 110, 152	0
All	All	4195/4365 (96%)	-0.70	1 (0%) 100   100	41, 79, 134, 246	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	ALA	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	TPO	B	893	11/12	0.59	0.12	268,280,340,343	6
2	TPO	E	893	11/12	0.64	0.12	202,242,288,292	6
2	TPO	H	893	11/12	0.84	0.12	199,220,274,274	6

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

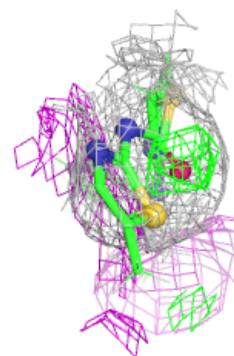
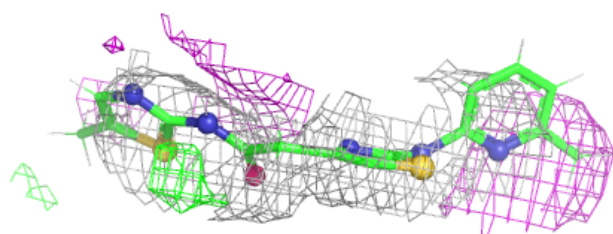
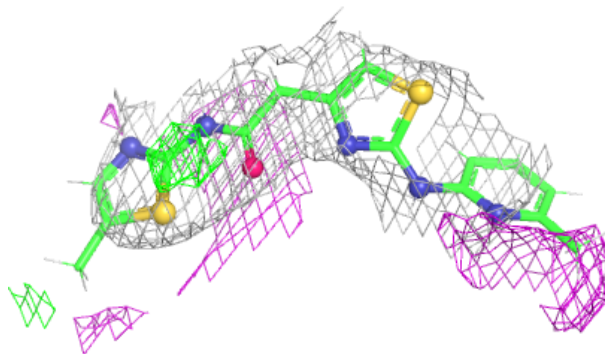
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	CIT	H	1101	13/13	0.44	0.15	136,192,218,245	5
4	CIT	I	301	13/13	0.50	0.07	163,196,208,213	5
4	CIT	H	1102	13/13	0.52	0.07	159,195,235,235	5
4	CIT	C	301	13/13	0.65	0.07	148,190,230,230	5
4	CIT	D	1201	13/13	0.71	0.06	162,203,220,246	5
4	CIT	F	301	13/13	0.75	0.07	124,186,207,226	5
4	CIT	A	1201	13/13	0.76	0.08	183,204,262,262	5
5	RPW	D	1202	23/23	0.92	0.14	144,216,263,274	15
5	RPW	G	1201	23/23	0.92	0.17	144,203,262,274	15
5	RPW	B	1101	23/23	0.94	0.10	144,203,259,274	15

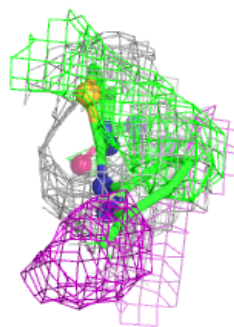
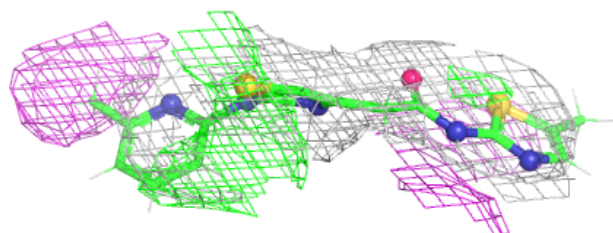
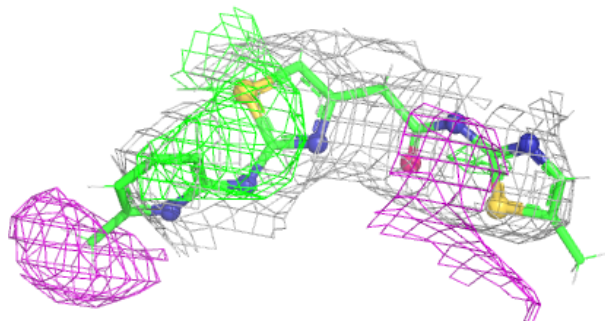
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

