



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 03:10 am BST

PDB ID : 3MKS
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

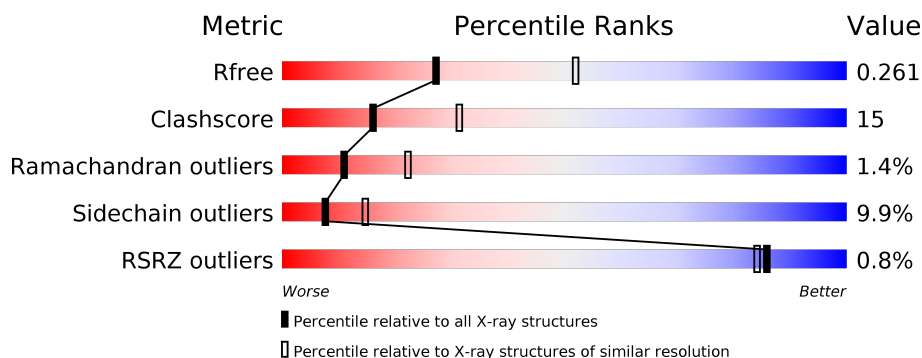
1 Overall quality at a glance ⓘ

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on 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	<div> <div>3%</div> <div> <div></div> <div>50%</div> <div>28%</div> <div>•</div> <div>21%</div> </div> </div>
1	C	169	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>21%</div> <div>• •</div> <div>22%</div> </div> </div>
2	B	464	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>32%</div> <div>5%</div> <div>• • •</div> </div> </div>
2	D	464	<div> <div></div> <div> <div></div> <div>66%</div> <div>24%</div> <div>5%</div> <div>• • •</div> </div> </div>

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

Continued on next page...

Continued from previous page...

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:

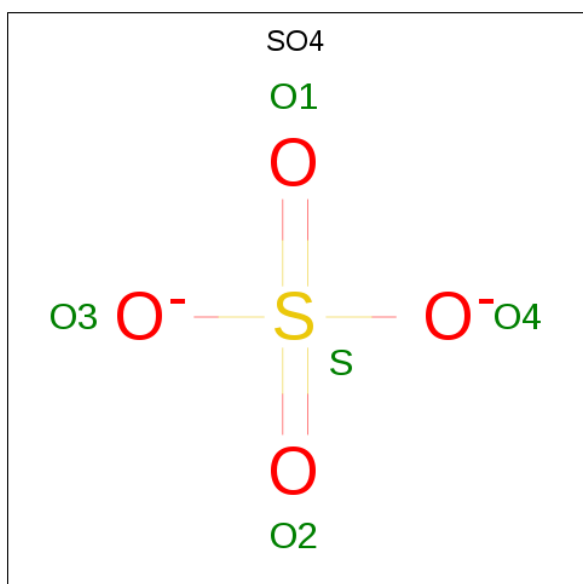
Chain	Residue	Modelled	Actual	Comment	Reference
B	261	GLY	-	EXPRESSION TAG	UNP P07834
B	262	ALA	-	EXPRESSION TAG	UNP P07834
B	460	GLU	LYS	SEE REMARK 999	UNP P07834
B	?	-	ASN	DELETION	UNP P07834
B	?	-	ILE	DELETION	UNP P07834
B	?	-	TRP	DELETION	UNP P07834
B	?	-	ASN	DELETION	UNP P07834
B	?	-	CYS	DELETION	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

Continued on next page...

Continued from previous page...

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 (three-letter code: SO4) (formula: O₄S).



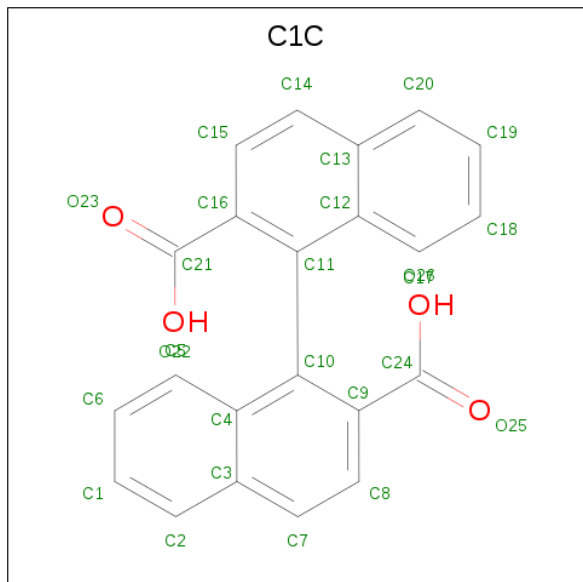
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

