Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 11:46 AM EDT

PDB ID	:	3ZWY
Title	:	Crystal structure of ADP-ribosyl cyclase complexed with 8-bromo-ADP- ribose and cyclic 8-bromo-cyclic-ADP-ribose
Authors	:	Kotaka, M.; Graeff, R.; Zhang, L.H.; Lee, H.C.; Hao, Q.
Deposited on	:	2011-08-03
Resolution	:	2.40 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

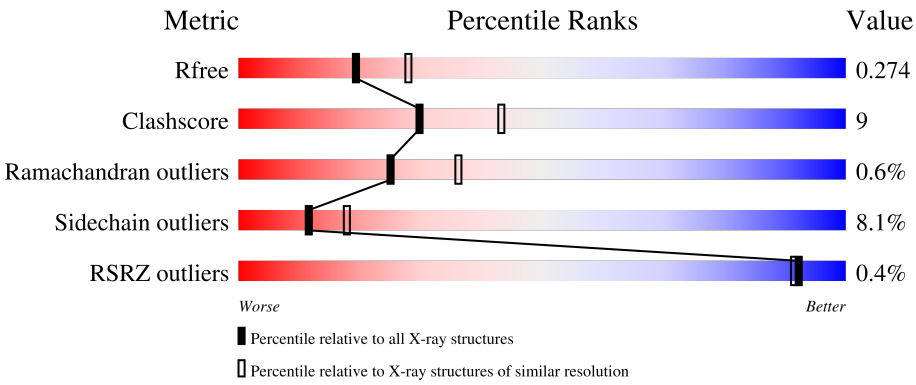
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	260	73% 20% • •
1	B	260	% 77% 18% • •
1	C	260	70% 25% • •
1	D	260	75% 20% • •
1	E	260	% 73% 20% • •

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Mol	Chain	Length	Quality of chain
1	F	260	69% 23%
1	G	260	74% 20%
1	H	260	72% 22%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16759 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 ADP-RIBOSYL CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	251	2012	1288	342	368	14	0	0	0
1	B	252	2017	1291	343	369	14	0	0	0
1	C	252	2017	1291	343	369	14	0	0	0
1	D	252	2017	1291	343	369	14	0	0	0
1	E	251	2012	1288	342	368	14	0	0	0
1	F	251	2012	1288	342	368	14	0	0	0
1	G	251	2012	1288	342	368	14	0	0	0
1	H	251	2012	1288	342	368	14	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP P29241
A	0	ALA	-	expression tag	UNP P29241
B	-1	ALA	-	expression tag	UNP P29241
B	0	ALA	-	expression tag	UNP P29241
C	-1	ALA	-	expression tag	UNP P29241
C	0	ALA	-	expression tag	UNP P29241
D	-1	ALA	-	expression tag	UNP P29241
D	0	ALA	-	expression tag	UNP P29241
E	-1	ALA	-	expression tag	UNP P29241
E	0	ALA	-	expression tag	UNP P29241
F	-1	ALA	-	expression tag	UNP P29241
F	0	ALA	-	expression tag	UNP P29241
G	-1	ALA	-	expression tag	UNP P29241

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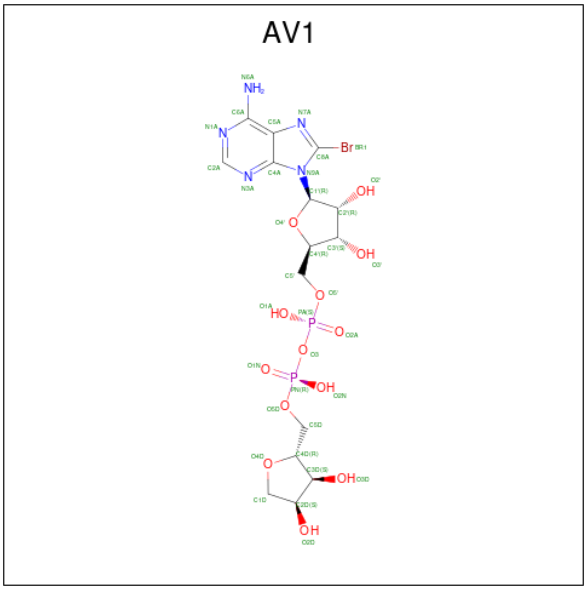
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	ALA	-	expression tag	UNP P29241
H	-1	ALA	-	expression tag	UNP P29241
H	0	ALA	-	expression tag	UNP P29241

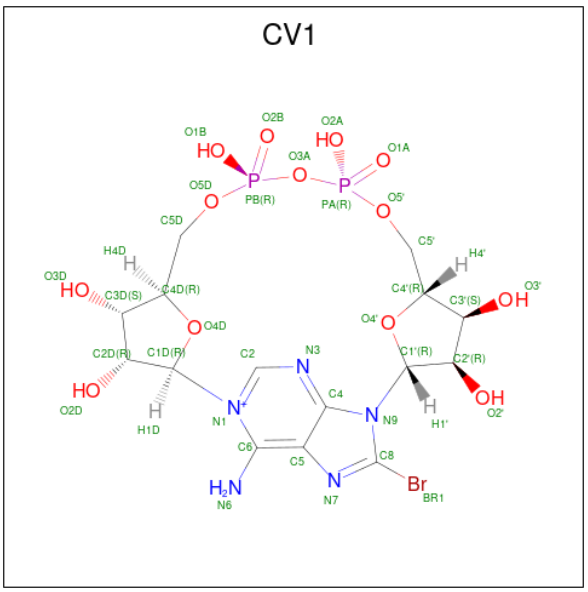
- Molecule 2 is [(2R,3S,4R,5R)-5-(6-amino-8-bromo-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl [(2R,3S,4S)-3,4-dihydroxytetrahydrofuran-2-yl]methyl dihydrogen diphosphate (three-letter code: AV1) (formula: $C_{15}H_{22}BrN_5O_{13}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	N	O	P		
2	A	1	36	1	15	5	13	2	0	0
2	B	1	36	1	15	5	13	2	0	0
2	C	1	36	1	15	5	13	2	0	0
2	E	1	36	1	15	5	13	2	0	0
2	F	1	36	1	15	5	13	2	0	0
2	G	1	36	1	15	5	13	2	0	0
2	H	1	36	1	15	5	13	2	0	0

- Molecule 3 is (2R,3R,4S,5R,13R,14S,15R,16R)-24-amino-18-bromo-3,4,14,15-tetrahydroxy-7,9,11,25,26-pentaoxa-17,19,22-triaza-1-azonia-8 ,10-diphosphapentacyclo[18.3.1.1^2,5^.1^13,16^.0^17,21^]hexacosa-1(24),18,20,22-tetraene-8,10-diolate 8,10-dioxide (three-letter code:

CV1) (formula: $C_{15}H_{21}BrN_5O_{13}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	N	O	P		
3	D	1	36	1	15	5	13	2	0	0

- Molecule 4 is water.

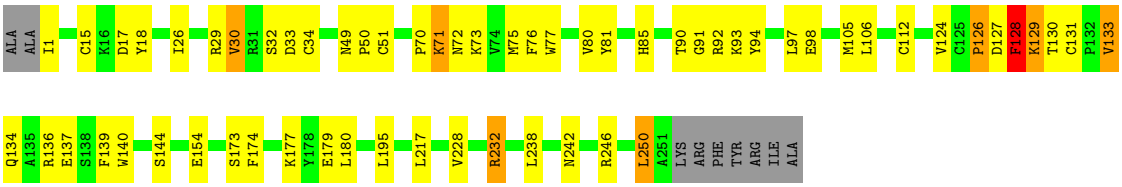
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	41	41	41	0	0
4	B	61	61	61	0	0
4	C	60	60	60	0	0
4	D	52	52	52	0	0
4	E	50	50	50	0	0
4	F	34	34	34	0	0
4	G	41	41	41	0	0
4	H	21	21	21	0	0

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.

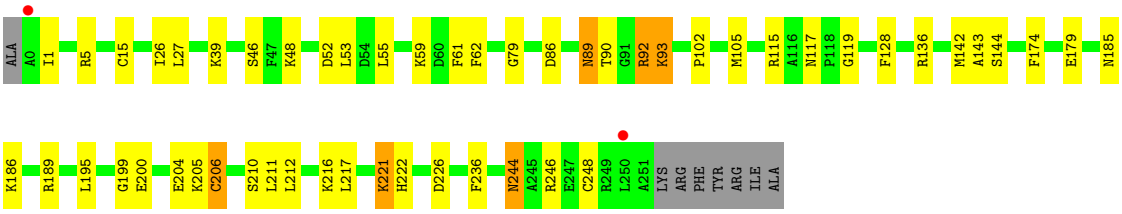
• Molecule 1: ADP-RIBOSYL CYCLASE

Chain A:



• Molecule 1: ADP-RIBOSYL CYCLASE

Chain B:

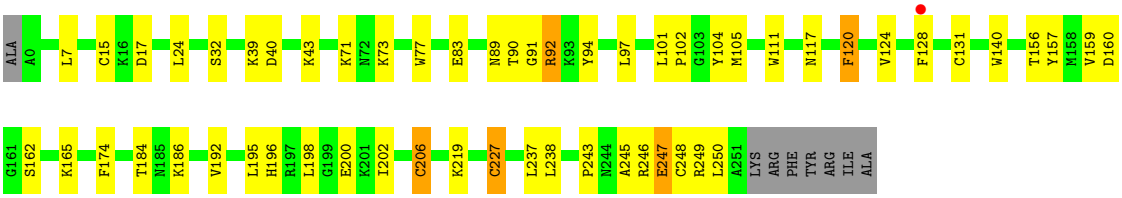


• Molecule 1: ADP-RIBOSYL CYCLASE

Chain C:

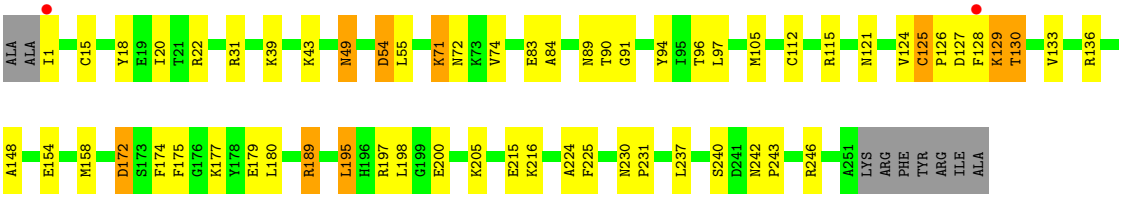
• Molecule 1: ADP-RIBOSYL CYCLASE

Chain D:



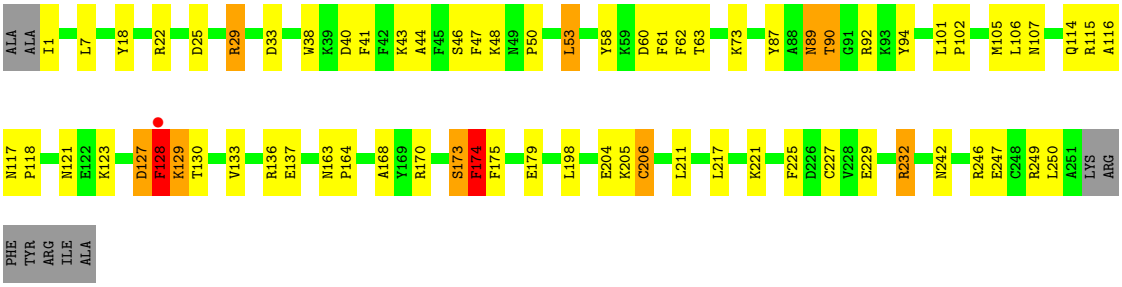
• Molecule 1: ADP-RIBOSYL CYCLASE

Chain E:



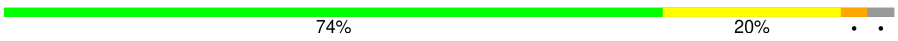
• Molecule 1: ADP-RIBOSYL CYCLASE

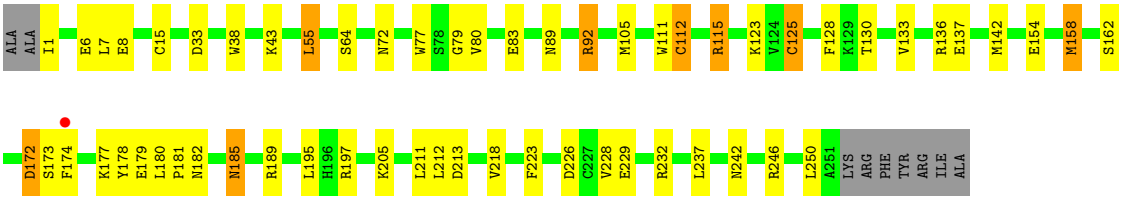
Chain F:



