



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:00 am BST

PDB ID : 4PL5  
Title : Crystal structure of murine IRE1 in complex with OICR573 inhibitor  
Authors : Sanches, M.; Duffy, N.; Talukdar, M.; Thevakumaran, N.; Chiovitti, D.; Al-  
awar, R.; Patterson, J.B.; Sicheri, F.  
Deposited on : 2014-05-16  
Resolution : 3.40 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

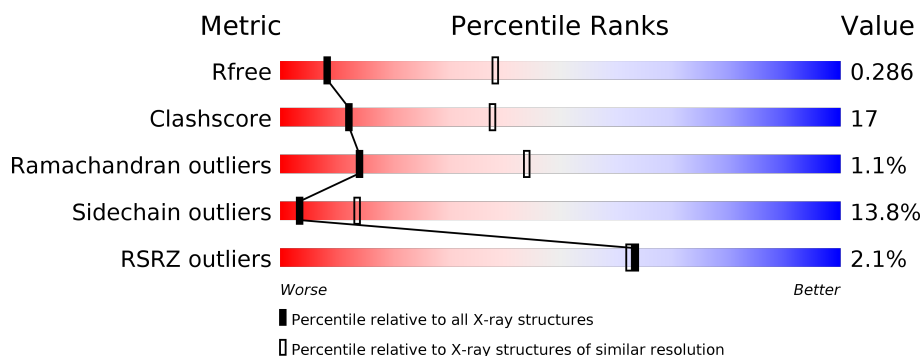
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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  $\geq 3$ , 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	435	
1	B	435	
1	C	435	
1	D	435	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12629 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 Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	383	Total	C	N	O	S	0	0	0
			3117	1993	550	555	19			
1	A	386	Total	C	N	O	S	0	0	0
			3124	2000	547	558	19			
1	C	386	Total	C	N	O	S	0	0	0
			3133	2003	554	557	19			
1	D	385	Total	C	N	O	S	0	0	0
			3090	1973	542	556	19			

There are 32 discrepancies between the modelled and reference sequences:

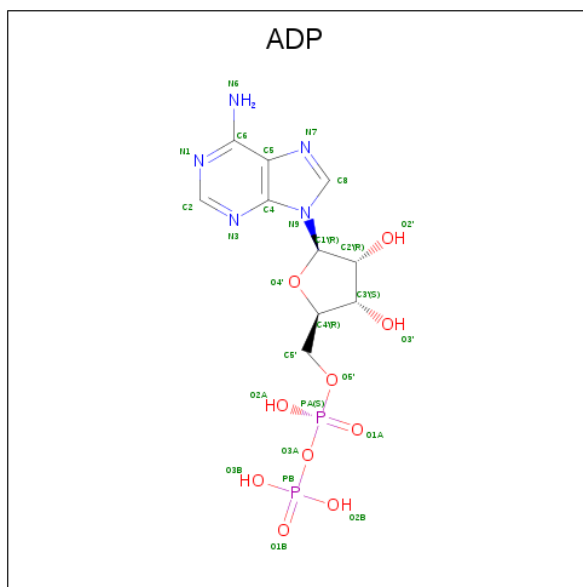
Chain	Residue	Modelled	Actual	Comment	Reference
B	543	GLY	-	expression tag	UNP Q9EQY0
B	544	ALA	-	expression tag	UNP Q9EQY0
B	545	MET	-	expression tag	UNP Q9EQY0
B	546	ASP	-	expression tag	UNP Q9EQY0
B	547	PRO	-	expression tag	UNP Q9EQY0
B	548	GLU	-	expression tag	UNP Q9EQY0
B	549	PHE	-	expression tag	UNP Q9EQY0
B	772	TYR	ASN	engineered mutation	UNP Q9EQY0
A	543	GLY	-	expression tag	UNP Q9EQY0
A	544	ALA	-	expression tag	UNP Q9EQY0
A	545	MET	-	expression tag	UNP Q9EQY0
A	546	ASP	-	expression tag	UNP Q9EQY0
A	547	PRO	-	expression tag	UNP Q9EQY0
A	548	GLU	-	expression tag	UNP Q9EQY0
A	549	PHE	-	expression tag	UNP Q9EQY0
A	772	TYR	ASN	engineered mutation	UNP Q9EQY0
C	543	GLY	-	expression tag	UNP Q9EQY0
C	544	ALA	-	expression tag	UNP Q9EQY0
C	545	MET	-	expression tag	UNP Q9EQY0
C	546	ASP	-	expression tag	UNP Q9EQY0
C	547	PRO	-	expression tag	UNP Q9EQY0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	548	GLU	-	expression tag	UNP Q9EQY0
C	549	PHE	-	expression tag	UNP Q9EQY0
C	772	TYR	ASN	engineered mutation	UNP Q9EQY0
D	543	GLY	-	expression tag	UNP Q9EQY0
D	544	ALA	-	expression tag	UNP Q9EQY0
D	545	MET	-	expression tag	UNP Q9EQY0
D	546	ASP	-	expression tag	UNP Q9EQY0
D	547	PRO	-	expression tag	UNP Q9EQY0
D	548	GLU	-	expression tag	UNP Q9EQY0
D	549	PHE	-	expression tag	UNP Q9EQY0
D	772	TYR	ASN	engineered mutation	UNP Q9EQY0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

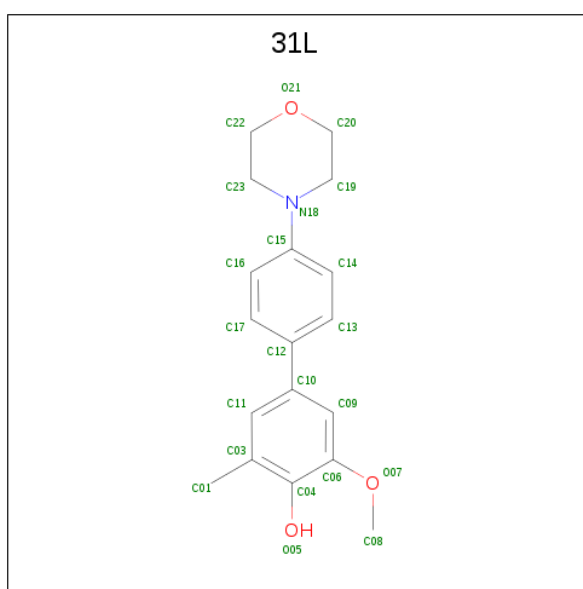


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

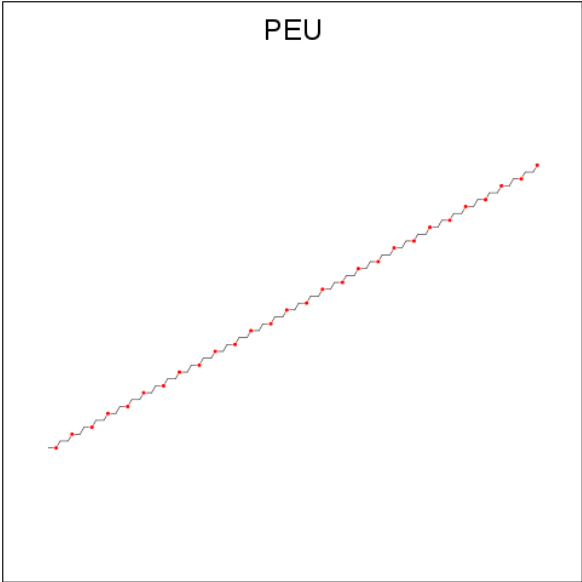
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is 3-methoxy-5-methyl-4'-(morpholin-4-yl)biphenyl-4-ol (three-letter code: 31L) (formula:  $C_{18}H_{21}NO_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 22 18 1 3	0	0

- Molecule 5 is 2,5,8,11,14,17,20,23,26,29,32,35,38,41,44,47,50,53,56,59,62,65,68,71,74,77,80-HEPTACOSAOXADOCTACONTAN-82-OL (three-letter code: PEU) (formula:  $C_{55}H_{112}O_{28}$ ).

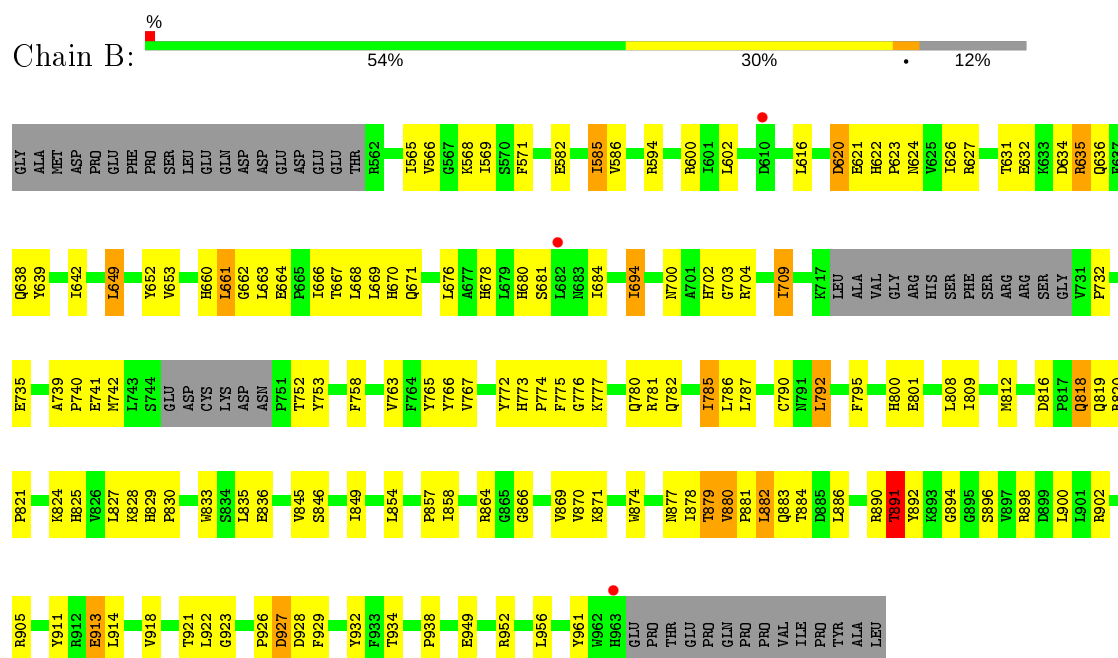


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	31	20	11	0	0

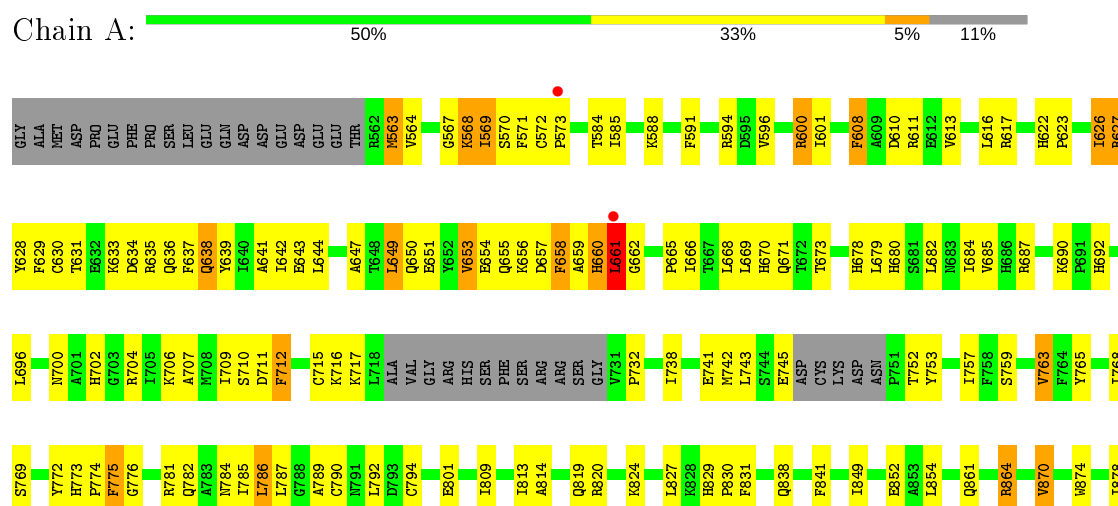
### 3 Residue-property plots

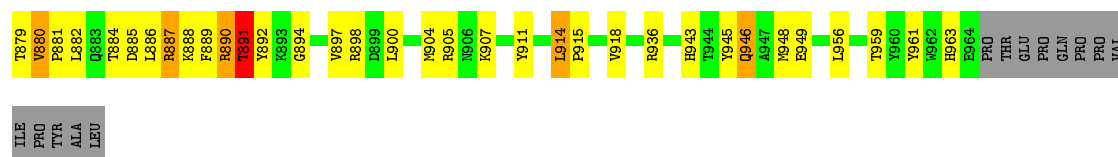
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Serine/threonine-protein kinase/endoribonuclease IRE1

