



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:05 PM UTC

PDB ID : 1VKG / pdb_00001vkg
Title : Crystal Structure of Human HDAC8 complexed with CRA-19156
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Wynands, R.; Leahy, E.M.; Dougan, D.R.; Snell, G.; Navre, M.; Knuth, M.W.;
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Deposited on : 2004-05-13
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 ⓘ 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

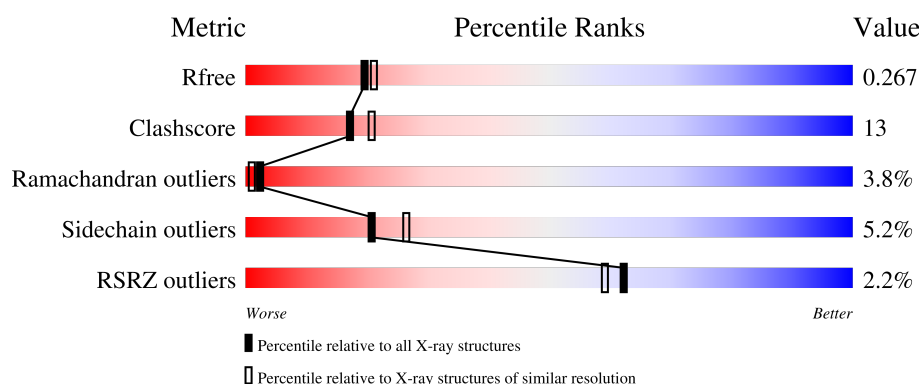
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	377	2% 48% 34% 9% • 8%
1	B	377	2% 54% 30% 8% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11640 atoms, of which 5898 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 Histone deacetylase 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	348	Total	C	H	N	O	S	0	3	0
			5401	1742	2684	454	503	18			
1	B	348	Total	C	H	N	O	S	0	0	0
			5397	1740	2682	454	503	18			

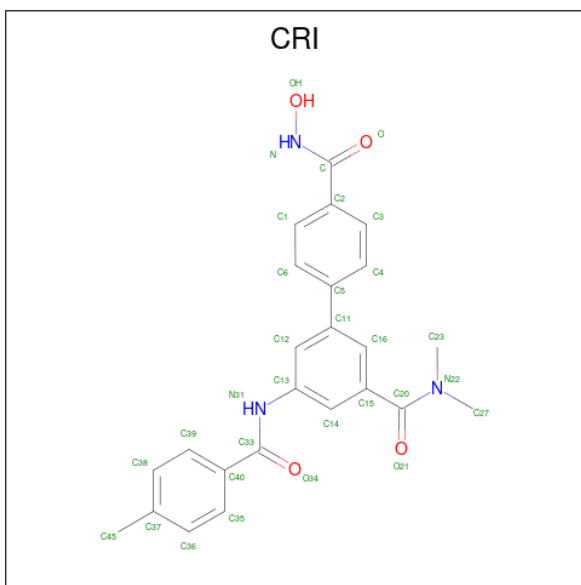
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is 5-(4-METHYL-BENZOYLAMINO)-BIPHENYL-3,4'-DICARBOXYLIC ACID 3-DIMETHYLAMIDE-4'-HYDROXYAMIDE (CCD ID: CRI) (formula: C₂₄H₂₃N₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 24	H 22	N 3	O 4	0	0
4	B	1	Total 53	C 24	H 22	N 3	O 4	0	0

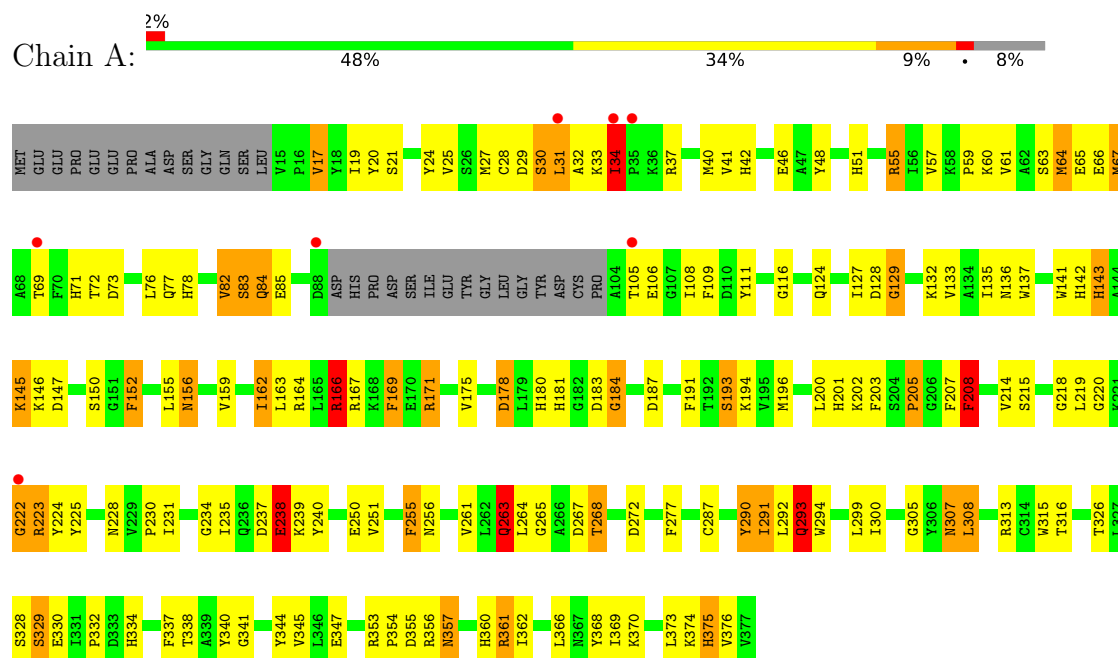
- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	129	Total 387	H 258	O 129	0	0
5	B	115	Total 345	H 230	O 115	0	0

