



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2022 – 12:14 PM JST

PDB ID : 7DXM
Title : Crystal structure of DltD
Authors : Yan, X.X.; Zeng, Q.; Tian, L.F.
Deposited on : 2021-01-19
Resolution : 2.96 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 : 4.02b-467
Mogul : ?? (???), CSD ??CSD?? (????)
Xtriage (Phenix) : 1.13
EDS : 2.29
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) : 2.29

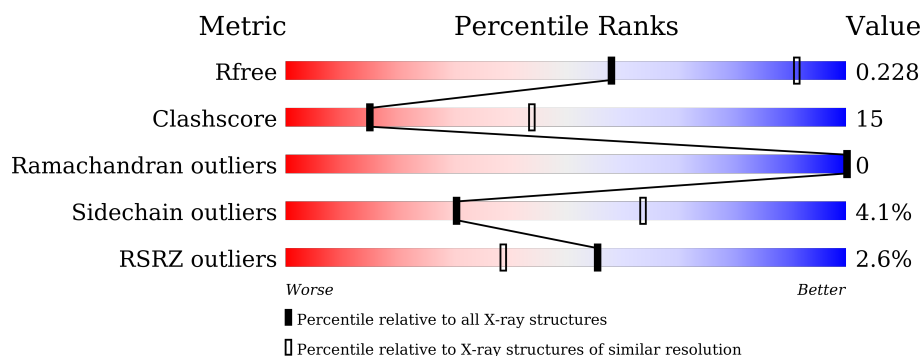
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	397	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>..</div> </div> </div>
1	B	397	<div> <div></div> <div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
1	C	397	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>32%</div> <div>..</div> </div> </div>
1	D	397	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>27%</div> <div>..</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12785 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 Protein DltD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3186	2028	540	609	9			
1	B	392	Total	C	N	O	S	0	0	0
			3191	2028	541	613	9			
1	C	389	Total	C	N	O	S	0	0	0
			3171	2017	538	607	9			
1	D	392	Total	C	N	O	S	0	0	0
			3178	2021	536	612	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	423	ASP	-	expression tag	UNP Q5M4V2
A	424	GLU	-	expression tag	UNP Q5M4V2
B	423	ASP	-	expression tag	UNP Q5M4V2
B	424	GLU	-	expression tag	UNP Q5M4V2
C	423	ASP	-	expression tag	UNP Q5M4V2
C	424	GLU	-	expression tag	UNP Q5M4V2
D	423	ASP	-	expression tag	UNP Q5M4V2
D	424	GLU	-	expression tag	UNP Q5M4V2

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



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

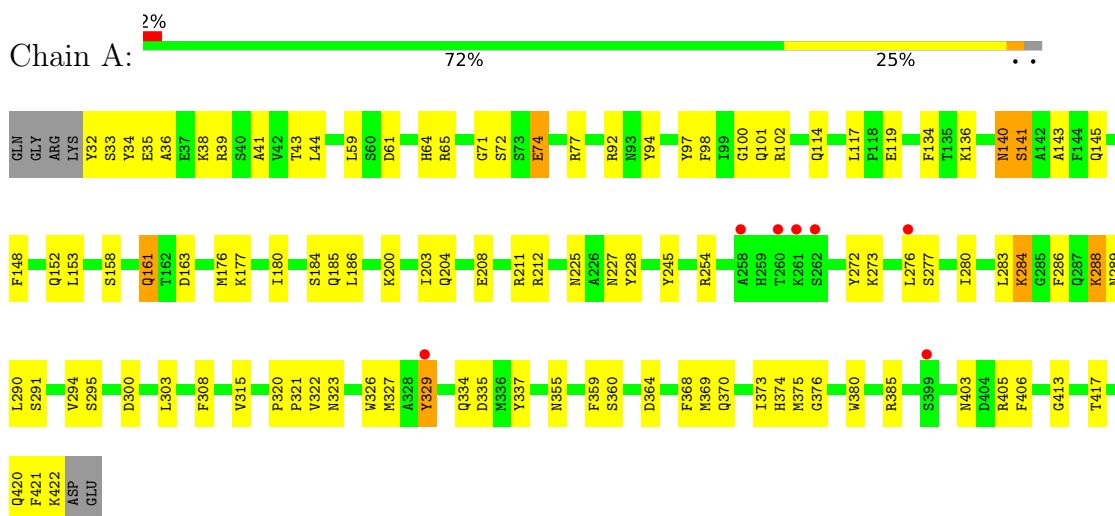
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		
3	B	10	Total	O	0	0
			10	10		
3	C	7	Total	O	0	0
			7	7		
3	D	9	Total	O	0	0
			9	9		

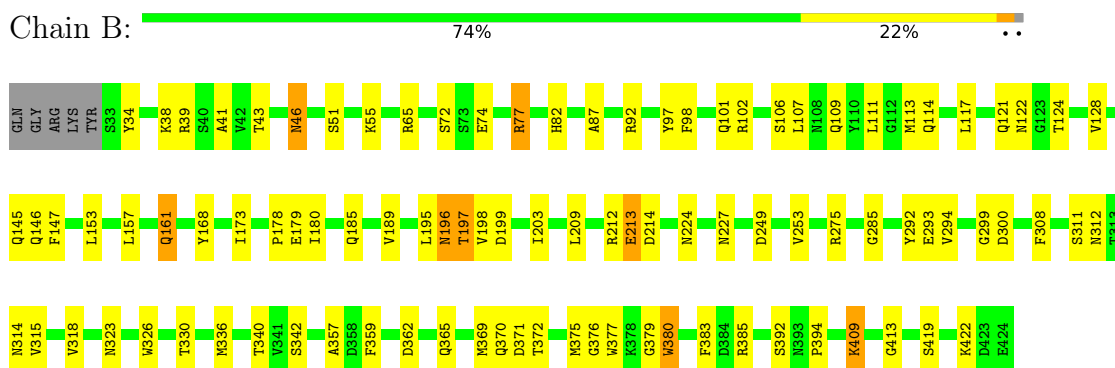
3 Residue-property plots

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.