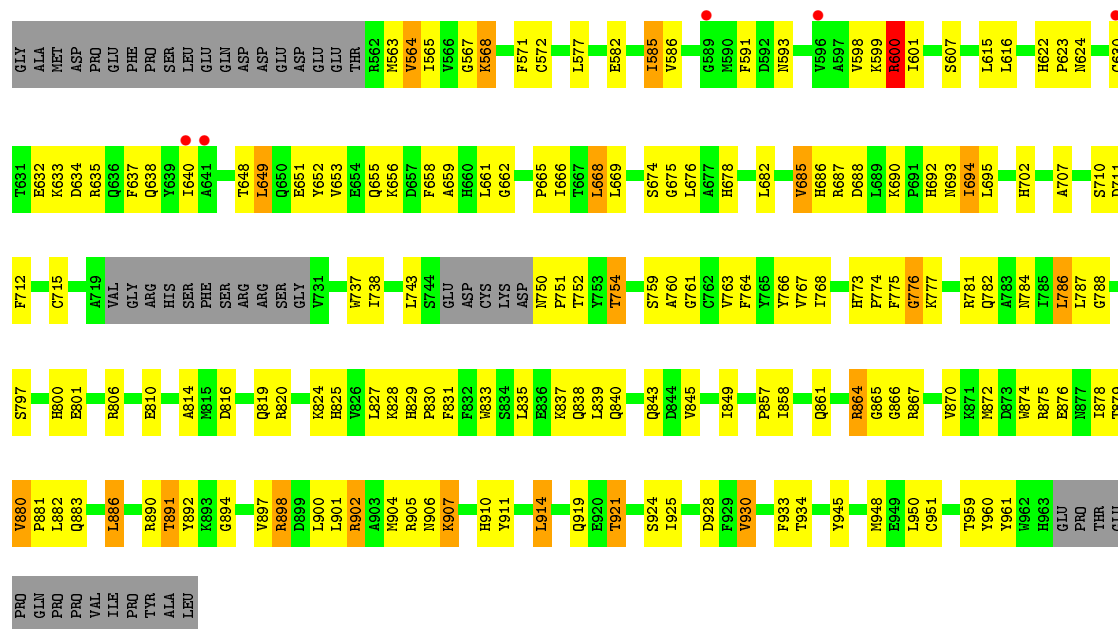


- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

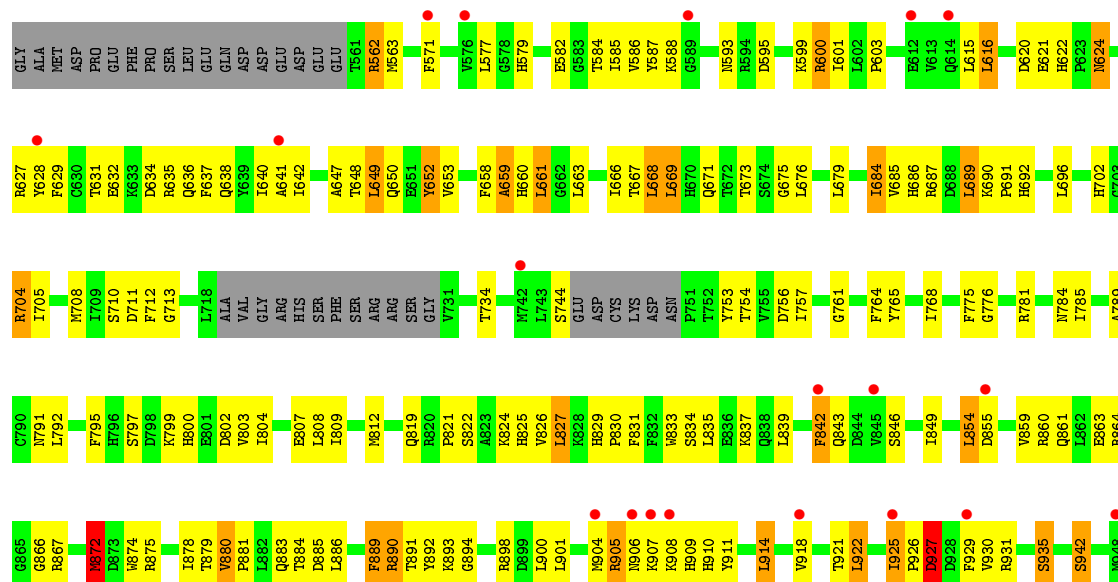




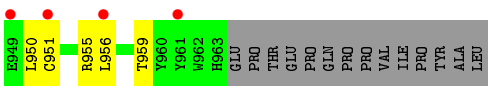
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1



• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	319.22Å 63.03Å 140.78Å 90.00° 99.49° 90.00°	Depositor
Resolution (Å)	48.27 – 3.40 48.27 – 3.40	Depositor EDS
% Data completeness (in resolution range)	75.2 (48.27-3.40) 75.3 (48.27-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1175)	Depositor
R, $R_{free}$	0.222 , 0.285 0.222 , 0.286	Depositor DCC
$R_{free}$ test set	1207 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.2	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 65.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	12629	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEU, MG, ADP, 31L

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	0.36	0/3202	0.60	3/4327 (0.1%)
1	B	0.34	0/3195	0.57	1/4315 (0.0%)
1	C	0.31	0/3211	0.55	2/4339 (0.0%)
1	D	0.33	0/3165	0.56	1/4281 (0.0%)
All	All	0.33	0/12773	0.57	7/17262 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	661	LEU	CA-CB-CG	5.91	128.89	115.30
1	A	891	THR	N-CA-C	5.80	126.65	111.00
1	A	775	PHE	N-CA-C	5.35	125.44	111.00
1	D	616	LEU	CA-CB-CG	5.27	127.42	115.30
1	B	891	THR	N-CA-C	5.24	125.15	111.00
1	C	891	THR	N-CA-C	5.22	125.11	111.00
1	C	600	ARG	CG-CD-NE	5.12	122.55	111.80

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	3124	0	3066	112	0
1	B	3117	0	3073	91	0
1	C	3133	0	3088	103	0
1	D	3090	0	3012	118	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	1	0
2	D	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	22	0	18	3	0
5	A	31	0	40	0	0
All	All	12629	0	12345	424	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 17.

