



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:59 PM UTC

PDB ID : 4BC1 / pdb_00004bc1
Title : Structure of mouse acetylcholinesterase inhibited by CBDP (30-min soak): cr
esyl-saligenin-phosphoserine adduct
Authors : Carletti, E.; Colletier, J.-P.; Schopfer, L.M.; Santoni, G.; Masson, P.; Lock-
ridge, O.; Nachon, F.; Weik, M.
Deposited on : 2012-09-30
Resolution : 2.95 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

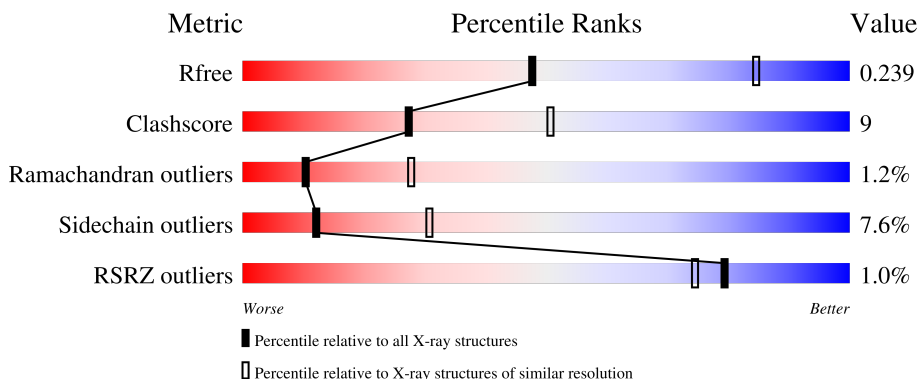
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



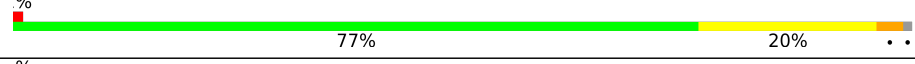

The reported resolution of this entry is 2.95 Å.

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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	543	 77% 20% ..
1	B	543	 70% 26% ..
1	C	543	 77% 20% ..
1	D	543	 72% 25% ..

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
2	TQV	C	600	-	-	X	-
4	CL	A	1544	-	-	X	-

2 Entry composition [i](#)

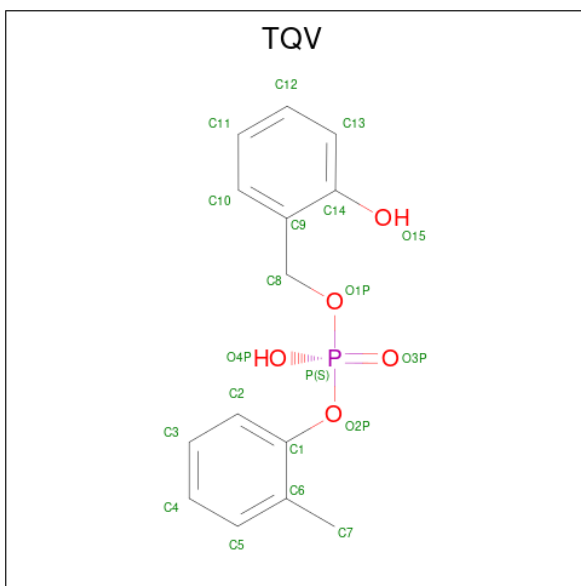
There are 6 unique types of molecules in this entry. The entry contains 17994 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	540	Total 4224	C 2712	N 732	O 766	S 14	0	3	0
1	B	539	Total 4202	C 2698	N 728	O 762	S 14	0	1	0
1	C	540	Total 4230	C 2716	N 732	O 768	S 14	0	4	0
1	D	540	Total 4243	C 2723	N 741	O 765	S 14	0	5	0

- Molecule 2 is O-CRESYL-SALIGENIN PHOSPHATE (CCD ID: TQV) (formula: C₁₄H₁₅O₅P).



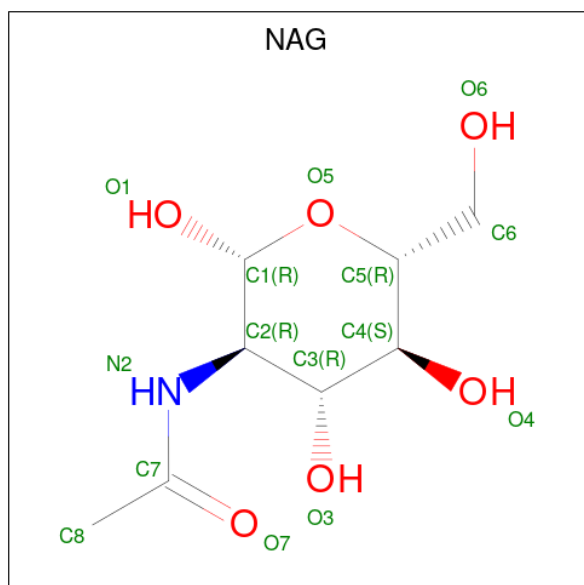
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	Total 19	C 14	O 4	P 1	0	0
2	B	1	Total 19	C 14	O 4	P 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	0
			19	14	4	1		
2	D	1	Total	C	O	P	0	0
			19	14	4	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

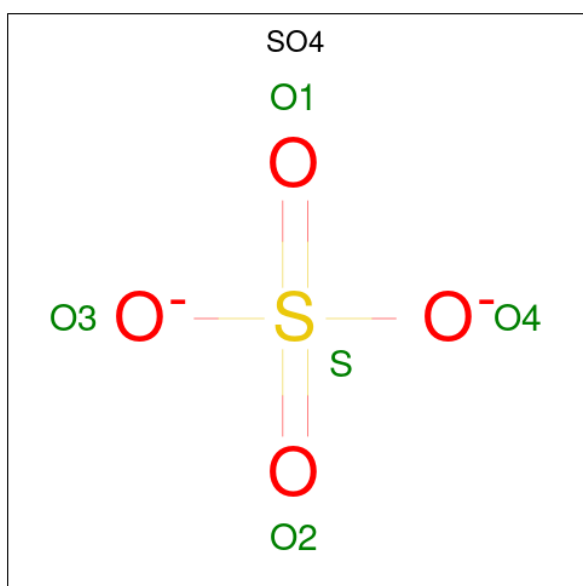


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Cl 3 3	0	0
4	B	1	Total Cl 1 1	0	0
4	C	4	Total Cl 4 4	0	0
4	D	3	Total Cl 3 3	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

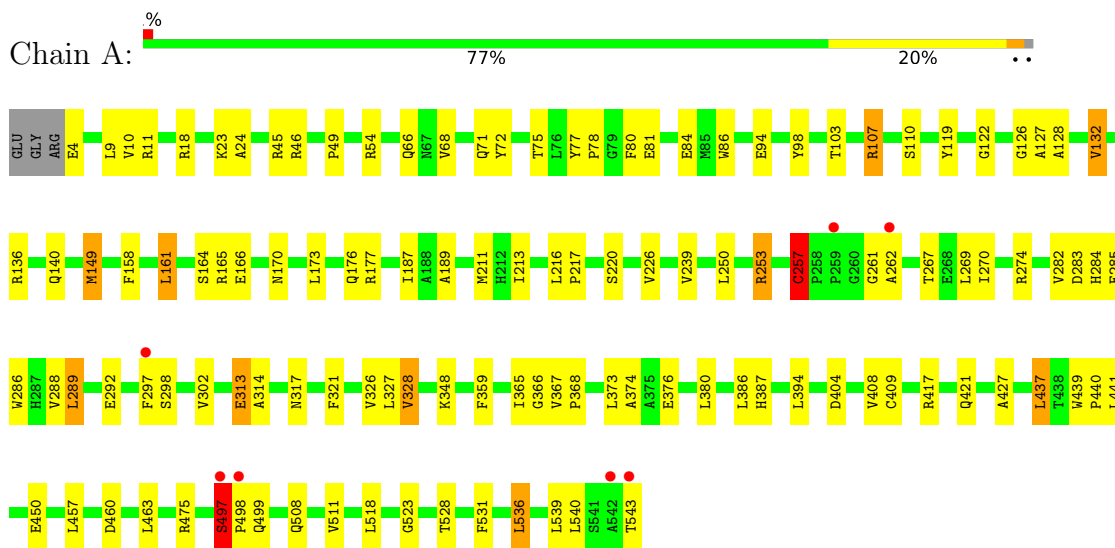
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	247	Total O 247 247	0	0
6	B	144	Total O 144 144	0	0
6	C	258	Total O 258 258	0	0
6	D	186	Total O 186 186	0	0

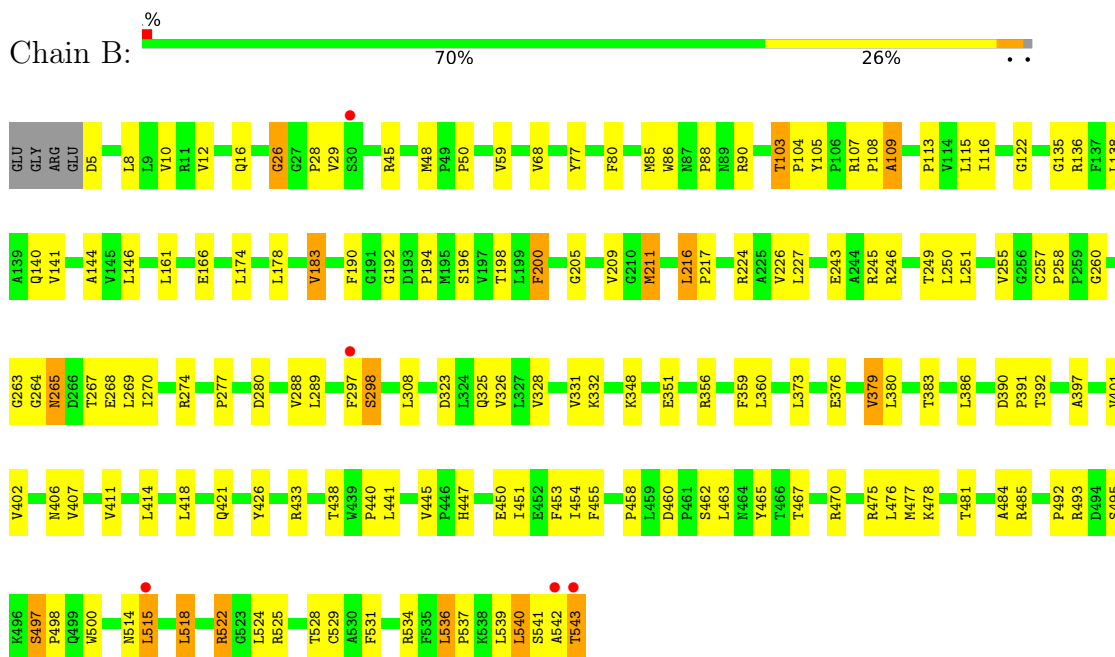
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

