



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 06:03 PM BST

PDB ID : 2VGJ
Title : Crystal structure of Actinomadura R39 DD-peptidase complexed with a peptidoglycan-mimetic cephalosporin
Authors : Sauvage, E.; kerff, F.; Herman, R.; Charlier, P.
Deposited on : 2007-11-14
Resolution : 2.40 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 : 2.13
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) : 2.13

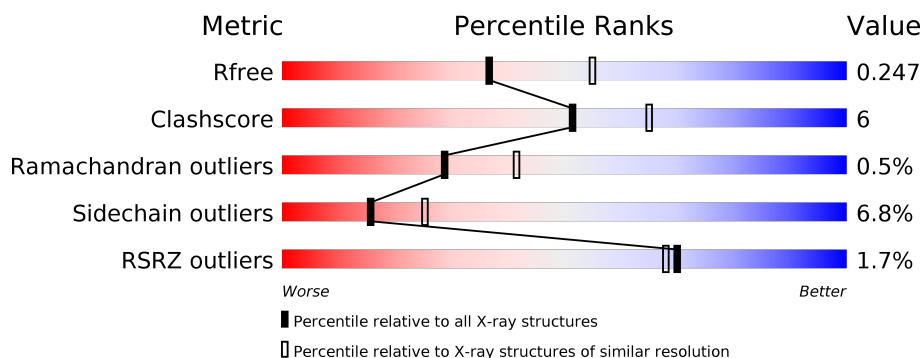
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	489	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• •</div> </div> </div>
1	B	489	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	C	489	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>• 5%</div> </div> </div>
1	D	489	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• •</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	601	-	-	X	-
3	SO4	B	602	-	-	-	X

2 Entry composition [i](#)

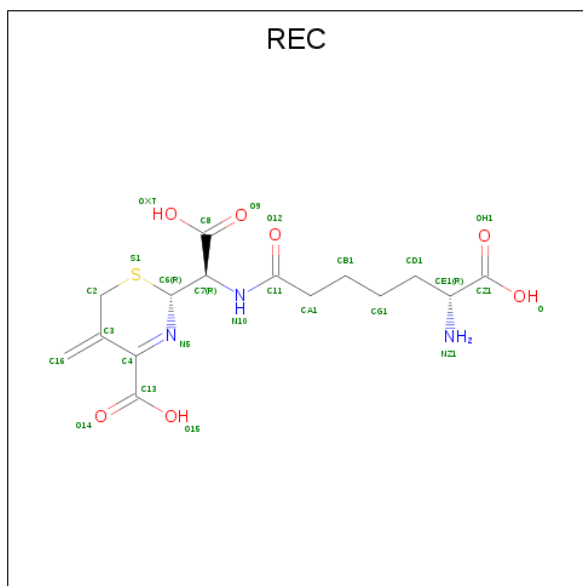
There are 5 unique types of molecules in this entry. The entry contains 14096 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-ALANYL-D-ALANINE CARBOXYPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	1
			3353	2076	565	706	6			
1	B	466	Total	C	N	O	S	0	0	1
			3344	2071	564	703	6			
1	C	466	Total	C	N	O	S	0	0	1
			3344	2071	564	703	6			
1	D	467	Total	C	N	O	S	0	0	1
			3353	2076	565	706	6			

- Molecule 2 is CEPHALOSPORIN (three-letter code: REC) (formula: C₁₅H₂₁N₃O₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			25	15	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			25	15	3	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			25	15	3	6	1		
2	D	1	Total	C	N	O	S	0	0
			25	15	3	6	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

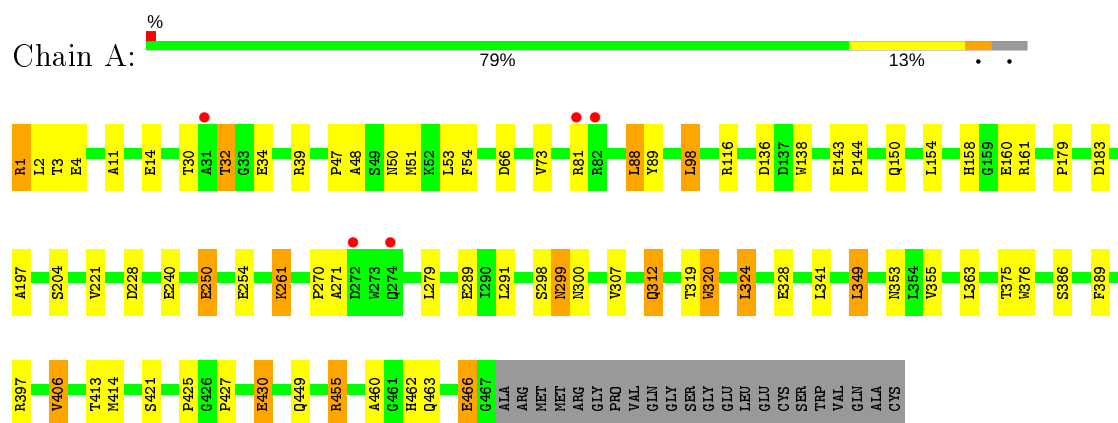
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	163	Total	O	0	0
			163	163		
5	B	118	Total	O	0	0
			118	118		
5	C	105	Total	O	0	0
			105	105		
5	D	134	Total	O	0	0
			134	134		

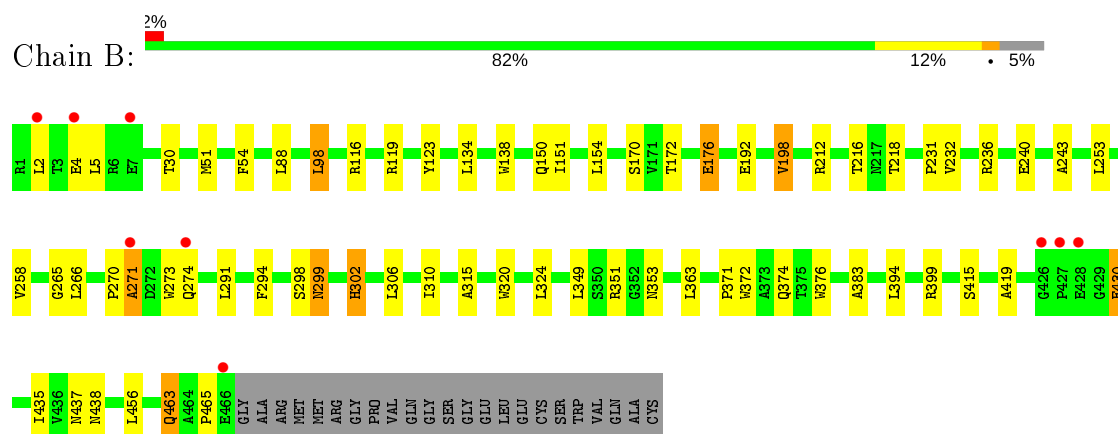
3 Residue-property plots

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.