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 (three-letter code: 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		

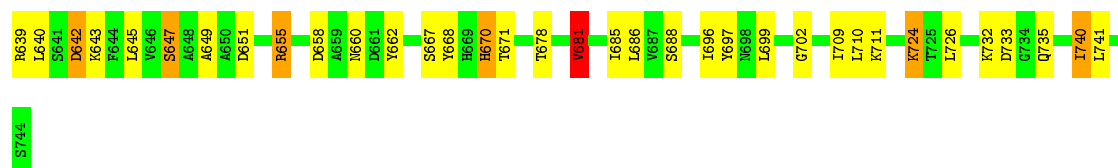
- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

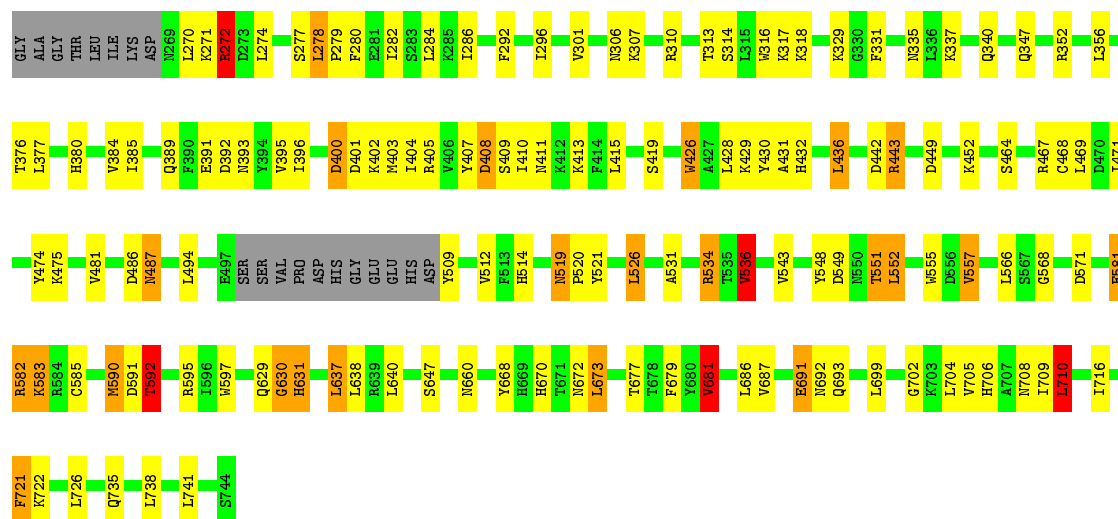
- Molecule 6 is water.

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 2: Cell division control protein 4

