



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:40 PM UTC

PDB ID : 5LY1 / pdb_00005ly1
Title : JMJD2A/ KDM4A COMPLEXED WITH NI(II) AND Macrocyclic PEPTIDE Inhibitor CP2 (13-mer)
Authors : King, O.N.F.; Chowdhury, R.; Kawamura, A.; Schofield, C.J.
Deposited on : 2016-09-23
Resolution : 2.50 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 ⓘ](#)) 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
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

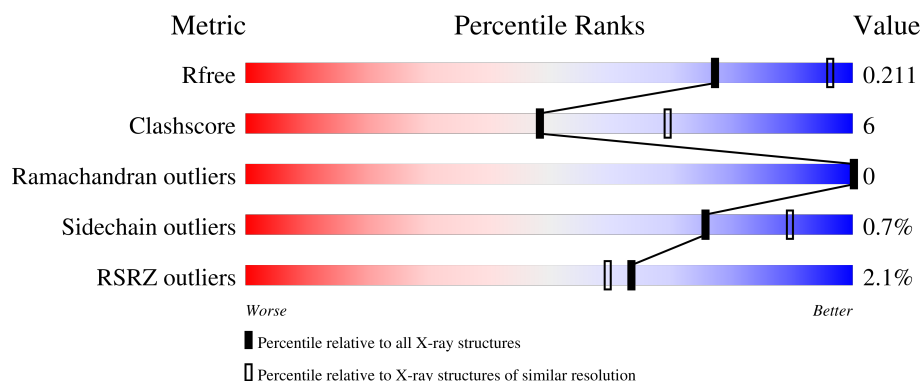
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	381	2% 82% 10% 8%
1	B	381	3% 77% 13% 9%
1	C	381	2% 78% 12% 10%
1	D	381	0% 81% 10% 9%
2	E	14	7% 43% 50% 7%

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
6	GOL	B	503	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11711 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 Lysine-specific demethylase 4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2803	1814	462	512	15			
1	B	346	Total	C	N	O	S	0	0	0
			2765	1795	456	500	14			
1	C	342	Total	C	N	O	S	0	0	0
			2768	1796	461	496	15			
1	D	347	Total	C	N	O	S	0	0	0
			2779	1802	460	503	14			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP O75164
A	-20	HIS	-	expression tag	UNP O75164
A	-19	HIS	-	expression tag	UNP O75164
A	-18	HIS	-	expression tag	UNP O75164
A	-17	HIS	-	expression tag	UNP O75164
A	-16	HIS	-	expression tag	UNP O75164
A	-15	HIS	-	expression tag	UNP O75164
A	-14	SER	-	expression tag	UNP O75164
A	-13	SER	-	expression tag	UNP O75164
A	-12	GLY	-	expression tag	UNP O75164
A	-11	VAL	-	expression tag	UNP O75164
A	-10	ASP	-	expression tag	UNP O75164
A	-9	LEU	-	expression tag	UNP O75164
A	-8	GLY	-	expression tag	UNP O75164
A	-7	THR	-	expression tag	UNP O75164
A	-6	GLU	-	expression tag	UNP O75164
A	-5	ASN	-	expression tag	UNP O75164
A	-4	LEU	-	expression tag	UNP O75164
A	-3	TYR	-	expression tag	UNP O75164
A	-2	PHE	-	expression tag	UNP O75164
A	-1	GLN	-	expression tag	UNP O75164