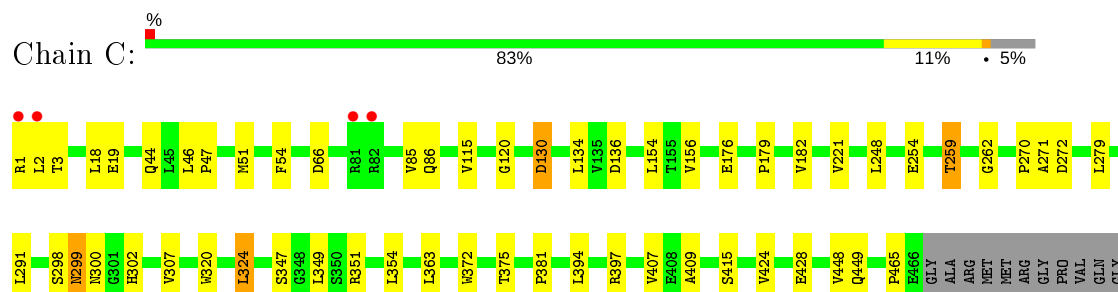
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

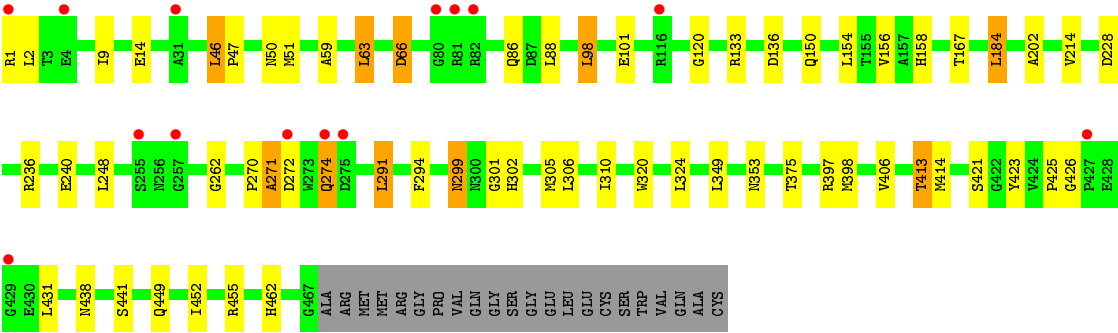
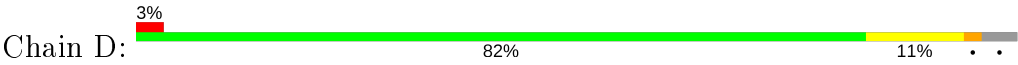


• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



SER
GLY
GLU
LEU
GLU
CYS
SER
TRP
VAL
GLN
ALA
CYS

● Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.03Å 93.25Å 108.16Å 90.00° 94.21° 90.00°	Depositor
Resolution (Å)	16.03 – 2.40 16.03 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (16.03-2.40) 99.9 (16.03-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.248 0.196 , 0.247	Depositor DCC
R_{free} test set	4073 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.034 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14096	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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: REC, MG, 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	0.74	1/3412 (0.0%)	0.81	2/4668 (0.0%)
1	B	0.66	0/3403	0.78	4/4656 (0.1%)
1	C	0.66	0/3403	0.77	1/4656 (0.0%)
1	D	0.70	1/3412 (0.0%)	0.78	2/4668 (0.0%)
All	All	0.69	2/13630 (0.0%)	0.78	9/18648 (0.0%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	136	ASP	CB-CG	5.58	1.63	1.51
1	A	466	GLU	C-N	-5.47	1.23	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	98	LEU	CA-CB-CG	6.74	130.79	115.30
1	A	98	LEU	CA-CB-CG	6.03	129.16	115.30
1	B	198	VAL	CB-CA-C	-6.01	99.99	111.40
1	A	228	ASP	CB-CG-OD1	5.57	123.32	118.30
1	B	351	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	D	98	LEU	CA-CB-CG	5.34	127.57	115.30
1	C	46	LEU	CA-CB-CG	5.31	127.50	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	D	291	LEU	CA-CB-CG	5.10	127.02	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	426	GLY	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	3353	0	3200	48	0
1	B	3344	0	3194	32	0
1	C	3344	0	3194	24	0
1	D	3353	0	3200	43	0
2	A	25	0	18	2	0
2	B	25	0	18	0	0
2	C	25	0	18	0	0
2	D	25	0	18	2	0
3	A	20	0	0	2	0
3	B	20	0	0	1	0
3	C	20	0	0	0	0
3	D	20	0	0	1	0
4	A	1	0	0	0	1
4	D	1	0	0	0	0
5	A	163	0	0	8	1
5	B	118	0	0	5	0
5	C	105	0	0	3	0
5	D	134	0	0	8	0
All	All	14096	0	12860	148	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (148) 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:161:ARG:HD2	5:A:2062:HOH:O	1.63	0.97
1:D:1:ARG:HD3	1:D:455:ARG:HH22	1.28	0.95
1:C:136:ASP:HB3	5:C:2032:HOH:O	1.68	0.91
1:A:414:MET:HG2	2:A:500:REC:HB11	1.63	0.79
1:D:306:LEU:HD23	5:D:2094:HOH:O	1.82	0.79
1:B:172:THR:HG22	1:B:231:PRO:HB3	1.68	0.76
1:A:406:VAL:HG21	1:A:462:HIS:CE1	2.22	0.74
1:B:119:ARG:HG2	1:B:119:ARG:HH11	1.53	0.72
1:B:294:PHE:HB2	1:B:302:HIS:HD2	1.55	0.72
1:C:1:ARG:HB2	5:C:2001:HOH:O	1.90	0.71
1:D:1:ARG:HD3	1:D:455:ARG:NH2	2.06	0.71
1:A:319:THR:HG22	5:A:2115:HOH:O	1.93	0.68
1:D:167:THR:OG1	1:D:184:LEU:O	2.12	0.67
1:D:413:THR:CG2	5:D:2115:HOH:O	2.42	0.67
1:A:270:PRO:O	1:A:271:ALA:HB3	1.95	0.66
1:D:406:VAL:HG13	1:D:425:PRO:HD2	1.78	0.64
1:B:399:ARG:HD3	5:B:2107:HOH:O	1.97	0.64
1:A:427:PRO:HD2	1:A:460:ALA:O	1.99	0.63
1:D:270:PRO:O	1:D:271:ALA:CB	2.46	0.63
1:D:120:GLY:O	1:D:262:GLY:HA3	1.99	0.63
1:A:47:PRO:HG3	1:A:51:MET:CE	2.29	0.62
1:C:300:ASN:HA	1:C:347:SER:HB2	1.81	0.62
1:B:151:ILE:HA	5:B:2045:HOH:O	1.98	0.62
1:A:32:THR:OG1	1:A:34:GLU:HB2	2.00	0.61
1:D:270:PRO:O	1:D:271:ALA:HB3	2.03	0.59
1:B:243:ALA:HB2	1:B:266:LEU:HD11	1.85	0.58
1:B:306:LEU:O	1:B:310:ILE:HG13	2.04	0.58
1:D:214:VAL:HG13	5:D:2069:HOH:O	2.04	0.58
1:D:397:ARG:HH12	1:D:449:GLN:HE21	1.52	0.57
1:C:3:THR:HG22	5:C:2002:HOH:O	2.05	0.56
1:B:51:MET:CE	1:B:353:ASN:HB3	2.36	0.56
1:A:1:ARG:HH22	1:A:455:ARG:HH22	1.54	0.56
1:B:192:GLU:HB2	1:B:218:THR:HA	1.88	0.55
1:B:465:PRO:HG2	5:B:2108:HOH:O	2.05	0.55
1:A:150:GLN:HE22	1:A:240:GLU:H	1.55	0.55
1:A:47:PRO:HG3	1:A:51:MET:HE2	1.87	0.55
1:D:66:ASP:HB3	5:D:2012:HOH:O	2.06	0.55
1:B:371:PRO:HD2	5:B:2009:HOH:O	2.07	0.55
1:B:54:PHE:CD2	1:B:363:LEU:HD22	2.42	0.54
1:D:133:ARG:HB3	1:D:150:GLN:HB3	1.89	0.54
1:D:214:VAL:HG12	5:D:2035:HOH:O	2.08	0.54
1:C:372:TRP:O	1:C:375:THR:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:MET:HE2	1:B:353:ASN:HB3	1.89	0.54
1:C:156:VAL:HG21	1:C:248:LEU:HD12	1.90	0.53
1:A:341:LEU:CD2	1:A:355:VAL:HG12	2.39	0.53
1:A:349:LEU:HD22	5:A:2122:HOH:O	2.09	0.53
1:B:253:LEU:HB3	1:B:258:VAL:HB	1.91	0.53
1:D:47:PRO:HG3	1:D:51:MET:CE	2.38	0.53
1:D:414:MET:HB3	2:D:500:REC:HB11	1.90	0.53
1:B:119:ARG:HG2	1:B:119:ARG:NH1	2.18	0.53
1:D:1:ARG:CD	1:D:455:ARG:HH22	2.11	0.53
1:B:138:TRP:HB3	5:B:2039:HOH:O	2.09	0.53
1:B:270:PRO:O	1:B:271:ALA:HB3	2.10	0.52
1:C:254:GLU:OE1	1:C:259:THR:HA	2.10	0.52
2:D:500:REC:O14	2:D:500:REC:H161	2.10	0.51
1:D:236:ARG:NH2	3:D:602:SO4:O3	2.40	0.51
1:A:299:ASN:HD22	1:A:299:ASN:C	2.13	0.51
1:A:158:HIS:HD2	5:A:2160:HOH:O	1.92	0.51
1:D:406:VAL:HG21	1:D:462:HIS:CE1	2.46	0.51
1:A:320:TRP:O	1:A:324:LEU:HB2	2.10	0.51
1:A:413:THR:O	2:A:500:REC:HA12	2.11	0.50
1:D:150:GLN:NE2	1:D:240:GLU:H	2.09	0.50
1:D:294:PHE:HB2	1:D:302:HIS:HD2	1.76	0.50
1:D:47:PRO:HG3	1:D:51:MET:HE3	1.93	0.50
1:D:413:THR:HG22	5:D:2115:HOH:O	2.09	0.50
1:A:143:GLU:N	1:A:144:PRO:CD	2.75	0.50
1:D:150:GLN:HE22	1:D:240:GLU:H	1.58	0.50
1:A:143:GLU:N	1:A:144:PRO:HD3	2.26	0.49
1:D:14:GLU:HA	1:D:14:GLU:OE1	2.12	0.49
1:C:18:LEU:HD11	1:C:448:VAL:HG11	1.95	0.48
1:A:51:MET:HE3	1:A:353:ASN:HB3	1.95	0.48
1:A:50:ASN:ND2	1:A:421:SER:OG	2.46	0.48
1:A:261:LYS:HB3	1:A:261:LYS:HE3	1.40	0.48
1:D:413:THR:HG23	5:D:2115:HOH:O	2.11	0.48
1:D:50:ASN:ND2	1:D:421:SER:OG	2.46	0.48
1:D:397:ARG:HH12	1:D:449:GLN:NE2	2.11	0.48
1:D:301:GLY:O	1:D:305:MET:HG3	2.13	0.48
1:D:158:HIS:HD2	5:D:2049:HOH:O	1.96	0.48
1:A:73:VAL:HA	1:A:89:TYR:O	2.14	0.47
1:C:182:VAL:HG21	1:C:221:VAL:HG21	1.96	0.47
1:B:170:SER:HA	1:B:232:VAL:O	2.15	0.47
1:D:46:LEU:N	1:D:46:LEU:HD23	2.29	0.47
1:C:44:GLN:HB3	1:C:354:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:ARG:O	1:D:398:MET:HB2	2.14	0.46
1:D:156:VAL:HG21	1:D:248:LEU:HD12	1.96	0.46
1:B:5:LEU:HD11	1:B:456:LEU:HD23	1.98	0.46
1:A:1:ARG:NH2	1:A:455:ARG:HH22	2.14	0.46
1:A:81:ARG:NH1	1:A:81:ARG:HB3	2.31	0.46
1:C:115:VAL:HG21	1:C:279:LEU:HD13	1.98	0.46
1:B:123:TYR:HA	1:B:265:GLY:O	2.15	0.46
1:B:419:ALA:HA	1:B:435:ILE:O	2.15	0.46
1:B:236:ARG:NH1	3:B:602:SO4:O4	2.43	0.46
1:B:176:GLU:H	1:B:176:GLU:HG2	1.25	0.46
1:C:86:GLN:O	1:C:120:GLY:N	2.45	0.46
1:A:197:ALA:HB2	1:A:221:VAL:HG12	1.97	0.45
1:A:312:GLN:HE21	1:A:312:GLN:CA	2.29	0.45
1:C:51:MET:HG3	1:C:51:MET:O	2.15	0.45
1:D:51:MET:HE3	1:D:353:ASN:HB3	1.99	0.45
1:B:270:PRO:HG2	1:B:273:TRP:CE2	2.52	0.45
1:D:299:ASN:HD22	1:D:299:ASN:C	2.20	0.44
1:D:9:ILE:HG12	1:D:452:ILE:HG23	1.99	0.44
1:A:39:ARG:HD3	5:A:2008:HOH:O	2.17	0.44
1:C:85:VAL:HG12	1:C:86:GLN:N	2.33	0.44
1:B:116:ARG:NH2	1:B:116:ARG:HB3	2.33	0.44
1:C:351:ARG:HH12	1:C:415:SER:HB2	1.82	0.44
1:B:437:ASN:C	1:B:438:ASN:HD22	2.21	0.44
1:B:150:GLN:HE22	1:B:240:GLU:H	1.66	0.43
1:C:299:ASN:ND2	1:C:302:HIS:H	2.16	0.43
1:A:160:GLU:HG2	3:A:601:SO4:O3	2.18	0.43
1:A:270:PRO:O	1:A:271:ALA:CB	2.60	0.43
1:A:11:ALA:O	1:A:14:GLU:HB2	2.19	0.43
1:C:270:PRO:O	1:C:271:ALA:HB3	2.19	0.43
1:D:202:ALA:HA	1:D:228:ASP:OD1	2.19	0.43
1:D:274:GLN:HE21	1:D:274:GLN:HB3	1.68	0.43
1:A:161:ARG:HG3	3:A:601:SO4:O1	2.19	0.42
1:B:212:ARG:NH1	1:B:216:THR:O	2.53	0.42
1:B:383:ALA:HA	1:B:394:LEU:HB3	2.00	0.42
1:D:59:ALA:O	1:D:63:LEU:HB2	2.18	0.42
1:B:150:GLN:NE2	1:B:240:GLU:H	2.17	0.42
1:B:463:GLN:HB2	1:B:463:GLN:HE21	1.59	0.42
1:D:423:TYR:HA	1:D:431:LEU:O	2.19	0.42
1:A:179:PRO:HB3	5:A:2081:HOH:O	2.18	0.42
1:A:341:LEU:HD21	1:A:355:VAL:HG12	2.01	0.42
1:A:51:MET:CE	1:A:353:ASN:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:TRP:HB3	5:A:2050:HOH:O	2.20	0.42
1:A:160:GLU:HG3	1:A:389:PHE:HZ	1.84	0.42
1:A:4:GLU:HB2	5:A:2003:HOH:O	2.19	0.42
1:A:307:VAL:HG11	1:A:320:TRP:CD1	2.55	0.41
1:D:406:VAL:CG2	1:D:462:HIS:CE1	3.03	0.41
1:A:397:ARG:HH12	1:A:449:GLN:NE2	2.18	0.41
1:A:88:LEU:HD21	1:A:279:LEU:HD12	2.02	0.41
1:C:397:ARG:HH12	1:C:449:GLN:NE2	2.18	0.41
1:C:47:PRO:HG3	1:C:51:MET:HE2	2.01	0.41
1:A:250:GLU:O	1:A:254:GLU:HB2	2.20	0.41
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.84	0.41
1:A:307:VAL:HG11	1:A:320:TRP:HD1	1.86	0.41
1:D:306:LEU:O	1:D:310:ILE:HG13	2.21	0.41
1:A:54:PHE:CD2	1:A:363:LEU:HD22	2.56	0.41
1:D:294:PHE:CD2	1:D:302:HIS:HB2	2.56	0.41
1:B:299:ASN:C	1:B:299:ASN:HD22	2.24	0.40
1:C:324:LEU:HA	1:C:324:LEU:HD12	1.96	0.40
1:C:407:VAL:HG22	1:C:424:VAL:HG22	2.02	0.40
1:A:299:ASN:HD22	1:A:300:ASN:N	2.18	0.40
1:A:425:PRO:HA	1:A:430:GLU:HG2	2.03	0.40
1:C:381:PRO:HD2	1:C:409:ALA:O	2.22	0.40
1:C:120:GLY:O	1:C:262:GLY:HA3	2.21	0.40
1:A:1:ARG:HH22	1:A:455:ARG:NH2	2.19	0.40
1:C:54:PHE:CD2	1:C:363:LEU:HD22	2.57	0.40