Chain D: 66% 24% 5%



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 20.45 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (93.66-2.60) 99.9 (20.45-2.60)	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 0.209 , 0.261	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)	0.32 , 20.0	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	0.76	0/1101	0.83	0/1487
1	C	1.04	2/1091 (0.2%)	1.04	3/1473 (0.2%)
2	B	0.88	1/3663 (0.0%)	0.96	11/4957 (0.2%)
2	D	0.97	3/3672 (0.1%)	1.03	16/4969 (0.3%)
All	All	0.93	6/9527 (0.1%)	0.98	30/12886 (0.2%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	156	GLU	CG-CD	8.81	1.65	1.51
2	D	721	PHE	CE2-CZ	6.29	1.49	1.37
2	D	391	GLU	CD-OE2	5.71	1.31	1.25
2	D	581	GLU	CG-CD	5.61	1.60	1.51
1	C	156	GLU	CB-CG	5.58	1.62	1.52
2	B	697	TYR	CE2-CZ	5.01	1.45	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	ARG	NE-CZ-NH2	-8.66	115.97	120.30
2	D	681	VAL	CB-CA-C	-7.25	97.62	111.40
2	D	571	ASP	CB-CG-OD1	6.94	124.54	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	356	LEU	CB-CG-CD1	-6.92	99.23	111.00
1	C	141	LEU	CA-CB-CG	6.50	130.26	115.30
2	B	408	ASP	CB-CG-OD2	6.45	124.10	118.30
2	B	273	ASP	CB-CG-OD1	6.40	124.06	118.30
2	D	408	ASP	CB-CG-OD1	6.40	124.06	118.30
2	D	590	MET	CG-SD-CE	6.34	110.35	100.20
2	D	673	LEU	CA-CB-CG	-6.31	100.79	115.30
2	D	536	VAL	CB-CA-C	-6.25	99.53	111.40
2	B	378	ARG	NE-CZ-NH1	6.11	123.35	120.30
2	D	571	ASP	CB-CG-OD2	-6.05	112.86	118.30
2	D	710	LEU	CA-CB-CG	5.88	128.82	115.30
2	B	681	VAL	CB-CA-C	-5.86	100.27	111.40
1	C	118	SER	N-CA-C	5.85	126.80	111.00
2	D	637	LEU	CA-CB-CG	5.62	128.23	115.30
2	B	608	LEU	CA-CB-CG	5.60	128.17	115.30
2	B	273	ASP	CB-CG-OD2	-5.58	113.28	118.30
2	D	436	LEU	CA-CB-CG	5.56	128.09	115.30
2	B	655	ARG	NE-CZ-NH1	5.55	123.07	120.30
2	D	582	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	B	655	ARG	NE-CZ-NH2	-5.39	117.60	120.30
2	D	436	LEU	CB-CG-CD2	-5.38	101.85	111.00
2	B	374	ARG	NE-CZ-NH2	-5.37	117.62	120.30
2	B	582	ARG	NE-CZ-NH2	-5.35	117.63	120.30
2	D	469	LEU	CA-CB-CG	5.30	127.49	115.30
2	D	272	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	D	630	GLY	N-CA-C	-5.10	100.34	113.10
2	B	639	ARG	NE-CZ-NH1	-5.03	117.79	120.30

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	38	0
1	C	1073	0	1082	39	0
2	B	3582	0	3581	119	0
2	D	3591	0	3589	94	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	273	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 (273) 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
1:C:86:VAL:HG22	1:C:130:MET:HE1	1.20	1.14
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:CE	1.87	1.05
1:C:31:ASN:O	1:C:33:LEU:HA	1.58	1.01
1:A:86:VAL:HG22	1:A:130:MET:HE3	0.99	0.97
1:A:86:VAL:CG2	1:A:130:MET:HE3	1.94	0.96
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: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
1:C:86:VAL:HG22	1:C:130:MET:HE3	1.54	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
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:C	2:D:519:ASN:HD22	1.84	0.81
1:C:86:VAL:CG2	1:C:130:MET:CE	2.53	0.81
2:D:519:ASN:ND2	2:D:521:TYR:H	1.78	0.81
1:C:86:VAL:CG2	1:C:130:MET:HE1	2.09	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:86:VAL:CG2	1:C:130:MET:HE3	2.19	0.72
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
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:557:VAL:HG13	2:B:560:MET:HE1	1.78	0.64
2:B:491:VAL:HG11	2:B:560:MET:HE1	1.79	0.63
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:D:519:ASN:ND2	2:D:519:ASN:C	2.50	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:491:VAL:HG11	2:B:560:MET:CE	2.34	0.56
