



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:55 AM UTC

PDB ID : 6JVU / pdb_00006jvu
Title : Crystal structure of Klebsiella pneumoniae CysE in complex with L-cysteine
Authors : Verma, D.; Gupta, V.
Deposited on : 2019-04-17
Resolution : 2.80 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

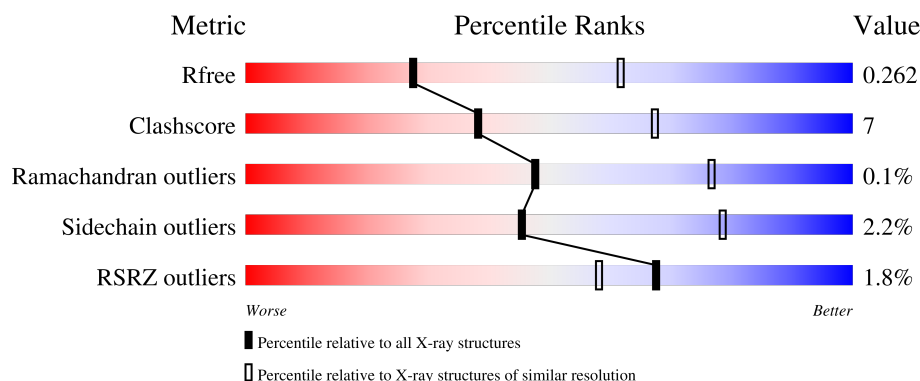
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	281	0% 78% 12% • 9%
1	B	281	73% 16% • 10%
1	C	281	3% 79% 10% • 10%
1	D	281	2% 78% 11% • 9%
1	E	281	0% 75% 13% • 11%

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Mol	Chain	Length	Quality of chain
1	F	281	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CYS	E	601	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10987 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 Serine acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	1	0
			1855	1172	328	344	11			
1	B	253	Total	C	N	O	S	0	1	0
			1868	1184	329	344	11			
1	C	252	Total	C	N	O	S	0	0	0
			1813	1146	317	340	10			
1	D	255	Total	C	N	O	S	0	0	0
			1842	1161	323	348	10			
1	E	251	Total	C	N	O	S	0	0	0
			1812	1142	321	339	10			
1	F	251	Total	C	N	O	S	0	0	0
			1691	1053	299	330	9			

There are 48 discrepancies between the modelled and reference sequences:

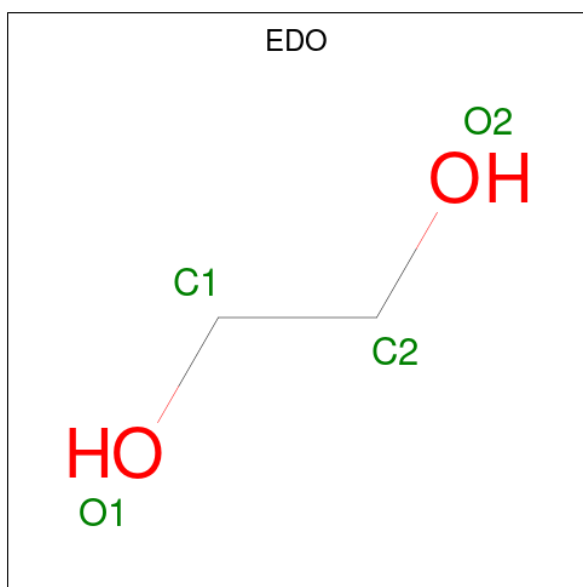
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ALA	-	expression tag	UNP Q0ZB96
A	-6	SER	-	expression tag	UNP Q0ZB96
A	-5	HIS	-	expression tag	UNP Q0ZB96
A	-4	HIS	-	expression tag	UNP Q0ZB96
A	-3	HIS	-	expression tag	UNP Q0ZB96
A	-2	HIS	-	expression tag	UNP Q0ZB96
A	-1	HIS	-	expression tag	UNP Q0ZB96
A	0	HIS	-	expression tag	UNP Q0ZB96
B	-7	ALA	-	expression tag	UNP Q0ZB96
B	-6	SER	-	expression tag	UNP Q0ZB96
B	-5	HIS	-	expression tag	UNP Q0ZB96
B	-4	HIS	-	expression tag	UNP Q0ZB96
B	-3	HIS	-	expression tag	UNP Q0ZB96
B	-2	HIS	-	expression tag	UNP Q0ZB96
B	-1	HIS	-	expression tag	UNP Q0ZB96
B	0	HIS	-	expression tag	UNP Q0ZB96
C	-7	ALA	-	expression tag	UNP Q0ZB96

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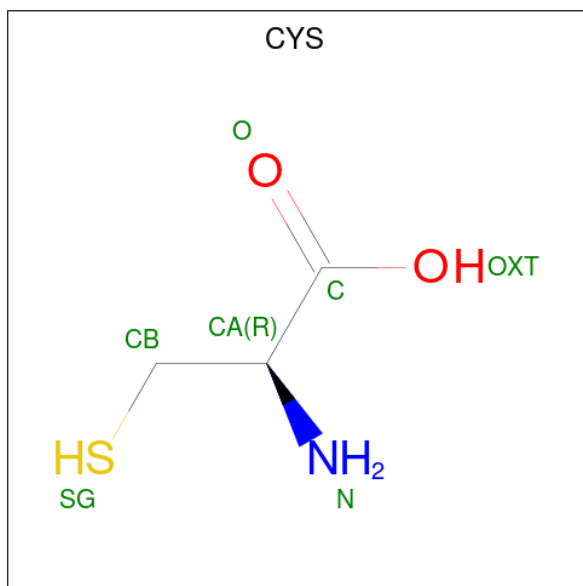
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	SER	-	expression tag	UNP Q0ZB96
C	-5	HIS	-	expression tag	UNP Q0ZB96
C	-4	HIS	-	expression tag	UNP Q0ZB96
C	-3	HIS	-	expression tag	UNP Q0ZB96
C	-2	HIS	-	expression tag	UNP Q0ZB96
C	-1	HIS	-	expression tag	UNP Q0ZB96
C	0	HIS	-	expression tag	UNP Q0ZB96
D	-7	ALA	-	expression tag	UNP Q0ZB96
D	-6	SER	-	expression tag	UNP Q0ZB96
D	-5	HIS	-	expression tag	UNP Q0ZB96
D	-4	HIS	-	expression tag	UNP Q0ZB96
D	-3	HIS	-	expression tag	UNP Q0ZB96
D	-2	HIS	-	expression tag	UNP Q0ZB96
D	-1	HIS	-	expression tag	UNP Q0ZB96
D	0	HIS	-	expression tag	UNP Q0ZB96
E	-7	ALA	-	expression tag	UNP Q0ZB96
E	-6	SER	-	expression tag	UNP Q0ZB96
E	-5	HIS	-	expression tag	UNP Q0ZB96
E	-4	HIS	-	expression tag	UNP Q0ZB96
E	-3	HIS	-	expression tag	UNP Q0ZB96
E	-2	HIS	-	expression tag	UNP Q0ZB96
E	-1	HIS	-	expression tag	UNP Q0ZB96
E	0	HIS	-	expression tag	UNP Q0ZB96
F	-7	ALA	-	expression tag	UNP Q0ZB96
F	-6	SER	-	expression tag	UNP Q0ZB96
F	-5	HIS	-	expression tag	UNP Q0ZB96
F	-4	HIS	-	expression tag	UNP Q0ZB96
F	-3	HIS	-	expression tag	UNP Q0ZB96
F	-2	HIS	-	expression tag	UNP Q0ZB96
F	-1	HIS	-	expression tag	UNP Q0ZB96
F	0	HIS	-	expression tag	UNP Q0ZB96

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CYSTEINE (CCD ID: CYS) (formula: $C_3H_7NO_2S$) (labeled as "Ligand of Interest" by depositor).



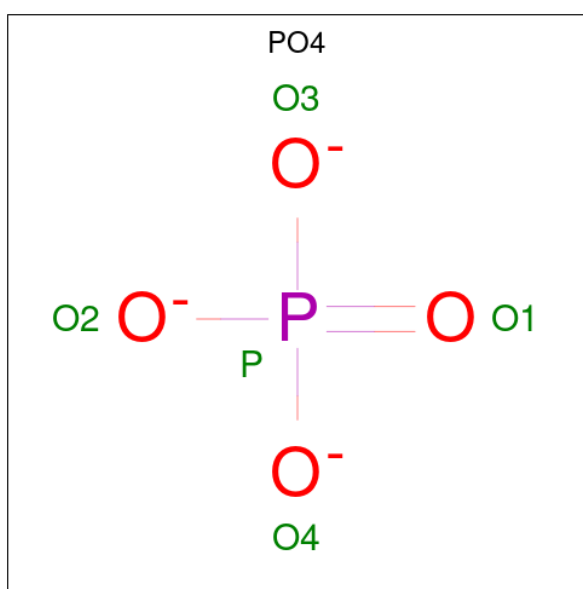
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
3	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
3	D	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
3	E	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
3	E	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

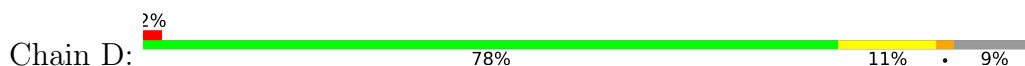
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	O	0	0
			12	12		
5	B	14	Total	O	0	0
			14	14		
5	C	3	Total	O	0	0
			3	3		