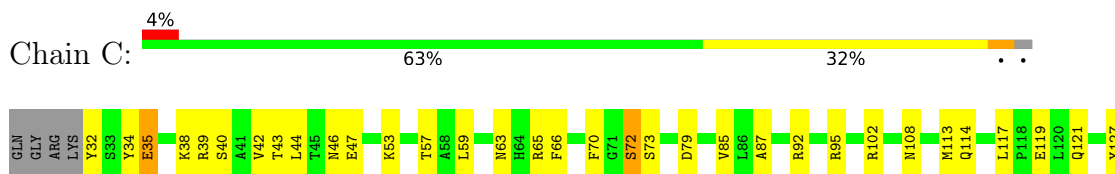
• Molecule 1: Protein DltD

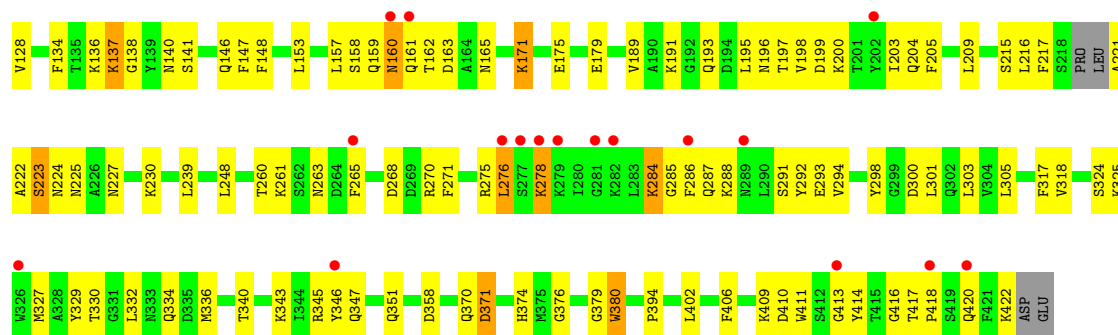


• Molecule 1: Protein DltD

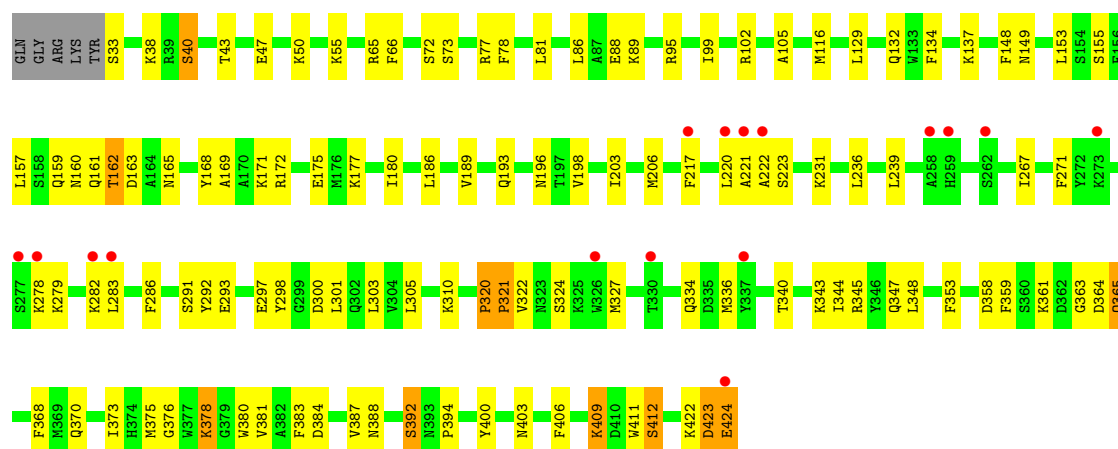


• Molecule 1: Protein DltD





● Molecule 1: Protein DltD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.27Å 109.92Å 282.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.96 39.98 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.1 (40.00-2.96) 98.2 (39.98-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.12	Depositor
R, R_{free}	0.216 , 0.228 0.198 , 0.228	Depositor DCC
R_{free} test set	1887 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	69.8	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12785	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: 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	0.59	0/3266	0.69	1/4415 (0.0%)
1	B	0.59	0/3270	0.68	0/4420
1	C	0.52	0/3249	0.67	1/4389 (0.0%)
1	D	0.55	0/3257	0.72	4/4405 (0.1%)
All	All	0.56	0/13042	0.69	6/17629 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	320	PRO	CB-CA-C	-11.48	83.29	112.00
1	D	160	ASN	CB-CA-C	-8.55	93.30	110.40
1	A	140	ASN	CB-CA-C	-6.64	97.11	110.40
1	D	321	PRO	CB-CA-C	-6.63	95.41	112.00
1	C	72	SER	N-CA-C	5.93	127.01	111.00
1	D	160	ASN	N-CA-C	5.23	125.12	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3186	0	3070	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3191	0	3071	78	0
1	C	3171	0	3051	132	0
1	D	3178	0	3045	89	0
2	A	10	0	0	2	0
2	B	5	0	0	1	0
2	D	5	0	0	1	0
3	A	13	0	0	1	0
3	B	10	0	0	0	0
3	C	7	0	0	0	0
3	D	9	0	0	1	0
All	All	12785	0	12237	378	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (378) 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:208:GLU:HG3	1:A:212:ARG:NH1	1.55	1.20
1:C:275:ARG:C	1:C:276:LEU:HD23	1.68	1.12
1:A:273:LYS:HD2	3:A:605:HOH:O	1.50	1.10
1:C:268:ASP:OD2	1:C:270:ARG:HG2	1.54	1.05
1:A:208:GLU:CG	1:A:212:ARG:NH1	2.27	0.97
1:A:71:GLY:O	1:A:100:GLY:HA3	1.63	0.97
1:A:208:GLU:HG3	1:A:212:ARG:HH11	1.17	0.97
1:D:320:PRO:O	1:D:320:PRO:HG2	1.66	0.95
1:C:287:GLN:HG3	1:C:330:THR:HB	1.49	0.94
1:C:221:ALA:HA	1:C:222:ALA:HB2	1.51	0.93
1:A:208:GLU:CG	1:A:212:ARG:HH11	1.80	0.92
1:C:161:GLN:HB2	1:C:162:THR:HA	1.52	0.92
1:D:267:ILE:HD11	1:D:271:PHE:CD1	2.06	0.91
1:C:161:GLN:HB2	1:C:162:THR:CA	2.02	0.89
1:C:284:LYS:HD2	1:C:285:GLY:N	1.88	0.89
1:C:161:GLN:HB2	1:C:162:THR:OG1	1.72	0.89
1:B:196:ASN:OD1	1:B:197:THR:N	2.07	0.88
1:D:267:ILE:HD11	1:D:271:PHE:HD1	1.35	0.87
1:A:294:VAL:HG13	1:A:413:GLY:HA2	1.61	0.83
1:D:365:GLN:HE22	1:D:378:LYS:HG2	1.43	0.83
1:D:322:VAL:HB	1:D:327:MET:HE2	1.58	0.83
1:C:284:LYS:CD	1:C:285:GLY:N	2.41	0.83
1:C:161:GLN:CG	1:C:162:THR:OG1	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:VAL:HB	1:B:413:GLY:HA2	1.62	0.81
1:D:409:LYS:H	1:D:409:LYS:HD2	1.46	0.80
1:A:161:GLN:HG3	1:A:163:ASP:OD2	1.82	0.79
1:C:287:GLN:OE1	1:C:332:LEU:HD12	1.82	0.79
1:D:161:GLN:HE22	1:D:310:LYS:HE2	1.48	0.79
1:B:213:GLU:OE2	1:C:209:LEU:HD12	1.82	0.78
1:C:222:ALA:HB1	1:C:224:ASN:N	1.98	0.78
1:B:293:GLU:HG3	1:B:340:THR:HG22	1.65	0.77
1:C:276:LEU:HD23	1:C:276:LEU:N	2.00	0.77
1:C:161:GLN:HB2	1:C:162:THR:CB	2.14	0.76
1:B:293:GLU:CG	1:B:340:THR:HG22	2.15	0.76
1:C:222:ALA:HA	1:C:223:SER:CB	2.15	0.75
1:B:122:ASN:HD22	1:B:312:ASN:HD22	1.34	0.75
1:C:285:GLY:O	1:C:288:LYS:HE2	1.86	0.75
1:A:161:GLN:O	1:A:161:GLN:HG2	1.86	0.75
1:A:185:GLN:HG2	1:A:203:ILE:HD11	1.68	0.75
1:A:321:PRO:HD2	1:A:375:MET:CE	2.16	0.75
1:C:161:GLN:CB	1:C:162:THR:OG1	2.34	0.74
1:C:87:ALA:HA	1:C:92:ARG:HD2	1.69	0.74
1:C:300:ASP:O	1:C:303:LEU:HB2	1.89	0.73
1:C:371:ASP:HB2	1:C:374:HIS:HB2	1.69	0.73
1:C:265:PHE:CD1	1:C:325:LYS:HB3	2.24	0.72
1:D:365:GLN:HE22	1:D:378:LYS:CG	2.03	0.72
1:B:161:GLN:O	1:B:161:GLN:OE1	2.07	0.72
1:A:208:GLU:HG3	1:A:212:ARG:HH12	1.52	0.72
1:B:196:ASN:OD1	1:B:198:VAL:N	2.22	0.72
1:A:327:MET:HE1	1:A:334:GLN:HB2	1.71	0.71
1:D:196:ASN:ND2	1:D:198:VAL:HG12	2.05	0.71
1:C:327:MET:SD	1:C:334:GLN:NE2	2.64	0.71
1:C:221:ALA:CA	1:C:222:ALA:HB2	2.22	0.70
1:C:294:VAL:HG12	1:C:413:GLY:HA2	1.73	0.69
1:D:161:GLN:NE2	1:D:310:LYS:HE2	2.07	0.69
1:C:284:LYS:HD3	1:C:285:GLY:H	1.57	0.68
1:B:102:ARG:NH1	1:C:63:ASN:OD1	2.27	0.67
1:B:41:ALA:HB1	1:B:97:TYR:HA	1.76	0.67
1:D:77:ARG:NH1	2:D:501:SO4:O4	2.28	0.67
1:D:388:ASN:O	1:D:392:SER:HB2	1.94	0.67
1:C:161:GLN:HG3	1:C:162:THR:OG1	1.92	0.67
1:D:327:MET:SD	1:D:334:GLN:HG2	2.35	0.66
1:B:275:ARG:NH1	2:B:501:SO4:O2	2.28	0.66
1:D:161:GLN:HE22	1:D:310:LYS:CE	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ARG:O	1:B:43:THR:HG23	1.95	0.66
1:C:225:ASN:HB3	1:C:227:ASN:H	1.60	0.65
1:B:128:VAL:HG22	1:B:318:VAL:HB	1.77	0.65
1:B:409:LYS:HE2	1:B:409:LYS:N	2.12	0.65
1:C:275:ARG:O	1:C:276:LEU:HD23	1.96	0.65
1:A:43:THR:O	1:A:225:ASN:ND2	2.30	0.65
1:A:77:ARG:HH11	1:A:374:HIS:CE1	2.14	0.65
1:B:370:GLN:HB2	1:B:376:GLY:HA3	1.79	0.65
1:A:140:ASN:HB3	1:A:143:ALA:H	1.62	0.64
1:A:177:LYS:HD3	1:A:180:ILE:HD12	1.79	0.64
1:D:40:SER:HA	1:D:43:THR:HG23	1.80	0.64
1:D:423:ASP:O	1:D:424:GLU:HB2	1.97	0.64
1:C:140:ASN:OD1	1:C:141:SER:N	2.31	0.64
1:C:222:ALA:HA	1:C:223:SER:HB3	1.79	0.64
1:A:368:PHE:HD2	1:A:369:MET:HE3	1.64	0.63
1:B:46:ASN:HD22	1:B:146:GLN:HB2	1.64	0.63
1:C:65:ARG:NH2	1:C:394:PRO:HG3	2.14	0.63
1:C:287:GLN:HG3	1:C:330:THR:CB	2.26	0.63
1:D:168:TYR:CZ	1:D:172:ARG:HD3	2.34	0.63
1:D:153:LEU:HD22	1:D:180:ILE:HD11	1.81	0.62
1:A:225:ASN:HB3	1:A:227:ASN:H	1.65	0.62
1:D:293:GLU:O	1:D:343:LYS:NZ	2.33	0.62
1:C:158:SER:C	1:C:159:GLN:HG3	2.20	0.61
1:D:171:LYS:O	1:D:175:GLU:HG3	2.00	0.61
1:C:345:ARG:HD2	1:C:358:ASP:OD2	2.01	0.61
1:D:222:ALA:O	1:D:223:SER:HB2	2.00	0.61
1:B:109:GLN:O	1:B:113:MET:HG3	2.01	0.61
1:D:320:PRO:O	1:D:320:PRO:CG	2.28	0.61
1:B:336:MET:O	1:B:340:THR:HG23	2.00	0.61
1:C:161:GLN:CB	1:C:162:THR:HA	2.18	0.61
1:C:284:LYS:HD3	1:C:329:TYR:O	2.00	0.61
1:D:148:PHE:CZ	1:D:153:LEU:HB2	2.36	0.61
1:C:292:TYR:HB2	1:C:340:THR:HG21	1.81	0.60
1:C:265:PHE:HD1	1:C:325:LYS:HB3	1.64	0.60
1:A:153:LEU:HD11	1:A:186:LEU:HD11	1.82	0.60
1:A:211:ARG:NH1	2:A:502:SO4:O1	2.34	0.60
1:A:370:GLN:HB2	1:A:376:GLY:HA3	1.82	0.60
1:B:46:ASN:ND2	1:B:146:GLN:OE1	2.33	0.60
1:D:162:THR:HG23	1:D:189:VAL:HG13	1.84	0.60
