



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:11 PM UTC

PDB ID : 8DI0 / pdb_00008di0
Title : Bfo2290: Tannerella forsythia chondroitin sulfate A sulfatase
Authors : Suits, M.D.L.
Deposited on : 2022-06-28
Resolution : 2.85 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

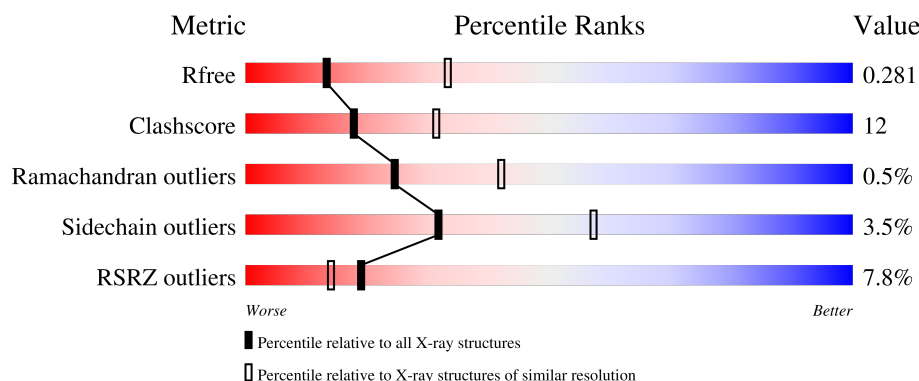
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	516	6% 62% 23% • 14%
1	B	516	10% 53% 28% • 17%
1	C	516	4% 62% 27% • 10%

2 Entry composition [i](#)

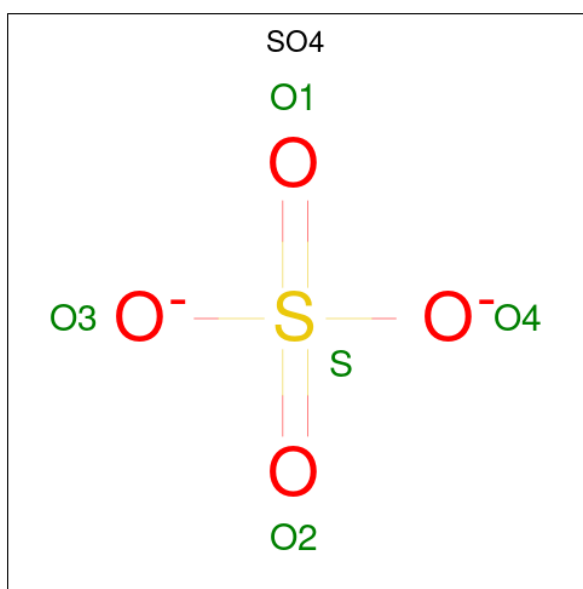
There are 3 unique types of molecules in this entry. The entry contains 10773 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Arylsulfatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3563	2259	618	667	19			
1	B	426	Total	C	N	O	S	0	0	0
			3441	2180	600	642	19			
1	C	463	Total	C	N	O	S	0	0	0
			3745	2370	650	706	19			

