Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 03:43 pm GMT

PDB ID	:	1UNL
Title	:	Structural mechanism for the inhibition of CD5-p25 from the roscovitine, aloisine and indirubin.
Authors	:	Mapelli, M.; Crovace, C.; Massimiliano, L.; Musacchio, A.
Deposited on	:	2003-09-10
Resolution	:	2.20 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:

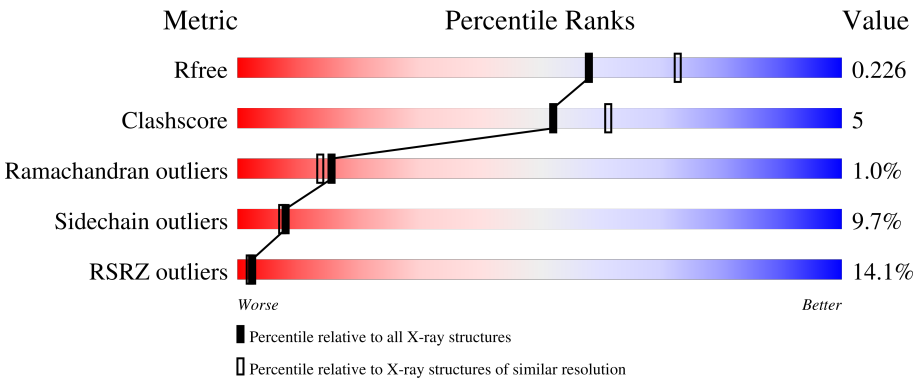
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	292	8%, 77%, 18%, • •
1	B	292	17%, 78%, 17%, • •
2	D	208	62%, 8%, •, 28%
2	E	208	25%, 55%, 14%, •, 28%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7424 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 CYCLIN-DEPENDENT KINASE 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	292	2346	1505	403	426	12	0	0	0
1	B	292	2346	1505	403	426	12	0	0	0

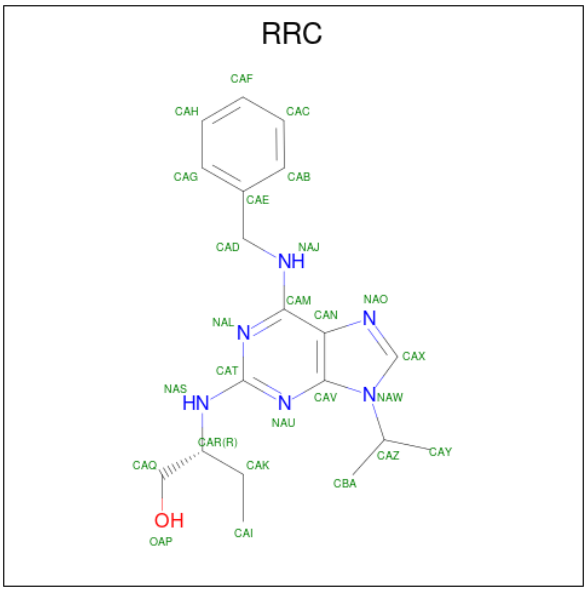
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	ASN	ASP	engineered mutation	UNP Q00535
B	144	ASN	ASP	engineered mutation	UNP Q00535

- Molecule 2 is a protein called CYCLIN-DEPENDENT KINASE 5 ACTIVATOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	150	1202	771	199	221	11	0	0	1
2	E	150	1202	771	199	221	11	0	0	1

- Molecule 3 is R-ROSCOVITINE (three-letter code: RRC) (formula: $C_{19}H_{26}N_6O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	26	19	6	1	0	0

- Molecule 4 is water.

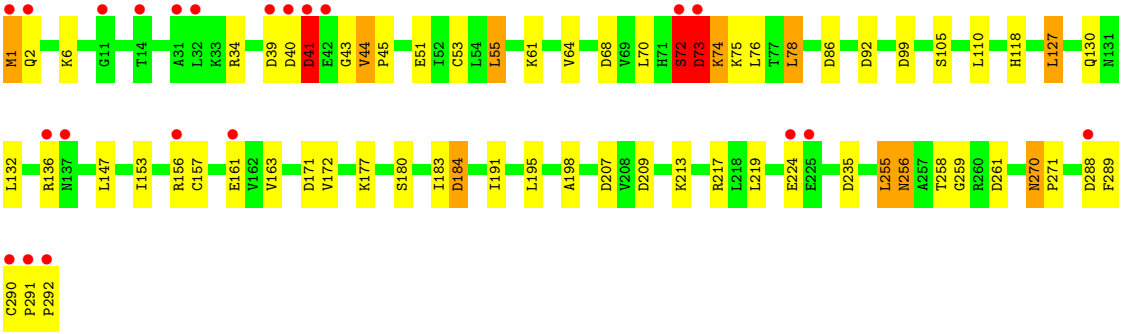
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	142	142	142	0	0
4	B	80	80	80	0	0
4	D	58	58	58	0	0
4	E	22	22	22	0	0

