



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:49 AM UTC

PDB ID : 3MKS / pdb_00003mks
Title : Crystal Structure of yeast Cdc4/Skp1 in complex with an allosteric inhibitor SCF-I2
Authors : Orlicky, S.; Sicheri, F.; Tyers, M.; Tang, X.
Deposited on : 2010-04-15
Resolution : 2.60 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
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

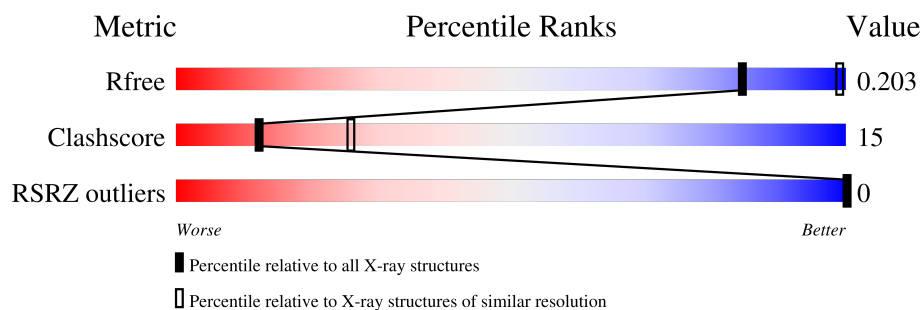
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	169	
1	C	169	
2	B	464	
2	D	464	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9456 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 Suppressor of kinetochore protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	0	0
			1083	686	188	205	4			
1	C	132	Total	C	N	O	S	0	0	0
			1073	681	189	199	4			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P52286
A	-1	ALA	-	expression tag	UNP P52286
A	0	HIS	-	expression tag	UNP P52286
A	1	MET	-	expression tag	UNP P52286
A	?	-	HIS	deletion	UNP P52286
A	?	-	ASP	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	?	-	LEU	deletion	UNP P52286
A	?	-	GLN	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	ASP	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	GLU	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	ASP	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	ASP	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	GLU	deletion	UNP P52286
A	?	-	THR	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	?	-	HIS	deletion	UNP P52286

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	LYS	deletion	UNP P52286
A	?	-	ASP	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
C	-2	GLY	-	expression tag	UNP P52286
C	-1	ALA	-	expression tag	UNP P52286
C	0	HIS	-	expression tag	UNP P52286
C	1	MET	-	expression tag	UNP P52286
C	?	-	HIS	deletion	UNP P52286
C	?	-	ASP	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286
C	?	-	LEU	deletion	UNP P52286
C	?	-	GLN	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	ASP	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	GLU	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	ASP	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	ASP	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	GLU	deletion	UNP P52286
C	?	-	THR	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286
C	?	-	HIS	deletion	UNP P52286
C	?	-	LYS	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	LYS	deletion	UNP P52286
C	?	-	ASP	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286

- Molecule 2 is a protein called Cell division control protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	444	Total	C	N	O	S	0	0	0
			3582	2296	618	656	12			
2	D	445	Total	C	N	O	S	0	0	0
			3591	2301	620	658	12			

There are 46 discrepancies between the modelled and reference sequences:

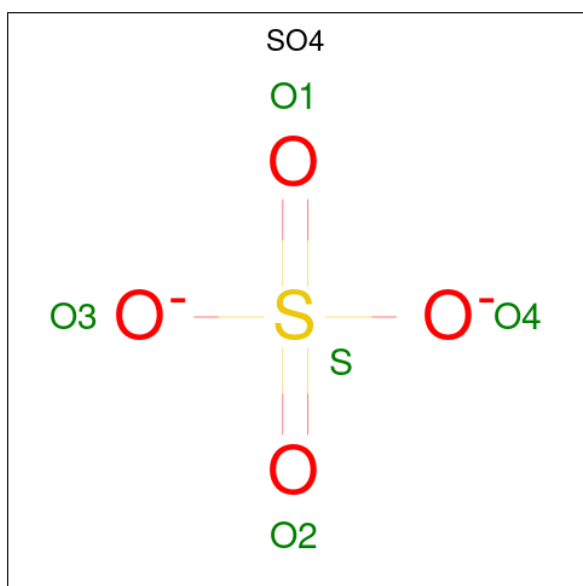
Chain	Residue	Modelled	Actual	Comment	Reference
B	261	GLY	-	expression tag	UNP P07834
B	262	ALA	-	expression tag	UNP P07834
B	460	GLU	LYS	SEE REMARK 999	UNP P07834
B	?	-	ASN	deletion	UNP P07834
B	?	-	ILE	deletion	UNP P07834
B	?	-	TRP	deletion	UNP P07834
B	?	-	ASN	deletion	UNP P07834
B	?	-	CYS	deletion	UNP P07834
B	?	-	SER	deletion	UNP P07834
B	?	-	TYR	deletion	UNP P07834
B	?	-	ALA	deletion	UNP P07834
B	?	-	THR	deletion	UNP P07834
B	?	-	ASN	deletion	UNP P07834
B	?	-	SER	deletion	UNP P07834
B	?	-	ALA	deletion	UNP P07834
B	?	-	SER	deletion	UNP P07834
B	?	-	PRO	deletion	UNP P07834
B	?	-	CYS	deletion	UNP P07834
B	?	-	ALA	deletion	UNP P07834
B	?	-	LYS	deletion	UNP P07834
B	?	-	ILE	deletion	UNP P07834
B	?	-	GLY	deletion	UNP P07834
B	?	-	ALA	deletion	UNP P07834
D	261	GLY	-	expression tag	UNP P07834
D	262	ALA	-	expression tag	UNP P07834
D	460	GLU	LYS	SEE REMARK 999	UNP P07834
D	?	-	ASN	deletion	UNP P07834
D	?	-	ILE	deletion	UNP P07834
D	?	-	TRP	deletion	UNP P07834
D	?	-	ASN	deletion	UNP P07834
D	?	-	CYS	deletion	UNP P07834
D	?	-	SER	deletion	UNP P07834
D	?	-	TYR	deletion	UNP P07834
D	?	-	ALA	deletion	UNP P07834
D	?	-	THR	deletion	UNP P07834

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASN	deletion	UNP P07834
D	?	-	SER	deletion	UNP P07834
D	?	-	ALA	deletion	UNP P07834
D	?	-	SER	deletion	UNP P07834
D	?	-	PRO	deletion	UNP P07834
D	?	-	CYS	deletion	UNP P07834
D	?	-	ALA	deletion	UNP P07834
D	?	-	LYS	deletion	UNP P07834
D	?	-	ILE	deletion	UNP P07834
D	?	-	GLY	deletion	UNP P07834
D	?	-	ALA	deletion	UNP P07834