1:D:279:LYS:HB2	1:D:283:LEU:HD11	1.82	0.60
1:A:35:GLU:HB3	1:A:39:ARG:HH12	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ALA:HA	1:C:222:ALA:CB	2.19	0.60
1:C:284:LYS:HD3	1:C:285:GLY:N	2.15	0.59
1:C:222:ALA:HA	1:C:223:SER:OG	2.02	0.59
1:B:153:LEU:CD1	1:B:180:ILE:HD11	2.32	0.59
1:D:81:LEU:HD22	1:D:381:VAL:HG22	1.84	0.58
1:A:101:GLN:HG3	1:A:102:ARG:H	1.68	0.58
1:A:284:LYS:HG2	1:A:329:TYR:CE2	2.38	0.58
1:A:321:PRO:HG3	1:A:359:PHE:O	2.04	0.58
1:A:44:LEU:O	1:A:101:GLN:NE2	2.37	0.58
1:A:321:PRO:HD3	1:A:359:PHE:O	2.03	0.58
1:C:34:TYR:CZ	1:C:38:LYS:HD2	2.39	0.57
1:A:35:GLU:OE1	1:A:38:LYS:NZ	2.26	0.57
1:D:161:GLN:NE2	1:D:310:LYS:CE	2.67	0.57
1:C:114:GLN:HA	1:C:117:LEU:HD13	1.87	0.57
1:D:383:PHE:CZ	1:D:387:VAL:HG21	2.39	0.57
1:C:161:GLN:HE21	1:C:195:LEU:HD12	1.69	0.57
1:D:132:GLN:OE1	1:D:132:GLN:N	2.28	0.57
1:C:34:TYR:CE2	1:C:38:LYS:HD2	2.40	0.57
1:B:213:GLU:OE2	1:C:209:LEU:CD1	2.51	0.56
1:B:122:ASN:ND2	1:B:312:ASN:HD22	2.02	0.56
1:B:419:SER:O	1:B:422:LYS:NZ	2.39	0.56
1:A:321:PRO:HB3	1:A:360:SER:O	2.06	0.56
1:B:362:ASP:CG	1:B:365:GLN:HE22	2.09	0.56
1:B:369:MET:CE	1:B:375:MET:HG3	2.36	0.56
1:A:101:GLN:HG3	1:A:102:ARG:N	2.21	0.56
1:C:148:PHE:HZ	1:C:153:LEU:HB2	1.71	0.56
1:B:179:GLU:HA	1:C:160:ASN:HD21	1.71	0.55
1:C:287:GLN:HB2	1:C:330:THR:O	2.05	0.55
1:D:38:LYS:NZ	3:D:601:HOH:O	2.38	0.55
1:D:370:GLN:HB2	1:D:376:GLY:HA3	1.88	0.55
1:A:77:ARG:NH1	2:A:501:SO4:O2	2.38	0.55
1:C:160:ASN:OD1	1:C:160:ASN:N	2.39	0.55
1:C:196:ASN:OD1	1:C:197:THR:N	2.40	0.55
1:C:284:LYS:HD2	1:C:284:LYS:C	2.26	0.55
1:D:221:ALA:O	1:D:222:ALA:HB3	2.05	0.55
1:A:33:SER:HB3	1:A:36:ALA:HB3	1.87	0.55
1:C:222:ALA:CA	1:C:223:SER:CB	2.84	0.55
1:B:65:ARG:NH2	1:B:394:PRO:HG3	2.21	0.55
1:B:409:LYS:CE	1:B:409:LYS:H	2.20	0.54
1:B:293:GLU:HG2	1:B:340:THR:HG22	1.88	0.54
1:C:43:THR:HB	1:C:225:ASN:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LYS:O	1:A:204:GLN:HG2	2.07	0.54
1:C:137:LYS:HD2	1:C:138:GLY:O	2.08	0.54
1:A:272:TYR:OH	1:A:280:ILE:HD13	2.07	0.54
1:D:132:GLN:HE21	1:D:373:ILE:HG12	1.72	0.54
1:A:35:GLU:HB3	1:A:39:ARG:NH1	2.23	0.54
1:C:200:LYS:O	1:C:204:GLN:HG2	2.07	0.54
1:B:121:GLN:HA	1:B:311:SER:O	2.08	0.53
1:C:275:ARG:C	1:C:276:LEU:CD2	2.60	0.53
1:C:370:GLN:HB2	1:C:376:GLY:HA3	1.90	0.53
1:A:300:ASP:HA	1:A:303:LEU:HD12	1.91	0.53
1:A:369:MET:HE1	1:A:375:MET:HB3	1.89	0.53
1:C:159:GLN:HA	1:C:160:ASN:HB3	1.90	0.53
1:C:35:GLU:HG3	1:C:39:ARG:HH12	1.73	0.53
1:C:414:TYR:CE1	1:C:416:GLY:HA3	2.43	0.53
1:C:217:PHE:CZ	1:D:206:MET:HB2	2.44	0.53
1:C:265:PHE:CE1	1:C:325:LYS:HB3	2.44	0.52
1:C:291:SER:OG	1:C:293:GLU:HG3	2.10	0.52
1:B:369:MET:HE2	1:B:375:MET:HG3	1.92	0.52
1:D:347:GLN:HG3	1:D:406:PHE:CD2	2.45	0.52
1:D:65:ARG:NH2	1:D:394:PRO:HG3	2.25	0.52
1:D:169:ALA:HB2	1:D:303:LEU:HD21	1.92	0.52
1:D:47:GLU:OE1	1:D:221:ALA:HB1	2.10	0.52
1:B:178:PRO:HG2	1:C:121:GLN:NE2	2.25	0.52
1:C:114:GLN:HA	1:C:117:LEU:CD1	2.41	0.51
1:B:362:ASP:CB	1:B:365:GLN:NE2	2.73	0.51
1:C:53:LYS:O	1:C:57:THR:OG1	2.20	0.51
1:D:50:LYS:HB2	1:D:149:ASN:ND2	2.25	0.51
1:B:409:LYS:N	1:B:409:LYS:CE	2.73	0.51
1:A:119:GLU:OE1	1:A:119:GLU:N	2.43	0.51
1:A:177:LYS:HD3	1:A:180:ILE:CD1	2.40	0.51
1:A:321:PRO:CG	1:A:359:PHE:O	2.57	0.51
1:C:171:LYS:O	1:C:175:GLU:HG3	2.10	0.51
1:B:209:LEU:HD13	1:C:205:PHE:CD1	2.45	0.51
1:D:165:ASN:OD1	1:D:303:LEU:HD23	2.11	0.51
1:D:217:PHE:O	1:D:220:LEU:HB3	2.11	0.51
1:D:301:LEU:O	1:D:305:LEU:HG	2.11	0.51
1:A:322:VAL:HG13	1:A:373:ILE:HG22	1.92	0.51
1:A:283:LEU:HD22	1:A:286:PHE:CE2	2.46	0.51
1:B:153:LEU:HD11	1:B:180:ILE:HD11	1.93	0.51
1:D:267:ILE:HD11	1:D:271:PHE:CE1	2.45	0.51
1:C:347:GLN:O	1:C:351:GLN:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:TYR:C	1:D:340:THR:HG21	2.32	0.50
1:B:249:ASP:OD2	1:B:385:ARG:NH2	2.39	0.50
1:D:88:GLU:HG3	1:D:236:LEU:HD21	1.93	0.50
1:A:290:LEU:HD12	1:A:291:SER:N	2.27	0.50
1:D:155:SER:O	1:D:159:GLN:OE1	2.30	0.50
1:A:208:GLU:HA	1:A:211:ARG:NH1	2.26	0.50
1:B:51:SER:O	1:B:55:LYS:HG2	2.11	0.49
1:B:153:LEU:HD12	1:B:180:ILE:HD11	1.94	0.49
1:D:99:ILE:HD13	1:D:116:MET:HE1	1.94	0.49
1:D:221:ALA:O	1:D:223:SER:N	2.40	0.49
1:B:196:ASN:OD1	1:B:196:ASN:C	2.50	0.49
1:C:148:PHE:CZ	1:C:153:LEU:HB2	2.48	0.49
1:A:284:LYS:HG2	1:A:329:TYR:CD2	2.48	0.49
1:B:362:ASP:HB3	1:B:365:GLN:NE2	2.27	0.49
1:D:66:PHE:HA	1:D:95:ARG:O	2.13	0.49
1:A:134:PHE:O	1:A:295:SER:HB2	2.13	0.49
1:D:383:PHE:CE2	1:D:387:VAL:HG21	2.47	0.49
1:C:271:PHE:CE1	1:C:275:ARG:HG3	2.48	0.48
1:C:414:TYR:CE1	1:C:416:GLY:N	2.81	0.48
1:D:168:TYR:OH	1:D:172:ARG:HD3	2.13	0.48
1:A:141:SER:OG	1:A:176:MET:O	2.30	0.48
1:C:59:LEU:HB2	1:C:119:GLU:HG2	1.94	0.48
1:D:293:GLU:HA	1:D:340:THR:HG22	1.96	0.48
1:A:369:MET:HA	1:A:375:MET:HA	1.94	0.48
1:B:145:GLN:O	1:B:145:GLN:HG3	2.14	0.48
1:C:222:ALA:HB1	1:C:223:SER:C	2.34	0.48
1:A:77:ARG:HE	1:A:374:HIS:CG	2.31	0.48
1:B:409:LYS:H	1:B:409:LYS:HE3	1.79	0.48
1:A:273:LYS:HA	1:A:277:SER:HB2	1.95	0.48
1:B:43:THR:HG21	1:B:224:ASN:HA	1.96	0.47
1:C:191:LYS:HE2	1:C:193:GLN:OE1	2.15	0.47
1:C:346:TYR:CG	1:C:418:PRO:HB3	2.50	0.47
1:D:221:ALA:C	1:D:223:SER:H	2.17	0.47
1:A:368:PHE:HD2	1:A:369:MET:CE	2.26	0.47
1:B:185:GLN:HG2	1:B:203:ILE:HD11	1.96	0.47
1:C:414:TYR:OH	1:C:420:GLN:O	2.32	0.47
1:B:377:TRP:O	1:B:380:TRP:N	2.48	0.47
1:D:163:ASP:OD1	1:D:165:ASN:HB3	2.15	0.47
1:D:292:TYR:HB2	1:D:340:THR:HG21	1.96	0.47
1:C:199:ASP:O	1:C:203:ILE:HG12	2.15	0.47
1:A:417:THR:CG2	1:A:420:GLN:HB2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:VAL:CG2	1:C:195:LEU:HD11	2.44	0.47
1:D:368:PHE:HE1	1:D:375:MET:HE2	1.80	0.47
1:D:81:LEU:HD22	1:D:381:VAL:CG2	2.45	0.47
1:D:406:PHE:HD1	1:D:411:TRP:CG	2.32	0.47
1:B:323:ASN:HB3	1:B:326:TRP:HB3	1.97	0.46
1:B:377:TRP:O	1:B:379:GLY:N	2.48	0.46
1:D:409:LYS:HA	1:D:412:SER:HB3	1.97	0.46
1:A:32:TYR:HE1	1:A:61:ASP:HA	1.80	0.46
1:C:134:PHE:CD1	1:C:134:PHE:N	2.84	0.46
1:D:40:SER:HA	1:D:43:THR:CG2	2.46	0.46
1:C:414:TYR:CE1	1:C:416:GLY:CA	2.99	0.46
1:A:41:ALA:HA	1:A:97:TYR:CD2	2.51	0.46
1:A:322:VAL:O	1:A:323:ASN:C	2.52	0.46
1:B:34:TYR:CZ	1:B:38:LYS:HD2	2.51	0.46
1:C:216:LEU:HD12	1:C:216:LEU:O	2.16	0.46
1:D:134:PHE:HD2	1:D:298:TYR:CE1	2.34	0.46
1:C:260:THR:O	1:C:260:THR:CG2	2.61	0.46
1:A:34:TYR:CE2	1:A:38:LYS:HD2	2.51	0.46