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



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

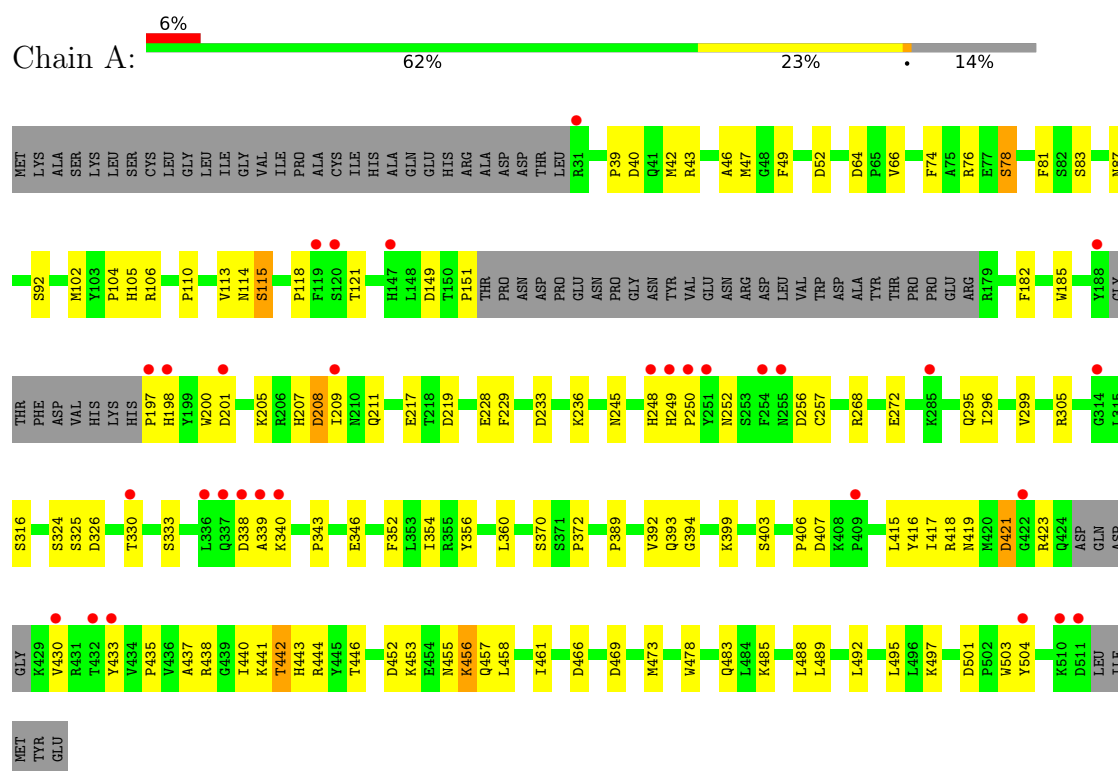
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total 5	O 5	0	0
3	B	10	Total 10	O 10	0	0
3	C	4	Total 4	O 4	0	0

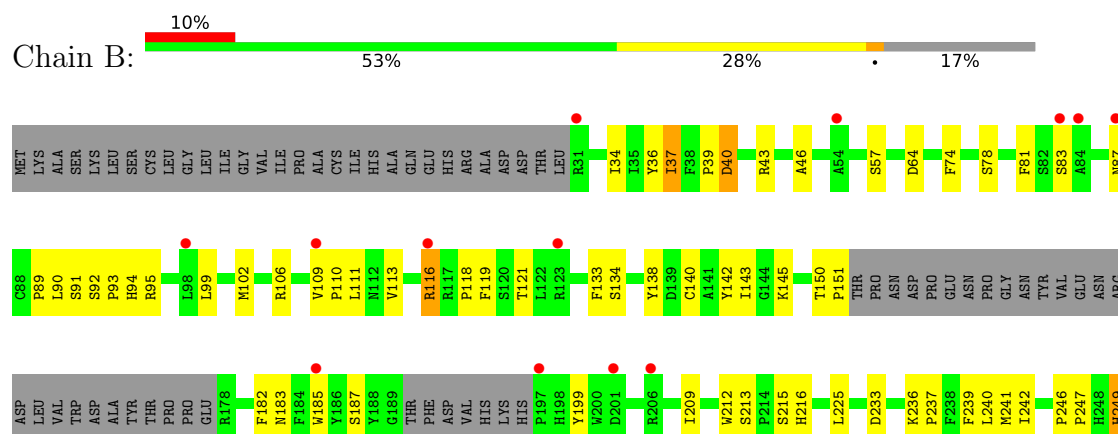
3 Residue-property plots [i](#)

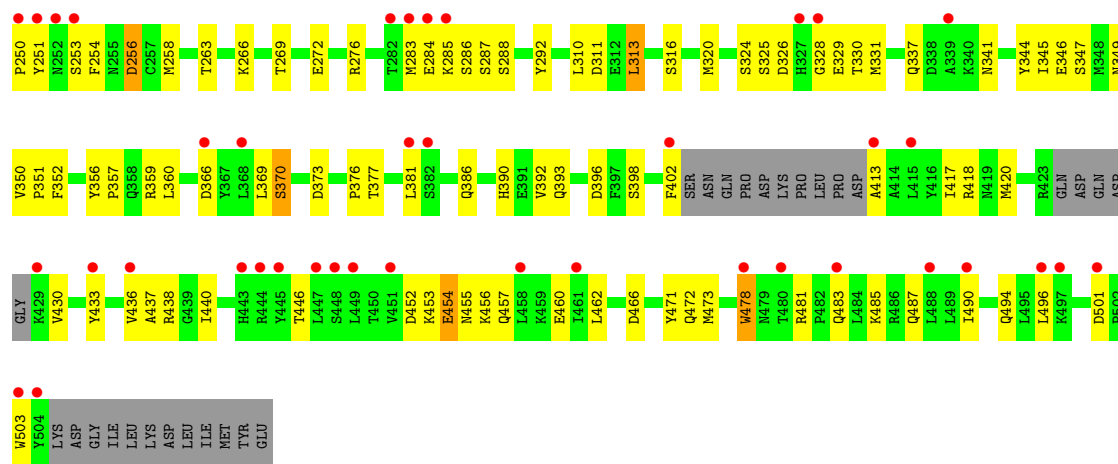
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Arylsulfatase