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



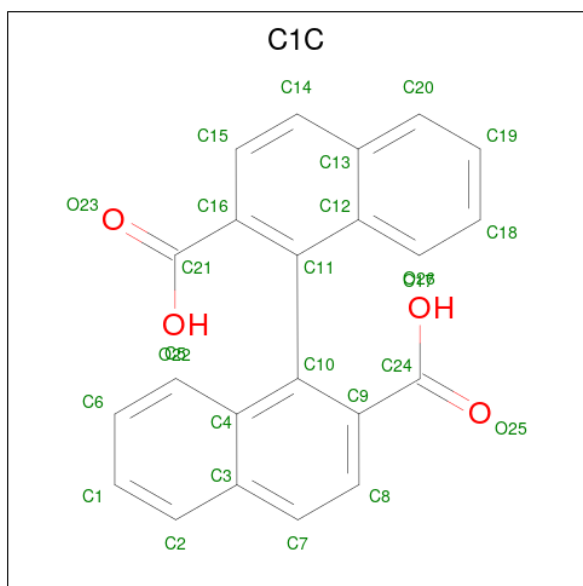
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,1'-binaphthalene-2,2'-dicarboxylic acid (CCD ID: C1C) (formula: $C_{22}H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			26	22	4		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



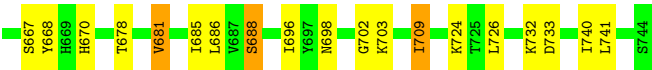
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

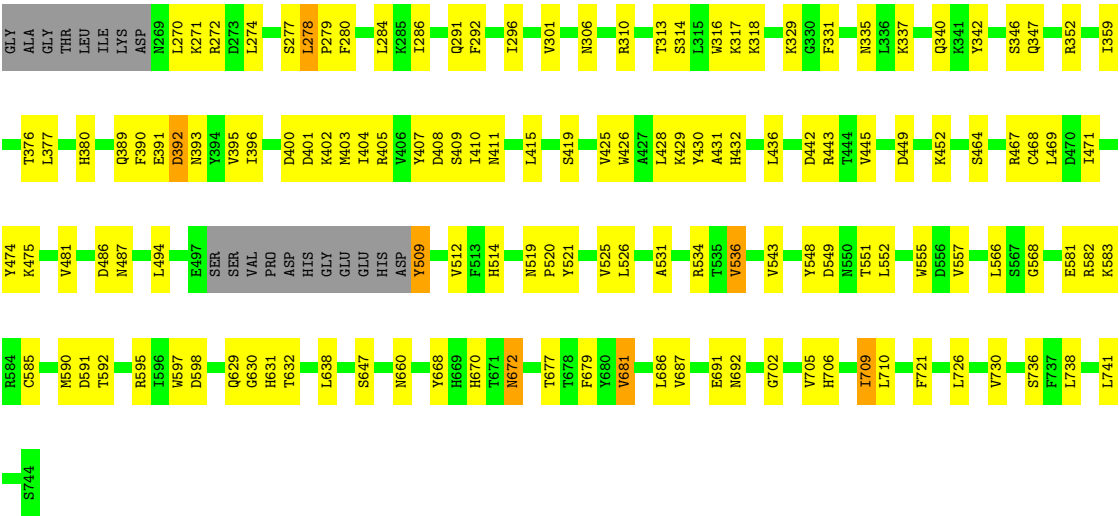
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	O	0	0
			4	4		
6	B	22	Total	O	0	0
			22	22		
6	C	4	Total	O	0	0
			4	4		
6	D	10	Total	O	0	0
			10	10		

- Molecule 1: Suppressor of kinetochore protein 1





● Molecule 2: Cell division control protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	108.28Å 108.28Å 165.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	93.66 – 2.60 93.66 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (93.66-2.60) 99.7 (93.66-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.211 , 0.266 (Not available) , 0.203	Depositor DCC
R_{free} test set	3375 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 24.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.210 for -h,-k,l 0.076 for h,-h-k,-l 0.075 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9456	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: C1C, GOL, SO4

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	0.95	2/1101 (0.2%)	1.22	6/1487 (0.4%)
1	C	1.25	6/1091 (0.5%)	1.29	8/1473 (0.5%)
2	B	1.07	3/3663 (0.1%)	1.19	13/4957 (0.3%)
2	D	1.15	1/3672 (0.0%)	1.26	19/4969 (0.4%)
All	All	1.11	12/9527 (0.1%)	1.23	46/12886 (0.4%)