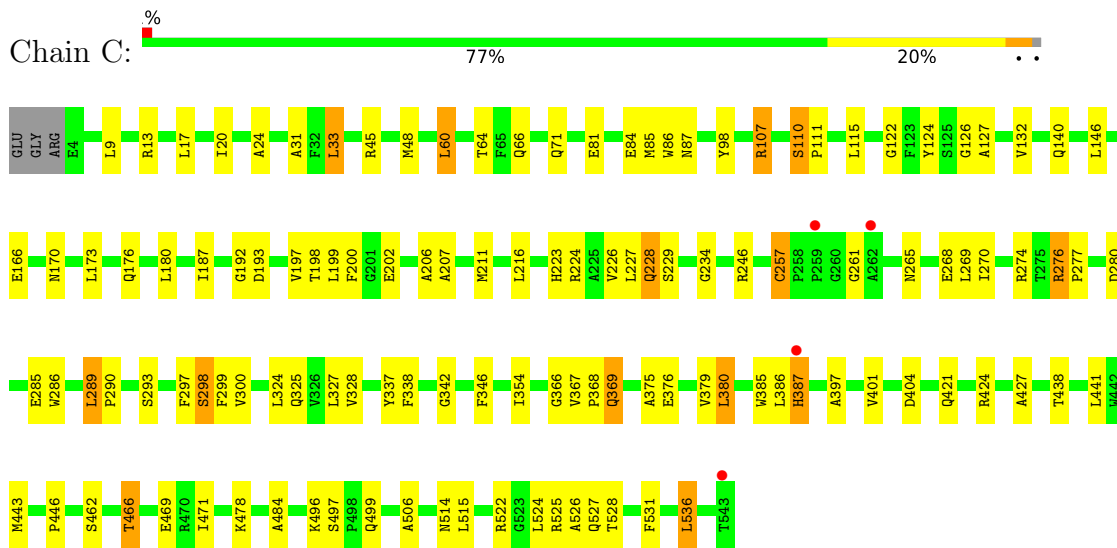
• Molecule 1: ACETYLCHOLINESTERASE



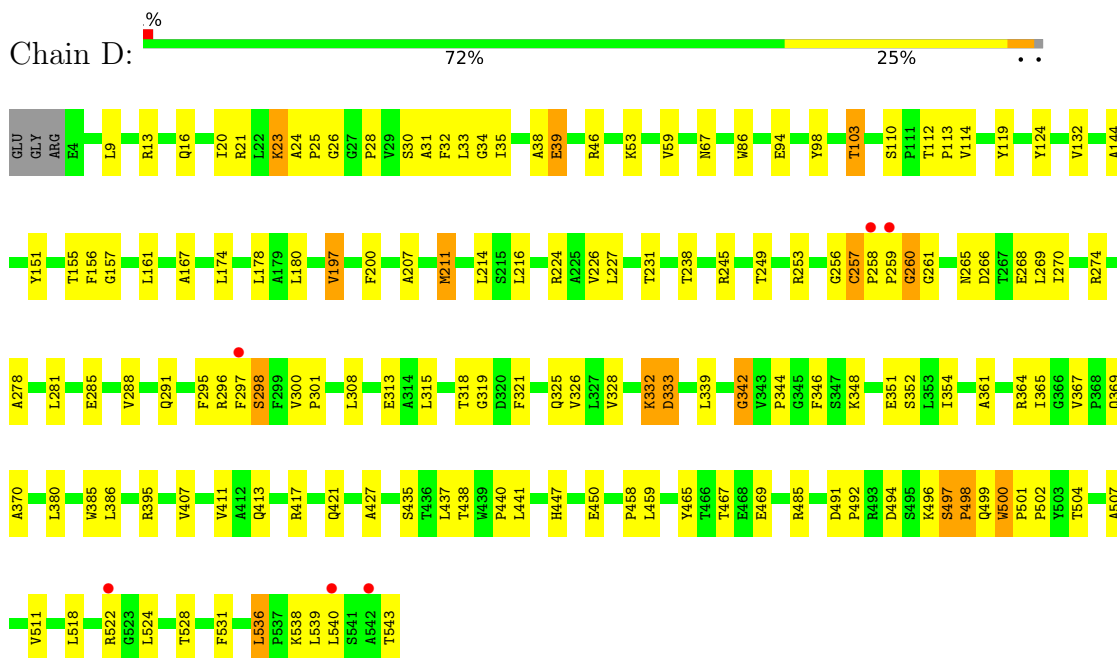
• Molecule 1: ACETYLCHOLINESTERASE



• Molecule 1: ACETYLCHOLINESTERASE



● Molecule 1: ACETYLCHOLINESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.54Å 173.25Å 224.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.28 – 2.95 48.28 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.28-2.95) 99.7 (48.28-2.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.96Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.186 , 0.238 0.189 , 0.239	Depositor DCC
R_{free} test set	3345 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.9	Xtrriage
Anisotropy	0.289	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17994	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: NAG, CL, SO4, TQV

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	0.62	0/4358	1.04	24/5955 (0.4%)
1	B	0.52	0/4329	0.92	10/5916 (0.2%)
1	C	0.61	0/4367	1.03	18/5968 (0.3%)
1	D	0.57	0/4382	0.97	11/5984 (0.2%)
All	All	0.58	0/17436	0.99	63/23823 (0.3%)

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

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

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	257	CYS	CA-C-N	-15.45	104.46	120.38
1	A	257	CYS	C-N-CA	-15.45	104.46	120.38
1	C	257	CYS	CA-C-N	-12.23	107.79	120.38
1	C	257	CYS	C-N-CA	-12.23	107.79	120.38
1	D	257	CYS	CA-C-N	-9.35	110.75	120.38
1	D	257	CYS	C-N-CA	-9.35	110.75	120.38
1	C	367	VAL	CA-C-N	7.18	127.18	119.28
1	C	367	VAL	C-N-CA	7.18	127.18	119.28
1	A	367	VAL	CA-C-N	6.83	126.63	119.05
1	A	367	VAL	C-N-CA	6.83	126.63	119.05
1	C	285	GLU	N-CA-C	6.77	119.49	111.71
1	B	298	SER	N-CA-C	6.57	118.98	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	450	GLU	N-CA-C	-6.34	106.18	114.04
1	D	500	TRP	CA-C-N	6.33	126.91	120.38
1	D	500	TRP	C-N-CA	6.33	126.91	120.38
1	A	161	LEU	CA-C-N	6.33	127.76	119.84
1	A	161	LEU	C-N-CA	6.33	127.76	119.84
1	A	285	GLU	N-CA-C	6.23	118.08	111.28
1	A	409	CYS	CA-C-N	-6.15	112.15	118.85
1	A	409	CYS	C-N-CA	-6.15	112.15	118.85
1	B	514	ASN	N-CA-C	6.10	116.65	108.23
1	C	87	ASN	CA-C-N	6.01	126.03	119.90
1	C	87	ASN	C-N-CA	6.01	126.03	119.90
1	B	289	LEU	CA-C-N	5.98	125.19	118.97
1	B	289	LEU	C-N-CA	5.98	125.19	118.97
1	C	276	ARG	CA-C-N	5.92	125.94	119.90
1	C	276	ARG	C-N-CA	5.92	125.94	119.90
1	A	289	LEU	CA-C-N	5.92	125.46	119.19
1	A	289	LEU	C-N-CA	5.92	125.46	119.19
1	A	49	PRO	O-C-N	5.84	124.00	121.31
1	A	54	ARG	CA-C-N	5.81	127.10	119.84
1	A	54	ARG	C-N-CA	5.81	127.10	119.84
1	B	540	LEU	N-CA-C	-5.80	106.04	113.23
1	B	257	CYS	N-CA-C	5.73	120.04	109.10
1	C	293	SER	N-CA-C	5.70	117.51	108.79
1	D	167	ALA	CA-C-N	5.67	126.75	120.45
1	D	167	ALA	C-N-CA	5.67	126.75	120.45
1	D	24	ALA	CA-C-N	5.61	126.86	119.84
1	D	24	ALA	C-N-CA	5.61	126.86	119.84
1	C	497	SER	CA-C-N	5.60	126.84	119.84
1	C	497	SER	C-N-CA	5.60	126.84	119.84
1	A	158	PHE	N-CA-C	5.60	121.36	113.02
1	A	110	SER	CA-C-N	5.49	126.70	119.84
1	A	110	SER	C-N-CA	5.49	126.70	119.84
1	B	258	PRO	CA-C-N	-5.48	112.99	119.84
1	B	258	PRO	C-N-CA	-5.48	112.99	119.84
1	B	77	TYR	CA-C-N	5.45	126.30	119.98
1	B	77	TYR	C-N-CA	5.45	126.30	119.98
1	D	39	GLU	CA-C-N	5.42	125.96	120.38
1	D	39	GLU	C-N-CA	5.42	125.96	120.38
1	C	300	VAL	CA-C-N	-5.36	114.23	119.76
1	C	300	VAL	C-N-CA	-5.36	114.23	119.76
1	A	387	HIS	CA-C-N	5.23	124.84	119.56
1	A	387	HIS	C-N-CA	5.23	124.84	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	GLU	N-CA-C	-5.20	106.89	114.12
1	A	457	LEU	CA-C-N	-5.17	114.38	120.12
1	A	457	LEU	C-N-CA	-5.17	114.38	120.12
1	C	289	LEU	CA-C-N	5.11	124.61	119.19
1	C	289	LEU	C-N-CA	5.11	124.61	119.19
1	C	526	ALA	N-CA-C	5.08	116.51	111.07
1	A	103	THR	CA-C-N	-5.04	115.37	120.21
1	A	103	THR	C-N-CA	-5.04	115.37	120.21
1	C	497	SER	N-CA-C	-5.01	101.43	109.04

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	257	CYS	Peptide

5.2 Too-close contacts [i](#)

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	4224	0	4111	64	0
1	B	4202	0	4089	85	0
1	C	4230	0	4116	69	0
1	D	4243	0	4146	91	0
2	A	19	0	12	4	0
2	B	19	0	11	3	0
2	C	19	0	12	7	0
2	D	19	0	12	4	0
3	A	14	0	13	0	0
3	B	28	0	26	0	0
3	C	14	0	13	0	0
3	D	42	0	39	0	0
4	A	3	0	0	2	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	3	0	0	1	0
5	A	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	15	0	0	0	0
5	C	15	0	0	1	0
5	D	15	0	0	0	0
6	A	247	0	0	18	0
6	B	144	0	0	6	0
6	C	258	0	0	9	0
6	D	186	0	0	12	0
All	All	17994	0	16600	307	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 9.