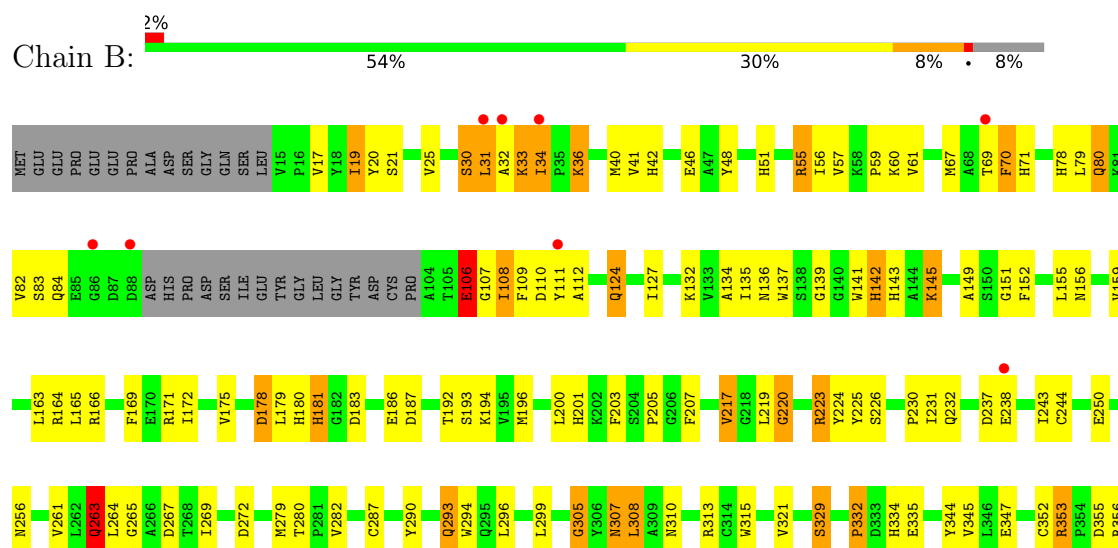
3 Residue-property plots

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: Histone deacetylase 8



• Molecule 1: Histone deacetylase 8



N357	
H360	
R361	
I365	
L366	
N367	
Y368	
I369	
K370	
G371	
N372	
L373	
K374	
H375	
V376	
V377	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.63Å 92.71Å 98.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20 7.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.5 (7.00-2.20) 93.0 (7.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.65 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.851, X-PLOR 3.851	Depositor
R, R_{free}	0.237 , 0.304 0.256 , 0.267	Depositor DCC
R_{free} test set	1872 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 117.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11640	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ZN, CRI

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	1.90	33/2807 (1.2%)	1.81	66/3802 (1.7%)
1	B	1.94	37/2780 (1.3%)	1.86	63/3767 (1.7%)
All	All	1.92	70/5587 (1.3%)	1.83	129/7569 (1.7%)

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	11
1	B	0	7
All	All	0	18

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	19	ILE	CA-CB	8.73	1.63	1.53
1	A	78	HIS	CG-ND1	-8.62	1.28	1.38
1	B	34	ILE	CA-CB	8.55	1.62	1.53
1	B	143	HIS	CG-ND1	-8.36	1.29	1.38
1	A	143	HIS	CG-ND1	-8.29	1.29	1.38
1	B	78	HIS	CG-ND1	-8.24	1.29	1.38
1	B	282	VAL	CA-CB	8.23	1.65	1.54
1	A	375	HIS	CG-ND1	-8.06	1.29	1.38
1	A	42	HIS	CG-ND1	-7.76	1.29	1.38
1	B	71	HIS	CG-ND1	-7.75	1.29	1.38
1	B	201	HIS	CG-ND1	-7.60	1.29	1.38
1	A	201	HIS	CG-ND1	-7.58	1.29	1.38
1	B	375	HIS	CG-ND1	-7.57	1.29	1.38
1	B	42	HIS	CG-ND1	-7.42	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	360	HIS	CG-ND1	-7.41	1.30	1.38
1	A	334	HIS	CG-ND1	-7.40	1.30	1.38
1	B	360	HIS	CG-ND1	-7.34	1.30	1.38
1	A	51	HIS	CG-ND1	-7.31	1.30	1.38
1	B	181	HIS	CG-ND1	-7.30	1.30	1.38
1	A	181	HIS	CG-ND1	-7.24	1.30	1.38
1	A	71	HIS	CG-ND1	-7.21	1.30	1.38
1	B	139	GLY	N-CA	7.19	1.50	1.44
1	A	41	VAL	CA-CB	7.14	1.62	1.54
1	B	51	HIS	CG-ND1	-6.96	1.30	1.38
1	B	334	HIS	CG-ND1	-6.90	1.30	1.38
1	A	180	HIS	CD2-NE2	-6.84	1.30	1.37
1	B	180	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	142	HIS	CD2-NE2	-6.43	1.30	1.37
1	B	142	HIS	CG-ND1	-6.25	1.31	1.38
1	B	142	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	51	HIS	CD2-NE2	-6.12	1.31	1.37
1	B	238	GLU	CD-OE2	5.98	1.36	1.25
1	A	238	GLU	CD-OE2	5.94	1.36	1.25
1	A	162	ILE	CA-CB	5.88	1.60	1.54
1	A	181	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	208	PHE	CA-CB	5.85	1.62	1.53
1	A	142	HIS	CG-ND1	-5.82	1.31	1.38
1	B	201	HIS	CA-CB	5.74	1.62	1.53
1	B	51	HIS	CD2-NE2	-5.70	1.31	1.37
1	A	142	HIS	CB-CG	5.67	1.58	1.50
1	B	181	HIS	CD2-NE2	-5.66	1.31	1.37
1	A	34	ILE	CA-CB	5.53	1.61	1.54
1	A	334	HIS	CD2-NE2	-5.49	1.31	1.37
1	A	201	HIS	CD2-NE2	-5.49	1.31	1.37
1	A	105	THR	CA-CB	5.49	1.62	1.53
1	A	30	SER	CA-C	5.48	1.55	1.52
1	B	334	HIS	CD2-NE2	-5.48	1.31	1.37
1	A	360	HIS	CD2-NE2	-5.41	1.31	1.37
1	B	41	VAL	CA-CB	5.39	1.60	1.54
1	A	78	HIS	CD2-NE2	-5.35	1.31	1.37
1	A	71	HIS	CD2-NE2	-5.31	1.32	1.37
1	B	108	ILE	N-CA	5.27	1.52	1.46
1	B	375	HIS	CD2-NE2	-5.26	1.32	1.37
1	B	34	ILE	CA-C	5.24	1.57	1.53
1	B	135	ILE	CA-CB	5.23	1.61	1.54
1	B	142	HIS	CB-CG	5.23	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	TRP	CG-CD2	-5.21	1.34	1.43
1	A	375	HIS	CD2-NE2	-5.21	1.32	1.37
1	B	143	HIS	CD2-NE2	-5.21	1.32	1.37
1	B	78	HIS	CD2-NE2	-5.19	1.32	1.37
1	A	178	ASP	N-CA	5.14	1.52	1.45
1	B	71	HIS	CD2-NE2	-5.13	1.32	1.37
1	A	34	ILE	CA-C	5.12	1.58	1.52
1	A	362	ILE	CA-CB	5.12	1.60	1.54
1	B	139	GLY	CA-C	5.12	1.57	1.52
1	B	201	HIS	CD2-NE2	-5.10	1.32	1.37
1	B	360	HIS	CD2-NE2	-5.07	1.32	1.37
1	B	296	LEU	N-CA	5.06	1.51	1.45
1	A	353	ARG	CA-C	5.06	1.57	1.52
1	B	36	LYS	N-CA	5.00	1.52	1.46