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

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	116	VAL	N-CA	6.59	1.54	1.46
1	C	116	VAL	CA-C	6.57	1.61	1.52
1	C	116	VAL	CA-CB	6.27	1.62	1.54
1	A	9	VAL	CA-CB	6.14	1.61	1.54
1	A	172	ILE	CA-CB	5.90	1.62	1.54
1	C	156	GLU	N-CA	5.81	1.53	1.46
1	C	86	VAL	CA-CB	5.75	1.61	1.54
2	D	359	ILE	CA-CB	-5.29	1.47	1.54
1	C	156	GLU	CG-CD	5.25	1.65	1.52
2	B	361	ILE	CA-CB	-5.09	1.47	1.54
2	B	703	LYS	CA-C	-5.09	1.46	1.52
2	B	688	SER	CA-C	-5.04	1.46	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	709	ILE	N-CA-C	10.06	120.88	110.62
2	B	509	TYR	CA-C-N	-9.63	107.80	119.84
2	B	509	TYR	C-N-CA	-9.63	107.80	119.84
2	D	342	TYR	CA-C-N	-9.49	110.06	119.64
2	D	342	TYR	C-N-CA	-9.49	110.06	119.64
1	C	177	THR	CA-C-N	-7.81	110.69	119.28
1	C	177	THR	C-N-CA	-7.81	110.69	119.28
2	B	311	LYS	N-CA-C	-7.81	103.64	113.01
1	C	118	SER	N-CA-C	7.51	126.80	110.80
2	D	681	VAL	CB-CA-C	-7.50	97.62	110.30
1	A	184	ILE	N-CA-C	7.47	120.39	109.63
1	A	77	MET	CA-C-N	7.36	127.12	119.76
1	A	77	MET	C-N-CA	7.36	127.12	119.76
2	B	331	PHE	N-CA-C	7.21	118.83	110.97
1	C	119	TRP	N-CA-C	-7.00	104.21	112.89
2	D	536	VAL	CB-CA-C	-6.98	99.53	110.69
2	D	278	LEU	CA-C-N	-6.95	112.80	119.89
2	D	278	LEU	C-N-CA	-6.95	112.80	119.89
2	D	672	ASN	N-CA-C	-6.87	100.82	110.50
2	B	632	THR	N-CA-C	-6.40	106.19	112.97
2	D	632	THR	N-CA-C	-5.98	99.60	108.99
2	B	709	ILE	CB-CA-C	-5.94	104.25	112.04
2	D	509	TYR	CA-C-N	5.90	127.21	119.84
2	D	509	TYR	C-N-CA	5.90	127.21	119.84
2	B	681	VAL	N-CA-C	5.87	118.31	108.81
2	B	450	ILE	CB-CA-C	-5.84	104.50	111.97
2	D	672	ASN	CA-C-N	-5.84	111.75	122.31
2	D	672	ASN	C-N-CA	-5.84	111.75	122.31
2	B	681	VAL	CB-CA-C	-5.83	100.27	110.71
2	B	476	ASN	N-CA-C	5.64	122.82	110.80
2	D	392	ASP	CB-CA-C	-5.54	104.03	111.89
2	D	736	SER	N-CA-C	5.51	119.21	109.96
2	D	730	VAL	N-CA-C	5.38	116.66	108.80
1	A	162	SER	CA-C-N	5.35	124.81	119.24
1	A	162	SER	C-N-CA	5.35	124.81	119.24
2	D	525	VAL	CB-CA-C	-5.35	102.68	110.81
1	A	134	ILE	CB-CA-C	-5.35	105.13	111.97
2	B	302	SER	N-CA-C	5.30	116.59	108.42
1	C	116	VAL	N-CA-C	5.28	120.33	109.34
1	C	144	LYS	CA-C-N	-5.18	113.69	119.19
1	C	144	LYS	C-N-CA	-5.18	113.69	119.19
2	B	272	ARG	N-CA-C	5.18	117.13	108.99
2	B	454	CYS	N-CA-C	5.12	116.31	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	GLU	N-CA-C	5.11	116.85	111.28
2	D	445	VAL	N-CA-C	-5.02	101.14	108.17
2	D	291	GLN	N-CA-C	-5.01	103.92	110.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	509	TYR	Peptide

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	1083	0	1084	41	0
1	C	1073	0	1082	39	0
2	B	3582	0	3581	126	0
2	D	3591	0	3589	100	0
3	B	25	0	0	2	0
3	D	30	0	0	0	0
4	D	26	0	12	0	0
5	D	6	0	8	0	0
6	A	4	0	0	1	0
6	B	22	0	0	2	0
6	C	4	0	0	0	0
6	D	10	0	0	0	0
All	All	9456	0	9356	289	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 15.