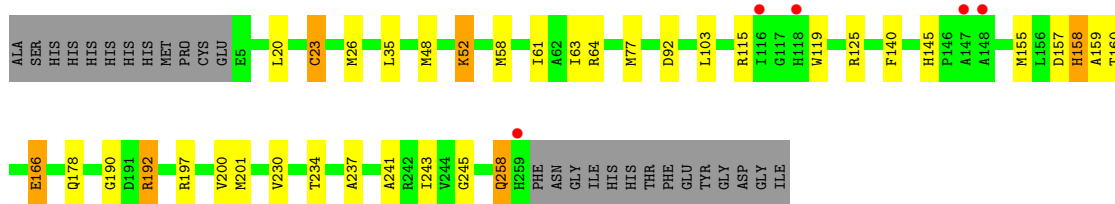
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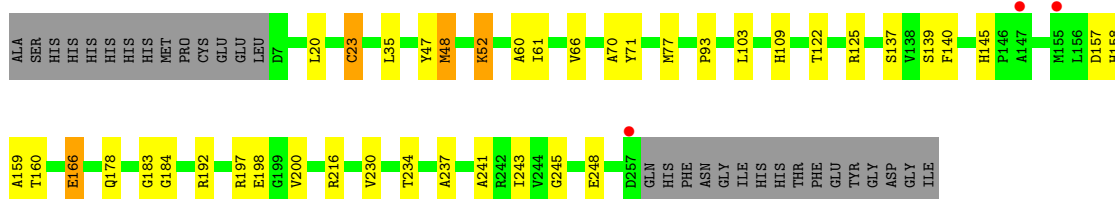
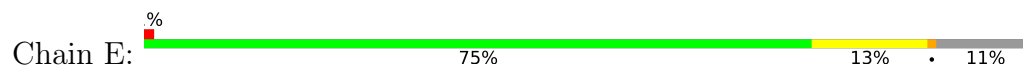
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	6	Total 6	O 6	0	0
5	E	5	Total 5	O 5	0	0
5	F	10	Total 10	O 10	0	0

- Molecule 1: Serine acetyltransferase

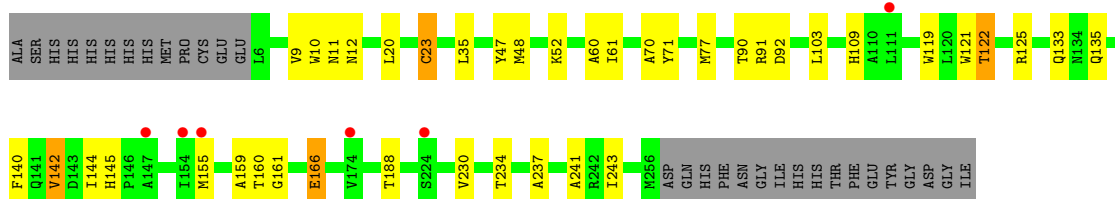
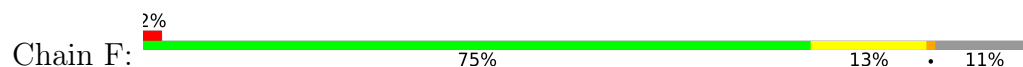




• Molecule 1: Serine acetyltransferase



• Molecule 1: Serine acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.77Å 110.75Å 101.79Å 90.00° 96.62° 90.00°	Depositor
Resolution (Å)	101.11 – 2.80 101.11 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (101.11-2.80) 99.2 (101.11-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.223 , 0.257 0.227 , 0.262	Depositor DCC
R_{free} test set	1766 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	90.6	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 109.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10987	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.09	1/1896 (0.1%)	1.16	8/2582 (0.3%)
1	B	1.07	1/1909 (0.1%)	1.11	6/2598 (0.2%)
1	C	0.97	0/1848	1.10	5/2519 (0.2%)
1	D	1.04	0/1877	1.13	5/2558 (0.2%)
1	E	1.07	2/1846 (0.1%)	1.13	5/2513 (0.2%)
1	F	1.06	0/1722	1.16	5/2357 (0.2%)
All	All	1.05	4/11098 (0.0%)	1.13	34/15127 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	139	SER	C-O	-5.65	1.17	1.24
1	E	139	SER	C-O	-5.64	1.17	1.24
1	A	258	GLN	CA-CB	5.46	1.62	1.53
1	E	137	SER	CA-C	-5.03	1.46	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	GLU	N-CA-C	10.41	123.93	111.33
1	A	48[A]	MET	CA-CB-CG	7.16	128.42	114.10
1	A	48[B]	MET	CA-CB-CG	7.16	128.42	114.10
1	E	166	GLU	N-CA-C	6.39	119.06	111.33
1	F	230	VAL	CA-C-N	-6.20	113.99	120.38
1	F	230	VAL	C-N-CA	-6.20	113.99	120.38
1	D	166	GLU	N-CA-C	6.17	118.80	111.33
1	F	166	GLU	N-CA-C	6.03	118.63	111.33
1	B	245	GLY	N-CA-C	5.92	118.85	110.74
1	D	245	GLY	N-CA-C	5.86	118.06	110.45
1	F	135	GLN	CB-CG-CD	-5.85	102.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	GLY	N-CA-C	-5.84	107.33	114.92
1	A	230	VAL	CA-C-N	-5.73	114.47	120.38
1	A	230	VAL	C-N-CA	-5.73	114.47	120.38
1	F	125	ARG	N-CA-C	-5.72	101.65	109.71
1	D	125	ARG	N-CA-C	-5.71	101.67	109.71
1	A	125	ARG	N-CA-C	-5.66	101.73	109.71
1	B	230	VAL	CA-C-N	-5.64	114.57	120.38
1	B	230	VAL	C-N-CA	-5.64	114.57	120.38
1	C	245	GLY	N-CA-C	5.52	117.63	110.45
1	B	166	GLU	N-CA-C	5.42	117.89	111.33
1	C	166	GLU	N-CA-C	5.42	117.89	111.33
1	E	125	ARG	N-CA-C	-5.38	102.12	109.71
1	C	230	VAL	CA-C-N	-5.33	114.89	120.38
1	C	230	VAL	C-N-CA	-5.33	114.89	120.38
1	C	125	ARG	N-CA-C	-5.32	102.20	109.71
1	D	230	VAL	CA-C-N	-5.25	114.98	120.38
1	D	230	VAL	C-N-CA	-5.25	114.98	120.38
1	B	7	ASP	N-CA-C	5.19	116.63	111.07
1	B	125	ARG	N-CA-C	-5.13	102.47	109.71
1	E	230	VAL	CA-C-N	-5.08	115.14	120.38
1	E	230	VAL	C-N-CA	-5.08	115.14	120.38
1	A	245	GLY	N-CA-C	5.04	117.00	110.45
1	E	245	GLY	N-CA-C	5.01	117.89	110.42

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	1855	0	1826	34	2
1	B	1868	0	1875	33	0
1	C	1813	0	1770	15	0
1	D	1842	0	1777	26	0
1	E	1812	0	1763	29	2
1	F	1691	0	1493	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	6	0	0
3	A	7	0	4	0	0
3	B	7	0	4	0	0
3	C	7	0	4	0	0
3	D	7	0	4	2	0
3	E	14	0	8	6	0
4	A	5	0	0	0	0
4	E	5	0	0	0	0
5	A	12	0	0	0	0
5	B	14	0	0	0	0
5	C	3	0	0	0	0
5	D	6	0	0	0	0
5	E	5	0	0	0	0
5	F	10	0	0	0	0
All	All	10987	0	10534	147	2

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 7.

