Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 12:55 am GMT

PDB ID	:	1UNG
Title	:	Structural mechanism for the inhibition of CDK5-p25 by roscovitine, aloisine and indirubin.
Authors	:	Mapelli, M.; Crovace, C.; Massimiliano, L.; Musacchio, A.
Deposited on	:	2003-09-10
Resolution	:	2.30 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:

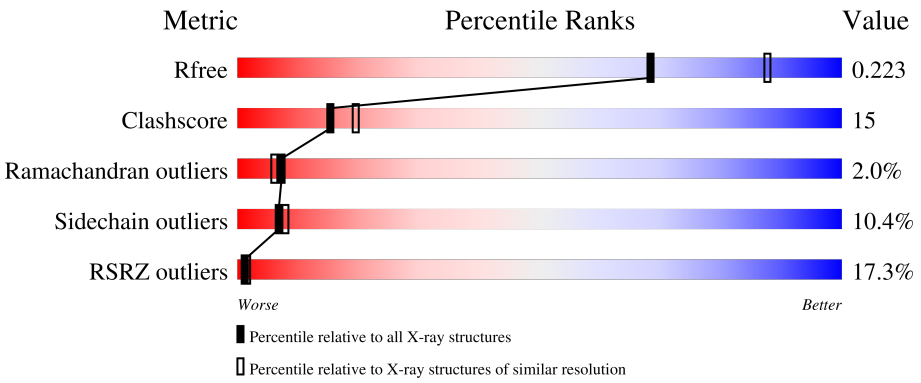
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

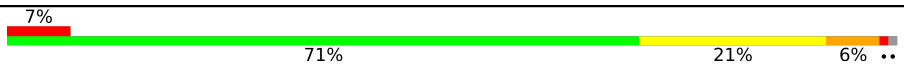
The reported resolution of this entry is 2.30 Å.

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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ALH	A	1293	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ALH	B	1288	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7204 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 CELL DIVISION PROTEIN KINASE 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2322	1492	399	419	12	0	0	0
1	B	269	2155	1391	373	381	10	0	0	1

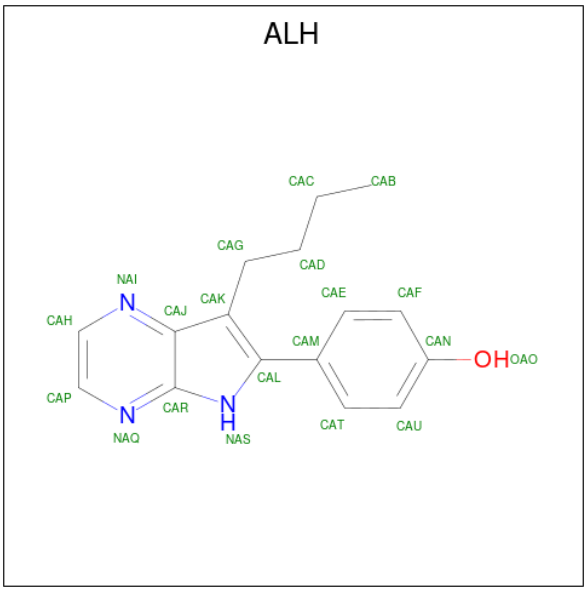
There are 2 discrepancies between the modelled and reference sequences:

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	148	1191	765	197	218	11	0	0	1

- Molecule 3 is 6-PHENYL[5H]PYRROLO[2,3-B]PYRAZINE (three-letter code: ALH) (formula: $C_{16}H_{17}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	20	16	3	1	0	0
3	B	1	20	16	3	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	146	146	146	0	0
4	B	76	76	76	0	0
4	D	61	61	61	0	0
4	E	11	11	11	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.72Å 117.72Å 156.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.76 – 2.30 19.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.5 (19.76-2.30) 95.5 (19.73-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.216 , 0.225 0.213 , 0.223	Depositor DCC
R_{free} test set	2713 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 64.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7204	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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.

4 Model quality (i)

4.1 Standard geometry (i)

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

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	1.01	2/2377 (0.1%)	1.08	19/3216 (0.6%)
1	B	0.80	0/2203	0.95	12/2979 (0.4%)
2	D	1.03	1/1230 (0.1%)	1.01	5/1669 (0.3%)
2	E	0.92	2/1219 (0.2%)	0.97	11/1654 (0.7%)
All	All	0.94	5/7029 (0.1%)	1.01	47/9518 (0.5%)

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	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	171	PRO	N-CD	20.82	1.76	1.47
1	A	117	CYS	CB-SG	-5.98	1.72	1.81
1	A	135	ASN	CB-CG	-5.75	1.37	1.51
2	D	145	GLN	C-O	-5.37	1.13	1.23
2	E	210	ASP	N-CA	-5.16	1.36	1.46

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	65	ARG	NE-CZ-NH2	-11.86	114.37	120.30
2	D	209	ARG	NE-CZ-NH2	-11.57	114.52	120.30
2	E	171	PRO	CA-N-CD	-10.23	97.17	111.50
1	A	288	ASP	CB-CG-OD2	8.45	125.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	97	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	65	ARG	NE-CZ-NH1	7.46	124.03	120.30
2	E	278	ASP	CB-CG-OD2	7.32	124.89	118.30
1	B	210	ASP	CB-CG-OD2	7.30	124.87	118.30
1	A	207	ASP	CB-CG-OD2	7.24	124.82	118.30
2	E	293	SER	O-C-N	-7.08	111.17	123.20
1	A	184	ASP	CB-CG-OD2	6.88	124.49	118.30
2	E	182	ASP	CB-CG-OD2	6.76	124.39	118.30
1	A	68	ASP	CB-CG-OD2	6.68	124.31	118.30
1	B	38	ASP	CB-CG-OD2	6.65	124.29	118.30
1	B	75	LYS	N-CA-CB	6.57	122.42	110.60
1	A	261	ASP	CB-CG-OD2	6.53	124.18	118.30
1	A	198	ALA	N-CA-CB	6.48	119.18	110.10
2	D	209	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	207	ASP	CB-CG-OD2	6.35	124.01	118.30
1	A	92	ASP	CB-CG-OD2	6.29	123.97	118.30
1	B	99	ASP	CB-CG-OD2	6.20	123.88	118.30
2	D	260	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	A	171	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	168	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	126	ASP	CB-CG-OD2	5.84	123.55	118.30
2	D	182	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	210	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	99	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	235	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	84	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	168	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	38	ASP	CB-CG-OD2	5.51	123.26	118.30
2	E	155	LEU	CA-CB-CG	5.40	127.71	115.30
1	A	86	ASP	CB-CG-OD1	5.38	123.14	118.30
2	E	288	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	171	ASP	CB-CG-OD2	5.34	123.10	118.30
2	E	173	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	84	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	73	ASP	CB-CG-OD2	5.22	123.00	118.30
2	E	212	ILE	N-CA-C	5.19	125.02	111.00
1	B	184	ASP	CB-CG-OD2	5.17	122.95	118.30
2	E	259	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	34	ARG	NE-CZ-NH1	-5.16	117.72	120.30
2	E	211	VAL	C-N-CA	5.12	134.49	121.70
2	E	171	PRO	N-CA-CB	5.05	109.36	103.30
2	D	206	MET	CG-SD-CE	-5.04	92.13	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	73	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	244	ALA	Peptide