• Molecule 1: ADP-RIBOSYL CYCLASE

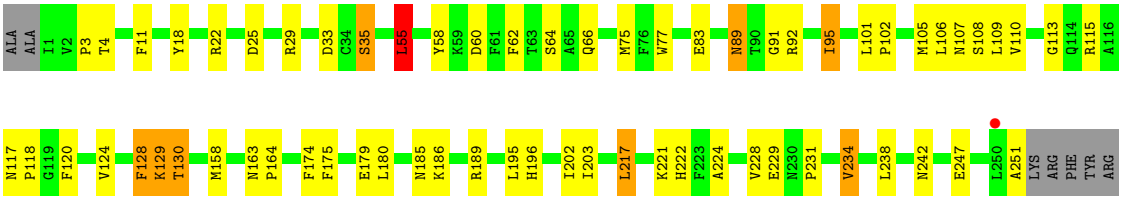
Chain G:





• Molecule 1: ADP-RIBOSYL CYCLASE

Chain H:



ILE
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.29Å 77.01Å 140.34Å 87.50° 89.27° 88.99°	Depositor
Resolution (Å)	30.00 – 2.40 26.25 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.4 (30.00-2.40) 96.5 (26.25-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.215 , 0.283 0.209 , 0.274	Depositor DCC
R_{free} test set	4730 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 13.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.099 for h,-k,-l 0.014 for -h,k,-l 0.011 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16759	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: AV1, CV1

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	0.92	0/2064	0.88	1/2793 (0.0%)
1	B	1.02	2/2069 (0.1%)	0.94	2/2800 (0.1%)
1	C	0.98	1/2069 (0.0%)	0.94	3/2800 (0.1%)
1	D	0.95	1/2069 (0.0%)	0.91	3/2800 (0.1%)
1	E	0.97	2/2064 (0.1%)	0.94	3/2793 (0.1%)
1	F	0.74	1/2064 (0.0%)	0.82	1/2793 (0.0%)
1	G	0.90	0/2064	0.87	3/2793 (0.1%)
1	H	0.74	0/2064	0.77	0/2793
All	All	0.91	7/16527 (0.0%)	0.88	16/22365 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	125	CYS	CB-SG	-8.17	1.68	1.82
1	D	104	TYR	CE1-CZ	5.70	1.46	1.38
1	F	48	LYS	CD-CE	5.59	1.65	1.51
1	B	248	CYS	CB-SG	5.49	1.91	1.82
1	B	206	CYS	CB-SG	5.22	1.91	1.82
1	C	15	CYS	CB-SG	-5.17	1.73	1.81
1	E	174	PHE	CE1-CZ	5.05	1.47	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	125	CYS	CA-CB-SG	-15.08	86.85	114.00
1	G	125	CYS	CA-CB-SG	-8.87	98.04	114.00
1	D	17	ASP	CB-CG-OD1	7.99	125.49	118.30
1	C	29	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	E	195	LEU	CB-CG-CD2	-7.00	99.10	111.00
1	D	160	ASP	CB-CG-OD1	6.23	123.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	206	CYS	CA-CB-SG	-6.03	103.15	114.00
1	C	86	ASP	CB-CG-OD1	5.77	123.49	118.30
1	C	206	CYS	CA-CB-SG	5.76	124.36	114.00
1	B	53	LEU	CA-CB-CG	5.75	128.51	115.30
1	G	55	LEU	CB-CG-CD1	5.69	120.67	111.00
1	G	172	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	E	54	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	86	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	206	CYS	N-CA-CB	-5.18	101.28	110.60
1	A	17	ASP	CB-CG-OD1	5.08	122.87	118.30