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	SER	N-CA-C	11.38	128.30	111.34
1	B	357	ASN	CA-CB-CG	-10.43	102.17	112.60
1	A	200	LEU	N-CA-C	-10.21	92.63	109.07
1	B	78	HIS	CA-CB-CG	-9.60	104.20	113.80
1	A	61	VAL	N-CA-C	-9.51	94.85	108.17
1	A	30	SER	N-CA-C	8.95	123.25	108.48
1	B	200	LEU	N-CA-C	-8.40	95.55	109.07
1	A	42	HIS	CA-CB-CG	-8.20	105.60	113.80
1	B	223	ARG	N-CA-C	-8.06	98.35	110.28
1	A	261	VAL	N-CA-C	-7.92	96.05	107.77
1	B	106	GLU	N-CA-C	-7.88	98.80	110.46
1	A	29	ASP	N-CA-C	-7.87	101.72	112.03
1	B	374	LYS	N-CA-C	-7.86	103.30	113.12
1	B	261	VAL	N-CA-C	-7.82	96.19	107.77
1	B	61	VAL	N-CA-C	-7.77	97.20	109.17
1	A	132	LYS	N-CA-C	-7.61	102.20	113.61
1	A	299	LEU	N-CA-C	-7.59	96.85	109.07
1	B	307	ASN	N-CA-C	-7.47	91.91	107.37
1	B	60	LYS	N-CA-C	-7.41	98.48	109.81
1	A	78	HIS	CA-CB-CG	-7.28	106.52	113.80
1	B	329	SER	N-CA-C	-7.22	103.45	111.82
1	A	256	ASN	CA-CB-CG	-7.19	105.41	112.60
1	A	300	ILE	N-CA-CB	-7.18	102.42	111.46
1	A	272	ASP	CA-CB-CG	-7.17	105.43	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	ARG	N-CA-C	-6.97	97.36	108.73
1	B	55	ARG	N-CA-C	-6.95	97.89	109.07
1	A	357	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	A	326	THR	N-CA-C	-6.83	98.11	109.24
1	B	36	LYS	N-CA-C	6.78	125.24	110.80
1	A	29	ASP	CA-CB-CG	6.77	119.37	112.60
1	B	299	LEU	N-CA-C	-6.76	97.87	108.90
1	B	42	HIS	CA-CB-CG	-6.68	107.12	113.80
1	A	228	ASN	CA-CB-CG	-6.68	105.92	112.60
1	B	243	ILE	N-CA-C	-6.68	104.14	110.42
1	B	156	ASN	CA-CB-CG	-6.67	105.93	112.60
1	B	367	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	A	355	ASP	N-CA-C	-6.64	97.90	108.73
1	B	193	SER	N-CA-C	-6.63	104.50	112.59
1	B	267	ASP	CA-CB-CG	6.50	119.10	112.60
1	B	321	VAL	N-CA-C	-6.50	104.19	110.42
1	B	207	PHE	CA-CB-CG	-6.41	107.39	113.80
1	B	256	ASN	CA-CB-CG	-6.40	106.20	112.60
1	B	186	GLU	N-CA-C	-6.37	103.02	111.24
1	B	217	VAL	N-CA-C	6.36	118.21	112.17
1	B	124	GLN	OE1-CD-NE2	-6.35	116.25	122.60
1	A	169	PHE	CA-CB-CG	-6.25	107.55	113.80
1	A	316	THR	N-CA-C	-6.24	104.55	111.36
1	B	46	GLU	N-CA-C	-6.23	104.41	111.07
1	B	141	TRP	NE1-CE2-CZ2	6.17	139.36	130.10
1	B	367	ASN	CA-CB-CG	-6.15	106.45	112.60
1	B	149	ALA	N-CA-C	-6.14	101.43	110.52
1	A	287	CYS	N-CA-C	-6.09	104.72	111.36
1	A	293	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	A	268	THR	CA-CB-OG1	-6.02	100.56	109.60
1	B	308	LEU	N-CA-C	5.99	118.33	111.02
1	A	67	MET	N-CA-C	-5.99	104.84	111.36
1	A	136	ASN	CA-CB-CG	-5.96	106.64	112.60
1	A	202	LYS	N-CA-C	-5.94	99.99	109.96
1	A	137	TRP	NE1-CE2-CZ2	5.93	139.00	130.10
1	B	80	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	A	156	ASN	CA-CB-CG	-5.84	106.76	112.60
1	A	337	PHE	N-CA-C	5.84	118.11	111.11
1	B	294	TRP	NE1-CE2-CZ2	5.79	138.79	130.10
1	B	287	CYS	N-CA-C	-5.78	103.97	111.02
1	A	330	GLU	N-CA-C	-5.77	99.32	108.73
1	A	57	VAL	N-CA-C	-5.76	99.48	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	TRP	NE1-CE2-CZ2	5.75	138.73	130.10
1	B	226	SER	N-CA-C	-5.75	99.03	108.41
1	A	124	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	A	60	LYS	N-CA-C	-5.71	101.75	110.14
1	B	181	HIS	CE1-NE2-CD2	-5.68	103.32	109.00
1	A	137	TRP	CG-CD1-NE1	-5.64	102.86	110.20
1	A	141	TRP	NE1-CE2-CZ2	5.63	138.55	130.10
1	A	237	ASP	CA-CB-CG	-5.60	107.00	112.60
1	A	374	LYS	N-CA-C	-5.59	106.16	112.87
1	A	291	ILE	N-CA-C	-5.58	105.66	110.74
1	B	71	HIS	CE1-NE2-CD2	-5.58	103.42	109.00
1	A	193	SER	N-CA-C	-5.51	105.17	112.94
1	A	328	SER	N-CA-C	-5.50	103.27	110.53
1	A	48	TYR	N-CA-C	-5.50	106.16	112.92
1	A	152	PHE	CA-CB-CG	-5.47	108.33	113.80
1	A	51	HIS	CE1-NE2-CD2	-5.46	103.54	109.00
1	A	82	VAL	N-CA-CB	-5.44	104.18	110.55
1	A	329	SER	N-CA-C	-5.42	105.88	112.88
1	A	207	PHE	CA-CB-CG	-5.41	108.39	113.80
1	B	141	TRP	CG-CD1-NE1	-5.39	103.19	110.20
1	B	305	GLY	N-CA-C	-5.39	100.41	113.18
1	A	17	VAL	N-CA-C	-5.37	100.75	108.48
1	B	175	VAL	N-CA-C	-5.37	100.75	108.53
1	B	263	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	A	135	ILE	N-CA-C	5.35	116.19	108.48
1	B	70	PHE	CA-CB-CG	-5.33	108.47	113.80
1	B	294	TRP	CG-CD1-NE1	-5.33	103.27	110.20
1	A	255	PHE	CA-CB-CG	-5.33	108.47	113.80
1	B	280	THR	N-CA-C	-5.32	99.83	109.09
1	B	180	HIS	ND1-CG-CD2	5.30	111.40	106.10
1	B	335	GLU	N-CA-C	5.28	119.21	112.34
1	B	143	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
1	A	175	VAL	N-CA-C	-5.27	100.89	108.48
1	A	78	HIS	CE1-NE2-CD2	-5.26	103.74	109.00
1	A	178	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	375	HIS	CE1-NE2-CD2	-5.26	103.74	109.00
1	B	56	ILE	N-CA-C	-5.22	100.89	108.36
1	A	64	MET	N-CA-C	-5.21	104.85	111.11
1	B	132	LYS	N-CA-C	-5.21	107.30	113.97
1	A	116	GLY	N-CA-C	-5.20	106.35	112.64
1	A	294	TRP	NE1-CE2-CZ2	5.20	137.90	130.10
1	A	178	ASP	N-CA-C	-5.18	103.69	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	ASN	CA-CB-CG	-5.17	107.43	112.60
1	B	34	ILE	N-CA-C	-5.17	102.43	107.55
1	A	136	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	B	181	HIS	CB-CG-ND1	5.14	130.41	122.70
1	B	137	TRP	CG-CD1-NE1	-5.13	103.53	110.20
1	B	134	ALA	N-CA-C	-5.13	100.09	108.76
1	B	137	TRP	NE1-CE2-CZ2	5.13	137.79	130.10
1	A	46	GLU	N-CA-C	-5.12	105.61	111.14
1	A	369	ILE	N-CA-CB	-5.11	105.25	110.62
1	B	79	LEU	N-CA-C	-5.10	105.61	111.07
1	B	315	TRP	NE1-CE2-CZ2	5.09	137.74	130.10
1	B	372	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	B	244	CYS	CA-CB-SG	5.08	126.09	114.40
1	A	187	ASP	CA-CB-CG	-5.08	107.52	112.60
1	A	294	TRP	CG-CD1-NE1	-5.08	103.60	110.20
1	A	263	GLN	N-CA-C	-5.07	100.90	109.07
1	B	357	ASN	O-C-N	5.06	128.27	122.55
1	A	290	TYR	CA-CB-CG	-5.06	104.80	113.90
1	A	222	GLY	N-CA-C	-5.05	101.22	113.18
1	B	355	ASP	N-CA-C	-5.03	101.51	109.76
1	A	77	GLN	OE1-CD-NE2	-5.00	117.60	122.60