4.2 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	2322	0	2345	69	0
1	B	2155	0	2200	68	0
2	D	1202	0	1187	32	0
2	E	1191	0	1177	46	0
3	A	20	0	16	9	0
3	B	20	0	16	7	0
4	A	146	0	0	5	0
4	B	76	0	0	3	1
4	D	61	0	0	8	0
4	E	11	0	0	2	0
All	All	7204	0	6941	206	1

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 15.

All (206) 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)
2:E:171:PRO:N	2:E:171:PRO:CD	1.77	1.27
1:B:56:LYS:NZ	2:E:265:ILE:HG22	1.52	1.24
1:A:53:CYS:SG	4:D:2004:HOH:O	1.95	1.20
1:A:53:CYS:HB3	4:D:2004:HOH:O	1.51	1.10
2:D:158:PHE:HB2	2:D:292:GLU:HG3	1.37	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HB2	1:A:34:ARG:HH22	1.21	1.05
2:D:269:SER:HA	2:D:272:MET:HE3	1.39	1.05
1:A:53:CYS:CB	4:D:2004:HOH:O	1.97	1.01
2:D:254:LYS:HE2	2:D:258:TRP:HE1	1.25	0.98
1:A:156:ARG:HG3	1:A:156:ARG:HH11	1.29	0.95
1:B:250:ASN:HD22	1:B:250:ASN:H	1.15	0.95
1:B:56:LYS:HZ1	2:E:265:ILE:HG22	1.13	0.94
3:B:1288:ALH:HAG1	3:B:1288:ALH:HAT	1.49	0.93
1:B:44:VAL:H	1:B:45:PRO:CD	1.82	0.93
1:A:37:LEU:O	2:D:254:LYS:NZ	2.04	0.89
1:B:56:LYS:NZ	2:E:265:ILE:CG2	2.36	0.89
3:A:1293:ALH:HAG1	3:A:1293:ALH:HAT	1.53	0.89
1:B:56:LYS:HZ3	2:E:265:ILE:HG22	1.35	0.88
1:A:153:ILE:HG23	1:A:154:PRO:HD2	1.55	0.88
1:B:256:ASN:HD22	1:B:256:ASN:H	1.21	0.88
1:A:73:ASP:CG	1:A:74:LYS:H	1.77	0.87
2:E:211:VAL:HG12	2:E:212:ILE:CD1	2.10	0.82
1:A:156:ARG:HG3	1:A:156:ARG:NH1	1.93	0.82
1:B:250:ASN:H	1:B:250:ASN:ND2	1.77	0.81
1:A:85:GLN:HA	3:A:1293:ALH:CAF	2.12	0.79
1:B:250:ASN:HD22	1:B:250:ASN:N	1.79	0.79
2:D:209:ARG:HD2	4:D:2030:HOH:O	1.80	0.79
1:B:256:ASN:HD22	1:B:256:ASN:N	1.81	0.78
1:B:44:VAL:H	1:B:45:PRO:HD3	1.45	0.78
1:A:223:THR:H	1:A:226:GLN:HE21	1.31	0.77
1:A:290:CYS:C	1:A:292:PRO:HD2	2.04	0.77
2:E:198:PRO:O	2:E:202:VAL:HG12	1.85	0.77
1:A:144:ASN:HD21	3:A:1293:ALH:HAC2	1.48	0.75
3:B:1288:ALH:HAT	3:B:1288:ALH:CAG	2.16	0.75
1:B:36:ARG:HG2	1:B:36:ARG:HH11	1.52	0.74
1:A:1:MET:HB2	1:A:34:ARG:NH2	2.01	0.73
1:B:118:HIS:HD2	4:B:2074:HOH:O	1.72	0.72
1:B:56:LYS:HZ3	2:E:265:ILE:CG2	2.01	0.72
2:D:289:LEU:O	2:D:292:GLU:HB2	1.90	0.72
1:A:127:LEU:HD22	1:A:191:ILE:CD1	2.19	0.72
2:E:260:ARG:O	2:E:264:VAL:HG23	1.90	0.72
1:A:85:GLN:HA	3:A:1293:ALH:HAF	1.72	0.72
2:D:153:ARG:NH1	2:D:293:SER:HB2	2.04	0.72
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.70	0.71
1:B:85:GLN:HA	3:B:1288:ALH:CAF	2.20	0.71
1:A:44:VAL:HB	1:A:45:PRO:HD3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:170:SER:C	2:E:171:PRO:CD	2.59	0.71
1:B:85:GLN:HA	3:B:1288:ALH:HAF	1.71	0.71
1:B:256:ASN:H	1:B:256:ASN:ND2	1.87	0.71
1:A:289:PHE:CE2	1:A:291:PRO:HG2	2.26	0.70
1:B:36:ARG:HH11	1:B:36:ARG:CG	2.04	0.70
2:E:170:SER:HA	2:E:171:PRO:CD	2.21	0.70
1:A:34:ARG:NH1	1:A:75:LYS:HE3	2.08	0.68
1:A:101:GLU:OE2	4:A:2052:HOH:O	2.11	0.68
1:B:44:VAL:N	1:B:45:PRO:HD3	2.08	0.67
2:D:153:ARG:HH12	2:D:293:SER:HB2	1.58	0.66
1:A:73:ASP:CG	1:A:74:LYS:N	2.41	0.66
1:B:34:ARG:HD3	1:B:75:LYS:HE2	1.78	0.66
1:B:57:GLU:OE2	2:E:269:SER:OG	2.13	0.66
2:E:190:TRP:HA	4:E:2002:HOH:O	1.95	0.66
1:B:220:GLY:HA3	1:B:244:ALA:HA	1.77	0.65
3:A:1293:ALH:HAT	3:A:1293:ALH:CAG	2.27	0.65