All (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:MET:HE1	1:A:119:TRP:HB2	1.23	1.15
1:E:184:GLY:N	3:E:601:CYS:SG	2.21	1.12
1:D:77:MET:HE1	1:D:119:TRP:HB2	1.25	1.09
1:A:48[B]:MET:SD	1:A:49:LEU:HG	1.97	1.05
1:A:48[B]:MET:HE1	1:A:49:LEU:CD2	1.88	1.04
1:A:48[B]:MET:HE1	1:A:49:LEU:HD23	1.00	0.98
1:F:121:TRP:CE3	1:F:121:TRP:CH2	2.44	0.98
1:A:48[B]:MET:CE	1:A:49:LEU:HD23	1.94	0.97
1:A:77:MET:CE	1:A:119:TRP:HB2	2.02	0.89
1:B:92:ASP:OD2	1:B:95:VAL:HG23	1.74	0.88
1:B:253:ALA:O	1:B:256:MET:HE3	1.76	0.84
1:D:77:MET:CE	1:D:119:TRP:HB2	2.06	0.84
1:C:77:MET:HE1	1:C:119:TRP:HB2	1.59	0.83
1:A:77:MET:HE1	1:A:119:TRP:CB	2.08	0.80
1:D:77:MET:HE1	1:D:119:TRP:CB	2.11	0.79
1:B:77:MET:HE1	1:B:116:ILE:HD13	1.62	0.79
1:F:133:GLN:HG3	1:F:144:ILE:O	1.89	0.72
1:B:34:THR:HB	1:B:48[B]:MET:HE1	1.70	0.72
1:F:9:VAL:O	1:F:12:ASN:N	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:ASP:OD1	1:D:158:HIS:N	2.25	0.70
1:B:77:MET:CE	1:B:116:ILE:HD13	2.22	0.69
1:B:18:ARG:HG2	1:B:36:LEU:HD21	1.76	0.67
1:A:48[B]:MET:SD	1:A:49:LEU:CG	2.82	0.66
1:A:48[B]:MET:SD	1:A:49:LEU:N	2.68	0.66
1:B:175:SER:HB2	1:B:256:MET:HE1	1.76	0.66
1:D:157:ASP:O	1:D:159:ALA:N	2.28	0.64
1:A:61:ILE:HD11	1:D:64:ARG:HD2	1.80	0.63
1:B:47:TYR:CE1	1:F:61:ILE:HG23	2.34	0.63
1:A:222:ALA:O	1:B:225:VAL:HG21	1.99	0.62
1:A:48[B]:MET:CE	1:A:49:LEU:HA	2.30	0.62
1:F:9:VAL:O	1:F:10:TRP:C	2.40	0.62
1:F:70:ALA:HB1	1:F:77:MET:HE1	1.83	0.60
1:B:61:ILE:HG23	1:F:47:TYR:CE1	2.37	0.60
1:E:93:PRO:HG2	3:E:602:CYS:O	2.02	0.59
1:E:70:ALA:HB1	1:E:77:MET:HE1	1.84	0.59
1:E:48:MET:HE3	1:E:52:LYS:HG3	1.84	0.59
1:F:142:VAL:O	1:F:142:VAL:HG12	2.01	0.59
1:D:157:ASP:OD2	3:E:601:CYS:N	2.35	0.59
1:B:61:ILE:HD12	1:F:60:ALA:HB1	1.84	0.58
1:B:92:ASP:HB2	1:B:155:MET:CE	2.34	0.58
1:A:48[B]:MET:HE1	1:A:49:LEU:HA	1.86	0.57
1:D:52:LYS:HB3	1:D:140:PHE:HZ	1.68	0.57
1:F:52:LYS:HB3	1:F:140:PHE:HZ	1.69	0.57
1:C:60:ALA:HB1	1:E:61:ILE:HD12	1.87	0.56
1:C:52:LYS:HB3	1:C:140:PHE:HZ	1.71	0.56
1:A:52:LYS:HB3	1:A:140:PHE:HZ	1.71	0.55
1:D:190:GLY:O	1:D:192:ARG:HD3	2.07	0.54
1:A:92:ASP:HB2	1:A:155:MET:CE	2.36	0.54
1:C:92:ASP:HB2	1:C:155:MET:CE	2.38	0.54
1:D:92:ASP:HB2	1:D:155:MET:CE	2.37	0.54
1:F:92:ASP:HB2	1:F:155:MET:CE	2.38	0.54
1:B:60:ALA:HB1	1:F:61:ILE:HD12	1.88	0.53
1:E:52:LYS:HB3	1:E:140:PHE:HZ	1.73	0.53
1:C:35:LEU:HD11	1:C:103:LEU:HD21	1.91	0.52
1:D:157:ASP:OD1	1:D:158:HIS:CD2	2.62	0.52
1:E:71:TYR:CD2	1:E:77:MET:HE3	2.44	0.52
1:F:35:LEU:HD11	1:F:103:LEU:HD21	1.91	0.52
1:A:35:LEU:HD11	1:A:103:LEU:HD21	1.93	0.51
1:B:253:ALA:O	1:B:256:MET:CE	2.54	0.51
1:F:9:VAL:O	1:F:11:ASN:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:THR:HG22	1:D:243:ILE:HG23	1.93	0.51
1:B:52:LYS:HB3	1:B:140:PHE:HZ	1.76	0.51
1:C:61:ILE:HG23	1:E:47:TYR:CE1	2.45	0.51
1:E:198:GLU:OE1	1:E:216:ARG:NH2	2.44	0.51
1:E:35:LEU:HD11	1:E:103:LEU:HD21	1.93	0.50
1:E:234:THR:HG22	1:E:243:ILE:HG23	1.93	0.50
1:A:60:ALA:HB1	1:D:61:ILE:HD12	1.93	0.50
1:B:234:THR:HG22	1:B:243:ILE:HG23	1.93	0.50
1:B:35:LEU:HD11	1:B:103:LEU:HD21	1.93	0.50
1:E:71:TYR:HD2	1:E:77:MET:HE3	1.76	0.50
1:A:234:THR:HG22	1:A:243:ILE:HG23	1.94	0.49
1:B:18:ARG:HG2	1:B:36:LEU:CD2	2.40	0.49
1:E:183:GLY:CA	3:E:601:CYS:SG	3.00	0.49
1:F:234:THR:HG22	1:F:243:ILE:HG23	1.94	0.49
1:D:192:ARG:NH1	3:D:501:CYS:O	2.42	0.49
1:B:92:ASP:CG	1:B:95:VAL:HG23	2.37	0.48
1:F:52:LYS:HE3	1:F:109:HIS:CE1	2.48	0.48
1:A:77:MET:HE2	1:A:115:ARG:O	2.13	0.48
1:C:47:TYR:CE1	1:E:61:ILE:HG23	2.48	0.48
1:C:234:THR:HG22	1:C:243:ILE:HG23	1.96	0.48
1:D:35:LEU:HD11	1:D:103:LEU:HD21	1.94	0.48
1:F:90:THR:HG23	1:F:91:ARG:HG3	1.96	0.48
1:D:201:MET:SD	1:D:258:GLN:NE2	2.87	0.48
1:D:145:HIS:CE1	1:D:166:GLU:HG3	2.50	0.47
1:B:77:MET:HE1	1:B:116:ILE:CD1	2.39	0.47
1:A:48[B]:MET:CE	1:A:49:LEU:CA	2.92	0.47
1:E:145:HIS:CE1	1:E:166:GLU:HG3	2.49	0.47
1:E:157:ASP:OD2	3:E:602:CYS:N	2.48	0.46
1:F:71:TYR:HD1	1:F:77:MET:HE3	1.79	0.46
1:B:145:HIS:CE1	1:B:166:GLU:HG3	2.50	0.46
1:F:71:TYR:CD1	1:F:77:MET:HE3	2.50	0.46
1:F:145:HIS:CE1	1:F:166:GLU:HG3	2.51	0.46
1:D:192:ARG:NE	3:D:501:CYS:O	2.47	0.46
1:A:178:GLN:HE21	1:B:181:THR:HG21	1.82	0.45
1:D:77:MET:HE2	1:D:115:ARG:O	2.15	0.45
1:A:48[B]:MET:CE	1:A:49:LEU:CD2	2.73	0.45
1:C:58:MET:HE3	1:C:63:ILE:HG13	1.99	0.44
1:B:92:ASP:HB2	1:B:155:MET:HE1	1.98	0.44
1:E:48:MET:CE	1:E:52:LYS:HG3	2.48	0.44
1:E:184:GLY:HA2	1:E:192:ARG:O	2.18	0.44
1:A:159:ALA:O	1:A:160:THR:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ALA:O	1:D:160:THR:C	2.61	0.43
1:C:61:ILE:HD12	1:E:60:ALA:HB1	1.99	0.43
1:F:119:TRP:O	1:F:122:THR:HB	2.19	0.43
1:B:20:LEU:HA	1:B:23:CYS:HB2	2.00	0.42
1:F:20:LEU:HA	1:F:23:CYS:HB2	2.01	0.42
1:C:20:LEU:HA	1:C:23:CYS:HB2	2.01	0.42
1:B:237:ALA:O	1:B:241:ALA:HA	2.20	0.42
1:D:20:LEU:HA	1:D:23:CYS:HB2	2.00	0.42
1:A:77:MET:CE	1:A:115:ARG:O	2.67	0.42
1:A:237:ALA:O	1:A:241:ALA:HA	2.19	0.42
1:B:159:ALA:O	1:B:160:THR:C	2.61	0.42
1:E:237:ALA:O	1:E:241:ALA:HA	2.20	0.42
1:A:48[B]:MET:CE	1:A:49:LEU:N	2.83	0.42
1:B:77:MET:HE3	1:B:115:ARG:HB3	2.00	0.42
1:B:197:ARG:O	1:B:200:VAL:HG23	2.20	0.42
1:C:237:ALA:O	1:C:241:ALA:HA	2.20	0.42
1:D:237:ALA:O	1:D:241:ALA:HA	2.20	0.42
1:A:222:ALA:O	1:B:225:VAL:HG11	2.20	0.42
1:C:159:ALA:O	1:C:160:THR:C	2.61	0.42
1:D:197:ARG:O	1:D:200:VAL:HG23	2.20	0.42
1:F:237:ALA:O	1:F:241:ALA:HA	2.20	0.42
1:A:197:ARG:O	1:A:200:VAL:HG23	2.20	0.41
1:D:26:MET:HE1	1:E:66:VAL:CG2	2.51	0.41
1:A:184:GLY:HA2	1:A:192:ARG:O	2.20	0.41
1:E:20:LEU:HA	1:E:23:CYS:HB2	2.01	0.41
1:E:159:ALA:O	1:E:160:THR:C	2.62	0.41
1:E:48:MET:C	1:E:48:MET:HE2	2.45	0.41
1:D:58:MET:HE3	1:D:63:ILE:HG13	2.01	0.41
1:A:133:GLN:OE1	1:A:145:HIS:HA	2.21	0.41
1:A:183:GLY:O	1:A:209:LEU:HA	2.21	0.41
1:B:165:GLY:HA3	1:B:193:HIS:CD2	2.56	0.41
1:D:158:HIS:HB2	1:D:178:GLN:OE1	2.21	0.41
1:B:183:GLY:O	1:B:209:LEU:HA	2.21	0.41
1:E:160:THR:HG21	1:F:161:GLY:HA2	2.03	0.40
1:F:159:ALA:O	1:F:160:THR:C	2.62	0.40
1:C:48:MET:SD	1:C:109:HIS:CD2	3.15	0.40
1:E:158:HIS:HB2	1:E:178:GLN:OE1	2.21	0.40
1:C:197:ARG:O	1:C:200:VAL:HG23	2.20	0.40
1:E:197:ARG:O	1:E:200:VAL:HG23	2.21	0.40
1:B:158:HIS:HB2	1:B:178:GLN:OE1	2.22	0.40
1:E:48:MET:SD	1:E:109:HIS:CD2	3.14	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:GLY:C	3:E:601:CYS:SG	3.00	0.40
1:B:48[A]:MET:SD	1:B:109:HIS:CD2	3.15	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ARG:NH1	1:E:248:GLU:CG[1_556]	1.63	0.57
1:A:216:ARG:NH2	1:E:248:GLU:OE2[1_556]	2.16	0.04