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	ARG	Sidechain
1	A	166	ARG	Sidechain
1	A	167	ARG	Sidechain
1	A	171	ARG	Sidechain
1	A	208	PHE	Peptide
1	A	223	ARG	Sidechain
1	A	313	ARG	Sidechain
1	A	356	ARG	Sidechain
1	A	361	ARG	Sidechain
1	A	37	ARG	Sidechain
1	A	55	ARG	Sidechain
1	B	171	ARG	Sidechain
1	B	223	ARG	Sidechain
1	B	313	ARG	Sidechain
1	B	353	ARG	Sidechain
1	B	356	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	361	ARG	Sidechain
1	B	55	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2717	2684	2656	82	1
1	B	2715	2682	2679	58	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	22	23	1	0
4	B	31	22	22	0	0
5	A	129	258	0	1	0
5	B	115	230	0	0	1
All	All	5742	5898	5380	132	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 13.

All (132) 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:33:LYS:CB	1:B:33:LYS:HG3	1.66	1.24
1:A:33:LYS:HB3	1:B:33:LYS:CG	1.70	1.20
1:A:33:LYS:HB3	1:B:33:LYS:HG3	0.88	0.86
1:A:69:THR:HG22	1:A:163:LEU:HD13	1.61	0.83
1:A:263:GLN:HE21	1:A:263:GLN:C	1.95	0.74
1:B:366:LEU:O	1:B:370:LYS:HG3	1.90	0.71
1:A:178:ASP:HB2	1:A:263:GLN:HE22	1.57	0.69
1:A:193:SER:HB2	1:A:225:TYR:CE2	2.31	0.65
1:B:194:LYS:HA	1:B:194:LYS:HE2	1.77	0.65
1:A:33:LYS:HB3	1:B:33:LYS:CB	2.26	0.65
1:A:194:LYS:HE3	5:A:471:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:GLN:NE2	1:B:164:ARG:HE	1.96	0.62
1:A:366:LEU:O	1:A:370[A]:LYS:HG3	1.99	0.61
1:A:366:LEU:O	1:A:370[B]:LYS:HG3	1.99	0.60
1:A:64:MET:SD	1:A:76:LEU:HB3	2.42	0.59
1:B:112:ALA:HB1	1:B:155:LEU:HB2	1.85	0.57
1:A:145:LYS:HZ3	1:A:145:LYS:HA	1.69	0.57
1:B:31:LEU:HG	1:B:111:TYR:CD2	2.40	0.56
1:A:31:LEU:O	1:A:33:LYS:N	2.39	0.56
1:B:70:PHE:CD1	1:B:159:VAL:HG11	2.41	0.55
1:B:69:THR:HG22	1:B:163:LEU:HD13	1.89	0.55
1:A:30:SER:N	1:A:34:ILE:HG21	2.22	0.54
1:A:329:SER:O	1:A:345:VAL:HA	2.06	0.54
1:B:31:LEU:O	1:B:33:LYS:N	2.41	0.53
1:A:145:LYS:CE	1:A:184:GLY:HA2	2.38	0.53
1:A:290:TYR:O	1:A:293:GLN:HG3	2.07	0.53
1:B:203:PHE:CB	1:B:230:PRO:HB3	2.40	0.52
1:A:203:PHE:HB3	1:A:230:PRO:HB3	1.91	0.51
1:B:263:GLN:C	1:B:263:GLN:HE21	2.18	0.51
1:A:20:TYR:CD1	1:A:21:SER:N	2.79	0.51
1:A:203:PHE:CB	1:A:230:PRO:HB3	2.41	0.51
1:B:106:GLU:N	1:B:106:GLU:CD	2.69	0.51
1:B:178:ASP:HB2	1:B:263:GLN:OE1	2.11	0.51
1:A:293:GLN:C	1:A:293:GLN:HE21	2.18	0.50
1:A:250:GLU:HG3	1:A:370[A]:LYS:HG2	1.94	0.50
1:A:250:GLU:HG3	1:A:370[B]:LYS:HG2	1.94	0.50
1:A:143:HIS:O	1:A:150:SER:HB3	2.12	0.50
1:A:191:PHE:CE2	1:A:219:LEU:HB2	2.47	0.50
1:A:225:TYR:CE2	1:A:376:VAL:HG13	2.46	0.49
1:B:106:GLU:CD	1:B:106:GLU:H	2.21	0.49
1:A:145:LYS:HA	1:A:145:LYS:NZ	2.27	0.49
1:B:69:THR:HG22	1:B:163:LEU:CD1	2.43	0.49
1:B:107:GLY:O	1:B:110:ASP:N	2.46	0.49
1:B:290:TYR:O	1:B:293:GLN:HG3	2.13	0.49
1:B:290:TYR:O	1:B:293:GLN:CG	2.61	0.48
1:A:31:LEU:HG	1:A:111:TYR:CD2	2.49	0.48
1:B:181:HIS:CD2	1:B:183:ASP:HB3	2.49	0.48
1:A:263:GLN:NE2	1:A:265:GLY:H	2.12	0.48
1:B:17:VAL:HG13	1:B:57:VAL:CG2	2.43	0.48
1:B:48:TYR:CE2	1:B:332:PRO:HD2	2.48	0.48
1:A:178:ASP:HB2	1:A:263:GLN:NE2	2.27	0.48
1:A:205:PRO:O	1:B:353:ARG:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LYS:NZ	1:B:33:LYS:HB3	2.29	0.47
1:A:307:ASN:O	1:A:308:LEU:C	2.57	0.47
1:A:208:PHE:CE1	4:A:402:CRI:H26	2.50	0.47