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.

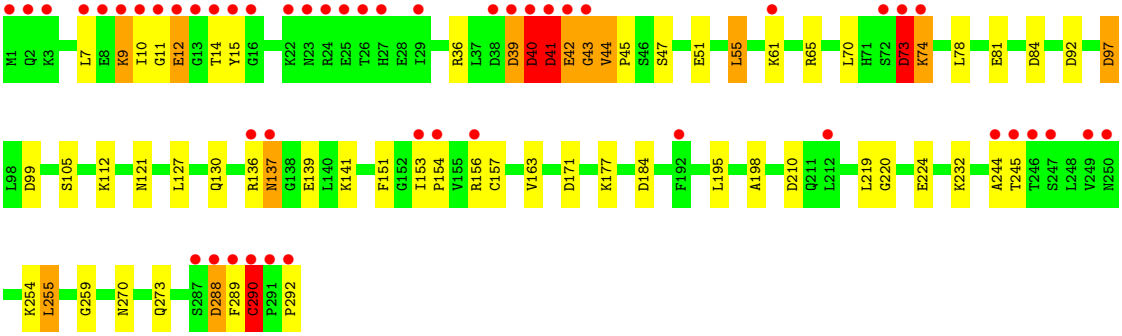
• Molecule 1: CYCLIN-DEPENDENT KINASE 5

Chain A:



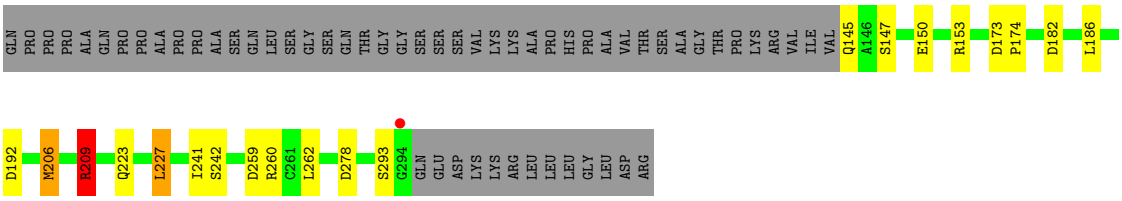
• Molecule 1: CYCLIN-DEPENDENT KINASE 5

Chain B:



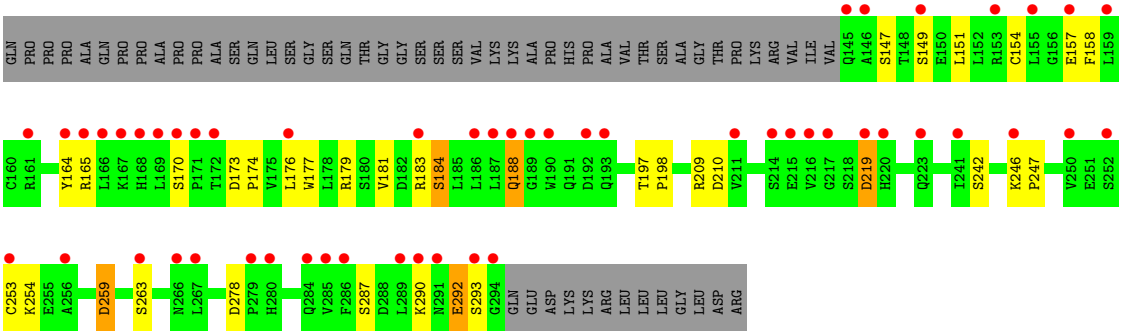
• Molecule 2: CYCLIN-DEPENDENT KINASE 5 ACTIVATOR 1

Chain D:



• Molecule 2: CYCLIN-DEPENDENT KINASE 5 ACTIVATOR 1

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.99Å 117.99Å 156.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.76 – 2.20 19.66 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.4 (19.76-2.20) 94.4 (19.66-2.20)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.216 , 0.219 0.218 , 0.226	Depositor DCC
R_{free} test set	3057 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 65.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7424	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: RRC

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	0.84	5/2402 (0.2%)	0.97	16/3251 (0.5%)
1	B	0.68	1/2402 (0.0%)	0.92	16/3251 (0.5%)
2	D	0.79	0/1230	0.86	8/1669 (0.5%)
2	E	0.44	0/1230	0.67	4/1669 (0.2%)
All	All	0.72	6/7264 (0.1%)	0.89	44/9840 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	ASP	C-N	-6.98	1.18	1.34
1	B	43	GLY	N-CA	6.62	1.55	1.46
1	A	53	CYS	CB-SG	-6.08	1.72	1.82
1	A	180	SER	CB-OG	5.44	1.49	1.42
1	A	74	LYS	N-CA	-5.30	1.35	1.46
1	A	256	ASN	CG-OD1	5.08	1.35	1.24

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	ALA	N-CA-CB	11.59	126.33	110.10
1	A	72	SER	C-N-CA	-9.02	99.15	121.70
1	B	198	ALA	N-CA-CB	8.85	122.48	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	209	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	A	235	ASP	CB-CG-OD2	8.12	125.61	118.30
1	A	92	ASP	CB-CG-OD2	7.81	125.33	118.30
1	B	41	ASP	CA-C-N	-7.20	101.37	117.20
1	A	74	LYS	N-CA-C	-6.95	92.25	111.00
1	A	261	ASP	CB-CG-OD2	6.76	124.39	118.30
2	D	209	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	B	92	ASP	CB-CG-OD2	6.68	124.31	118.30
1	B	42	GLU	N-CA-C	-6.56	93.29	111.00
1	A	184	ASP	CB-CG-OD2	6.54	124.18	118.30
1	B	40	ASP	CA-CB-CG	-6.49	99.11	113.40
1	B	184	ASP	CB-CG-OD2	6.45	124.10	118.30
1	A	68	ASP	CB-CG-OD2	6.41	124.06	118.30
2	D	206	MET	CG-SD-CE	6.36	110.38	100.20
1	B	288	ASP	CB-CG-OD2	6.30	123.97	118.30
2	E	210	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	207	ASP	CB-CG-OD2	6.10	123.79	118.30
1	B	84	ASP	CB-CG-OD2	5.90	123.61	118.30
2	D	192	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	99	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	41	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	99	ASP	CB-CG-OD2	5.52	123.27	118.30
2	E	278	ASP	CB-CG-OD2	5.41	123.17	118.30
2	D	259	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	78	LEU	CA-CB-CG	5.37	127.66	115.30
2	D	182	ASP	CB-CG-OD2	5.36	123.13	118.30
1	B	41	ASP	CB-CA-C	5.33	121.06	110.40
1	B	41	ASP	CA-CB-CG	-5.33	101.69	113.40
2	E	219	ASP	CB-CG-OD2	5.30	123.07	118.30
2	D	260	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	E	259	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	209	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	40	ASP	CB-CA-C	-5.23	99.95	110.40
2	D	278	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	86	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	73	ASP	CA-C-N	-5.15	105.87	117.20
1	B	171	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	97	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	40	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	171	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	210	ASP	CB-CG-OD2	5.05	122.84	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	41	ASP	Peptide
1	A	72	SER	Peptide

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	2346	0	2364	34	0
1	B	2346	0	2365	31	0
2	D	1202	0	1187	8	0
2	E	1202	0	1187	10	0
3	A	26	0	26	1	0
4	A	142	0	0	2	0
4	B	80	0	0	2	0
4	D	58	0	0	1	0
4	E	22	0	0	1	0
All	All	7424	0	7129	78	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 5.