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	254/281 (90%)	240 (94%)	14 (6%)	0	100	100
1	B	252/281 (90%)	239 (95%)	13 (5%)	0	100	100
1	C	250/281 (89%)	237 (95%)	13 (5%)	0	100	100
1	D	253/281 (90%)	241 (95%)	11 (4%)	1 (0%)	30	60
1	E	249/281 (89%)	237 (95%)	12 (5%)	0	100	100
1	F	249/281 (89%)	235 (94%)	14 (6%)	0	100	100
All	All	1507/1686 (89%)	1429 (95%)	77 (5%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	158	HIS

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	182/220 (83%)	177 (97%)	5 (3%)	39	74
1	B	189/220 (86%)	185 (98%)	4 (2%)	47	79
1	C	178/220 (81%)	176 (99%)	2 (1%)	65	87
1	D	177/220 (80%)	172 (97%)	5 (3%)	38	73
1	E	173/220 (79%)	169 (98%)	4 (2%)	44	78
1	F	141/220 (64%)	136 (96%)	5 (4%)	32	67
All	All	1040/1320 (79%)	1015 (98%)	25 (2%)	45	77

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	CYS
1	A	48[A]	MET
1	A	48[B]	MET
1	A	52	LYS
1	A	61	ILE
1	B	23	CYS
1	B	48[A]	MET
1	B	48[B]	MET
1	B	149	LYS
1	C	23	CYS
1	C	52	LYS
1	D	23	CYS
1	D	48	MET
1	D	52	LYS
1	D	192	ARG
1	D	258	GLN
1	E	23	CYS
1	E	48	MET
1	E	52	LYS
1	E	122	THR
1	F	23	CYS
1	F	48	MET

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Mol	Chain	Res	Type
1	F	122	THR
1	F	142	VAL
1	F	188	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	134	ASN
1	B	12	ASN
1	B	109	HIS
1	C	109	HIS
1	C	133	GLN
1	D	12	ASN
1	D	145	HIS
1	E	145	HIS
1	E	233	HIS
1	F	32	HIS

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](#)

9 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	CYS	E	601	-	5,6,6	1.30	0	3,7,7	3.82	1 (33%)
4	PO4	E	603	-	4,4,4	0.87	0	6,6,6	0.83	0
4	PO4	A	303	-	4,4,4	0.98	0	6,6,6	0.53	0
3	CYS	D	501	-	5,6,6	1.19	1 (20%)	3,7,7	1.81	1 (33%)
2	EDO	A	301	-	3,3,3	0.46	0	2,2,2	0.44	0
3	CYS	A	302	-	5,6,6	1.47	2 (40%)	3,7,7	1.47	1 (33%)
3	CYS	C	501	-	5,6,6	1.32	1 (20%)	3,7,7	2.64	3 (100%)
3	CYS	B	701	-	5,6,6	1.07	0	3,7,7	1.95	1 (33%)
3	CYS	E	602	-	5,6,6	2.08	3 (60%)	3,7,7	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYS	E	601	-	-	3/6/6/6	-
3	CYS	D	501	-	-	1/6/6/6	-
2	EDO	A	301	-	-	1/1/1/1	-
3	CYS	A	302	-	-	1/6/6/6	-
3	CYS	C	501	-	-	2/6/6/6	-
3	CYS	B	701	-	-	1/6/6/6	-
3	CYS	E	602	-	-	4/6/6/6	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	CYS	CB-CA	2.99	1.56	1.53
3	E	602	CYS	O-C	2.83	1.30	1.22
3	C	501	CYS	OXT-C	-2.42	1.22	1.30
3	A	302	CYS	CB-CA	2.33	1.55	1.53
3	D	501	CYS	CB-CA	-2.19	1.50	1.53
3	E	602	CYS	CB-SG	2.15	1.85	1.81
3	A	302	CYS	O-C	2.10	1.28	1.22

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	CYS	CB-CA-C	6.21	116.08	109.89
3	C	501	CYS	CB-CA-C	2.99	112.87	109.89
3	D	501	CYS	OXT-C-O	-2.82	117.67	124.08
3	C	501	CYS	CA-CB-SG	2.59	119.92	114.40
3	B	701	CYS	CB-CA-C	2.58	112.46	109.89
3	C	501	CYS	OXT-C-O	-2.29	118.88	124.08
3	A	302	CYS	CB-CA-C	2.08	111.96	109.89

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	602	CYS	C-CA-CB-SG
3	E	601	CYS	O-C-CA-N
3	E	601	CYS	N-CA-CB-SG
3	C	501	CYS	C-CA-CB-SG
2	A	301	EDO	O1-C1-C2-O2
3	B	701	CYS	OXT-C-CA-N
3	E	602	CYS	O-C-CA-N
3	E	602	CYS	N-CA-CB-SG
3	E	602	CYS	OXT-C-CA-N
3	E	601	CYS	OXT-C-CA-N
3	C	501	CYS	N-CA-CB-SG
3	A	302	CYS	OXT-C-CA-N
3	D	501	CYS	OXT-C-CA-N

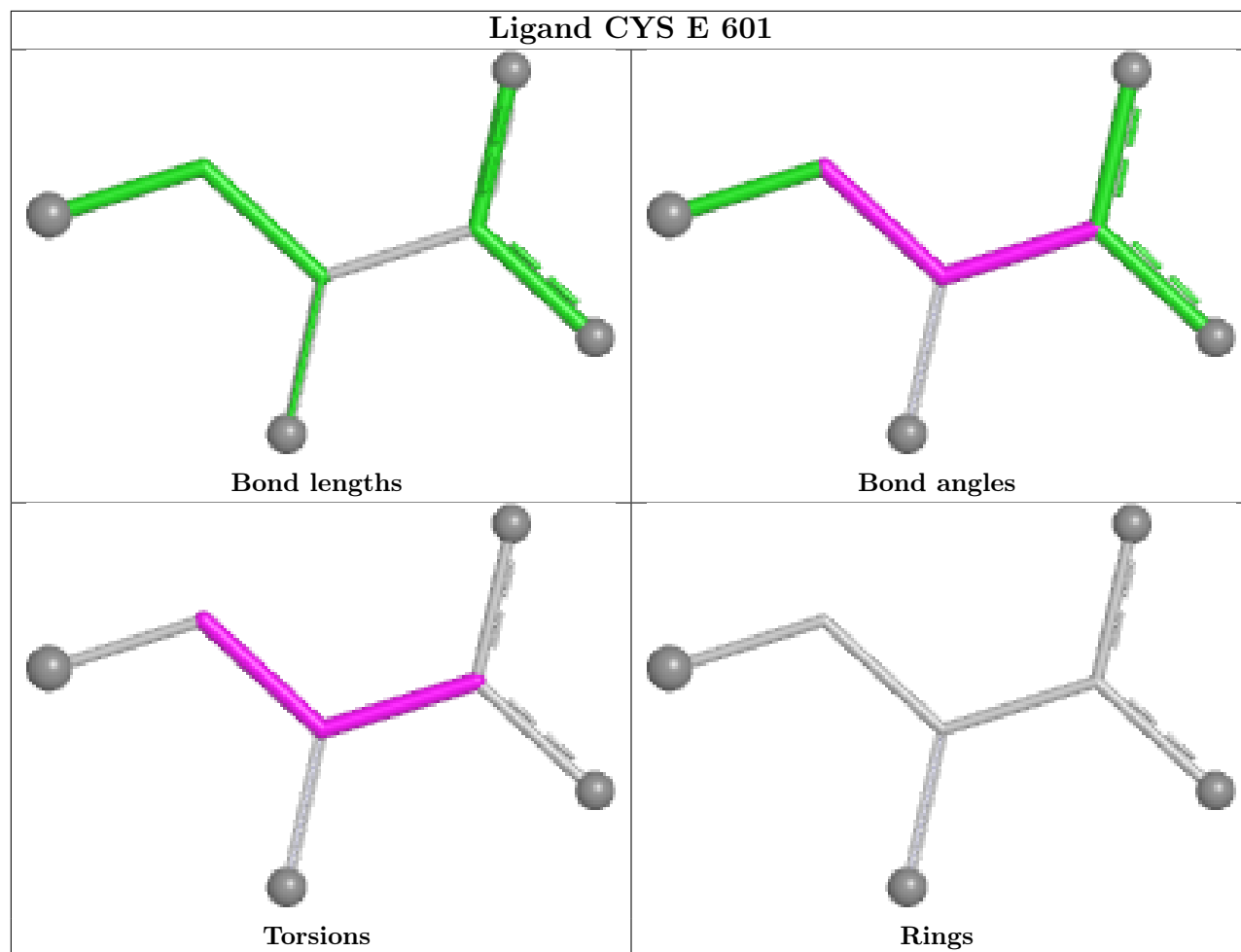
There are no ring outliers.