1:A:347:GLU:H	1:A:347:GLU:CD	2.21	0.47
1:B:67:MET:HE1	1:B:109:PHE:CZ	2.49	0.47
1:A:65:GLU:HG3	1:A:66:GLU:N	2.30	0.47
1:A:225:TYR:CZ	1:A:376:VAL:HG13	2.50	0.47
1:A:196:MET:SD	1:A:251:VAL:HG13	2.55	0.47
1:B:30:SER:O	1:B:31:LEU:C	2.58	0.47
1:A:33:LYS:HB2	1:B:33:LYS:HG3	1.81	0.46
1:A:205:PRO:HG2	1:B:352:CYS:O	2.16	0.46
1:A:84:GLN:HG2	1:A:85:GLU:H	1.81	0.46
1:A:193:SER:HB2	1:A:225:TYR:CZ	2.50	0.46
1:A:223:ARG:HG2	1:A:224:TYR:CE1	2.51	0.46
1:B:127:ILE:HD11	1:B:165:LEU:HA	1.97	0.46
1:B:124:GLN:NE2	1:B:164:ARG:HH21	2.14	0.46
1:B:196:MET:HE2	1:B:225:TYR:HA	1.96	0.45
1:A:341:GLY:HA2	1:A:344:TYR:CE1	2.51	0.45
1:B:264:LEU:O	1:B:265:GLY:C	2.59	0.45
1:A:83:SER:O	1:A:106:GLU:HA	2.16	0.45
1:B:361:ARG:HE	1:B:365:ILE:HD11	1.81	0.45
1:B:367:ASN:O	1:B:368:TYR:C	2.58	0.45
1:B:40:MET:SD	1:B:308:LEU:HB3	2.55	0.45
1:B:375:HIS:CD2	1:B:375:HIS:N	2.84	0.45
1:A:231:ILE:CG2	1:A:357:ASN:HD21	2.28	0.45
1:B:263:GLN:C	1:B:263:GLN:NE2	2.75	0.45
1:A:24:TYR:CE1	1:A:28:CYS:SG	3.10	0.45
1:A:205:PRO:O	1:B:353:ARG:CD	2.65	0.45
1:A:218:GLY:HA3	1:A:222:GLY:O	2.17	0.45
1:A:40:MET:HE2	1:A:40:MET:HB3	1.89	0.45
1:A:128:ASP:O	1:A:129:GLY:C	2.60	0.45
1:B:225:TYR:CZ	1:B:376:VAL:HG13	2.52	0.45
1:A:162:ILE:O	1:A:163:LEU:C	2.57	0.44
1:A:166:ARG:HA	1:A:169:PHE:O	2.17	0.44
1:A:146:LYS:HG3	1:A:147:ASP:N	2.32	0.44
1:A:82:VAL:O	1:A:84:GLN:N	2.50	0.44
1:A:19:ILE:CG2	1:A:59:PRO:HB3	2.48	0.44
1:A:183:ASP:O	1:A:184:GLY:C	2.61	0.44
1:A:340:TYR:CD1	1:A:340:TYR:N	2.86	0.44
1:B:48:TYR:CZ	1:B:332:PRO:HD3	2.53	0.44
1:B:329:SER:O	1:B:345:VAL:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:TYR:CG	1:A:21:SER:N	2.86	0.43
1:A:235:ILE:HD11	1:A:240:TYR:HA	2.00	0.43
1:A:20:TYR:CE1	1:A:25:VAL:HG21	2.53	0.43
1:A:64:MET:HA	1:A:67:MET:HE3	2.01	0.43
1:A:214:VAL:HG22	1:A:368:TYR:CD2	2.53	0.43
1:B:20:TYR:CE1	1:B:25:VAL:HG21	2.54	0.43
1:A:72:THR:O	1:A:73:ASP:C	2.61	0.42
1:A:163:LEU:O	1:A:166:ARG:HB2	2.19	0.42
1:A:291:ILE:O	1:A:292:LEU:C	2.62	0.42
1:B:80:GLN:HA	1:B:109:PHE:CG	2.54	0.42
1:A:24:TYR:O	1:A:27:MET:HB3	2.20	0.42
1:A:171:ARG:HD2	1:A:255:PHE:O	2.19	0.42
1:B:352:CYS:O	1:B:352:CYS:SG	2.77	0.42
1:A:127:ILE:HD13	1:A:169:PHE:CE1	2.55	0.42
1:A:67:MET:HE1	1:A:109:PHE:CZ	2.55	0.41
1:A:373:LEU:C	1:A:375:HIS:N	2.76	0.41
1:B:269:ILE:HA	1:B:279:MET:O	2.20	0.41
1:A:223:ARG:HG2	1:A:224:TYR:CD1	2.55	0.41
1:B:145:LYS:HZ2	1:B:145:LYS:HB3	1.84	0.41
1:A:156:ASN:CG	1:A:159:VAL:HG23	2.46	0.41
1:A:231:ILE:HG22	1:A:357:ASN:HD21	1.86	0.41
1:A:234:GLY:HA3	1:A:354:PRO:O	2.20	0.41
1:B:372:ASN:C	1:B:374:LYS:H	2.29	0.41
1:A:264:LEU:O	1:A:265:GLY:C	2.62	0.41
1:B:217:VAL:O	1:B:224:TYR:N	2.50	0.41
1:A:145:LYS:NZ	1:A:184:GLY:HA2	2.35	0.41
1:B:82:VAL:C	1:B:84:GLN:N	2.79	0.41
1:B:151:GLY:O	1:B:152:PHE:HB2	2.21	0.41
1:B:219:LEU:O	1:B:220:GLY:C	2.64	0.41
1:B:347:GLU:N	1:B:347:GLU:CD	2.79	0.41
1:B:250:GLU:HG3	1:B:370:LYS:HG2	2.03	0.41
1:A:63:SER:O	1:A:64:MET:C	2.64	0.40
1:B:169:PHE:HB2	1:B:172:ILE:HD11	2.03	0.40
1:A:178:ASP:CB	1:A:263:GLN:HE22	2.29	0.40
1:A:268:THR:HA	1:A:277:PHE:HB2	2.04	0.40
1:B:19:ILE:CG2	1:B:59:PRO:HB3	2.51	0.40
1:B:232:GLN:HE21	1:B:232:GLN:HA	1.87	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)
1:A:376:VAL:O	5:B:472:HOH:H1[2_564]	1.50	0.10