2:E:175:VAL:HG12	2:E:179:ARG:HG2	1.77	0.64
2:E:208:CYS:HA	2:E:211:VAL:HG23	1.79	0.64
1:B:56:LYS:HZ1	2:E:265:ILE:CG2	1.98	0.63
2:E:228:THR:HG21	2:E:260:ARG:HD2	1.81	0.63
1:B:137:ASN:OD1	1:B:139:GLU:HG3	1.98	0.62
1:B:6:LYS:HD3	1:B:19:PHE:CE2	2.35	0.62
1:B:20:LYS:HG3	1:B:82:PHE:CE2	2.34	0.61
2:E:197:THR:HG22	2:E:200:ASN:H	1.65	0.61
1:A:73:ASP:OD2	1:A:74:LYS:N	2.33	0.61
1:A:144:ASN:HD21	3:A:1293:ALH:CAC	2.15	0.60
1:A:290:CYS:O	1:A:292:PRO:HD2	2.02	0.60
1:A:168:ARG:HD3	1:A:172:VAL:HG12	1.85	0.59
1:A:118:HIS:HD2	4:A:2142:HOH:O	1.84	0.59
1:A:144:ASN:ND2	3:A:1293:ALH:HAC2	2.16	0.59
1:B:127:LEU:HB3	1:B:187:SER:HB3	1.86	0.57
1:B:81:GLU:OE2	1:B:141:LYS:HE3	2.04	0.57
1:B:164:THR:HG22	4:B:2030:HOH:O	2.04	0.57
1:A:1:MET:HE3	1:A:3:LYS:HB3	1.86	0.57
1:A:152:GLY:HA3	2:D:276:ASN:O	2.05	0.57
2:D:246:LYS:HB3	2:D:247:PRO:HD3	1.87	0.56
2:E:211:VAL:HG12	2:E:212:ILE:HD11	1.87	0.56
1:B:2:GLN:HE22	1:B:70:LEU:HD11	1.70	0.56
1:B:57:GLU:OE1	2:E:270:SER:HB3	2.06	0.56
2:D:173:ASP:HB2	2:D:174:PRO:HD3	1.87	0.56
1:A:50:ARG:HG2	1:A:50:ARG:HH11	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ASN:ND2	4:B:2014:HOH:O	2.40	0.55
1:A:153:ILE:HG23	1:A:154:PRO:CD	2.34	0.55
1:A:156:ARG:HH11	1:A:156:ARG:CG	2.09	0.55
1:B:103:VAL:HG13	1:B:195:LEU:HB3	1.87	0.55
1:B:34:ARG:HH11	1:B:34:ARG:HG3	1.72	0.55
1:A:256:ASN:ND2	4:A:2124:HOH:O	2.40	0.55
2:E:211:VAL:HG12	2:E:212:ILE:HG12	1.89	0.55
1:B:6:LYS:HD3	1:B:19:PHE:CD2	2.42	0.54
1:B:153:ILE:HD11	2:E:237:MET:HE2	1.89	0.54
2:D:269:SER:CA	2:D:272:MET:HE3	2.26	0.54
2:E:170:SER:CA	2:E:171:PRO:CD	2.85	0.54
1:A:162:VAL:O	1:A:163:VAL:HG23	2.07	0.54
1:B:127:LEU:CD1	1:B:142:LEU:HD21	2.39	0.53
1:B:153:ILE:HG23	2:E:276:ASN:HA	1.91	0.53
1:A:1:MET:HE3	1:A:3:LYS:CB	2.38	0.53
2:D:150:GLU:OE2	2:D:153:ARG:CZ	2.57	0.53
2:E:211:VAL:HG12	2:E:212:ILE:CG1	2.38	0.53
3:A:1293:ALH:HAG1	3:A:1293:ALH:CAT	2.34	0.53
1:B:196:ALA:O	1:B:254:LYS:HB2	2.08	0.53
2:E:162:ARG:HH11	2:E:162:ARG:HG2	1.73	0.53
1:A:2:GLN:O	1:A:24:ARG:NH1	2.41	0.53
1:A:39:ASP:OD1	1:A:40:ASP:N	2.40	0.53
1:A:1:MET:O	1:A:3:LYS:N	2.43	0.52
1:B:18:VAL:C	1:B:19:PHE:CD1	2.82	0.52
1:B:65:ARG:HG2	1:B:65:ARG:HH11	1.74	0.52
1:B:90:TYR:HE2	1:B:98:LEU:HD22	1.74	0.52
1:A:118:HIS:HE1	1:A:184:ASP:OD1	1.92	0.52
2:D:245:LEU:HD22	2:D:254:LYS:HE3	1.92	0.52
1:A:290:CYS:C	1:A:292:PRO:CD	2.75	0.52
1:B:20:LYS:HG2	1:B:20:LYS:O	2.08	0.52
2:D:158:PHE:HB2	2:D:292:GLU:CG	2.24	0.52
1:B:109:GLN:HA	1:B:112:LYS:HE3	1.91	0.52
1:B:156:ARG:O	1:B:157:CYS:HB3	2.09	0.52
1:B:99:ASP:HB3	1:B:102:ILE:HG13	1.92	0.52
1:A:50:ARG:NH1	1:A:146:GLY:O	2.36	0.51
2:D:150:GLU:OE2	2:D:153:ARG:NH2	2.43	0.51
1:B:157:CYS:SG	2:E:239:ASN:ND2	2.83	0.51
1:B:44:VAL:H	1:B:45:PRO:HD2	1.70	0.51
2:D:145:GLN:N	2:D:150:GLU:HG2	2.25	0.51
1:A:1:MET:C	1:A:1:MET:SD	2.89	0.51
2:D:246:LYS:HD2	4:D:2041:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ILE:HD11	1:A:78:LEU:CD2	2.41	0.51
2:D:209:ARG:CD	4:D:2030:HOH:O	2.48	0.50
1:B:99:ASP:HB3	1:B:102:ILE:CG1	2.42	0.49
2:E:251:GLU:OE2	2:E:256:ALA:HB3	2.12	0.49
2:D:245:LEU:CD2	2:D:254:LYS:HE3	2.43	0.49
1:B:36:ARG:CG	1:B:36:ARG:NH1	2.70	0.49
1:B:63:ILE:O	1:B:64:VAL:C	2.50	0.49