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	2012	0	1968	36	0
1	B	2017	0	1973	28	0
1	C	2017	0	1973	47	0
1	D	2017	0	1973	34	0
1	E	2012	0	1968	41	0
1	F	2012	0	1968	43	0
1	G	2012	0	1968	43	0
1	H	2012	0	1968	41	0
2	A	36	0	20	3	0
2	B	36	0	20	4	0
2	C	36	0	20	1	0
2	E	36	0	20	1	0
2	F	36	0	20	3	0
2	G	36	0	20	3	0
2	H	36	0	20	2	0
3	D	36	0	19	4	0
4	A	41	0	0	2	0
4	B	61	0	0	2	0
4	C	60	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	52	0	0	3	0
4	E	50	0	0	6	0
4	F	34	0	0	7	0
4	G	41	0	0	4	0
4	H	21	0	0	1	0
All	All	16759	0	15918	304	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (304) 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:G:128:PHE:O	1:G:136:ARG:HD3	1.52	1.09
1:C:127:ASP:O	1:C:130:THR:HG22	1.56	1.06
1:E:121:ASN:OD1	1:E:124:VAL:O	1.77	1.02
1:F:33:ASP:HB3	4:F:2009:HOH:O	1.58	1.02
1:D:198:LEU:HD22	1:D:247:GLU:HG3	1.39	1.02
1:C:128:PHE:O	1:C:136:ARG:HD3	1.64	0.96
1:A:129:LYS:HZ1	1:A:129:LYS:H	1.18	0.90
1:G:128:PHE:O	1:G:136:ARG:CD	2.18	0.90
1:C:127:ASP:O	1:C:130:THR:CG2	2.19	0.89
1:G:1:ILE:HG22	1:G:125:CYS:O	1.74	0.87
1:G:80:VAL:HG21	1:G:158:MET:HG2	1.56	0.87
1:C:128:PHE:O	1:C:136:ARG:CD	2.23	0.86
1:A:127:ASP:O	1:A:130:THR:HG22	1.77	0.85
1:C:133:VAL:HB	1:G:177:LYS:HB2	1.61	0.81
1:A:129:LYS:H	1:A:129:LYS:NZ	1.78	0.81
1:D:97:LEU:HD23	3:D:303:CV1:N6	1.97	0.79
1:G:115:ARG:HH11	1:G:115:ARG:HG2	1.47	0.79
1:D:198:LEU:CD2	1:D:247:GLU:HG3	2.13	0.78
1:F:174:PHE:CD1	2:F:1682:AV1:O1N	2.35	0.78
1:G:115:ARG:HH11	1:G:115:ARG:CG	1.96	0.78
1:D:97:LEU:HD23	3:D:303:CV1:HN6	1.51	0.73
1:H:89:ASN:OD1	1:H:92:ARG:HD3	1.90	0.71
1:H:107:ASN:OD1	2:H:1682:AV1:H2A	1.93	0.69
1:F:43:LYS:N	4:F:2010:HOH:O	2.22	0.68
1:C:80:VAL:HG21	1:C:158:MET:HG2	1.76	0.68
1:G:83:GLU:HG2	1:G:195:LEU:HD21	1.76	0.68
1:A:195:LEU:HD11	1:A:238:LEU:HD21	1.77	0.66
1:D:246:ARG:O	1:D:249:ARG:HD3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:180:LEU:HD21	1:H:217:LEU:HD22	1.77	0.66
1:G:133:VAL:HA	1:G:136:ARG:HG3	1.79	0.64
1:F:40:ASP:O	4:F:2011:HOH:O	2.15	0.64
1:C:134:GLN:HG2	1:G:55:LEU:HD23	1.80	0.64
1:F:41:PHE:C	4:F:2010:HOH:O	2.36	0.63
1:E:49:ASN:HB2	4:E:2012:HOH:O	1.97	0.63
1:B:92:ARG:HH22	1:B:93:LYS:NZ	1.96	0.63
1:F:43:LYS:HA	1:F:46:SER:HG	1.64	0.63
1:E:128:PHE:O	1:E:136:ARG:CD	2.48	0.62
2:E:1682:AV1:BR1	2:E:1682:AV1:O4'	2.72	0.62
1:E:125:CYS:SG	1:E:126:PRO:HD2	2.39	0.62
1:H:107:ASN:O	1:H:108:SER:HB2	1.98	0.62
1:C:134:GLN:HG2	1:G:55:LEU:CD2	2.30	0.62
1:E:128:PHE:O	1:E:136:ARG:HD2	1.98	0.62
1:A:85:HIS:NE2	1:A:98:GLU:OE1	2.32	0.62
1:B:204:GLU:OE2	1:B:210:SER:OG	2.11	0.61
1:D:117:ASN:ND2	4:D:2029:HOH:O	2.31	0.61
1:D:174:PHE:HB2	3:D:303:CV1:O5D	2.00	0.61
1:D:198:LEU:HD22	1:D:247:GLU:CG	2.22	0.61
1:H:77:TRP:O	2:H:1682:AV1:H5DA	1.99	0.61
1:F:1:ILE:N	4:F:2001:HOH:O	2.12	0.61
1:H:33:ASP:OD2	1:H:35:SER:HB2	2.01	0.61
1:D:157:TYR:CE2	1:D:159:VAL:HG11	2.36	0.60
1:A:30:VAL:HG13	4:A:2012:HOH:O	2.00	0.60
1:B:128:PHE:HD2	1:B:136:ARG:HA	1.66	0.60
1:C:174:PHE:HZ	4:C:2050:HOH:O	1.84	0.60
1:H:117:ASN:OD1	1:H:118:PRO:HA	2.01	0.60
1:C:118:PRO:HB2	1:C:120:PHE:CE1	2.35	0.59
1:C:79:GLY:N	2:C:1682:AV1:O1A	2.33	0.59
1:F:127:ASP:O	1:F:129:LYS:HE2	2.02	0.59
1:E:133:VAL:HA	1:E:136:ARG:HG3	1.83	0.59
1:F:107:ASN:OD1	2:F:1682:AV1:H2A	2.02	0.59
1:A:34:CYS:HB2	4:A:2013:HOH:O	2.03	0.59
1:G:8:GLU:HG3	1:G:38:TRP:CE2	2.38	0.58
1:E:90:THR:O	1:E:90:THR:HG22	2.03	0.58
1:D:15:CYS:HB2	1:D:105:MET:SD	2.43	0.58
1:E:49:ASN:ND2	4:E:2012:HOH:O	2.37	0.57
1:E:124:VAL:O	1:E:125:CYS:SG	2.62	0.57
1:B:174:PHE:HB2	2:B:1682:AV1:PN	2.45	0.57
1:C:80:VAL:HG11	1:C:195:LEU:CD1	2.34	0.57
1:E:127:ASP:OD1	1:E:129:LYS:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:ASN:HA	1:G:154:GLU:O	2.05	0.56
1:A:128:PHE:CD2	1:A:129:LYS:HE3	2.40	0.56
1:C:62:PHE:CZ	1:C:143:ALA:HB2	2.40	0.56
1:G:1:ILE:N	4:G:2001:HOH:O	2.37	0.56
1:C:48:LYS:HB3	1:C:52:ASP:HB3	1.87	0.56
1:C:114:GLN:HG2	1:C:120:PHE:C	2.26	0.56
1:A:91:GLY:HA2	1:A:94:TYR:O	2.06	0.55
1:G:55:LEU:HD12	1:G:142:MET:HB2	1.88	0.55
1:D:245:ALA:HB3	1:D:248:CYS:SG	2.47	0.55
1:E:127:ASP:O	1:E:130:THR:HG23	2.06	0.55
1:E:1:ILE:N	4:E:2001:HOH:O	2.38	0.55
1:A:174:PHE:HB2	2:A:1682:AV1:PN	2.47	0.55
1:C:80:VAL:HG11	1:C:195:LEU:HD12	1.88	0.55
1:D:140:TRP:HB3	1:D:174:PHE:HE2	1.73	0.54
1:C:196:HIS:CE1	1:C:229:GLU:HB3	2.43	0.54
1:F:47:PHE:HA	1:F:114:GLN:O	2.08	0.54
1:D:140:TRP:CB	1:D:174:PHE:HE2	2.21	0.54
1:F:43:LYS:HA	1:F:46:SER:OG	2.07	0.54
1:A:15:CYS:HB2	1:A:105:MET:SD	2.48	0.53
1:G:7:LEU:HD22	4:G:2002:HOH:O	2.08	0.53
4:G:2041:HOH:O	1:H:251:ALA:N	2.41	0.53
1:H:128:PHE:C	1:H:130:THR:N	2.62	0.53
1:A:144:SER:HB3	1:A:179:GLU:HG2	1.90	0.53
1:C:246:ARG:O	1:C:249:ARG:HG3	2.08	0.53
1:H:4:THR:HG21	1:H:109:LEU:HD22	1.89	0.53
1:H:128:PHE:C	1:H:130:THR:H	2.12	0.53
1:A:232:ARG:HH22	1:B:244:ASN:HD22	1.55	0.53
1:G:179:GLU:OE2	2:G:1682:AV1:O2D	2.24	0.53
1:B:48:LYS:CE	1:B:52:ASP:O	2.57	0.52
4:B:2027:HOH:O	1:D:165:LYS:NZ	2.41	0.52
1:B:92:ARG:HH22	1:B:93:LYS:HZ2	1.55	0.52
1:C:206:CYS:HB2	1:C:229:GLU:OE2	2.10	0.52
1:F:168:ALA:H	1:F:204:GLU:HG3	1.74	0.52
1:B:48:LYS:HE2	1:B:52:ASP:O	2.09	0.52
1:G:115:ARG:CG	1:G:115:ARG:NH1	2.63	0.52
1:H:55:LEU:O	1:H:55:LEU:HG	2.09	0.52
1:G:15:CYS:HB2	1:G:105:MET:SD	2.50	0.52
1:C:114:GLN:NE2	1:C:116:ALA:O	2.27	0.51
1:C:204:GLU:OE2	1:C:210:SER:OG	2.23	0.51
1:C:10:VAL:O	1:C:14:ARG:HG3	2.10	0.51
1:A:133:VAL:HA	1:A:136:ARG:HE	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:GLY:HA2	1:B:246:ARG:HH21	1.75	0.51
1:C:130:THR:O	1:G:181:PRO:HB3	2.11	0.51
1:H:18:TYR:HA	1:H:22:ARG:HB2	1.93	0.51
1:E:18:TYR:HA	1:E:22:ARG:CG	2.41	0.51
1:F:174:PHE:CD1	1:F:174:PHE:N	2.71	0.51
1:A:71:LYS:O	1:A:72:ASN:HB2	2.11	0.51
1:H:174:PHE:O	1:H:179:GLU:HG3	2.11	0.50
1:B:117:ASN:ND2	4:B:2044:HOH:O	2.44	0.50
1:D:89:ASN:OD1	1:D:92:ARG:HD3	2.11	0.50
1:G:79:GLY:N	2:G:1682:AV1:O1A	2.44	0.50
1:G:179:GLU:O	1:G:180:LEU:C	2.49	0.50
1:D:157:TYR:CE2	1:D:159:VAL:CG1	2.95	0.50
1:E:198:LEU:HD12	1:E:242:ASN:HB3	1.93	0.50
1:G:137:GLU:HG2	1:G:174:PHE:CZ	2.47	0.50
1:A:75:MET:HG2	1:A:76:PHE:N	2.27	0.50
1:D:184:THR:OG1	1:D:186:LYS:HE2	2.12	0.50
1:E:84:ALA:HA	1:E:158:MET:CE	2.42	0.50
1:G:250:LEU:C	4:G:2041:HOH:O	2.50	0.49
1:C:8:GLU:HG3	1:C:38:TRP:CE2	2.47	0.49
1:B:205:LYS:O	1:B:211:LEU:HD12	2.12	0.49
1:B:217:LEU:HD11	1:E:129:LYS:HB2	1.94	0.49
1:D:90:THR:HG22	1:D:90:THR:O	2.13	0.49
1:D:219:LYS:HG2	4:D:2048:HOH:O	2.11	0.49
1:E:15:CYS:HB2	1:E:105:MET:SD	2.53	0.49
1:F:217:LEU:O	1:F:221:LYS:HG3	2.12	0.49
1:A:70:PRO:HG2	1:A:73:LYS:HB2	1.94	0.48
1:D:243:PRO:HD2	4:D:2050:HOH:O	2.13	0.48
1:F:44:ALA:HB2	4:F:2011:HOH:O	2.13	0.48
1:F:87:TYR:CE2	1:F:94:TYR:HE2	2.31	0.48
1:C:232:ARG:NH1	1:D:250:LEU:HD12	2.28	0.48
1:G:89:ASN:O	1:G:92:ARG:HB2	2.13	0.48
1:F:18:TYR:O	1:F:29:ARG:NH1	2.47	0.48
1:F:205:LYS:NZ	1:F:229:GLU:OE1	2.46	0.48
1:E:189:ARG:HB2	1:E:224:ALA:HB3	1.94	0.48
1:E:54:ASP:HB2	4:E:2013:HOH:O	2.13	0.48
1:C:54:ASP:HB2	4:C:2021:HOH:O	2.12	0.48
1:F:198:LEU:HD22	1:F:247:GLU:HB2	1.96	0.48
1:E:55:LEU:O	1:E:55:LEU:HG	2.12	0.48
1:C:54:ASP:O	1:C:138:SER:OG	2.28	0.48
1:C:217:LEU:HD23	4:C:2054:HOH:O	2.14	0.48