All (289) 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:C:86:VAL:HG22	1:C:130:MET:CE	1.63	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:VAL:CG2	1:C:130:MET:HE1	1.74	1.18
1:C:121:ARG:HG3	1:C:121:ARG:HH11	0.99	1.12
2:D:629:GLN:HG2	2:D:630:GLY:HA3	1.34	1.08
1:A:86:VAL:HG22	1:A:130:MET:HE1	1.11	1.07
1:A:86:VAL:HG22	1:A:130:MET:CE	1.87	1.05
1:C:31:ASN:O	1:C:33:LEU:HA	1.58	1.01
1:C:86:VAL:HG22	1:C:130:MET:HE1	1.01	1.00
2:B:491:VAL:HG11	2:B:560:MET:HE1	1.43	0.98
2:D:630:GLY:O	2:D:631:HIS:HB2	1.61	0.96
1:C:121:ARG:HG3	1:C:121:ARG:NH1	1.77	0.95
1:A:86:VAL:CG2	1:A:130:MET:HE1	1.99	0.92
1:C:33:LEU:HB3	1:C:34:ASN:HA	1.52	0.91
1:C:33:LEU:H	1:C:34:ASN:HB2	1.36	0.90
2:D:591:ASP:O	2:D:592:THR:HB	1.69	0.88
2:D:549:ASP:OD1	2:D:551:THR:HB	1.76	0.86
2:B:303:GLN:HA	2:B:303:GLN:HE21	1.38	0.85
2:D:519:ASN:C	2:D:519:ASN:HD22	1.84	0.84
1:C:177:THR:OG1	1:C:180:GLU:HG2	1.77	0.83
2:B:314:SER:HB2	3:B:1:SO4:O2	1.79	0.81
2:D:519:ASN:ND2	2:D:521:TYR:H	1.78	0.81
1:A:130:MET:HE2	1:A:134:ILE:HG13	1.62	0.80
2:D:272:ARG:HG2	2:D:274:LEU:HD23	1.65	0.79
2:D:629:GLN:CG	2:D:630:GLY:HA3	2.12	0.79
2:B:412:LYS:HG2	2:B:740:ILE:HG12	1.66	0.77
2:D:393:ASN:ND2	2:D:410:ILE:HD11	2.01	0.76
1:A:15:ARG:HD3	6:A:198:HOH:O	1.87	0.74
1:C:169:THR:O	2:D:271:LYS:HE2	1.86	0.74
2:B:740:ILE:HD12	2:B:741:LEU:N	2.04	0.73
2:B:681:VAL:HG13	2:B:686:LEU:HD13	1.71	0.71
2:B:529:HIS:NE2	2:B:545:SER:OG	2.21	0.71
2:B:539:HIS:HB3	6:B:19:HOH:O	1.90	0.71
2:D:630:GLY:O	2:D:631:HIS:CB	2.39	0.71
2:B:405:ARG:HH11	2:B:417:GLN:NE2	1.90	0.68
2:B:467:ARG:HG2	2:B:534:ARG:HH21	1.59	0.68
2:D:591:ASP:O	2:D:592:THR:CB	2.42	0.68
2:D:486:ASP:O	2:D:487:ASN:HB2	1.94	0.67
2:B:484:SER:HB3	2:B:486:ASP:OD1	1.94	0.67
1:C:127:ASP:OD2	2:D:270:LEU:HD13	1.94	0.67
1:A:8:LEU:HD21	1:A:29:LEU:HD11	1.77	0.66
2:D:519:ASN:HD22	2:D:520:PRO:N	1.92	0.66
2:B:631:HIS:ND1	2:B:649:ALA:HB2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:HIS:HE1	2:B:397:THR:OG1	1.79	0.65
1:C:121:ARG:HH11	1:C:121:ARG:CG	1.91	0.65
2:D:306:ASN:HD21	2:D:310:ARG:HE	1.44	0.65
2:D:638:LEU:HD23	2:D:647:SER:HB2	1.79	0.65
2:B:491:VAL:CG1	2:B:560:MET:HE1	2.25	0.64
2:D:408:ASP:HB2	2:D:415:LEU:HD11	1.80	0.63
2:D:486:ASP:O	2:D:487:ASN:CB	2.47	0.63
2:B:303:GLN:HA	2:B:303:GLN:NE2	2.13	0.62
2:B:544:VAL:HG22	2:B:554:VAL:HG22	1.81	0.62
2:D:534:ARG:HG2	2:D:548:TYR:CE1	2.36	0.61
2:B:670:HIS:HE1	2:B:688:SER:OG	1.85	0.60
2:B:740:ILE:HD12	2:B:740:ILE:C	2.26	0.60
2:B:484:SER:C	2:B:486:ASP:H	2.09	0.60
1:C:130:MET:HE3	1:C:130:MET:HA	1.84	0.60
2:B:462:HIS:NE2	2:B:482:THR:CG2	2.65	0.60
2:D:468:CYS:SG	2:D:536:VAL:HG22	2.42	0.59
2:D:519:ASN:C	2:D:519:ASN:ND2	2.50	0.59
2:B:389:GLN:HE21	2:B:430:TYR:H	1.50	0.59
2:D:393:ASN:HA	2:D:409:SER:OG	2.02	0.59
2:B:681:VAL:HG13	2:B:686:LEU:CD1	2.32	0.59
2:D:681:VAL:HG13	2:D:686:LEU:HD13	1.84	0.59
2:B:586:ILE:HD13	2:B:645:LEU:HD13	1.85	0.59
2:B:513:PHE:CE2	2:B:520:PRO:HD2	2.39	0.58
2:B:696:ILE:HD12	2:B:709:ILE:HD12	1.86	0.58
2:D:705:VAL:HG12	2:D:706:HIS:CD2	2.38	0.58
2:B:473:GLU:O	2:B:540:GLY:HA2	2.05	0.57
2:B:696:ILE:HD12	2:B:709:ILE:CD1	2.35	0.57
2:D:292:PHE:O	2:D:296:ILE:HD12	2.03	0.57
1:A:161:ARG:HD2	1:A:165:GLU:OE2	2.05	0.57
1:C:161:ARG:NH2	1:C:165:GLU:HB3	2.21	0.56
2:D:403:MET:SD	2:D:419:SER:HB3	2.46	0.56
2:D:534:ARG:HG2	2:D:548:TYR:CZ	2.41	0.56
2:B:393:ASN:HA	2:B:409:SER:OG	2.06	0.56
2:B:462:HIS:CE1	2:B:484:SER:HB2	2.41	0.56
2:B:635:VAL:HG11	2:B:647:SER:HB2	1.89	0.56
2:B:586:ILE:HG21	2:B:645:LEU:HD11	1.88	0.55
2:B:589:SER:HB3	2:B:591:ASP:OD1	2.06	0.55
2:B:462:HIS:NE2	2:B:482:THR:HG22	2.21	0.55
2:B:525:VAL:O	2:B:526:LEU:HD12	2.06	0.55
2:B:685:ILE:HG13	3:B:7:SO4:O2	2.06	0.55
1:C:33:LEU:N	1:C:34:ASN:HB2	2.16	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:LYS:HG2	2:B:740:ILE:CG1	2.37	0.55
2:D:726:LEU:HD23	2:D:741:LEU:HD12	1.88	0.54
2:B:590:MET:HA	2:B:634:LEU:HB3	1.88	0.54
2:B:316:TRP:CZ2	2:B:352:ARG:HD3	2.43	0.54
2:B:569:HIS:HE1	2:B:587:SER:OG	1.90	0.54
2:B:412:LYS:HE3	2:B:740:ILE:HD11	1.90	0.54
2:D:442:ASP:C	2:D:443:ARG:HG2	2.33	0.54
2:D:306:ASN:ND2	2:D:310:ARG:HE	2.05	0.54
2:D:306:ASN:HD21	2:D:310:ARG:HH21	1.56	0.53
1:A:163:PRO:HB3	2:B:300:GLY:O	2.08	0.53
1:C:132:TYR:CE1	2:D:278:LEU:HD13	2.44	0.53
2:B:732:LYS:O	2:B:733:ASP:C	2.52	0.53
2:B:534:ARG:HG2	2:B:574:TYR:HA	1.91	0.53
2:D:313:THR:HG21	2:D:347:GLN:OE1	2.08	0.53
2:D:552:LEU:HB2	2:D:566:LEU:HB2	1.90	0.53
2:B:468:CYS:SG	2:B:536:VAL:HG23	2.49	0.53
1:C:33:LEU:CB	1:C:34:ASN:HA	2.33	0.53
2:B:631:HIS:ND1	2:B:649:ALA:CB	2.72	0.52
2:B:534:ARG:HD2	2:B:548:TYR:CE1	2.45	0.52
1:C:137:ALA:O	1:C:141:LEU:HB2	2.09	0.52
2:B:696:ILE:CD1	2:B:709:ILE:HD12	2.39	0.52