1:B:357:ALA:HB1	1:B:359:PHE:CE1	2.51	0.45
1:C:275:ARG:O	1:C:276:LEU:CD2	2.62	0.45
1:A:39:ARG:HG2	1:A:228:TYR:HB3	1.98	0.45
1:B:106:SER:HA	1:B:109:GLN:HB2	1.97	0.45
1:B:285:GLY:HA2	1:B:330:THR:O	2.16	0.45
1:B:111:LEU:HD21	1:B:173:ILE:HD11	1.98	0.45
1:A:405:ARG:HB3	1:A:421:PHE:HE2	1.81	0.45
1:B:213:GLU:O	1:B:214:ASP:C	2.52	0.45
1:B:380:TRP:HA	1:B:380:TRP:CE3	2.52	0.45
1:B:82:HIS:HE1	1:B:98:PHE:CZ	2.35	0.45
1:B:87:ALA:HA	1:B:92:ARG:HD2	1.98	0.45
1:C:406:PHE:HD1	1:C:411:TRP:CE2	2.35	0.45
1:D:157:LEU:HA	1:D:157:LEU:HD23	1.78	0.45
1:B:101:GLN:HB3	1:B:147:PHE:CE1	2.52	0.45
1:C:159:GLN:HA	1:C:160:ASN:CB	2.44	0.45
1:D:220:LEU:HG	1:D:220:LEU:O	2.16	0.45
1:C:72:SER:OG	1:C:73:SER:N	2.50	0.45
1:A:308:PHE:CD2	1:A:315:VAL:HG21	2.52	0.45
1:A:322:VAL:HG23	1:A:337:TYR:CZ	2.52	0.44
1:B:109:GLN:HA	1:B:109:GLN:OE1	2.17	0.44
1:B:196:ASN:O	1:B:199:ASP:HB2	2.17	0.44
1:D:162:THR:HG21	1:D:193:GLN:O	2.16	0.44
1:B:77:ARG:NE	1:B:371:ASP:OD2	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LEU:HB2	1:B:300:ASP:OD2	2.18	0.44
1:B:376:GLY:O	1:B:377:TRP:C	2.56	0.44
1:C:278:LYS:HD3	1:C:278:LYS:H	1.83	0.44
1:D:278:LYS:HG3	1:D:279:LYS:HG3	1.99	0.44
1:D:324:SER:OG	1:D:363:GLY:C	2.56	0.44
1:A:43:THR:HG23	1:A:225:ASN:ND2	2.32	0.44
1:C:327:MET:CE	1:C:332:LEU:HD22	2.47	0.44
1:D:72:SER:OG	1:D:73:SER:N	2.49	0.44
1:D:353:PHE:CE1	1:D:400:TYR:CE1	3.05	0.44
1:A:34:TYR:CD1	1:A:64:HIS:CG	3.05	0.44
1:B:380:TRP:O	1:B:383:PHE:HB3	2.17	0.44
1:A:44:LEU:HD21	1:A:98:PHE:HB3	2.00	0.44
1:A:148:PHE:HA	1:A:152:GLN:OE1	2.17	0.44
1:C:46:ASN:OD1	1:C:146:GLN:HB3	2.17	0.44
1:C:196:ASN:O	1:C:199:ASP:HB2	2.18	0.44
1:C:286:PHE:CG	1:C:286:PHE:O	2.71	0.44
1:D:221:ALA:C	1:D:223:SER:N	2.72	0.44
1:A:59:LEU:HB2	1:A:119:GLU:HG2	2.00	0.44
1:A:290:LEU:HD12	1:A:291:SER:H	1.83	0.44
1:B:72:SER:O	1:B:74:GLU:N	2.51	0.44
1:B:185:GLN:O	1:B:189:VAL:HG23	2.18	0.44
1:D:86:LEU:HD12	1:D:384:ASP:OD2	2.18	0.44
1:D:89:LYS:HE2	1:D:239:LEU:HB2	2.00	0.44
1:D:291:SER:HA	1:D:336:MET:HG3	2.00	0.44
1:A:288:LYS:HG2	1:A:289:ASN:N	2.32	0.43
1:D:55:LYS:HD2	1:D:116:MET:HE1	2.00	0.43
1:A:280:ILE:HA	1:A:283:LEU:HD12	2.00	0.43
1:A:315:VAL:O	1:A:355:ASN:HB2	2.18	0.43
1:A:403:ASN:HB3	1:A:406:PHE:CE2	2.54	0.43
1:C:113:MET:O	1:C:117:LEU:HD13	2.18	0.43
1:C:127:TYR:O	1:C:317:PHE:HA	2.18	0.43
1:C:351:GLN:OE1	1:C:402:LEU:HA	2.19	0.43
1:D:134:PHE:N	1:D:134:PHE:CD1	2.87	0.43
1:D:186:LEU:HD23	1:D:186:LEU:HA	1.85	0.43
1:A:44:LEU:HD21	1:A:98:PHE:CB	2.48	0.43
1:C:414:TYR:OH	1:C:417:THR:O	2.36	0.43
1:C:158:SER:HB3	1:C:159:GLN:NE2	2.34	0.43
1:A:136:LYS:HD2	1:A:136:LYS:HA	1.82	0.43
1:A:417:THR:HG23	1:A:420:GLN:HB2	2.01	0.43
1:B:124:THR:HA	1:B:314:ASN:O	2.18	0.43
1:C:179:GLU:OE2	1:D:47:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:PRO:HB3	1:D:359:PHE:O	2.18	0.43
1:C:248:LEU:HD23	1:C:248:LEU:HA	1.79	0.43
1:C:301:LEU:O	1:C:305:LEU:HG	2.18	0.43
1:A:114:GLN:HA	1:A:117:LEU:CD1	2.49	0.43
1:D:129:LEU:HD11	1:D:348:LEU:HD11	2.01	0.43
1:A:321:PRO:HB3	1:A:360:SER:C	2.40	0.43
1:C:47:GLU:OE1	1:D:177:LYS:NZ	2.50	0.43
1:C:222:ALA:CB	1:C:224:ASN:CG	2.87	0.43
1:D:157:LEU:HB3	1:D:203:ILE:HD13	2.00	0.43
1:A:376:GLY:HA2	1:A:380:TRP:CD1	2.54	0.42
1:B:292:TYR:HB2	1:B:340:THR:HG21	2.01	0.42
1:C:261:LYS:HE3	1:C:261:LYS:HB3	1.82	0.42
1:D:105:ALA:HB1	1:D:297:GLU:OE2	2.19	0.42
1:B:195:LEU:HD23	1:B:195:LEU:HA	1.73	0.42
1:C:85:VAL:HG12	1:C:239:LEU:HD11	2.01	0.42
1:A:208:GLU:CD	1:A:212:ARG:NH1	2.72	0.42
1:A:321:PRO:CD	1:A:359:PHE:O	2.65	0.42
1:B:122:ASN:ND2	1:B:312:ASN:HB3	2.34	0.42
1:C:42:VAL:O	1:C:44:LEU:HD12	2.19	0.42
1:C:221:ALA:CA	1:C:222:ALA:CB	2.88	0.42
1:D:300:ASP:O	1:D:303:LEU:HB2	2.20	0.42
1:A:145:GLN:OE1	1:A:177:LYS:HE3	2.19	0.42
1:C:380:TRP:HA	1:C:380:TRP:CE3	2.55	0.42
1:B:308:PHE:CE2	1:B:315:VAL:HG21	2.54	0.42
1:C:66:PHE:HA	1:C:95:ARG:O	2.19	0.42
1:C:113:MET:O	1:C:117:LEU:CD1	2.67	0.42
1:C:40:SER:HA	1:C:43:THR:HG23	2.02	0.42
1:D:422:LYS:HA	1:D:423:ASP:HA	1.65	0.42
1:A:92:ARG:C	1:A:94:TYR:H	2.23	0.41
1:C:79:ASP:O	1:C:85:VAL:HG21	2.20	0.41
1:C:158:SER:O	1:C:159:GLN:HG3	2.20	0.41
1:C:196:ASN:CG	1:C:198:VAL:HG12	2.40	0.41
1:D:78:PHE:HD2	1:D:231:LYS:HD3	1.85	0.41
1:C:128:VAL:HG22	1:C:318:VAL:HB	2.01	0.41
1:C:303:LEU:HD23	1:C:303:LEU:HA	1.93	0.41
1:C:409:LYS:H	1:C:409:LYS:HG2	1.61	0.41
1:D:345:ARG:NH1	1:D:358:ASP:OD2	2.47	0.41
1:B:153:LEU:CD2	1:B:157:LEU:HD11	2.50	0.41
1:B:168:TYR:CZ	1:B:299:GLY:HA3	2.56	0.41
1:B:326:TRP:CD1	1:B:372:THR:HB	2.55	0.41
1:C:163:ASP:OD1	1:C:165:ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:SER:O	1:A:74:GLU:N	2.53	0.41
1:D:321:PRO:O	1:D:321:PRO:HG2	2.20	0.41
1:C:298:TYR:CZ	1:C:343:LYS:HD3	2.56	0.41
1:C:336:MET:O	1:C:340:THR:HG23	2.20	0.41
1:C:371:ASP:CB	1:C:374:HIS:HB2	2.45	0.41
1:D:409:LYS:H	1:D:409:LYS:CD	2.18	0.41
1:B:43:THR:O	1:B:227:ASN:ND2	2.53	0.41
1:C:59:LEU:CB	1:C:119:GLU:HG2	2.51	0.41
1:C:108:ASN:ND2	1:C:147:PHE:HB2	2.36	0.41
1:A:320:PRO:HG2	1:A:320:PRO:O	2.20	0.41
1:A:321:PRO:HD2	1:A:375:MET:HE1	2.01	0.41
1:B:168:TYR:OH	1:B:299:GLY:HA3	2.21	0.41
1:C:157:LEU:HD23	1:C:157:LEU:HA	1.85	0.41
1:C:422:LYS:H	1:C:422:LYS:HG2	1.56	0.41
1:A:364:ASP:OD1	1:A:364:ASP:N	2.54	0.41
1:C:263:ASN:OD1	1:C:265:PHE:HB2	2.21	0.41
1:D:81:LEU:O	1:D:380:TRP:HB3	2.21	0.41
1:C:70:PHE:HB2	1:C:127:TYR:CD2	2.56	0.41
1:C:284:LYS:CD	1:C:284:LYS:C	2.85	0.41
1:B:114:GLN:HA	1:B:117:LEU:HD13	2.02	0.40
1:C:275:ARG:CB	1:C:276:LEU:HD23	2.52	0.40
1:D:129:LEU:HD13	1:D:344:ILE:HG21	2.04	0.40
1:B:249:ASP:O	1:B:253:VAL:HG13	2.21	0.40
1:C:376:GLY:O	1:C:379:GLY:N	2.52	0.40
1:A:245:TYR:HB3	1:A:385:ARG:NH2	2.37	0.40
1:A:65:ARG:NH1	1:A:94:TYR:HB3	2.36	0.40
1:A:276:LEU:HD13	1:A:326:TRP:CH2	2.56	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	389/397 (98%)	361 (93%)	28 (7%)	0	100	100
1	B	390/397 (98%)	362 (93%)	28 (7%)	0	100	100
1	C	385/397 (97%)	353 (92%)	32 (8%)	0	100	100
1	D	390/397 (98%)	358 (92%)	32 (8%)	0	100	100
All	All	1554/1588 (98%)	1434 (92%)	120 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	345/350 (99%)	334 (97%)	11 (3%)	39	71
1	B	346/350 (99%)	335 (97%)	11 (3%)	39	71
1	C	343/350 (98%)	326 (95%)	17 (5%)	24	57
1	D	343/350 (98%)	326 (95%)	17 (5%)	24	57
All	All	1377/1400 (98%)	1321 (96%)	56 (4%)	30	64