All (307) 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)
4:A:1544:CL:CL	6:A:2034:HOH:O	2.19	0.98
2:C:600:TQV:H2	2:C:600:TQV:H8	1.47	0.95
1:D:112:THR:HG21	1:D:144:ALA:HA	1.59	0.85
1:D:249:THR:HG22	1:D:253:ARG:HH21	1.44	0.82
1:A:126:GLY:HA2	6:A:2086:HOH:O	1.82	0.79
1:C:387[A]:HIS:ND1	6:C:2216:HOH:O	2.16	0.78
2:C:600:TQV:H2	2:C:600:TQV:C8	2.15	0.77
1:A:72:TYR:O	6:A:2052:HOH:O	2.02	0.77
1:B:135:GLY:HA3	1:B:146:LEU:HD22	1.67	0.77
1:B:224:ARG:HG2	1:B:325:GLN:HB2	1.67	0.77
1:C:387[A]:HIS:ND1	6:C:2215:HOH:O	2.19	0.75
1:D:227:LEU:HB2	1:D:328:VAL:HG12	1.70	0.73
1:D:39:GLU:OE2	6:D:2019:HOH:O	2.07	0.72
1:A:4:GLU:N	6:A:2001:HOH:O	2.23	0.71
1:D:497:SER:OG	6:D:2169:HOH:O	2.07	0.71
1:C:387[B]:HIS:ND1	6:C:2214:HOH:O	2.22	0.71
1:B:138:LEU:HD21	1:B:455:PHE:HA	1.72	0.70
1:D:155:THR:O	6:D:2080:HOH:O	2.09	0.70
1:B:265:ASN:HB3	1:B:268:GLU:HB2	1.73	0.70
1:C:122:GLY:N	2:C:600:TQV:O3P	2.24	0.70
1:C:227:LEU:HB2	1:C:328:VAL:HG12	1.72	0.70
1:A:165:ARG:NH2	4:A:1544:CL:CL	2.62	0.69
1:C:48:MET:HE3	1:C:166:GLU:HA	1.75	0.69
1:C:86:TRP:CD2	2:C:600:TQV:H5	2.28	0.68
1:C:274:ARG:NH1	6:C:2041:HOH:O	2.17	0.68
1:D:86:TRP:CD2	2:D:600:TQV:H5	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:VAL:HG22	1:B:107:ARG:HH21	1.62	0.65
1:A:508:GLN:NE2	6:A:2228:HOH:O	2.18	0.65
1:B:48:MET:HE3	1:B:166:GLU:HA	1.78	0.65
1:A:4:GLU:OE1	1:A:18:ARG:NH1	2.28	0.64
1:A:161:LEU:HD11	1:A:269:LEU:HD23	1.78	0.64
1:B:103:THR:HG21	1:B:190:PHE:O	1.97	0.64
1:D:259:PRO:HB2	6:D:2124:HOH:O	1.99	0.63
1:A:166:GLU:HB2	1:A:270:ILE:HD13	1.81	0.62
1:D:265:ASN:HB3	1:D:268:GLU:HB2	1.82	0.62
1:B:528:THR:O	1:B:531:PHE:HB3	1.99	0.62
1:D:380:LEU:HA	1:D:385:TRP:HZ2	1.65	0.62
1:C:265:ASN:HB3	1:C:268:GLU:H	1.66	0.61
1:D:380:LEU:HB3	6:D:2154:HOH:O	1.98	0.61
1:C:86:TRP:CE3	2:C:600:TQV:H5	2.36	0.61
1:B:122:GLY:N	2:B:600:TQV:O3P	2.33	0.61
1:C:366:GLY:O	1:C:368:PRO:HD3	2.00	0.61
1:B:166:GLU:HG2	1:B:274:ARG:HH22	1.66	0.60
1:A:46:ARG:O	1:A:274:ARG:NH1	2.34	0.60
1:C:107:ARG:HG2	1:C:107:ARG:HH11	1.65	0.60
1:C:337:TYR:HA	1:C:443:MET:HE2	1.82	0.60
1:D:214:LEU:HD22	1:D:315:LEU:HB3	1.84	0.60
1:A:250:LEU:HG	1:A:288:VAL:HG12	1.85	0.58
1:A:366:GLY:O	1:A:368:PRO:HD3	2.04	0.58
1:D:348:LYS:O	1:D:440:PRO:HG3	2.03	0.58
1:B:541:SER:O	1:B:543:THR:N	2.36	0.58
1:D:86:TRP:CE3	2:D:600:TQV:H5	2.38	0.58
1:C:197:VAL:H	1:C:223:HIS:HD2	1.51	0.58
1:D:332:LYS:HB3	1:D:333:ASP:OD1	2.04	0.58
1:C:380:LEU:HA	1:C:385:TRP:HZ2	1.69	0.57
1:A:149:MET:HE2	1:A:176:GLN:HA	1.87	0.57
1:B:166:GLU:OE1	1:B:267:THR:HG22	2.05	0.57
1:B:260:GLY:HA2	1:C:286:TRP:CG	2.39	0.57
1:B:498:PRO:HD2	1:B:518:LEU:HB3	1.87	0.57
1:A:107:ARG:NH2	6:A:2010:HOH:O	2.28	0.56
1:B:460:ASP:HB3	1:B:463:LEU:HD12	1.87	0.56
1:D:224:ARG:HG2	1:D:325:GLN:HB2	1.87	0.56
1:B:263:GLY:O	1:B:265:ASN:N	2.38	0.56
1:A:68:VAL:HG13	1:A:127:ALA:HB2	1.88	0.56
1:B:113:PRO:HG3	1:B:485:ARG:HB3	1.88	0.55
1:C:71:GLN:NE2	1:C:126:GLY:O	2.37	0.55
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:THR:HG23	1:C:469:GLU:OE1	2.07	0.55
1:B:475:ARG:NH2	6:B:2131:HOH:O	2.30	0.54
1:A:321:PHE:HD2	1:A:421:GLN:HB3	1.73	0.54
1:A:161:LEU:HD12	1:A:270:ILE:HD11	1.89	0.54
1:B:260:GLY:HA2	1:C:286:TRP:CD1	2.42	0.54
1:C:180:LEU:HD21	1:C:199:LEU:HD21	1.90	0.54
1:B:450:GLU:OE1	6:B:2061:HOH:O	2.18	0.54
1:A:177:ARG:NH2	1:A:217:PRO:HG2	2.23	0.54
1:A:497:SER:H	1:A:498:PRO:HA	1.73	0.54
1:D:30:SER:HB2	1:D:103:THR:HG23	1.90	0.54
1:B:5:ASP:OD2	1:B:105:TYR:OH	2.23	0.53
1:D:333:ASP:OD1	1:D:333:ASP:N	2.40	0.53
1:D:256:GLY:O	1:D:259:PRO:HB3	2.09	0.53
1:D:266:ASP:O	1:D:270:ILE:HG12	2.09	0.53
1:A:348:LYS:HA	1:A:440:PRO:HG3	1.91	0.53
1:B:525:ARG:O	1:B:529:CYS:HB2	2.08	0.53
1:C:115:LEU:HD23	1:C:198:THR:HB	1.90	0.53
1:D:39:GLU:HG2	1:D:53:LYS:HA	1.91	0.53
1:D:370:ALA:HA	1:D:540:LEU:HD11	1.91	0.53
1:A:71:GLN:HA	6:A:2050:HOH:O	2.09	0.53
1:A:226:VAL:HG13	1:A:327:LEU:HB3	1.90	0.53
1:B:348:LYS:O	1:B:440:PRO:HG3	2.09	0.53
1:C:200:PHE:HB2	1:C:226:VAL:HB	1.91	0.53
1:D:119:TYR:O	1:D:151:TYR:OH	2.21	0.52
1:C:115:LEU:HD21	1:C:484:ALA:HB2	1.91	0.52
1:C:187:ILE:HG13	1:C:192:GLY:HA3	1.91	0.52
1:D:38:ALA:HB2	1:D:178:LEU:HD23	1.91	0.52
1:D:435:SER:HG	1:D:469:GLU:CD	2.17	0.52
1:A:122:GLY:N	2:A:600:TQV:O3P	2.36	0.52
1:C:246:ARG:NH2	1:C:290:PRO:HG3	2.25	0.52
1:C:298:SER:HB3	1:C:299:PHE:CD2	2.44	0.52
1:D:249:THR:HG22	1:D:253:ARG:NH2	2.20	0.52
1:D:511:VAL:HB	1:D:518:LEU:HD22	1.91	0.52
1:B:28:PRO:HG2	1:B:105:TYR:HB3	1.92	0.52
1:B:356:ARG:O	1:B:360:LEU:HG	2.10	0.51
1:B:373:LEU:HD23	1:B:539:LEU:HD11	1.92	0.51
1:B:323:ASP:N	1:B:323:ASP:OD1	2.43	0.51
1:D:214:LEU:HD22	1:D:315:LEU:CB	2.41	0.51
1:B:534:ARG:NH1	6:B:2141:HOH:O	2.33	0.51
1:A:166:GLU:HB3	1:A:274:ARG:HH22	1.75	0.51
1:A:380:LEU:HB3	6:A:2246:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:THR:O	1:A:531:PHE:HB3	2.10	0.51
1:D:157:GLY:O	6:D:2081:HOH:O	2.20	0.51
1:A:292:GLU:HB2	1:D:249:THR:HG21	1.93	0.51
1:C:166:GLU:OE1	1:C:166:GLU:N	2.40	0.51
1:D:458:PRO:HA	1:D:465:TYR:CD2	2.46	0.50
1:D:21:ARG:HH11	1:D:28:PRO:HB3	1.76	0.50
1:D:297[A]:PHE:CG	1:D:298:SER:N	2.79	0.50
1:A:66:GLN:HG3	1:A:98:TYR:CD2	2.47	0.50
1:A:128:ALA:HB3	6:A:2072:HOH:O	2.10	0.50
1:B:68:VAL:HG11	1:B:88:PRO:HB3	1.93	0.50
1:B:454:ILE:HD12	1:B:476:LEU:HD13	1.94	0.49
1:C:31:ALA:HB1	1:C:33:LEU:HD21	1.93	0.49
1:D:313:GLU:HG2	1:D:417[B]:ARG:HH12	1.76	0.49
1:D:342:GLY:O	1:D:344:PRO:HD3	2.11	0.49
1:D:407:VAL:O	1:D:411:VAL:HG23	2.11	0.49
1:A:66:GLN:HG3	1:A:98:TYR:CG	2.48	0.49
1:B:243:GLU:OE2	1:B:246:ARG:NH2	2.42	0.49
1:C:404:ASP:OD2	1:C:525:ARG:NH2	2.45	0.49
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.95	0.49
1:C:424:ARG:HD2	6:C:2225:HOH:O	2.12	0.49
1:D:34:GLY:HA2	1:D:98:TYR:HB3	1.94	0.49
1:B:113:PRO:HA	1:B:196:SER:HB3	1.94	0.49
1:B:332:LYS:HB3	1:B:445:VAL:HB	1.95	0.48
1:A:289:LEU:O	1:D:253:ARG:NH1	2.45	0.48
1:A:286:TRP:CG	1:D:260:GLY:HA2	2.49	0.48
1:B:379:VAL:O	1:B:383:THR:OG1	2.15	0.48
1:D:326:VAL:HG12	1:D:328:VAL:HG13	1.95	0.48
1:A:475:ARG:NH2	6:A:2220:HOH:O	2.47	0.48
1:D:16:GLN:HB2	1:D:59:VAL:HG22	1.96	0.48
1:B:116:ILE:HD11	1:B:183:VAL:HG11	1.95	0.48
1:D:211:MET:HG2	1:D:308:LEU:HD21	1.95	0.48
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.94	0.48
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.96	0.47
1:D:67:ASN:ND2	6:D:2041:HOH:O	2.46	0.47
1:A:107:ARG:HG2	1:A:107:ARG:HH11	1.79	0.47
1:B:407:VAL:O	1:B:411:VAL:HG23	2.15	0.47
1:B:200:PHE:CB	1:B:226:VAL:HB	2.44	0.47
1:B:453:PHE:HB3	1:B:476:LEU:HD12	1.96	0.47
1:D:528:THR:O	1:D:531:PHE:HB3	2.14	0.47
1:B:103:THR:HG22	1:B:104:PRO:HD2	1.96	0.47
1:D:497:SER:N	1:D:498:PRO:HA	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:LEU:HA	1:D:174:LEU:HD23	1.74	0.47
1:B:115:LEU:HD23	1:B:198:THR:HB	1.97	0.47
1:C:346:PHE:CZ	1:C:354:ILE:HD13	2.49	0.47
1:D:156:PHE:CZ	1:D:278:ALA:HB1	2.50	0.47
1:C:24:ALA:HB3	1:C:140:GLN:HG3	1.97	0.47
1:C:338:PHE:CE2	2:C:600:TQV:H8A	2.49	0.47