1:A:105:SER:HA	1:A:289:PHE:HZ	1.79	0.48
1:B:153:ILE:HD11	2:E:237:MET:CE	2.43	0.47
1:A:283:HIS:CG	1:A:284:PRO:HD2	2.49	0.47
2:E:191:GLN:H	2:E:191:GLN:CD	2.17	0.47
1:A:255:LEU:HG	1:A:259:GLY:HA3	1.96	0.47
2:E:197:THR:O	2:E:201:VAL:HG23	2.15	0.47
3:B:1288:ALH:HAG1	3:B:1288:ALH:CAT	2.34	0.47
2:E:211:VAL:CG1	2:E:225:VAL:HG11	2.45	0.47
2:E:246:LYS:HB3	2:E:247:PRO:HD3	1.97	0.47
2:D:246:LYS:HD2	2:D:246:LYS:O	2.14	0.47
2:D:254:LYS:HE2	2:D:258:TRP:NE1	2.10	0.47
1:A:71:HIS:ND1	2:D:259:ASP:OD1	2.43	0.46
1:B:127:LEU:HB3	1:B:187:SER:CB	2.45	0.46
1:A:162:VAL:C	1:A:163:VAL:HG23	2.36	0.46
2:E:176:LEU:O	2:E:180:SER:HB2	2.15	0.46
2:E:181:VAL:HG12	2:E:227:LEU:HD11	1.98	0.46
2:D:268:MET:HB2	2:D:272:MET:HE2	1.98	0.46
1:A:84:ASP:O	3:A:1293:ALH:HAF	2.16	0.46
1:B:226:GLN:HE21	1:B:226:GLN:HB3	1.58	0.45
1:B:279:GLU:O	1:B:279:GLU:HG3	2.15	0.45
1:B:123:LEU:HD22	1:B:181:THR:HA	1.99	0.45
1:B:34:ARG:HG3	1:B:34:ARG:NH1	2.30	0.45
2:E:191:GLN:HG3	4:E:2003:HOH:O	2.17	0.45
1:A:85:GLN:NE2	4:A:2039:HOH:O	2.22	0.44
2:E:208:CYS:HA	2:E:211:VAL:CG2	2.47	0.44
1:A:24:ARG:HG3	1:A:24:ARG:HH11	1.82	0.44
2:E:162:ARG:HG2	2:E:162:ARG:NH1	2.32	0.44
2:E:211:VAL:HG12	2:E:212:ILE:HD13	1.96	0.44
1:A:51:GLU:HG3	1:A:55:LEU:HD22	2.00	0.43
1:B:275:ILE:HG13	1:B:279:GLU:HG2	2.01	0.43
3:B:1288:ALH:CAG	3:B:1288:ALH:CAT	2.92	0.43
2:E:196:ILE:H	2:E:196:ILE:HG13	1.44	0.43
1:A:270:ASN:HD22	1:A:270:ASN:C	2.20	0.43
1:A:290:CYS:CB	1:A:291:PRO:CD	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:LEU:HG	1:B:259:GLY:HA3	2.01	0.43
1:A:38:ASP:HA	2:D:254:LYS:NZ	2.34	0.43
1:B:176:ALA:HB2	1:B:233:LEU:HD22	1.99	0.43
1:A:9:LYS:HB2	1:A:9:LYS:HE2	1.66	0.43
1:B:250:ASN:ND2	1:B:250:ASN:N	2.46	0.43
1:A:223:THR:OG1	1:A:226:GLN:HG3	2.18	0.43
2:E:199:ALA:O	2:E:202:VAL:HG13	2.18	0.43
1:A:50:ARG:HD2	1:A:148:ALA:O	2.19	0.43
2:D:251:GLU:CD	2:D:260:ARG:HH22	2.22	0.43
1:A:34:ARG:HH11	1:A:75:LYS:HE3	1.83	0.42
2:E:170:SER:HA	2:E:171:PRO:HD2	2.00	0.42
1:B:227:TRP:CD2	1:B:230:MET:HB3	2.55	0.42
2:D:216:VAL:HG11	2:D:222:LEU:HB2	2.01	0.42
2:E:263:SER:HA	2:E:266:ASN:HD22	1.84	0.42
1:B:108:PHE:CE2	1:B:112:LYS:HD3	2.55	0.42
2:D:167:LYS:NZ	4:D:2011:HOH:O	2.48	0.42
1:B:81:GLU:O	3:B:1288:ALH:HAP	2.20	0.42
1:A:51:GLU:CG	1:A:55:LEU:HD22	2.50	0.41
2:D:152:LEU:HD11	2:D:196:ILE:HG21	2.01	0.41
1:A:50:ARG:HG2	1:A:50:ARG:NH1	2.33	0.41
1:B:19:PHE:CD1	1:B:19:PHE:N	2.89	0.41
1:B:59:LYS:HD2	1:B:65:ARG:CZ	2.49	0.41
2:E:193:GLN:HE21	2:E:193:GLN:HB3	1.56	0.41
2:E:211:VAL:CG1	2:E:225:VAL:CG1	2.98	0.41
1:A:105:SER:HA	1:A:289:PHE:CZ	2.56	0.41
2:E:281:TYR:O	2:E:285:VAL:HG23	2.21	0.41
1:B:17:THR:HG23	1:B:18:VAL:HG23	2.01	0.41
2:D:223:GLN:HG2	2:D:227:LEU:HD22	2.03	0.41
1:A:157:CYS:HB2	1:A:177:LYS:HB3	2.03	0.41
1:A:7:LEU:HB2	1:A:20:LYS:HG2	2.02	0.40
1:A:39:ASP:CB	4:A:2009:HOH:O	2.69	0.40
1:B:270:ASN:C	1:B:270:ASN:HD22	2.25	0.40
1:A:50:ARG:NH1	1:A:50:ARG:CG	2.84	0.40
2:D:190:TRP:O	2:D:240:GLU:HG3	2.21	0.40
1:A:76:LEU:HA	1:A:76:LEU:HD12	1.66	0.40
1:A:270:ASN:HA	1:A:271:PRO:HD2	1.95	0.40
2:D:161:ARG:HD2	4:D:2009:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2019:HOH:O	4:B:2019:HOH:O[5_555]	1.91	0.29