1:E:18:TYR:HA	1:E:22:ARG:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:HD21	1:B:236:PHE:CE1	2.49	0.47
1:B:221:LYS:O	1:B:222:HIS:HB2	2.14	0.47
1:F:58:TYR:O	1:F:62:PHE:HD2	1.97	0.47
1:D:192:VAL:HB	1:D:227:CYS:HB2	1.96	0.47
1:B:189:ARG:HD3	1:B:226:ASP:OD2	2.14	0.47
1:A:140:TRP:HB3	1:A:174:PHE:HE2	1.80	0.47
1:B:179:GLU:OE2	2:B:1682:AV1:H1D	2.13	0.47
1:H:58:TYR:O	1:H:62:PHE:HD2	1.97	0.47
1:H:185:ASN:OD1	1:H:186:LYS:HE2	2.14	0.47
1:G:137:GLU:OE1	1:G:178:TYR:OH	2.23	0.47
1:H:83:GLU:HG2	1:H:238:LEU:HD21	1.96	0.47
1:D:40:ASP:HA	1:D:43:LYS:HD3	1.97	0.47
1:E:179:GLU:O	1:E:180:LEU:C	2.53	0.47
1:E:215:GLU:HG3	1:E:225:PHE:CD2	2.49	0.47
1:C:101:LEU:HB3	1:C:102:PRO:HD3	1.96	0.47
1:G:211:LEU:HD23	1:G:211:LEU:HA	1.76	0.47
1:H:89:ASN:O	1:H:92:ARG:HG2	2.15	0.47
1:H:91:GLY:HA2	1:H:95:ILE:HD12	1.96	0.47
1:A:106:LEU:HG	1:A:139:PHE:CZ	2.49	0.47
1:C:197:ARG:HG2	1:C:197:ARG:HH11	1.80	0.47
1:F:101:LEU:N	1:F:102:PRO:HD2	2.30	0.47
1:A:50:PRO:HB2	1:A:126:PRO:HG2	1.97	0.46
1:F:50:PRO:O	1:F:53:LEU:HD21	2.15	0.46
1:E:74:VAL:HB	4:E:2019:HOH:O	2.15	0.46
1:E:128:PHE:HD2	1:E:136:ARG:HA	1.80	0.46
1:G:173:SER:O	1:G:177:LYS:HG2	2.16	0.46
1:B:79:GLY:N	2:B:1682:AV1:O1A	2.44	0.46
1:E:205:LYS:HB3	1:E:205:LYS:HE2	1.71	0.46
1:G:137:GLU:HG2	1:G:174:PHE:HZ	1.80	0.46
1:B:217:LEU:HD23	1:B:217:LEU:HA	1.65	0.46
1:C:128:PHE:O	1:C:136:ARG:HD2	2.13	0.46
1:D:7:LEU:HD22	1:D:111:TRP:HB3	1.98	0.46
1:E:115:ARG:HD2	4:E:2012:HOH:O	2.16	0.46
1:F:101:LEU:HD12	1:F:105:MET:HG3	1.98	0.46
1:E:243:PRO:O	1:F:232:ARG:NH2	2.48	0.46
1:C:71:LYS:HG3	1:C:152:GLU:HB2	1.98	0.46
1:D:195:LEU:HD11	1:D:238:LEU:HD21	1.97	0.46
1:A:140:TRP:CB	1:A:174:PHE:HE2	2.29	0.46
1:C:198:LEU:HD12	1:C:242:ASN:HB3	1.98	0.46
1:H:3:PRO:HA	1:H:110:VAL:HB	1.98	0.45
1:C:242:ASN:ND2	4:C:2058:HOH:O	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:HZ1	1:A:129:LYS:N	2.00	0.45
1:B:174:PHE:HB2	2:B:1682:AV1:O5D	2.17	0.45
1:F:7:LEU:HD23	1:F:38:TRP:HH2	1.82	0.45
1:F:40:ASP:C	4:F:2010:HOH:O	2.53	0.45
1:A:49:ASN:C	1:A:51:CYS:H	2.19	0.45
1:D:91:GLY:HA2	1:D:94:TYR:O	2.16	0.45
1:G:80:VAL:HG23	1:G:80:VAL:O	2.17	0.45
1:H:175:PHE:HA	1:H:179:GLU:HG3	1.98	0.45
1:C:120:PHE:N	1:C:120:PHE:CD1	2.85	0.45
1:G:128:PHE:HD2	1:G:136:ARG:HA	1.82	0.45
1:F:206:CYS:SG	1:F:211:LEU:HD13	2.57	0.44
1:B:89:ASN:C	1:B:89:ASN:HD22	2.19	0.44
1:G:77:TRP:O	2:G:1682:AV1:H5DA	2.17	0.44
1:E:20:ILE:HG22	1:E:20:ILE:O	2.16	0.44
1:E:91:GLY:HA2	1:E:94:TYR:O	2.18	0.44
1:H:11:PHE:CD1	1:H:11:PHE:C	2.90	0.44
1:B:55:LEU:HD12	1:B:142:MET:HB2	2.00	0.44
1:F:117:ASN:OD1	1:F:118:PRO:HA	2.18	0.44
1:D:83:GLU:CD	1:D:83:GLU:H	2.21	0.44
1:F:33:ASP:C	1:F:33:ASP:OD1	2.56	0.44
1:G:218:VAL:HG13	1:G:223:PHE:HB2	1.99	0.44
1:H:60:ASP:HB2	4:H:2007:HOH:O	2.18	0.44
1:H:231:PRO:HG2	1:H:234:VAL:HB	2.00	0.44
1:A:128:PHE:CD1	1:A:128:PHE:C	2.90	0.44
1:C:28:PRO:HG2	1:C:67:GLN:HB3	2.00	0.44
1:C:183:LEU:HD22	1:C:187:VAL:HG21	2.00	0.44
1:G:83:GLU:HG2	1:G:195:LEU:CD2	2.47	0.44
1:H:196:HIS:NE2	1:H:202:ILE:HG23	2.33	0.43
1:C:127:ASP:O	1:C:130:THR:HG23	2.10	0.43
1:E:125:CYS:SG	1:E:126:PRO:CD	3.06	0.43
1:E:175:PHE:HA	1:E:179:GLU:HB2	1.99	0.43
1:H:101:LEU:N	1:H:102:PRO:HD2	2.32	0.43
1:A:136:ARG:HB3	1:A:137:GLU:HG3	1.99	0.43
1:B:62:PHE:CZ	1:B:143:ALA:HB2	2.52	0.43
1:F:106:LEU:O	1:F:107:ASN:C	2.57	0.43
1:H:128:PHE:H	1:H:130:THR:CG2	2.31	0.43
1:H:195:LEU:HD11	1:H:238:LEU:HD11	2.01	0.43
1:D:73:LYS:O	1:D:94:TYR:HB3	2.18	0.43
1:E:172:ASP:O	1:E:177:LYS:HD2	2.18	0.43
1:D:24:LEU:HD23	1:D:24:LEU:HA	1.84	0.43
1:E:230:ASN:O	1:E:231:PRO:C	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:ARG:O	1:F:29:ARG:NH2	2.46	0.43
1:F:89:ASN:O	1:F:90:THR:C	2.57	0.43
1:G:205:LYS:HA	1:G:229:GLU:OE2	2.18	0.43
1:H:163:ASN:HA	1:H:164:PRO:HD3	1.83	0.43
1:A:80:VAL:O	1:A:81:TYR:C	2.57	0.43
1:B:61:PHE:CE2	1:B:102:PRO:HB3	2.53	0.43
1:C:174:PHE:CZ	4:C:2050:HOH:O	2.57	0.43
1:E:128:PHE:O	1:E:136:ARG:HD3	2.18	0.43
1:E:189:ARG:HA	1:E:224:ALA:O	2.19	0.43
1:C:43:LYS:NZ	1:C:60:ASP:OD2	2.42	0.43
1:A:85:HIS:CE1	1:A:98:GLU:OE1	2.72	0.43
1:E:124:VAL:HG22	1:E:125:CYS:N	2.33	0.43
1:C:221:LYS:O	1:C:222:HIS:HB2	2.19	0.42
1:G:128:PHE:O	1:G:136:ARG:HD2	2.10	0.42
1:H:101:LEU:O	1:H:105:MET:HG3	2.18	0.42
1:A:97:LEU:HD23	2:A:1682:AV1:H1D	2.02	0.42
1:F:47:PHE:HD1	1:F:115:ARG:O	2.02	0.42
1:F:174:PHE:CD1	2:F:1682:AV1:PN	3.12	0.42
1:F:232:ARG:H	1:F:232:ARG:HG2	1.33	0.42
1:A:180:LEU:HD12	1:A:180:LEU:O	2.20	0.42
1:C:106:LEU:O	1:C:107:ASN:C	2.58	0.42
1:H:228:VAL:HG22	1:H:229:GLU:N	2.35	0.42
1:H:228:VAL:CG2	1:H:229:GLU:N	2.83	0.42
1:A:77:TRP:O	2:A:1682:AV1:H5DA	2.20	0.42
1:D:77:TRP:O	3:D:303:CV1:H5DA	2.19	0.42
1:D:94:TYR:HE2	1:D:156:THR:HG1	1.67	0.42
1:H:77:TRP:HA	1:H:158:MET:O	2.20	0.42
1:G:185:ASN:C	1:G:185:ASN:ND2	2.73	0.42
1:H:128:PHE:H	1:H:130:THR:HG23	1.85	0.42
1:G:177:LYS:HG3	1:G:178:TYR:CE2	2.55	0.41
1:H:62:PHE:O	1:H:66:GLN:HB2	2.19	0.41
1:H:106:LEU:HD13	1:H:109:LEU:HD12	2.02	0.41
1:C:133:VAL:HA	1:C:136:ARG:HG3	2.01	0.41
1:E:96:THR:O	1:E:97:LEU:C	2.58	0.41
1:G:162:SER:HB2	1:G:197:ARG:HG3	2.02	0.41
1:H:106:LEU:HD13	1:H:106:LEU:HA	1.82	0.41
1:A:232:ARG:HH22	1:B:244:ASN:ND2	2.18	0.41
1:B:144:SER:HB3	1:B:179:GLU:CG	2.49	0.41
1:F:170:ARG:HB2	1:F:173:SER:HB3	2.02	0.41
1:H:221:LYS:O	1:H:222:HIS:HB2	2.20	0.41
1:B:26:ILE:HG22	1:B:27:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:LEU:HD23	1:C:12:LEU:HA	1.89	0.41
1:D:120:PHE:HD1	1:D:120:PHE:H	1.69	0.41
1:H:189:ARG:HA	1:H:224:ALA:O	2.21	0.41
1:C:97:LEU:O	1:C:103:GLY:HA3	2.20	0.41
1:F:198:LEU:CD2	1:F:247:GLU:HB2	2.50	0.41
1:A:50:PRO:HB3	1:A:112:CYS:HB2	2.03	0.41
1:A:18:TYR:CD1	1:A:18:TYR:C	2.93	0.41
1:C:80:VAL:HG11	1:C:195:LEU:HD13	2.03	0.41
1:D:196:HIS:NE2	1:D:202:ILE:HG23	2.35	0.41
1:E:148:ALA:HB2	1:E:179:GLU:HG2	2.02	0.41
1:A:173:SER:O	1:A:177:LYS:HB2	2.21	0.41
1:B:15:CYS:HB2	1:B:105:MET:SD	2.60	0.41
1:F:127:ASP:O	1:F:128:PHE:HB2	2.21	0.41
1:H:106:LEU:O	1:H:107:ASN:C	2.59	0.41
1:A:72:ASN:HA	1:A:154:GLU:O	2.21	0.41
1:B:46:SER:HA	1:B:119:GLY:O	2.20	0.41
1:F:60:ASP:O	1:F:61:PHE:C	2.60	0.41
1:F:225:PHE:CD1	1:F:225:PHE:C	2.95	0.41
1:D:101:LEU:HB3	1:D:102:PRO:CD	2.51	0.40
1:G:111:TRP:C	1:G:112:CYS:SG	2.98	0.40
1:F:163:ASN:HA	1:F:164:PRO:HD2	1.82	0.40
1:G:212:LEU:O	1:G:213:ASP:C	2.58	0.40
1:C:101:LEU:N	1:C:102:PRO:HD2	2.36	0.40
1:E:83:GLU:OE2	1:E:197:ARG:NH1	2.54	0.40
1:F:116:ALA:O	1:F:117:ASN:C	2.60	0.40
1:F:175:PHE:HA	1:F:179:GLU:HB2	2.03	0.40
1:G:178:TYR:O	1:G:182:ASN:HB2	2.22	0.40
1:E:72:ASN:HA	1:E:154:GLU:O	2.22	0.40
1:G:189:ARG:HD3	1:G:226:ASP:OD2	2.21	0.40
1:H:113:GLY:HA2	1:H:120:PHE:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	249/260 (96%)	233 (94%)	14 (6%)	2 (1%)	19	29
1	B	250/260 (96%)	239 (96%)	10 (4%)	1 (0%)	34	48
1	C	250/260 (96%)	236 (94%)	13 (5%)	1 (0%)	34	48
1	D	250/260 (96%)	239 (96%)	11 (4%)	0	100	100
1	E	249/260 (96%)	238 (96%)	10 (4%)	1 (0%)	34	48
1	F	249/260 (96%)	226 (91%)	20 (8%)	3 (1%)	13	19
1	G	249/260 (96%)	237 (95%)	12 (5%)	0	100	100
1	H	249/260 (96%)	230 (92%)	15 (6%)	4 (2%)	9	13
All	All	1995/2080 (96%)	1878 (94%)	105 (5%)	12 (1%)	25	36