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP O75164
B	-21	MET	-	initiating methionine	UNP O75164
B	-20	HIS	-	expression tag	UNP O75164
B	-19	HIS	-	expression tag	UNP O75164
B	-18	HIS	-	expression tag	UNP O75164
B	-17	HIS	-	expression tag	UNP O75164
B	-16	HIS	-	expression tag	UNP O75164
B	-15	HIS	-	expression tag	UNP O75164
B	-14	SER	-	expression tag	UNP O75164
B	-13	SER	-	expression tag	UNP O75164
B	-12	GLY	-	expression tag	UNP O75164
B	-11	VAL	-	expression tag	UNP O75164
B	-10	ASP	-	expression tag	UNP O75164
B	-9	LEU	-	expression tag	UNP O75164
B	-8	GLY	-	expression tag	UNP O75164
B	-7	THR	-	expression tag	UNP O75164
B	-6	GLU	-	expression tag	UNP O75164
B	-5	ASN	-	expression tag	UNP O75164
B	-4	LEU	-	expression tag	UNP O75164
B	-3	TYR	-	expression tag	UNP O75164
B	-2	PHE	-	expression tag	UNP O75164
B	-1	GLN	-	expression tag	UNP O75164
B	0	SER	-	expression tag	UNP O75164
C	-21	MET	-	initiating methionine	UNP O75164
C	-20	HIS	-	expression tag	UNP O75164
C	-19	HIS	-	expression tag	UNP O75164
C	-18	HIS	-	expression tag	UNP O75164
C	-17	HIS	-	expression tag	UNP O75164
C	-16	HIS	-	expression tag	UNP O75164
C	-15	HIS	-	expression tag	UNP O75164
C	-14	SER	-	expression tag	UNP O75164
C	-13	SER	-	expression tag	UNP O75164
C	-12	GLY	-	expression tag	UNP O75164
C	-11	VAL	-	expression tag	UNP O75164
C	-10	ASP	-	expression tag	UNP O75164
C	-9	LEU	-	expression tag	UNP O75164
C	-8	GLY	-	expression tag	UNP O75164
C	-7	THR	-	expression tag	UNP O75164
C	-6	GLU	-	expression tag	UNP O75164
C	-5	ASN	-	expression tag	UNP O75164
C	-4	LEU	-	expression tag	UNP O75164
C	-3	TYR	-	expression tag	UNP O75164

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PHE	-	expression tag	UNP O75164
C	-1	GLN	-	expression tag	UNP O75164
C	0	SER	-	expression tag	UNP O75164
D	-21	MET	-	initiating methionine	UNP O75164
D	-20	HIS	-	expression tag	UNP O75164
D	-19	HIS	-	expression tag	UNP O75164
D	-18	HIS	-	expression tag	UNP O75164
D	-17	HIS	-	expression tag	UNP O75164
D	-16	HIS	-	expression tag	UNP O75164
D	-15	HIS	-	expression tag	UNP O75164
D	-14	SER	-	expression tag	UNP O75164
D	-13	SER	-	expression tag	UNP O75164
D	-12	GLY	-	expression tag	UNP O75164
D	-11	VAL	-	expression tag	UNP O75164
D	-10	ASP	-	expression tag	UNP O75164
D	-9	LEU	-	expression tag	UNP O75164
D	-8	GLY	-	expression tag	UNP O75164
D	-7	THR	-	expression tag	UNP O75164
D	-6	GLU	-	expression tag	UNP O75164
D	-5	ASN	-	expression tag	UNP O75164
D	-4	LEU	-	expression tag	UNP O75164
D	-3	TYR	-	expression tag	UNP O75164
D	-2	PHE	-	expression tag	UNP O75164
D	-1	GLN	-	expression tag	UNP O75164
D	0	SER	-	expression tag	UNP O75164

- Molecule 2 is a protein called CP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	S	0	0	0
			135	88	24	22	1			

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Ni 1 1	0	0

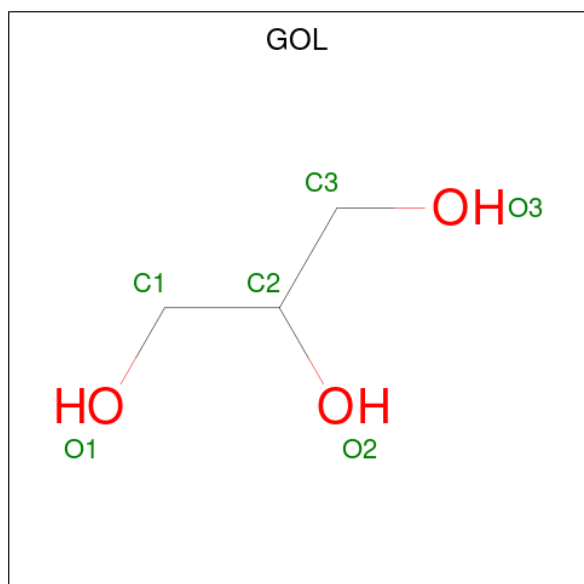
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