4.3 Torsion angles (i)

4.3.1 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	284/292 (97%)	261 (92%)	17 (6%)	6 (2%)	7 5
1	B	261/292 (89%)	240 (92%)	17 (6%)	4 (2%)	10 10
2	D	148/208 (71%)	146 (99%)	2 (1%)	0	100 100
2	E	146/208 (70%)	113 (77%)	26 (18%)	7 (5%)	2 1
All	All	839/1000 (84%)	760 (91%)	62 (7%)	17 (2%)	7 6

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	44	VAL
1	B	44	VAL
2	E	170	SER
1	A	42	GLU
1	B	163	VAL
2	E	195	PHE
1	A	163	VAL
1	A	290	CYS
1	A	291	PRO
2	E	156	GLY
2	E	168	HIS
1	B	154	PRO
2	E	211	VAL
2	E	293	SER
1	B	64	VAL
2	E	217	GLY

4.3.2 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	258/260 (99%)	239 (93%)	19 (7%)	13 17
1	B	239/260 (92%)	216 (90%)	23 (10%)	8 10
2	D	138/186 (74%)	132 (96%)	6 (4%)	29 40
2	E	137/186 (74%)	105 (77%)	32 (23%)	1 0
All	All	772/892 (86%)	692 (90%)	80 (10%)	7 8

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLN
1	A	9	LYS
1	A	17	THR
1	A	24	ARG
1	A	55	LEU
1	A	65	ARG
1	A	72	SER
1	A	73	ASP
1	A	127	LEU
1	A	130	GLN
1	A	132	LEU
1	A	141	LYS
1	A	156	ARG
1	A	195	LEU
1	A	219	LEU
1	A	237	LYS
1	A	255	LEU
1	A	270	ASN
1	B	2	GLN
1	B	9	LYS
1	B	29	ILE
1	B	36	ARG
1	B	46	SER

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Mol	Chain	Res	Type
1	B	95	ASN
1	B	132	LEU
1	B	142	LEU
1	B	155	VAL
1	B	195	LEU
1	B	197	ASN
1	B	219	LEU
1	B	223	THR
1	B	226	GLN
1	B	232	LYS
1	B	237	LYS
1	B	250	ASN
1	B	254	LYS
1	B	255	LEU
1	B	256	ASN
1	B	258	THR
1	B	270	ASN
1	B	279	GLU
2	D	167	LYS
2	D	186	LEU
2	D	209	ARG
2	D	227	LEU
2	D	241	ILE
2	D	292	GLU
2	E	148	THR
2	E	150	GLU
2	E	163	CYS
2	E	164	TYR
2	E	168	HIS
2	E	170	SER
2	E	171	PRO
2	E	172	THR
2	E	177	TRP
2	E	180	SER
2	E	185	LEU
2	E	191	GLN
2	E	192	ASP
2	E	193	GLN
2	E	196	ILE
2	E	197	THR
2	E	202	VAL
2	E	209	ARG

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Mol	Chain	Res	Type
2	E	212	ILE
2	E	214	SER
2	E	216	VAL
2	E	218	SER
2	E	219	ASP
2	E	220	HIS
2	E	223	GLN
2	E	235	SER
2	E	246	LYS
2	E	252	SER
2	E	260	ARG
2	E	263	SER
2	E	275	ILE
2	E	283	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	62	ASN
1	A	118	HIS
1	A	135	ASN
1	A	144	ASN
1	A	226	GLN
1	A	270	ASN
1	B	2	GLN
1	B	71	HIS
1	B	95	ASN
1	B	118	HIS
1	B	131	ASN
1	B	197	ASN
1	B	250	ASN
1	B	256	ASN
1	B	270	ASN
1	B	273	GLN
2	D	188	GLN
2	E	191	GLN
2	E	193	GLN
2	E	239	ASN
2	E	266	ASN

4.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

2 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	ALH	A	1293	-	19,22,22	1.97	3 (15%)	15,30,30	1.42	3 (20%)
3	ALH	B	1288	-	19,22,22	1.93	2 (10%)	15,30,30	0.72	0

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	ALH	A	1293	-	-	2/4/8/8	0/3/3/3
3	ALH	B	1288	-	-	0/4/8/8	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1288	ALH	CAJ-NAI	5.61	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1293	ALH	CAR-NAQ	5.26	1.44	1.37
3	A	1293	ALH	CAJ-NAI	5.18	1.43	1.37
3	B	1288	ALH	CAR-NAQ	4.89	1.43	1.37
3	A	1293	ALH	OAO-CAN	-2.65	1.30	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1293	ALH	CAD-CAG-CAK	3.31	121.28	112.88
3	A	1293	ALH	CAT-CAM-CAE	2.14	120.55	118.65
3	A	1293	ALH	CAE-CAF-CAN	-2.04	117.80	120.15

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1293	ALH	CAB-CAC-CAD-CAG
3	A	1293	ALH	CAC-CAD-CAG-CAK

