



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:33 PM UTC

PDB ID : 2VGJ / pdb_00002vgj
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 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

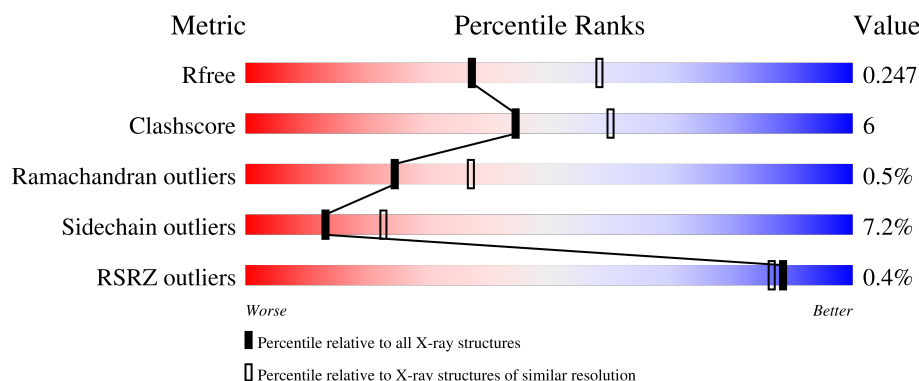
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	489	 77% 15% . .
1	B	489	 81% 13% . 5%
1	C	489	 82% 12% . 5%
1	D	489	 80% 13% . .

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	SO4	A	601	-	-	X	-

2 Entry composition [i](#)

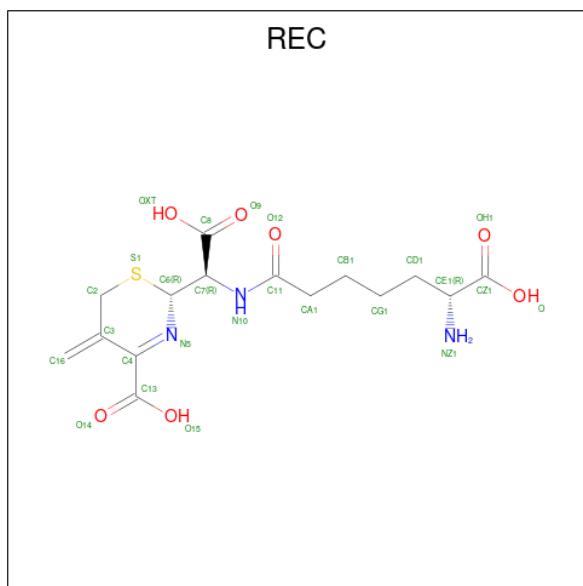
There are 5 unique types of molecules in this entry. The entry contains 14096 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: REC) (formula: C₁₅H₂₁N₃O₇S).



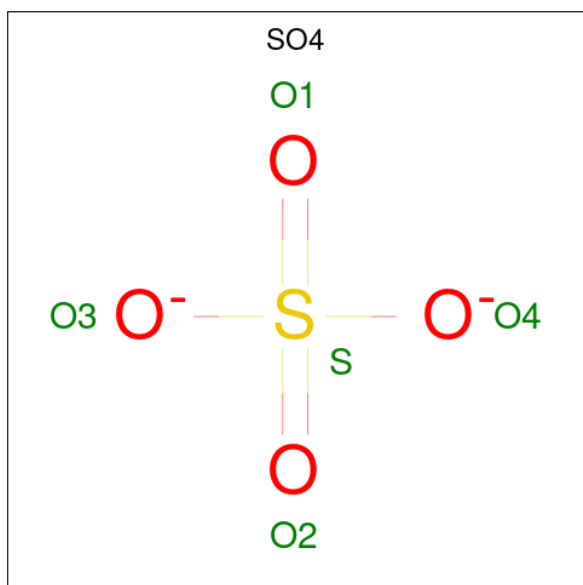
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			25	15	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			25	15	3	6	1		

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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 (CCD ID: 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 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

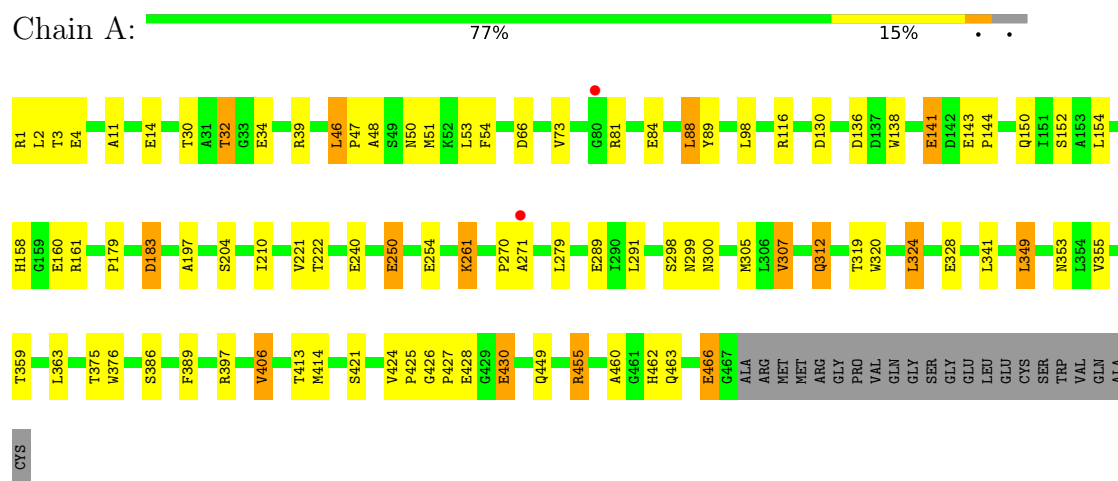
- Molecule 5 is water.