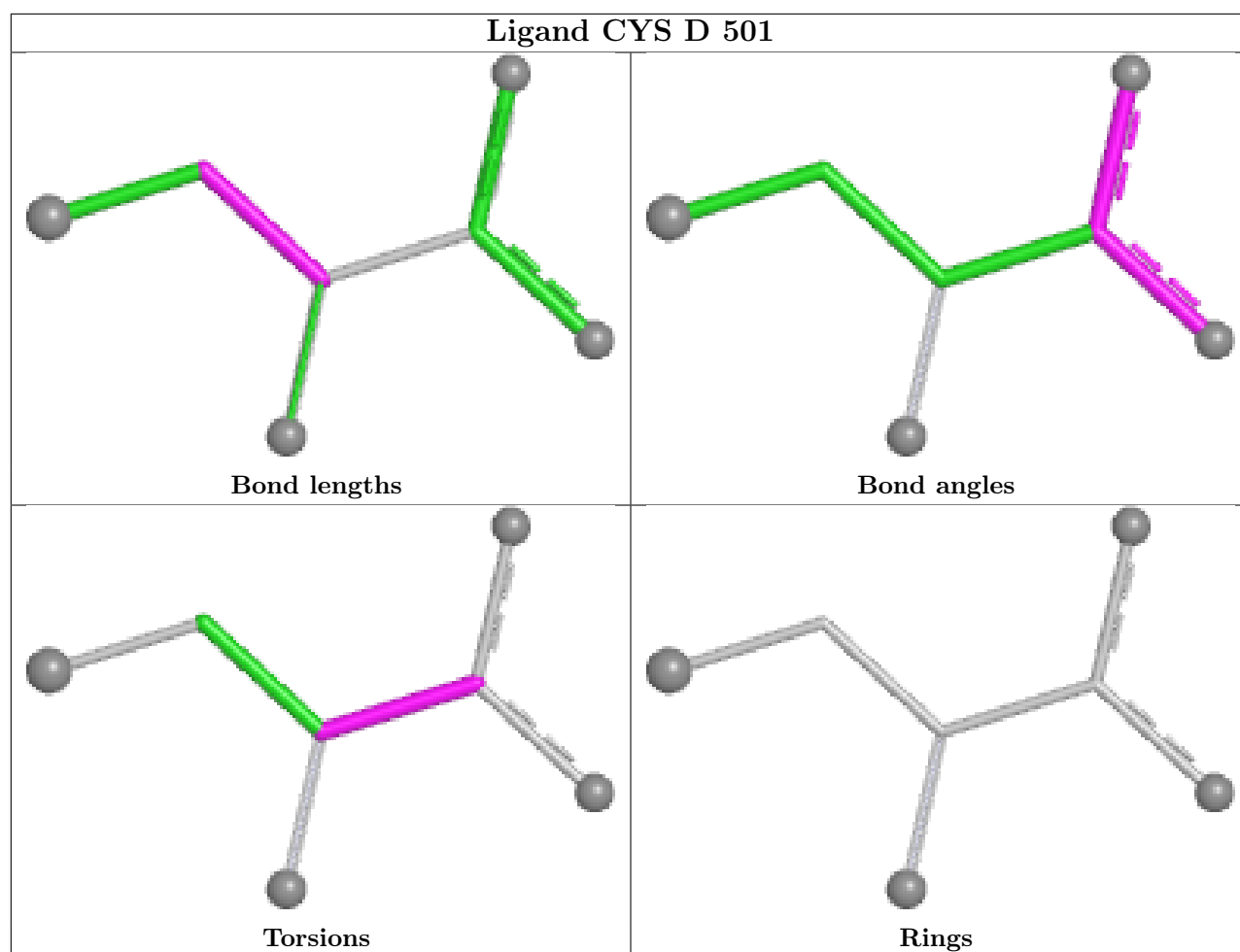
3 monomers are involved in 8 short contacts:

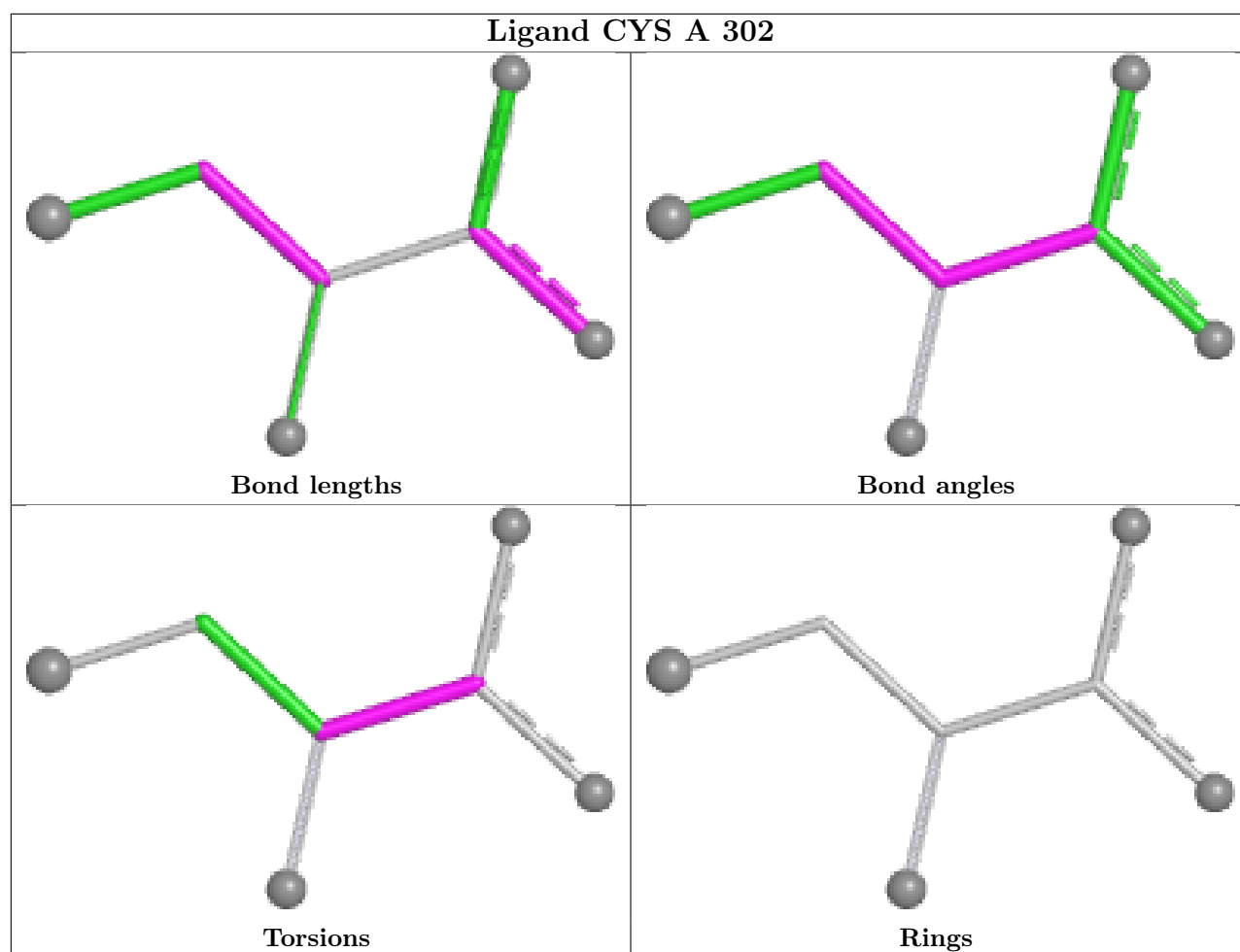
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	CYS	4	0
3	D	501	CYS	2	0
3	E	602	CYS	2	0

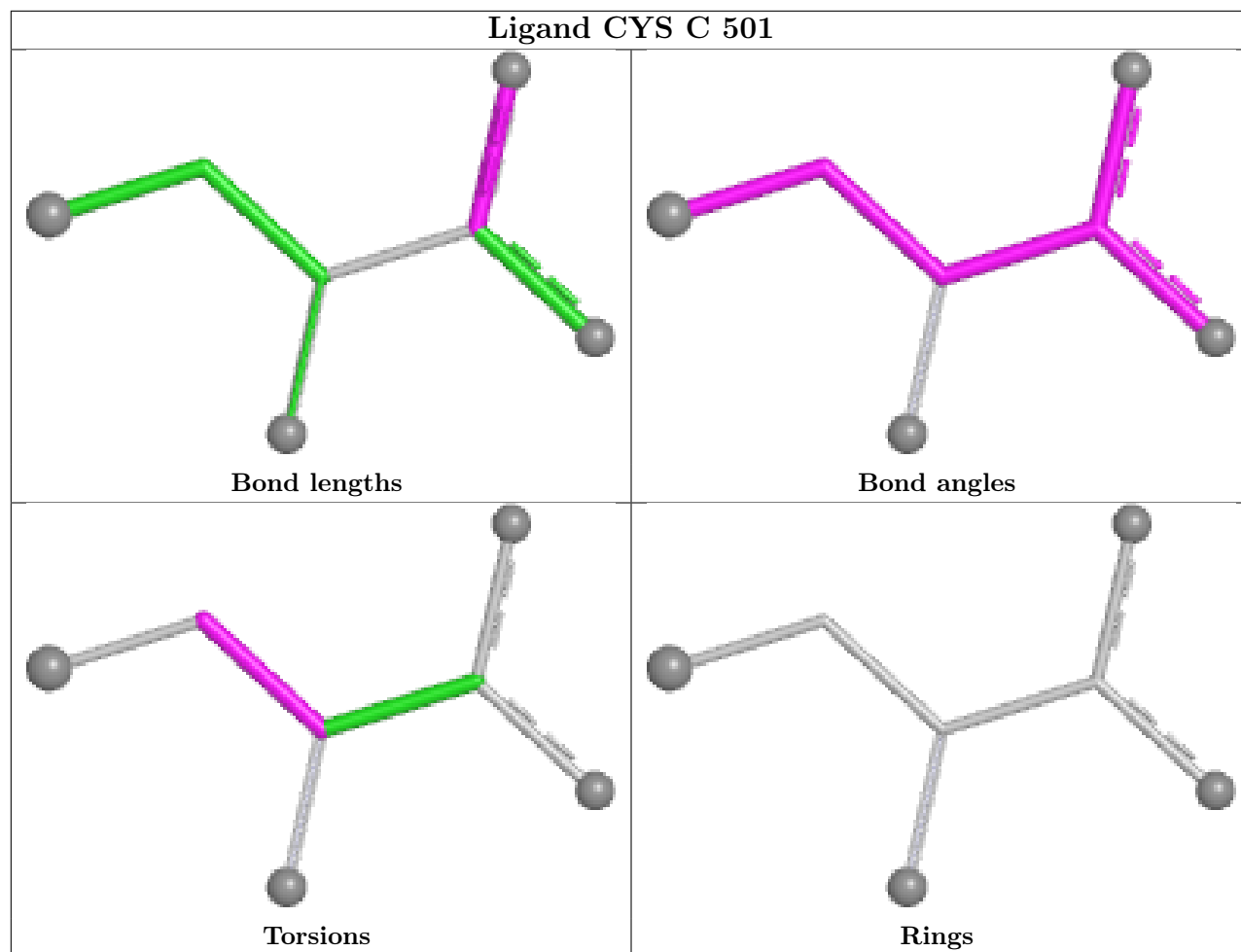
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