1:C:197:VAL:H	1:C:223:HIS:CD2	2.31	0.47
1:A:373:LEU:HD23	1:A:539:LEU:HD11	1.97	0.46
1:B:447:HIS:HD2	2:B:600:TQV:C2	2.28	0.46
1:B:522:ARG:HB3	6:B:2138:HOH:O	2.15	0.46
1:B:537:PRO:C	1:B:539:LEU:H	2.23	0.46
1:B:543:THR:O	1:B:543:THR:OG1	2.29	0.46
1:C:528:THR:O	1:C:531:PHE:HB3	2.15	0.46
1:D:339:LEU:HD13	1:D:346:PHE:CE2	2.50	0.46
1:A:75:THR:O	1:A:78:PRO:HD3	2.15	0.46
1:D:32:PHE:HB3	1:D:35:ILE:HD11	1.97	0.46
1:D:124:TYR:HB3	1:D:297[A]:PHE:CD2	2.50	0.46
1:A:11:ARG:N	6:A:2011:HOH:O	2.35	0.46
1:A:86:TRP:CD2	2:A:600:TQV:H5	2.50	0.46
1:B:26:GLY:HA3	1:B:140:GLN:OE1	2.16	0.46
1:B:109:ALA:HB3	6:B:2035:HOH:O	2.15	0.46
1:C:124:TYR:HB3	1:C:297[A]:PHE:CE2	2.50	0.46
1:D:249:THR:CG2	1:D:253:ARG:HH21	2.22	0.46
1:C:289:LEU:HA	1:C:290:PRO:HD3	1.78	0.46
1:A:239:VAL:HG23	1:A:302:VAL:HG23	1.98	0.46
1:B:277:PRO:HG2	1:B:280:ASP:CG	2.41	0.46
1:B:216:LEU:HB3	1:B:217:PRO:HD3	1.98	0.46
1:B:297[A]:PHE:CG	1:B:298:SER:N	2.82	0.46
1:B:397:ALA:O	1:B:401:VAL:HG23	2.16	0.46
1:A:536:LEU:HD23	6:A:2240:HOH:O	2.16	0.46
1:C:66:GLN:HG3	1:C:98:TYR:CD2	2.51	0.46
1:C:111:PRO:HB2	1:C:193:ASP:HB2	1.98	0.46
1:C:276:ARG:N	1:C:276:ARG:HD2	2.29	0.46
1:D:300:VAL:HB	1:D:301:PRO:HD2	1.97	0.46
1:D:328:VAL:O	1:D:427:ALA:HA	2.15	0.46
1:C:270:ILE:O	1:C:274:ARG:HG3	2.16	0.45
1:D:113:PRO:HG3	1:D:485:ARG:HG2	1.97	0.45
1:D:369:GLN:HB2	6:D:2139:HOH:O	2.17	0.45
1:A:166:GLU:HG2	6:A:2144:HOH:O	2.15	0.45
1:B:414:LEU:O	1:B:418:LEU:HG	2.17	0.45
1:C:346:PHE:HZ	1:C:354:ILE:HD13	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:VAL:HB	1:D:197:VAL:HG22	1.97	0.45
1:D:245:ARG:NH2	1:D:266:ASP:OD1	2.50	0.45
1:B:192:GLY:O	1:B:194:PRO:HD3	2.16	0.45
1:C:443:MET:HB3	1:C:446:PRO:HG3	1.98	0.45
1:D:31:ALA:HB1	1:D:33:LEU:HD21	1.99	0.45
1:A:499:GLN:HB3	6:A:2223:HOH:O	2.15	0.45
1:B:86:TRP:CD2	2:B:600:TQV:H5	2.52	0.45
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.97	0.45
1:C:515:LEU:HD23	1:C:515:LEU:HA	1.72	0.45
1:D:207:ALA:O	1:D:211:MET:HE3	2.17	0.45
1:A:46:ARG:HD2	1:A:274:ARG:HG2	1.99	0.44
1:C:81:GLU:HG3	6:C:2076:HOH:O	2.17	0.44
1:D:161:LEU:HD11	1:D:269:LEU:HD23	1.99	0.44
1:D:231:THR:HG21	1:D:411:VAL:HA	1.99	0.44
1:B:426:TYR:HB3	1:B:500:TRP:NE1	2.33	0.44
1:D:112:THR:CG2	1:D:144:ALA:HA	2.40	0.44
1:D:539:LEU:O	1:D:543:THR:HG22	2.17	0.44
1:A:45:ARG:NH1	6:A:2034:HOH:O	2.48	0.44
1:A:77:TYR:O	1:A:80:PHE:HB3	2.18	0.44
1:B:166:GLU:HB3	1:B:274:ARG:HH12	1.83	0.44
1:C:170:ASN:O	1:C:173:LEU:HB2	2.18	0.44
1:D:346:PHE:CE1	1:D:354:ILE:HG21	2.53	0.44
1:D:447:HIS:HD2	2:D:600:TQV:C2	2.30	0.44
1:D:522[B]:ARG:H	1:D:522[B]:ARG:HE	1.66	0.44
1:C:274:ARG:HD3	6:C:2041:HOH:O	2.17	0.44
1:A:313:GLU:HG3	1:A:314:ALA:N	2.32	0.44
1:C:527:GLN:N	5:C:1547:SO4:O3	2.44	0.44
1:C:536:LEU:HD23	1:C:536:LEU:HA	1.74	0.44
1:C:173:LEU:O	1:C:176:GLN:HB2	2.18	0.44
1:C:338:PHE:HE2	2:C:600:TQV:H8A	1.83	0.44
1:D:238:THR:HG22	1:D:301:PRO:HB2	2.00	0.44
1:B:402:VAL:O	1:B:406:ASN:HB2	2.18	0.43
1:C:81:GLU:O	1:C:85:MET:HG2	2.18	0.43
1:C:297[A]:PHE:CG	1:C:298:SER:N	2.86	0.43
1:D:504:THR:OG1	1:D:507:ALA:HB3	2.17	0.43
1:B:174:LEU:HA	1:B:174:LEU:HD23	1.86	0.43
1:B:390:ASP:HA	1:B:391:PRO:HD2	1.84	0.43
1:D:23:LYS:HG3	6:D:2012:HOH:O	2.18	0.43
1:D:313:GLU:HG3	6:D:2160:HOH:O	2.18	0.43
1:C:202:GLU:HA	1:C:228:GLN:O	2.19	0.43
1:C:328:VAL:O	1:C:427:ALA:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ASN:OD1	1:B:267:THR:OG1	2.36	0.43
1:A:404:ASP:HA	1:A:408:VAL:HB	2.00	0.43
1:D:501:PRO:HA	1:D:502:PRO:HD3	1.95	0.43
1:A:282:VAL:O	1:A:284:HIS:N	2.52	0.43
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.99	0.43
1:A:107:ARG:NH1	1:A:189:ALA:O	2.52	0.43
2:A:600:TQV:H2	2:A:600:TQV:O1P	2.18	0.43
1:B:115:LEU:HD21	1:B:484:ALA:HB2	2.00	0.43
1:B:531:PHE:CD1	1:B:531:PHE:C	2.97	0.43
1:B:531:PHE:CE1	1:B:536:LEU:HG	2.54	0.43
1:C:234:GLY:O	6:C:2150:HOH:O	2.21	0.43
1:C:277:PRO:O	1:C:280:ASP:HB3	2.18	0.43
1:A:253:ARG:NH2	4:D:1991:CL:CL	2.89	0.43
1:B:458:PRO:HG3	1:B:465:TYR:CD2	2.54	0.43
1:D:352:SER:O	1:D:395:ARG:HG3	2.19	0.43
1:D:492:PRO:O	1:D:494:ASP:N	2.44	0.43
1:C:397:ALA:O	1:C:401:VAL:HG23	2.19	0.42
1:D:46:ARG:O	1:D:274:ARG:HD3	2.19	0.42
1:C:200:PHE:CB	1:C:226:VAL:HB	2.48	0.42
1:A:119:TYR:CE1	1:A:126:GLY:HA3	2.55	0.42
1:A:328:VAL:O	1:A:427:ALA:HA	2.20	0.42
1:A:460:ASP:HB3	1:A:463:LEU:HD12	1.99	0.42
1:D:200:PHE:CB	1:D:226:VAL:HB	2.49	0.42
1:D:296:ARG:N	2:D:600:TQV:H12	2.33	0.42
1:D:435:SER:OG	1:D:469:GLU:OE1	2.29	0.42
1:C:45:ARG:HA	1:C:45:ARG:HD2	1.78	0.42
1:C:206:ALA:O	1:C:207:ALA:C	2.63	0.42
1:D:46:ARG:NH2	1:D:94:GLU:OE2	2.50	0.42
1:B:68:VAL:HG23	1:B:90:ARG:HB2	2.02	0.42
1:B:144:ALA:HA	6:B:2037:HOH:O	2.20	0.42
1:C:17:LEU:HB3	1:C:60:LEU:HB3	2.02	0.42
1:B:85:MET:HE3	1:B:85:MET:HB2	1.90	0.42
1:D:200:PHE:HB2	1:D:226:VAL:HB	2.02	0.42
1:B:326:VAL:HG12	1:B:328:VAL:HG13	2.01	0.42
1:C:369[A]:GLN:HG2	6:C:2152:HOH:O	2.20	0.42
1:D:361:ALA:O	1:D:365:ILE:HG13	2.20	0.42
1:B:433:ARG:HH12	1:B:441:LEU:HA	1.83	0.42
1:B:359:PHE:HD2	1:B:360:LEU:HD23	1.84	0.41
1:B:467:THR:HG22	1:B:470:ARG:NH2	2.34	0.41
1:D:258:PRO:HD2	1:D:259:PRO:HA	2.01	0.41
1:D:494:ASP:HB2	6:D:2172:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ARG:HH22	1:B:440:PRO:C	2.27	0.41
1:A:94:GLU:HA	6:A:2016:HOH:O	2.20	0.41
1:C:376:GLU:OE1	1:D:538:LYS:HD2	2.21	0.41
1:D:295:PHE:O	1:D:296:ARG:HD3	2.19	0.41
1:C:375:ALA:O	1:C:379:VAL:HG23	2.21	0.41
1:D:531:PHE:CZ	1:D:536:LEU:HD23	2.56	0.41
1:A:86:TRP:HB3	6:A:2061:HOH:O	2.21	0.41
1:A:374:ALA:HA	1:A:539:LEU:HD23	2.02	0.41
1:A:86:TRP:CE2	2:A:600:TQV:H5	2.56	0.41
1:C:224:ARG:HG2	1:C:325:GLN:HB2	2.01	0.41
1:D:26:GLY:N	6:D:2013:HOH:O	2.31	0.41
1:A:187:ILE:HD12	1:A:187:ILE:HA	1.91	0.41
1:D:288:VAL:HG23	1:D:298:SER:HB3	2.03	0.41
1:B:205:GLY:O	1:B:209:VAL:HG23	2.21	0.41
1:C:33:LEU:HB2	1:C:64:THR:O	2.20	0.41
1:A:297[A]:PHE:CG	1:A:298:SER:N	2.88	0.41
1:A:437:LEU:HD12	1:A:439:TRP:H	1.86	0.41
1:B:50:PRO:HB2	1:B:178:LEU:HD22	2.03	0.41
1:B:104:PRO:HG2	1:B:108:PRO:HD3	2.02	0.41
1:B:515:LEU:H	1:B:515:LEU:HG	1.58	0.41
1:C:66:GLN:HG3	1:C:98:TYR:CG	2.56	0.41
1:D:500:TRP:HA	1:D:501:PRO:HD2	1.92	0.41
1:A:132:VAL:HG22	6:A:2060:HOH:O	2.21	0.41
1:B:138:LEU:HD13	1:B:477:MET:HE3	2.02	0.41
1:A:359:PHE:CG	1:A:394:LEU:HD22	2.56	0.40
1:A:511:VAL:HB	1:A:518:LEU:HD22	2.03	0.40
1:C:324:LEU:HD12	1:C:324:LEU:HA	1.91	0.40
1:D:319:GLY:HA3	1:D:321:PHE:CZ	2.57	0.40
1:B:80:PHE:CD1	1:B:348:LYS:HE2	2.57	0.40
1:B:460:ASP:OD2	1:B:462:SER:OG	2.35	0.40
1:B:481:THR:O	1:B:485:ARG:HG2	2.21	0.40
1:A:170:ASN:HB3	1:A:173:LEU:HD12	2.03	0.40
1:B:250:LEU:HG	1:B:288:VAL:HG12	2.03	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	541/543 (100%)	500 (92%)	35 (6%)	6 (1%)	11	29
1	B	538/543 (99%)	485 (90%)	45 (8%)	8 (2%)	8	23
1	C	542/543 (100%)	500 (92%)	36 (7%)	6 (1%)	11	29
1	D	543/543 (100%)	503 (93%)	34 (6%)	6 (1%)	11	29
All	All	2164/2172 (100%)	1988 (92%)	150 (7%)	26 (1%)	10	28