2:D:481:VAL:HG21	2:D:543:VAL:HG21	1.91	0.52
2:B:594:ILE:HB	2:B:628:LEU:HB2	1.91	0.52
2:D:408:ASP:OD2	2:D:411:ASN:HB2	2.08	0.52
1:C:7:VAL:HB	1:C:76:VAL:HG22	1.91	0.52
1:A:18:VAL:HG22	1:A:19:ASP:H	1.75	0.52
2:B:327:SER:O	2:B:328:PRO:C	2.49	0.52
2:B:535:THR:HG21	2:B:575:SER:N	2.24	0.52
1:A:26:SER:HB3	1:A:29:LEU:HB2	1.92	0.51
2:B:457:HIS:CD2	2:B:495:PRO:HG2	2.45	0.51
2:B:696:ILE:CD1	2:B:709:ILE:CD1	2.87	0.51
2:B:590:MET:HG3	2:B:634:LEU:HD22	1.92	0.51
2:D:709:ILE:HG22	2:D:710:LEU:HD13	1.93	0.51
2:B:445:VAL:HB	2:B:459:PHE:HB2	1.93	0.50
2:B:483:GLY:HA2	2:B:489:LEU:HD23	1.93	0.50
2:B:310:ARG:C	2:B:312:SER:H	2.19	0.50
2:B:635:VAL:CG1	2:B:647:SER:HB2	2.41	0.50
2:D:474:TYR:O	2:D:475:LYS:C	2.54	0.50
1:C:97:HIS:HE1	1:C:120:ASP:OD1	1.95	0.50
1:C:135:ILE:HG23	1:C:147:LEU:HD12	1.94	0.50
1:C:154:VAL:HG11	2:D:286:ILE:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:487:ASN:ND2	2:D:531:ALA:HA	2.26	0.50
1:A:89:LYS:HG2	1:A:123:PHE:CE1	2.47	0.49
1:C:161:ARG:CZ	1:C:165:GLU:HB3	2.42	0.49
2:D:337:LYS:HA	2:D:340:GLN:HE21	1.77	0.49
2:D:585:CYS:HB3	2:D:597:TRP:HB2	1.94	0.49
1:A:161:ARG:NH1	1:A:165:GLU:OE2	2.45	0.49
2:B:299:LEU:HD23	2:B:306:ASN:HA	1.94	0.49
2:D:449:ASP:OD1	2:D:452:LYS:HE3	2.11	0.49
2:D:668:TYR:OH	2:D:702:GLY:HA2	2.12	0.49
2:B:487:ASN:N	2:B:487:ASN:HD22	2.09	0.49
2:D:335:ASN:ND2	2:D:347:GLN:HE21	2.11	0.49
2:D:526:LEU:HG	2:D:555:TRP:CE3	2.48	0.49
2:B:487:ASN:HA	2:B:531:ALA:O	2.12	0.49
2:B:655:ARG:HG2	2:B:667:SER:HB3	1.93	0.49
2:D:317:LYS:HG3	2:D:331:PHE:CZ	2.48	0.49
2:B:591:ASP:O	2:B:592:THR:HG22	2.13	0.49
2:D:392:ASP:O	2:D:393:ASN:HB2	2.13	0.49
1:A:6:VAL:HG12	1:A:7:VAL:N	2.27	0.48
1:A:132:TYR:CE1	2:B:278:LEU:HD13	2.49	0.48
2:D:389:GLN:HE21	2:D:430:TYR:H	1.61	0.48
2:D:568:GLY:HA3	2:D:595:ARG:NH1	2.28	0.48
2:B:726:LEU:HB3	2:B:741:LEU:HB2	1.95	0.48
2:B:670:HIS:CE1	2:B:688:SER:OG	2.66	0.48
1:A:128:GLN:HB3	2:B:274:LEU:HD11	1.94	0.48
1:A:172:ILE:HD11	2:B:302:SER:HB2	1.96	0.48
2:D:278:LEU:O	2:D:279:PRO:C	2.55	0.48
1:A:130:MET:HE2	1:A:134:ILE:CG1	2.40	0.48
2:B:448:TRP:CZ3	2:B:455:CYS:HB2	2.48	0.48
2:B:547:SER:HB3	2:B:549:ASP:OD1	2.13	0.48
2:D:426:TRP:HD1	2:D:467:ARG:CD	2.27	0.48
2:D:677:THR:O	2:D:677:THR:HG22	2.12	0.48
1:A:162:SER:OG	1:A:165:GLU:HG3	2.14	0.48
1:C:132:TYR:CD1	2:D:278:LEU:HD13	2.49	0.48
1:A:167:ARG:CG	1:A:172:ILE:O	2.62	0.48
1:A:177:THR:O	1:A:178:PRO:C	2.57	0.47
2:D:691:GLU:O	2:D:692:ASN:HB2	2.13	0.47
2:B:483:GLY:CA	2:B:489:LEU:HD23	2.44	0.47
1:C:25:ARG:HH21	1:C:102:PHE:HD1	1.62	0.47
2:D:389:GLN:HG2	2:D:428:LEU:CD1	2.43	0.47
2:B:526:LEU:HD11	2:B:560:MET:SD	2.54	0.47
1:C:117:ASP:N	1:C:117:ASP:OD1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:329:LYS:HD3	2:D:581:GLU:HG3	1.96	0.47
2:D:512:VAL:HG11	2:D:514:HIS:CE1	2.49	0.47
2:B:586:ILE:HG12	2:B:596:ILE:HD12	1.97	0.47
1:A:93:TRP:CE2	1:A:97:HIS:CD2	3.02	0.47
2:B:272:ARG:O	2:B:274:LEU:HD12	2.15	0.47
1:C:33:LEU:HB3	1:C:34:ASN:CA	2.33	0.47
2:B:534:ARG:O	2:B:534:ARG:HG3	2.15	0.47
2:D:592:THR:O	2:D:592:THR:CG2	2.62	0.47
2:B:464:SER:OG	2:B:465:THR:N	2.46	0.47
2:D:590:MET:HE3	2:D:590:MET:HA	1.96	0.47
1:C:166:ILE:HG21	2:D:301:VAL:HG21	1.97	0.47
1:A:128:GLN:NE2	2:B:271:LYS:HB3	2.29	0.47
2:B:459:PHE:HB3	2:B:492:TRP:CZ3	2.50	0.47
2:D:429:LYS:HG2	2:D:471:ILE:HD12	1.96	0.47
2:D:557:VAL:O	2:D:557:VAL:HG13	2.15	0.47
1:A:171:ASN:O	1:A:171:ASN:CG	2.58	0.46
2:B:489:LEU:HD21	2:B:533:VAL:HG11	1.98	0.46
1:C:121:ARG:NH1	1:C:121:ARG:CG	2.60	0.46
2:D:395:VAL:C	2:D:396:ILE:HG13	2.40	0.46
2:D:592:THR:O	2:D:592:THR:HG23	2.14	0.46
2:D:389:GLN:HG2	2:D:428:LEU:HD12	1.96	0.46
1:A:6:VAL:HG11	1:A:77:MET:SD	2.56	0.46
1:C:97:HIS:CE1	1:C:120:ASP:OD1	2.69	0.46
2:B:473:GLU:HG3	2:B:478:LYS:HG3	1.98	0.46
2:D:481:VAL:HG11	2:D:543:VAL:HG11	1.98	0.46
2:B:484:SER:C	2:B:486:ASP:N	2.74	0.46
2:D:401:ASP:O	2:D:402:LYS:HB2	2.15	0.46
1:A:170:PHE:HB3	2:B:272:ARG:O	2.16	0.46
2:D:380:HIS:NE2	2:D:405:ARG:HG3	2.31	0.46
2:D:431:ALA:O	2:D:432:HIS:C	2.59	0.46
2:B:487:ASN:HB3	2:B:529:HIS:O	2.15	0.46
2:B:519:ASN:ND2	2:B:521:TYR:H	2.13	0.46
2:D:670:HIS:O	2:D:672:ASN:O	2.33	0.46
2:D:721:PHE:HB3	2:D:726:LEU:CD1	2.46	0.46
2:B:298:SER:HB3	2:B:305:TRP:CZ3	2.52	0.45
2:B:380:HIS:CE1	2:B:397:THR:OG1	2.66	0.45
2:D:429:LYS:CG	2:D:471:ILE:HD12	2.47	0.45
1:A:184:ILE:HD12	1:A:184:ILE:HA	1.78	0.45
2:B:482:THR:HB	2:B:492:TRP:HE1	1.81	0.45
2:B:303:GLN:O	2:B:307:LYS:HB2	2.17	0.45
1:A:80:PRO:O	1:A:82:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:C	1:A:80:PRO:HD3	2.42	0.45
1:C:89:LYS:HG2	1:C:134:ILE:HD11	1.98	0.45
2:D:487:ASN:HD22	2:D:531:ALA:C	2.24	0.45
1:A:154:VAL:HG11	2:B:286:ILE:HD13	1.99	0.45