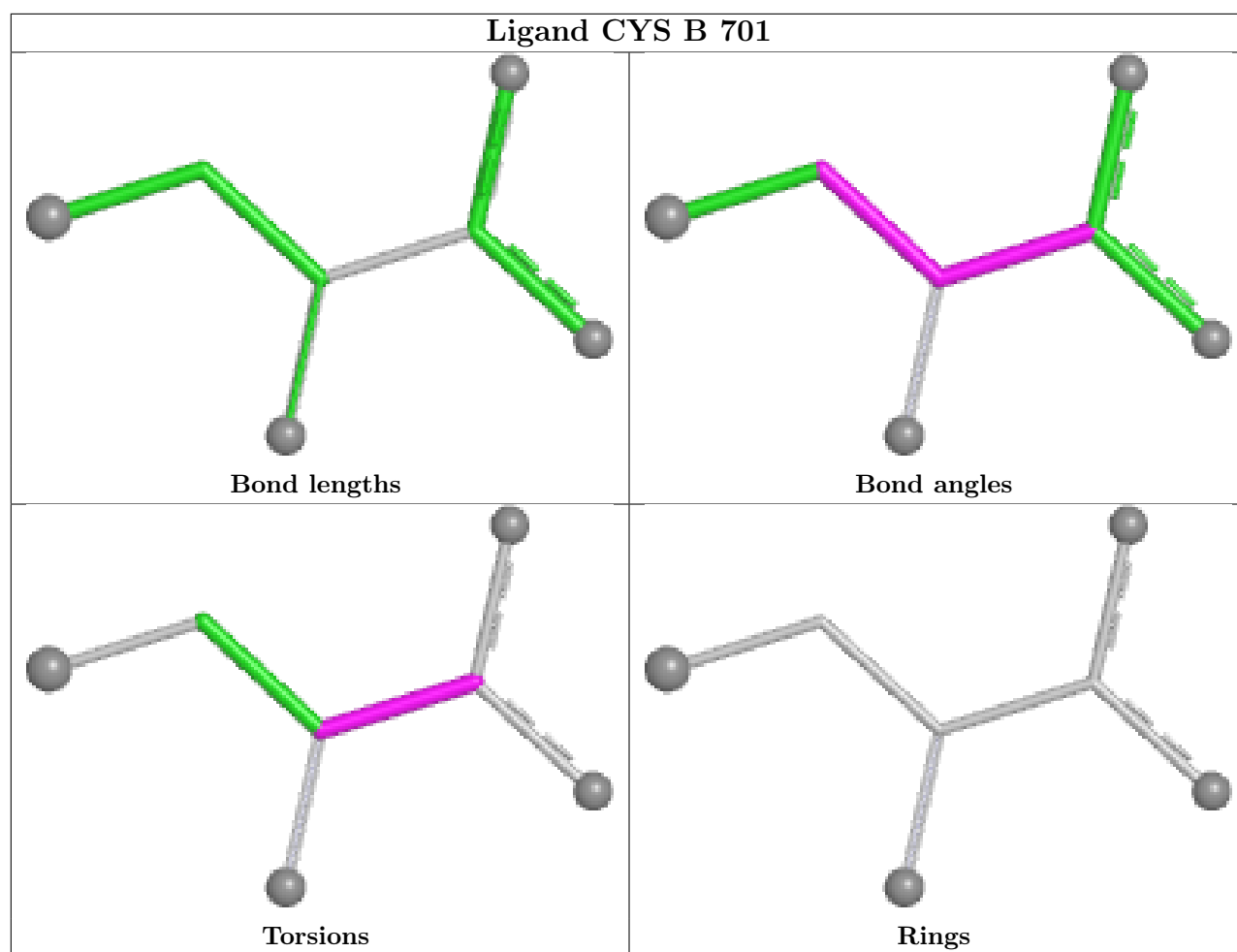
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

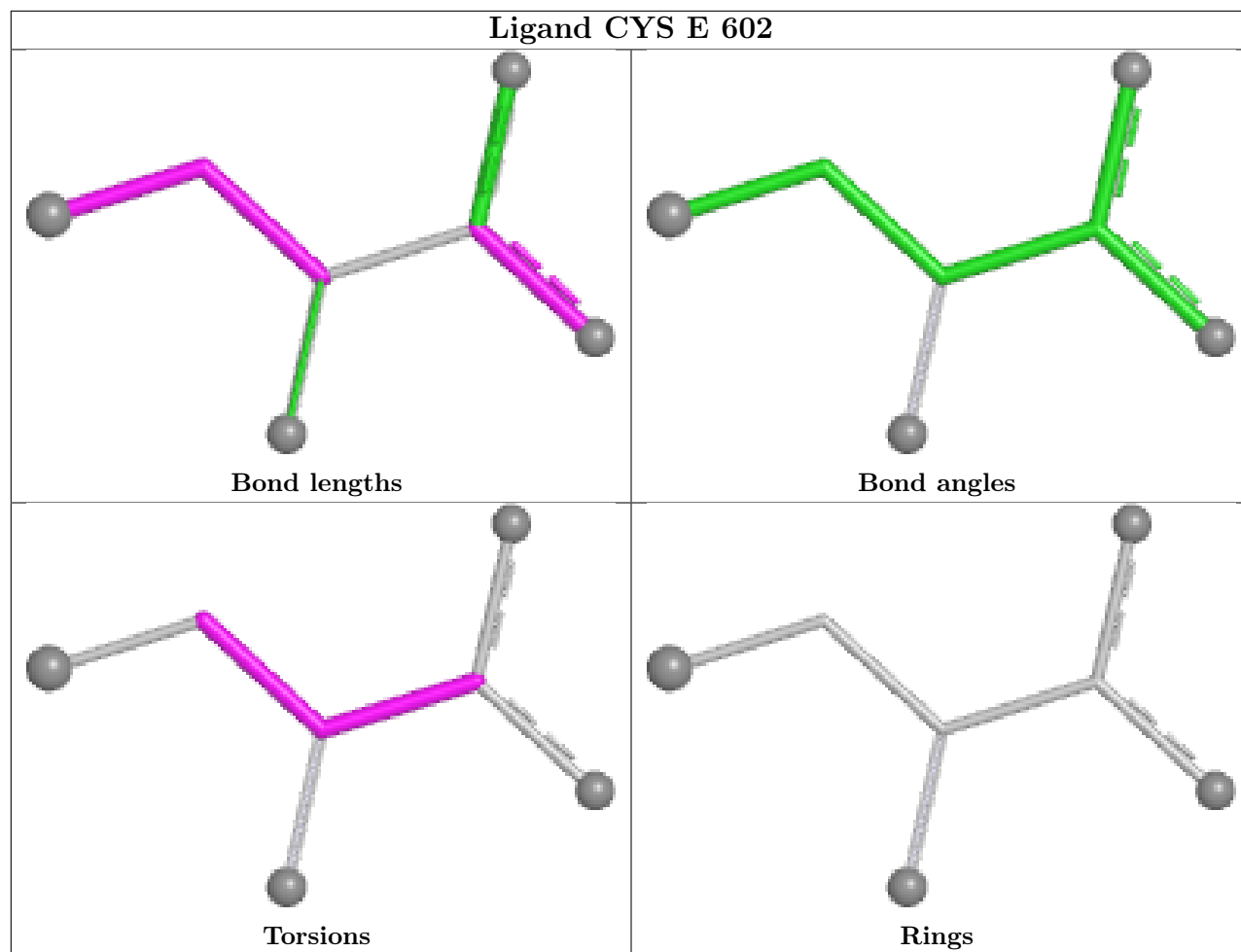












5.7 Other polymers [i](#)

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

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	255/281 (90%)	-0.13	4 (1%) 70 61	62, 113, 152, 174	1 (0%)
1	B	253/281 (90%)	-0.19	1 (0%) 88 84	58, 107, 150, 171	1 (0%)
1	C	252/281 (89%)	0.07	8 (3%) 50 40	68, 130, 193, 233	0
1	D	255/281 (90%)	-0.07	5 (1%) 65 56	65, 113, 169, 195	0
1	E	251/281 (89%)	-0.06	3 (1%) 76 68	68, 112, 147, 176	0
1	F	251/281 (89%)	0.16	6 (2%) 59 49	78, 139, 194, 223	0
All	All	1517/1686 (89%)	-0.04	27 (1%) 67 58	58, 117, 175, 233	2 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	147	ALA	3.7
1	A	258	GLN	3.5
1	E	257	ASP	3.4
1	C	30	PHE	3.3
1	F	147	ALA	3.1
1	F	111	LEU	2.9
1	A	48[A]	MET	2.8
1	F	174	VAL	2.8
1	C	85	ILE	2.6
1	C	209	LEU	2.6
1	B	257	ASP	2.6
1	F	224	SER	2.5
1	C	27	LEU	2.5
1	C	111	LEU	2.4
1	D	148	ALA	2.4
1	A	100	THR	2.3
1	F	154	ILE	2.3
1	E	155	MET	2.2
1	A	222	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	147	ALA	2.2
1	C	184	GLY	2.1
1	F	155	MET	2.0
1	D	259	HIS	2.0
1	D	118	HIS	2.0
1	D	116	ILE	2.0
1	C	94	ALA	2.0
1	C	31	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