All (78) 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:73:ASP:OD1	1:A:74:LYS:N	1.85	1.08
1:A:73:ASP:OD1	1:A:75:LYS:N	1.89	1.04
1:A:72:SER:O	1:A:73:ASP:HB3	1.62	0.96
1:B:40:ASP:N	1:B:40:ASP:OD1	1.81	0.96
1:B:40:ASP:CG	1:B:41:ASP:N	2.30	0.85
1:A:73:ASP:CG	1:A:74:LYS:N	2.30	0.83
1:A:1:MET:HG3	1:A:70:LEU:HD13	1.61	0.82
1:B:40:ASP:CG	1:B:41:ASP:H	1.71	0.78
1:B:39:ASP:HB3	1:B:40:ASP:OD1	1.83	0.77
1:B:220:GLY:HA3	1:B:244:ALA:HB2	1.66	0.76
2:E:181:VAL:HA	4:E:2006:HOH:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLU:OE1	1:B:141:LYS:HE2	1.88	0.74
1:A:256:ASN:HD21	1:A:258:THR:HB	1.57	0.70
1:A:157:CYS:HB2	1:A:177:LYS:HB3	1.75	0.68
1:B:9:LYS:HB3	1:B:12:GLU:OE2	1.94	0.67
1:B:43:GLY:HA3	2:E:242:SER:HB3	1.76	0.66
2:D:209:ARG:HD2	4:D:2021:HOH:O	1.95	0.66
1:B:177:LYS:HE2	4:B:2040:HOH:O	1.96	0.66
1:A:72:SER:O	1:A:73:ASP:CB	2.29	0.64
1:A:73:ASP:OD1	1:A:74:LYS:C	2.37	0.63
1:A:290:CYS:HB2	1:A:291:PRO:HD3	1.82	0.61
1:A:291:PRO:HB2	1:A:292:PRO:HD3	1.83	0.61
1:B:137:ASN:HD22	1:B:139:GLU:HG3	1.66	0.60
2:E:173:ASP:HB2	2:E:174:PRO:HD3	1.84	0.60
1:B:41:ASP:O	1:B:44:VAL:CG2	2.50	0.59
1:A:43:GLY:HA3	2:D:242:SER:HB2	1.84	0.58
1:A:256:ASN:ND2	1:A:258:THR:HB	2.17	0.58
2:E:174:PRO:HA	2:E:177:TRP:CE3	2.40	0.57
2:D:145:GLN:HA	2:D:150:GLU:HG2	1.87	0.57
1:B:157:CYS:HB2	1:B:177:LYS:HB3	1.90	0.54
2:E:184:SER:O	2:E:188:GLN:HB2	2.08	0.52
2:E:246:LYS:HB3	2:E:247:PRO:HD3	1.91	0.52
1:B:121:ASN:HA	1:B:151:PHE:CE1	2.45	0.52
1:B:40:ASP:O	1:B:42:GLU:N	2.41	0.52
1:B:41:ASP:O	1:B:44:VAL:HG22	2.10	0.51
1:A:73:ASP:H	1:A:75:LYS:H	1.58	0.51
1:B:41:ASP:O	1:B:44:VAL:HG23	2.11	0.51
1:A:172:VAL:HG21	1:A:183:ILE:HD12	1.93	0.51
2:D:241:ILE:HG13	2:D:242:SER:N	2.26	0.50
1:B:156:ARG:HH12	2:E:197:THR:HG21	1.76	0.50
1:A:64:VAL:HG21	3:A:1293:RRC:HAY2	1.94	0.49
1:A:270:ASN:HD22	1:A:270:ASN:C	2.16	0.49
1:A:6:LYS:HE3	1:A:34:ARG:HD2	1.96	0.48
2:D:173:ASP:HB2	2:D:174:PRO:HD3	1.96	0.48
1:A:288:ASP:HB3	4:A:2141:HOH:O	2.13	0.48
1:B:44:VAL:N	1:B:45:PRO:CD	2.77	0.47
1:B:39:ASP:C	1:B:40:ASP:OD1	2.47	0.47
2:E:151:LEU:HD12	2:E:198:PRO:HA	1.96	0.47
1:B:43:GLY:CA	2:E:242:SER:HB3	2.45	0.47
1:B:105:SER:HA	1:B:289:PHE:CZ	2.50	0.47
1:A:255:LEU:HG	1:A:259:GLY:HA3	1.97	0.47
2:E:158:PHE:HB2	2:E:292:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:HIS:HE1	1:A:184:ASP:OD1	1.99	0.46
1:B:10:ILE:O	1:B:12:GLU:N	2.47	0.46
1:B:15:TYR:OH	1:B:51:GLU:OE2	2.23	0.46
1:A:51:GLU:HG3	1:A:55:LEU:HD22	1.98	0.46
1:B:273:GLN:NE2	4:B:2071:HOH:O	2.48	0.46
1:B:43:GLY:H	1:B:45:PRO:HD2	1.80	0.46
2:D:223:GLN:HG2	2:D:227:LEU:HD22	1.97	0.46
1:A:289:PHE:HB3	4:A:2142:HOH:O	2.16	0.45
1:B:97:ASP:OD2	1:B:254:LYS:NZ	2.44	0.45
1:A:44:VAL:N	1:A:45:PRO:CD	2.80	0.45
1:B:290:CYS:C	1:B:292:PRO:HD2	2.37	0.45
1:B:51:GLU:O	1:B:55:LEU:HB2	2.17	0.45
1:A:76:LEU:HD11	2:D:262:LEU:HD11	1.98	0.45
1:B:73:ASP:HB3	1:B:74:LYS:H	1.16	0.44
2:D:153:ARG:HH12	2:D:293:SER:HB2	1.83	0.44
1:A:127:LEU:HD22	1:A:191:ILE:CD1	2.48	0.43
1:B:255:LEU:HG	1:B:259:GLY:HA3	2.01	0.43
1:A:110:LEU:HD11	1:A:127:LEU:HD21	2.01	0.42
1:A:73:ASP:N	1:A:75:LYS:H	2.17	0.42
1:A:73:ASP:OD1	1:A:75:LYS:HG3	2.19	0.42
1:B:78:LEU:N	1:B:78:LEU:HD23	2.33	0.42
1:A:213:LYS:O	1:A:217:ARG:HB2	2.20	0.42
1:A:270:ASN:HD22	1:A:271:PRO:N	2.17	0.42
1:A:270:ASN:HD22	1:A:271:PRO:HD2	1.85	0.42
1:A:105:SER:HA	1:A:289:PHE:CZ	2.56	0.41
1:A:105:SER:HA	1:A:289:PHE:HZ	1.86	0.41