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	264	GLY
1	B	495	SER
1	B	542	ALA
1	D	497	SER
1	A	283	ASP
1	C	496	LYS
1	D	260	GLY
1	A	257	CYS
1	A	261	GLY
1	A	497	SER
1	C	127	ALA
1	A	262	ALA
1	B	109	ALA
1	B	492	PRO
1	B	497	SER
1	C	110	SER
1	C	342	GLY
1	D	25	PRO
1	D	261	GLY
1	B	26	GLY
1	C	261	GLY
1	C	506	ALA

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Mol	Chain	Res	Type
1	A	523	GLY
1	D	342	GLY
1	B	255	VAL
1	D	498	PRO

5.3.2 Protein sidechains [i](#)

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	444/443 (100%)	413 (93%)	31 (7%)	14	34
1	B	441/443 (100%)	404 (92%)	37 (8%)	10	26
1	C	445/443 (100%)	409 (92%)	36 (8%)	11	28
1	D	446/443 (101%)	414 (93%)	32 (7%)	13	33
All	All	1776/1772 (100%)	1640 (92%)	136 (8%)	12	30

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	10	VAL
1	A	23	LYS
1	A	81	GLU
1	A	84	GLU
1	A	107	ARG
1	A	132	VAL
1	A	136	ARG
1	A	149	MET
1	A	164	SER
1	A	211	MET
1	A	213	ILE
1	A	216	LEU
1	A	220	SER
1	A	253	ARG
1	A	257	CYS
1	A	267	THR

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Mol	Chain	Res	Type
1	A	313	GLU
1	A	317	ASN
1	A	326	VAL
1	A	328	VAL
1	A	365	ILE
1	A	376	GLU
1	A	386	LEU
1	A	417	ARG
1	A	437	LEU
1	A	441	LEU
1	A	497	SER
1	A	536	LEU
1	A	540	LEU
1	A	543	THR
1	B	8	LEU
1	B	12	VAL
1	B	16	GLN
1	B	29	VAL
1	B	45	ARG
1	B	59	VAL
1	B	103	THR
1	B	136	ARG
1	B	141	VAL
1	B	183	VAL
1	B	200	PHE
1	B	211	MET
1	B	216	LEU
1	B	245	ARG
1	B	249	THR
1	B	251	LEU
1	B	265	ASN
1	B	331	VAL
1	B	351	GLU
1	B	376	GLU
1	B	379	VAL
1	B	380	LEU
1	B	386	LEU
1	B	392	THR
1	B	421	GLN
1	B	438	THR
1	B	451	ILE
1	B	478	LYS

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Mol	Chain	Res	Type
1	B	493	ARG
1	B	497	SER
1	B	515	LEU
1	B	518	LEU
1	B	522	ARG
1	B	524	LEU
1	B	536	LEU
1	B	540	LEU
1	B	543	THR
1	C	9	LEU
1	C	13	ARG
1	C	20	ILE
1	C	33	LEU
1	C	60	LEU
1	C	84	GLU
1	C	107	ARG
1	C	110	SER
1	C	132	VAL
1	C	146	LEU
1	C	211	MET
1	C	216	LEU
1	C	228	GLN
1	C	229	SER
1	C	257	CYS
1	C	269	LEU
1	C	298	SER
1	C	327	LEU
1	C	369[A]	GLN
1	C	369[B]	GLN
1	C	380	LEU
1	C	386	LEU
1	C	387[A]	HIS
1	C	387[B]	HIS
1	C	421	GLN
1	C	438	THR
1	C	441	LEU
1	C	462	SER
1	C	466	THR
1	C	471	ILE
1	C	478	LYS
1	C	499	GLN
1	C	514	ASN