All (1) 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)
4:A:611:MG:MG	5:A:2074:HOH:O[2_546]	1.54	0.66

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	465/489 (95%)	435 (94%)	28 (6%)	2 (0%)	34	48
1	B	464/489 (95%)	439 (95%)	21 (4%)	4 (1%)	17	25
1	C	464/489 (95%)	442 (95%)	19 (4%)	3 (1%)	25	36
1	D	465/489 (95%)	433 (93%)	31 (7%)	1 (0%)	47	62
All	All	1858/1956 (95%)	1749 (94%)	99 (5%)	10 (0%)	29	41

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	130	ASP
1	D	271	ALA
1	A	48	ALA
1	A	204	SER
1	B	271	ALA
1	C	179	PRO
1	C	465	PRO
1	B	315	ALA
1	B	430	GLU
1	B	372	TRP

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	339/356 (95%)	308 (91%)	31 (9%)	9	14
1	B	338/356 (95%)	316 (94%)	22 (6%)	17	27
1	C	338/356 (95%)	320 (95%)	18 (5%)	22	37
1	D	339/356 (95%)	318 (94%)	21 (6%)	18	29
All	All	1354/1424 (95%)	1262 (93%)	92 (7%)	16	25

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ARG
1	A	2	LEU
1	A	3	THR
1	A	30	THR
1	A	32	THR
1	A	66	ASP
1	A	88	LEU
1	A	98	LEU
1	A	116	ARG
1	A	136	ASP
1	A	154	LEU
1	A	183	ASP
1	A	250	GLU
1	A	261	LYS
1	A	289	GLU
1	A	291	LEU
1	A	298	SER
1	A	299	ASN
1	A	312	GLN
1	A	320	TRP
1	A	324	LEU
1	A	328	GLU
1	A	349	LEU
1	A	375	THR
1	A	376	TRP
1	A	386	SER
1	A	406	VAL
1	A	430	GLU
1	A	455	ARG
1	A	463	GLN
1	A	466	GLU
1	B	2	LEU
1	B	4	GLU
1	B	30	THR
1	B	88	LEU
1	B	98	LEU
1	B	134	LEU
1	B	154	LEU
1	B	176	GLU
1	B	198	VAL
1	B	274	GLN
1	B	291	LEU
1	B	298	SER

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Mol	Chain	Res	Type
1	B	299	ASN
1	B	302	HIS
1	B	320	TRP
1	B	324	LEU
1	B	349	LEU
1	B	374	GLN
1	B	376	TRP
1	B	415	SER
1	B	430	GLU
1	B	463	GLN
1	C	2	LEU
1	C	19	GLU
1	C	66	ASP
1	C	130	ASP
1	C	134	LEU
1	C	154	LEU
1	C	176	GLU
1	C	259	THR
1	C	272	ASP
1	C	291	LEU
1	C	298	SER
1	C	299	ASN
1	C	307	VAL
1	C	320	TRP
1	C	324	LEU
1	C	349	LEU
1	C	394	LEU
1	C	428	GLU
1	D	2	LEU
1	D	46	LEU
1	D	63	LEU
1	D	66	ASP
1	D	86	GLN
1	D	88	LEU
1	D	98	LEU
1	D	101	GLU
1	D	154	LEU
1	D	184	LEU
1	D	272	ASP
1	D	274	GLN
1	D	291	LEU
1	D	299	ASN

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Mol	Chain	Res	Type
1	D	320	TRP
1	D	324	LEU
1	D	349	LEU
1	D	375	THR
1	D	413	THR
1	D	438	ASN
1	D	441	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	150	GLN
1	A	158	HIS
1	A	299	ASN
1	A	312	GLN
1	A	437	ASN
1	A	449	GLN
1	A	463	GLN
1	B	44	GLN
1	B	50	ASN
1	B	150	GLN
1	B	299	ASN
1	B	302	HIS
1	B	396	ASN
1	B	437	ASN
1	B	449	GLN
1	B	463	GLN
1	C	44	GLN
1	C	50	ASN
1	C	299	ASN
1	C	302	HIS
1	C	437	ASN
1	C	449	GLN
1	D	44	GLN
1	D	50	ASN
1	D	150	GLN
1	D	158	HIS
1	D	274	GLN
1	D	299	ASN
1	D	302	HIS
1	D	366	GLN

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Mol	Chain	Res	Type
1	D	449	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	$\# Z > 2$
3	SO4	D	603	-	4,4,4	0.26	0	6,6,6	0.40	0
3	SO4	A	603	-	4,4,4	0.13	0	6,6,6	0.37	0
2	REC	D	500	1	14,25,26	1.20	2 (14%)	11,33,35	2.25	1 (9%)
3	SO4	C	603	-	4,4,4	0.14	0	6,6,6	0.44	0
3	SO4	C	602	-	4,4,4	0.14	0	6,6,6	0.13	0
3	SO4	D	600	-	4,4,4	0.23	0	6,6,6	0.33	0
3	SO4	B	600	-	4,4,4	0.20	0	6,6,6	0.28	0
3	SO4	A	602	-	4,4,4	0.14	0	6,6,6	0.25	0
2	REC	A	500	1	14,25,26	1.15	2 (14%)	11,33,35	2.67	3 (27%)
2	REC	C	500	1	14,25,26	1.38	2 (14%)	11,33,35	2.64	1 (9%)
3	SO4	C	601	-	4,4,4	0.14	0	6,6,6	0.19	0
2	REC	B	500	1	14,25,26	1.13	1 (7%)	11,33,35	2.17	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	601	-	4,4,4	0.20	0	6,6,6	0.32	0
3	SO4	B	601	-	4,4,4	0.12	0	6,6,6	0.21	0
3	SO4	D	602	-	4,4,4	0.13	0	6,6,6	0.20	0
3	SO4	A	600	-	4,4,4	0.17	0	6,6,6	0.52	0
3	SO4	D	601	-	4,4,4	0.22	0	6,6,6	0.22	0
3	SO4	B	602	-	4,4,4	0.15	0	6,6,6	0.13	0
3	SO4	C	600	-	4,4,4	0.19	0	6,6,6	0.67	0
3	SO4	B	603	-	4,4,4	0.08	0	6,6,6	0.40	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
2	REC	C	500	1	-	0/11/38/40	0/0/1/1
2	REC	B	500	1	-	0/11/38/40	0/0/1/1
2	REC	D	500	1	-	1/11/38/40	0/0/1/1
2	REC	A	500	1	-	1/11/38/40	0/0/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	REC	C13-C4	-3.76	1.46	1.52
2	D	500	REC	C13-C4	-3.29	1.47	1.52
2	A	500	REC	C13-C4	-3.15	1.47	1.52
2	B	500	REC	C13-C4	-3.14	1.47	1.52
2	D	500	REC	C2-S1	-2.49	1.76	1.82
2	C	500	REC	C2-S1	-2.46	1.76	1.82
2	A	500	REC	C2-S1	-2.22	1.77	1.82