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	347/377 (92%)	292 (84%)	43 (12%)	12 (4%)	3	1
1	B	344/377 (91%)	295 (86%)	35 (10%)	14 (4%)	2	1
All	All	691/754 (92%)	587 (85%)	78 (11%)	26 (4%)	2	1

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	ALA
1	A	83	SER
1	B	31	LEU
1	B	32	ALA
1	B	36	LYS
1	B	237	ASP
1	B	272	ASP
1	B	344	TYR
1	A	31	LEU
1	A	108	ILE
1	A	129	GLY
1	A	220	GLY
1	B	108	ILE
1	B	179	LEU
1	A	308	LEU
1	B	142	HIS
1	A	152	PHE
1	A	305	GLY
1	A	205	PRO
1	B	83	SER

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Mol	Chain	Res	Type
1	B	205	PRO
1	B	220	GLY
1	B	332	PRO
1	B	305	GLY
1	A	332	PRO
1	A	184	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/316 (93%)	277 (94%)	17 (6%)	18	22
1	B	291/316 (92%)	277 (95%)	14 (5%)	23	30
All	All	585/632 (93%)	554 (95%)	31 (5%)	21	26

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	34	ILE
1	A	84	GLN
1	A	133	VAL
1	A	145	LYS
1	A	155	LEU
1	A	166	ARG
1	A	215	SER
1	A	238	GLU
1	A	239[A]	LYS
1	A	239[B]	LYS
1	A	263	GLN
1	A	267	ASP
1	A	293	GLN
1	A	307	ASN
1	A	338	THR
1	A	361	ARG

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Mol	Chain	Res	Type
1	B	21	SER
1	B	33	LYS
1	B	34	ILE
1	B	106	GLU
1	B	145	LYS
1	B	166	ARG
1	B	178	ASP
1	B	187	ASP
1	B	192	THR
1	B	231	ILE
1	B	263	GLN
1	B	293	GLN
1	B	307	ASN
1	B	310	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	80	GLN
1	A	124	GLN
1	A	181	HIS
1	A	256	ASN
1	A	263	GLN
1	A	293	GLN
1	A	307	ASN
1	A	310	ASN
1	A	357	ASN
1	A	372	ASN
1	B	53	GLN
1	B	84	GLN
1	B	124	GLN
1	B	181	HIS
1	B	201	HIS
1	B	232	GLN
1	B	256	ASN
1	B	293	GLN
1	B	310	ASN
1	B	375	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CRI	A	402	2	33,33,33	2.31	6 (18%)	46,46,46	1.10	6 (13%)
4	CRI	B	402	2	33,33,33	2.21	6 (18%)	46,46,46	1.14	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CRI	A	402	2	-	4/26/26/26	0/3/3/3
4	CRI	B	402	2	-	6/26/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	402	CRI	C15-C20	-6.95	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	CRI	C15-C20	-5.73	1.40	1.50
4	B	402	CRI	C-N	5.57	1.39	1.32
4	A	402	CRI	C-N	5.35	1.39	1.32
4	A	402	CRI	C2-C	-5.13	1.38	1.50
4	A	402	CRI	C13-N31	-4.71	1.32	1.41
4	B	402	CRI	C40-C33	-4.60	1.40	1.50
4	B	402	CRI	C11-C5	-4.44	1.38	1.49
4	A	402	CRI	C11-C5	-4.43	1.38	1.49
4	A	402	CRI	C40-C33	-4.26	1.40	1.50
4	B	402	CRI	C13-N31	-4.24	1.33	1.41
4	B	402	CRI	C2-C	-4.20	1.41	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	CRI	C2-C-N	3.29	121.34	116.26
4	B	402	CRI	O-C-N	-2.85	117.65	122.90
4	B	402	CRI	C13-N31-C33	-2.67	119.58	126.61
4	A	402	CRI	C13-N31-C33	-2.58	119.81	126.61
4	A	402	CRI	C2-C-N	2.29	119.80	116.26
4	A	402	CRI	O21-C20-C15	-2.25	115.84	120.29
4	A	402	CRI	O-C-N	-2.12	119.00	122.90
4	B	402	CRI	C3-C2-C1	-2.03	115.98	118.57
4	A	402	CRI	C11-C16-C15	2.03	123.21	121.04
4	A	402	CRI	C14-C15-C20	2.02	124.61	120.13

There are no chirality outliers.