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	GLU
1	A	141	SER
1	A	158	SER
1	A	161	GLN
1	A	184	SER
1	A	254	ARG
1	A	284	LYS
1	A	288	LYS
1	A	329	TYR
1	A	335	ASP
1	A	422	LYS
1	B	46	ASN
1	B	77	ARG

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Mol	Chain	Res	Type
1	B	161	GLN
1	B	196	ASN
1	B	197	THR
1	B	212	ARG
1	B	213	GLU
1	B	342	SER
1	B	380	TRP
1	B	392	SER
1	B	409	LYS
1	C	32	TYR
1	C	35	GLU
1	C	102	ARG
1	C	136	LYS
1	C	137	LYS
1	C	160	ASN
1	C	171	LYS
1	C	215	SER
1	C	223	SER
1	C	230	LYS
1	C	276	LEU
1	C	278	LYS
1	C	284	LYS
1	C	324	SER
1	C	371	ASP
1	C	380	TRP
1	C	410	ASP
1	D	33	SER
1	D	40	SER
1	D	102	ARG
1	D	137	LYS
1	D	162	THR
1	D	282	LYS
1	D	286	PHE
1	D	361	LYS
1	D	364	ASP
1	D	365	GLN
1	D	378	LYS
1	D	392	SER
1	D	403	ASN
1	D	409	LYS
1	D	412	SER
1	D	423	ASP

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Mol	Chain	Res	Type
1	D	424	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	146	GLN
1	A	393	ASN
1	A	420	GLN
1	B	62	GLN
1	B	122	ASN
1	B	365	GLN
1	C	46	ASN
1	C	334	GLN
1	C	365	GLN
1	D	161	GLN
1	D	334	GLN
1	D	365	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 ⓘ