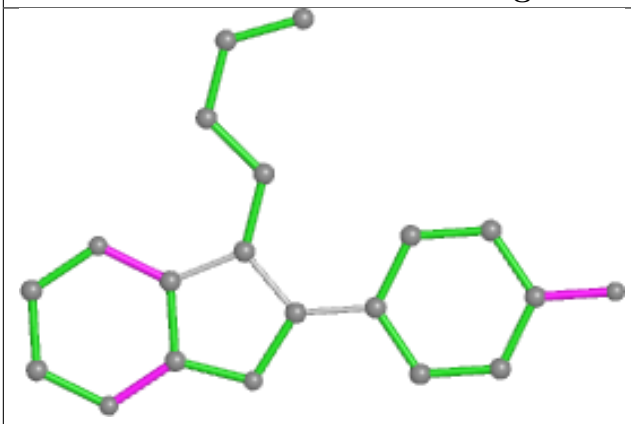
There are no ring outliers.

2 monomers are involved in 16 short contacts:

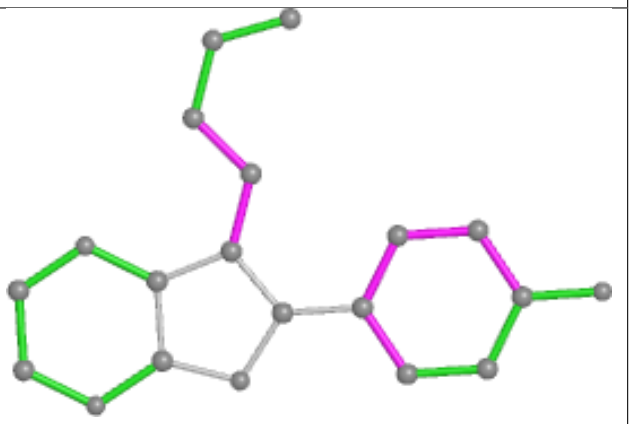
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1293	ALH	9	0
3	B	1288	ALH	7	0

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.