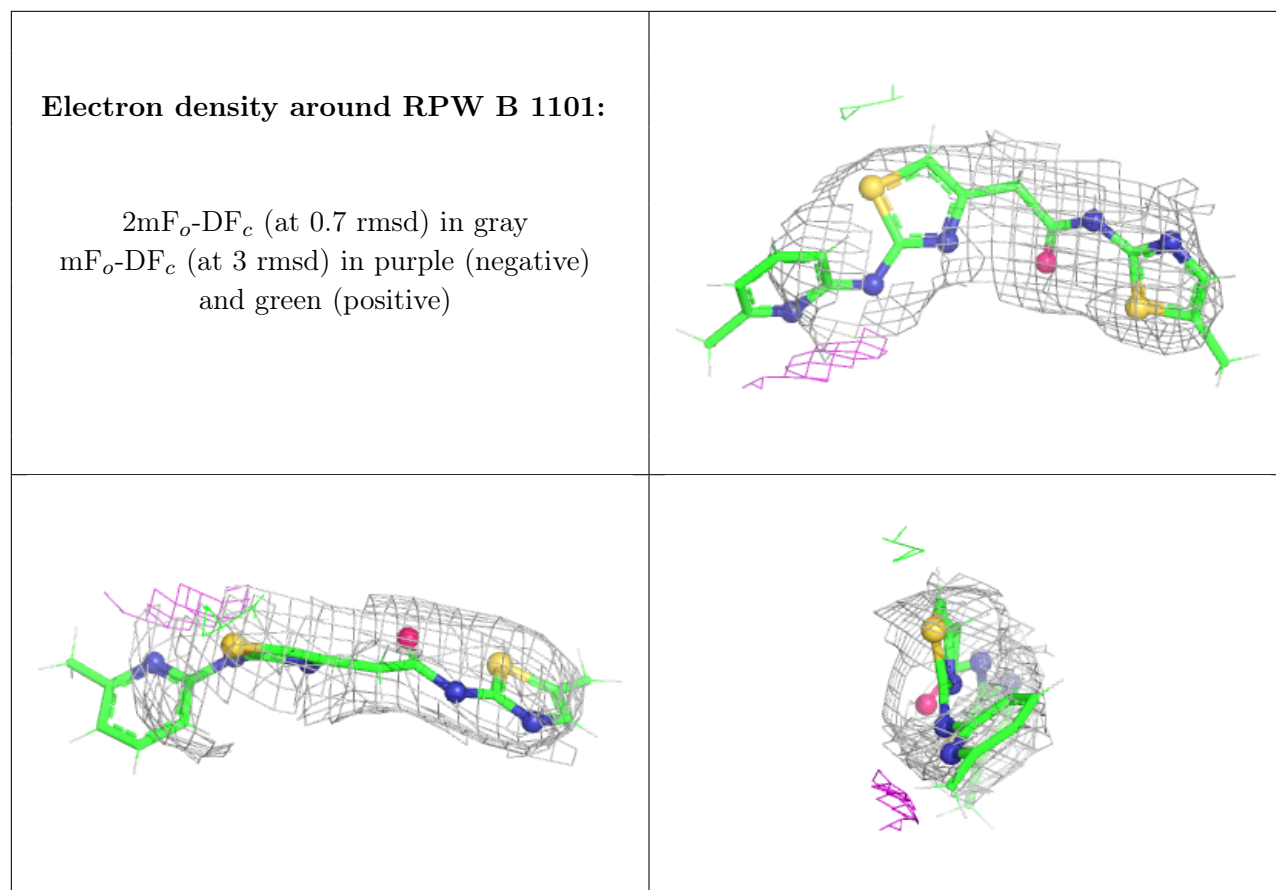
**Electron density around RPW D 1202:**

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

**Electron density around RPW G 1201:**

$2mF_o-DF_c$  (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.