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:740:ILE:HD12	2:B:740:ILE:C	2.26	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:484:SER:C	2:B:486:ASP:H	2.09	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
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:635:VAL:CG1	2:B:647:SER:HB2	2.41	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
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:HD22	2:B:487:ASN:N	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
1:A:130:MET:HE2	1:A:134:ILE:HG13	1.94	0.49
2:B:327:SER:O	2:B:328:PRO:C	2.49	0.49
2:D:442:ASP:C	2:D:443:ARG:HG2	2.33	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:130:MET:CE	1:A:134:ILE:HG13	2.43	0.48
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:732:LYS:O	2:B:733:ASP:C	2.52	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
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:OD1	1:C:117:ASP:N	2.46	0.47
2:D:512:VAL:HG11	2:D:514:HIS:CE1	2.49	0.47
2:D:329:LYS:HD3	2:D:581:GLU:HG3	1.96	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:HG3	2:B:534:ARG:O	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
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:HG13	2:D:557:VAL:O	2.15	0.47
2:B:489:LEU:HD21	2:B:533:VAL:HG11	1.98	0.46
1:C:121:ARG:CG	1:C:121:ARG:NH1	2.60	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:310:ARG:C	2:B:312:SER:H	2.19	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:HA	1:A:184:ILE:HD12	1.78	0.45
2:B:482:THR:HB	2:B:492:TRP:HE1	1.81	0.45
2:D:474:TYR:O	2:D:475:LYS:C	2.54	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
1:C:89:LYS:HG2	1:C:134:ILE:HD11	1.98	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
1:C:132:TYR:CE1	2:D:277:SER:HB3	2.52	0.44
2:D:557:VAL:O	2:D:557:VAL:CG1	2.65	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:481:VAL:HG21	2:B:543:VAL:HG21	1.99	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: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:N	2:B:651:ASP:OD1	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:278:LEU:O	2:D:279:PRO:C	2.55	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:443:ARG:HB3	2:D:464:SER:O	2.19	0.43
1:C:75:ILE:HG23	1:C:76:VAL:HG23	2.01	0.43
2:D:583:LYS:HB2	2:D:583:LYS:HE3	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
1:A:177:THR:O	1:A:178:PRO:C	2.57	0.43
2:B:637:LEU:HD21	2:B:678:THR:HA	2.01	0.43
2:B:327:SER:HB3	2:B:642:ASP:OD1	2.18	0.43
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:D:400:ASP:OD1	2:D:426:TRP:CZ3	2.72	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:335:ASN:OD1	2:B:347:GLN:NE2	2.45	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
1:A:171:ASN:CG	1:A:171:ASN:O	2.58	0.42
2:D:395:VAL:C	2:D:396:ILE:HG13	2.40	0.42
2:B:326:VAL:HG22	2:B:327:SER:N	2.34	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:B:484:SER:C	2:B:486:ASP:N	2.74	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:OE1	1:C:180:GLU:HA	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
2:D:431:ALA:O	2:D:432:HIS:C	2.59	0.41
2:B:554:VAL:O	2:B:563:LEU:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:HIS:CE1	2:B:440:SER:HB2	2.56	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
1:A:78:PRO:C	1:A:80:PRO:HD3	2.42	0.40
2:D:487:ASN:HD22	2:D:531:ALA:C	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	128/169 (76%)	112 (88%)	14 (11%)	2 (2%)	9	19
1	C	126/169 (75%)	119 (94%)	5 (4%)	2 (2%)	9	19
2	B	440/464 (95%)	404 (92%)	27 (6%)	9 (2%)	7	14
2	D	441/464 (95%)	418 (95%)	20 (4%)	3 (1%)	22	43
All	All	1135/1266 (90%)	1053 (93%)	66 (6%)	16 (1%)	11	22