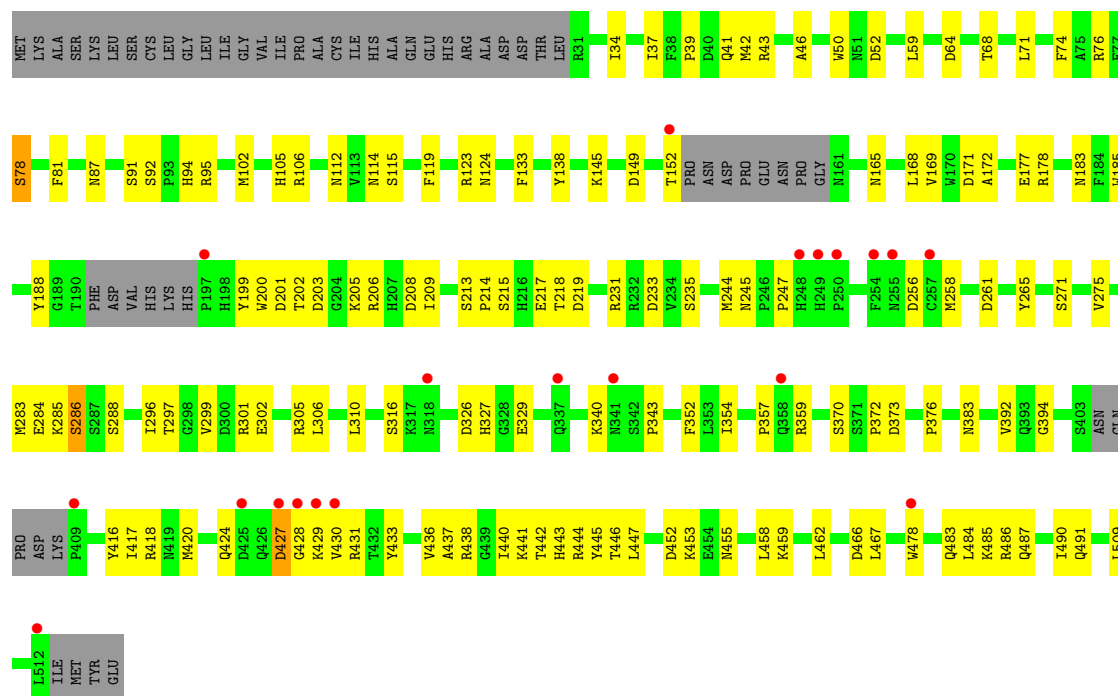


• Molecule 1: Arylsulfatase





• Molecule 1: Arylsulfatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.18Å 121.11Å 144.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.32 – 2.85 48.32 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.32-2.85) 99.9 (48.32-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.222 , 0.281 0.222 , 0.281	Depositor DCC
R_{free} test set	2355 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.3	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	0.92	EDS
Total number of atoms	10773	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: 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	0.17	0/3662	0.40	0/4971
1	B	0.17	0/3535	0.44	0/4794
1	C	0.14	0/3848	0.34	0/5225
All	All	0.16	0/11045	0.40	0/14990

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	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	116	ARG	Sidechain
1	B	454	GLU	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	3563	0	3409	71	0
1	B	3441	0	3293	100	0
1	C	3745	0	3579	88	0
2	B	5	0	0	1	0
3	A	5	0	0	0	0
3	B	10	0	0	1	0
3	C	4	0	0	2	0
All	All	10773	0	10281	258	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 12.