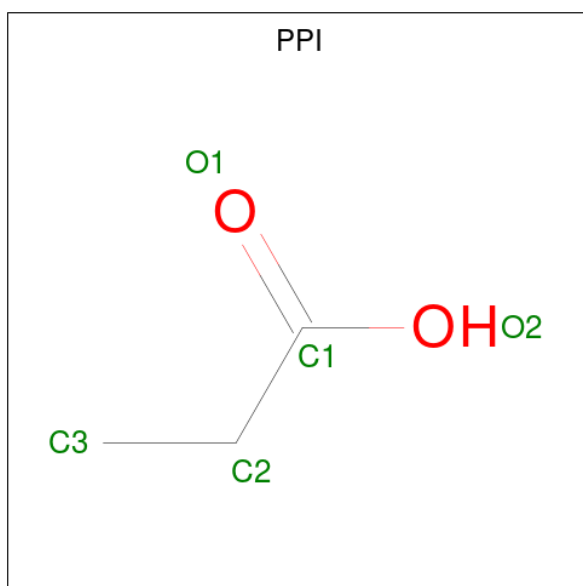
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0

- Molecule 7 is PROPANOIC ACID (CCD ID: PPI) (formula: $C_3H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 5 3 2	0	0
7	B	1	Total C O 5 3 2	0	0
7	D	1	Total C O 5 3 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	97	Total O 97 97	0	0
8	B	74	Total O 74 74	0	0

Continued on next page...

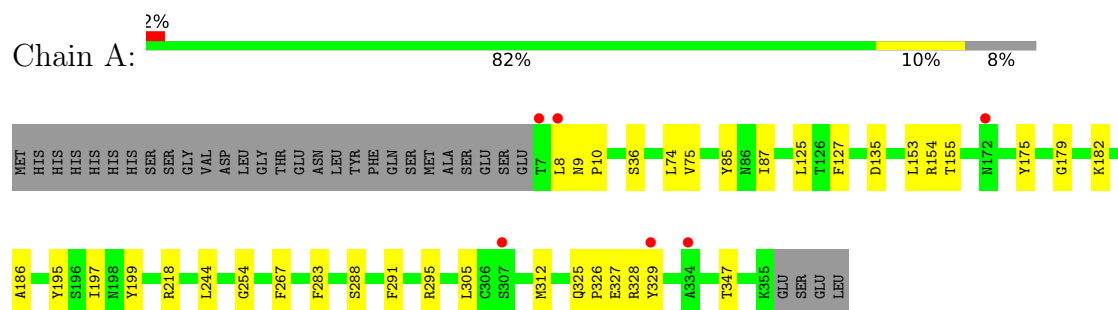
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	124	Total 124	O 124	0	0
8	D	103	Total 103	O 103	0	0
8	E	7	Total 7	O 7	0	0

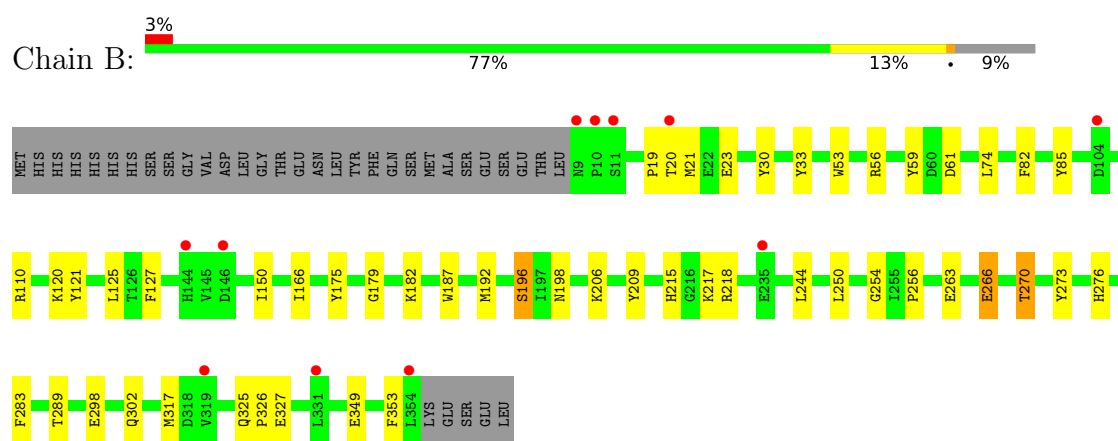
3 Residue-property plots [i](#)

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.