2:B:600:GLU:O	2:B:605:ASN:CB	2.63	0.45
2:D:442:ASP:O	2:D:443:ARG:HG2	2.16	0.45
1:A:31:ASN:O	1:A:32:TYR:CG	2.70	0.45
2:B:310:ARG:C	2:B:312:SER:N	2.73	0.44
1:C:132:TYR:CE1	2:D:277:SER:HB3	2.52	0.44
2:D:407:TYR:CD1	2:D:738:LEU:HD22	2.52	0.44
2:B:655:ARG:HD3	6:B:746:HOH:O	2.17	0.44
2:B:314:SER:O	2:B:315:LEU:C	2.57	0.44
2:B:481:VAL:HG21	2:B:543:VAL:HG21	1.99	0.44
2:D:346:SER:O	2:D:347:GLN:C	2.59	0.44
2:B:396:ILE:HG21	2:B:436:LEU:HD22	1.99	0.44
2:D:280:PHE:CZ	2:D:284:LEU:HD11	2.53	0.44
2:D:314:SER:O	2:D:318:LYS:HG3	2.17	0.44
1:A:12:GLU:HB2	1:A:84:SER:OG	2.17	0.44
2:B:317:LYS:O	2:B:321:ILE:HG13	2.18	0.44
2:B:668:TYR:OH	2:B:702:GLY:HA2	2.18	0.44
2:D:582:ARG:HD3	2:D:660:ASN:ND2	2.33	0.44
2:B:569:HIS:HD2	2:B:591:ASP:OD2	2.01	0.44
2:B:423:GLY:O	2:B:424:GLY:C	2.60	0.43
2:D:598:ASP:C	2:D:598:ASP:OD1	2.61	0.43
2:D:629:GLN:HG2	2:D:630:GLY:CA	2.24	0.43
2:B:631:HIS:CG	2:B:649:ALA:HB2	2.53	0.43
1:A:79:VAL:HG12	1:A:82:VAL:HB	2.00	0.43
2:B:651:ASP:OD1	2:B:651:ASP:N	2.50	0.43
2:B:658:ASP:O	2:B:662:TYR:HA	2.17	0.43
1:A:19:ASP:HB3	1:A:22:ILE:HD12	2.00	0.43
2:D:443:ARG:HB3	2:D:464:SER:O	2.19	0.43
2:B:698:ASN:OD1	2:B:698:ASN:C	2.61	0.43
1:C:75:ILE:HG23	1:C:76:VAL:HG23	2.01	0.43
2:D:583:LYS:HE3	2:D:583:LYS:HB2	1.72	0.43
2:B:298:SER:HB3	2:B:305:TRP:CE3	2.54	0.43
2:B:724:LYS:H	2:B:724:LYS:HG3	1.45	0.43
2:D:443:ARG:HD2	2:D:464:SER:HA	2.01	0.43
2:D:494:LEU:HD12	2:D:494:LEU:HA	1.88	0.43
2:B:327:SER:HB3	2:B:642:ASP:OD1	2.18	0.43
2:B:637:LEU:HD21	2:B:678:THR:HA	2.01	0.43
1:C:177:THR:O	1:C:178:PRO:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:ARG:O	2:B:348:GLN:HG2	2.19	0.42
2:B:342:TYR:HB3	2:B:345:LEU:HD12	2.01	0.42
1:C:19:ASP:HB3	1:C:22:ILE:HD12	2.00	0.42
1:A:172:ILE:HD11	2:B:302:SER:CB	2.48	0.42
2:B:552:LEU:HG	2:B:573:ILE:HD12	2.00	0.42
1:A:162:SER:O	1:A:166:ILE:HG13	2.18	0.42
2:B:395:VAL:HB	2:B:407:TYR:HB2	2.02	0.42
2:B:591:ASP:OD1	2:B:591:ASP:C	2.61	0.42
2:D:400:ASP:OD1	2:D:426:TRP:CZ3	2.72	0.42
1:A:182:ALA:C	1:A:184:ILE:H	2.27	0.42
1:C:7:VAL:HG11	1:C:15:ARG:HB3	2.01	0.42
1:A:8:LEU:HA	1:A:77:MET:O	2.20	0.42
2:B:605:ASN:OD1	2:B:605:ASN:C	2.63	0.42
2:B:335:ASN:OD1	2:B:347:GLN:NE2	2.45	0.42
2:B:523:VAL:CG1	2:B:560:MET:HE3	2.50	0.42
2:D:404:ILE:HG21	2:D:436:LEU:HD21	2.02	0.42
2:D:426:TRP:HD1	2:D:467:ARG:HD2	1.84	0.42
1:A:128:GLN:HE22	2:B:271:LYS:HB3	1.85	0.42
2:B:326:VAL:HG22	2:B:327:SER:N	2.34	0.41
1:C:86:VAL:CG2	1:C:130:MET:CE	2.53	0.41
2:D:487:ASN:ND2	2:D:531:ALA:CA	2.82	0.41
2:B:421:HIS:CE1	2:B:440:SER:CB	3.03	0.41
2:D:557:VAL:O	2:D:557:VAL:CG1	2.65	0.41
2:D:679:PHE:HA	2:D:687:VAL:O	2.21	0.41
1:C:135:ILE:HG23	1:C:147:LEU:CD1	2.50	0.41
2:D:376:THR:O	2:D:377:LEU:HD23	2.21	0.41
1:A:132:TYR:CZ	2:B:277:SER:HB3	2.56	0.41
1:C:180:GLU:HA	1:C:180:GLU:OE1	2.20	0.41
2:D:316:TRP:CZ2	2:D:352:ARG:HD3	2.55	0.41
2:B:353:LEU:HD22	2:B:353:LEU:HA	1.60	0.41
2:B:359:ILE:HD12	2:B:359:ILE:HA	1.93	0.41
2:B:480:ILE:HD11	2:B:494:LEU:HD12	2.03	0.41
1:A:83:ARG:O	1:A:84:SER:C	2.61	0.41
1:A:148:ASP:O	1:A:149:ALA:C	2.62	0.41
2:B:443:ARG:HG2	2:B:464:SER:C	2.46	0.41
2:B:554:VAL:O	2:B:563:LEU:HB2	2.21	0.41
2:D:469:LEU:C	2:D:469:LEU:HD12	2.46	0.41
2:B:421:HIS:CE1	2:B:440:SER:HB2	2.56	0.41
2:D:390:PHE:C	2:D:391:GLU:HG2	2.47	0.41
2:B:545:SER:O	2:B:552:LEU:HA	2.21	0.40
2:D:721:PHE:HB3	2:D:726:LEU:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:425:VAL:C	2:D:426:TRP:HE3	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	SO4	B	3	-	4,4,4	0.50	0	6,6,6	0.75	0
3	SO4	D	10	-	4,4,4	0.36	0	6,6,6	0.45	0
3	SO4	D	9	-	4,4,4	0.37	0	6,6,6	0.66	0
3	SO4	D	8	-	4,4,4	0.37	0	6,6,6	0.46	0
3	SO4	B	4	-	4,4,4	0.39	0	6,6,6	0.56	0
3	SO4	B	7	-	4,4,4	0.40	0	6,6,6	1.32	0
3	SO4	D	11	-	4,4,4	0.50	0	6,6,6	1.06	0
3	SO4	D	2	-	4,4,4	0.56	0	6,6,6	0.62	0
4	C1C	D	1	-	29,29,29	1.38	3 (10%)	42,42,42	1.39	7 (16%)
5	GOL	D	745	-	5,5,5	0.27	0	5,5,5	1.14	1 (20%)
3	SO4	D	5	-	4,4,4	0.43	0	6,6,6	0.47	0
3	SO4	B	6	-	4,4,4	0.24	0	6,6,6	0.56	0
3	SO4	B	1	-	4,4,4	0.40	0	6,6,6	0.62	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
4	C1C	D	1	-	-	4/12/12/12	0/4/4/4
5	GOL	D	745	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	C1C	C11-C10	-3.82	1.41	1.50
4	D	1	C1C	O26-C24	-2.47	1.23	1.30
4	D	1	C1C	C12-C13	-2.40	1.38	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	C1C	C9-C10-C4	-2.96	116.47	119.04
4	D	1	C1C	O25-C24-C9	-2.65	115.63	121.97
4	D	1	C1C	C8-C7-C3	-2.55	117.03	120.84
5	D	745	GOL	C3-C2-C1	-2.18	103.79	111.80
4	D	1	C1C	C7-C3-C2	-2.08	118.26	123.01
4	D	1	C1C	C9-C10-C11	2.07	125.15	122.48
4	D	1	C1C	C5-C4-C10	-2.06	119.42	122.44
4	D	1	C1C	O23-C21-C16	-2.03	117.12	121.97