All (258) 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:456:LYS:H	1:A:456:LYS:HD3	1.47	0.79
1:C:183:ASN:ND2	3:C:601:HOH:O	2.14	0.78
1:B:452:ASP:HB3	1:B:455:ASN:HB3	1.64	0.77
1:A:418:ARG:HB3	1:A:437:ALA:HB3	1.66	0.77
1:B:102:MET:HE3	1:B:106:ARG:HB3	1.65	0.76
1:B:418:ARG:HB3	1:B:437:ALA:HB3	1.67	0.75
1:C:37:ILE:HD11	1:C:306:LEU:HD12	1.69	0.74
1:B:99:LEU:HD21	1:B:241:MET:HE1	1.70	0.74
1:A:421:ASP:OD1	1:A:421:ASP:N	2.21	0.73
1:C:452:ASP:OD2	1:C:455:ASN:ND2	2.22	0.72
1:B:81:PHE:HB2	1:B:352:PHE:HB3	1.72	0.70
1:B:283:MET:HG3	1:B:285:LYS:H	1.57	0.70
1:B:118:PRO:HA	1:B:150:THR:HG21	1.74	0.69
1:C:124:ASN:OD1	1:C:178:ARG:NH1	2.24	0.69
1:B:325:SER:HB3	1:B:351:PRO:HD2	1.75	0.69
1:C:105:HIS:ND1	3:C:602:HOH:O	2.26	0.68
1:A:102:MET:HG2	1:A:393:GLN:HG3	1.75	0.68
1:A:440:ILE:HG23	1:A:492:LEU:HD13	1.75	0.67
1:C:41:GLN:HG3	1:C:327:HIS:CE1	2.30	0.67
1:C:203:ASP:OD2	1:C:231:ARG:NH2	2.28	0.67
1:B:283:MET:SD	1:B:284:GLU:N	2.68	0.67
1:A:52:ASP:OD2	1:A:76:ARG:NH2	2.28	0.66
1:A:219:ASP:OD1	1:A:305:ARG:NH2	2.25	0.66
1:B:142:TYR:OH	1:B:145:LYS:O	2.13	0.66
1:A:121:THR:HG23	1:A:149:ASP:HA	1.77	0.66
1:B:481:ARG:HB2	1:B:483:GLN:HE22	1.61	0.66
1:A:81:PHE:HB2	1:A:352:PHE:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:ARG:HB3	1:C:437:ALA:HB3	1.77	0.65
1:C:441:LYS:NZ	1:C:466:ASP:OD2	2.27	0.64
1:C:302:GLU:OE1	1:C:305:ARG:NH1	2.29	0.64
1:A:46:ALA:HA	1:A:64:ASP:HB2	1.79	0.64
1:A:201:ASP:HB2	1:A:205:LYS:HB2	1.78	0.64
1:C:81:PHE:HB2	1:C:352:PHE:HB3	1.80	0.64
1:C:427:ASP:OD1	1:C:427:ASP:N	2.30	0.64
1:C:420:MET:HE3	1:C:436:VAL:HG11	1.80	0.63
1:A:441:LYS:NZ	1:A:466:ASP:OD2	2.31	0.63
1:C:283:MET:O	1:C:286:SER:OG	2.16	0.63
1:C:74:PHE:O	1:C:78:SER:OG	2.12	0.63
1:B:373:ASP:O	1:B:377:THR:OG1	2.16	0.63
1:A:228:GLU:HA	1:C:258:MET:HE3	1.79	0.63
1:C:376:PRO:HG3	1:C:392:VAL:HG11	1.80	0.62
1:C:442:THR:HG23	1:C:445:TYR:H	1.65	0.62
1:C:428:GLY:O	1:C:431:ARG:NH1	2.33	0.61
1:B:102:MET:HB3	1:B:393:GLN:HG3	1.83	0.61
1:C:285:LYS:O	1:C:288:SER:OG	2.17	0.61
1:A:330:THR:HA	1:A:346:GLU:HB3	1.83	0.61
1:B:471:TYR:HB2	1:B:473:MET:HE2	1.82	0.61
1:B:359:ARG:HD3	1:B:402:PHE:HE1	1.66	0.60
1:A:443:HIS:HB2	1:A:444:ARG:HD3	1.82	0.60
1:A:415:LEU:HG	1:A:495:LEU:HD23	1.83	0.60