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

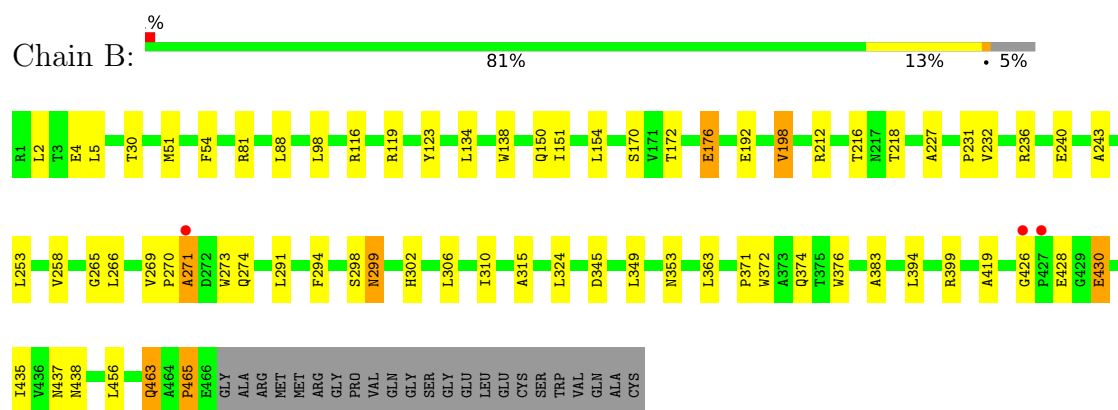
3 Residue-property plots

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.

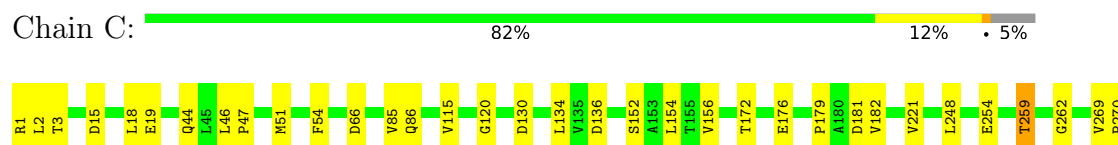
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



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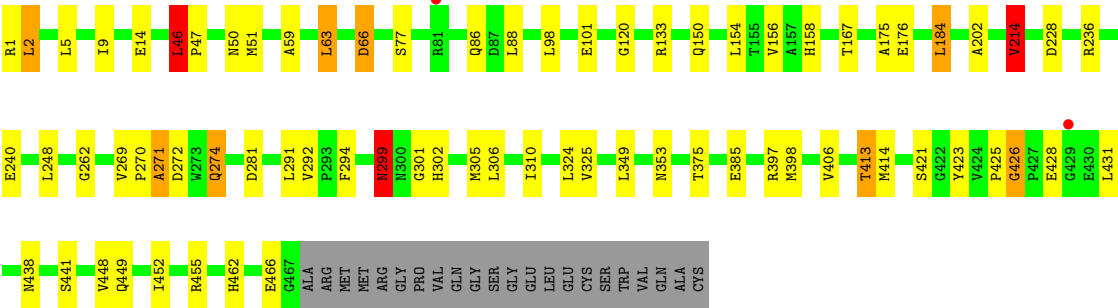
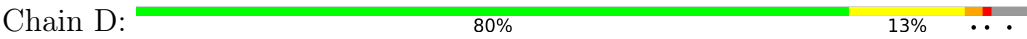


• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE





● 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) 99.5 (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)	0.42 , 52.5	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	0.96	2/3412 (0.1%)	1.12	5/4668 (0.1%)
1	B	0.88	2/3403 (0.1%)	1.04	4/4656 (0.1%)
1	C	0.86	1/3403 (0.0%)	1.06	8/4656 (0.2%)
1	D	0.93	3/3412 (0.1%)	1.10	11/4668 (0.2%)
All	All	0.91	8/13630 (0.1%)	1.08	28/18648 (0.2%)

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

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	GLU	C-N	-7.25	1.23	1.33
1	B	465	PRO	C-N	-6.72	1.24	1.33
1	D	466	GLU	C-N	-6.53	1.24	1.33
1	D	214	VAL	CA-CB	6.35	1.62	1.54
1	D	325	VAL	CA-CB	6.35	1.62	1.54
1	C	465	PRO	C-N	-6.17	1.24	1.33
1	B	227	ALA	CA-CB	-5.24	1.44	1.53
1	A	210	ILE	CA-CB	5.10	1.60	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	LEU	CA-C-N	10.02	129.76	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	LEU	C-N-CA	10.02	129.76	119.64
1	B	198	VAL	CB-CA-C	-7.83	99.99	111.19
1	D	269	VAL	CA-C-N	6.99	128.58	119.84
1	D	269	VAL	C-N-CA	6.99	128.58	119.84
1	C	269	VAL	CA-C-N	6.88	127.45	119.47
1	C	269	VAL	C-N-CA	6.88	127.45	119.47
1	C	181	ASP	CB-CA-C	-6.63	100.59	110.67
1	B	345	ASP	N-CA-C	6.29	116.75	107.88
1	A	426	GLY	CA-C-N	6.20	125.42	118.97
1	A	426	GLY	C-N-CA	6.20	125.42	118.97
1	D	292	VAL	CA-C-N	-5.84	113.60	119.56
1	D	292	VAL	C-N-CA	-5.84	113.60	119.56
1	D	2	LEU	N-CA-C	5.83	117.44	111.14
1	B	269	VAL	CA-C-N	5.81	126.21	119.47
1	B	269	VAL	C-N-CA	5.81	126.21	119.47
1	D	299	ASN	N-CA-C	5.48	117.39	108.63
1	D	385	GLU	CA-C-N	5.39	127.45	120.44
1	D	385	GLU	C-N-CA	5.39	127.45	120.44
1	D	46	LEU	CA-C-N	5.38	124.89	119.19
1	D	46	LEU	C-N-CA	5.38	124.89	119.19
1	C	46	LEU	CA-C-N	5.36	125.06	119.64
1	C	46	LEU	C-N-CA	5.36	125.06	119.64
1	C	430	GLU	N-CA-C	5.25	117.92	110.10
1	A	183	ASP	CB-CA-C	-5.21	100.72	109.48
1	C	15	ASP	CA-C-N	5.08	125.37	119.47
1	C	15	ASP	C-N-CA	5.08	125.37	119.47
1	D	281	ASP	N-CA-C	5.03	116.64	109.14