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	290/292 (99%)	273 (94%)	15 (5%)	2 (1%)	22	22
1	B	290/292 (99%)	265 (91%)	19 (7%)	6 (2%)	7	4
2	D	148/208 (71%)	146 (99%)	2 (1%)	0	100	100
2	E	148/208 (71%)	142 (96%)	5 (3%)	1 (1%)	22	22
All	All	876/1000 (88%)	826 (94%)	41 (5%)	9 (1%)	15	14

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	ASP
1	B	11	GLY
1	B	163	VAL
1	A	73	ASP
1	A	163	VAL
2	E	293	SER
1	B	41	ASP
1	B	154	PRO
1	B	290	CYS

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	260/260 (100%)	239 (92%)	21 (8%)	11	12
1	B	260/260 (100%)	230 (88%)	30 (12%)	5	5
2	D	138/186 (74%)	133 (96%)	5 (4%)	35	45
2	E	138/186 (74%)	117 (85%)	21 (15%)	3	2
All	All	796/892 (89%)	719 (90%)	77 (10%)	8	7

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLN

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Mol	Chain	Res	Type
1	A	39	ASP
1	A	41	ASP
1	A	44	VAL
1	A	55	LEU
1	A	61	LYS
1	A	78	LEU
1	A	127	LEU
1	A	130	GLN
1	A	132	LEU
1	A	136	ARG
1	A	147	LEU
1	A	153	ILE
1	A	156	ARG
1	A	161	GLU
1	A	195	LEU
1	A	219	LEU
1	A	224	GLU
1	A	255	LEU
1	A	270	ASN
1	B	7	LEU
1	B	9	LYS
1	B	12	GLU
1	B	14	THR
1	B	36	ARG
1	B	39	ASP
1	B	41	ASP
1	B	44	VAL
1	B	47	SER
1	B	55	LEU
1	B	61	LYS
1	B	65	ARG
1	B	70	LEU
1	B	73	ASP
1	B	74	LYS
1	B	112	LYS
1	B	127	LEU
1	B	130	GLN
1	B	136	ARG
1	B	137	ASN
1	B	153	ILE
1	B	195	LEU
1	B	219	LEU