1:A:455:ASN:O	1:A:457:GLN:N	2.35	0.60
1:A:483:GLN:OE1	1:A:483:GLN:N	2.32	0.59
1:B:345:ILE:HG13	1:B:349:ASN:HB2	1.84	0.59
1:B:356:TYR:HB3	1:B:360:LEU:HB2	1.83	0.59
1:A:249:HIS:ND1	1:A:250:PRO:HD3	2.17	0.59
1:A:87:ASN:HD21	1:A:370:SER:HB3	1.67	0.58
1:B:151:PRO:O	3:B:701:HOH:O	2.17	0.58
1:A:209:ILE:HG13	1:A:211:GLN:H	1.68	0.58
1:B:199:TYR:HH	1:B:213:SER:HG	1.51	0.58
1:B:478:TRP:HB2	1:B:485:LYS:HB2	1.85	0.58
1:A:104:PRO:HB3	1:A:110:PRO:HA	1.86	0.58
1:A:421:ASP:HB3	1:A:430:VAL:HG11	1.85	0.58
1:A:74:PHE:O	1:A:78:SER:OG	2.22	0.57
1:A:423:ARG:HA	1:A:430:VAL:HG22	1.85	0.57
1:A:201:ASP:OD2	1:A:207:HIS:NE2	2.38	0.56
1:A:356:TYR:HB3	1:A:360:LEU:HB2	1.87	0.56
1:B:74:PHE:O	1:B:78:SER:OG	2.18	0.56
1:C:92:SER:HB2	1:C:112:ASN:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:PRO:HG2	1:C:256:ASP:HB3	1.88	0.56
1:B:247:PRO:HB2	1:B:256:ASP:HB3	1.88	0.56
1:B:487:GLN:O	1:B:490:ILE:HG13	2.06	0.56
1:B:34:ILE:HG22	1:B:320:MET:HG2	1.88	0.56
1:C:233:ASP:OD1	1:C:235:SER:OG	2.22	0.55
1:C:453:LYS:HE3	1:C:459:LYS:NZ	2.21	0.55
1:C:41:GLN:HG3	1:C:327:HIS:HE1	1.70	0.55
1:B:251:TYR:CZ	1:B:285:LYS:HA	2.43	0.54
1:C:52:ASP:OD2	1:C:76:ARG:NH2	2.37	0.54
1:C:188:TYR:HB2	1:C:199:TYR:CE2	2.42	0.54
1:B:43:ARG:NH1	1:B:330:THR:O	2.40	0.54
1:C:261:ASP:CG	1:C:301:ARG:HH21	2.16	0.54
1:C:105:HIS:CD2	1:C:106:ARG:HG2	2.43	0.54
1:B:249:HIS:HB2	1:B:250:PRO:HD2	1.90	0.53
1:C:39:PRO:HG3	1:C:299:VAL:HG11	1.89	0.53
1:A:42:MET:HE3	1:A:296:ILE:HG23	1.91	0.53
1:B:81:PHE:CE2	1:B:369:LEU:HD12	2.43	0.53
1:B:496:LEU:HD12	1:B:501:ASP:HB3	1.91	0.53
1:A:115:SER:HB3	1:A:151:PRO:HG2	1.88	0.53
1:C:171:ASP:CG	1:C:172:ALA:H	2.16	0.52
1:C:217:GLU:OE2	1:C:245:ASN:ND2	2.42	0.52
1:B:455:ASN:OD1	1:B:457:GLN:HG3	2.08	0.52
1:C:114:ASN:OD1	1:C:115:SER:N	2.42	0.52
1:B:453:LYS:HG2	1:B:454:GLU:HG3	1.91	0.52
1:A:217:GLU:OE2	1:A:245:ASN:ND2	2.41	0.52
1:C:446:THR:OG1	1:C:466:ASP:OD2	2.27	0.51
1:A:197:PRO:HB2	1:A:198:HIS:CE1	2.44	0.51
1:C:359:ARG:NH2	1:C:383:ASN:OD1	2.43	0.51
1:A:453:LYS:N	1:A:453:LYS:HD3	2.25	0.51
1:B:390:HIS:H	1:B:390:HIS:CD2	2.28	0.51
1:A:47:MET:HE3	1:A:49:PHE:CE2	2.46	0.51
1:B:446:THR:OG1	1:B:466:ASP:OD2	2.29	0.50
1:A:399:LYS:O	1:A:403:SER:OG	2.28	0.50
1:B:43:ARG:HH21	1:B:64:ASP:CG	2.19	0.50