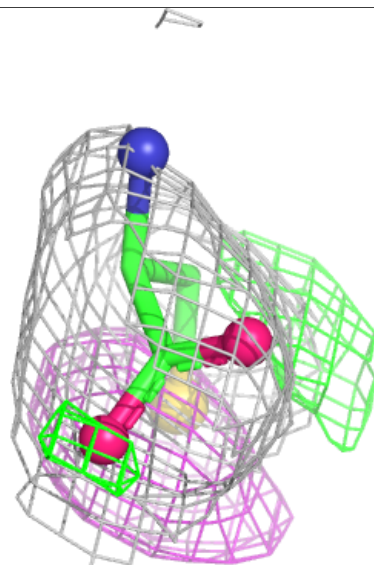
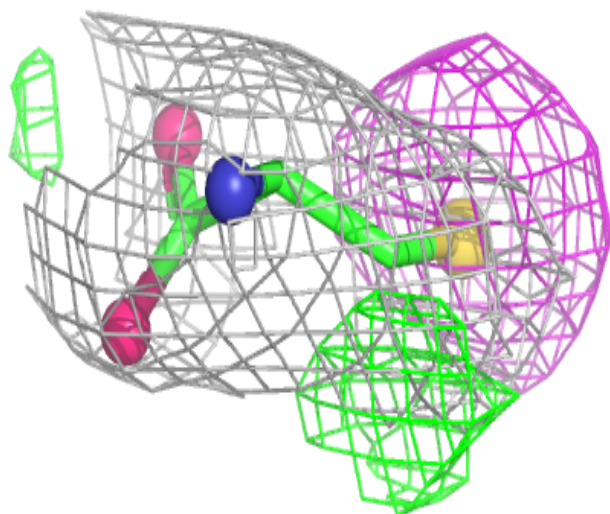
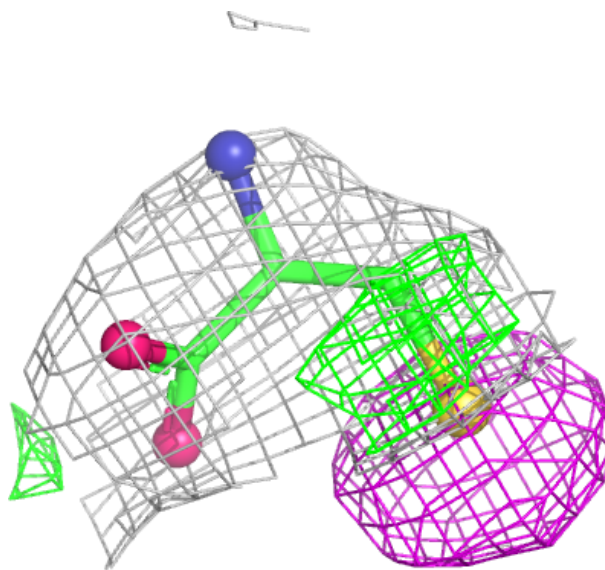
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CYS	E	601	7/7	0.58	0.16	97,99,103,109	0
4	PO4	E	603	5/5	0.81	0.09	110,121,136,158	0
2	EDO	A	301	4/4	0.83	0.14	98,101,102,104	0
4	PO4	A	303	5/5	0.86	0.08	101,105,132,147	0
3	CYS	A	302	7/7	0.86	0.11	110,114,119,124	0
3	CYS	C	501	7/7	0.87	0.12	115,120,125,131	0
3	CYS	D	501	7/7	0.90	0.08	110,120,123,128	0
3	CYS	E	602	7/7	0.91	0.09	115,120,124,130	0
3	CYS	B	701	7/7	0.94	0.07	94,97,105,119	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.

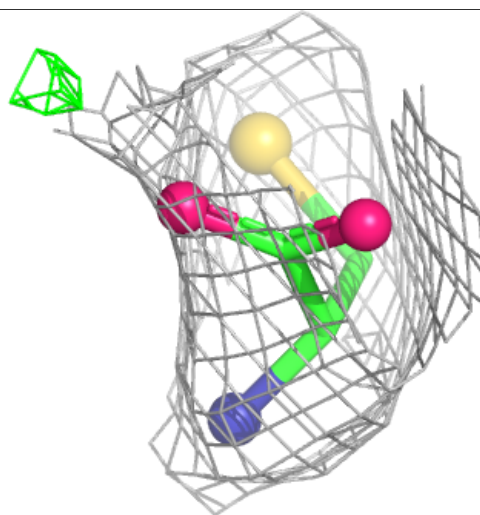
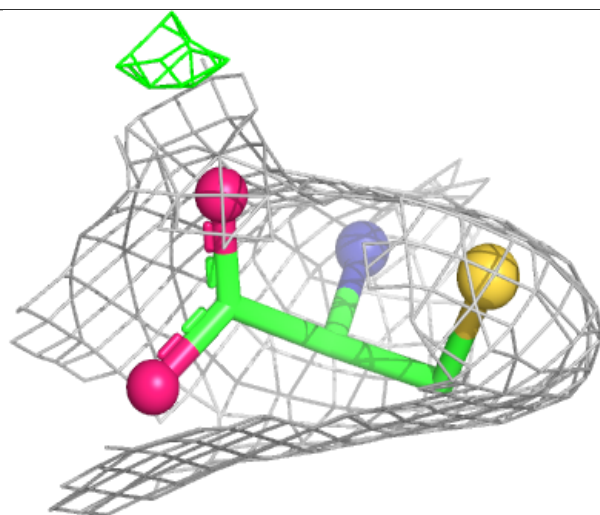
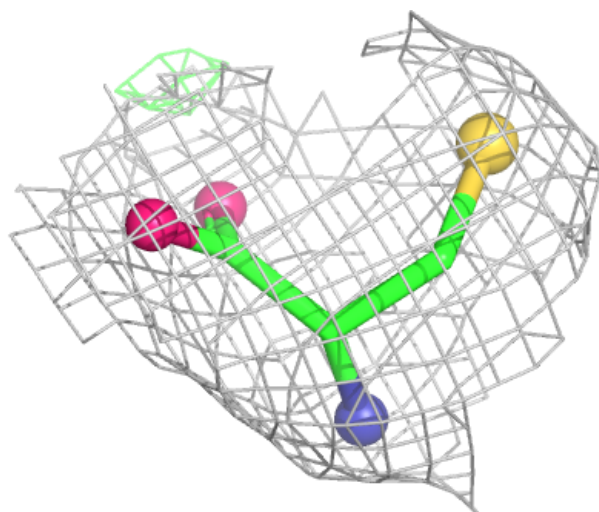
Electron density around CYS E 601:

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



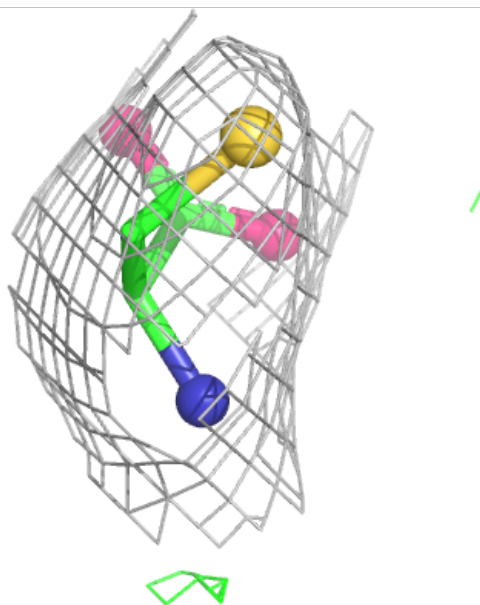
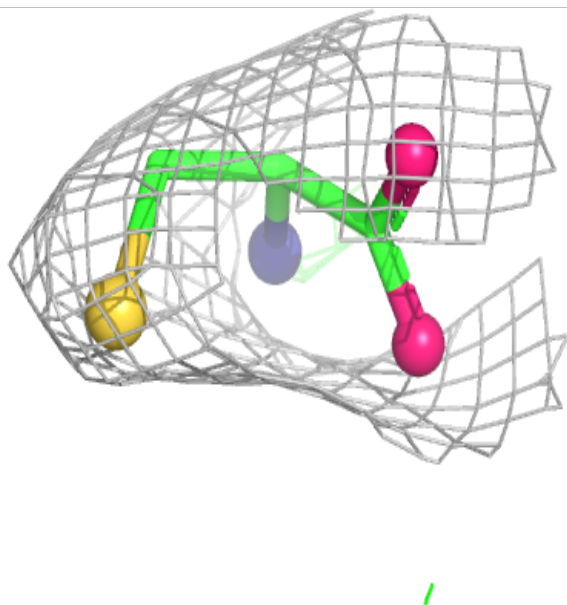
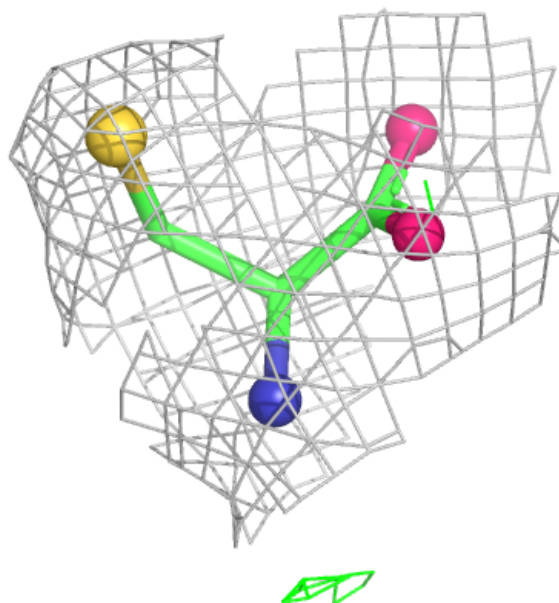
Electron density around CYS A 302:

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



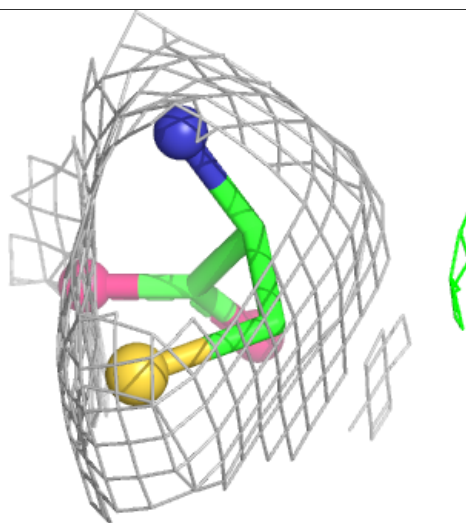
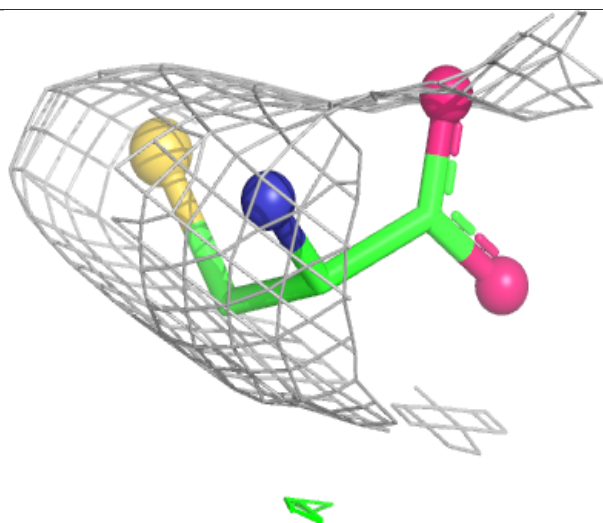
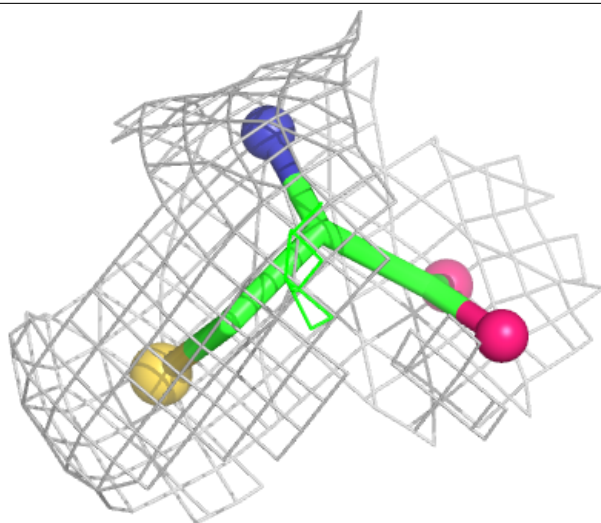
Electron density around CYS C 501:

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



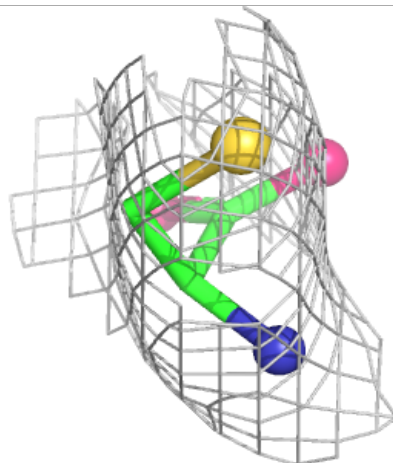
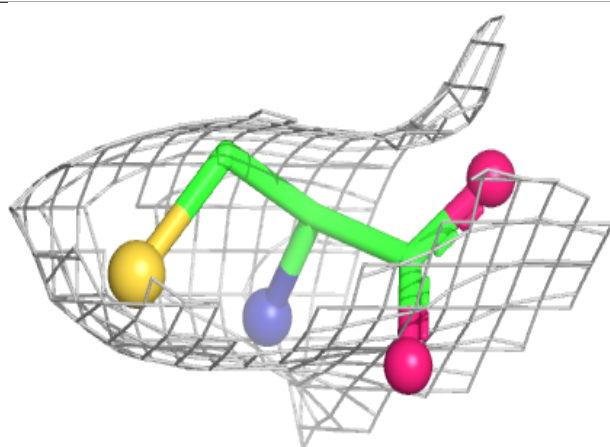
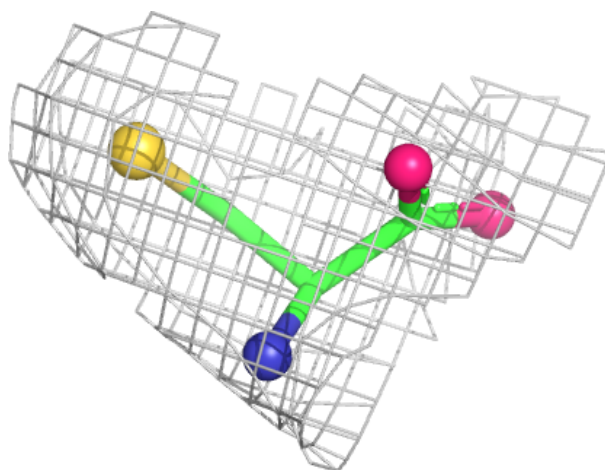
Electron density around CYS D 501:

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



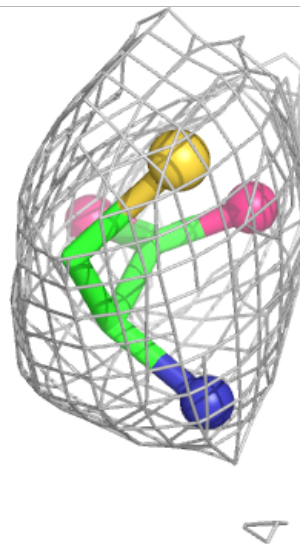
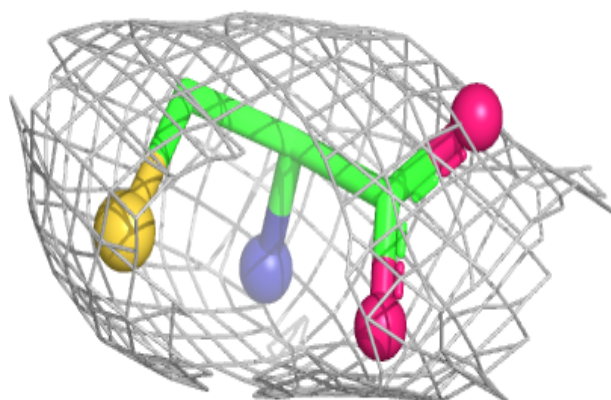
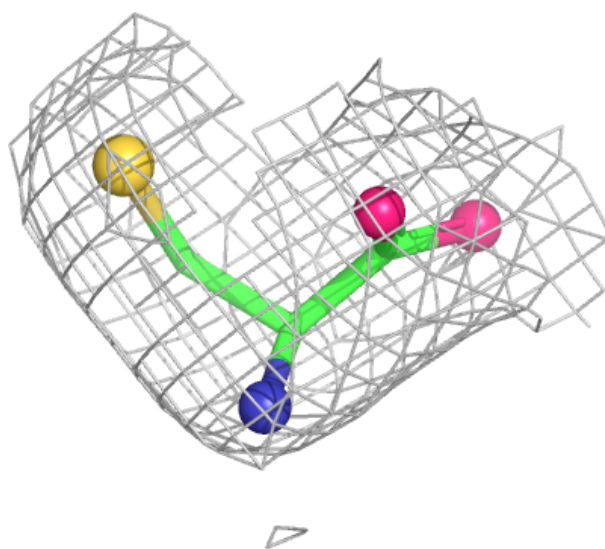
Electron density around CYS E 602:

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



Electron density around CYS B 701:

$2mF_o-DF_c$ (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.