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	PHE
1	A	126	PRO
1	F	174	PHE
1	H	128	PHE
1	F	127	ASP
1	H	129	LYS
1	F	128	PHE
1	H	55	LEU
1	B	185	ASN
1	E	71	LYS
1	C	1	ILE
1	H	247	GLU

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	220/226 (97%)	198 (90%)	22 (10%)	7	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	220/226 (97%)	203 (92%)	17 (8%)	13	20
1	C	220/226 (97%)	204 (93%)	16 (7%)	14	22
1	D	220/226 (97%)	206 (94%)	14 (6%)	17	28
1	E	220/226 (97%)	203 (92%)	17 (8%)	13	20
1	F	220/226 (97%)	196 (89%)	24 (11%)	6	8
1	G	220/226 (97%)	203 (92%)	17 (8%)	13	20
1	H	220/226 (97%)	204 (93%)	16 (7%)	14	22
All	All	1760/1808 (97%)	1617 (92%)	143 (8%)	11	18

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	26	ILE
1	A	29	ARG
1	A	30	VAL
1	A	32	SER
1	A	33	ASP
1	A	71	LYS
1	A	90	THR
1	A	92	ARG
1	A	93	LYS
1	A	124	VAL
1	A	128	PHE
1	A	129	LYS
1	A	131	CYS
1	A	133	VAL
1	A	134	GLN
1	A	217	LEU
1	A	228	VAL
1	A	232	ARG
1	A	242	ASN
1	A	246	ARG
1	A	250	LEU
1	B	1	ILE
1	B	5	ARG
1	B	39	LYS
1	B	59	LYS
1	B	89	ASN
1	B	90	THR

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Mol	Chain	Res	Type
1	B	92	ARG
1	B	93	LYS
1	B	115	ARG
1	B	186	LYS
1	B	195	LEU
1	B	200	GLU
1	B	206	CYS
1	B	212	LEU
1	B	216	LYS
1	B	221	LYS
1	B	244	ASN
1	C	21	THR
1	C	25	ASP
1	C	30	VAL
1	C	31	ARG
1	C	39	LYS
1	C	55	LEU
1	C	73	LYS
1	C	89	ASN
1	C	123	LYS
1	C	130	THR
1	C	134	GLN
1	C	172	ASP
1	C	195	LEU
1	C	200	GLU
1	C	228	VAL
1	C	242	ASN
1	D	32	SER
1	D	39	LYS
1	D	71	LYS
1	D	92	ARG
1	D	120	PHE
1	D	124	VAL
1	D	128	PHE
1	D	131	CYS
1	D	162	SER
1	D	200	GLU
1	D	206	CYS
1	D	227	CYS
1	D	237	LEU
1	D	247	GLU
1	E	31	ARG

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Mol	Chain	Res	Type
1	E	39	LYS
1	E	43	LYS
1	E	49	ASN
1	E	71	LYS
1	E	89	ASN
1	E	112	CYS
1	E	129	LYS
1	E	130	THR
1	E	172	ASP
1	E	189	ARG
1	E	195	LEU
1	E	200	GLU
1	E	216	LYS
1	E	237	LEU
1	E	240	SER
1	E	246	ARG
1	F	25	ASP
1	F	29	ARG
1	F	53	LEU
1	F	63	THR
1	F	73	LYS
1	F	89	ASN
1	F	90	THR
1	F	92	ARG
1	F	121	ASN
1	F	123	LYS
1	F	128	PHE
1	F	129	LYS
1	F	130	THR
1	F	133	VAL
1	F	136	ARG
1	F	137	GLU
1	F	173	SER
1	F	174	PHE
1	F	227	CYS
1	F	232	ARG
1	F	242	ASN
1	F	246	ARG
1	F	249	ARG
1	F	250	LEU
1	G	6	GLU
1	G	33	ASP

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Mol	Chain	Res	Type
1	G	43	LYS
1	G	64	SER
1	G	92	ARG
1	G	112	CYS
1	G	115	ARG
1	G	123	LYS
1	G	130	THR
1	G	158	MET
1	G	172	ASP
1	G	185	ASN
1	G	228	VAL
1	G	232	ARG
1	G	237	LEU
1	G	242	ASN
1	G	246	ARG
1	H	25	ASP
1	H	29	ARG
1	H	35	SER
1	H	55	LEU
1	H	64	SER
1	H	75	MET
1	H	89	ASN
1	H	95	ILE
1	H	115	ARG
1	H	124	VAL
1	H	129	LYS
1	H	130	THR
1	H	203	ILE
1	H	217	LEU
1	H	234	VAL
1	H	242	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	117	ASN
1	A	242	ASN
1	B	89	ASN
1	B	242	ASN
1	B	244	ASN
1	C	49	ASN

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Mol	Chain	Res	Type
1	C	89	ASN
1	C	196	HIS
1	C	242	ASN
1	D	117	ASN
1	D	242	ASN
1	D	244	ASN
1	E	242	ASN
1	F	89	ASN
1	F	242	ASN
1	G	107	ASN
1	G	185	ASN
1	G	242	ASN
1	H	242	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	CV1	D	303	-	35,40,40	2.01	7 (20%)	38,64,64	1.34	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AV1	C	1682	-	35,39,39	1.61	8 (22%)	39,60,60	2.57	7 (17%)
2	AV1	F	1682	-	35,39,39	1.49	2 (5%)	39,60,60	1.31	2 (5%)
2	AV1	A	1682	-	35,39,39	1.54	3 (8%)	39,60,60	1.76	6 (15%)
2	AV1	H	1682	-	35,39,39	1.72	5 (14%)	39,60,60	2.10	5 (12%)
2	AV1	B	1682	-	35,39,39	2.23	6 (17%)	39,60,60	3.16	10 (25%)
2	AV1	E	1682	-	35,39,39	1.39	5 (14%)	39,60,60	1.89	8 (20%)
2	AV1	G	1682	-	35,39,39	1.16	2 (5%)	39,60,60	2.72	8 (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
3	CV1	D	303	-	-	8/20/58/58	0/4/5/5
2	AV1	C	1682	-	-	6/18/51/51	0/4/4/4
2	AV1	F	1682	-	-	10/18/51/51	0/4/4/4
2	AV1	A	1682	-	-	7/18/51/51	0/4/4/4
2	AV1	H	1682	-	-	3/18/51/51	0/4/4/4
2	AV1	B	1682	-	-	6/18/51/51	0/4/4/4
2	AV1	E	1682	-	-	3/18/51/51	0/4/4/4
2	AV1	G	1682	-	-	3/18/51/51	0/4/4/4