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Mol	Chain	Res	Type
1	B	224	GLU
1	B	232	LYS
1	B	245	THR
1	B	255	LEU
1	B	270	ASN
1	B	288	ASP
1	B	290	CYS
2	D	147	SER
2	D	186	LEU
2	D	206	MET
2	D	209	ARG
2	D	227	LEU
2	E	147	SER
2	E	149	SER
2	E	154	CYS
2	E	157	GLU
2	E	164	TYR
2	E	165	ARG
2	E	170	SER
2	E	176	LEU
2	E	179	ARG
2	E	183	ARG
2	E	184	SER
2	E	188	GLN
2	E	209	ARG
2	E	219	ASP
2	E	253	CYS
2	E	254	LYS
2	E	259	ASP
2	E	263	SER
2	E	287	SER
2	E	290	LYS
2	E	292	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	62	ASN
1	A	67	HIS
1	A	118	HIS
1	A	135	ASN

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Mol	Chain	Res	Type
1	A	226	GLN
1	A	270	ASN
1	B	62	ASN
1	B	135	ASN
1	B	137	ASN
1	B	206	ASN
1	B	270	ASN
1	B	273	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	RRC	A	1293	-	25,28,28	0.86	2 (8%)	27,38,38	3.33	9 (33%)

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	RRC	A	1293	-	-	2/17/17/17	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1293	RRC	CAX-NAO	2.25	1.38	1.34
3	A	1293	RRC	CAN-CAV	-2.11	1.35	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1293	RRC	CAX-NAW-CAZ	11.13	136.35	125.42
3	A	1293	RRC	CAZ-NAW-CAV	-9.11	116.33	127.15
3	A	1293	RRC	NAU-CAT-NAL	-5.13	118.12	126.23
3	A	1293	RRC	NAS-CAT-NAL	4.15	123.41	117.18
3	A	1293	RRC	CAT-NAU-CAV	3.93	119.74	115.28
3	A	1293	RRC	CAT-NAL-CAM	2.69	122.55	116.39
3	A	1293	RRC	CAK-CAR-CAQ	-2.69	107.39	111.72
3	A	1293	RRC	CBA-CAZ-CAY	2.23	120.15	113.28
3	A	1293	RRC	CAY-CAZ-NAW	-2.03	106.98	110.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1293	RRC	CAI-CAK-CAR-CAQ
3	A	1293	RRC	CAI-CAK-CAR-NAS

There are no ring outliers.

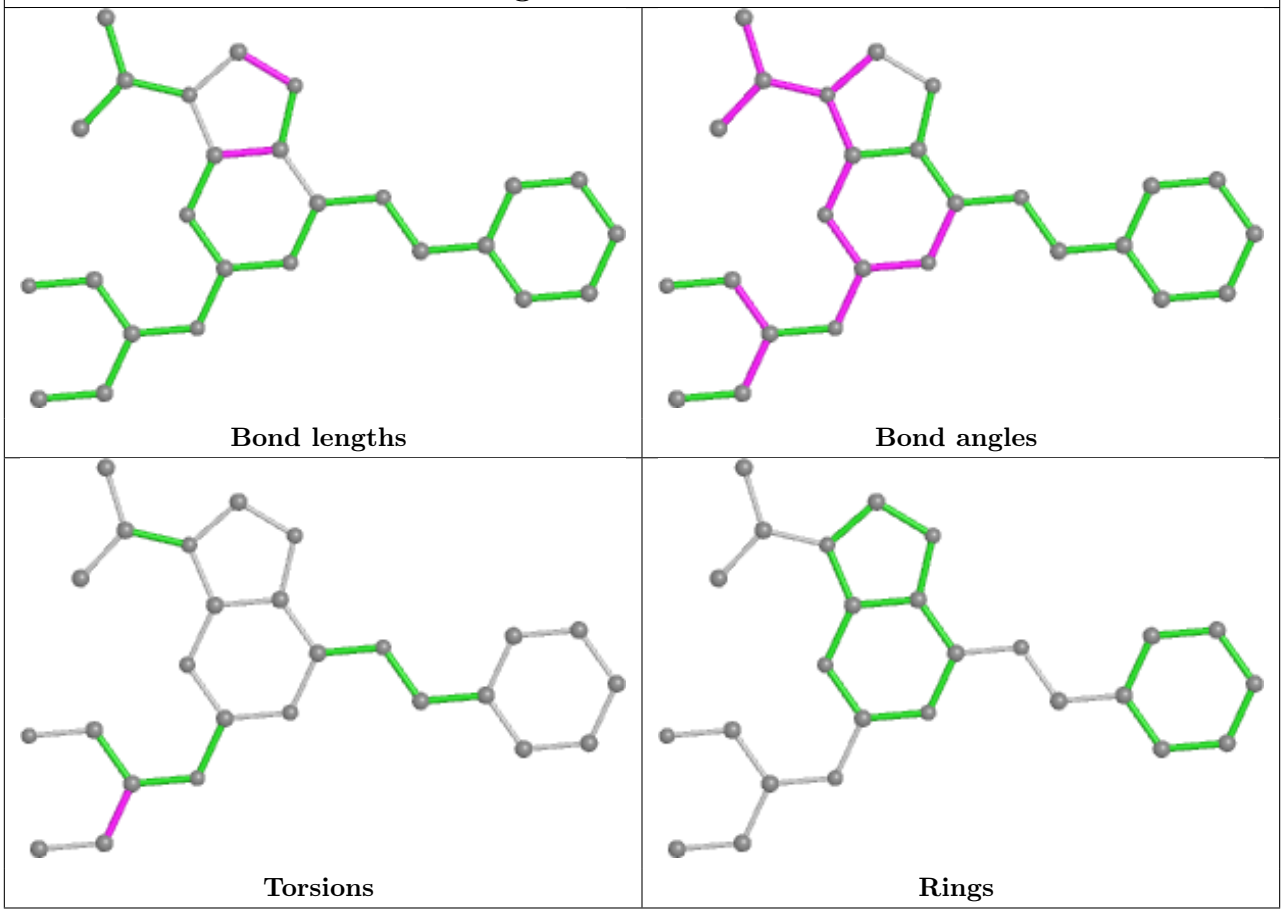
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1293	RRC	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 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 RRC A 1293