All (10) torsion outliers are listed below:

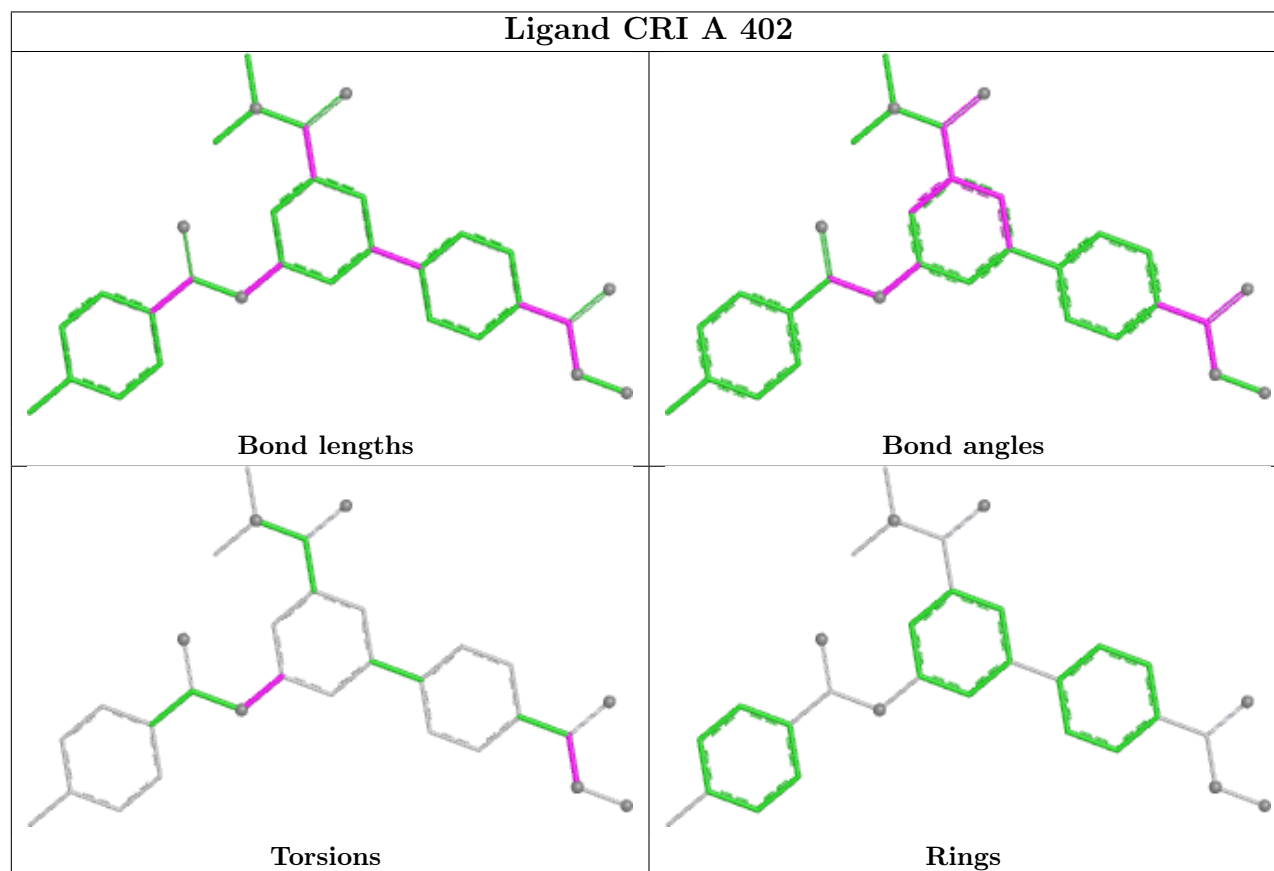
Mol	Chain	Res	Type	Atoms
4	A	402	CRI	O-C-N-OH
4	A	402	CRI	C2-C-N-OH
4	A	402	CRI	C14-C13-N31-C33
4	A	402	CRI	C12-C13-N31-C33
4	B	402	CRI	C14-C13-N31-C33
4	B	402	CRI	C12-C13-N31-C33
4	B	402	CRI	C16-C11-C5-C4
4	B	402	CRI	C12-C11-C5-C4
4	B	402	CRI	C12-C11-C5-C6
4	B	402	CRI	C16-C11-C5-C6