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	51	0
1	B	3344	0	3194	33	0
1	C	3344	0	3194	27	0
1	D	3353	0	3200	46	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	3	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	158	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 (158) 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:A:47:PRO:HG3	1:A:51:MET:HE2	1.63	0.78
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:51:MET:HE3	1:A:353:ASN:HB3	1.74	0.70
1:A:319:THR:HG22	5:A:2115:HOH:O	1.93	0.68
1:C:47:PRO:HG3	1:C:51:MET:HE2	1.76	0.68
1:D:167:THR:OG1	1:D:184:LEU:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:299:ASN:C	1:A:299:ASN:HD22	2.13	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:C:51:MET:HE3	1:C:353:ASN:HB3	1.87	0.55
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:D:51:MET:HE3	1:D:353:ASN:HB3	1.87	0.55
1:A:150:GLN:HE22	1:A:240:GLU:H	1.55	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:GLU:OE1	1:C:259:THR:HA	2.10	0.52
1:D:236:ARG:NH2	3:D:602:SO4:O3	2.40	0.51
2:D:500:REC:H161	2:D:500:REC:O14	2.10	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: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:152:SER:O	1:C:305:MET:HE3	2.12	0.49
1:B:437:ASN:C	1:B:438:ASN:HD22	2.21	0.48
1:C:18:LEU:HD11	1:C:448:VAL:HG11	1.95	0.48
1:D:299:ASN:C	1:D:299:ASN:HD22	2.20	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:50:ASN:ND2	1:D:421:SER:OG	2.46	0.48
1:D:413:THR:HG23	5:D:2115:HOH:O	2.11	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:D:414:MET:HE2	2:D:500:REC:HB11	1.97	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
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:HB3	1:A:81:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:GLN:O	1:C:120:GLY:N	2.45	0.46
1:B:51:MET:HE2	1:B:353:ASN:HB3	1.98	0.45
1:A:152:SER:O	1:A:305:MET:HE3	2.16	0.45
1:A:197:ALA:HB2	1:A:221:VAL:HG12	1.97	0.45
1:A:312:GLN:CA	1:A:312:GLN:HE21	2.29	0.45
1:B:299:ASN:HD22	1:B:299:ASN:C	2.24	0.45
1:C:51:MET:HG3	1:C:51:MET:O	2.15	0.45
1:B:270:PRO:HG2	1:B:273:TRP:CE2	2.52	0.45
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:HB3	1:B:116:ARG:NH2	2.33	0.44
1:C:351:ARG:HH12	1:C:415:SER:HB2	1.82	0.44
1:D:175:ALA:O	1:D:176:GLU:C	2.60	0.44
1:A:130:ASP:OD1	1:A:130:ASP:C	2.61	0.43
1:D:426:GLY:C	1:D:428:GLU:N	2.76	0.43
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:C:270:PRO:C	1:C:272:ASP:H	2.27	0.43
1:D:47:PRO:HG3	1:D:51:MET:HE2	2.00	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:HE21	1:B:463:GLN:HB2	1.59	0.42
1:D:423:TYR:HA	1:D:431:LEU:O	2.19	0.42
1:A:141:GLU:H	1:A:141:GLU:CD	2.27	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:158:HIS:CD2	1:A:158:HIS:C	2.98	0.42
1:A:4:GLU:HB2	5:A:2003:HOH:O	2.19	0.42
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:307:VAL:HG11	1:A:320:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:324:LEU:HD12	1:C:324:LEU:HA	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:B:426:GLY:C	1:B:428:GLU:H	2.28	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%)	30 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	464/489 (95%)	439 (95%)	21 (4%)	4 (1%)	14	22
1	C	464/489 (95%)	442 (95%)	19 (4%)	3 (1%)	21	32
1	D	465/489 (95%)	433 (93%)	31 (7%)	1 (0%)	43	58
All	All	1858/1956 (95%)	1749 (94%)	99 (5%)	10 (0%)	24	37

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%)	303 (89%)	36 (11%)	6	10
1	B	338/356 (95%)	318 (94%)	20 (6%)	18	31
1	C	338/356 (95%)	321 (95%)	17 (5%)	22	38
1	D	339/356 (95%)	315 (93%)	24 (7%)	13	23
All	All	1354/1424 (95%)	1257 (93%)	97 (7%)	13	23

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU

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Mol	Chain	Res	Type
1	A	3	THR
1	A	30	THR
1	A	32	THR
1	A	46	LEU
1	A	66	ASP
1	A	84	GLU
1	A	88	LEU
1	A	98	LEU
1	A	116	ARG
1	A	136	ASP
1	A	141	GLU
1	A	154	LEU
1	A	183	ASP
1	A	222	THR
1	A	250	GLU
1	A	261	LYS
1	A	289	GLU
1	A	291	LEU
1	A	298	SER
1	A	307	VAL
1	A	312	GLN
1	A	324	LEU
1	A	328	GLU
1	A	349	LEU
1	A	359	THR
1	A	375	THR
1	A	376	TRP
1	A	386	SER
1	A	406	VAL
1	A	424	VAL
1	A	428	GLU
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	81	ARG
1	B	88	LEU
1	B	98	LEU
1	B	134	LEU

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Mol	Chain	Res	Type
1	B	154	LEU
1	B	176	GLU
1	B	198	VAL
1	B	274	GLN
1	B	291	LEU
1	B	298	SER
1	B	299	ASN
1	B	324	LEU
1	B	349	LEU
1	B	374	GLN
1	B	376	TRP
1	B	430	GLU
1	B	463	GLN
1	C	2	LEU
1	C	19	GLU
1	C	66	ASP
1	C	134	LEU
1	C	154	LEU
1	C	172	THR
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	324	LEU
1	C	349	LEU
1	C	394	LEU
1	C	428	GLU
1	D	2	LEU
1	D	5	LEU
1	D	46	LEU
1	D	63	LEU
1	D	66	ASP
1	D	77	SER
1	D	86	GLN
1	D	88	LEU
1	D	98	LEU
1	D	101	GLU
1	D	154	LEU
1	D	184	LEU