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Mol	Chain	Res	Type
1	C	522	ARG
1	C	524	LEU
1	C	536	LEU
1	D	9	LEU
1	D	13	ARG
1	D	20	ILE
1	D	23	LYS
1	D	103	THR
1	D	110	SER
1	D	132	VAL
1	D	180	LEU
1	D	197	VAL
1	D	211	MET
1	D	216	LEU
1	D	281	LEU
1	D	285	GLU
1	D	291	GLN
1	D	298	SER
1	D	318	THR
1	D	332	LYS
1	D	333	ASP
1	D	351	GLU
1	D	364	ARG
1	D	367	VAL
1	D	386	LEU
1	D	413	GLN
1	D	437	LEU
1	D	438	THR
1	D	441	LEU
1	D	459	LEU
1	D	467	THR
1	D	491	ASP
1	D	496	LYS
1	D	499	GLN
1	D	536	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	67	ASN
1	A	140	GLN

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Mol	Chain	Res	Type
1	A	317	ASN
1	A	421	GLN
1	A	474	GLN
1	A	509	GLN
1	B	100	ASN
1	B	228	GLN
1	B	279	GLN
1	C	16	GLN
1	C	140	GLN
1	C	181	GLN
1	D	67	ASN
1	D	228	GLN
1	D	421	GLN

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](#)

Of 37 ligands modelled in this entry, 11 are monoatomic - leaving 26 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	B	1545	-	4,4,4	0.25	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	701	1	14,14,15	0.45	0	17,19,21	1.30	1 (5%)
5	SO4	A	1550	-	4,4,4	0.25	0	6,6,6	0.21	0
2	TQV	C	600	1	17,20,21	1.06	1 (5%)	21,26,29	1.48	1 (4%)
3	NAG	D	703	1	14,14,15	0.64	0	17,19,21	1.53	3 (17%)
5	SO4	B	1546	-	4,4,4	0.22	0	6,6,6	0.11	0
5	SO4	D	1546	-	4,4,4	0.21	0	6,6,6	0.16	0
5	SO4	A	1545	-	4,4,4	0.26	0	6,6,6	0.20	0
5	SO4	A	1547	-	4,4,4	0.27	0	6,6,6	0.31	0
5	SO4	D	1545	-	4,4,4	0.25	0	6,6,6	0.16	0
5	SO4	A	1546	-	4,4,4	0.23	0	6,6,6	0.09	0
2	TQV	D	600	1	17,20,21	1.20	1 (5%)	21,26,29	1.41	4 (19%)
3	NAG	B	701	1	14,14,15	0.48	0	17,19,21	1.65	3 (17%)
5	SO4	B	1547	-	4,4,4	0.26	0	6,6,6	0.13	0
3	NAG	D	701	1	14,14,15	0.40	0	17,19,21	2.04	2 (11%)
2	TQV	B	600	1	17,20,21	1.11	1 (5%)	21,26,29	1.28	4 (19%)
5	SO4	D	1547	-	4,4,4	0.24	0	6,6,6	0.11	0
5	SO4	C	1548	-	4,4,4	0.34	0	6,6,6	0.28	0
5	SO4	A	1549	-	4,4,4	0.27	0	6,6,6	0.29	0
3	NAG	B	702	1	14,14,15	0.50	0	17,19,21	2.14	2 (11%)
5	SO4	A	1548	-	4,4,4	0.25	0	6,6,6	0.23	0
3	NAG	A	701	1	14,14,15	0.47	0	17,19,21	1.05	1 (5%)
3	NAG	D	702	1	14,14,15	0.56	0	17,19,21	2.01	1 (5%)
5	SO4	C	1549	-	4,4,4	0.27	0	6,6,6	0.16	0
2	TQV	A	600	1	17,20,21	1.15	1 (5%)	21,26,29	1.00	1 (4%)
5	SO4	C	1547	-	4,4,4	0.24	0	6,6,6	0.14	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	NAG	C	701	1	-	4/6/23/26	0/1/1/1
2	TQV	C	600	1	-	0/6/9/11	0/2/2/2
3	NAG	B	702	1	-	4/6/23/26	0/1/1/1
3	NAG	D	703	1	-	4/6/23/26	0/1/1/1
3	NAG	A	701	1	-	0/6/23/26	0/1/1/1
3	NAG	D	702	1	-	4/6/23/26	0/1/1/1
2	TQV	D	600	1	-	0/6/9/11	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	701	1	-	4/6/23/26	0/1/1/1
2	TQV	A	600	1	-	1/6/9/11	0/2/2/2
3	NAG	D	701	1	-	1/6/23/26	0/1/1/1
2	TQV	B	600	1	-	0/6/9/11	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	TQV	C8-C9	-4.45	1.39	1.50
2	D	600	TQV	C8-C9	-4.44	1.39	1.50
2	B	600	TQV	C8-C9	-4.32	1.39	1.50
2	C	600	TQV	C8-C9	-4.15	1.40	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NAG	C1-O5-C5	7.60	122.37	112.19
3	D	702	NAG	C1-O5-C5	7.22	121.86	112.19
3	D	701	NAG	C1-O5-C5	7.05	121.63	112.19
2	C	600	TQV	O1P-C8-C9	4.70	118.04	109.36
3	C	701	NAG	C1-O5-C5	4.52	118.25	112.19
3	B	701	NAG	C2-N2-C7	4.31	128.68	122.90
3	D	703	NAG	C1-O5-C5	3.99	117.54	112.19
3	A	701	NAG	C1-O5-C5	3.69	117.13	112.19
3	B	701	NAG	C1-O5-C5	3.18	116.45	112.19
3	D	703	NAG	C1-C2-N2	2.85	114.92	110.43
2	D	600	TQV	C10-C9-C14	2.69	121.09	118.16
3	D	703	NAG	O5-C5-C6	2.61	112.74	107.66
3	D	701	NAG	C4-C3-C2	-2.40	107.50	111.02
2	D	600	TQV	C7-C6-C1	-2.40	117.55	120.94
2	B	600	TQV	O2P-C1-C6	-2.35	116.45	118.49
2	B	600	TQV	C10-C9-C14	2.27	120.63	118.16
2	B	600	TQV	O1P-C8-C9	2.26	113.53	109.36
2	D	600	TQV	O2P-C1-C6	-2.25	116.54	118.49
2	A	600	TQV	C10-C9-C14	2.15	120.50	118.16
3	B	702	NAG	O5-C5-C4	2.11	115.96	110.83
2	D	600	TQV	O1P-C8-C9	2.09	113.22	109.36
3	B	701	NAG	O7-C7-C8	-2.09	118.34	122.05
2	B	600	TQV	O2P-C1-C2	2.08	124.24	120.47

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	NAG	C8-C7-N2-C2
3	B	702	NAG	O7-C7-N2-C2
3	D	702	NAG	C8-C7-N2-C2
3	D	702	NAG	O7-C7-N2-C2
3	D	703	NAG	C1-C2-N2-C7
3	D	703	NAG	C8-C7-N2-C2
3	D	703	NAG	O7-C7-N2-C2
3	C	701	NAG	C8-C7-N2-C2
3	C	701	NAG	O7-C7-N2-C2
3	C	701	NAG	O5-C5-C6-O6
3	B	701	NAG	C8-C7-N2-C2
3	C	701	NAG	C4-C5-C6-O6
3	B	702	NAG	O5-C5-C6-O6
3	B	701	NAG	O7-C7-N2-C2
3	D	702	NAG	C4-C5-C6-O6
3	D	702	NAG	O5-C5-C6-O6
3	D	703	NAG	O5-C5-C6-O6
3	B	701	NAG	O5-C5-C6-O6
3	D	701	NAG	O5-C5-C6-O6
3	B	701	NAG	C3-C2-N2-C7
2	A	600	TQV	C1-O2P-P-O1P
3	B	702	NAG	C4-C5-C6-O6

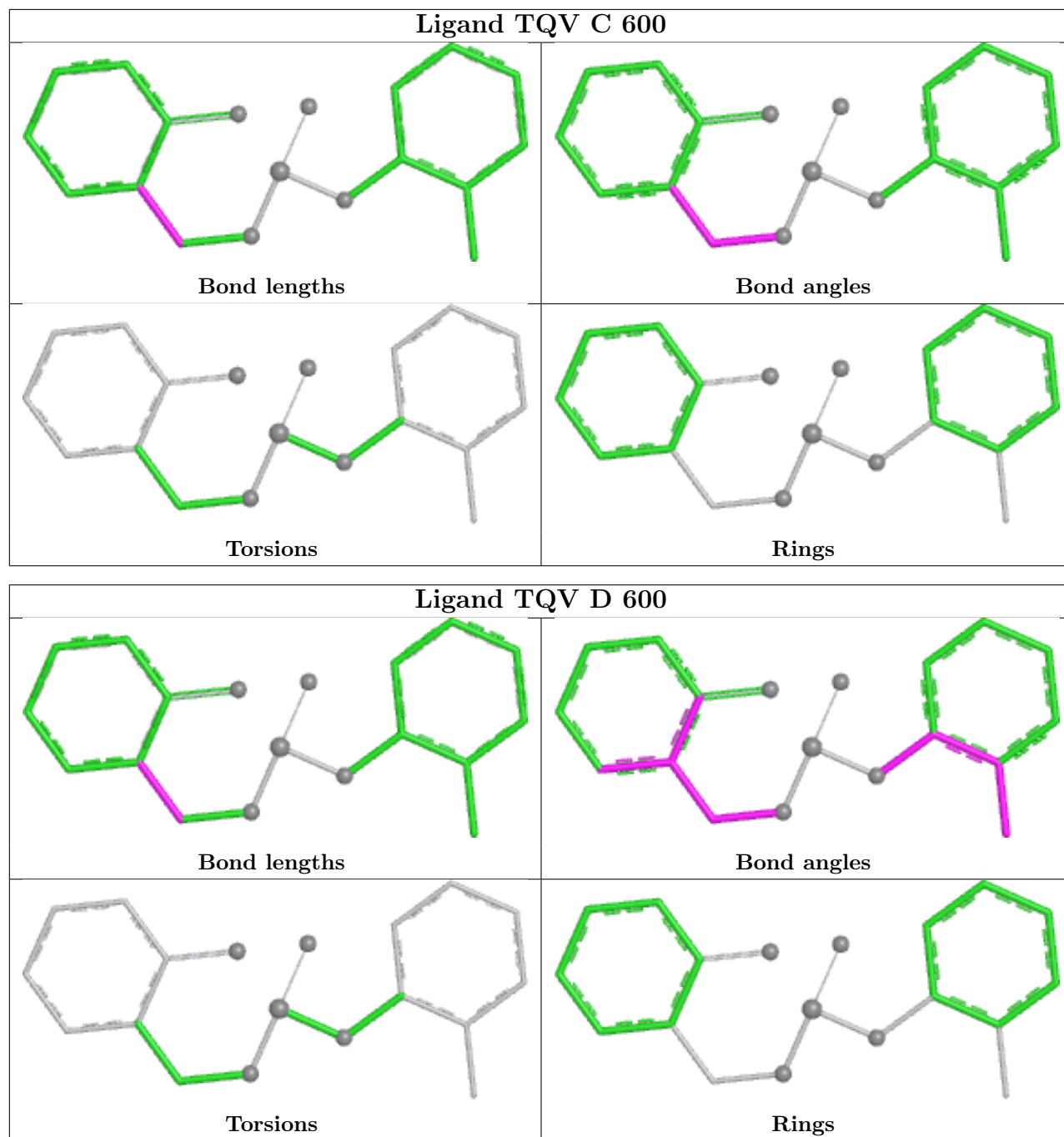
There are no ring outliers.