All (424) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:HIS:HB2	1:A:661:LEU:HA	1.53	0.90
1:B:649:LEU:HG	1:B:694:ILE:HD11	1.60	0.82
1:C:879:THR:HG21	1:C:921:THR:HG21	1.61	0.82
1:A:849:ILE:HD13	1:A:898:ARG:HG3	1.63	0.81
1:B:824:LYS:HE3	1:B:828:LYS:HD2	1.63	0.81
1:A:627:ARG:HH11	1:A:627:ARG:HG2	1.46	0.79
1:C:659:ALA:HB1	1:C:661:LEU:HG	1.61	0.79
1:D:753:TYR:HE2	1:D:822:SER:HA	1.49	0.77
1:A:784:ASN:HB3	1:A:789:ALA:HB3	1.67	0.77
1:A:617:ARG:NH2	1:A:628:TYR:O	2.17	0.76
1:A:680:HIS:CE1	1:A:753:TYR:HB2	2.20	0.76
1:C:816:ASP:HB3	1:C:819:GLN:HB2	1.68	0.76
1:C:688:ASP:O	1:C:693:ASN:ND2	2.18	0.76
1:B:773:HIS:HD2	1:B:774:PRO:HD2	1.49	0.75
1:B:782:GLN:HA	1:B:785:ILE:HG22	1.68	0.75
1:D:843:GLN:O	1:D:905:ARG:NH1	2.19	0.75
1:D:636:GLN:HG2	1:D:637:PHE:HD1	1.53	0.73
1:B:857:PRO:HG2	1:B:858:ILE:HD12	1.71	0.73
1:D:669:LEU:HD11	1:D:764:PHE:HA	1.72	0.72
1:A:591:PHE:HE1	1:A:630:CYS:HG	1.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:622:HIS:HD2	1:C:624:ASN:H	1.39	0.71
1:A:943:HIS:HD2	1:A:946:GLN:HE21	1.38	0.70
1:C:907:LYS:HG3	1:C:914:LEU:HD21	1.73	0.70
1:C:624:ASN:ND2	1:C:707:ALA:O	2.21	0.70
1:D:824:LYS:HA	1:D:827:LEU:HD22	1.74	0.70
1:D:834:SER:H	1:D:837:LYS:HE3	1.57	0.70
1:B:661:LEU:H	1:B:661:LEU:HD22	1.56	0.70
1:B:849:ILE:HD12	1:B:898:ARG:HG3	1.74	0.69
1:C:577:LEU:HB2	1:C:586:VAL:HG23	1.73	0.69
1:A:911:TYR:HA	1:A:914:LEU:HD22	1.75	0.69
1:D:889:PHE:HZ	1:D:907:LYS:HE2	1.57	0.68
1:B:773:HIS:HD2	1:B:774:PRO:CD	2.07	0.68
1:C:600:ARG:HG3	1:C:600:ARG:HH11	1.59	0.67
1:C:649:LEU:HG	1:C:694:ILE:HD11	1.74	0.67
1:A:690:LYS:HG3	1:A:692:HIS:H	1.60	0.67
1:D:791:ASN:OD1	1:D:792:LEU:N	2.24	0.66
1:A:636:GLN:HG2	1:A:637:PHE:HD1	1.59	0.66
1:A:627:ARG:NH1	1:A:643:GLU:OE2	2.28	0.66
1:A:679:LEU:HD21	1:A:712:PHE:HD2	1.61	0.66
1:A:880:VAL:HG13	1:A:881:PRO:HD3	1.78	0.65
1:D:587:TYR:HE2	1:D:600:ARG:HD2	1.61	0.65
1:A:889:PHE:HB3	4:A:1001:31L:H16	1.77	0.65
1:C:814:ALA:O	1:C:820:ARG:NH1	2.29	0.65
1:C:857:PRO:HG2	1:C:858:ILE:HD12	1.78	0.65
1:B:741:GLU:OE2	1:B:820:ARG:NH2	2.29	0.65
1:D:839:LEU:HD13	1:D:930:VAL:HG22	1.78	0.65
1:B:571:PHE:HE2	1:B:639:TYR:HE2	1.46	0.64
1:C:686:HIS:CD2	1:C:712:PHE:HB3	2.34	0.63
1:D:890:ARG:HB2	1:D:892:TYR:N	2.13	0.63
1:A:773:HIS:CD2	1:A:781:ARG:HD3	2.33	0.63
1:A:784:ASN:HA	1:A:787:LEU:HB2	1.81	0.63
1:A:626:ILE:HG12	1:A:643:GLU:OE2	2.00	0.62
1:C:634:ASP:OD1	1:C:635:ARG:N	2.32	0.62
1:D:666:ILE:HD12	1:D:666:ILE:H	1.65	0.61
1:D:846:SER:HB3	1:D:905:ARG:NH2	2.15	0.61
1:D:704:ARG:HB3	1:D:704:ARG:HH21	1.65	0.61
1:D:753:TYR:CE2	1:D:822:SER:HA	2.35	0.60
1:D:624:ASN:OD1	1:D:624:ASN:N	2.33	0.60
1:D:859:VAL:HG22	1:D:898:ARG:NH2	2.16	0.60
1:C:674:SER:HA	1:C:827:LEU:HD11	1.82	0.60
1:D:587:TYR:CE2	1:D:600:ARG:HD2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:THR:HG23	1:A:881:PRO:HD2	1.83	0.60
1:D:628:TYR:CD1	1:D:642:ILE:HD12	2.37	0.60
1:C:655:GLN:HG3	1:C:658:PHE:HB2	1.84	0.60
1:C:874:TRP:NE1	1:C:894:GLY:HA2	2.16	0.60
1:A:732:PRO:HG2	1:A:742:MET:HE3	1.83	0.60
1:B:680:HIS:CE1	1:B:753:TYR:HB2	2.37	0.60
1:A:765:TYR:O	1:A:769:SER:OG	2.16	0.59
1:C:568:LYS:NZ	1:C:632:GLU:OE2	2.34	0.59
1:C:880:VAL:HG13	1:C:881:PRO:HD3	1.83	0.59
1:D:634:ASP:OD1	1:D:635:ARG:N	2.34	0.59
1:D:658:PHE:HZ	1:D:696:LEU:HD11	1.66	0.59
1:B:773:HIS:CE1	1:B:781:ARG:HD3	2.38	0.59
1:B:660:HIS:N	1:B:661:LEU:HA	2.18	0.59
1:A:633:LYS:HD2	1:A:638:GLN:HG2	1.85	0.58
1:B:700:ASN:HD21	1:B:704:ARG:HB3	1.68	0.58
1:B:773:HIS:CD2	1:B:774:PRO:HD2	2.35	0.58
1:C:710:SER:OG	1:C:711:ASP:N	2.37	0.58
1:B:835:LEU:HD23	1:B:927:ASP:HA	1.85	0.58
1:D:890:ARG:HB2	1:D:892:TYR:H	1.68	0.58
1:A:824:LYS:HA	1:A:827:LEU:HD12	1.83	0.58
1:A:890:ARG:HB2	1:A:892:TYR:HB2	1.86	0.57
1:B:773:HIS:ND1	1:B:781:ARG:HD3	2.19	0.57
1:D:775:PHE:H	1:D:776:GLY:HA2	1.69	0.57
1:A:801:GLU:CD	1:A:801:GLU:H	2.06	0.57
1:C:754:THR:HG22	1:C:820:ARG:HE	1.69	0.57
1:A:743:LEU:HD23	1:A:786:LEU:HD11	1.85	0.57
1:A:773:HIS:CE1	1:A:775:PHE:HB2	2.40	0.57
1:C:874:TRP:CE2	1:C:894:GLY:HA2	2.40	0.56
1:A:563:MET:HG3	1:A:572:CYS:HB3	1.88	0.56
1:C:801:GLU:CD	1:C:801:GLU:H	2.09	0.56
1:D:833:TRP:CD1	1:D:837:LYS:HD2	2.40	0.56
1:D:659:ALA:HB1	1:D:661:LEU:HD23	1.87	0.56
1:B:890:ARG:HA	1:B:891:THR:HG22	1.88	0.56
1:C:615:LEU:HG	1:C:682:LEU:HD23	1.88	0.56
1:B:874:TRP:CD1	1:B:900:LEU:HB2	2.40	0.56
1:B:569:ILE:HG13	1:B:632:GLU:OE2	2.05	0.56
1:B:694:ILE:HG22	1:B:709:ILE:HG22	1.88	0.56
1:D:765:TYR:CE2	1:D:792:LEU:HA	2.41	0.56
1:A:650:GLN:O	1:A:654:GLU:HB3	2.05	0.56
1:C:775:PHE:N	1:C:776:GLY:HA2	2.21	0.56
1:A:765:TYR:HH	1:A:794:CYS:HG	1.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:LYS:HG2	1:A:569:ILE:HD13	1.87	0.55
1:D:648:THR:OG1	1:D:691:PRO:O	2.23	0.55
1:B:765:TYR:CE2	1:B:792:LEU:HA	2.41	0.55
1:B:801:GLU:CD	1:B:801:GLU:H	2.09	0.55
1:A:775:PHE:CE2	1:A:785:ILE:HA	2.41	0.55
1:D:577:LEU:HB2	1:D:586:VAL:HG12	1.87	0.55
1:D:878:ILE:HD11	1:D:883:GLN:HB3	1.87	0.55
1:D:880:VAL:HG13	1:D:881:PRO:HD3	1.89	0.55
1:A:890:ARG:HG3	1:A:892:TYR:H	1.70	0.55
1:B:824:LYS:HA	1:B:827:LEU:HD12	1.89	0.55
1:B:911:TYR:HA	1:B:914:LEU:HD12	1.88	0.55
1:C:687:ARG:NH1	1:C:751:PRO:HG3	2.22	0.55
1:D:600:ARG:HG3	1:D:637:PHE:HE2	1.72	0.54
1:A:814:ALA:O	1:A:820:ARG:NH1	2.40	0.54
1:C:775:PHE:H	1:C:776:GLY:HA2	1.72	0.54
1:D:926:PRO:O	1:D:930:VAL:HG23	2.07	0.54
1:B:766:TYR:HA	1:B:772:TYR:O	2.06	0.54
1:C:666:ILE:H	1:C:666:ILE:HD12	1.71	0.54
1:B:800:HIS:HB2	1:B:938:PRO:HA	1.89	0.54
1:A:710:SER:OG	1:A:711:ASP:N	2.41	0.54
1:C:649:LEU:HD22	1:C:653:VAL:HG23	1.91	0.53
1:A:627:ARG:HG2	1:A:643:GLU:OE2	2.08	0.53
1:B:821:PRO:HB2	1:B:825:HIS:HB3	1.90	0.53
1:D:628:TYR:OH	1:D:712:PHE:N	2.41	0.53
1:D:846:SER:HB3	1:D:905:ARG:CZ	2.38	0.53
1:A:660:HIS:CB	1:A:661:LEU:HA	2.31	0.53
1:C:634:ASP:HB3	1:C:637:PHE:HB2	1.91	0.53
1:A:643:GLU:OE1	1:A:643:GLU:N	2.28	0.53
1:A:870:VAL:HG12	1:A:874:TRP:HB3	1.91	0.53
1:D:931:ARG:O	1:D:935:SER:HB3	2.09	0.53
1:A:636:GLN:HG2	1:A:637:PHE:CD1	2.43	0.53
1:D:807:GLU:OE2	1:D:942:SER:HB3	2.09	0.52
1:A:765:TYR:CE2	1:A:792:LEU:HD13	2.44	0.52
1:B:816:ASP:OD1	1:B:818:GLN:NE2	2.41	0.52
1:D:849:ILE:HB	1:D:898:ARG:NH2	2.24	0.52
1:D:744:SER:OG	1:D:744:SER:O	2.25	0.52
1:A:775:PHE:N	1:A:776:GLY:HA2	2.25	0.52
1:A:775:PHE:H	1:A:776:GLY:HA2	1.74	0.52
1:D:775:PHE:N	1:D:776:GLY:HA2	2.25	0.52
1:B:870:VAL:HG12	1:B:874:TRP:HB3	1.92	0.52
1:D:918:VAL:HG12	1:D:922:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:784:ASN:O	1:C:788:GLY:N	2.30	0.52
1:D:669:LEU:HD22	1:D:831:PHE:HE2	1.74	0.52
1:C:773:HIS:CD2	1:C:781:ARG:HG2	2.45	0.52
1:A:715:CYS:SG	1:A:716:LYS:N	2.80	0.51
1:A:861:GLN:O	1:A:864:ARG:HB2	2.10	0.51
1:B:949:GLU:HG3	1:B:952:ARG:HH21	1.74	0.51
1:D:768:ILE:HD11	1:D:831:PHE:HZ	1.75	0.51
1:A:682:LEU:O	1:A:684:ILE:HG13	2.10	0.51
1:D:640:ILE:HG22	1:D:642:ILE:HD11	1.91	0.51
1:B:808:LEU:HD13	1:B:829:HIS:CD2	2.45	0.51
1:D:861:GLN:HA	1:D:864:ARG:HG2	1.93	0.51
1:C:806:ARG:HD3	1:D:872:MET:HG3	1.92	0.51
1:D:905:ARG:CZ	1:D:905:ARG:HB3	2.40	0.51
1:B:879:THR:HG22	1:B:882:LEU:HB2	1.93	0.50
1:D:890:ARG:HB3	1:D:892:TYR:CD2	2.45	0.50
1:B:830:PRO:HA	1:B:833:TRP:CD2	2.46	0.50
1:D:710:SER:OG	1:D:711:ASP:N	2.44	0.50
1:A:874:TRP:NE1	1:A:894:GLY:HA2	2.26	0.50
1:C:761:GLY:O	1:C:764:PHE:HB2	2.12	0.50
1:C:878:ILE:HD11	1:C:883:GLN:HB2	1.92	0.50
1:D:685:VAL:O	1:D:687:ARG:NH2	2.44	0.50
1:A:655:GLN:C	1:A:657:ASP:H	2.15	0.50
1:C:685:VAL:HG22	1:C:687:ARG:HG3	1.94	0.50
1:D:906:ASN:O	1:D:910:HIS:HB2	2.10	0.50
1:A:741:GLU:OE1	1:A:820:ARG:NH2	2.45	0.50
1:C:600:ARG:CG	1:C:600:ARG:HH11	2.24	0.49
1:C:833:TRP:CG	1:C:837:LYS:HG2	2.47	0.49
1:A:634:ASP:OD1	1:A:635:ARG:N	2.45	0.49
1:B:765:TYR:CD1	1:B:774:PRO:HD3	2.47	0.49
1:A:890:ARG:HA	1:A:891:THR:HG22	1.93	0.49
1:D:579:HIS:CD2	1:D:585:ILE:HD12	2.47	0.49
1:D:890:ARG:O	1:D:890:ARG:NE	2.45	0.49
1:B:880:VAL:HA	1:B:883:GLN:HG2	1.95	0.49
1:C:586:VAL:HG12	1:C:599:LYS:HB3	1.95	0.49
1:D:686:HIS:CD2	1:D:712:PHE:HB3	2.48	0.49
1:D:754:THR:O	1:D:757:ILE:HG22	2.13	0.49
1:D:795:PHE:HA	1:D:802:ASP:HB3	1.94	0.49
1:D:757:ILE:HD11	1:D:826:VAL:HG21	1.94	0.49
1:B:634:ASP:OD1	1:B:635:ARG:N	2.44	0.49
1:B:661:LEU:HD21	1:B:703:GLY:O	2.12	0.48
1:C:675:GLY:O	1:C:678:HIS:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:ARG:HG3	1:B:635:ARG:H	1.40	0.48
1:B:871:LYS:HD3	1:B:877:ASN:ND2	2.27	0.48
1:C:690:LYS:HG3	1:C:692:HIS:H	1.78	0.48
1:D:839:LEU:HA	1:D:842:PHE:CZ	2.48	0.48
1:B:732:PRO:HG2	1:B:742:MET:HE1	1.96	0.48
1:D:663:LEU:HD22	1:D:705:ILE:HG13	1.96	0.48
1:D:875:ARG:NH2	1:D:892:TYR:O	2.47	0.48
1:A:571:PHE:HE2	1:A:639:TYR:HE2	1.61	0.48
1:A:886:LEU:O	1:A:890:ARG:HB3	2.14	0.48
1:B:670:HIS:CE1	1:B:827:LEU:HD22	2.49	0.48
1:C:652:TYR:HA	1:C:658:PHE:CD2	2.49	0.48
1:D:886:LEU:HD23	1:D:889:PHE:HE1	1.78	0.48
1:A:666:ILE:H	1:A:666:ILE:HD12	1.79	0.48
1:B:923:GLY:HA3	1:B:928:ASP:HB3	1.95	0.48
1:C:824:LYS:HA	1:C:827:LEU:HB2	1.95	0.48
1:C:898:ARG:HH11	1:C:902:ARG:NH2	2.11	0.48
1:D:803:VAL:HG12	1:D:807:GLU:OE2	2.12	0.48
1:B:828:LYS:HE2	1:B:961:TYR:O	2.14	0.48
1:D:636:GLN:HG2	1:D:637:PHE:CD1	2.42	0.48
1:B:774:PRO:HB2	1:B:775:PHE:CD1	2.49	0.48
1:C:840:GLN:OE1	1:C:843:GLN:NE2	2.47	0.48
1:A:768:ILE:HD11	1:A:831:PHE:HZ	1.78	0.47
1:A:829:HIS:CG	1:A:830:PRO:HD2	2.49	0.47
1:D:563:MET:HG3	1:D:571:PHE:O	2.14	0.47
1:D:669:LEU:O	1:D:673:THR:HG22	2.14	0.47
1:A:627:ARG:NH1	1:A:627:ARG:HG2	2.22	0.47
1:A:596:VAL:HG22	1:A:629:PHE:HE2	1.79	0.47
1:A:943:HIS:CD2	1:A:946:GLN:HE21	2.25	0.47
1:C:828:LYS:HD3	1:C:961:TYR:C	2.34	0.47
1:D:808:LEU:O	1:D:812:MET:HG3	2.15	0.47
1:A:600:ARG:HG3	1:A:637:PHE:CE2	2.50	0.47