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Mol	Chain	Res	Type
1	D	214	VAL
1	D	272	ASP
1	D	274	GLN
1	D	291	LEU
1	D	299	ASN
1	D	324	LEU
1	D	349	LEU
1	D	375	THR
1	D	413	THR
1	D	438	ASN
1	D	441	SER
1	D	448	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	150	GLN
1	A	158	HIS
1	A	195	ASN
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	195	ASN
1	B	274	GLN
1	B	282	HIS
1	B	299	ASN
1	B	302	HIS
1	B	374	GLN
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	374	GLN

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Mol	Chain	Res	Type
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
1	D	449	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 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	C	602	-	4,4,4	0.24	0	6,6,6	0.12	0
2	REC	C	500	1	21,25,26	1.05	1 (4%)	19,33,35	4.21	3 (15%)
3	SO4	D	600	-	4,4,4	0.34	0	6,6,6	0.33	0
2	REC	A	500	1	21,25,26	1.08	3 (14%)	19,33,35	4.74	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	602	-	4,4,4	0.23	0	6,6,6	0.17	0
3	SO4	C	601	-	4,4,4	0.25	0	6,6,6	0.14	0
2	REC	D	500	1	21,25,26	1.03	1 (4%)	19,33,35	4.51	2 (10%)
3	SO4	B	600	-	4,4,4	0.30	0	6,6,6	0.25	0
3	SO4	A	603	-	4,4,4	0.21	0	6,6,6	0.41	0
3	SO4	D	603	-	4,4,4	0.36	0	6,6,6	0.37	0
3	SO4	B	601	-	4,4,4	0.22	0	6,6,6	0.21	0
3	SO4	A	600	-	4,4,4	0.22	0	6,6,6	0.50	0
3	SO4	A	601	-	4,4,4	0.32	0	6,6,6	0.25	0
3	SO4	A	602	-	4,4,4	0.25	0	6,6,6	0.25	0
3	SO4	B	602	-	4,4,4	0.26	0	6,6,6	0.16	0
3	SO4	C	603	-	4,4,4	0.24	0	6,6,6	0.44	0
3	SO4	D	601	-	4,4,4	0.32	0	6,6,6	0.24	0
3	SO4	C	600	-	4,4,4	0.28	0	6,6,6	0.62	0
3	SO4	B	603	-	4,4,4	0.17	0	6,6,6	0.38	0
2	REC	B	500	1	21,25,26	0.99	0	19,33,35	3.13	5 (26%)

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	-	3/18/38/40	0/0/1/1
2	REC	A	500	1	-	3/18/38/40	0/0/1/1
2	REC	D	500	1	-	4/18/38/40	0/0/1/1
2	REC	B	500	1	-	3/18/38/40	0/0/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	REC	C2-S1	-2.75	1.76	1.82
2	C	500	REC	C2-S1	-2.71	1.76	1.82
2	A	500	REC	C2-S1	-2.44	1.77	1.82
2	A	500	REC	C2-C3	2.24	1.53	1.50
2	A	500	REC	O-CZ1	-2.20	1.23	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	REC	C6-N5-C4	18.40	132.40	116.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	REC	C6-N5-C4	17.77	131.85	116.33
2	C	500	REC	C6-N5-C4	15.47	129.84	116.33
2	B	500	REC	C6-N5-C4	10.48	125.48	116.33
2	C	500	REC	C2-S1-C6	8.53	109.99	94.36
2	D	500	REC	C2-S1-C6	7.22	107.59	94.36
2	A	500	REC	C2-S1-C6	7.19	107.53	94.36
2	B	500	REC	C2-S1-C6	6.93	107.06	94.36
2	A	500	REC	C8-C7-N10	-3.11	104.89	109.80
2	B	500	REC	C2-C3-C16	-2.57	116.79	121.59
2	B	500	REC	C8-C7-N10	2.40	113.58	109.80
2	A	500	REC	O12-C11-N10	2.25	126.76	122.95
2	C	500	REC	C2-C3-C16	-2.24	117.40	121.59
2	B	500	REC	CD1-CE1-CZ1	-2.24	104.50	110.45

There are no chirality outliers.

All (13) torsion outliers are listed below:

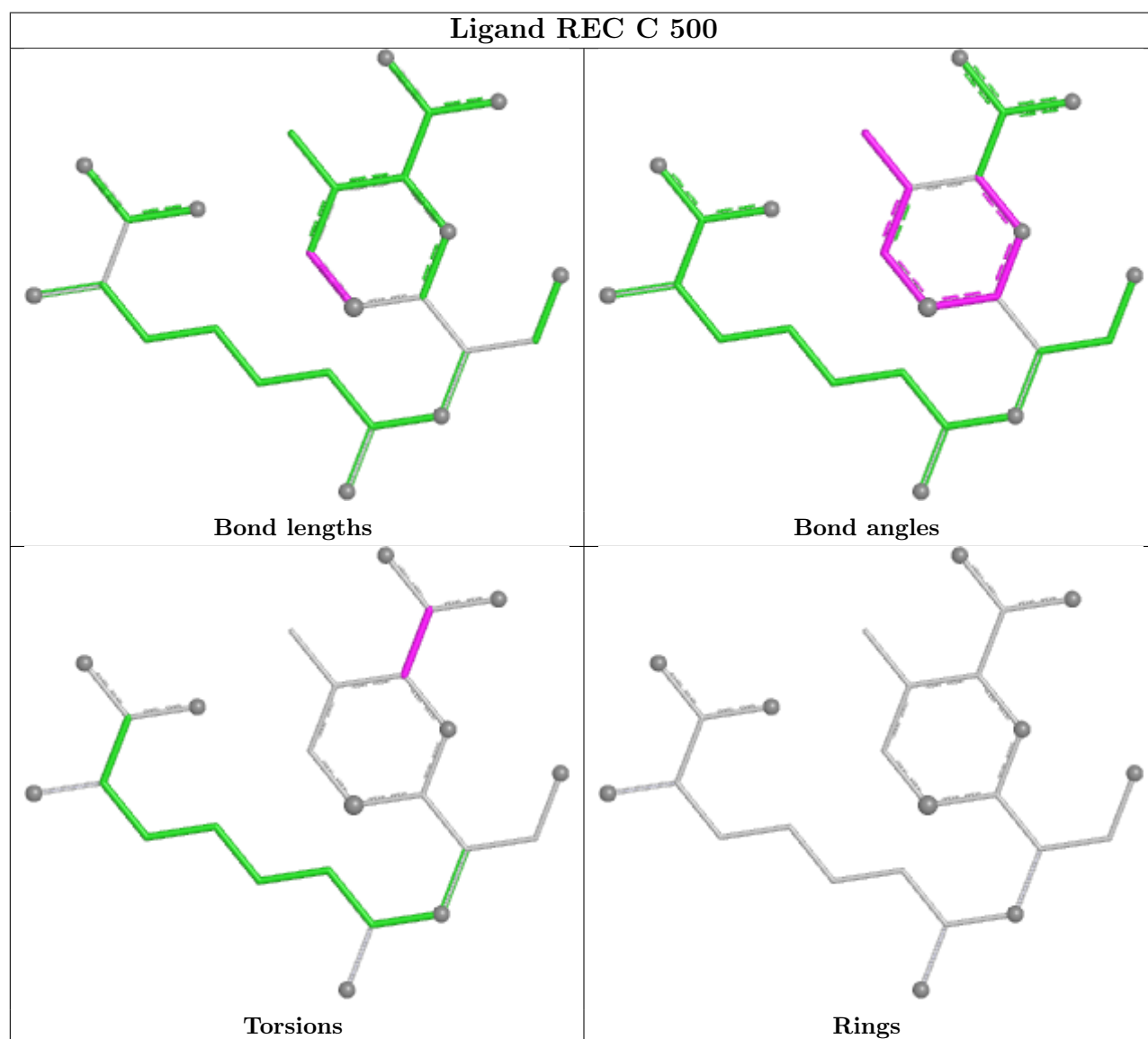
Mol	Chain	Res	Type	Atoms
2	C	500	REC	O14-C13-C4-N5
2	C	500	REC	O15-C13-C4-N5
2	A	500	REC	C11-CA1-CB1-CG1
2	C	500	REC	O14-C13-C4-C3
2	D	500	REC	O14-C13-C4-C3
2	D	500	REC	CG1-CD1-CE1-NZ1
2	A	500	REC	O15-C13-C4-N5
2	B	500	REC	O15-C13-C4-N5
2	B	500	REC	O14-C13-C4-N5
2	B	500	REC	O14-C13-C4-C3
2	A	500	REC	O14-C13-C4-C3
2	D	500	REC	CG1-CD1-CE1-CZ1
2	D	500	REC	O15-C13-C4-N5

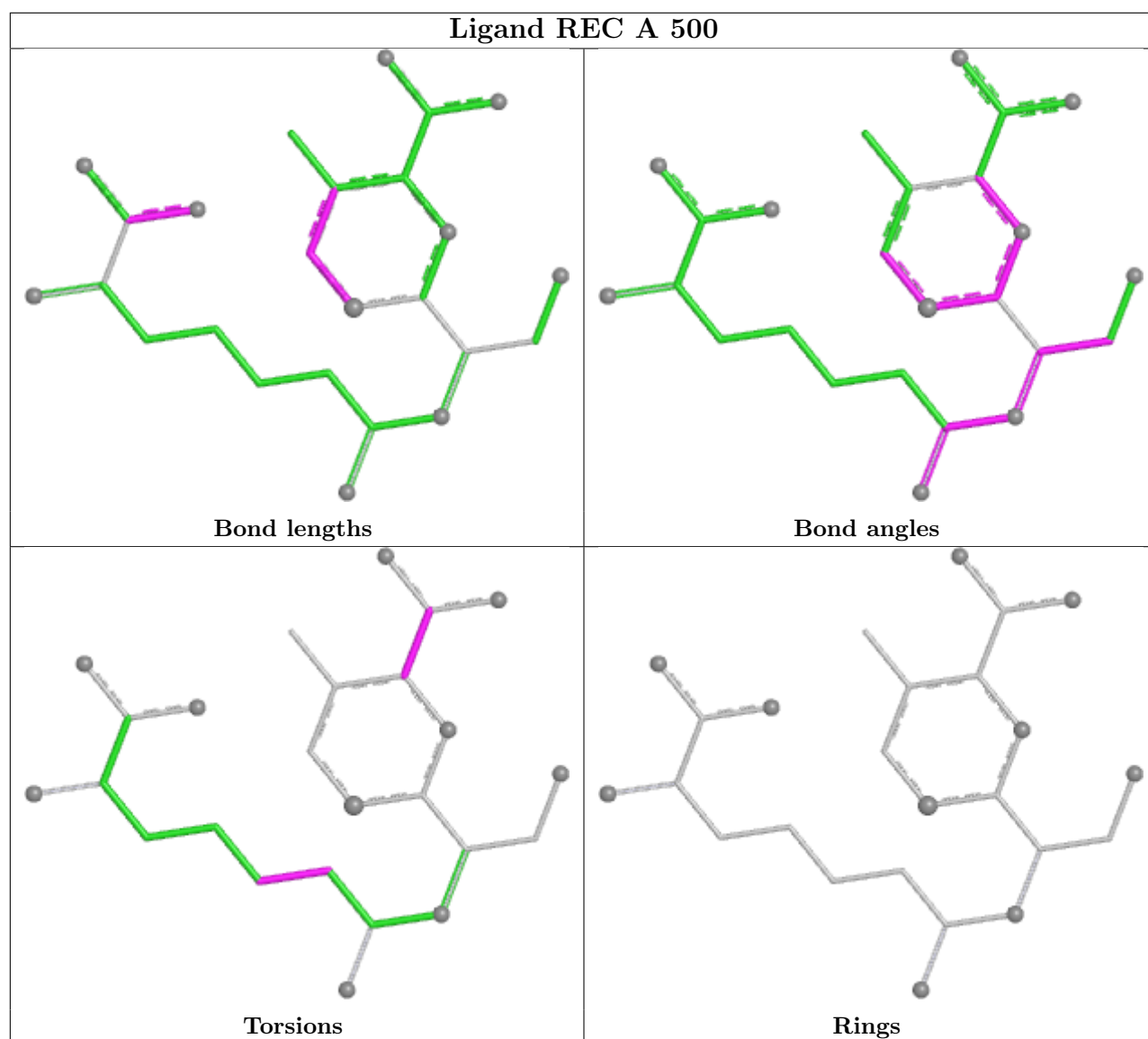
There are no ring outliers.