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	73:ASP	C	74:LYS	N	1.18

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	292/292 (100%)	0.30	22 (7%) 14 13	18, 23, 33, 53	0
1	B	292/292 (100%)	0.88	49 (16%) 1 1	18, 24, 32, 53	0
2	D	150/208 (72%)	-0.07	1 (0%) 87 86	19, 23, 29, 32	0
2	E	150/208 (72%)	1.66	53 (35%) 0 0	20, 24, 25, 26	0
All	All	884/1000 (88%)	0.66	125 (14%) 2 2	18, 24, 31, 53	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	290	CYS	10.6
1	A	292	PRO	10.3
1	A	291	PRO	10.3
1	A	290	CYS	9.3
1	B	43	GLY	9.0
1	B	291	PRO	8.8
2	E	187	LEU	8.6
1	B	292	PRO	8.5
1	B	1	MET	8.4
2	E	294	GLY	7.9
1	B	13	GLY	7.3
1	B	245	THR	7.2
1	B	73	ASP	7.2
2	E	189	GLY	6.6
1	B	244	ALA	6.5
2	E	168	HIS	5.9
2	E	250	VAL	5.8
1	B	39	ASP	5.6
1	B	11	GLY	5.6
1	B	26	THR	5.5
2	E	293	SER	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	288	ASP	5.4
2	E	183	ARG	5.4
1	B	14	THR	5.4
1	B	15	TYR	5.3
1	B	287	SER	5.2
1	B	288	ASP	5.1
1	B	10	ILE	5.0
2	E	291	ASN	4.9
2	E	167	LYS	4.9
2	E	252	SER	4.9
1	B	27	HIS	4.7
1	B	72	SER	4.7
2	E	241	ILE	4.7
2	E	166	LEU	4.6
1	B	41	ASP	4.5
2	E	170	SER	4.5
1	B	12	GLU	4.5
1	B	136	ARG	4.4
2	E	215	GLU	4.4
2	E	220	HIS	4.4
1	B	23	ASN	4.3
1	B	247	SER	4.1
1	B	154	PRO	4.1
1	B	2	GLN	4.0
1	B	8	GLU	4.0
2	E	161	ARG	4.0
2	E	172	THR	4.0
1	A	156	ARG	4.0
2	E	171	PRO	3.9
1	B	156	ARG	3.9
1	A	39	ASP	3.9
2	E	267	LEU	3.9
1	A	136	ARG	3.9
2	D	294	GLY	3.8
1	B	42	GLU	3.8
1	A	1	MET	3.7
2	E	192	ASP	3.7
2	E	217	GLY	3.7
2	E	186	LEU	3.6
1	A	2	GLN	3.6
2	E	169	LEU	3.6
1	B	40	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
2	E	159	LEU	3.6
1	A	40	ASP	3.6
2	E	279	PRO	3.6
1	B	74	LYS	3.6
2	E	253	CYS	3.5
2	E	146	ALA	3.4
2	E	216	VAL	3.3
1	B	289	PHE	3.3
2	E	176	LEU	3.3
2	E	188	GLN	3.3
1	B	153	ILE	3.3
1	A	14	THR	3.2
1	A	32	LEU	3.2
2	E	153	ARG	3.1
2	E	214	SER	3.1
1	B	24	ARG	3.1
2	E	263	SER	3.1
1	B	22	LYS	3.0
2	E	290	LYS	2.9
1	B	38	ASP	2.9
1	B	25	GLU	2.9
1	B	137	ASN	2.9
2	E	286	PHE	2.8
1	A	42	GLU	2.8
2	E	145	GLN	2.8
2	E	266	ASN	2.7
2	E	164	TYR	2.7
2	E	193	GLN	2.7
1	B	61	LYS	2.7
2	E	211	VAL	2.7
2	E	280	HIS	2.7
2	E	246	LYS	2.7
2	E	284	GLN	2.7
1	B	29	ILE	2.6
1	B	212	LEU	2.6
2	E	165	ARG	2.6
1	B	16	GLY	2.6
1	B	250	ASN	2.6
1	A	72	SER	2.6
1	B	249	VAL	2.5
2	E	289	LEU	2.4
1	A	225	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	31	ALA	2.4
1	B	9	LYS	2.4
2	E	256	ALA	2.4
1	B	192	PHE	2.4
2	E	157	GLU	2.4
1	A	11	GLY	2.4
1	A	224	GLU	2.3
1	A	161	GLU	2.3
2	E	190	TRP	2.3
2	E	155	LEU	2.2
1	A	137	ASN	2.2
1	B	246	THR	2.2
1	A	41	ASP	2.1
2	E	223	GLN	2.1
2	E	219	ASP	2.1
2	E	285	VAL	2.1
2	E	149	SER	2.1
1	A	73	ASP	2.0
1	B	7	LEU	2.0
1	B	3	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.