1:A:658:PHE:O	1:A:660:HIS:N	2.47	0.47
1:B:620:ASP:N	1:B:620:ASP:OD1	2.47	0.47
1:B:929:PHE:O	1:B:932:TYR:HB3	2.15	0.47
1:B:780:GLN:OE1	1:B:780:GLN:N	2.45	0.47
1:B:881:PRO:HA	1:B:884:THR:HG22	1.97	0.47
1:C:875:ARG:NH2	1:C:890:ARG:HB3	2.30	0.47
1:C:839:LEU:HB2	1:C:930:VAL:CG2	2.45	0.47
1:D:842:PHE:O	1:D:905:ARG:NH2	2.45	0.47
1:A:641:ALA:O	1:A:642:ILE:HD13	2.13	0.47
1:C:867:ARG:HD3	1:C:872:MET:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:689:LEU:CD1	1:D:756:ASP:HA	2.44	0.47
1:B:777:LYS:HD3	1:B:777:LYS:HA	1.50	0.47
1:C:874:TRP:CD1	1:C:900:LEU:HB2	2.50	0.47
1:D:669:LEU:HD22	1:D:831:PHE:CE2	2.50	0.47
1:A:571:PHE:HE2	1:A:639:TYR:CE2	2.32	0.47
1:A:712:PHE:H	1:A:712:PHE:HD1	1.63	0.47
1:D:689:LEU:HD13	1:D:756:ASP:HA	1.97	0.46
1:B:880:VAL:HG13	1:B:881:PRO:HD3	1.97	0.46
1:A:662:GLY:H	1:A:704:ARG:HD3	1.81	0.46
1:C:743:LEU:HD22	1:C:786:LEU:HD11	1.97	0.46
1:D:628:TYR:HH	1:D:712:PHE:N	2.12	0.46
1:A:775:PHE:HE2	1:A:785:ILE:HA	1.80	0.46
1:B:758:PHE:CZ	1:B:785:ILE:HD11	2.51	0.46
1:C:839:LEU:HB2	1:C:930:VAL:HG22	1.97	0.46
1:D:784:ASN:HB3	1:D:789:ALA:HB3	1.97	0.46
1:B:775:PHE:N	1:B:776:GLY:HA2	2.30	0.46
1:C:924:SER:N	1:C:928:ASP:HB2	2.31	0.46
1:D:636:GLN:OE1	1:D:636:GLN:N	2.48	0.46
1:B:874:TRP:NE1	1:B:894:GLY:HA2	2.30	0.46
1:C:777:LYS:HE3	1:C:777:LYS:HB2	1.63	0.46
1:D:833:TRP:CG	1:D:837:LYS:HD2	2.51	0.46
1:C:591:PHE:HE1	1:C:630:CYS:HG	1.64	0.46
1:C:651:GLU:O	1:C:655:GLN:HG2	2.16	0.46
1:B:836:GLU:HG3	1:B:926:PRO:HG2	1.97	0.46
1:C:773:HIS:CG	1:C:774:PRO:HD2	2.51	0.46
1:C:649:LEU:HB2	1:C:694:ILE:HG13	1.98	0.45
1:D:781:ARG:O	1:D:785:ILE:HG13	2.16	0.45
1:D:808:LEU:HB2	1:D:829:HIS:CE1	2.50	0.45
1:C:810:GLU:OE1	1:D:867:ARG:NH1	2.49	0.45
1:D:900:LEU:O	1:D:904:MET:HG3	2.15	0.45
1:A:782:GLN:HA	1:A:785:ILE:HG13	1.97	0.45
1:C:800:HIS:HE1	1:C:838:GLN:OE1	2.00	0.45
1:B:649:LEU:O	1:B:653:VAL:HG23	2.16	0.45
1:C:565:ILE:HG22	1:C:567:GLY:N	2.31	0.45
1:C:876:GLU:OE1	1:C:876:GLU:N	2.49	0.45
1:B:790:CYS:HB3	1:B:792:LEU:HD23	1.99	0.45
1:D:861:GLN:CD	1:D:950:LEU:HD11	2.37	0.45
1:A:690:LYS:HG3	1:A:692:HIS:N	2.28	0.45
1:B:795:PHE:HE2	1:B:809:ILE:HD12	1.81	0.45
1:C:830:PRO:HG3	1:C:945:TYR:CE2	2.51	0.45
1:B:870:VAL:CG1	1:B:874:TRP:HD1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:849:ILE:CD1	1:B:898:ARG:HG3	2.45	0.45
1:C:571:PHE:HB3	1:C:598:VAL:HG21	1.99	0.45
1:C:759:SER:O	1:C:763:VAL:HG13	2.17	0.45
1:A:673:THR:HG22	1:A:827:LEU:HG	1.98	0.45
1:D:854:LEU:HA	1:D:859:VAL:HG11	1.98	0.45
1:C:760:ALA:O	1:C:763:VAL:HG22	2.17	0.45
1:C:892:TYR:OH	1:C:906:ASN:ND2	2.47	0.45
1:B:568:LYS:H	1:B:568:LYS:HG2	1.49	0.45
1:A:870:VAL:HG22	1:A:897:VAL:HG13	1.99	0.44
1:A:900:LEU:O	1:A:904:MET:HG3	2.17	0.44
1:A:738:ILE:HG21	1:A:743:LEU:HD13	1.98	0.44
1:A:757:ILE:HD13	1:A:757:ILE:HA	1.85	0.44
1:B:652:TYR:HE1	1:B:660:HIS:CG	2.35	0.44
1:C:864:ARG:HG3	1:C:865:GLY:N	2.33	0.44
1:D:621:GLU:HG3	1:D:627:ARG:HD3	1.99	0.44
1:B:886:LEU:HD22	1:B:892:TYR:CE2	2.52	0.44
4:A:1001:31L:H20	4:A:1001:31L:H2	1.68	0.44
1:A:623:PRO:O	1:A:706:LYS:NZ	2.41	0.44
1:A:700:ASN:OD1	1:A:704:ARG:N	2.50	0.44
1:B:666:ILE:H	1:B:666:ILE:HD12	1.82	0.44
1:C:911:TYR:HE1	1:C:919:GLN:HE21	1.64	0.44
1:A:915:PRO:HB2	1:A:918:VAL:HG23	1.99	0.44
1:B:669:LEU:HD21	1:B:767:VAL:HG21	1.99	0.44
1:B:890:ARG:CB	1:B:892:TYR:H	2.31	0.44
1:C:901:LEU:HA	1:C:904:MET:HE3	2.00	0.44
1:D:667:THR:O	1:D:671:GLN:HG3	2.18	0.44
1:A:696:LEU:HA	1:A:696:LEU:HD23	1.81	0.44
1:A:759:SER:O	1:A:763:VAL:HG12	2.17	0.44
1:B:854:LEU:HD22	1:B:854:LEU:H	1.83	0.44
1:B:918:VAL:HA	1:B:921:THR:HG22	2.00	0.44
1:C:669:LEU:HD11	1:C:767:VAL:HG11	2.00	0.44
1:C:686:HIS:NE2	1:C:710:SER:O	2.49	0.44
1:B:565:ILE:HG13	1:B:566:VAL:H	1.83	0.44
1:C:773:HIS:CD2	1:C:775:PHE:HB2	2.53	0.44
1:D:687:ARG:HH12	1:D:713:GLY:N	2.16	0.43
4:A:1001:31L:H3	4:A:1001:31L:H9	1.70	0.43
1:A:838:GLN:O	1:A:841:PHE:HB3	2.18	0.43
1:C:661:LEU:N	1:C:662:GLY:HA2	2.33	0.43
1:C:738:ILE:HD11	1:C:782:GLN:NE2	2.33	0.43
1:A:830:PRO:HG3	1:A:945:TYR:CE2	2.53	0.43
1:B:634:ASP:HB2	1:B:639:TYR:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:LEU:CD2	1:B:662:GLY:HA3	2.48	0.43
1:C:763:VAL:HA	1:C:766:TYR:HB3	2.01	0.43
1:D:761:GLY:O	1:D:764:PHE:HB2	2.18	0.43
1:D:885:ASP:OD2	1:D:907:LYS:NZ	2.49	0.43
1:A:622:HIS:HB2	1:A:678:HIS:CD2	2.54	0.43
1:C:768:ILE:HD11	1:C:831:PHE:HZ	1.82	0.43
1:D:603:PRO:HD3	1:D:637:PHE:HA	2.01	0.43
1:C:883:GLN:O	1:C:886:LEU:N	2.51	0.43
1:D:584:THR:HG23	1:D:600:ARG:O	2.18	0.43
1:D:925:ILE:HG22	1:D:929:PHE:CD2	2.53	0.43
1:A:665:PRO:O	1:A:669:LEU:HG	2.19	0.43
1:B:624:ASN:OD1	1:B:671:GLN:HB3	2.17	0.43
1:C:879:THR:HG23	1:C:881:PRO:HD2	2.01	0.43
1:D:883:GLN:HA	1:D:886:LEU:HB2	2.01	0.43
1:D:562:ARG:H	1:D:562:ARG:HD2	1.83	0.43
1:D:800:HIS:O	1:D:804:ILE:HG12	2.19	0.43
1:D:859:VAL:HG13	1:D:898:ARG:NH1	2.34	0.43
1:B:765:TYR:HB3	1:B:774:PRO:HD3	2.01	0.43
1:C:687:ARG:CZ	1:C:751:PRO:HG3	2.48	0.43
1:C:648:THR:HG22	1:C:695:LEU:HD23	2.01	0.43
1:C:890:ARG:HA	1:C:892:TYR:N	2.33	0.43
1:C:910:HIS:O	1:C:914:LEU:HD13	2.18	0.43
1:D:799:LYS:O	1:D:803:VAL:HG23	2.19	0.43
1:A:830:PRO:HG3	1:A:945:TYR:CD2	2.54	0.43
1:B:828:LYS:HE3	1:B:828:LYS:HB3	1.75	0.43
1:C:665:PRO:O	1:C:668:LEU:HB3	2.19	0.43
1:D:599:LYS:NZ	2:D:1001:ADP:O2A	2.52	0.43
1:D:622:HIS:CD2	1:D:675:GLY:HA2	2.54	0.43
1:D:799:LYS:HD3	1:D:799:LYS:HA	1.81	0.43
1:D:927:ASP:OD1	1:D:927:ASP:N	2.45	0.43
1:D:588:LYS:HE2	1:D:595:ASP:HB3	2.01	0.42
1:A:588:LYS:HG3	1:A:644:LEU:HD22	2.01	0.42
1:A:651:GLU:O	1:A:655:GLN:HB2	2.19	0.42
1:A:907:LYS:HA	1:A:907:LYS:HD3	1.86	0.42
1:B:634:ASP:HB2	1:B:639:TYR:CE1	2.53	0.42
1:B:739:ALA:HA	1:B:740:PRO:HD3	1.84	0.42
2:C:1001:ADP:H5'2	2:C:1001:ADP:O2B	2.19	0.42
1:D:679:LEU:HG	1:D:684:ILE:HD11	2.01	0.42
1:A:949:GLU:HA	1:A:961:TYR:CE2	2.54	0.42
1:A:685:VAL:HG12	1:A:687:ARG:HG3	2.01	0.42
1:D:901:LEU:HD22	1:D:904:MET:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:CYS:HA	1:A:573:PRO:HD3	1.87	0.42
1:A:655:GLN:O	1:A:657:ASP:N	2.51	0.42
1:B:913:GLU:H	1:B:913:GLU:HG3	1.55	0.42
1:C:867:ARG:CD	1:C:872:MET:HA	2.50	0.42
1:A:637:PHE:HB3	1:A:638:GLN:H	1.72	0.42
1:A:911:TYR:O	1:A:914:LEU:HB2	2.19	0.42
1:D:648:THR:HG23	1:D:650:GLN:H	1.85	0.42
1:B:700:ASN:ND2	1:B:704:ARG:O	2.53	0.42
1:C:959:THR:HG23	1:C:960:TYR:CD1	2.55	0.42
1:D:641:ALA:O	1:D:642:ILE:HD13	2.20	0.42
1:D:893:LYS:HE2	1:D:893:LYS:HB3	1.75	0.42
1:D:830:PRO:HA	1:D:833:TRP:CD2	2.55	0.42
1:C:607:SER:OG	1:C:715:CYS:HB3	2.20	0.42
1:D:652:TYR:CE2	1:D:668:LEU:HD12	2.54	0.42
1:D:860:ARG:HB3	1:D:864:ARG:NH2	2.35	0.42
1:A:594:ARG:HD2	1:A:629:PHE:CE2	2.55	0.42
1:B:622:HIS:HA	1:B:623:PRO:HD3	1.78	0.42
1:B:678:HIS:O	1:B:681:SER:OG	2.25	0.42
1:B:812:MET:HB2	1:B:812:MET:HE2	1.80	0.42
1:C:669:LEU:CD2	1:C:764:PHE:HA	2.50	0.42
1:C:830:PRO:HA	1:C:833:TRP:CD2	2.55	0.42
1:C:829:HIS:CG	1:C:830:PRO:HD2	2.55	0.42
1:C:839:LEU:HD13	1:C:930:VAL:HG13	2.02	0.42
1:D:649:LEU:O	1:D:653:VAL:HG23	2.20	0.42
1:D:911:TYR:CE1	1:D:914:LEU:HD21	2.54	0.42
1:A:948:MET:O	1:A:961:TYR:HE2	2.03	0.41
1:B:845:VAL:O	1:B:849:ILE:HG23	2.20	0.41
1:C:585:ILE:HG13	1:C:586:VAL:N	2.35	0.41
1:D:690:LYS:HD3	1:D:734:THR:HG21	2.01	0.41
1:C:622:HIS:HA	1:C:623:PRO:HD3	1.92	0.41
1:C:890:ARG:CB	1:C:892:TYR:H	2.33	0.41
1:D:834:SER:O	1:D:837:LYS:HG2	2.20	0.41
1:D:854:LEU:HA	1:D:859:VAL:HG21	2.02	0.41
1:A:765:TYR:OH	1:A:794:CYS:SG	2.69	0.41
1:D:689:LEU:N	1:D:689:LEU:HD12	2.35	0.41
1:D:808:LEU:HB2	1:D:829:HIS:NE2	2.35	0.41
1:C:870:VAL:HG13	1:C:897:VAL:HG22	2.01	0.41
1:A:661:LEU:HA	1:A:662:GLY:HA2	1.72	0.41
1:C:737:TRP:CZ3	1:C:763:VAL:HG12	2.55	0.41
1:D:647:ALA:HB3	1:D:696:LEU:HD11	2.02	0.41
1:B:664:GLU:HB2	1:B:667:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:864:ARG:HH12	1:D:864:ARG:NH1	2.19	0.41
1:C:904:MET:HG2	1:C:933:PHE:CZ	2.56	0.41
1:A:849:ILE:HD13	1:A:898:ARG:CG	2.44	0.41
1:A:890:ARG:HB2	1:A:892:TYR:CB	2.50	0.41
1:C:845:VAL:HG21	1:C:948:MET:HG3	2.02	0.41
1:A:585:ILE:HD13	1:A:600:ARG:NH1	2.36	0.41
1:A:765:TYR:HB3	1:A:774:PRO:HD3	2.01	0.41
1:B:879:THR:HG23	1:B:881:PRO:HD2	2.02	0.41
1:B:866:GLY:O	1:B:869:VAL:HG12	2.21	0.41
1:D:879:THR:HB	1:D:881:PRO:HD2	2.03	0.41
1:D:908:LYS:NZ	1:D:925:ILE:HD13	2.35	0.41
1:A:671:GLN:OE1	1:A:707:ALA:N	2.47	0.41
1:A:772:TYR:N	1:A:772:TYR:CD1	2.89	0.41
1:B:709:ILE:HG12	1:B:709:ILE:H	1.55	0.41
1:A:596:VAL:HG11	1:A:641:ALA:HB1	2.02	0.40
1:A:647:ALA:HB1	1:A:651:GLU:HB2	2.02	0.40
1:A:649:LEU:O	1:A:653:VAL:HG13	2.20	0.40
1:B:765:TYR:CE2	1:B:792:LEU:HD13	2.56	0.40
1:B:879:THR:HG21	1:B:921:THR:OG1	2.21	0.40
1:C:563:MET:HG3	1:C:564:VAL:N	2.36	0.40
1:C:773:HIS:CD2	1:C:775:PHE:H	2.39	0.40
1:D:821:PRO:HB2	1:D:825:HIS:HB3	2.03	0.40
1:D:874:TRP:NE1	1:D:894:GLY:HA2	2.36	0.40
1:B:585:ILE:HG13	1:B:586:VAL:N	2.36	0.40
1:C:633:LYS:HB3	1:C:633:LYS:HE3	1.82	0.40
1:A:608:PHE:CE1	1:A:613:VAL:HG21	2.56	0.40
1:A:622:HIS:HA	1:A:623:PRO:HD3	1.86	0.40
1:C:861:GLN:NE2	1:C:950:LEU:HD11	2.36	0.40
1:A:809:ILE:O	1:A:813:ILE:HG12	2.21	0.40
1:A:943:HIS:O	1:A:946:GLN:HG3	2.21	0.40
1:B:758:PHE:CE2	1:B:785:ILE:HD11	2.57	0.40
1:B:846:SER:OG	1:B:902:ARG:HA	2.21	0.40
1:A:596:VAL:HG13	1:A:642:ILE:O	2.21	0.40
1:A:864:ARG:HA	1:A:864:ARG:HD2	1.85	0.40
1:A:887:ARG:HG2	1:A:888:LYS:N	2.35	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	380/435 (87%)	331 (87%)	44 (12%)	5 (1%)	12	39
1	B	377/435 (87%)	348 (92%)	27 (7%)	2 (0%)	29	61
1	C	380/435 (87%)	346 (91%)	31 (8%)	3 (1%)	19	51
1	D	379/435 (87%)	345 (91%)	27 (7%)	7 (2%)	8	32
All	All	1516/1740 (87%)	1370 (90%)	129 (8%)	17 (1%)	14	44