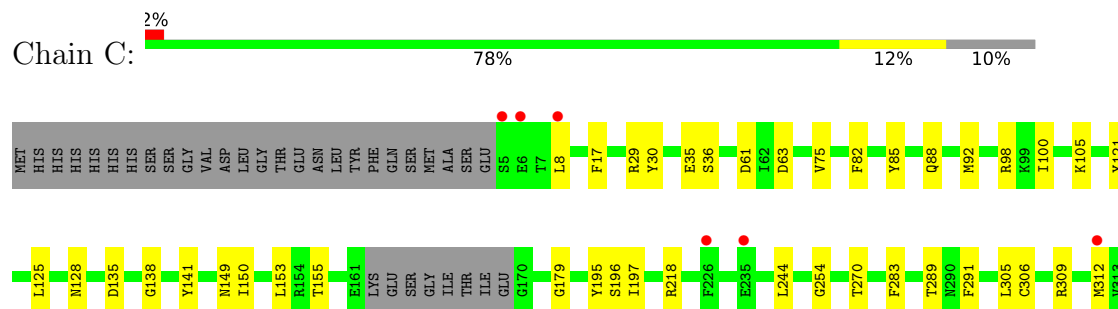
• Molecule 1: Lysine-specific demethylase 4A



• Molecule 1: Lysine-specific demethylase 4A

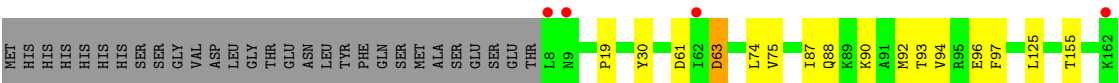
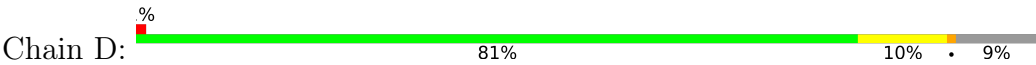


• Molecule 1: Lysine-specific demethylase 4A





● Molecule 1: Lysine-specific demethylase 4A



● Molecule 2: CP2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.27Å 101.48Å 140.33Å 90.00° 99.56° 90.00°	Depositor
Resolution (Å)	49.34 – 2.50 49.34 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.34-2.50) 98.1 (49.34-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.178 , 0.205 0.190 , 0.211	Depositor DCC
R_{free} test set	2721 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11711	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.05% 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: GOL, DTY, PPI, 48V, CL, NI, ZN

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	0.19	0/2890	0.41	0/3930
1	B	0.19	0/2852	0.41	0/3878
1	C	0.21	0/2854	0.44	0/3873
1	D	0.21	0/2866	0.42	0/3898
2	E	1.13	0/118	0.98	0/161
All	All	0.23	0/11580	0.43	0/15740

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2803	0	2646	25	0
1	B	2765	0	2603	37	0
1	C	2768	0	2645	33	0
1	D	2779	0	2610	30	0
2	E	135	0	115	14	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	1	0
6	A	6	0	8	0	0
6	B	12	0	16	6	0
6	C	12	0	16	2	0
7	A	5	0	5	0	0
7	B	5	0	5	0	0
7	D	5	0	5	0	0
8	A	97	0	0	0	0
8	B	74	0	0	3	0
8	C	124	0	0	0	0
8	D	103	0	0	0	0
8	E	7	0	0	0	0
All	All	11711	0	10674	121	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 6.