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	REC	C2-S1-C6	7.92	109.99	94.47
2	D	500	REC	C2-S1-C6	6.69	107.59	94.47
2	A	500	REC	C2-S1-C6	6.66	107.53	94.47
2	B	500	REC	C2-S1-C6	6.42	107.06	94.47
2	A	500	REC	C7-N10-C11	4.35	127.79	123.13
2	A	500	REC	O12-C11-N10	2.25	126.76	122.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

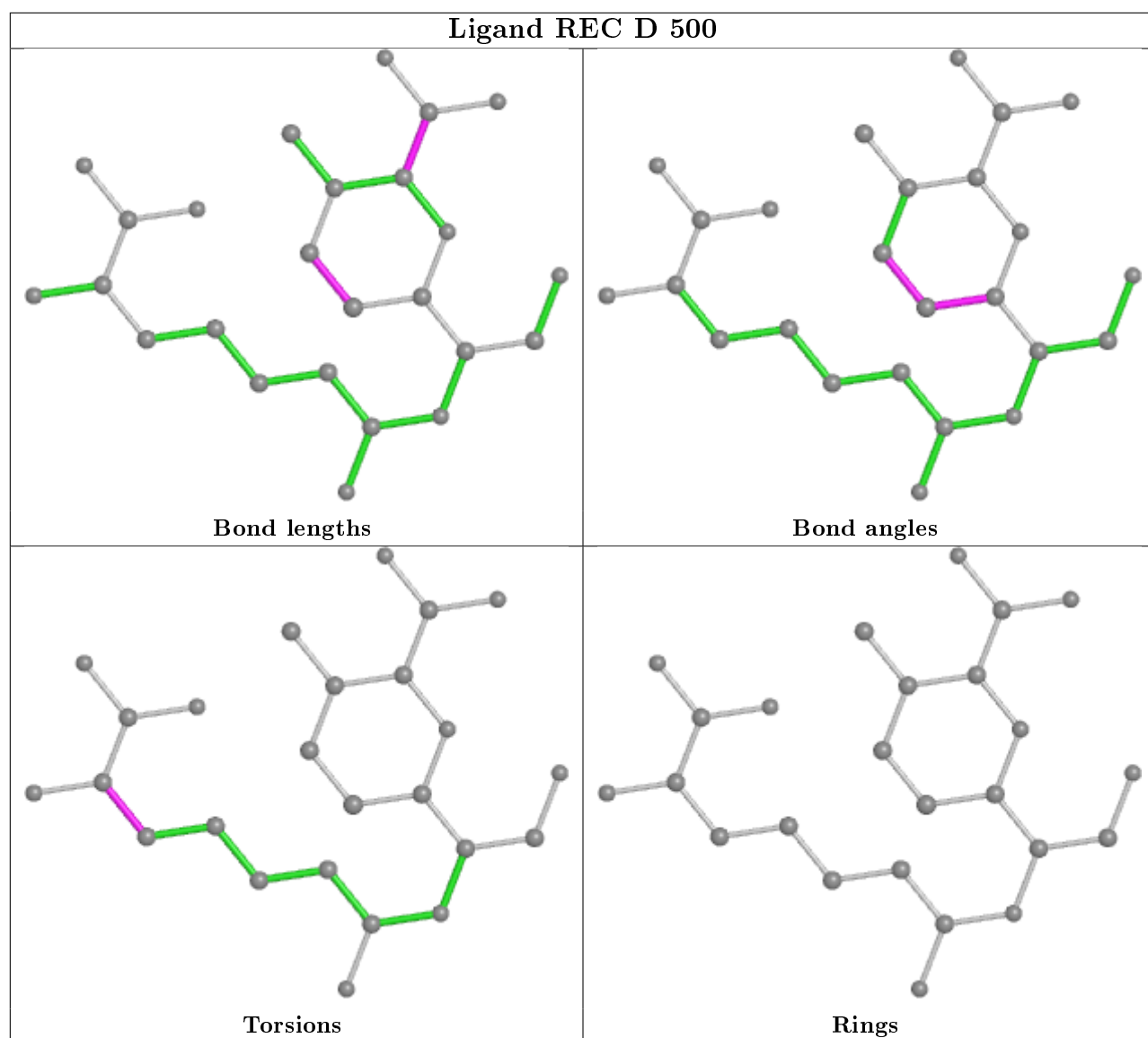
Mol	Chain	Res	Type	Atoms
2	A	500	REC	C11-CA1-CB1-CG1
2	D	500	REC	CG1-CD1-CE1-NZ1

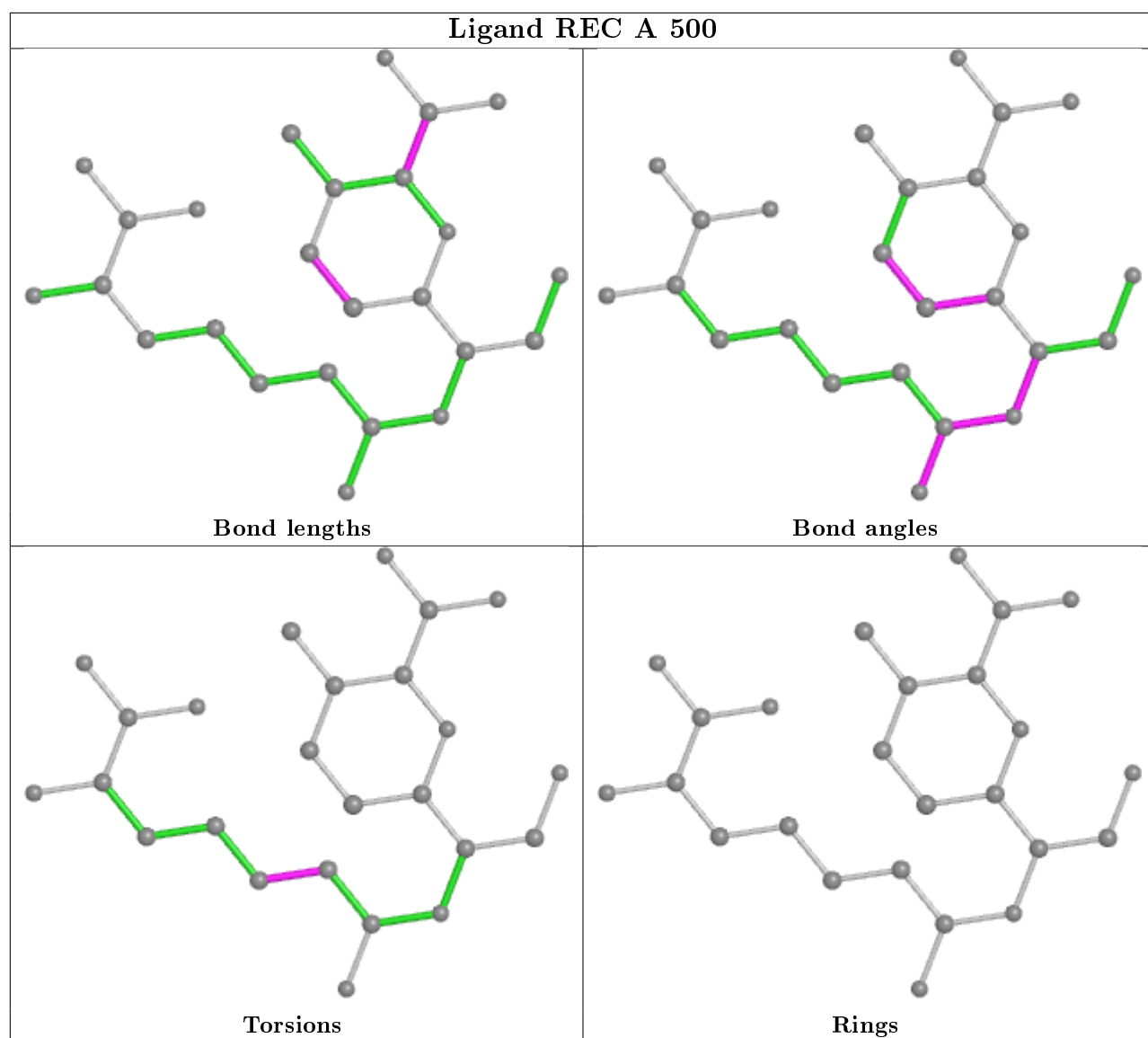
There are no ring outliers.