There are no chirality outliers.

All (6) torsion outliers are listed below:

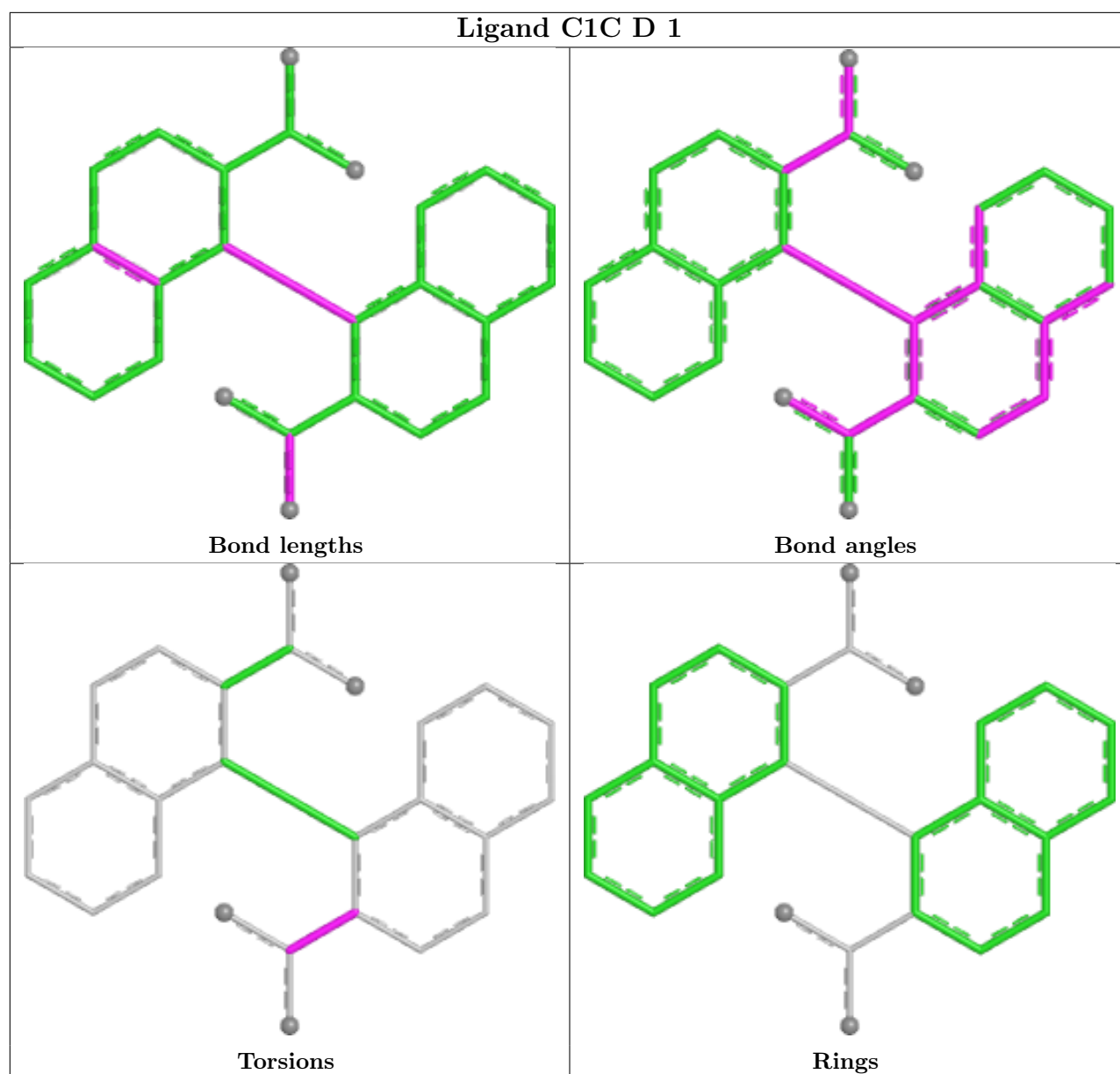
Mol	Chain	Res	Type	Atoms
5	D	745	GOL	O2-C2-C3-O3
5	D	745	GOL	C1-C2-C3-O3
4	D	1	C1C	O26-C24-C9-C8
4	D	1	C1C	O25-C24-C9-C8
4	D	1	C1C	O25-C24-C9-C10
4	D	1	C1C	O26-C24-C9-C10