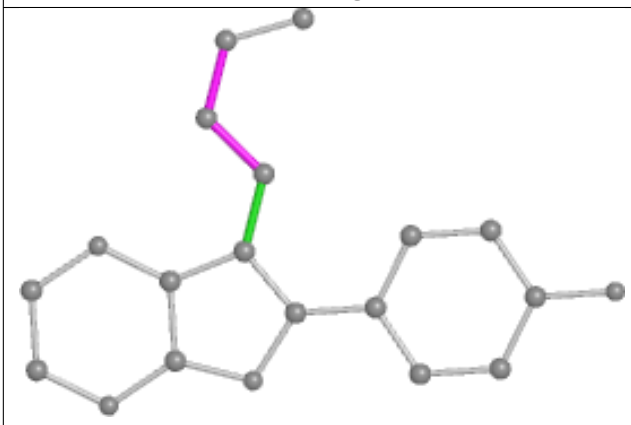
Ligand ALH A 1293



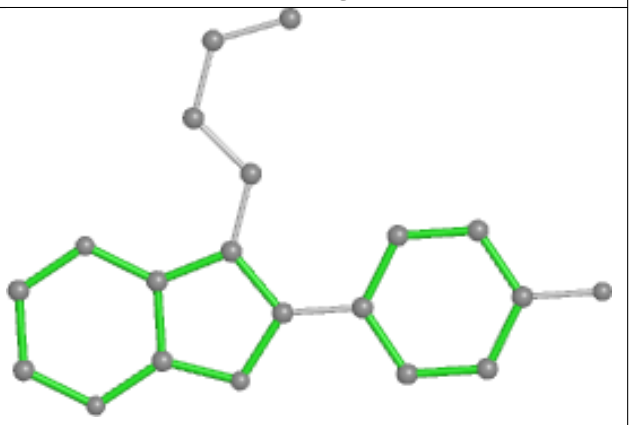
Bond lengths



Bond angles

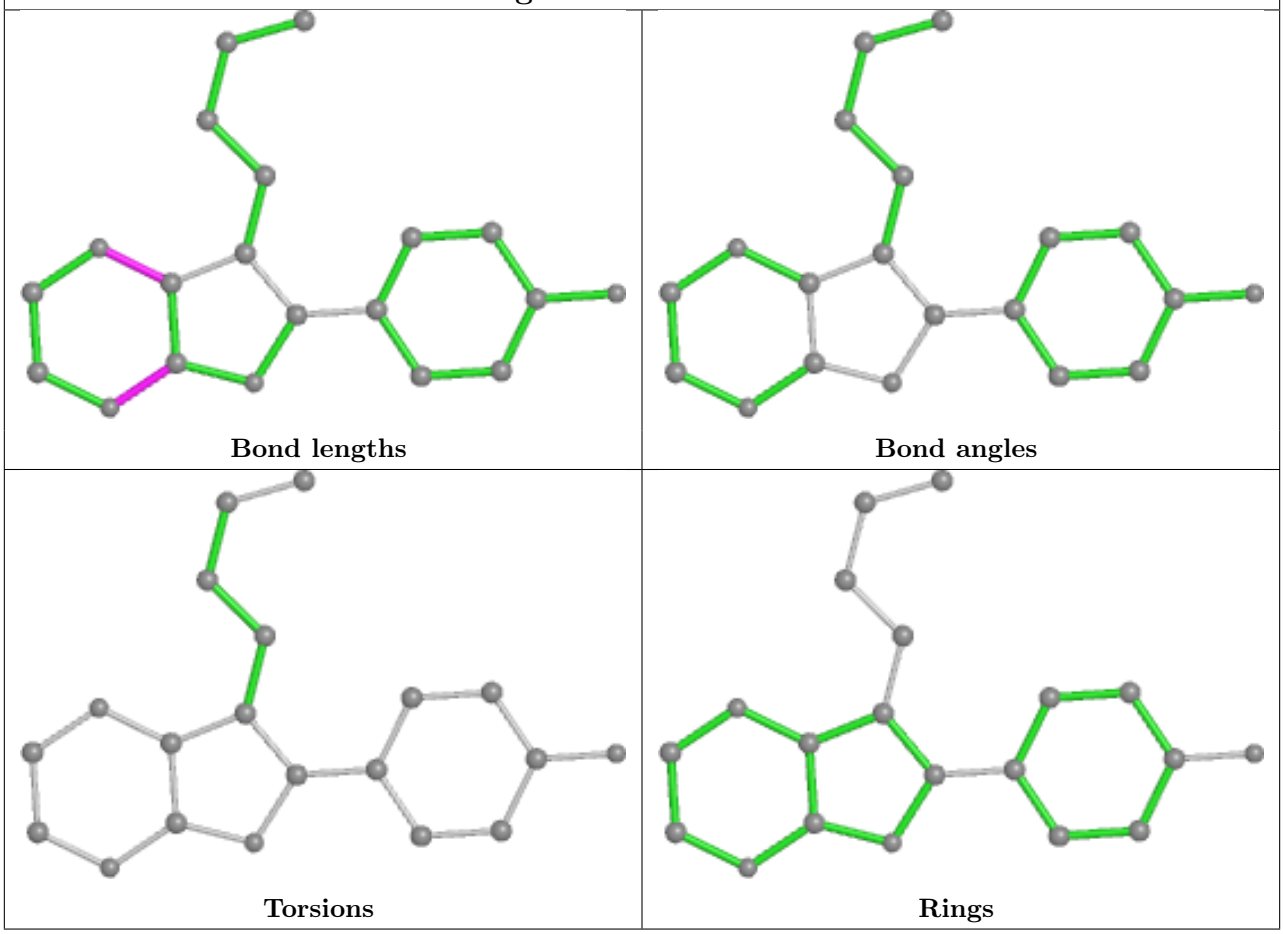


Torsions



Rings

Ligand ALH B 1288



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 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	288/292 (98%)	0.30	21 (7%) 15 20	14, 21, 38, 60	0
1	B	269/292 (92%)	0.52	29 (10%) 5 8	14, 24, 34, 41	0
2	D	150/208 (72%)	-0.05	5 (3%) 46 53	17, 21, 30, 33	0
2	E	148/208 (71%)	3.93	93 (62%) 0 0	16, 26, 30, 31	0
All	All	855/1000 (85%)	0.94	148 (17%) 1 1	14, 23, 34, 60	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	187	LEU	19.4
2	E	170	SER	13.5
2	E	151	LEU	13.0
2	E	168	HIS	11.1
2	E	186	LEU	11.1
2	E	160	CYS	11.0
2	E	171	PRO	10.9
2	E	293	SER	10.8
2	E	212	ILE	10.8
2	E	183	ARG	10.6
1	A	292	PRO	10.2
2	E	158	PHE	10.1
1	A	290	CYS	9.6
2	E	291	ASN	9.4
2	E	152	LEU	9.2
2	E	163	CYS	9.0
2	E	172	THR	8.9
2	E	156	GLY	8.8
2	E	211	VAL	8.7
2	E	149	SER	8.5
2	E	164	TYR	8.4

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Mol	Chain	Res	Type	RSRZ
2	E	294	GLY	8.3
2	E	166	LEU	8.3
2	E	148	THR	8.1
2	E	155	LEU	7.8
2	E	217	GLY	7.7
2	E	188	GLN	7.5
2	E	154	CYS	7.4
2	E	162	ARG	7.4
2	E	178	LEU	7.3
1	B	288	ASP	7.1
1	A	41	ASP	7.0
2	E	161	ARG	7.0
2	E	190	TRP	6.9
2	E	177	TRP	6.6
1	A	15	TYR	6.5
2	E	290	LYS	6.5
2	E	210	ASP	6.5
2	E	147	SER	6.4
1	B	2	GLN	6.3
2	E	174	PRO	6.3
2	E	169	LEU	6.3
2	E	153	ARG	6.2
2	E	292	GLU	5.9
2	E	167	LYS	5.8
1	B	43	GLY	5.5
2	E	175	VAL	5.5
2	E	215	GLU	5.5
1	A	291	PRO	5.4
2	E	159	LEU	5.2
2	E	165	ARG	5.2
2	E	220	HIS	5.1
1	B	44	VAL	5.1
2	E	173	ASP	5.1
1	B	245	THR	5.1
2	E	241	ILE	5.1
2	E	267	LEU	5.1
1	B	29	ILE	5.0
2	E	213	SER	5.0
1	A	136	ARG	4.7
1	B	136	ARG	4.7
2	E	150	GLU	4.6
1	B	73	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
2	E	214	SER	4.4
2	E	189	GLY	4.4
2	E	253	CYS	4.4
2	E	280	HIS	4.3
1	A	40	ASP	4.3
2	E	157	GLU	4.2
2	E	246	LYS	4.2
2	E	218	SER	4.1
2	E	281	TYR	4.0
2	E	216	VAL	4.0
2	E	263	SER	4.0
2	E	184	SER	4.0
2	E	288	ASP	3.9
2	E	249	LEU	3.9
1	B	4	TYR	3.8
2	E	205	TYR	3.7
2	E	209	ARG	3.7
1	B	9	LYS	3.7
1	B	156	ARG	3.7
2	E	179	ARG	3.7
1	B	154	PRO	3.6
2	E	194	GLY	3.6
1	B	244	ALA	3.5
2	E	286	PHE	3.5
2	E	289	LEU	3.5
2	E	287	SER	3.5
2	E	279	PRO	3.4
2	E	219	ASP	3.4
2	E	252	SER	3.4
2	E	196	ILE	3.3
1	A	160	ALA	3.3
2	E	247	PRO	3.3
1	A	154	PRO	3.2
2	E	180	SER	3.2
2	E	176	LEU	3.2
2	E	255	GLU	3.1
1	A	39	ASP	3.1
1	B	287	SER	3.1
1	A	161	GLU	3.1
1	A	1	MET	3.0
2	E	198	PRO	3.0
2	E	182	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	193	GLN	3.0
1	B	5	GLU	3.0
1	B	7	LEU	2.9
1	B	6	LYS	2.9
1	B	250	ASN	2.8
2	D	145	GLN	2.8
1	B	3	LYS	2.8
1	A	156	ARG	2.8
1	A	2	GLN	2.8
1	B	247	SER	2.8
1	B	137	ASN	2.8
2	E	251	GLU	2.8
1	A	288	ASP	2.8
1	B	17	THR	2.7
1	A	224	GLU	2.7
2	E	250	VAL	2.6
2	E	232	LEU	2.6
1	A	225	GLU	2.6
2	E	192	ASP	2.6
2	E	185	LEU	2.6
1	B	110	LEU	2.5
1	A	289	PHE	2.5
2	D	294	GLY	2.5
1	B	65	ARG	2.4
2	E	268	MET	2.4
1	B	32	LEU	2.4
2	E	242	SER	2.4
1	B	38	ASP	2.3
1	B	155	VAL	2.2
1	B	249	VAL	2.2
2	D	241	ILE	2.2
2	E	208	CYS	2.2
1	A	31	ALA	2.2
1	B	142	LEU	2.2
1	A	162	VAL	2.1
2	E	254	LYS	2.1
2	E	243	TYR	2.1
2	E	223	GLN	2.1
1	A	287	SER	2.1
2	D	252	SER	2.0
2	D	146	ALA	2.0
2	E	191	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	181	VAL	2.0