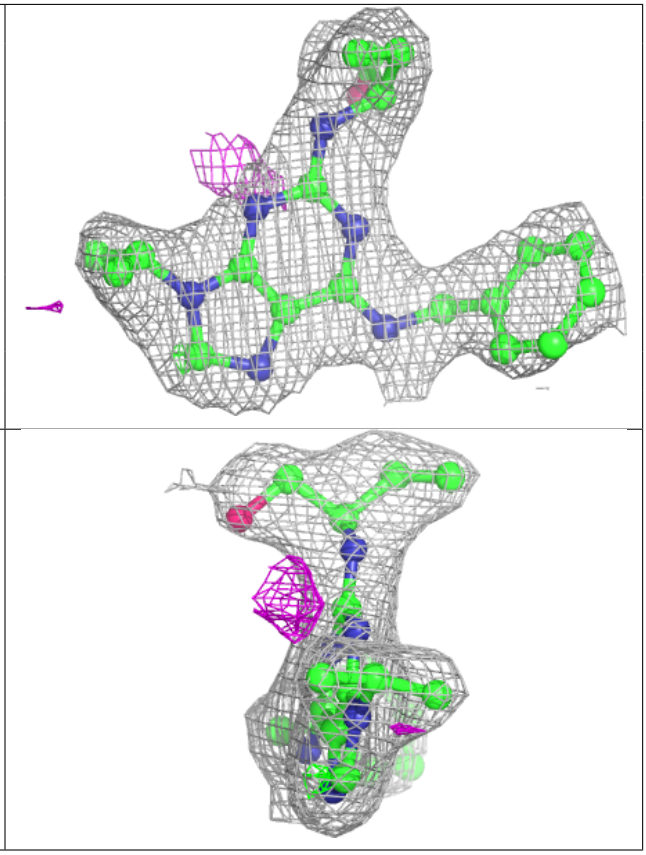
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	RRC	A	1293	26/26	0.88	0.16	19,23,24,25	0

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 RRC A 1293:

$2mF_o$-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.