All (121) 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:D:88:GLN:NE2	2:E:0:48V:H9	1.88	0.89
1:D:88:GLN:CD	2:E:0:48V:H9	1.98	0.88
1:C:135:ASP:OD2	2:E:7:SER:HB3	1.75	0.86
1:D:90:LYS:HB2	2:E:1:DTY:CE1	2.08	0.83
1:D:301:LYS:NZ	1:D:325:GLN:OE1	2.22	0.73
1:B:127:PHE:O	1:B:182:LYS:NZ	2.24	0.69
1:D:88:GLN:H	2:E:13:THR:HG22	1.60	0.66
1:D:196:SER:HB3	1:D:270:THR:HB	1.77	0.65
1:C:85:TYR:CD1	1:D:74:LEU:HD21	2.31	0.65
1:A:127:PHE:O	1:A:182:LYS:NZ	2.30	0.63
1:B:110:ARG:O	1:B:120:LYS:NZ	2.32	0.62
1:B:196:SER:HB3	1:B:270:THR:HB	1.82	0.61
1:D:181:TRP:CE2	1:D:182:LYS:HG3	2.35	0.61
1:B:33:TYR:CD1	6:B:503:GOL:H12	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:MET:HE2	1:B:317:MET:HE1	1.85	0.59
1:C:63:ASP:OD1	1:C:98:ARG:NH2	2.38	0.56
1:D:88:GLN:CD	2:E:0:48V:C08	2.76	0.55
1:A:218:ARG:NH2	1:A:254:GLY:O	2.41	0.54
1:D:63:ASP:HA	1:D:94:VAL:CG2	2.38	0.53
1:C:125:LEU:HD21	1:C:244:LEU:HD23	1.90	0.53
1:A:179:GLY:O	1:A:283:PHE:HA	2.09	0.52
1:C:92:MET:HE1	1:C:100:ILE:HD12	1.91	0.52
1:D:125:LEU:HD21	1:D:244:LEU:HD23	1.91	0.52
1:C:312:MET:HE3	1:C:314:LYS:HB2	1.91	0.51
1:D:74:LEU:HD13	1:D:87:ILE:HD12	1.91	0.51
1:D:179:GLY:O	1:D:283:PHE:HA	2.10	0.51
1:B:327:GLU:H	1:B:327:GLU:CD	2.18	0.51
1:B:23:GLU:OE1	6:B:503:GOL:O2	2.20	0.51
1:A:153:LEU:HD11	1:A:197:ILE:HG21	1.92	0.50
2:E:3:TYR:CE1	2:E:10:ARG:HD2	2.46	0.50
1:B:21:MET:HE1	1:B:53:TRP:HB2	1.94	0.50
1:C:105:LYS:O	1:C:128:ASN:ND2	2.45	0.50
1:B:166:ILE:HG12	1:C:138:GLY:HA2	1.93	0.49
1:C:179:GLY:O	1:C:283:PHE:HA	2.12	0.49
1:D:88:GLN:OE1	2:E:0:48V:H9	2.09	0.49
1:A:75:VAL:HG11	1:A:125:LEU:HG	1.94	0.49
1:C:61:ASP:OD1	1:C:61:ASP:N	2.42	0.49
1:B:198:ASN:OD1	8:B:601:HOH:O	2.20	0.49
1:B:150:ILE:HG23	1:B:289:THR:HG22	1.96	0.48
1:C:8:LEU:HD13	1:C:36:SER:O	2.13	0.48
1:C:135:ASP:CG	2:E:7:SER:HB3	2.39	0.48
1:C:341:ILE:HD12	6:C:405:GOL:H11	1.96	0.48
1:D:155:THR:OG1	1:D:292:ALA:O	2.31	0.48
1:A:135:ASP:HA	1:A:175:TYR:CD2	2.49	0.48
1:B:206:LYS:HE2	8:B:601:HOH:O	2.14	0.47
1:C:29:ARG:NH1	1:C:352:GLU:OE2	2.47	0.47
1:C:218:ARG:NH2	1:C:254:GLY:O	2.47	0.47
1:B:209:TYR:O	1:B:276:HIS:HA	2.15	0.47
1:D:229:GLY:N	5:D:503:CL:CL	2.85	0.47
1:D:92:MET:CE	1:D:97:PHE:HA	2.44	0.46