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	PRO
2	B	462	HIS
2	B	476	ASN
2	B	711	LYS
1	C	116	VAL
2	B	485	ARG
2	B	592	THR
1	C	98	ARG
2	D	631	HIS
2	B	605	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	424	GLY
2	B	630	GLY
2	D	487	ASN
1	A	75	ILE
2	D	592	THR
2	B	528	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	121/152 (80%)	110 (91%)	11 (9%)	9	18
1	C	120/152 (79%)	109 (91%)	11 (9%)	9	17
2	B	400/416 (96%)	352 (88%)	48 (12%)	5	9
2	D	401/416 (96%)	368 (92%)	33 (8%)	11	22
All	All	1042/1136 (92%)	939 (90%)	103 (10%)	8	15

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	98	ARG
1	A	99	ASP
1	A	112	LYS
1	A	121	ARG
1	A	122	GLU
1	A	141	LEU
1	A	144	LYS
1	A	172	ILE
1	A	179	GLU
1	A	184	ILE
2	B	278	LEU
2	B	282	ILE
2	B	284	LEU
2	B	285	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	302	SER
2	B	303	GLN
2	B	314	SER
2	B	329	LYS
2	B	333	SER
2	B	335	ASN
2	B	348	GLN
2	B	353	LEU
2	B	359	ILE
2	B	363	LYS
2	B	462	HIS
2	B	469	LEU
2	B	476	ASN
2	B	477	ILE
2	B	482	THR
2	B	485	ARG
2	B	492	TRP
2	B	493	LYS
2	B	496	LYS
2	B	508	ASP
2	B	509	TYR
2	B	519	ASN
2	B	525	VAL
2	B	535	THR
2	B	539	HIS
2	B	567	SER
2	B	571	ASP
2	B	592	THR
2	B	597	TRP
2	B	607	GLU
2	B	634	LEU
2	B	640	LEU
2	B	642	ASP
2	B	643	LYS
2	B	647	SER
2	B	660	ASN
2	B	670	HIS
2	B	671	THR
2	B	681	VAL
2	B	699	LEU
2	B	710	LEU
2	B	724	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	735	GLN
2	B	740	ILE
1	C	18	VAL
1	C	21	LYS
1	C	26	SER
1	C	89	LYS
1	C	98	ARG
1	C	116	VAL
1	C	117	ASP
1	C	121	ARG
1	C	141	LEU
1	C	168	ARG
1	C	185	ARG
2	D	272	ARG
2	D	278	LEU
2	D	282	ILE
2	D	307	LYS
2	D	384	VAL
2	D	385	ILE
2	D	400	ASP
2	D	413	LYS
2	D	426	TRP
2	D	443	ARG
2	D	519	ASN
2	D	526	LEU
2	D	534	ARG
2	D	536	VAL
2	D	551	THR
2	D	552	LEU
2	D	557	VAL
2	D	583	LYS
2	D	590	MET
2	D	592	THR
2	D	637	LEU
2	D	640	LEU
2	D	673	LEU
2	D	681	VAL
2	D	691	GLU
2	D	693	GLN
2	D	699	LEU
2	D	704	LEU
2	D	708	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	710	LEU
2	D	716	ILE
2	D	722	LYS
2	D	735	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	31	ASN
1	A	128	GLN
2	B	303	GLN
2	B	335	ASN
2	B	347	GLN
2	B	348	GLN
2	B	364	ASN
2	B	380	HIS
2	B	389	GLN
2	B	411	ASN
2	B	417	GLN
2	B	457	HIS
2	B	476	ASN
2	B	487	ASN
2	B	519	ASN
2	B	569	HIS
2	B	670	HIS
2	B	692	ASN
2	B	695	ASN
2	B	706	HIS
2	B	708	ASN
1	C	31	ASN
1	C	88	GLN
1	C	97	HIS
2	D	304	ASN
2	D	306	ASN
2	D	335	ASN
2	D	340	GLN
2	D	364	ASN
2	D	393	ASN
2	D	417	GLN
2	D	457	HIS
2	D	463	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	487	ASN
2	D	519	ASN
2	D	559	GLN
2	D	629	GLN
2	D	660	ASN
2	D	693	GLN
2	D	706	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	4	-	4,4,4	0.29	0	6,6,6	0.56	0
3	SO4	D	8	-	4,4,4	0.27	0	6,6,6	0.49	0
3	SO4	B	7	-	4,4,4	0.34	0	6,6,6	1.42	0
3	SO4	D	11	-	4,4,4	0.41	0	6,6,6	1.06	0
3	SO4	B	3	-	4,4,4	0.41	0	6,6,6	0.74	0
4	C1C	D	1	-	25,29,29	1.60	4 (16%)	34,42,42	1.65	9 (26%)
3	SO4	D	9	-	4,4,4	0.26	0	6,6,6	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	2	-	4,4,4	0.48	0	6,6,6	0.63	0
5	GOL	D	745	-	5,5,5	0.25	0	5,5,5	1.06	1 (20%)
3	SO4	B	1	-	4,4,4	0.29	0	6,6,6	0.61	0
3	SO4	B	6	-	4,4,4	0.16	0	6,6,6	0.60	0
3	SO4	D	5	-	4,4,4	0.33	0	6,6,6	0.47	0
3	SO4	D	10	-	4,4,4	0.26	0	6,6,6	0.44	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
5	GOL	D	745	-	-	2/4/4/4	-
4	C1C	D	1	-	-	0/4/12/12	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	C1C	C16-C21	3.73	1.51	1.47
4	D	1	C1C	C11-C10	-3.67	1.41	1.50
4	D	1	C1C	C9-C24	2.76	1.50	1.47
4	D	1	C1C	C12-C13	-2.45	1.38	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	C1C	C9-C10-C4	-3.71	116.47	119.63
4	D	1	C1C	C15-C16-C21	-3.34	115.23	120.20
4	D	1	C1C	C8-C9-C10	3.14	122.51	119.36
4	D	1	C1C	C8-C7-C3	-2.45	117.03	120.82
4	D	1	C1C	C16-C11-C12	-2.41	117.58	119.63
4	D	1	C1C	C9-C10-C11	2.13	125.15	121.47
4	D	1	C1C	C7-C3-C2	-2.11	118.26	123.19
4	D	1	C1C	C5-C4-C10	-2.07	119.42	122.47
5	D	745	GOL	C3-C2-C1	-2.04	103.79	111.70
4	D	1	C1C	C8-C9-C24	-2.01	117.21	120.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