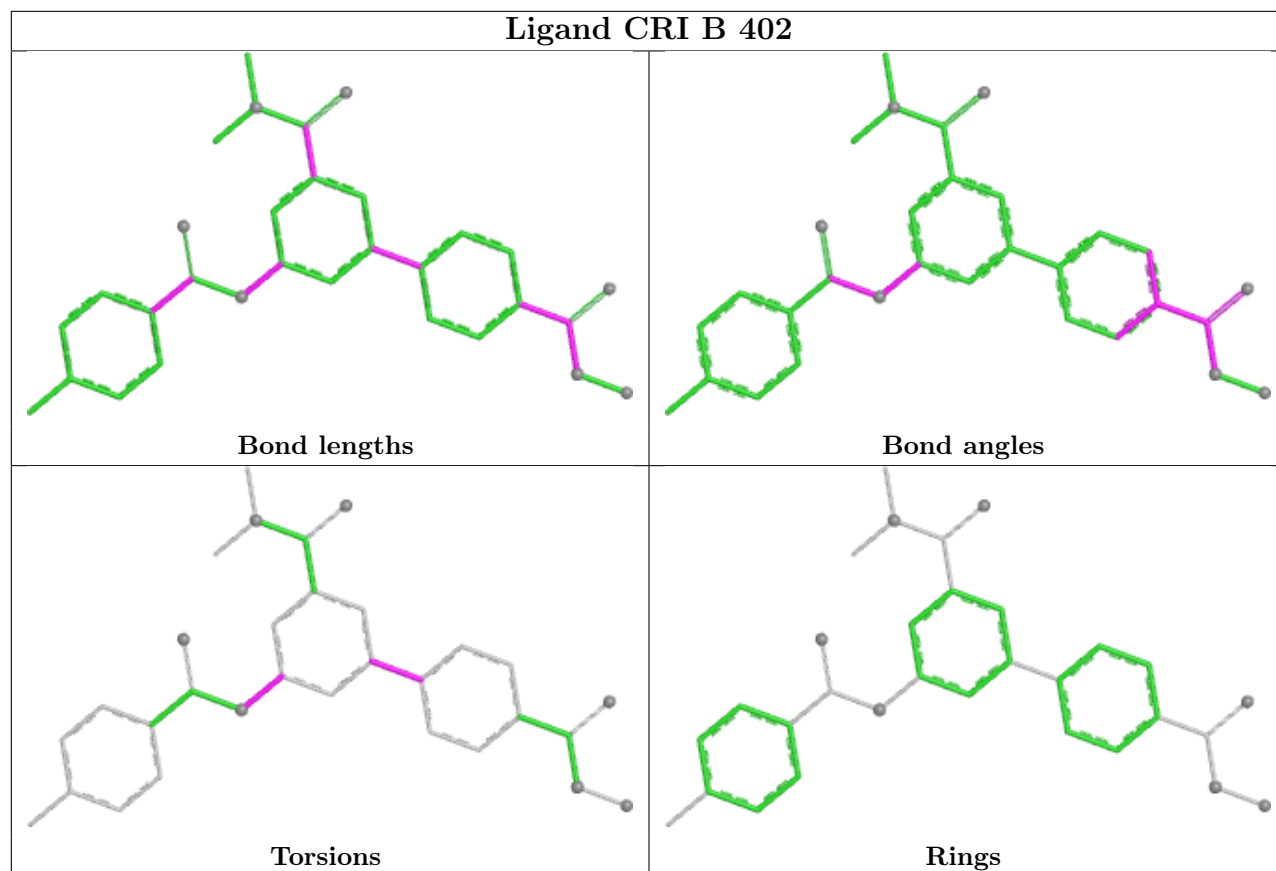
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	CRI	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [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	348/377 (92%)	-0.31	7 (2%) 65 62	22, 45, 82, 100	0
1	B	348/377 (92%)	-0.36	8 (2%) 61 58	17, 42, 76, 100	0
All	All	696/754 (92%)	-0.34	15 (2%) 62 59	17, 44, 79, 100	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	31	LEU	4.0
1	B	34	ILE	3.9
1	A	31	LEU	3.4
1	B	88	ASP	3.2
1	A	69	THR	3.2
1	A	34	ILE	2.9
1	A	88	ASP	2.8
1	A	35	PRO	2.5
1	B	32	ALA	2.5
1	B	69	THR	2.4
1	B	111	TYR	2.3
1	A	105	THR	2.1
1	A	222	GLY	2.1
1	B	86	GLY	2.1
1	B	238	GLU	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

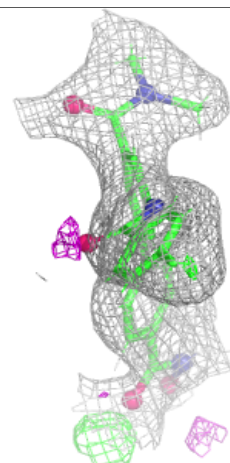
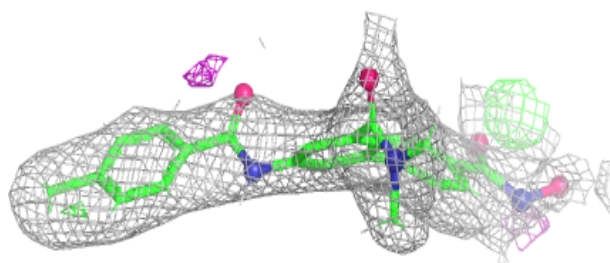
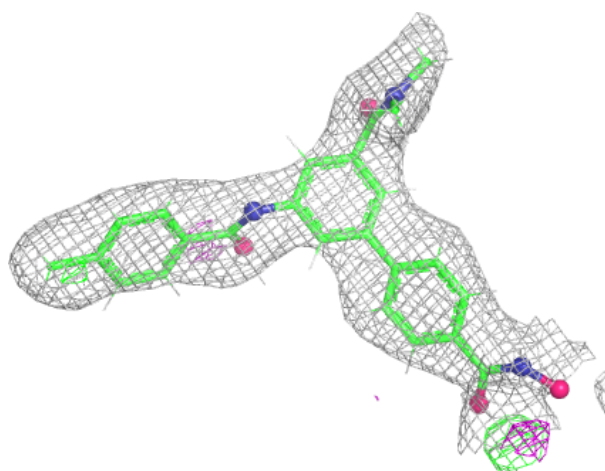
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NA	A	401	1/1	0.73	0.07	39,39,39,39	0
4	CRI	A	402	31/31	0.89	0.09	37,63,77,81	0
4	CRI	B	402	31/31	0.90	0.09	53,64,82,83	0
3	NA	B	401	1/1	0.94	0.06	30,30,30,30	0
2	ZN	A	400	1/1	0.99	0.10	36,36,36,36	0
2	ZN	B	400	1/1	0.99	0.06	44,44,44,44	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.

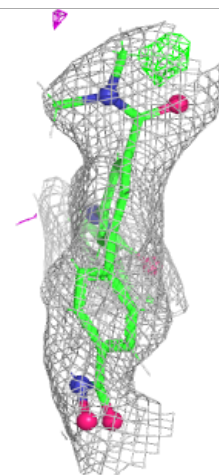
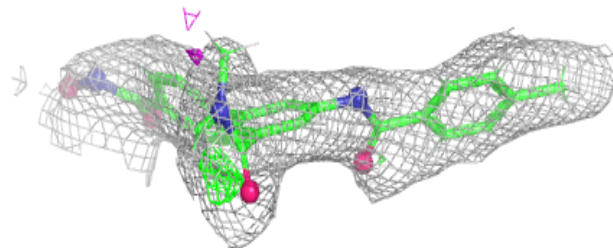
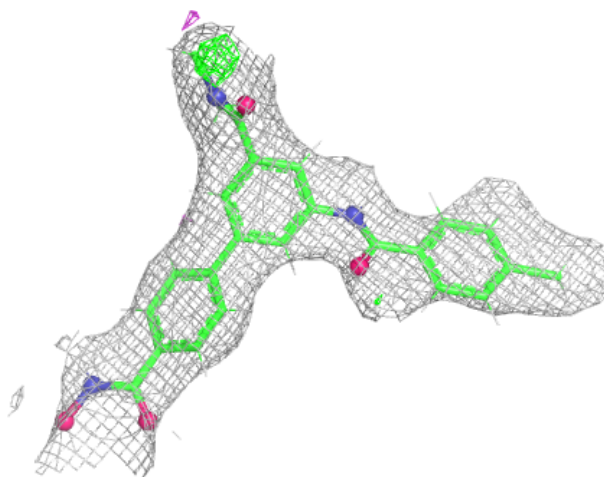
Electron density around CRI A 402:

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 CRI B 402:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.