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	659	ALA
1	C	866	GLY
1	D	661	LEU
1	B	735	GLU
1	B	927	ASP
1	A	567	GLY
1	A	658	PHE
1	A	660	HIS
1	D	593	ASN
1	D	866	GLY
1	D	872	MET
1	D	629	PHE
1	D	659	ALA
1	D	927	ASP
1	A	717	LYS
1	C	593	ASN
1	C	776	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	337/387 (87%)	287 (85%)	50 (15%)	3	12
1	B	338/387 (87%)	294 (87%)	44 (13%)	4	16
1	C	339/387 (88%)	298 (88%)	41 (12%)	5	18
1	D	331/387 (86%)	280 (85%)	51 (15%)	2	11
All	All	1345/1548 (87%)	1159 (86%)	186 (14%)	3	14

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	582	GLU
1	B	585	ILE
1	B	594	ARG
1	B	600	ARG
1	B	602	LEU
1	B	616	LEU
1	B	620	ASP
1	B	621	GLU
1	B	626	ILE
1	B	627	ARG
1	B	631	THR
1	B	635	ARG
1	B	636	GLN
1	B	638	GLN
1	B	642	ILE
1	B	649	LEU
1	B	661	LEU
1	B	663	LEU
1	B	668	LEU
1	B	676	LEU
1	B	684	ILE
1	B	694	ILE
1	B	702	HIS
1	B	709	ILE
1	B	752	THR
1	B	763	VAL
1	B	785	ILE
1	B	786	LEU

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Mol	Chain	Res	Type
1	B	787	LEU
1	B	792	LEU
1	B	818	GLN
1	B	819	GLN
1	B	864	ARG
1	B	878	ILE
1	B	879	THR
1	B	880	VAL
1	B	882	LEU
1	B	891	THR
1	B	896	SER
1	B	905	ARG
1	B	913	GLU
1	B	922	LEU
1	B	934	THR
1	B	956	LEU
1	A	563	MET
1	A	564	VAL
1	A	568	LYS
1	A	569	ILE
1	A	570	SER
1	A	584	THR
1	A	600	ARG
1	A	601	ILE
1	A	608	PHE
1	A	610	ASP
1	A	611	ARG
1	A	616	LEU
1	A	626	ILE
1	A	627	ARG
1	A	631	THR
1	A	638	GLN
1	A	649	LEU
1	A	653	VAL
1	A	656	LYS
1	A	661	LEU
1	A	668	LEU
1	A	670	HIS
1	A	702	HIS
1	A	709	ILE
1	A	712	PHE
1	A	745	GLU