4 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

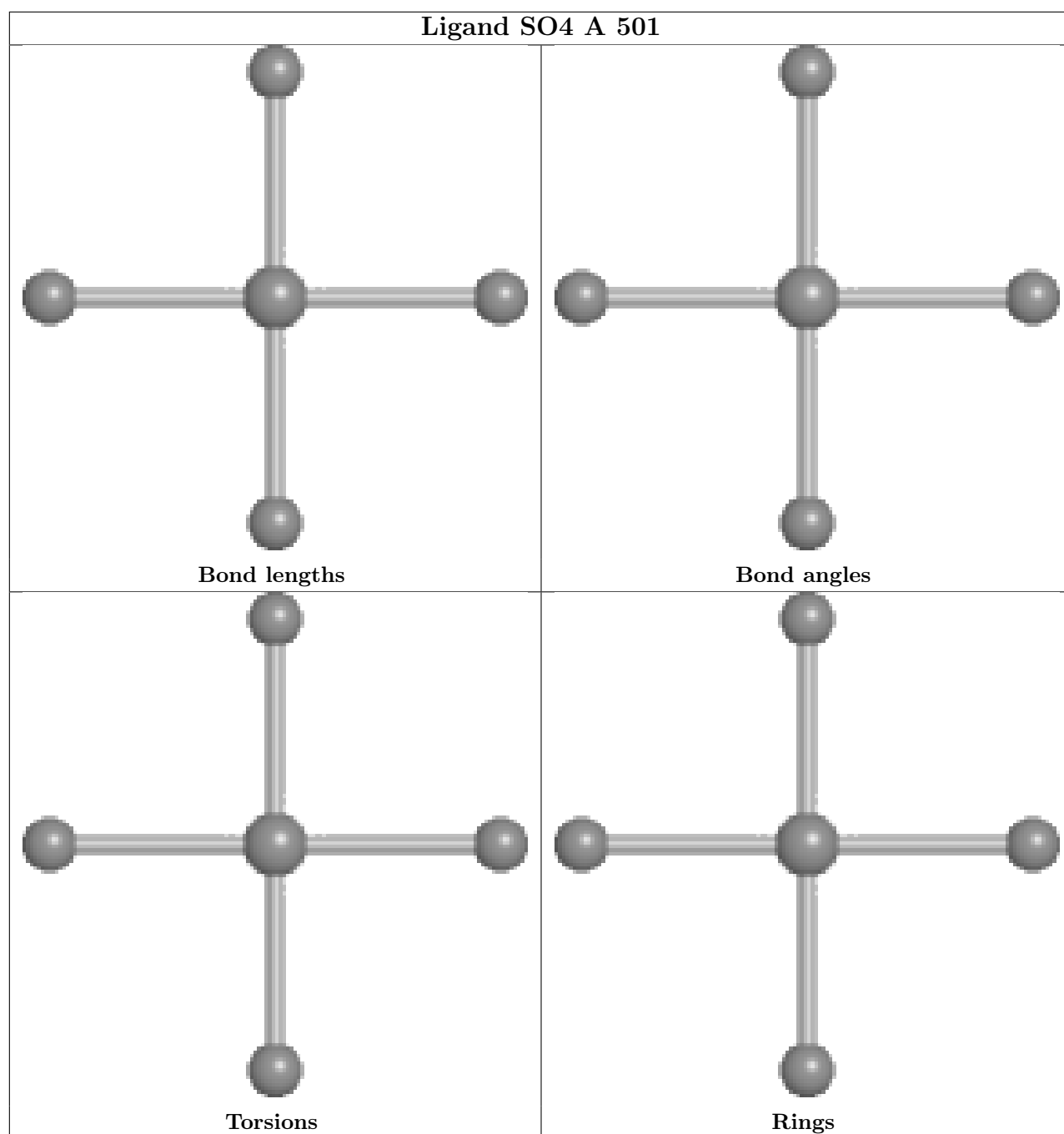
There are no chirality outliers.

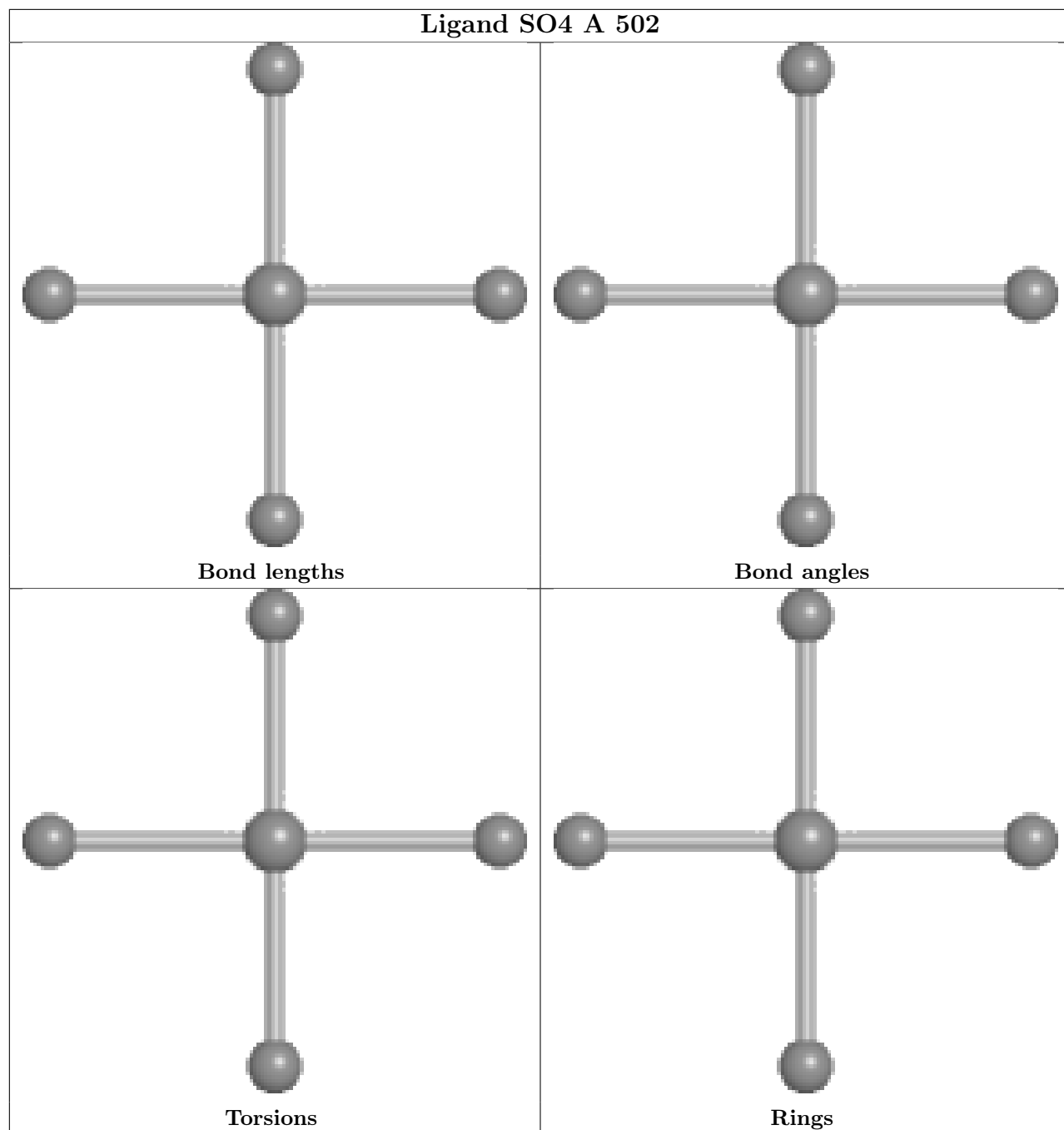
There are no torsion outliers.

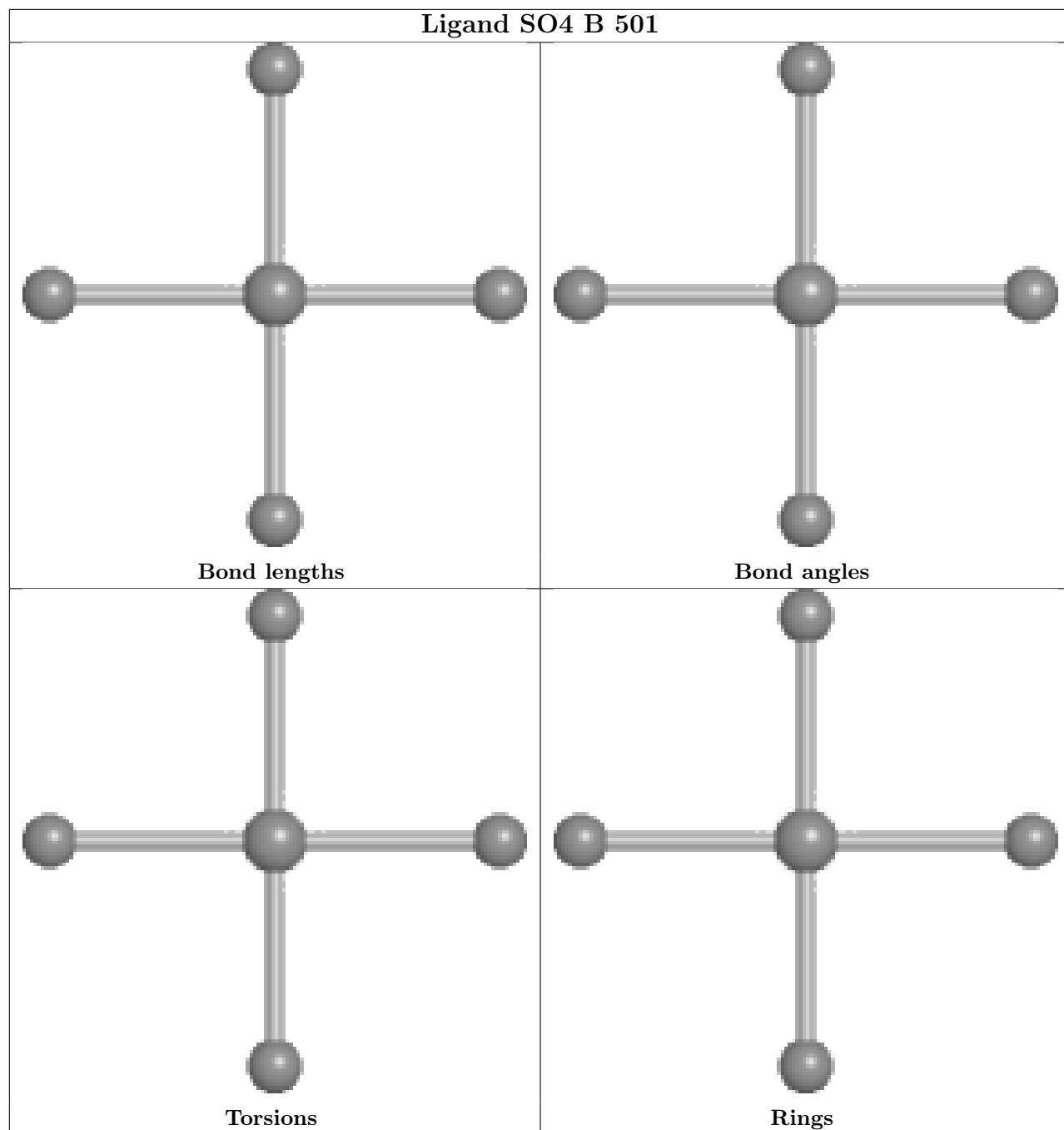
There are no ring outliers.