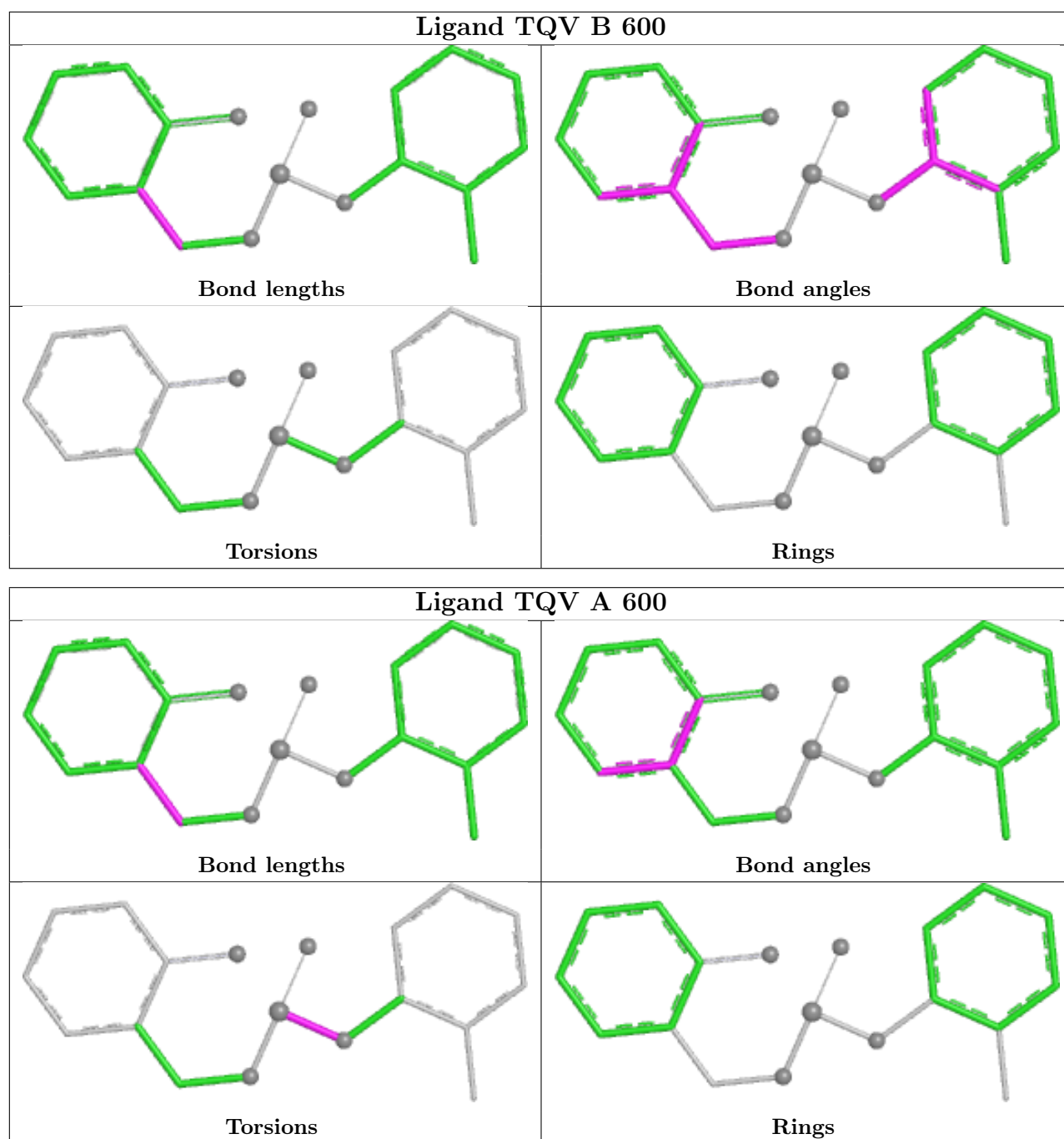
5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	600	TQV	7	0
2	D	600	TQV	4	0
2	B	600	TQV	3	0
2	A	600	TQV	4	0
5	C	1547	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	540/543 (99%)	-0.74	7 (1%) 75 69	14, 33, 69, 138	3 (0%)
1	B	539/543 (99%)	-0.28	5 (0%) 81 76	19, 61, 107, 165	1 (0%)
1	C	540/543 (99%)	-0.70	4 (0%) 84 80	11, 32, 72, 133	4 (0%)
1	D	540/543 (99%)	-0.56	6 (1%) 78 73	19, 43, 79, 146	5 (0%)
All	All	2159/2172 (99%)	-0.57	22 (1%) 79 74	11, 41, 94, 165	13 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	297[A]	PHE	4.2
1	B	297[A]	PHE	3.6
1	B	543	THR	3.2
1	A	542	ALA	3.1
1	A	297[A]	PHE	2.9
1	C	387[A]	HIS	2.8
1	B	30	SER	2.8
1	B	542	ALA	2.6
1	D	258	PRO	2.6
1	D	522[A]	ARG	2.5
1	A	259	PRO	2.5
1	C	543	THR	2.5
1	B	515	LEU	2.5
1	A	497	SER	2.4
1	C	259	PRO	2.4
1	A	262	ALA	2.4
1	C	262	ALA	2.4
1	D	259	PRO	2.1
1	A	498	PRO	2.1
1	D	540	LEU	2.0
1	A	543	THR	2.0
1	D	542	ALA	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.

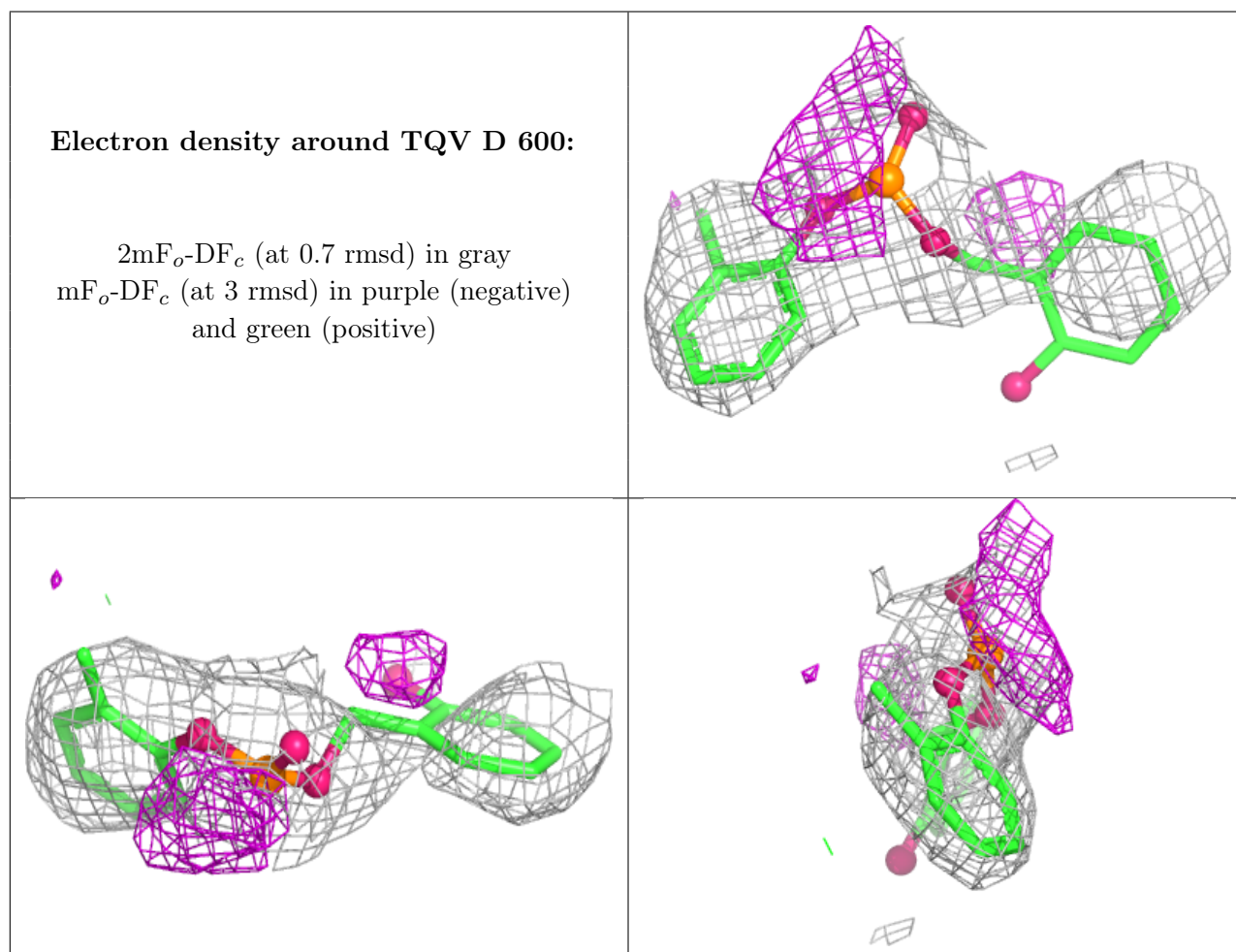
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	B	702	14/15	0.51	0.19	68,106,117,120	0
3	NAG	D	701	14/15	0.51	0.16	77,101,115,121	0
3	NAG	C	701	14/15	0.52	0.15	120,126,134,134	0
3	NAG	A	701	14/15	0.58	0.14	96,119,122,123	0
5	SO4	B	1546	5/5	0.60	0.14	166,166,167,169	0
3	NAG	D	703	14/15	0.62	0.15	109,127,137,141	0
3	NAG	B	701	14/15	0.64	0.16	98,103,107,110	0
5	SO4	C	1549	5/5	0.65	0.22	113,116,118,119	0
5	SO4	A	1550	5/5	0.71	0.35	122,123,127,131	0
3	NAG	D	702	14/15	0.75	0.14	60,102,109,110	0
5	SO4	A	1548	5/5	0.76	0.26	92,93,96,100	0
5	SO4	A	1549	5/5	0.79	0.17	106,116,120,121	0
4	CL	D	1991	1/1	0.79	0.12	82,82,82,82	0
4	CL	D	1544	1/1	0.81	0.13	84,84,84,84	0
5	SO4	B	1547	5/5	0.85	0.12	119,122,123,128	0
5	SO4	D	1546	5/5	0.85	0.30	116,119,120,123	0
5	SO4	D	1547	5/5	0.87	0.10	138,139,141,144	0
4	CL	C	1544	1/1	0.89	0.06	55,55,55,55	0
5	SO4	D	1545	5/5	0.90	0.09	68,69,72,79	0
4	CL	C	1546	1/1	0.91	0.10	72,72,72,72	0
4	CL	D	1990	1/1	0.91	0.06	57,57,57,57	0
5	SO4	B	1545	5/5	0.91	0.10	75,90,92,97	0
4	CL	A	1990	1/1	0.92	0.07	59,59,59,59	0
2	TQV	D	600	19/20	0.92	0.17	34,46,116,118	8
5	SO4	A	1546	5/5	0.93	0.11	110,110,112,115	0
5	SO4	A	1547	5/5	0.93	0.11	59,60,71,72	0
4	CL	B	1544	1/1	0.94	0.10	66,66,66,66	0