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Mol	Chain	Res	Type
1	A	752	THR
1	A	763	VAL
1	A	786	LEU
1	A	790	CYS
1	A	819	GLN
1	A	852	GLU
1	A	854	LEU
1	A	864	ARG
1	A	870	VAL
1	A	878	ILE
1	A	880	VAL
1	A	882	LEU
1	A	884	THR
1	A	885	ASP
1	A	887	ARG
1	A	890	ARG
1	A	891	THR
1	A	905	ARG
1	A	914	LEU
1	A	936	ARG
1	A	946	GLN
1	A	956	LEU
1	A	959	THR
1	A	963	HIS
1	C	564	VAL
1	C	568	LYS
1	C	572	CYS
1	C	582	GLU
1	C	585	ILE
1	C	600	ARG
1	C	601	ILE
1	C	616	LEU
1	C	638	GLN
1	C	640	ILE
1	C	649	LEU
1	C	656	LYS
1	C	668	LEU
1	C	676	LEU
1	C	685	VAL
1	C	694	ILE
1	C	702	HIS
1	C	750	ASN

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Mol	Chain	Res	Type
1	C	752	THR
1	C	754	THR
1	C	786	LEU
1	C	787	LEU
1	C	797	SER
1	C	825	HIS
1	C	835	LEU
1	C	849	ILE
1	C	864	ARG
1	C	880	VAL
1	C	882	LEU
1	C	886	LEU
1	C	891	THR
1	C	898	ARG
1	C	902	ARG
1	C	905	ARG
1	C	907	LYS
1	C	914	LEU
1	C	921	THR
1	C	925	ILE
1	C	930	VAL
1	C	934	THR
1	C	951	CYS
1	D	562	ARG
1	D	582	GLU
1	D	600	ARG
1	D	601	ILE
1	D	615	LEU
1	D	616	LEU
1	D	620	ASP
1	D	624	ASN
1	D	631	THR
1	D	632	GLU
1	D	638	GLN
1	D	649	LEU
1	D	652	TYR
1	D	660	HIS
1	D	668	LEU
1	D	669	LEU
1	D	676	LEU
1	D	684	ILE
1	D	689	LEU

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Mol	Chain	Res	Type
1	D	692	HIS
1	D	702	HIS
1	D	704	ARG
1	D	708	MET
1	D	797	SER
1	D	809	ILE
1	D	819	GLN
1	D	827	LEU
1	D	835	LEU
1	D	842	PHE
1	D	854	LEU
1	D	855	ASP
1	D	863	GLU
1	D	872	MET
1	D	880	VAL
1	D	884	THR
1	D	889	PHE
1	D	890	ARG
1	D	891	THR
1	D	905	ARG
1	D	909	HIS
1	D	914	LEU
1	D	921	THR
1	D	922	LEU
1	D	925	ILE
1	D	927	ASP
1	D	935	SER
1	D	942	SER
1	D	951	CYS
1	D	955	ARG
1	D	956	LEU
1	D	959	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	624	ASN
1	B	773	HIS
1	B	877	ASN
1	A	624	ASN
1	A	686	HIS
1	A	943	HIS

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Mol	Chain	Res	Type
1	C	773	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	ADP	A	1002	3	24,29,29	1.05	2 (8%)	29,45,45	1.52	3 (10%)
2	ADP	D	1001	3	24,29,29	1.01	1 (4%)	29,45,45	1.50	4 (13%)
5	PEU	A	1004	-	30,30,82	0.46	0	29,29,81	0.60	0
4	31L	A	1001	1	24,24,24	0.70	1 (4%)	32,33,33	2.56	8 (25%)
2	ADP	B	1001	3	24,29,29	0.98	1 (4%)	29,45,45	1.42	4 (13%)
2	ADP	C	1001	3	24,29,29	1.02	1 (4%)	29,45,45	1.30	2 (6%)

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	ADP	A	1002	3	-	0/12/32/32	0/3/3/3
2	ADP	D	1001	3	-	5/12/32/32	0/3/3/3
5	PEU	A	1004	-	-	12/28/28/80	-
4	31L	A	1001	1	-	2/10/18/18	0/3/3/3
2	ADP	B	1001	3	-	6/12/32/32	0/3/3/3
2	ADP	C	1001	3	-	8/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1002	ADP	C5-C4	2.82	1.48	1.40
2	B	1001	ADP	C5-C4	2.70	1.48	1.40
2	D	1001	ADP	C5-C4	2.69	1.48	1.40
2	C	1001	ADP	C5-C4	2.62	1.47	1.40
2	A	1002	ADP	C2-N3	2.22	1.35	1.32
4	A	1001	31L	C06-C04	-2.06	1.37	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	31L	O07-C06-C04	8.68	123.30	114.54
4	A	1001	31L	C20-C19-N18	-5.14	100.53	110.02
4	A	1001	31L	C22-C23-N18	-4.73	101.30	110.02
4	A	1001	31L	O07-C06-C09	-4.60	116.21	124.12
4	A	1001	31L	C19-N18-C23	4.51	121.47	111.52
2	D	1001	ADP	N3-C2-N1	-3.48	123.24	128.68
2	B	1001	ADP	C3'-C2'-C1'	3.47	106.20	100.98
2	A	1002	ADP	N3-C2-N1	-3.47	123.26	128.68
2	A	1002	ADP	PA-O3A-PB	-3.46	120.95	132.83
2	A	1002	ADP	C3'-C2'-C1'	3.36	106.04	100.98
2	D	1001	ADP	C3'-C2'-C1'	3.32	105.98	100.98
2	C	1001	ADP	C3'-C2'-C1'	3.22	105.82	100.98
2	B	1001	ADP	N3-C2-N1	-3.19	123.69	128.68
4	A	1001	31L	C08-O07-C06	3.18	122.33	117.53
2	C	1001	ADP	N3-C2-N1	-3.18	123.71	128.68
2	B	1001	ADP	PA-O3A-PB	-2.79	123.25	132.83
2	D	1001	ADP	PA-O3A-PB	-2.47	124.36	132.83
2	D	1001	ADP	C4-C5-N7	-2.35	106.95	109.40
2	B	1001	ADP	O3B-PB-O2B	2.19	116.02	107.64
4	A	1001	31L	C10-C09-C06	-2.18	117.17	120.13
4	A	1001	31L	C09-C10-C11	2.14	121.47	118.31

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1001	ADP	C5'-O5'-PA-O1A
2	D	1001	ADP	C5'-O5'-PA-O2A
2	D	1001	ADP	C5'-O5'-PA-O3A
2	D	1001	ADP	O4'-C4'-C5'-O5'
2	D	1001	ADP	C3'-C4'-C5'-O5'
2	B	1001	ADP	C5'-O5'-PA-O3A
2	B	1001	ADP	O4'-C4'-C5'-O5'
2	C	1001	ADP	C5'-O5'-PA-O1A
2	C	1001	ADP	C5'-O5'-PA-O3A
2	C	1001	ADP	O4'-C4'-C5'-O5'
2	C	1001	ADP	C3'-C4'-C5'-O5'
4	A	1001	31L	C04-C06-O07-C08
2	B	1001	ADP	C3'-C4'-C5'-O5'
4	A	1001	31L	C09-C06-O07-C08
5	A	1004	PEU	OAK-CAL-CAM-OAN
5	A	1004	PEU	OAB-CAC-CAD-OAE
5	A	1004	PEU	OAZ-CBA-CBB-OBC
5	A	1004	PEU	OAH-CAI-CAJ-OAK
5	A	1004	PEU	CAI-CAJ-OAK-CAL
5	A	1004	PEU	CAP-CAO-OAN-CAM
5	A	1004	PEU	CAR-CAS-OAT-CAU
5	A	1004	PEU	CAX-CAY-OAZ-CBA
5	A	1004	PEU	CBA-CBB-OBC-CCG
2	C	1001	ADP	PB-O3A-PA-O1A
5	A	1004	PEU	CBB-CBA-OAZ-CAY
2	B	1001	ADP	C5'-O5'-PA-O1A
2	B	1001	ADP	C5'-O5'-PA-O2A
2	C	1001	ADP	C5'-O5'-PA-O2A
5	A	1004	PEU	OAQ-CAR-CAS-OAT
2	B	1001	ADP	PA-O3A-PB-O1B
2	C	1001	ADP	PA-O3A-PB-O3B
5	A	1004	PEU	OAE-CAF-CAG-OAH
2	C	1001	ADP	PB-O3A-PA-O2A

There are no ring outliers.

3 monomers are involved in 5 short contacts:

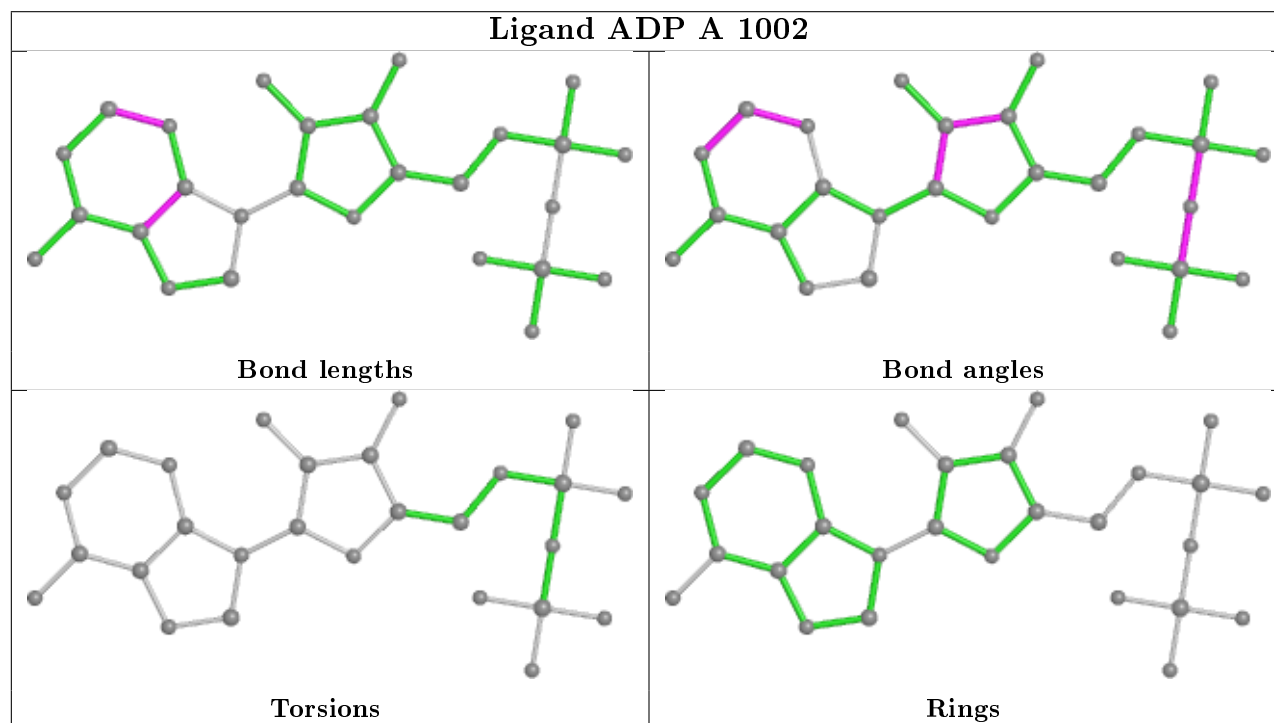
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1001	ADP	1	0
4	A	1001	31L	3	0