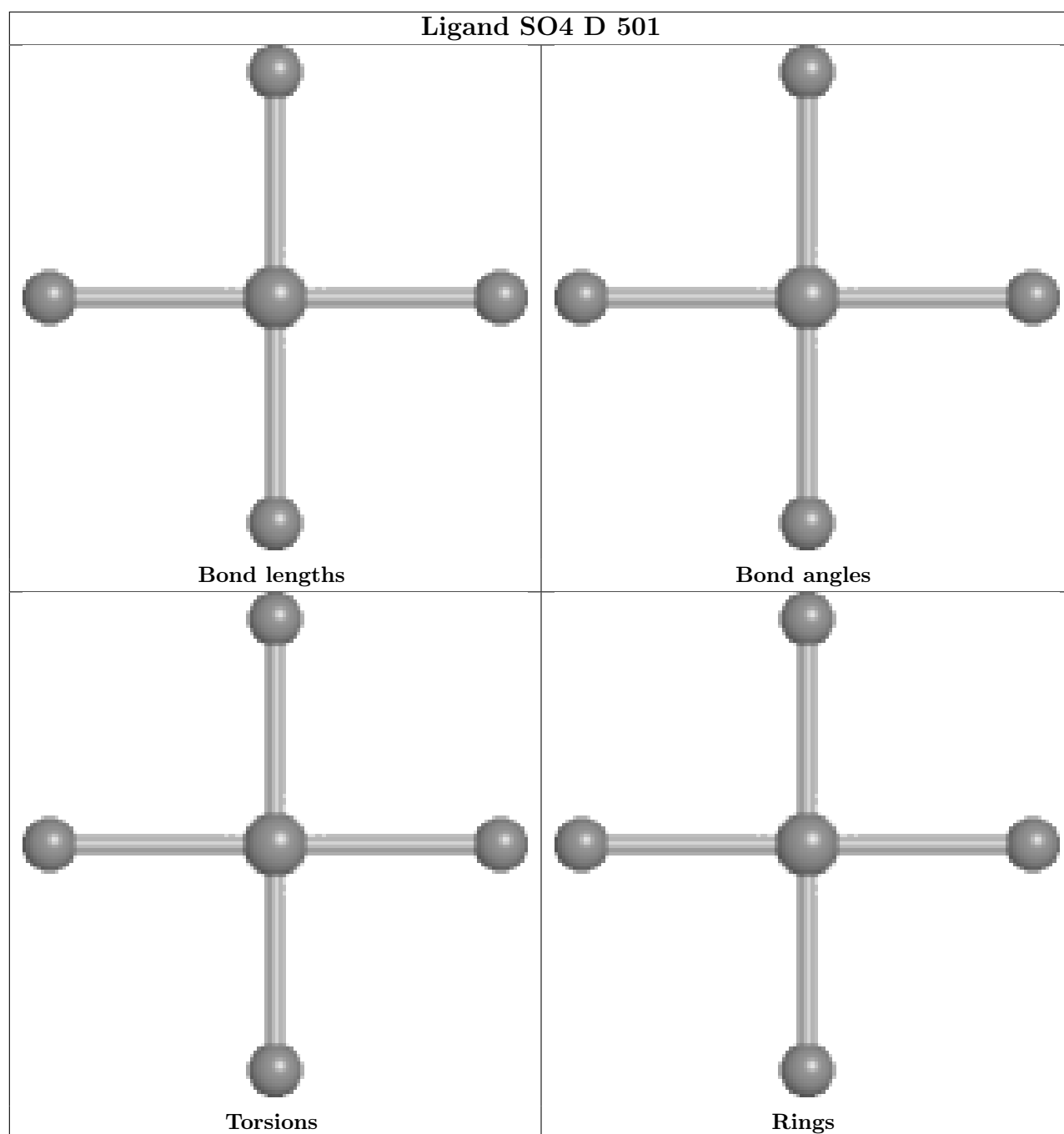
No monomer is involved in short contacts.

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	391/397 (98%)	0.01	7 (1%) 68 51	37, 54, 78, 97	0
1	B	392/397 (98%)	-0.14	0 100 100	37, 52, 73, 87	0
1	C	389/397 (97%)	0.12	17 (4%) 34 21	38, 65, 99, 119	0
1	D	392/397 (98%)	0.19	16 (4%) 37 24	38, 64, 95, 104	0
All	All	1564/1588 (98%)	0.05	40 (2%) 56 39	37, 57, 92, 119	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	220	LEU	5.0
1	D	424	GLU	4.2
1	D	262	SER	4.0
1	D	283	LEU	4.0
1	C	277	SER	3.9
1	C	286	PHE	3.8
1	A	329	TYR	3.8
1	A	262	SER	3.7
1	A	258	ALA	3.6
1	C	282	LYS	3.6
1	D	337	TYR	3.4
1	C	160	ASN	3.2
1	D	259	HIS	3.1
1	D	258	ALA	3.1
1	D	326	TRP	3.1
1	D	330	THR	3.0
1	C	279	LYS	2.9
1	C	413	GLY	2.8
1	C	326	TRP	2.7
1	D	273	LYS	2.7
1	C	265	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	418	PRO	2.6
1	A	261	LYS	2.6
1	C	161	GLN	2.5
1	C	346	TYR	2.5
1	D	277	SER	2.4
1	D	282	LYS	2.4
1	C	420	GLN	2.3
1	C	278	LYS	2.3
1	C	276	LEU	2.3
1	D	217	PHE	2.2
1	D	221	ALA	2.2
1	D	278	LYS	2.2
1	C	281	GLY	2.1
1	A	276	LEU	2.1
1	C	202	TYR	2.1
1	A	260	THR	2.1
1	A	399	SER	2.0
1	D	222	ALA	2.0
1	C	289	ASN	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](#)

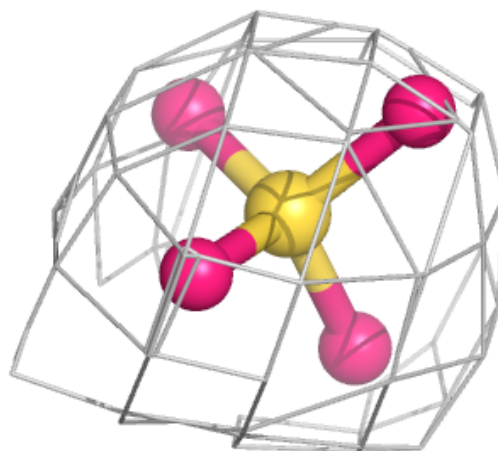
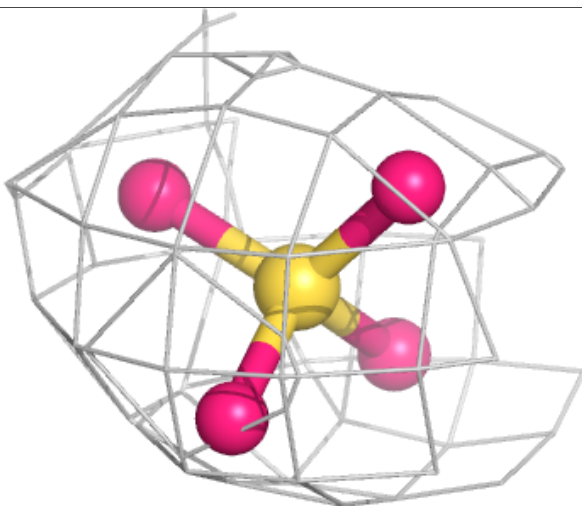
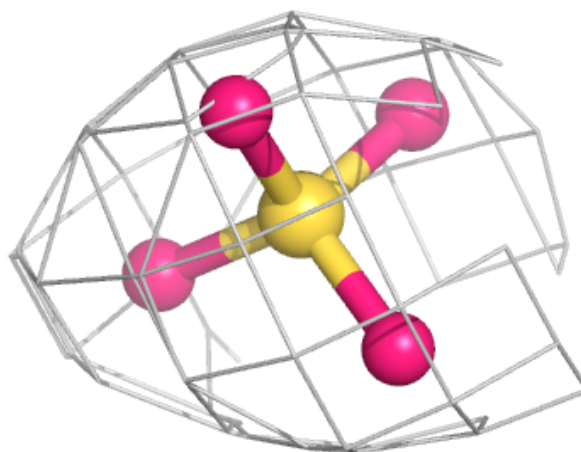
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	D	501	5/5	0.88	0.20	76,79,93,96	0
2	SO4	A	501	5/5	0.95	0.15	56,56,73,73	0
2	SO4	B	501	5/5	0.96	0.17	51,53,56,78	0
2	SO4	A	502	5/5	0.96	0.20	62,71,79,90	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.