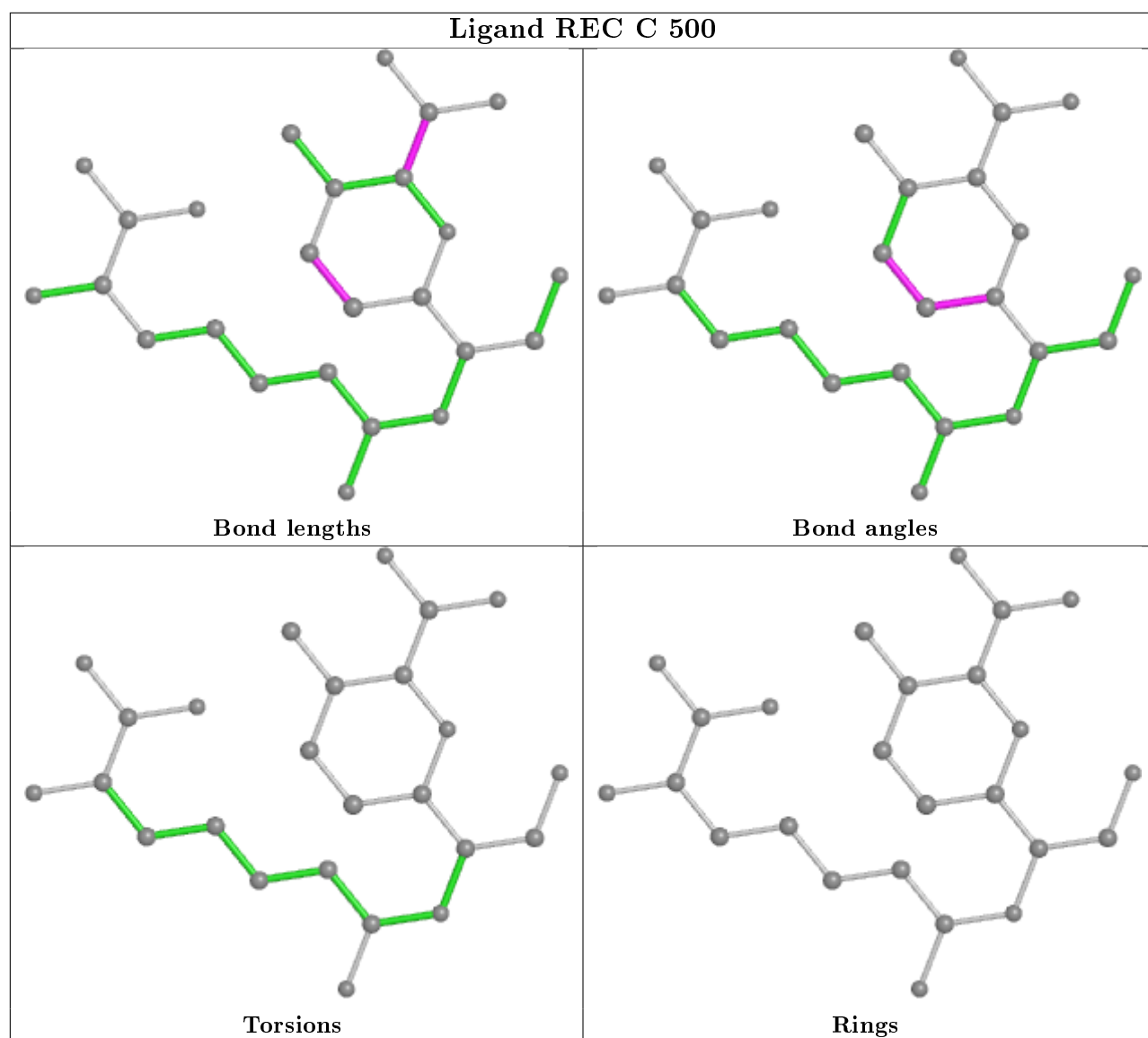
5 monomers are involved in 8 short contacts:

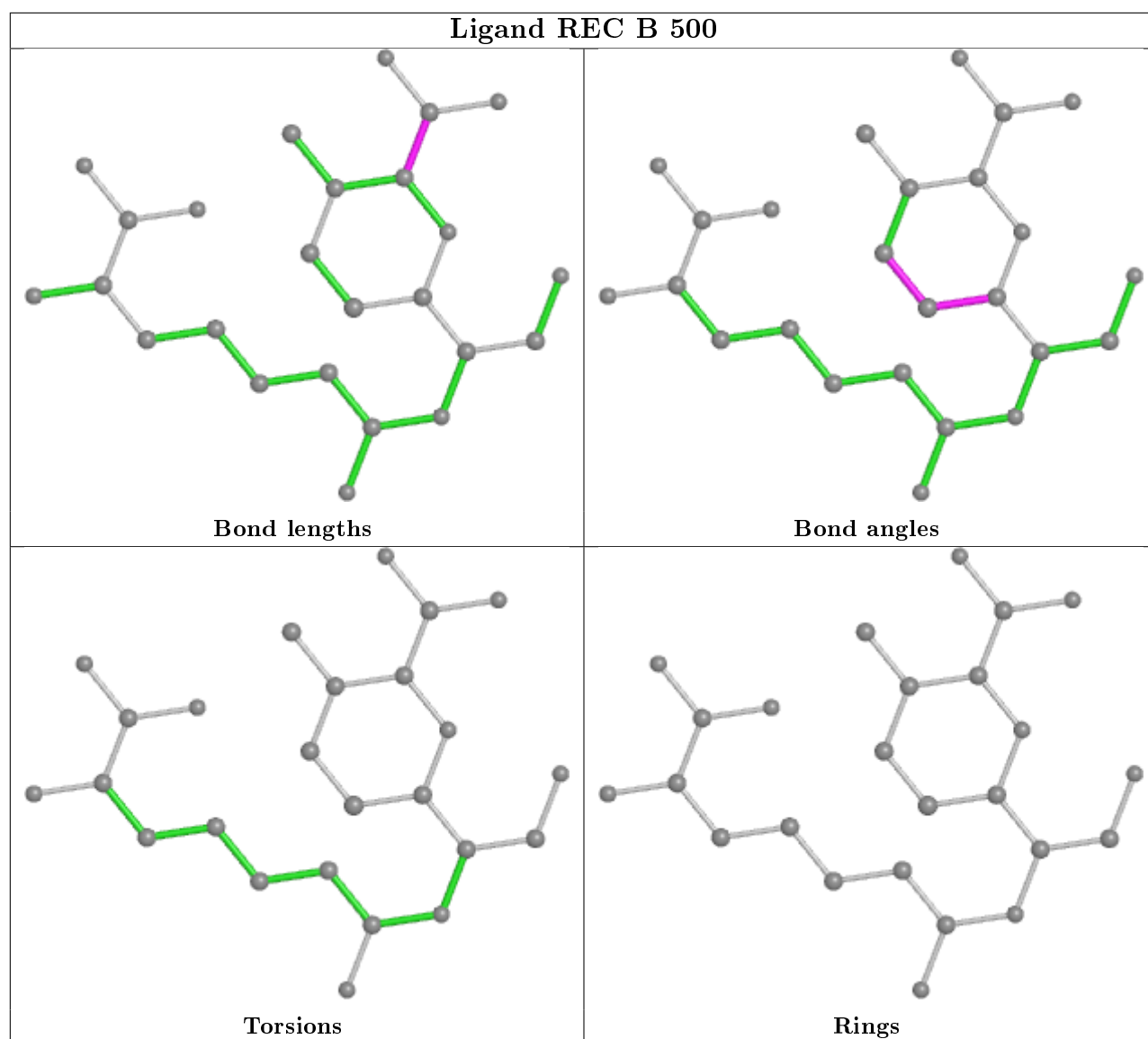
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	REC	2	0
2	A	500	REC	2	0
3	A	601	SO4	2	0
3	D	602	SO4	1	0
3	B	602	SO4	1	0