1:D:88:GLN:OE1	2:E:0:48V:C08	2.64	0.46
1:A:186:ALA:HA	1:A:244:LEU:HD23	1.97	0.46
1:B:206:LYS:CE	8:B:601:HOH:O	2.64	0.46
1:A:154:ARG:HG3	1:A:154:ARG:O	2.16	0.46
1:C:306:CYS:O	1:C:312:MET:SD	2.73	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:GLU:OE2	1:A:327:GLU:N	2.49	0.46
1:B:349:GLU:OE1	1:B:349:GLU:N	2.49	0.46
1:C:196:SER:HB3	1:C:270:THR:OG1	2.15	0.45
2:E:1:DTY:CE2	2:E:2:VAL:HG12	2.46	0.45
1:D:219:LEU:HA	1:D:255:ILE:HD13	1.99	0.45
1:A:199:TYR:HB2	1:A:267:PHE:CE1	2.52	0.45
1:A:155:THR:HG21	1:A:291:PHE:HB2	1.99	0.45
1:C:121:TYR:CZ	1:C:125:LEU:HD13	2.52	0.45
1:C:135:ASP:OD1	2:E:7:SER:HB2	2.17	0.45
1:C:341:ILE:CD1	6:C:405:GOL:H11	2.47	0.45
1:C:153:LEU:HD11	1:C:197:ILE:HG21	1.99	0.44
1:A:329:TYR:C	1:A:329:TYR:CD1	2.95	0.44
1:A:9:ASN:N	1:A:10:PRO:HD3	2.32	0.44
1:C:85:TYR:CG	1:D:74:LEU:HD21	2.53	0.44
1:A:325:GLN:N	1:A:326:PRO:CD	2.80	0.44
1:A:74:LEU:HD11	1:B:85:TYR:HB2	2.00	0.44
1:A:74:LEU:HD11	1:B:85:TYR:CB	2.48	0.44
1:B:33:TYR:CD1	6:B:503:GOL:C1	3.00	0.44
1:B:263:GLU:O	1:B:266:GLU:HB2	2.18	0.43
1:C:309:ARG:HG3	2:E:9:TRP:CZ2	2.52	0.43
1:B:33:TYR:CE1	6:B:503:GOL:H12	2.52	0.43
1:B:33:TYR:CG	6:B:503:GOL:H12	2.53	0.43
1:B:61:ASP:OD1	1:B:61:ASP:N	2.47	0.43
1:C:35:GLU:OE2	1:C:195:TYR:OH	2.26	0.43
1:D:63:ASP:HA	1:D:94:VAL:HG23	2.00	0.43
1:A:295:ARG:HB2	1:A:347:THR:HA	2.01	0.43
1:C:88:GLN:CD	2:E:3:TYR:HH	2.22	0.43
1:D:209:TYR:O	1:D:276:HIS:HA	2.19	0.43
1:B:217:LYS:HD2	1:B:273:TYR:OH	2.19	0.43
1:B:327:GLU:OE2	1:B:327:GLU:N	2.39	0.42
1:B:325:GLN:N	1:B:326:PRO:CD	2.82	0.42
1:D:195:TYR:HB3	1:D:291:PHE:CZ	2.54	0.42
1:B:353:PHE:CE2	6:B:503:GOL:H11	2.54	0.42
1:B:19:PRO:HB3	1:B:30:TYR:CZ	2.55	0.42
1:B:56:ARG:HD3	1:B:59:TYR:CE1	2.54	0.42
1:B:82:PHE:HB2	1:B:244:LEU:HB2	2.01	0.42
1:B:179:GLY:O	1:B:283:PHE:HA	2.19	0.42
1:C:17:PHE:HB3	1:C:30:TYR:OH	2.19	0.42
1:A:8:LEU:HD13	1:A:36:SER:O	2.20	0.42
1:B:218:ARG:NH2	1:B:254:GLY:O	2.52	0.42
1:C:150:ILE:HG23	1:C:289:THR:HG22	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:TYR:CE2	1:C:149:ASN:HA	2.54	0.42
1:A:197:ILE:O	1:A:288:SER:HA	2.20	0.41
1:A:74:LEU:HD11	1:A:87:ILE:HD11	2.02	0.41
1:A:85:TYR:CD1	1:B:74:LEU:HD11	2.56	0.41
1:A:305:LEU:HB3	1:A:312:MET:HE3	2.01	0.41