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	7	SO4	1	0
3	B	1	SO4	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	134/169 (79%)	-0.99	0 100 100	45, 73, 108, 119	0
1	C	132/169 (78%)	-1.46	0 100 100	32, 49, 83, 98	0
2	B	444/464 (95%)	-1.40	0 100 100	32, 56, 89, 110	0
2	D	445/464 (95%)	-1.60	0 100 100	28, 43, 65, 89	0
All	All	1155/1266 (91%)	-1.43	0 100 100	28, 51, 89, 119	0

There are no RSRZ outliers to report.

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 [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	SO4	D	2	5/5	0.97	0.16	68,70,73,74	0
3	SO4	B	3	5/5	0.98	0.07	73,77,79,79	0
3	SO4	B	1	5/5	0.98	0.06	74,76,77,77	0
3	SO4	B	6	5/5	0.99	0.03	57,58,58,59	0

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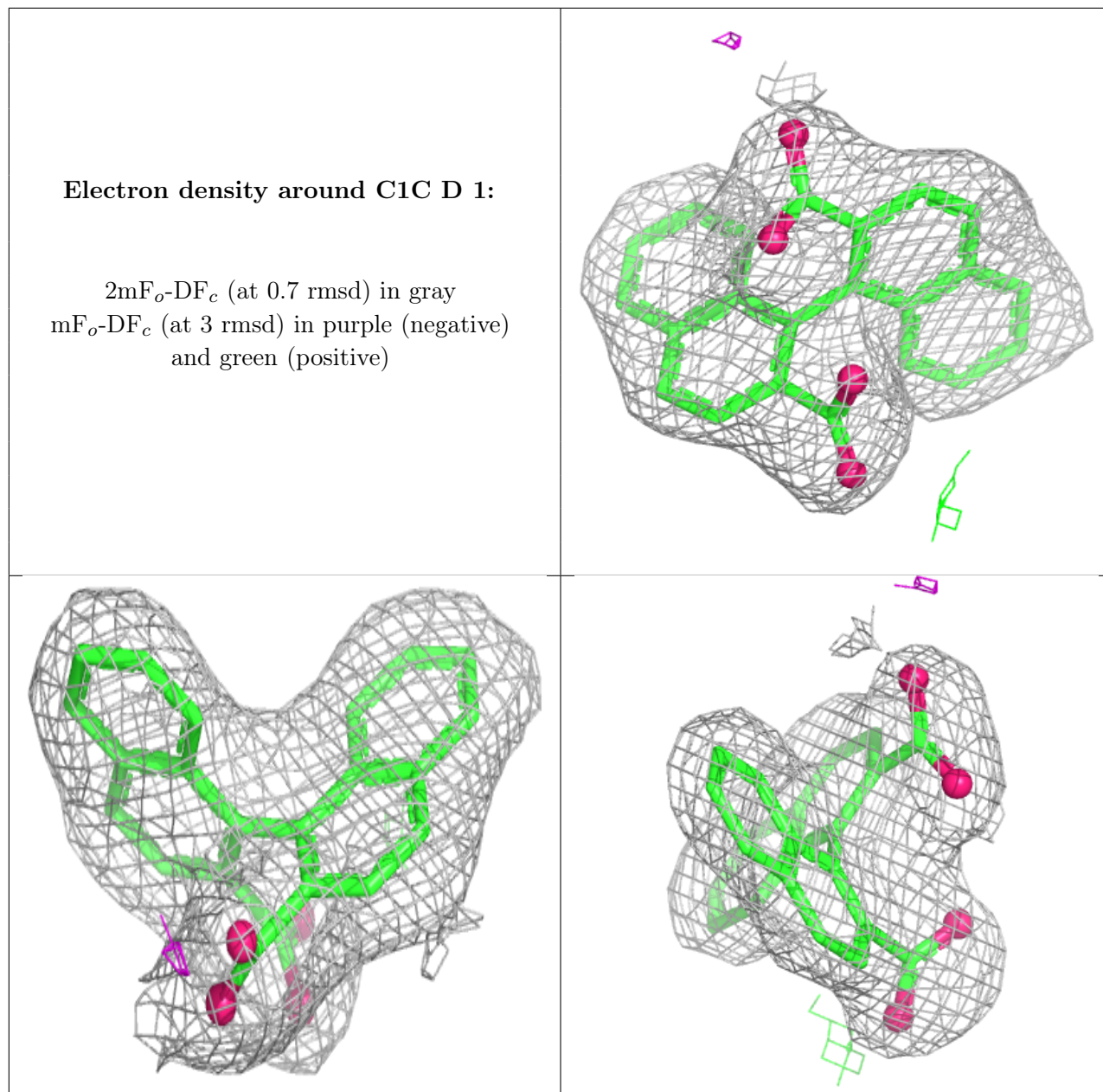
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	7	5/5	0.99	0.09	53,59,61,62	0
3	SO4	B	4	5/5	0.99	0.04	60,61,64,66	0
3	SO4	D	8	5/5	0.99	0.03	65,66,69,69	0
3	SO4	D	10	5/5	0.99	0.05	68,71,73,74	0
3	SO4	D	11	5/5	0.99	0.06	71,74,76,76	0
4	C1C	D	1	26/26	0.99	0.03	37,42,50,57	0
5	GOL	D	745	6/6	0.99	0.05	43,44,47,51	0
3	SO4	D	5	5/5	1.00	0.04	53,56,57,57	0
3	SO4	D	9	5/5	1.00	0.03	75,75,75,76	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 C1C D 1:

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

**6.5 Other polymers** [i](#)

There are no such residues in this entry.