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 ⓘ

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	467/489 (95%)	-0.50	5 (1%) 80 79	10, 23, 41, 60	0
1	B	466/489 (95%)	-0.36	9 (1%) 66 64	15, 28, 50, 74	0
1	C	466/489 (95%)	-0.40	4 (0%) 84 82	16, 28, 47, 66	0
1	D	467/489 (95%)	-0.31	14 (2%) 50 49	12, 27, 53, 72	0
All	All	1866/1956 (95%)	-0.39	32 (1%) 70 68	10, 26, 50, 74	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	427	PRO	4.5
1	C	81	ARG	4.3
1	B	426	GLY	4.3
1	C	82	ARG	3.7
1	D	31	ALA	3.6
1	D	81	ARG	3.4
1	A	31	ALA	3.3
1	D	429	GLY	3.3
1	D	274	GLN	3.2
1	B	428	GLU	3.0
1	D	4	GLU	3.0
1	B	466	GLU	2.9
1	D	1	ARG	2.7
1	A	81	ARG	2.7
1	B	4	GLU	2.7
1	A	274	GLN	2.7
1	C	2	LEU	2.5
1	D	257	GLY	2.5
1	D	427	PRO	2.4
1	D	255	SER	2.4
1	D	275	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	82	ARG	2.4
1	D	272	ASP	2.3
1	A	272	ASP	2.3
1	B	274	GLN	2.3
1	B	7	GLU	2.2
1	B	271	ALA	2.2
1	B	2	LEU	2.2
1	A	82	ARG	2.2
1	D	80	GLY	2.1
1	D	116	ARG	2.1
1	C	1	ARG	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

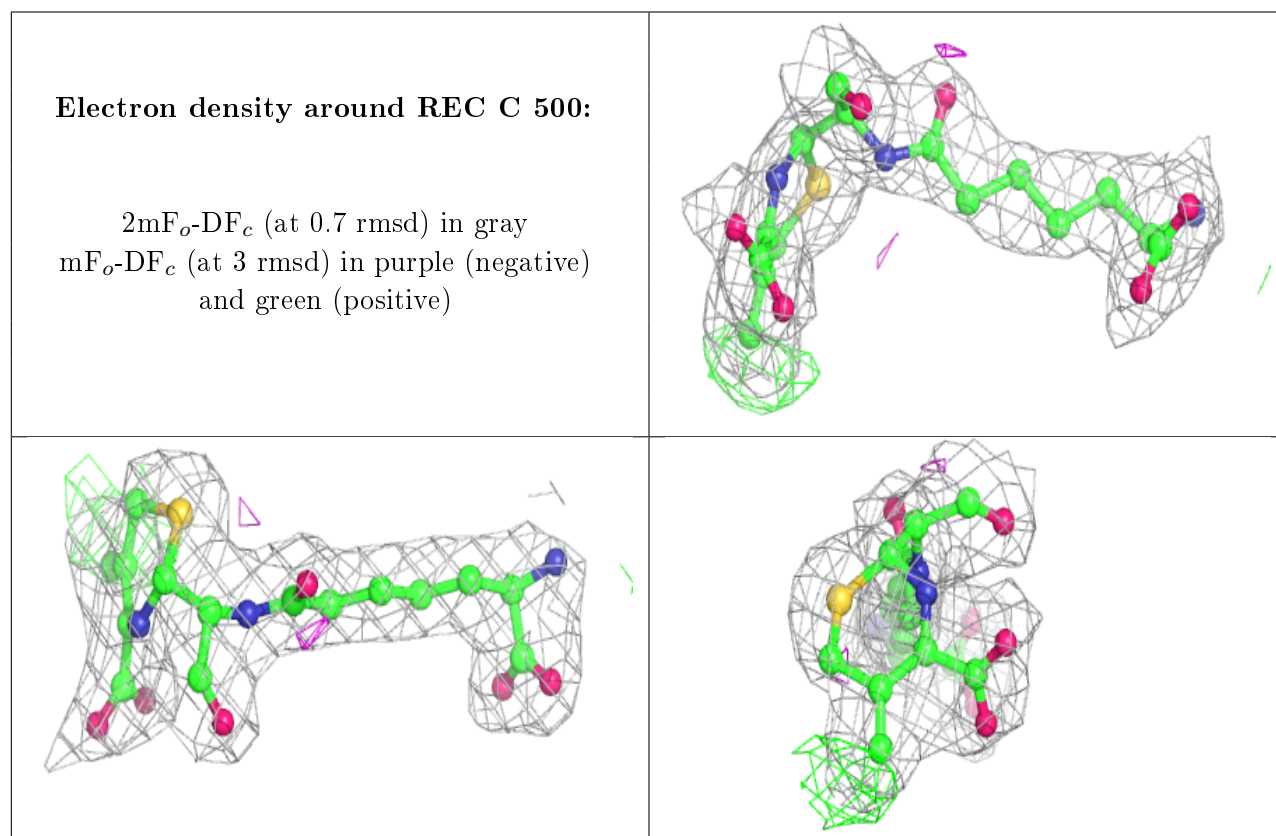
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	602	5/5	0.80	0.52	136,136,136,136	0
3	SO4	B	601	5/5	0.86	0.20	90,91,91,91	0
3	SO4	D	601	5/5	0.92	0.20	72,72,73,73	0
3	SO4	D	602	5/5	0.93	0.22	67,68,69,69	0
3	SO4	C	601	5/5	0.93	0.23	71,72,72,73	0
3	SO4	C	602	5/5	0.93	0.42	95,95,96,96	0
2	REC	C	500	25/26	0.95	0.10	23,28,36,36	0
3	SO4	A	602	5/5	0.95	0.26	82,83,83,83	0
2	REC	D	500	25/26	0.96	0.10	14,20,28,31	0
3	SO4	B	600	5/5	0.96	0.14	44,44,45,46	0
2	REC	A	500	25/26	0.96	0.10	15,20,27,27	0
3	SO4	C	600	5/5	0.96	0.18	41,42,42,45	0