1:B:187:TRP:CZ2	1:B:250:LEU:HD11	2.55	0.41
1:C:328:ARG:NH1	1:C:339:THR:OG1	2.53	0.41
1:A:195:TYR:HB3	1:A:291:PHE:CE1	2.56	0.41
1:D:190:GLU:HG3	1:D:196:SER:HB2	2.02	0.41
1:B:121:TYR:CZ	1:B:125:LEU:HD13	2.56	0.41
1:C:75:VAL:HG11	1:C:125:LEU:HG	2.03	0.41
1:A:328:ARG:O	1:A:329:TYR:C	2.62	0.41
1:B:298:GLU:OE1	1:B:302:GLN:NE2	2.54	0.41
1:D:260:VAL:HG11	1:D:268:MET:HE2	2.03	0.41
1:D:19:PRO:HB3	1:D:30:TYR:CZ	2.56	0.41
1:A:325:GLN:N	1:A:326:PRO:HD3	2.36	0.40
1:B:215:HIS:CE1	1:B:256:PRO:HG2	2.56	0.40
1:C:82:PHE:HB2	1:C:244:LEU:HB2	2.02	0.40
1:C:305:LEU:HB3	1:C:312:MET:HE1	2.02	0.40
1:D:93:THR:OG1	1:D:96:GLU:HG3	2.22	0.40
1:C:155:THR:HG21	1:C:291:PHE:HB2	2.03	0.40
1:D:75:VAL:HG11	1:D:125:LEU:HG	2.03	0.40
1:D:155:THR:HG21	1:D:291:PHE:HB2	2.02	0.40
1:B:20:THR:OG1	1:B:23:GLU:HG2	2.20	0.40
1:D:296:TRP:O	1:D:297:ILE:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	347/381 (91%)	342 (99%)	5 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	344/381 (90%)	341 (99%)	3 (1%)	0	100	100
1	C	338/381 (89%)	334 (99%)	4 (1%)	0	100	100
1	D	345/381 (91%)	341 (99%)	4 (1%)	0	100	100
2	E	11/14 (79%)	11 (100%)	0	0	100	100
All	All	1385/1538 (90%)	1369 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	290/335 (87%)	290 (100%)	0	100	100
1	B	281/335 (84%)	277 (99%)	4 (1%)	59	81
1	C	287/335 (86%)	287 (100%)	0	100	100
1	D	281/335 (84%)	277 (99%)	4 (1%)	59	81
2	E	11/11 (100%)	11 (100%)	0	100	100
All	All	1150/1351 (85%)	1142 (99%)	8 (1%)	76	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	175	TYR
1	B	196	SER
1	B	266	GLU
1	B	270	THR
1	D	61	ASP
1	D	63	ASP
1	D	182	LYS
1	D	235	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	302	GLN
1	B	72	GLN
1	B	137	ASN
1	C	128	ASN
1	C	137	ASN
1	D	124	ASN
1	D	198	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
2	48V	E	0	2	9,9,10	0.87	0	8,10,12	1.27	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	48V	E	0	2	-	5/8/9/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	0	48V	C03-C02-N01	2.31	118.04	109.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	0	48V	C06-C02-C03-N05
2	E	0	48V	C03-C02-C06-S07
2	E	0	48V	N01-C02-C03-O04
2	E	0	48V	C06-C02-C03-O04
2	E	0	48V	C09-C08-S07-C06