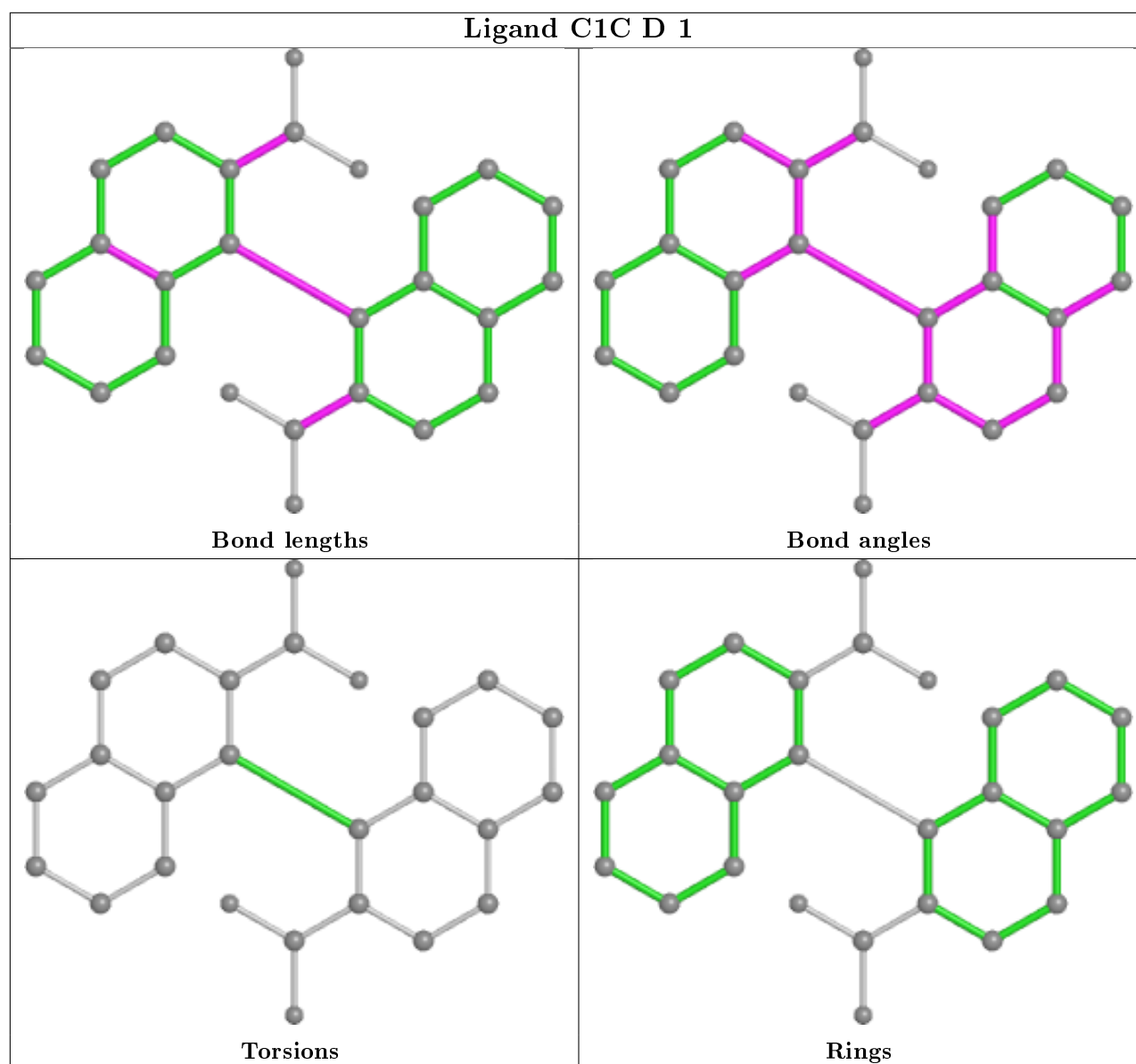
Mol	Chain	Res	Type	Atoms
5	D	745	GOL	O2-C2-C3-O3
5	D	745	GOL	C1-C2-C3-O3