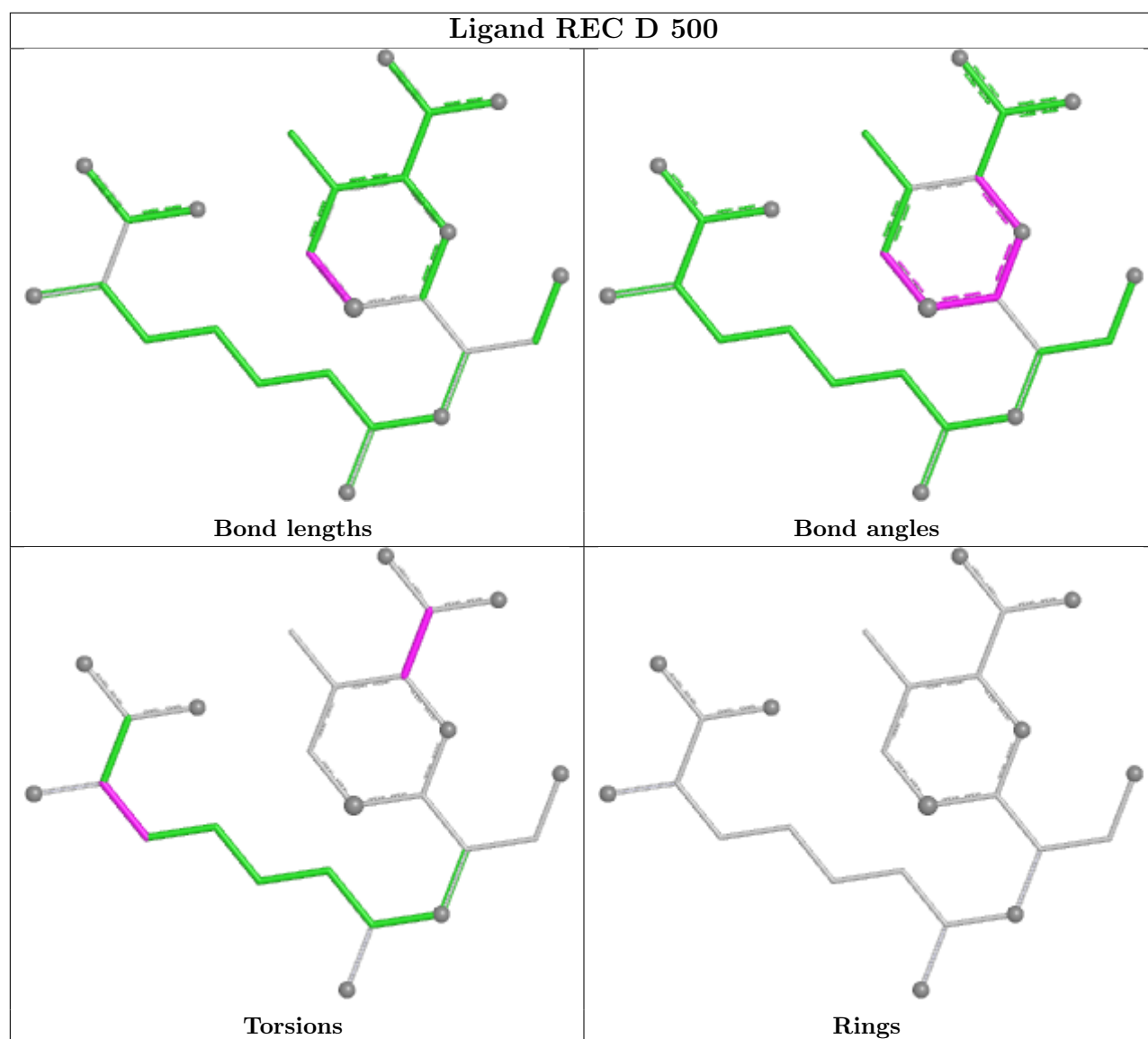
5 monomers are involved in 9 short contacts:

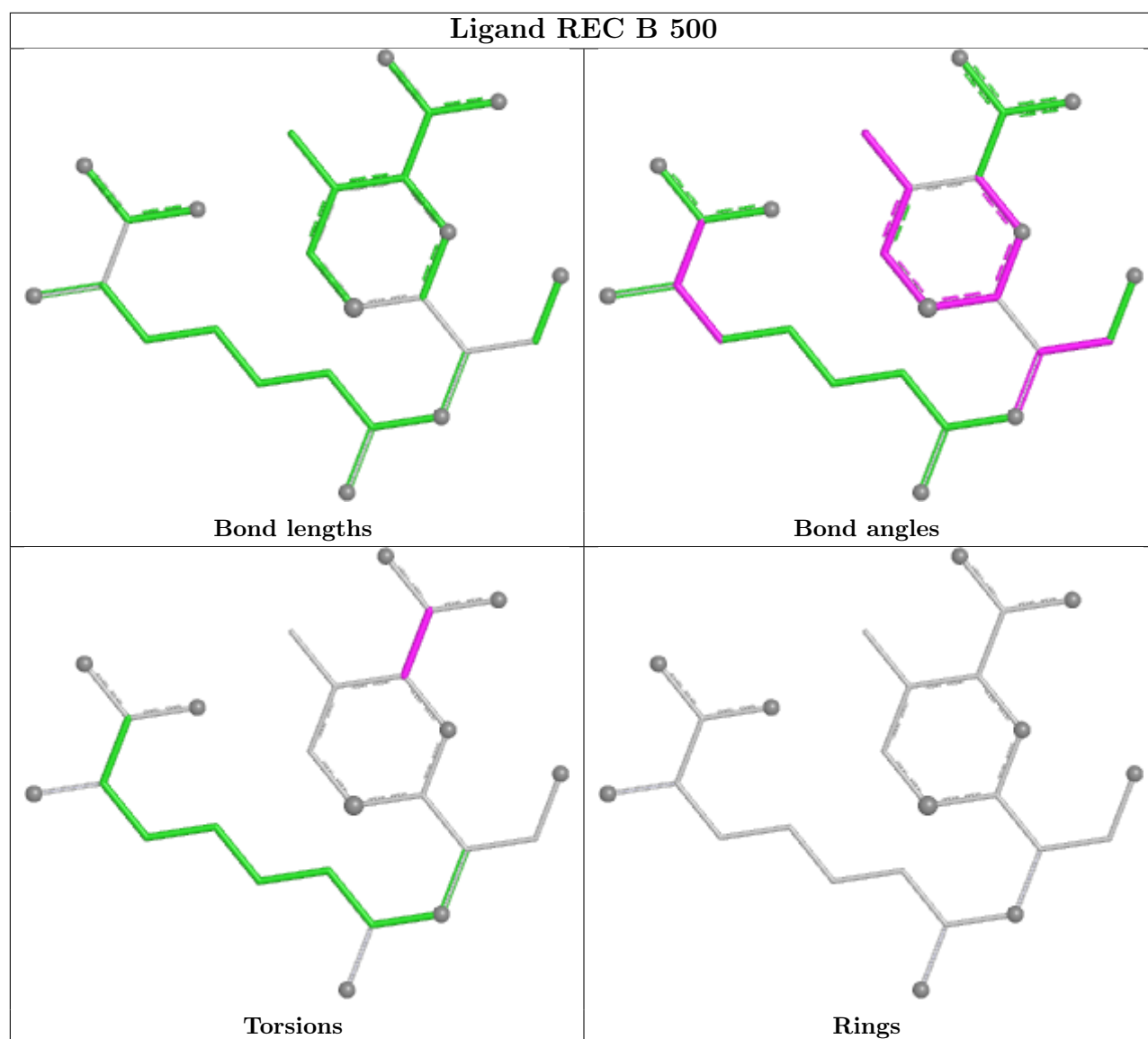
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	REC	2	0
3	D	602	SO4	1	0
2	D	500	REC	3	0
3	A	601	SO4	2	0
3	B	602	SO4	1	0

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 [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	467/489 (95%)	-0.65	2 (0%) 88 86	10, 23, 41, 60	0
1	B	466/489 (95%)	-0.51	3 (0%) 85 83	15, 28, 50, 74	0
1	C	466/489 (95%)	-0.56	0 100 100	16, 28, 47, 66	0
1	D	467/489 (95%)	-0.48	2 (0%) 88 86	12, 27, 53, 72	0
All	All	1866/1956 (95%)	-0.55	7 (0%) 88 86	10, 26, 50, 74	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	429	GLY	3.0
1	D	81	ARG	2.8
1	A	80	GLY	2.2
1	B	426	GLY	2.2
1	B	427	PRO	2.1
1	B	271	ALA	2.0
1	A	271	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 ⓘ

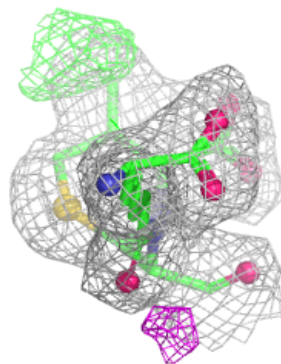
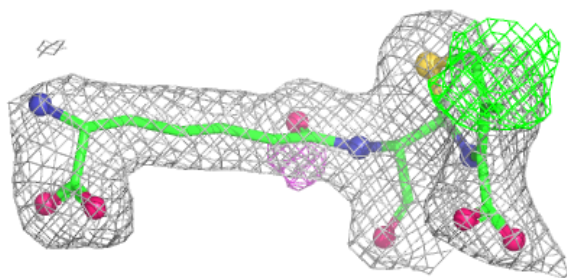
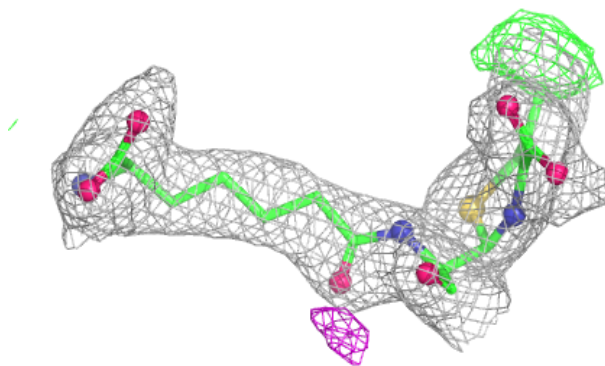
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.71	0.15	136,136,136,136	0
3	SO4	B	601	5/5	0.83	0.12	90,91,91,91	0
3	SO4	D	601	5/5	0.84	0.12	72,72,73,73	0
3	SO4	C	602	5/5	0.87	0.14	95,95,96,96	0
3	SO4	C	601	5/5	0.88	0.11	71,72,72,73	0
3	SO4	D	602	5/5	0.88	0.12	67,68,69,69	0
3	SO4	A	602	5/5	0.89	0.12	82,83,83,83	0
3	SO4	A	601	5/5	0.91	0.10	60,60,60,61	0
2	REC	C	500	25/26	0.92	0.07	23,28,36,36	0
3	SO4	C	600	5/5	0.95	0.09	41,42,42,45	0
3	SO4	D	600	5/5	0.95	0.07	47,48,50,50	0
4	MG	A	611	1/1	0.95	0.07	38,38,38,38	0
3	SO4	C	603	5/5	0.96	0.08	37,39,40,40	0
2	REC	D	500	25/26	0.96	0.05	14,20,28,31	0
3	SO4	A	603	5/5	0.96	0.11	39,40,41,44	0
3	SO4	B	600	5/5	0.96	0.08	44,44,45,46	0
2	REC	B	500	25/26	0.96	0.06	16,23,32,34	0
3	SO4	B	603	5/5	0.97	0.10	31,32,34,35	0
2	REC	A	500	25/26	0.97	0.05	15,20,27,27	0
3	SO4	A	600	5/5	0.97	0.07	34,36,38,39	0
3	SO4	D	603	5/5	0.98	0.09	23,25,27,27	0
4	MG	D	611	1/1	0.98	0.07	17,17,17,17	0