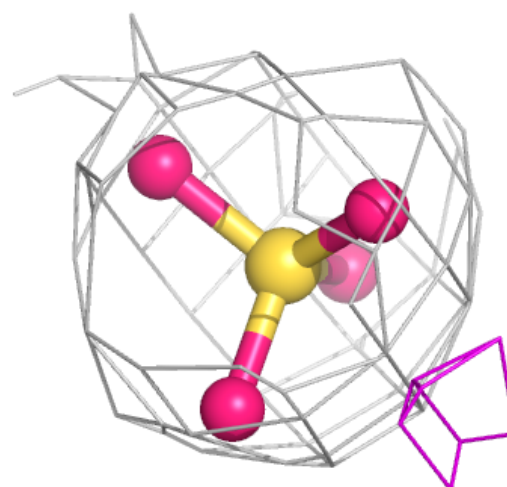
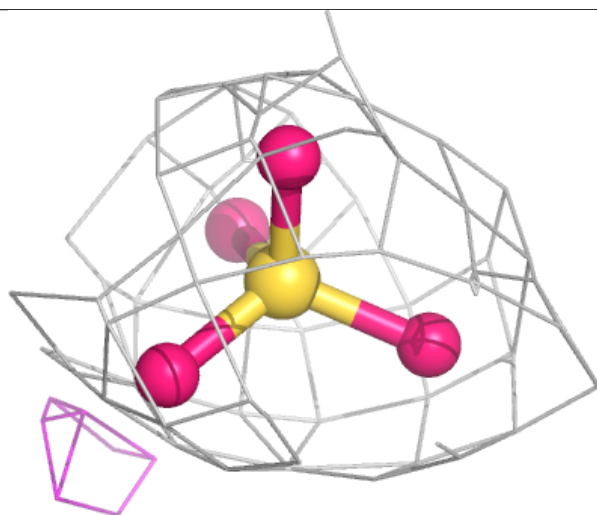
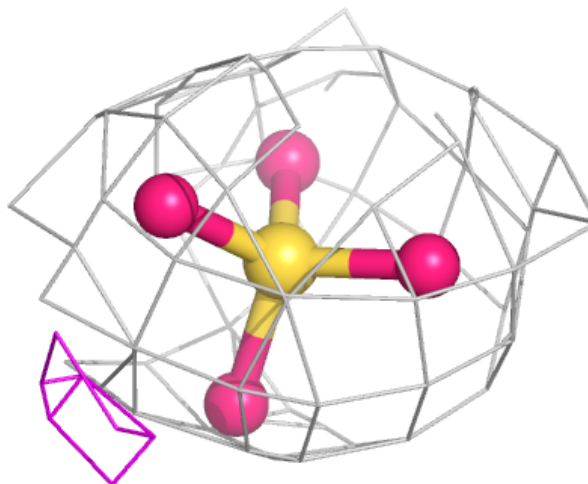
Electron density around SO4 D 501:

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



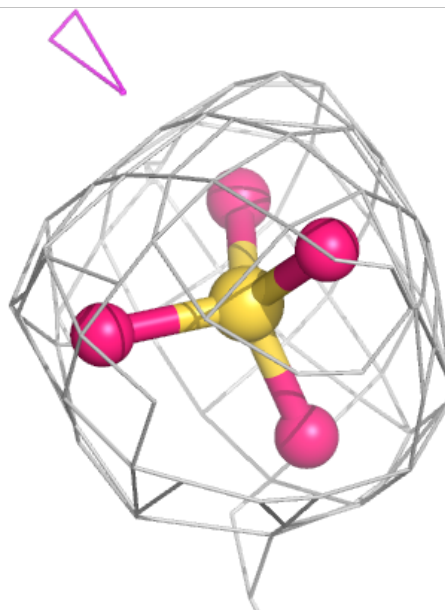
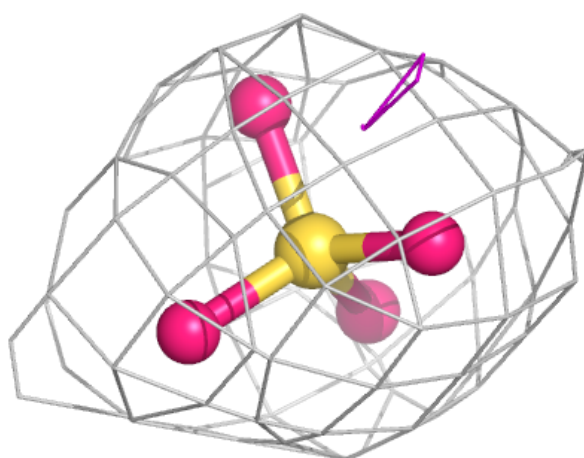
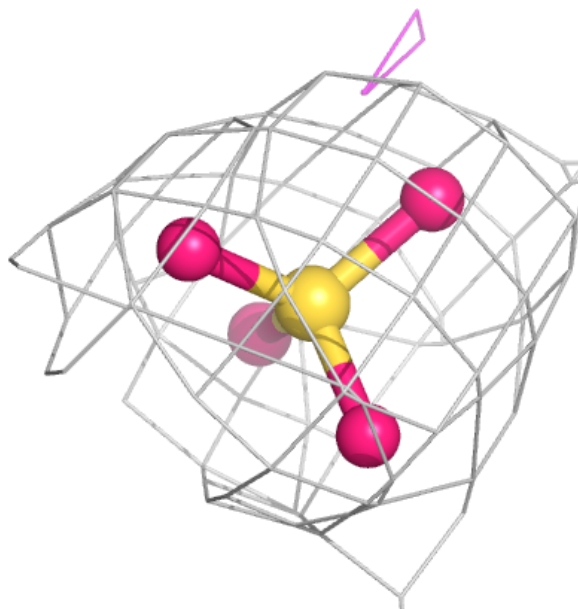
Electron density around SO4 A 501:

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



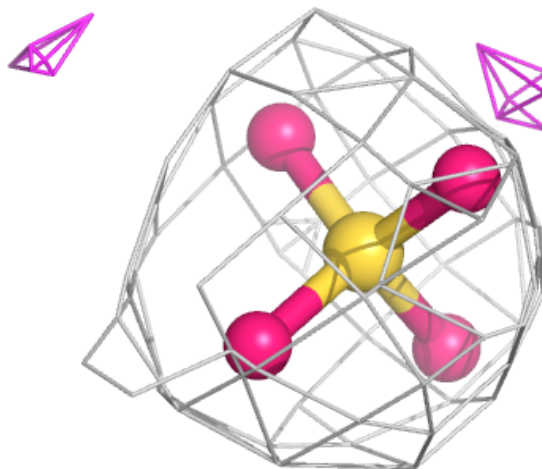
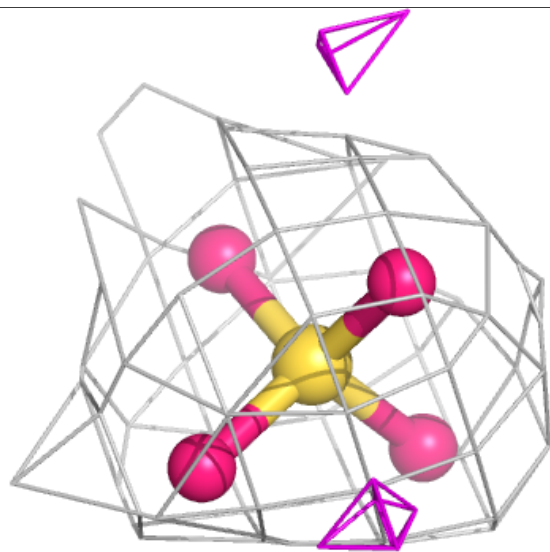
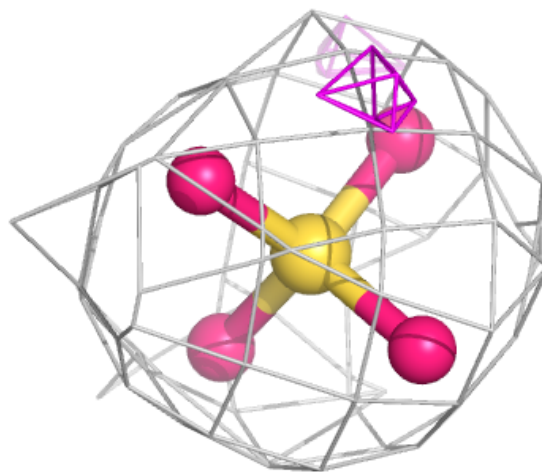
Electron density around SO4 B 501:

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



Electron density around SO4 A 502:

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.