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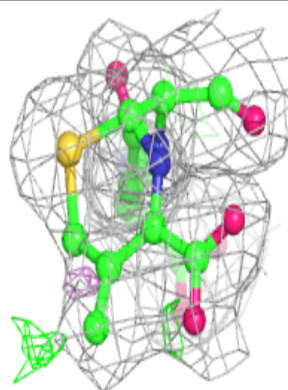
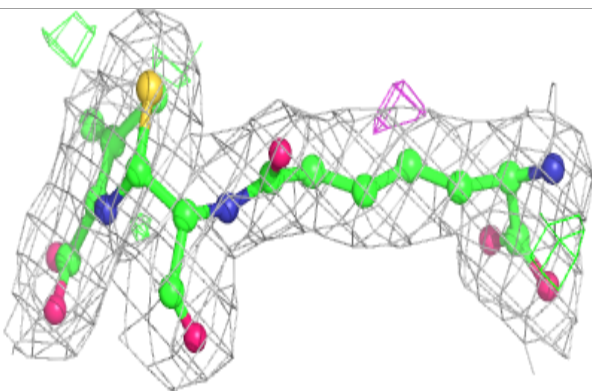
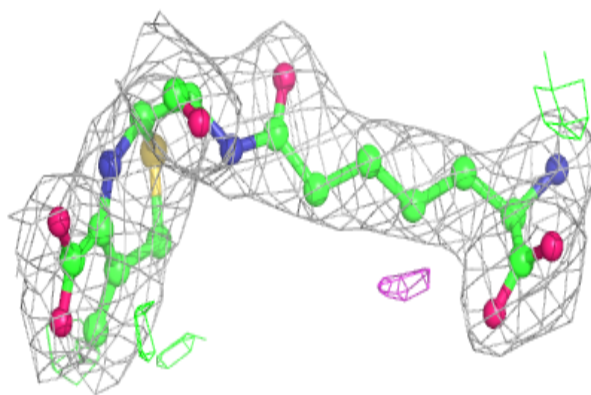
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	D	611	1/1	0.97	0.12	17,17,17,17	0
2	REC	B	500	25/26	0.97	0.08	16,23,32,34	0
3	SO4	A	601	5/5	0.97	0.18	60,60,60,61	0
3	SO4	D	600	5/5	0.98	0.19	47,48,50,50	0
4	MG	A	611	1/1	0.98	0.10	38,38,38,38	0
3	SO4	A	600	5/5	0.98	0.11	34,36,38,39	0
3	SO4	D	603	5/5	0.98	0.13	23,25,27,27	0
3	SO4	C	603	5/5	0.98	0.14	37,39,40,40	0
3	SO4	A	603	5/5	0.99	0.18	39,40,41,44	0
3	SO4	B	603	5/5	0.99	0.16	31,32,34,35	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.

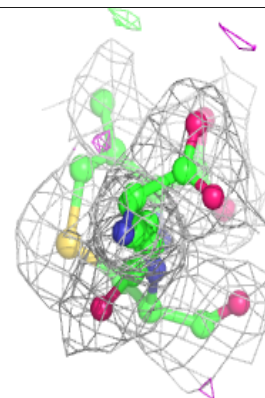
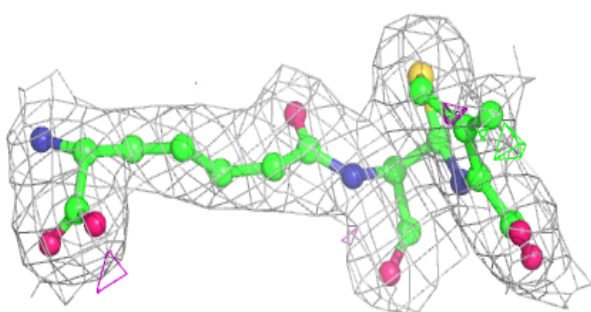
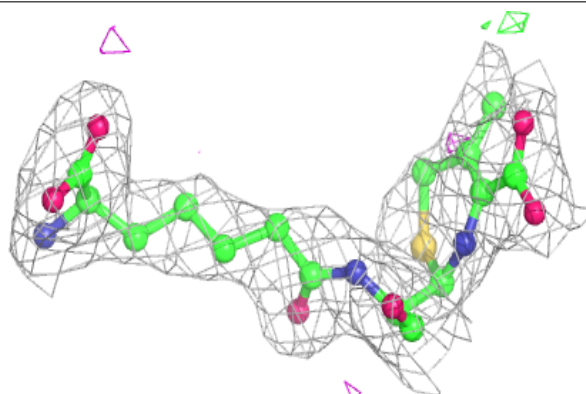


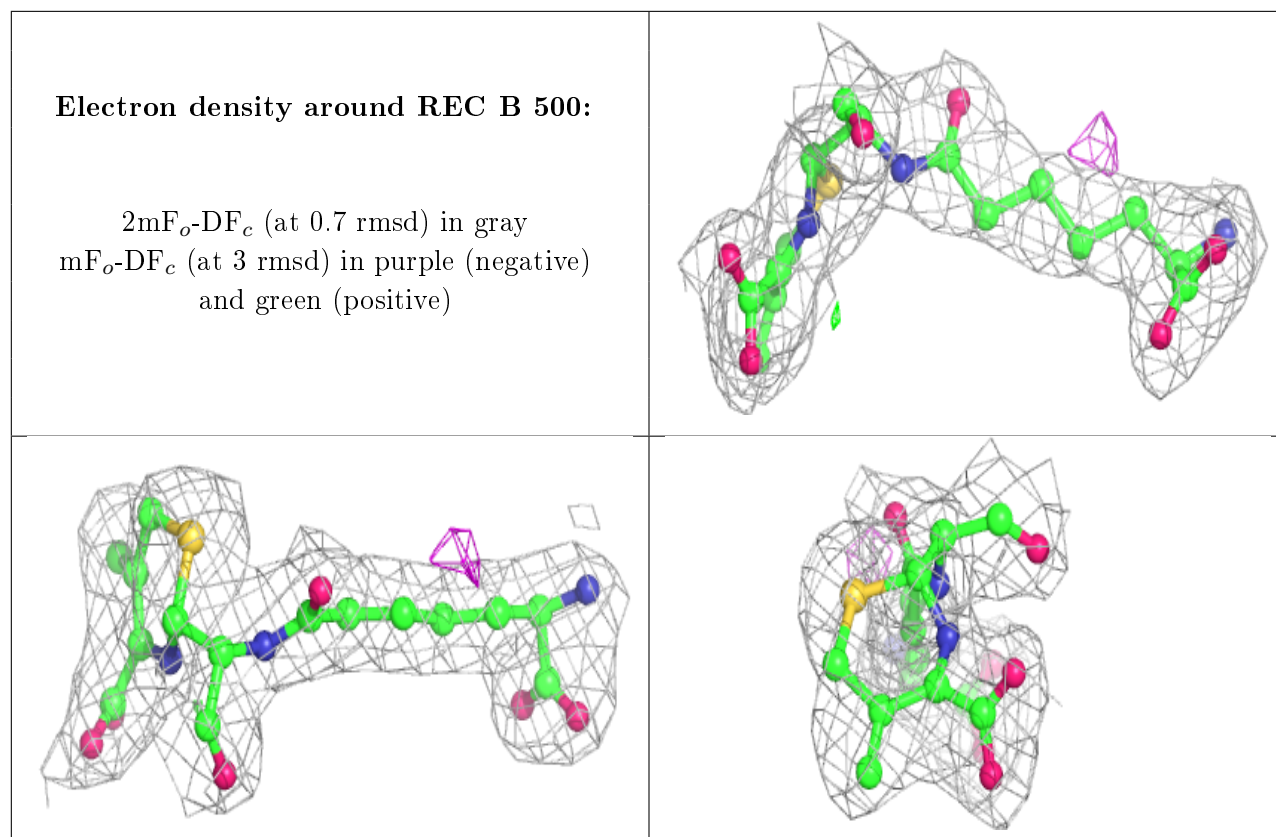
Electron density around REC D 500:

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

**Electron density around REC A 500:**

$2mF_o-DF_c$ (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.