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	0	48V	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 11 are monoatomic - leaving 8 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	$\# Z > 2$
6	GOL	B	503	-	5,5,5	0.26	0	5,5,5	0.31	0
6	GOL	B	504	-	5,5,5	0.38	0	5,5,5	0.28	0
6	GOL	C	405	-	5,5,5	0.38	0	5,5,5	0.27	0
7	PPI	D	504	-	4,4,4	1.00	0	4,4,4	1.05	0
7	PPI	A	505	-	4,4,4	1.01	0	4,4,4	1.13	0
6	GOL	C	401	-	5,5,5	0.41	0	5,5,5	0.28	0
7	PPI	B	505	-	4,4,4	1.01	0	4,4,4	1.08	0
6	GOL	A	504	-	5,5,5	0.47	0	5,5,5	0.29	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
6	GOL	B	503	-	-	0/4/4/4	-
6	GOL	B	504	-	-	0/4/4/4	-
6	GOL	C	405	-	-	0/4/4/4	-
7	PPI	D	504	-	-	0/2/2/2	-
7	PPI	A	505	-	-	0/2/2/2	-
6	GOL	C	401	-	-	0/4/4/4	-
7	PPI	B	505	-	-	0/2/2/2	-
6	GOL	A	504	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	503	GOL	6	0
6	C	405	GOL	2	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	349/381 (91%)	0.15	6 (1%) 69 65	31, 49, 88, 127	0
1	B	346/381 (90%)	0.32	11 (3%) 50 46	28, 54, 91, 109	0
1	C	342/381 (89%)	-0.10	7 (2%) 65 61	27, 42, 71, 104	0
1	D	347/381 (91%)	0.10	5 (1%) 73 70	27, 47, 84, 98	0
2	E	12/14 (85%)	0.89	1 (8%) 17 15	55, 65, 69, 70	0
All	All	1396/1538 (90%)	0.13	30 (2%) 63 59	27, 49, 85, 127	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	8	LEU	4.8
1	B	235	GLU	4.0
1	B	354	LEU	3.9
1	D	9	ASN	3.4
1	A	8	LEU	3.1
1	B	11	SER	3.0
1	B	10	PRO	2.9
1	A	329	TYR	2.7
1	B	9	ASN	2.7
1	B	146	ASP	2.7
1	A	7	THR	2.6
1	B	144	HIS	2.4
1	A	172	ASN	2.4
1	D	62	ILE	2.4
1	C	6	GLU	2.4
1	C	312	MET	2.3
1	A	334	ALA	2.2
1	C	354	LEU	2.2
1	B	319	VAL	2.2
1	D	164	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	235	GLU	2.2
1	C	8	LEU	2.2
1	C	5	SER	2.1
1	D	162	LYS	2.1
1	B	20	THR	2.1
2	E	13	THR	2.1
1	B	104	ASP	2.1
1	B	331	LEU	2.1
1	C	226	PHE	2.0
1	A	307	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	48V	E	0	10/11	0.47	0.17	80,83,84,85	0
2	DTY	E	1	12/13	0.81	0.16	57,75,76,77	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
6	GOL	B	503	6/6	0.55	0.22	84,85,86,87	0
6	GOL	A	504	6/6	0.77	0.19	73,75,76,76	0
7	PPI	B	505	5/5	0.79	0.20	46,47,47,48	0
6	GOL	C	405	6/6	0.81	0.22	77,81,82,82	0
7	PPI	A	505	5/5	0.84	0.18	47,47,48,48	0
7	PPI	D	504	5/5	0.85	0.16	46,47,47,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	D	503	1/1	0.88	0.13	80,80,80,80	0
6	GOL	B	504	6/6	0.88	0.12	72,74,74,74	0
6	GOL	C	401	6/6	0.89	0.13	69,70,71,71	0
5	CL	A	503	1/1	0.90	0.10	74,74,74,74	0
5	CL	C	404	1/1	0.93	0.08	66,66,66,66	0
3	NI	B	501	1/1	0.98	0.04	63,63,63,63	0
4	ZN	D	502	1/1	0.99	0.03	45,45,45,45	0
3	NI	A	501	1/1	0.99	0.03	62,62,62,62	0
3	NI	C	402	1/1	0.99	0.04	62,62,62,62	0
3	NI	D	501	1/1	0.99	0.04	68,68,68,68	0
4	ZN	A	502	1/1	0.99	0.03	50,50,50,50	0
4	ZN	B	502	1/1	0.99	0.02	50,50,50,50	0
4	ZN	C	403	1/1	1.00	0.01	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.