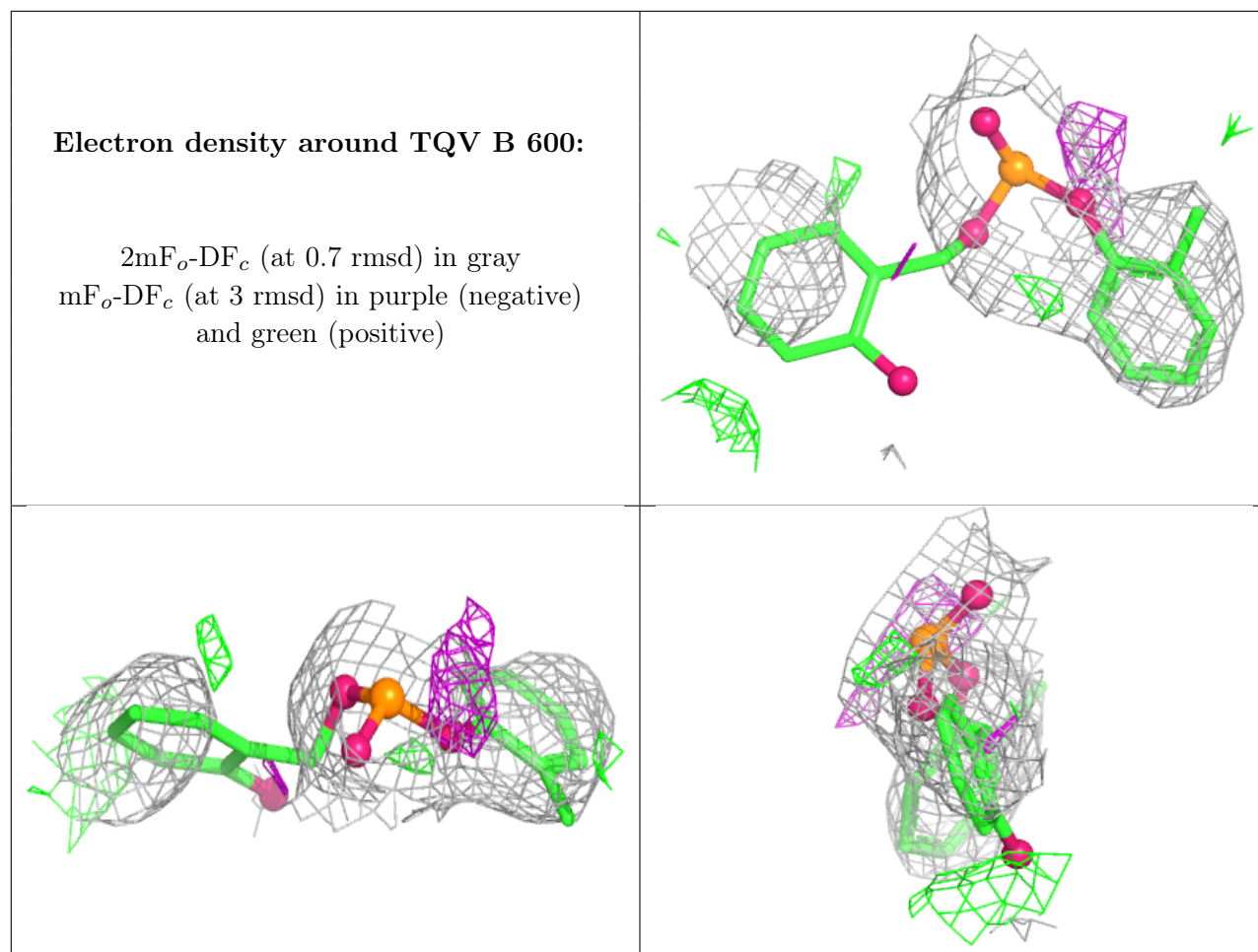
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TQV	B	600	19/20	0.94	0.17	42,60,97,97	8
4	CL	A	1991	1/1	0.95	0.10	66,66,66,66	0
5	SO4	A	1545	5/5	0.95	0.06	70,73,74,75	0
2	TQV	A	600	19/20	0.96	0.11	27,44,57,59	8
5	SO4	C	1547	5/5	0.96	0.05	75,82,83,87	0
2	TQV	C	600	19/20	0.96	0.13	22,49,83,83	8
4	CL	A	1544	1/1	0.97	0.03	67,67,67,67	0
5	SO4	C	1548	5/5	0.97	0.08	54,56,62,66	0
4	CL	C	1990	1/1	0.97	0.07	50,50,50,50	0
4	CL	C	1545	1/1	0.98	0.04	35,35,35,35	0

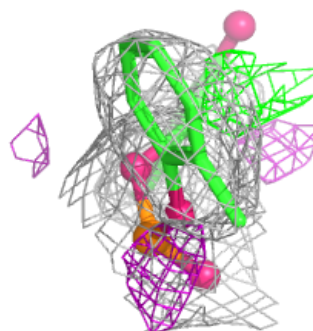
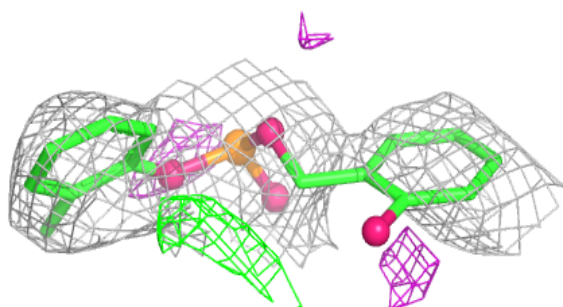
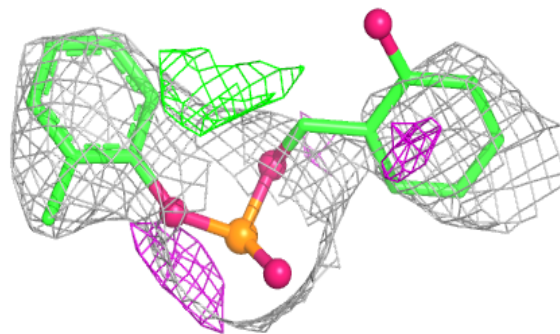
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



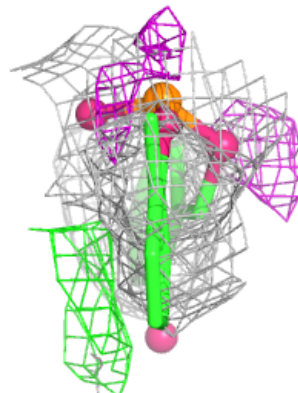
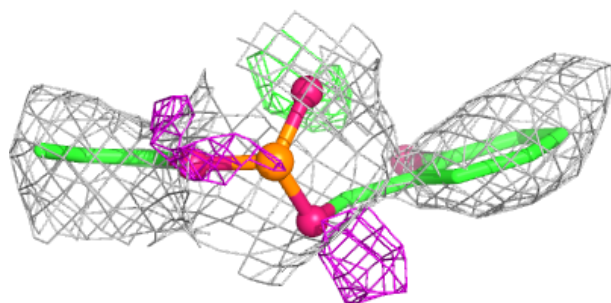
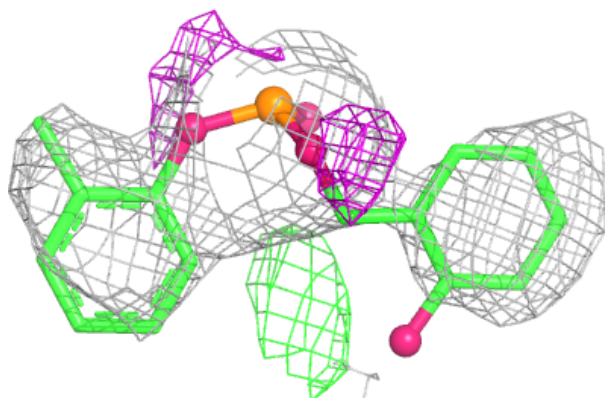


Electron density around TQV A 600:

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

**Electron density around TQV C 600:**

$2mF_o-DF_c$ (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.