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%)	0.08	5 (3%) 41 34	45, 73, 108, 119	0
1	C	132/169 (78%)	-0.09	1 (0%) 86 84	32, 49, 83, 98	0
2	B	444/464 (95%)	-0.07	3 (0%) 87 86	32, 56, 89, 110	0
2	D	445/464 (95%)	-0.12	0 100 100	28, 43, 65, 89	0
All	All	1155/1266 (91%)	-0.07	9 (0%) 86 84	28, 51, 89, 119	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	631	HIS	3.6
2	B	509	TYR	3.2
1	A	104	ASP	3.1
1	A	75	ILE	2.9
2	B	533	VAL	2.9
1	A	103	PRO	2.7
1	A	168	ARG	2.1
1	A	112	LYS	2.1
1	C	184	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

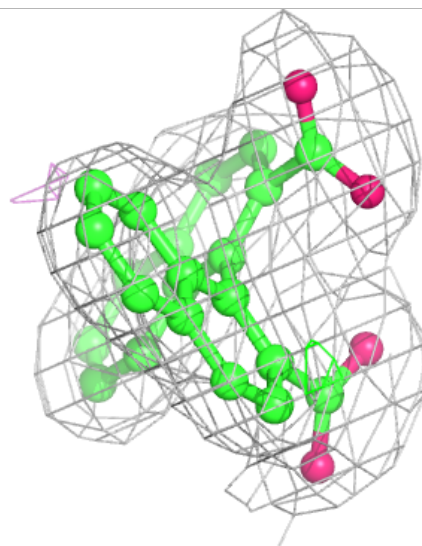
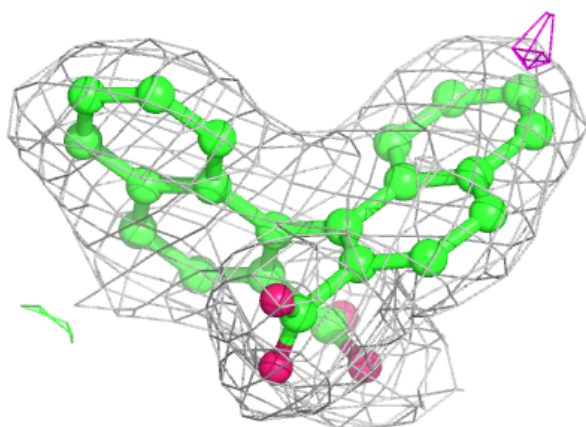
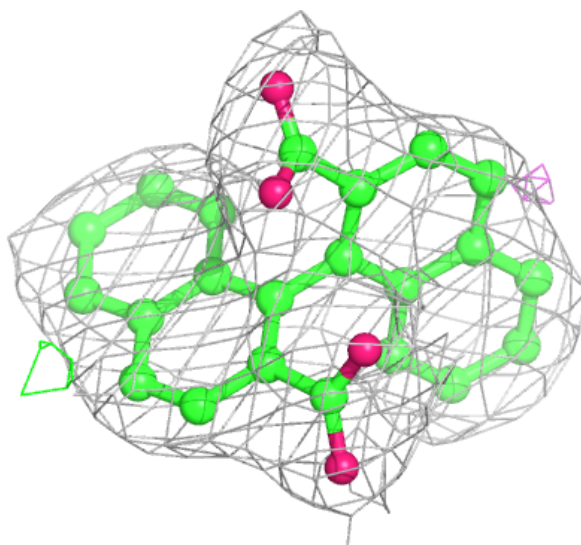
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	B	3	5/5	0.88	0.19	73,77,79,79	0
5	GOL	D	745	6/6	0.92	0.18	43,44,47,51	0
3	SO4	B	1	5/5	0.93	0.16	74,76,77,77	0
3	SO4	D	10	5/5	0.93	0.13	68,71,73,74	0
3	SO4	B	4	5/5	0.94	0.11	60,61,64,66	0
3	SO4	D	9	5/5	0.95	0.15	75,75,75,76	0
3	SO4	D	2	5/5	0.95	0.35	68,70,73,74	0
3	SO4	D	8	5/5	0.95	0.13	65,66,69,69	0
3	SO4	B	7	5/5	0.95	0.14	53,59,61,62	0
3	SO4	D	11	5/5	0.95	0.14	71,74,76,76	0
3	SO4	B	6	5/5	0.98	0.12	57,58,58,59	0
3	SO4	D	5	5/5	0.98	0.13	53,56,57,57	0
4	C1C	D	1	26/26	0.98	0.15	37,42,50,57	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.