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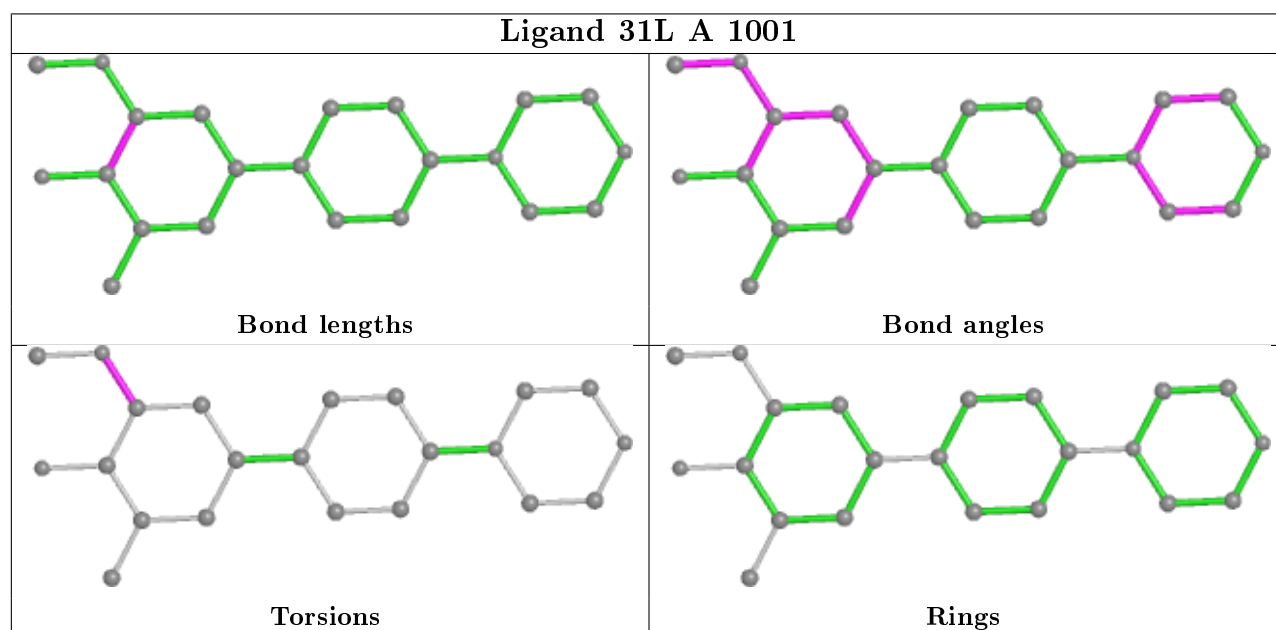
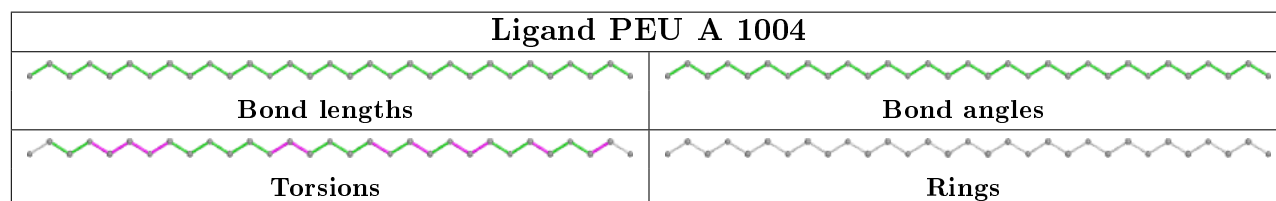
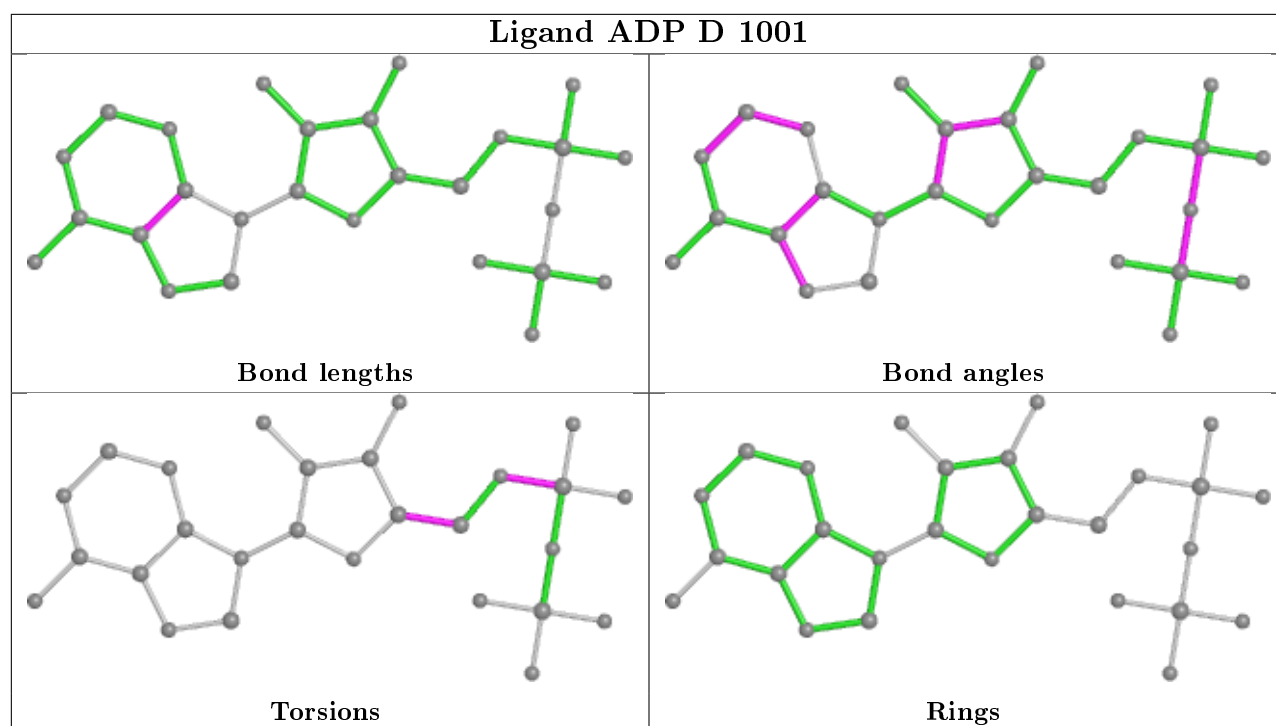
*Continued from previous page...*

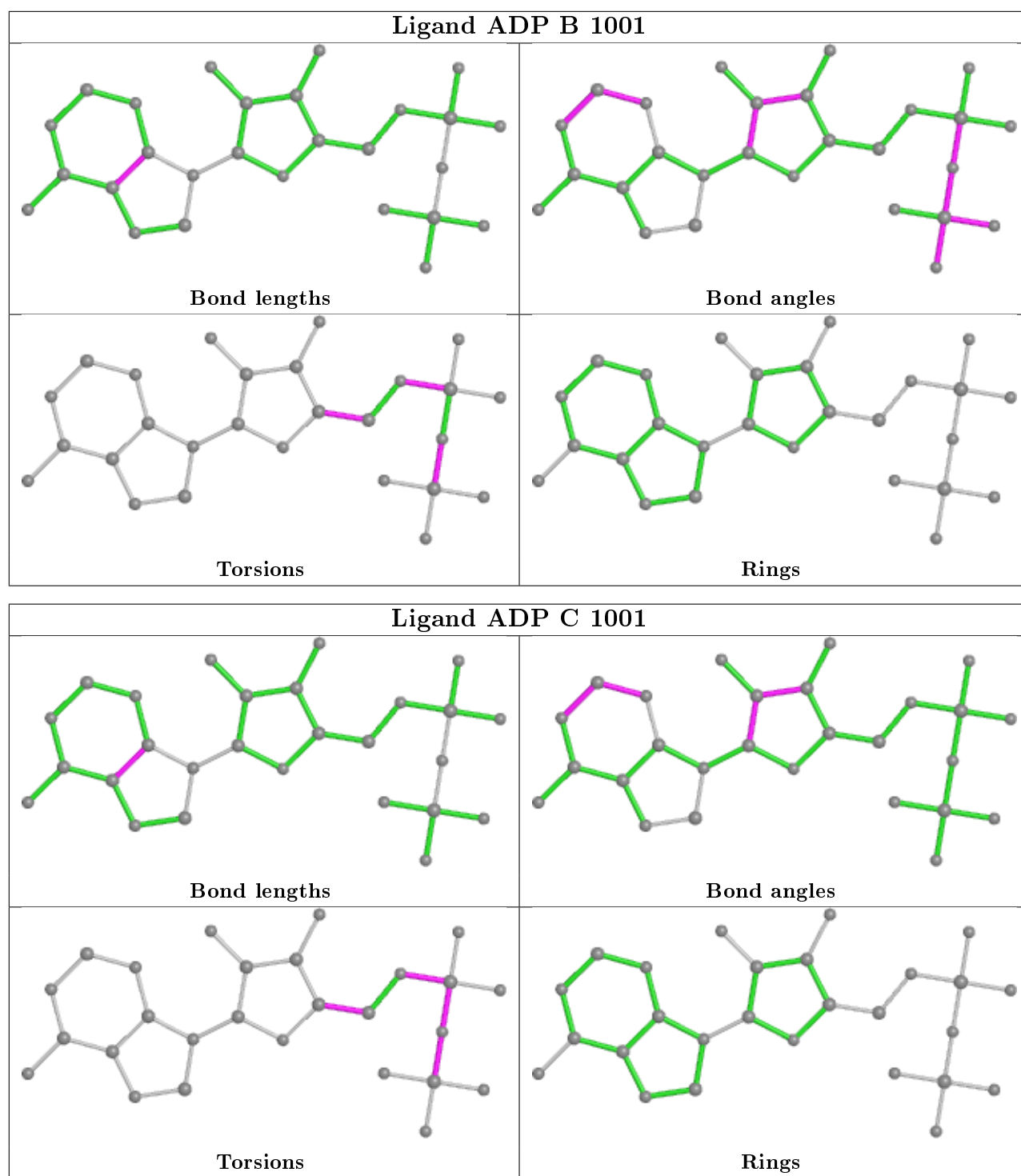
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	ADP	1	0

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 ⓘ

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, 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	386/435 (88%)	-0.11	2 (0%) 91 90	13, 62, 119, 153	0
1	B	383/435 (88%)	-0.06	3 (0%) 86 85	20, 68, 114, 134	0
1	C	386/435 (88%)	-0.13	5 (1%) 77 76	29, 74, 122, 164	0
1	D	385/435 (88%)	0.37	23 (5%) 21 23	55, 105, 155, 183	0
All	All	1540/1740 (88%)	0.02	33 (2%) 63 62	13, 78, 135, 183	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	907	LYS	4.6
1	C	596	VAL	4.4
1	D	906	ASN	4.3
1	D	589	GLY	4.1
1	D	641	ALA	3.8
1	D	628	TYR	3.8
1	C	630	CYS	3.5
1	D	845	VAL	3.4
1	D	908	LYS	3.4
1	D	951	CYS	3.2
1	C	589	GLY	3.1
1	D	918	VAL	3.0
1	D	956	LEU	3.0
1	D	948	MET	2.9
1	D	842	PHE	2.8
1	D	576	VAL	2.7
1	D	612	GLU	2.7
1	D	929	PHE	2.7
1	D	571	PHE	2.6
1	D	855	ASP	2.5
1	B	610	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	925	ILE	2.3
1	C	640	ILE	2.2
1	D	742	MET	2.2
1	C	641	ALA	2.2
1	A	573	PRO	2.2
1	B	963	HIS	2.2
1	D	961	TYR	2.1
1	D	904	MET	2.1
1	D	614	GLN	2.0
1	A	661	LEU	2.0
1	D	949	GLU	2.0
1	B	682	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 ⓘ