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1682	AV1	PN-O3	7.40	1.67	1.59
3	D	303	CV1	O4'-C1'	7.20	1.50	1.40
2	B	1682	AV1	O4'-C1'	7.03	1.50	1.40
2	H	1682	AV1	O4'-C1'	6.60	1.49	1.40
2	F	1682	AV1	O4'-C1'	6.47	1.49	1.40
2	B	1682	AV1	PA-O3	5.81	1.65	1.59
2	E	1682	AV1	O4'-C1'	5.60	1.48	1.40
2	A	1682	AV1	PA-O3	5.55	1.65	1.59
2	A	1682	AV1	PN-O3	4.90	1.64	1.59
2	C	1682	AV1	O4'-C1'	4.68	1.47	1.40
3	D	303	CV1	PB-O3A	4.56	1.64	1.59
2	H	1682	AV1	C1'-N9A	4.13	1.61	1.49
3	D	303	CV1	O4D-C1D	3.82	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1682	AV1	O4D-C4D	3.61	1.50	1.44
2	F	1682	AV1	C1'-N9A	3.56	1.59	1.49
3	D	303	CV1	PA-O3A	3.39	1.63	1.59
2	C	1682	AV1	PN-O3	3.34	1.63	1.59
2	G	1682	AV1	O4'-C1'	3.25	1.45	1.40
2	B	1682	AV1	C1'-N9A	3.12	1.58	1.49
2	H	1682	AV1	PA-O3	2.91	1.62	1.59
2	A	1682	AV1	O4'-C1'	2.91	1.44	1.40
2	C	1682	AV1	C1'-N9A	2.67	1.57	1.49
2	E	1682	AV1	BR1-C8A	2.61	1.95	1.88
2	H	1682	AV1	PN-O3	2.47	1.62	1.59
2	G	1682	AV1	PN-O5D	2.47	1.69	1.59
2	C	1682	AV1	BR1-C8A	2.43	1.94	1.88
2	E	1682	AV1	C5D-C4D	2.36	1.58	1.51
3	D	303	CV1	C6-N1	2.35	1.41	1.36
2	E	1682	AV1	PN-O3	2.29	1.62	1.59
2	C	1682	AV1	PA-O3	2.27	1.62	1.59
2	C	1682	AV1	PN-O2N	2.22	1.65	1.55
2	E	1682	AV1	O4D-C4D	2.20	1.48	1.44
3	D	303	CV1	C5'-C4'	2.18	1.58	1.51
2	B	1682	AV1	BR1-C8A	2.14	1.94	1.88
2	C	1682	AV1	C1D-C2D	2.14	1.55	1.51
2	H	1682	AV1	C5'-C4'	2.11	1.57	1.51
2	B	1682	AV1	PN-O2N	2.04	1.64	1.55
3	D	303	CV1	C2-N1	2.01	1.41	1.36

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1682	AV1	O4'-C1'-N9A	13.30	126.38	108.75
2	B	1682	AV1	C4'-O4'-C1'	-10.42	100.38	109.92
2	G	1682	AV1	O4'-C1'-N9A	10.35	122.47	108.75
2	C	1682	AV1	O4'-C1'-N9A	10.10	122.13	108.75
2	H	1682	AV1	O4'-C1'-N9A	9.39	121.20	108.75
2	G	1682	AV1	C4'-O4'-C1'	-9.12	101.57	109.92
2	C	1682	AV1	C4'-O4'-C1'	-7.62	102.94	109.92
2	A	1682	AV1	C4'-O4'-C1'	-7.13	103.39	109.92
2	E	1682	AV1	C4'-O4'-C1'	-6.54	103.93	109.92
2	E	1682	AV1	N3A-C2A-N1A	-5.56	121.12	128.67
2	C	1682	AV1	N3A-C2A-N1A	-5.23	121.57	128.67
2	A	1682	AV1	N3A-C2A-N1A	-5.21	121.60	128.67
2	G	1682	AV1	N3A-C2A-N1A	-5.15	121.69	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1682	AV1	N3A-C2A-N1A	-5.11	121.73	128.67
2	F	1682	AV1	N3A-C2A-N1A	-4.62	122.40	128.67
2	H	1682	AV1	N3A-C2A-N1A	-4.52	122.54	128.67
2	F	1682	AV1	O4'-C1'-N9A	4.49	114.70	108.75
3	D	303	CV1	C2-N3-C4	4.41	122.22	116.59
2	B	1682	AV1	O4D-C4D-C3D	4.40	108.69	104.63
2	H	1682	AV1	C4'-O4'-C1'	-4.39	105.91	109.92
2	C	1682	AV1	C5D-C4D-C3D	-4.29	99.78	115.21
2	G	1682	AV1	C5'-C4'-C3'	-3.96	100.97	115.21
2	B	1682	AV1	O4'-C4'-C5'	3.61	120.89	109.33
2	G	1682	AV1	O4D-C1D-C2D	-3.15	100.33	105.76
2	G	1682	AV1	O5'-PA-O2A	3.15	121.41	108.94
2	G	1682	AV1	C5D-C4D-C3D	-2.94	104.64	115.21
2	A	1682	AV1	C5D-C4D-C3D	-2.89	104.83	115.21
2	H	1682	AV1	C5D-C4D-C3D	-2.79	105.17	115.21
2	B	1682	AV1	C5D-C4D-C3D	-2.74	105.36	115.21
2	A	1682	AV1	O4'-C1'-N9A	2.72	112.35	108.75
2	E	1682	AV1	O4'-C4'-C5'	2.72	118.04	109.33
2	E	1682	AV1	C5'-C4'-C3'	-2.70	105.50	115.21
2	C	1682	AV1	O4D-C4D-C3D	2.69	107.11	104.63
3	D	303	CV1	O4D-C1D-N1	2.68	112.30	108.75
2	A	1682	AV1	O4D-C4D-C3D	2.67	107.09	104.63
2	E	1682	AV1	O4'-C1'-N9A	2.63	112.23	108.75
3	D	303	CV1	O4'-C1'-N9	-2.63	105.26	108.75
2	H	1682	AV1	O4D-C4D-C3D	2.62	107.05	104.63
2	E	1682	AV1	O4D-C1D-C2D	-2.53	101.40	105.76
2	B	1682	AV1	O4'-C4'-C3'	-2.50	100.19	105.15
2	A	1682	AV1	C5'-C4'-C3'	-2.44	106.41	115.21
2	E	1682	AV1	O5'-PA-O2A	2.39	118.40	108.94
2	G	1682	AV1	O2D-C2D-C3D	-2.35	106.80	111.43
2	C	1682	AV1	O1A-PA-O3	-2.31	101.02	107.27
3	D	303	CV1	C2'-C3'-C4'	2.29	107.04	102.61
2	B	1682	AV1	C5'-C4'-C3'	-2.27	107.05	115.21
2	B	1682	AV1	C1D-C2D-C3D	2.26	105.24	101.63
2	B	1682	AV1	C4A-C5A-N7A	-2.23	107.09	109.40
2	E	1682	AV1	O5D-PN-O1N	2.05	117.08	108.94
2	C	1682	AV1	O4'-C4'-C5'	2.01	115.76	109.33

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1682	AV1	C5'-O5'-PA-O3
2	A	1682	AV1	C5'-O5'-PA-O2A
2	B	1682	AV1	O4'-C4'-C5'-O5'
2	C	1682	AV1	C5'-O5'-PA-O3
2	C	1682	AV1	C5'-O5'-PA-O2A
2	E	1682	AV1	C5'-O5'-PA-O3
2	E	1682	AV1	C5'-O5'-PA-O2A
2	F	1682	AV1	C5D-O5D-PN-O3
2	F	1682	AV1	C5D-O5D-PN-O1N
2	F	1682	AV1	C5D-O5D-PN-O2N
2	F	1682	AV1	C3'-C4'-C5'-O5'
2	G	1682	AV1	PN-O3-PA-O5'
2	H	1682	AV1	PN-O3-PA-O5'
3	D	303	CV1	C5D-O5D-PB-O1B
3	D	303	CV1	C5D-O5D-PB-O3A
2	B	1682	AV1	C3'-C4'-C5'-O5'
2	C	1682	AV1	C3'-C4'-C5'-O5'
2	C	1682	AV1	O4'-C4'-C5'-O5'
2	F	1682	AV1	O4'-C4'-C5'-O5'
2	H	1682	AV1	C3'-C4'-C5'-O5'
2	H	1682	AV1	O4'-C4'-C5'-O5'
2	G	1682	AV1	C4'-C5'-O5'-PA
2	A	1682	AV1	C3'-C4'-C5'-O5'
2	F	1682	AV1	C3D-C4D-C5D-O5D
3	D	303	CV1	O4D-C4D-C5D-O5D
2	A	1682	AV1	O4'-C4'-C5'-O5'
2	F	1682	AV1	O4D-C4D-C5D-O5D
3	D	303	CV1	C3D-C4D-C5D-O5D
3	D	303	CV1	PA-O3A-PB-O2B
2	B	1682	AV1	PN-O3-PA-O5'
2	F	1682	AV1	PN-O3-PA-O5'
2	G	1682	AV1	C4D-C5D-O5D-PN
2	E	1682	AV1	C4D-C5D-O5D-PN
2	A	1682	AV1	C5'-O5'-PA-O1A
2	B	1682	AV1	C5'-O5'-PA-O2A
3	D	303	CV1	C5D-O5D-PB-O2B
2	A	1682	AV1	C4'-C5'-O5'-PA
2	B	1682	AV1	C4D-C5D-O5D-PN
2	C	1682	AV1	C4D-C5D-O5D-PN
2	B	1682	AV1	C3D-C4D-C5D-O5D
3	D	303	CV1	O4'-C4'-C5'-O5'
3	D	303	CV1	PA-O3A-PB-O1B
2	A	1682	AV1	PA-O3-PN-O5D

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Mol	Chain	Res	Type	Atoms
2	F	1682	AV1	PA-O3-PN-O1N
2	C	1682	AV1	PA-O3-PN-O2N
2	F	1682	AV1	PA-O3-PN-O2N

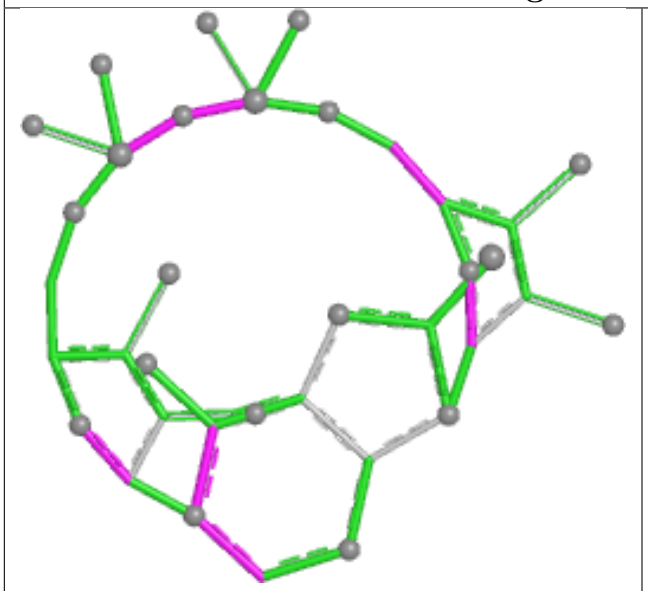
There are no ring outliers.

8 monomers are involved in 21 short contacts:

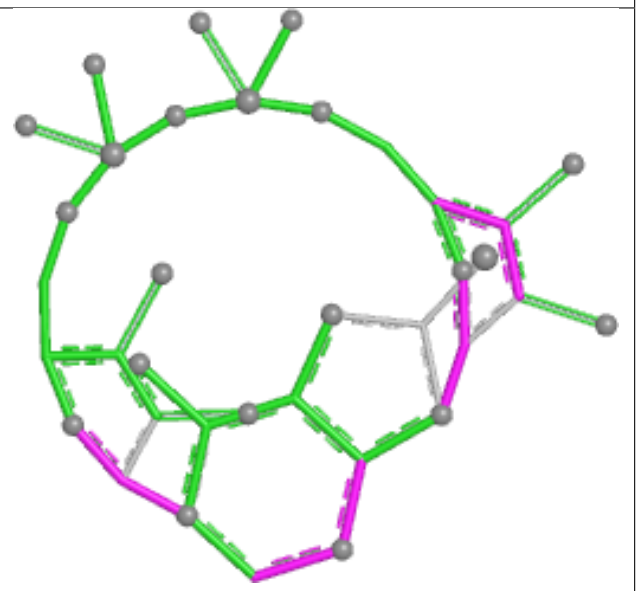
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	303	CV1	4	0
2	C	1682	AV1	1	0
2	F	1682	AV1	3	0
2	A	1682	AV1	3	0
2	H	1682	AV1	2	0
2	B	1682	AV1	4	0
2	E	1682	AV1	1	0
2	G	1682	AV1	3	0

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 then 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.