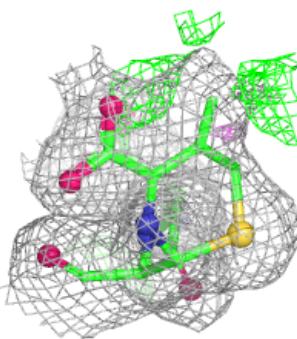
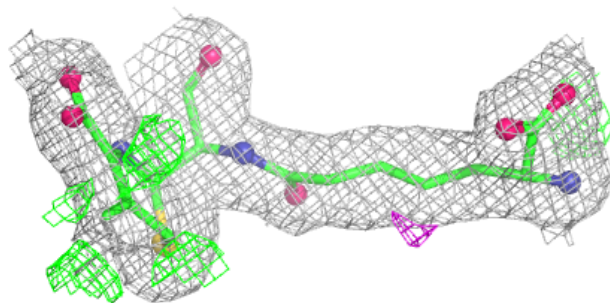
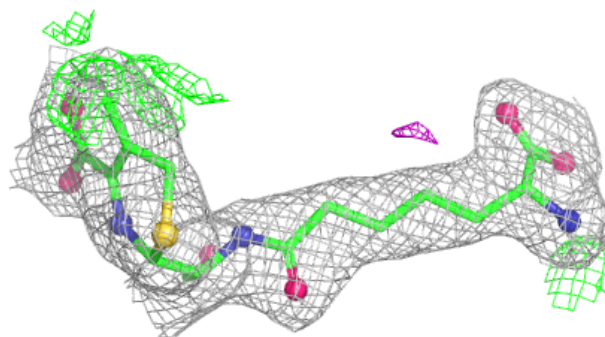
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around REC C 500:

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

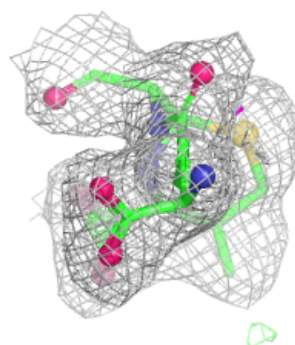
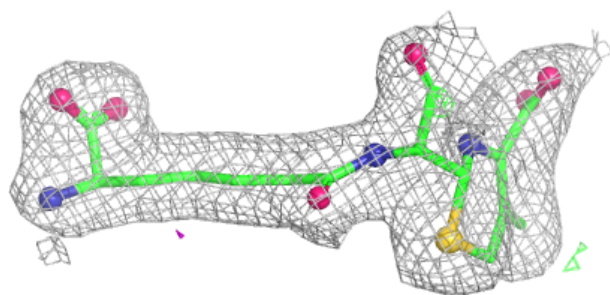
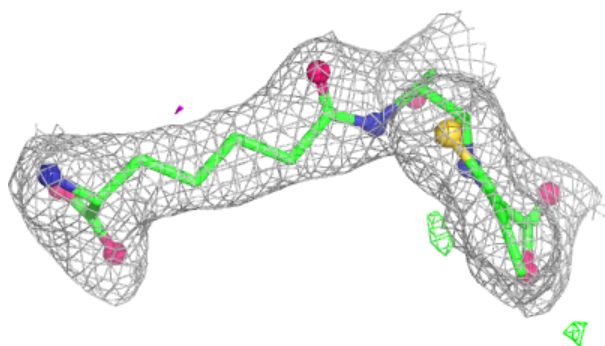
**Electron density around REC D 500:**

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

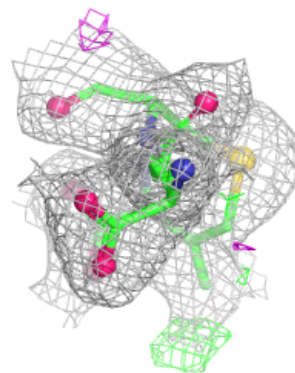
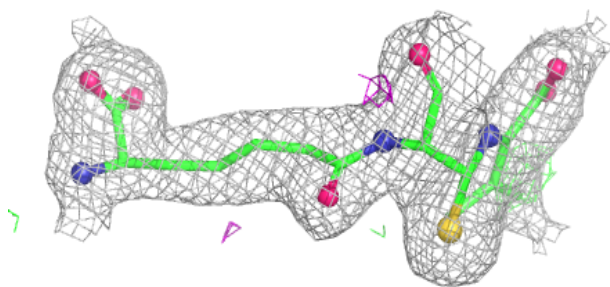
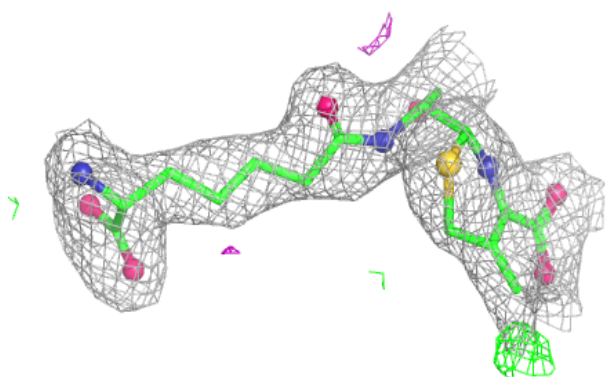


Electron density around REC B 500:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.