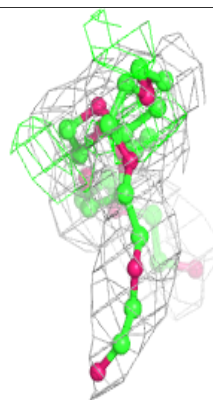
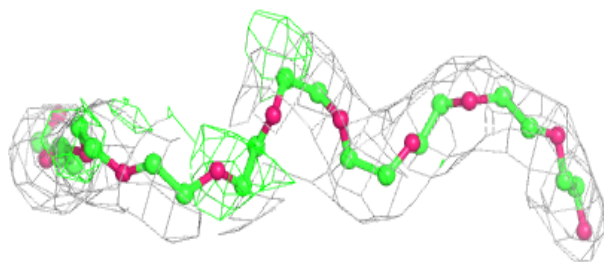
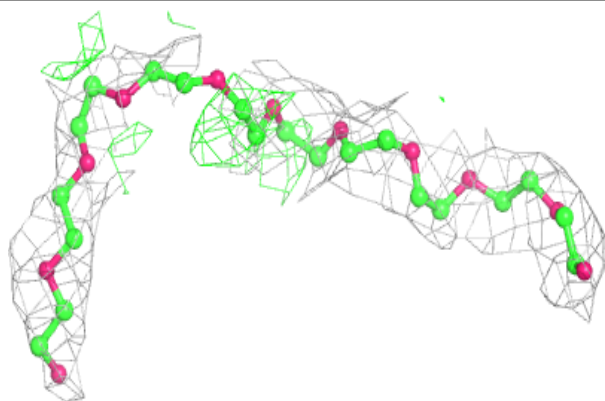
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	PEU	A	1004	31/83	0.82	0.26	36,76,91,98	0
2	ADP	D	1001	27/27	0.87	0.25	64,85,125,184	0
4	31L	A	1001	22/22	0.90	0.39	71,96,107,115	0
3	MG	B	1002	1/1	0.94	0.24	35,35,35,35	0
2	ADP	B	1001	27/27	0.94	0.20	25,54,79,132	0
2	ADP	C	1001	27/27	0.94	0.21	56,66,81,91	0
2	ADP	A	1002	27/27	0.96	0.20	21,46,74,154	0
3	MG	C	1002	1/1	0.96	0.23	34,34,34,34	0
3	MG	D	1002	1/1	0.97	0.27	109,109,109,109	0
3	MG	A	1003	1/1	0.98	0.25	46,46,46,46	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.

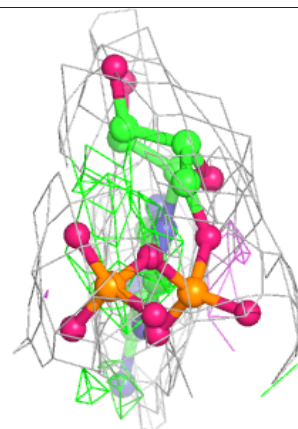
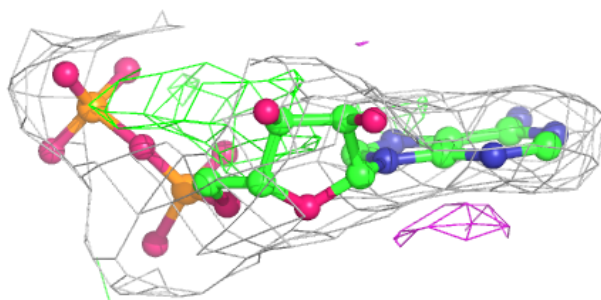
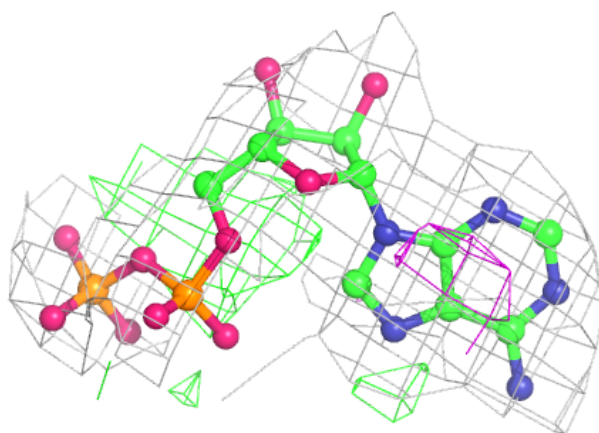
**Electron density around PEU A 1004:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

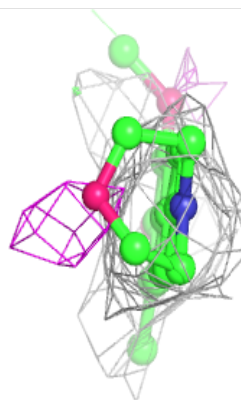
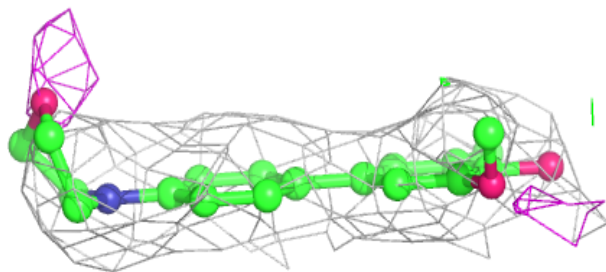
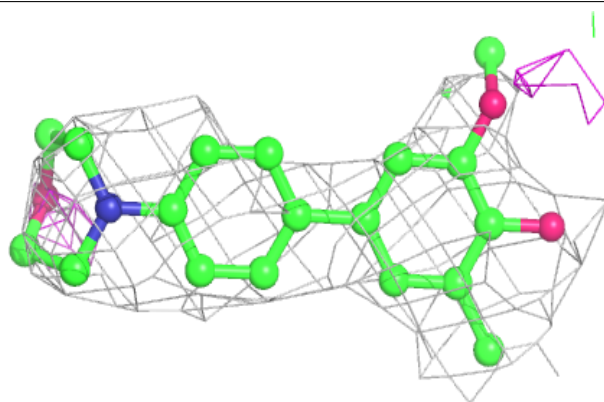


**Electron density around ADP D 1001:**

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

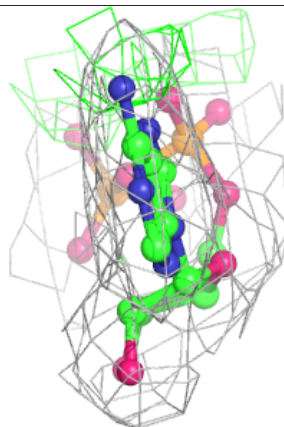
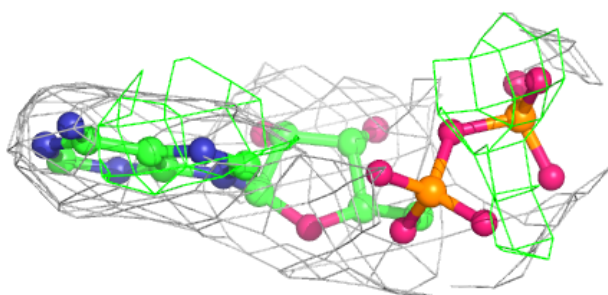
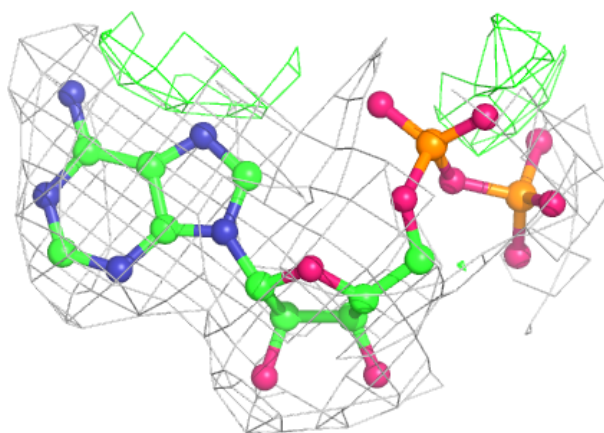
**Electron density around 31L A 1001:**

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



**Electron density around ADP B 1001:**

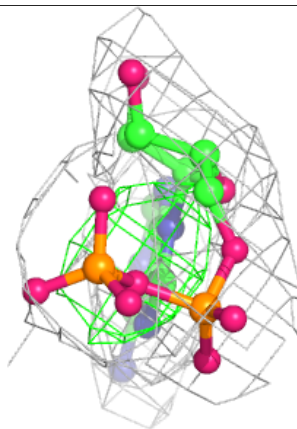
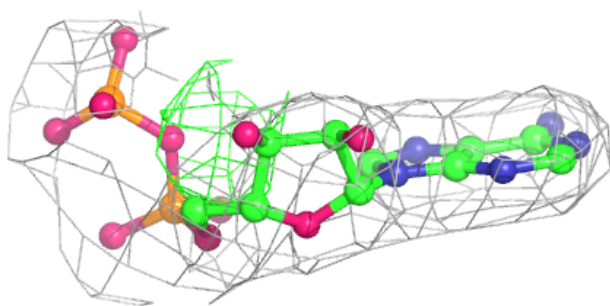
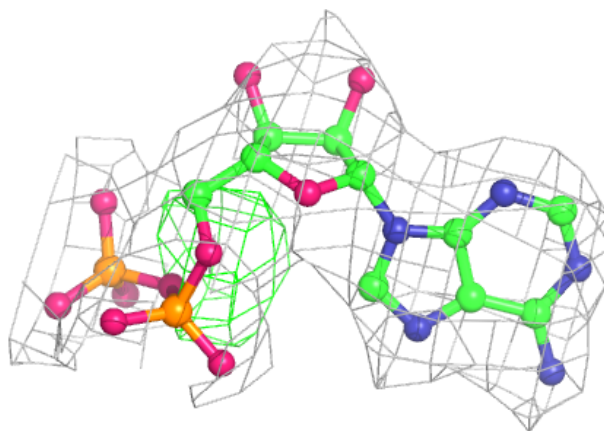
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



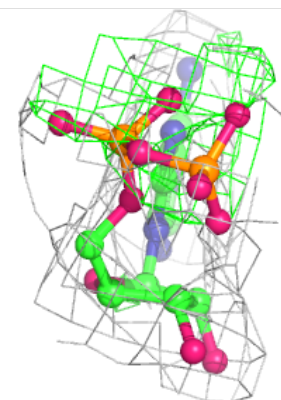
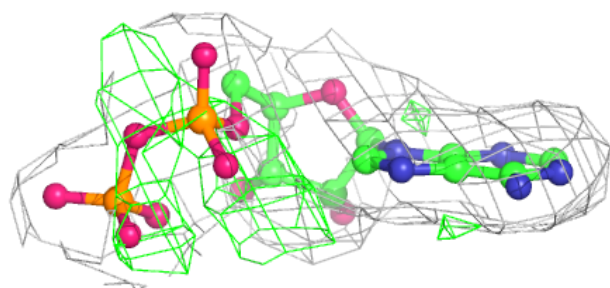
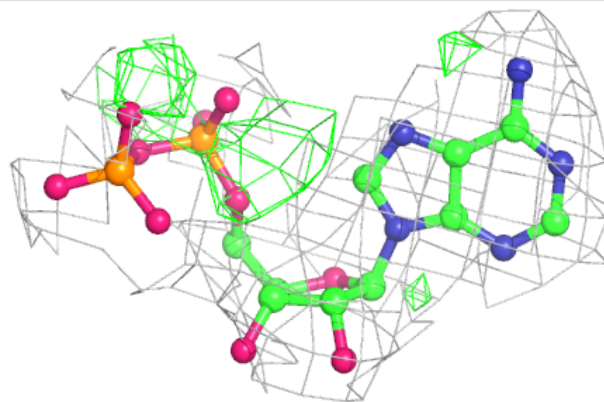


**Electron density around ADP C 1001:**

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

**Electron density around ADP A 1002:**

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



## 6.5 Other polymers

There are no such residues in this entry.