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

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

5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

5.4 Ligands (i)

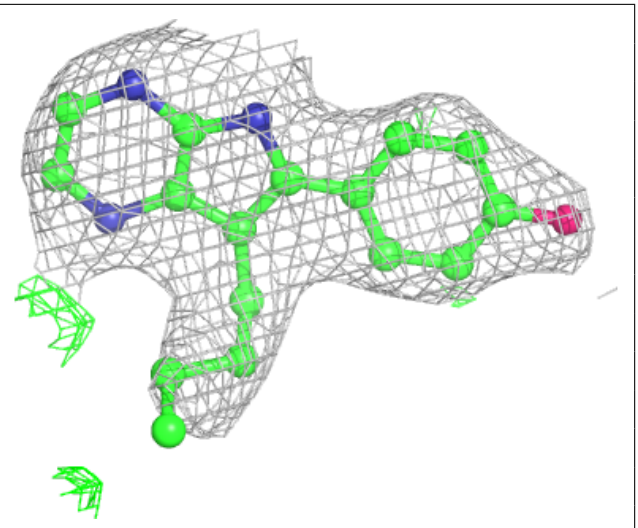
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

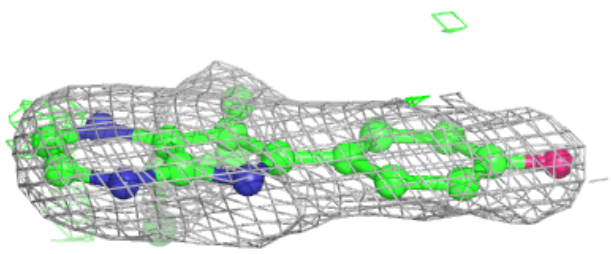
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ALH	B	1288	20/20	0.86	0.15	22,26,31,32	0
3	ALH	A	1293	20/20	0.94	0.14	18,23,29,34	0

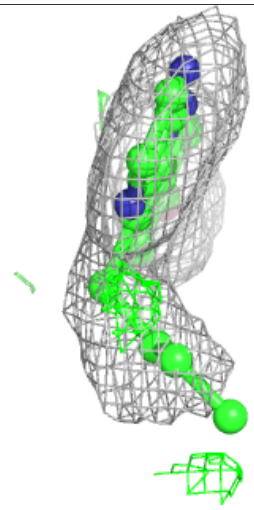
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ALH B 1288:

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

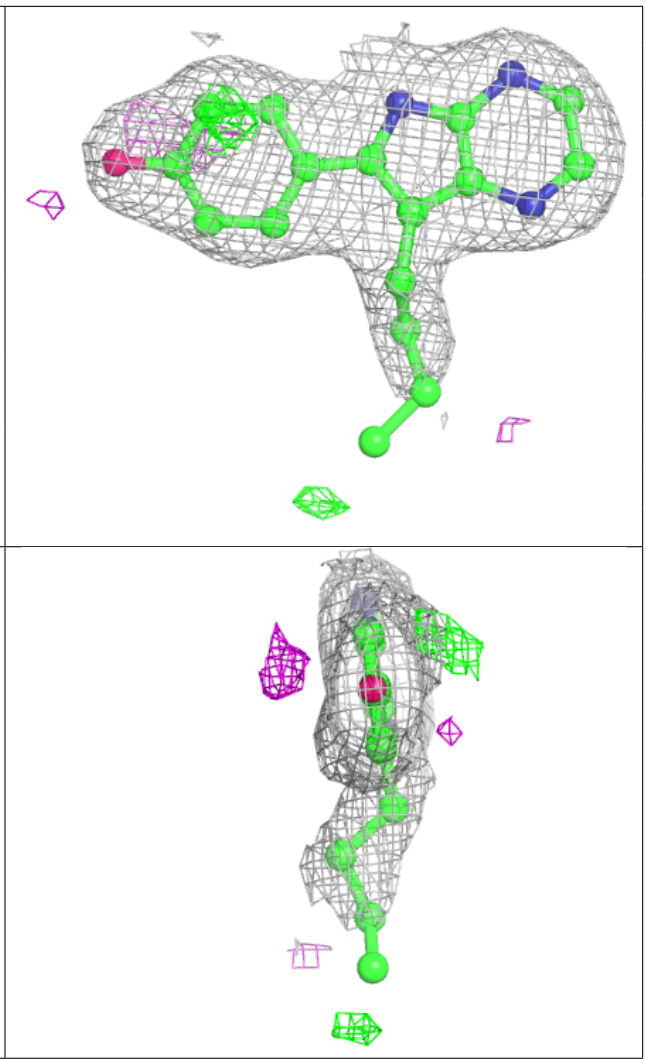






Electron density around ALH A 1293:

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



5.5 Other polymers (i)

There are no such residues in this entry.