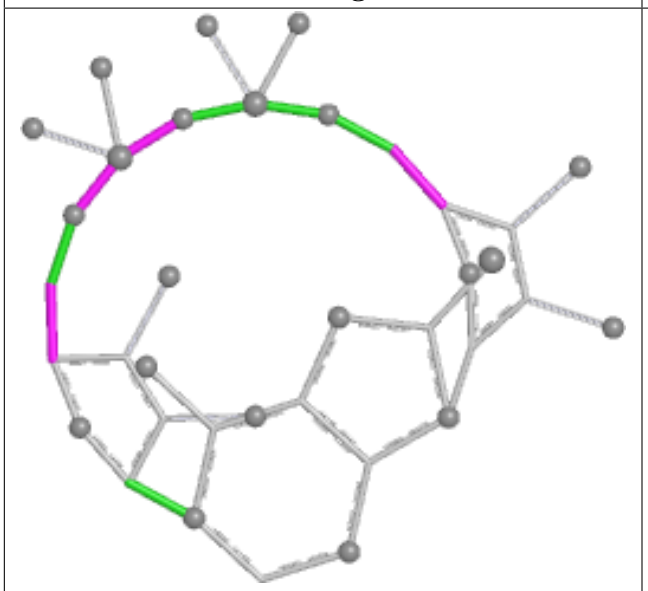
Ligand CV1 D 303



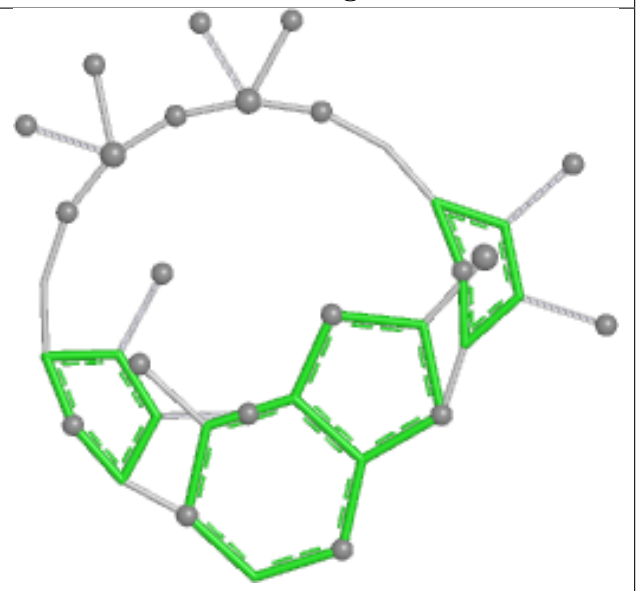
Bond lengths



Bond angles

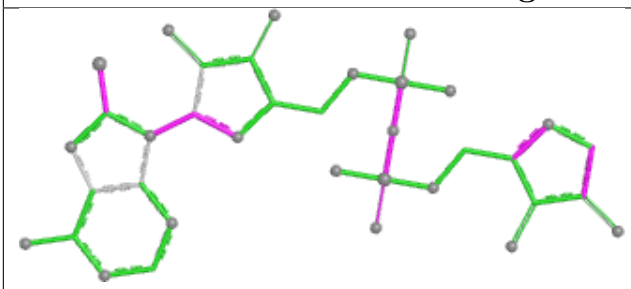


Torsions

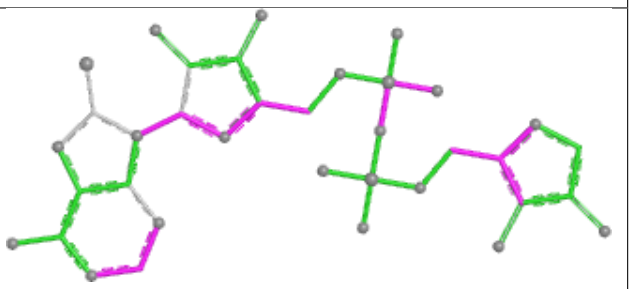


Rings

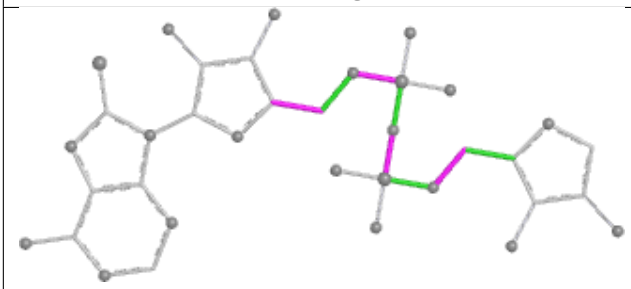
Ligand AV1 C 1682



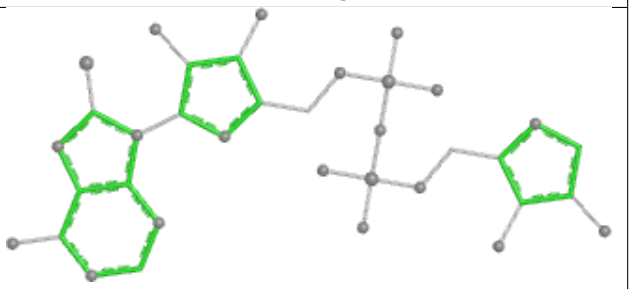
Bond lengths



Bond angles

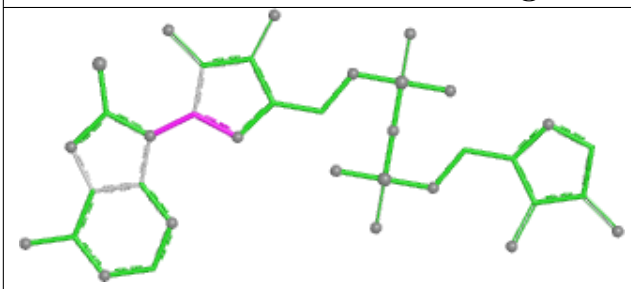


Torsions

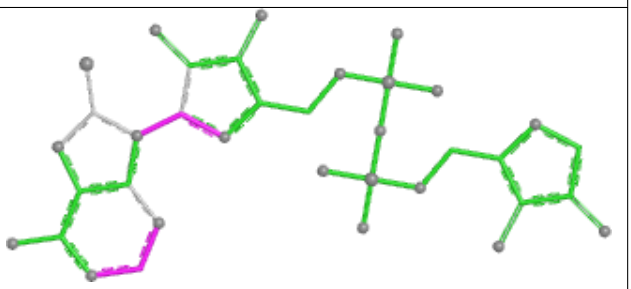


Rings

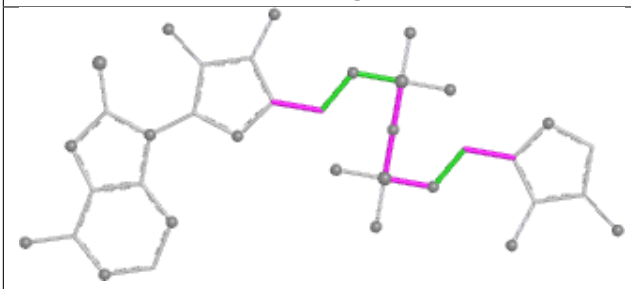
Ligand AV1 F 1682



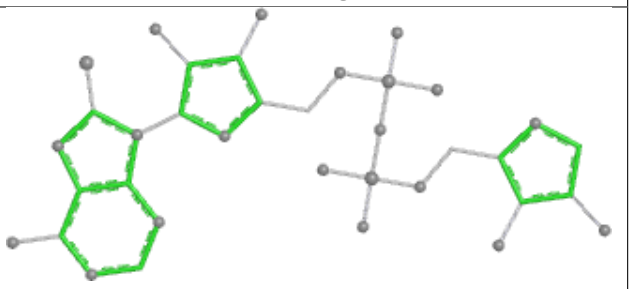
Bond lengths



Bond angles

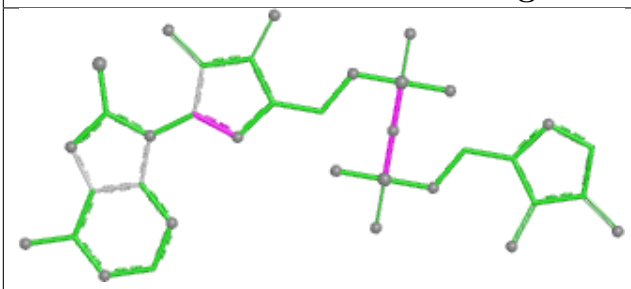


Torsions

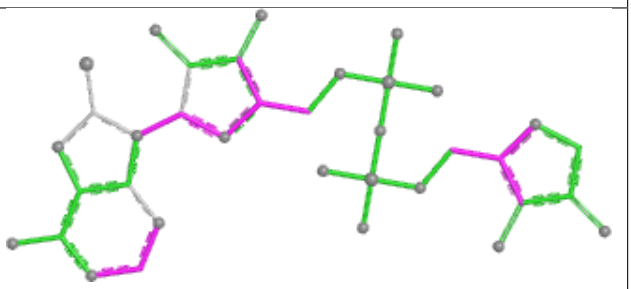


Rings

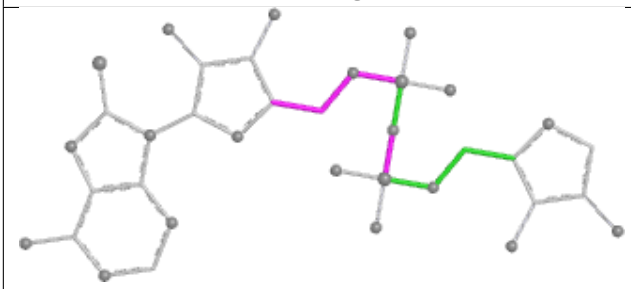
Ligand AV1 A 1682



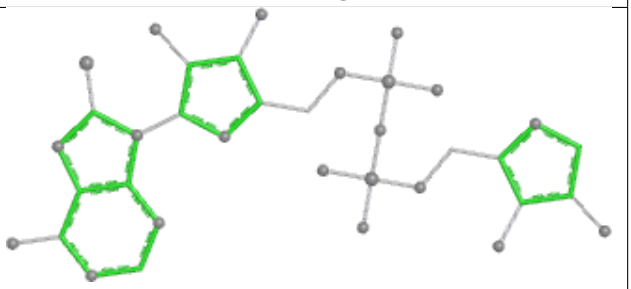
Bond lengths



Bond angles

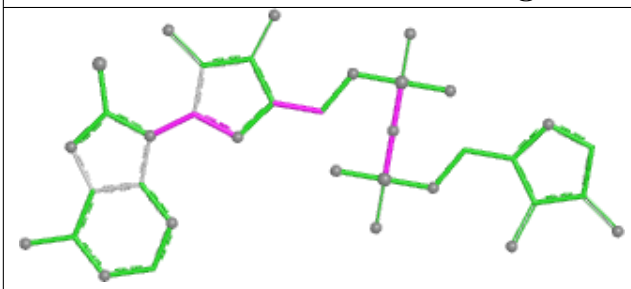


Torsions

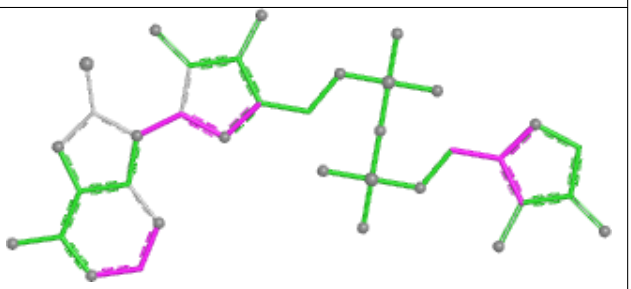


Rings

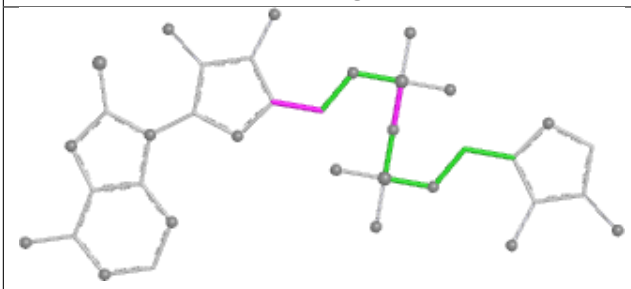
Ligand AV1 H 1682



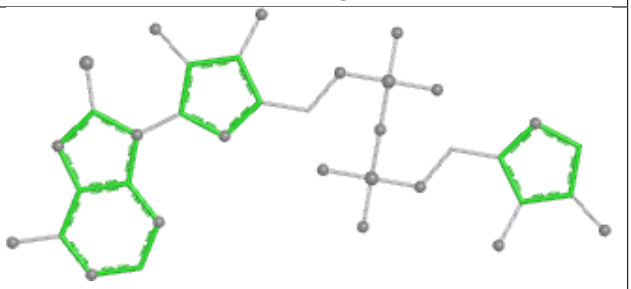
Bond lengths



Bond angles

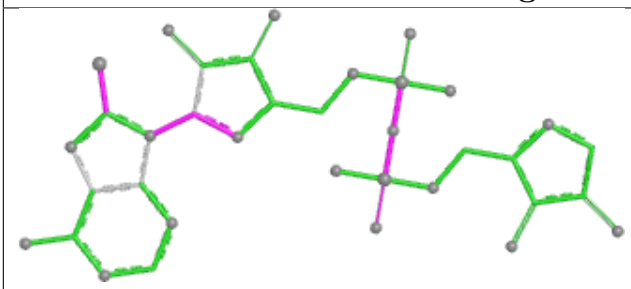


Torsions

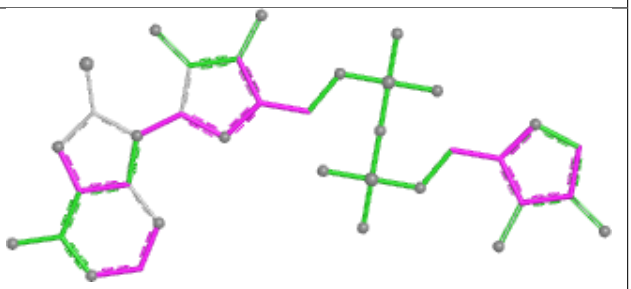


Rings

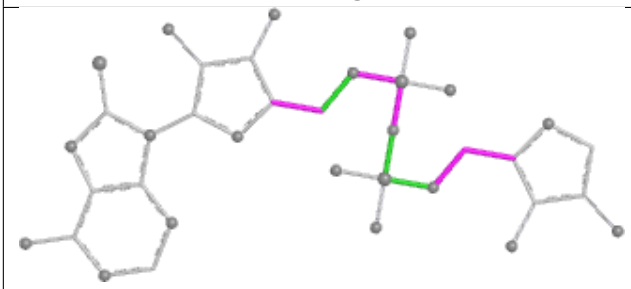
Ligand AV1 B 1682



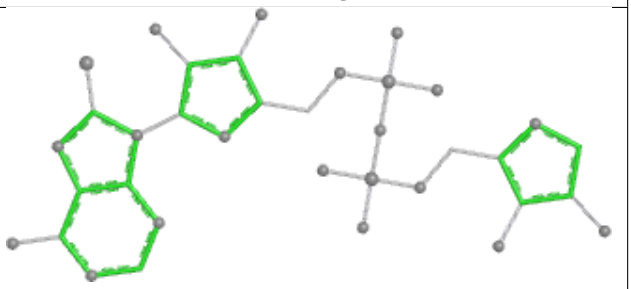
Bond lengths



Bond angles

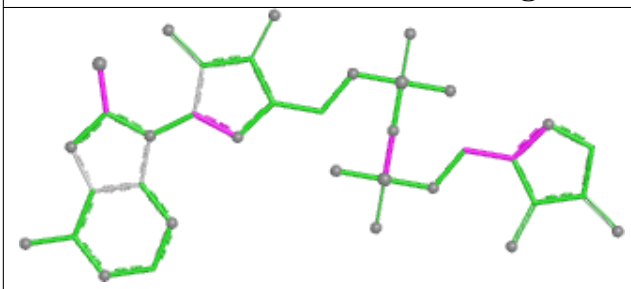


Torsions

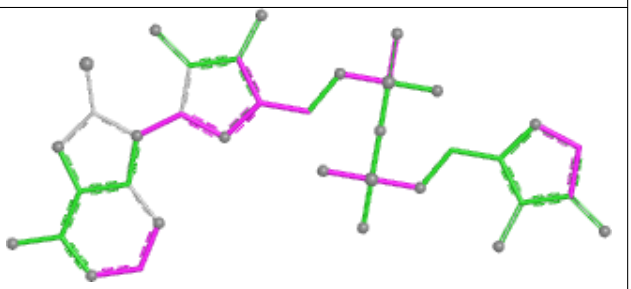


Rings

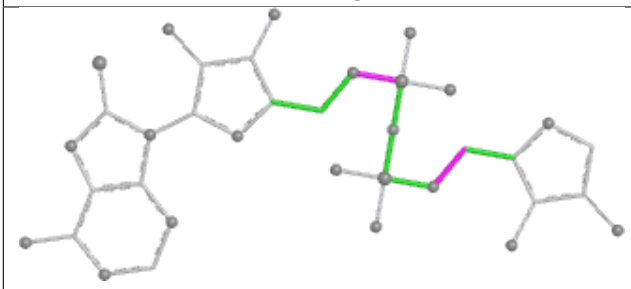
Ligand AV1 E 1682



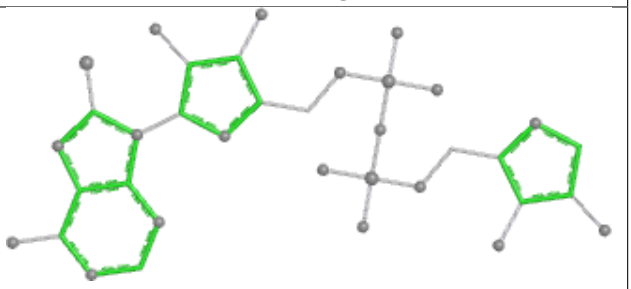
Bond lengths



Bond angles

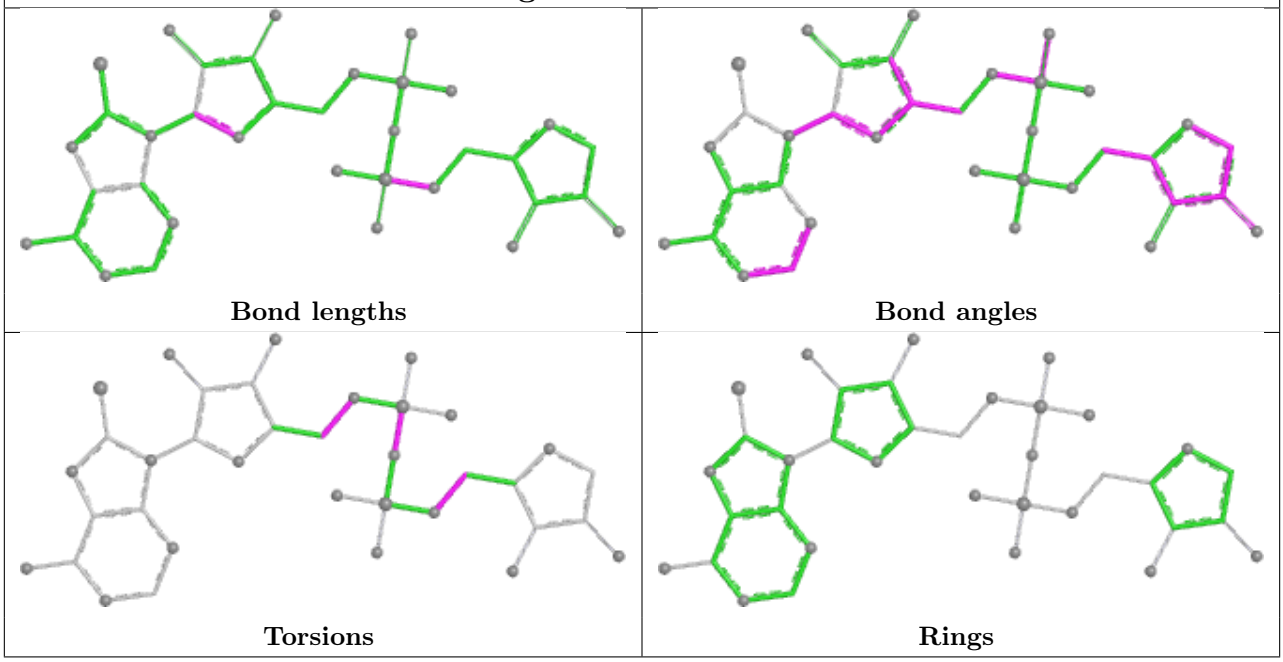


Torsions



Rings

Ligand AV1 G 1682



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	251/260 (96%)	-0.60	0	100	100	34, 50, 73, 87	0
1	B	252/260 (96%)	-0.57	2 (0%)	86	84	32, 45, 66, 78	0
1	C	252/260 (96%)	-0.60	1 (0%)	92	91	32, 48, 67, 79	0
1	D	252/260 (96%)	-0.58	1 (0%)	92	91	34, 48, 73, 91	0
1	E	251/260 (96%)	-0.51	2 (0%)	86	84	34, 49, 70, 89	0
1	F	251/260 (96%)	-0.35	1 (0%)	92	91	49, 71, 91, 108	0
1	G	251/260 (96%)	-0.50	1 (0%)	92	91	38, 52, 72, 91	0
1	H	251/260 (96%)	-0.41	1 (0%)	92	91	50, 67, 89, 98	0
All	All	2011/2080 (96%)	-0.52	9 (0%)	92	91	32, 53, 82, 108	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	128	PHE	6.1
1	E	1	ILE	3.7
1	B	0	ALA	2.7
1	E	128	PHE	2.6
1	B	250	LEU	2.5
1	F	128	PHE	2.5
1	C	250	LEU	2.3
1	G	174	PHE	2.2
1	H	250	LEU	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

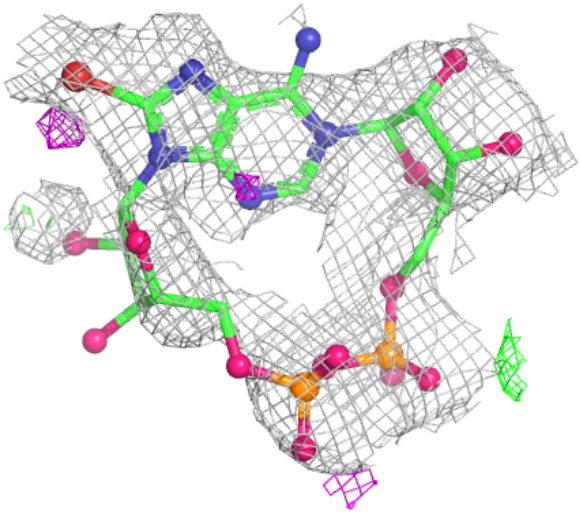
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

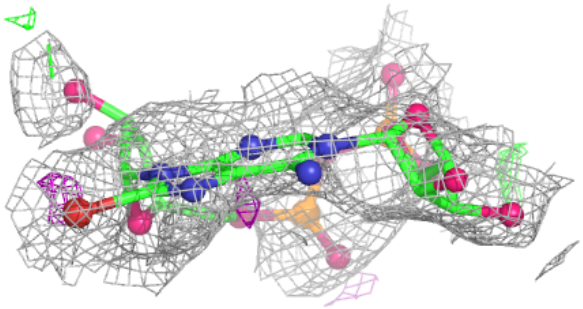
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CV1	D	303	36/36	0.73	0.21	147,153,159,160	0
2	AV1	F	1682	36/36	0.74	0.19	110,132,141,146	0
2	AV1	A	1682	36/36	0.78	0.20	119,140,150,153	0
2	AV1	C	1682	36/36	0.80	0.18	66,112,126,136	0
2	AV1	B	1682	36/36	0.82	0.19	72,105,128,138	0
2	AV1	H	1682	36/36	0.84	0.14	96,122,130,134	0
2	AV1	E	1682	36/36	0.88	0.14	66,90,117,126	0
2	AV1	G	1682	36/36	0.90	0.12	54,78,99,113	0

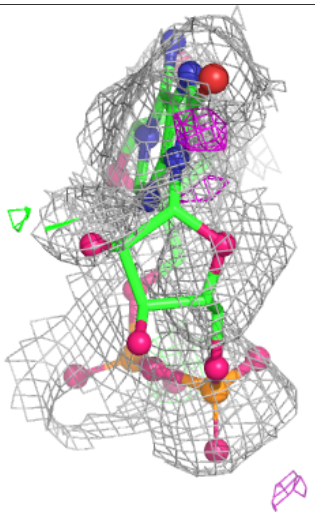
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CV1 D 303:

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

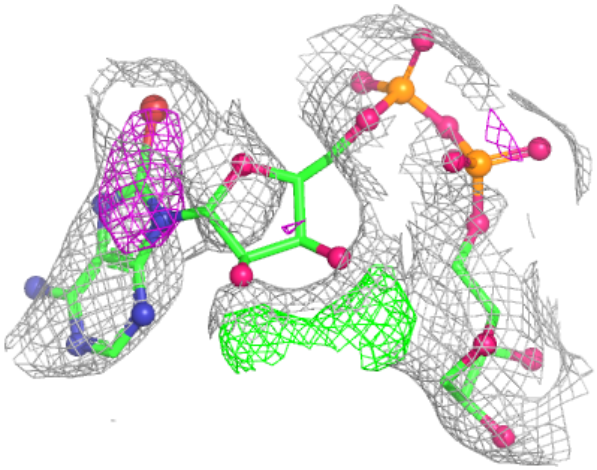


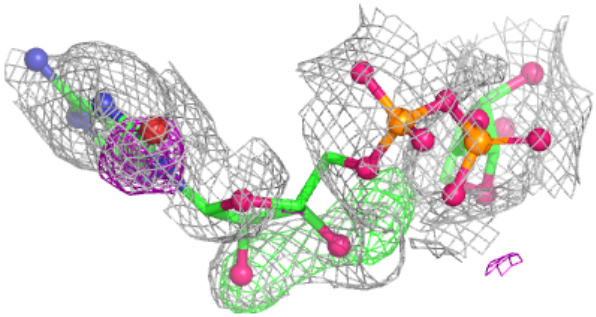


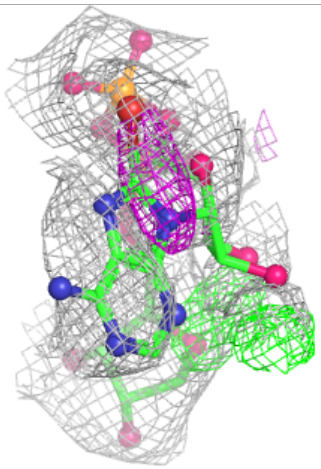


Electron density around AV1 F 1682:

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

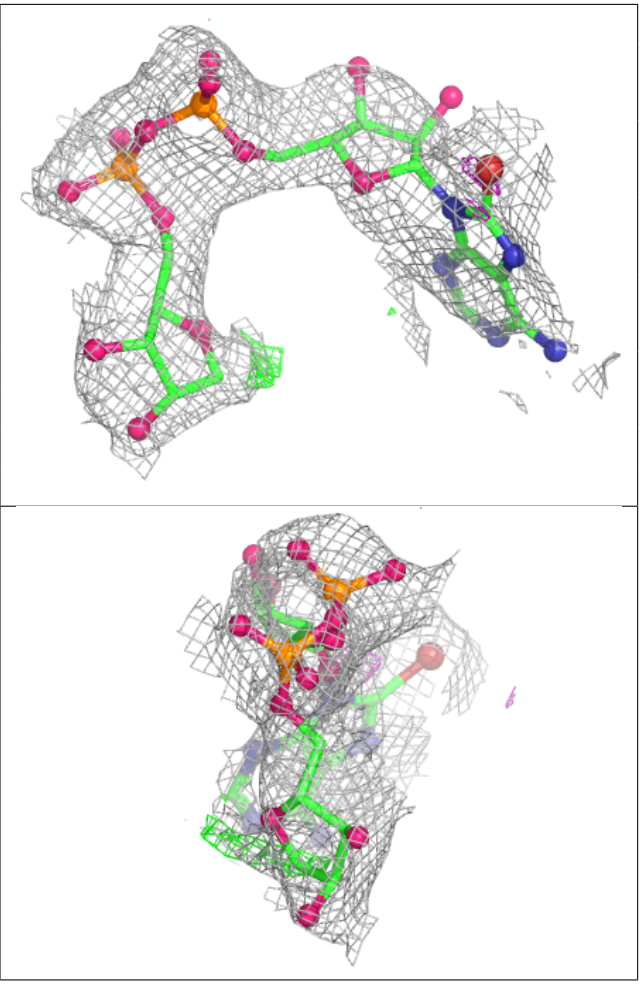






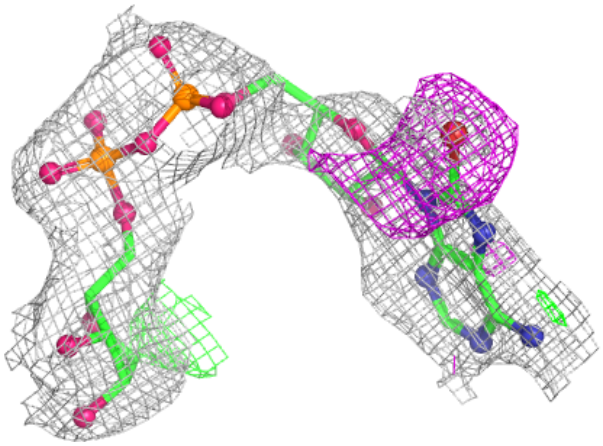
Electron density around AV1 A 1682:

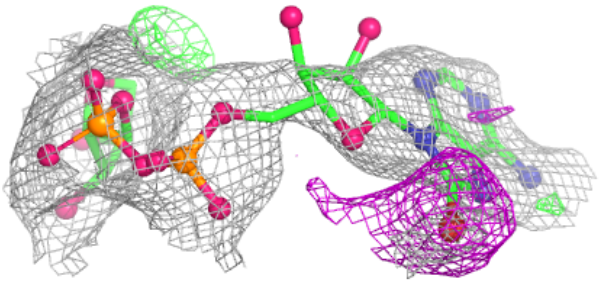
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

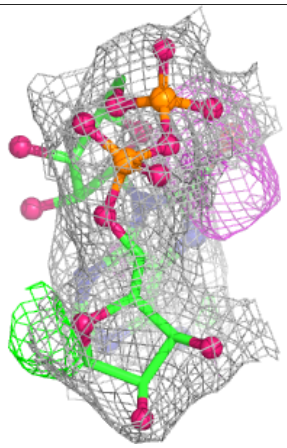


Electron density around AV1 C 1682:

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

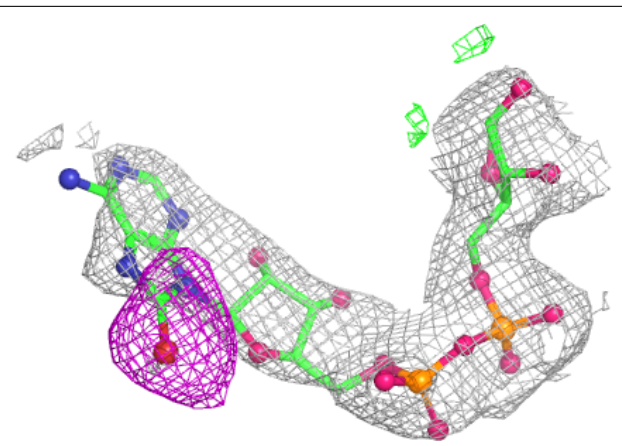


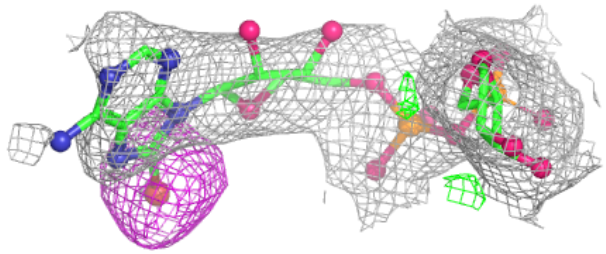


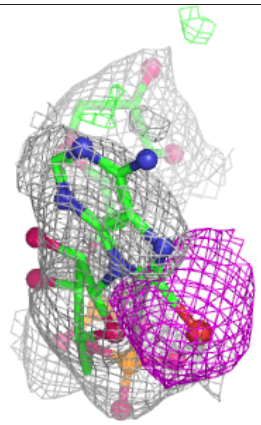


Electron density around AV1 B 1682:

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

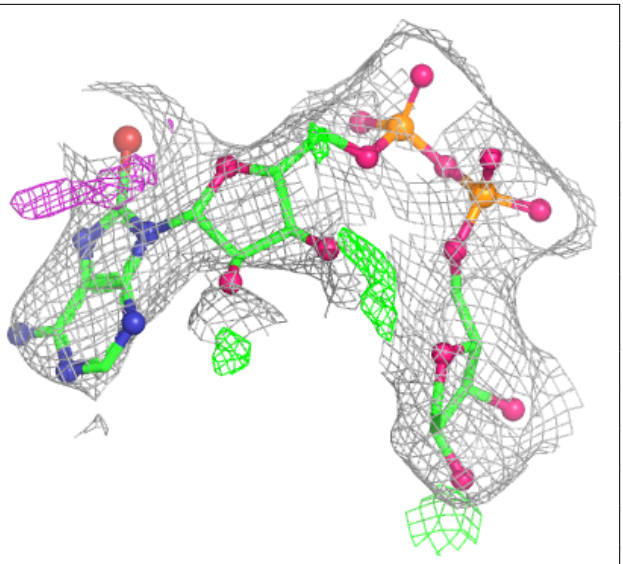


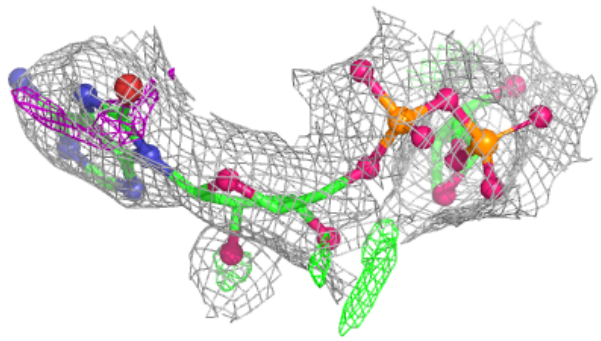


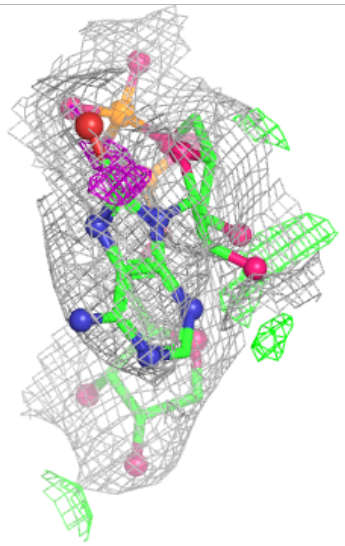


Electron density around AV1 H 1682:

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

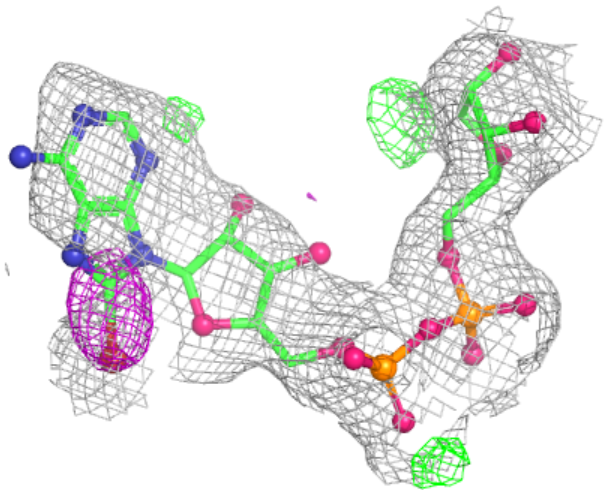


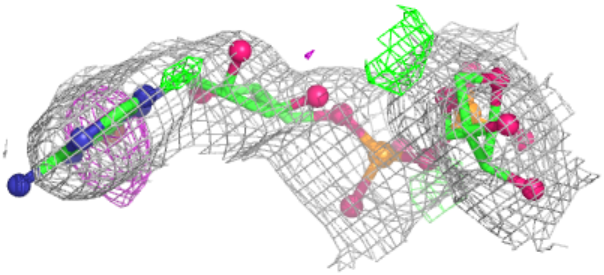


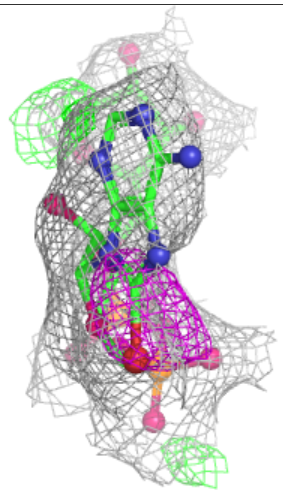


Electron density around AV1 E 1682:

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

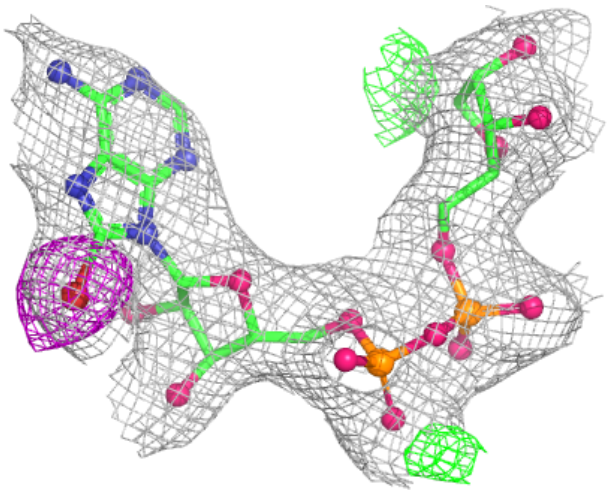


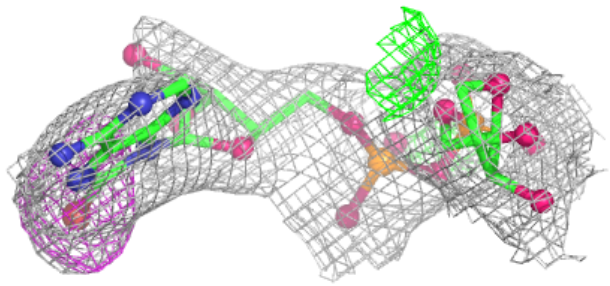


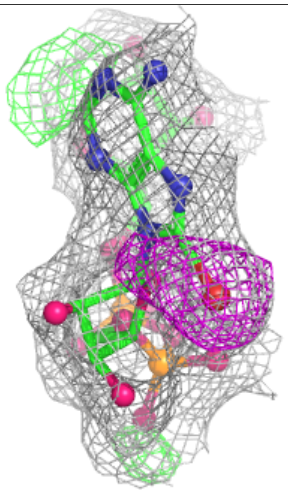


Electron density around AV1 G 1682:

$2mF_o$-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.