1:B:133:PHE:O	1:B:138:TYR:HB2	2.11	0.50
1:C:214:PRO:HB3	1:C:244:MET:HE3	1.94	0.50
1:C:424:GLN:HG2	1:C:430:VAL:HG23	1.94	0.50
1:C:106:ARG:O	1:C:123:ARG:NH1	2.45	0.50
1:C:177:GLU:H	1:C:177:GLU:CD	2.17	0.50
1:C:486:ARG:O	1:C:490:ILE:HG12	2.12	0.49
1:C:102:MET:HE2	1:C:106:ARG:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:SER:HB3	1:A:113:VAL:HG23	1.94	0.49
1:B:455:ASN:OD1	1:B:456:LYS:N	2.41	0.49
1:C:218:THR:HG23	1:C:306:LEU:HG	1.93	0.49
1:B:438:ARG:NH2	1:B:501:ASP:OD1	2.45	0.48
1:C:68:THR:HG22	1:C:68:THR:O	2.12	0.48
1:C:359:ARG:HH22	1:C:383:ASN:HD21	1.60	0.48
1:B:46:ALA:HA	1:B:64:ASP:HB2	1.95	0.48
1:B:116:ARG:C	1:B:118:PRO:HD3	2.39	0.48
1:B:249:HIS:HB2	1:B:250:PRO:CD	2.43	0.48
1:C:343:PRO:HG3	1:C:416:TYR:CE2	2.49	0.48
1:B:377:THR:O	1:B:381:LEU:HD23	2.13	0.48
1:C:145:LYS:H	1:C:245:ASN:HD21	1.60	0.48
1:A:43:ARG:NH2	1:A:64:ASP:OD1	2.39	0.48
1:A:442:THR:OG1	1:A:443:HIS:N	2.45	0.48
1:B:143:ILE:HD12	1:B:240:LEU:HD11	1.95	0.48
1:B:34:ILE:HD11	1:B:239:PHE:HD1	1.78	0.48
1:B:316:SER:O	1:B:357:PRO:HG2	2.14	0.48
1:C:165:ASN:HA	1:C:168:LEU:HD12	1.96	0.47
1:C:185:TRP:HB3	1:C:202:THR:HA	1.96	0.47
1:A:417:ILE:HG23	1:A:438:ARG:CZ	2.44	0.47
1:A:452:ASP:HB3	1:A:455:ASN:O	2.14	0.47
1:B:249:HIS:HE1	1:B:256:ASP:CG	2.23	0.47
1:C:119:PHE:CZ	1:C:433:TYR:HB3	2.49	0.47
1:B:344:TYR:HD1	1:B:472:GLN:HE21	1.62	0.47
1:C:442:THR:OG1	1:C:443:HIS:N	2.47	0.47
1:B:183:ASN:OD1	1:B:183:ASN:N	2.45	0.47
1:A:118:PRO:HD2	1:A:430:VAL:O	2.15	0.47
1:B:87:ASN:ND2	1:B:370:SER:OG	2.41	0.47
1:A:43:ARG:HH21	1:A:64:ASP:CG	2.21	0.47
1:B:292:TYR:HB2	1:B:331:MET:HE3	1.97	0.47
1:C:244:MET:HE2	1:C:299:VAL:HG13	1.96	0.46
1:A:352:PHE:HE2	1:A:354:ILE:HD11	1.81	0.46
1:B:283:MET:CG	1:B:285:LYS:H	2.26	0.46
1:A:182:PHE:CD2	1:A:185:TRP:HZ3	2.34	0.46
1:A:458:LEU:HD21	1:A:461:ILE:HD11	1.98	0.46
1:C:458:LEU:HD13	1:C:509:LEU:HD21	1.97	0.46
1:C:42:MET:HG3	1:C:296:ILE:HD13	1.97	0.46
1:C:94:HIS:CD2	1:C:326:ASP:HA	2.50	0.46
1:C:352:PHE:HE1	1:C:354:ILE:HD11	1.81	0.46
1:C:453:LYS:HE3	1:C:459:LYS:HZ3	1.80	0.46
1:A:389:PRO:HB2	1:A:392:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:TRP:NE1	1:B:256:ASP:O	2.47	0.46
1:C:201:ASP:HB2	1:C:205:LYS:H	1.81	0.46
1:A:497:LYS:HE3	1:A:504:TYR:CE2	2.51	0.45
1:B:337:GLN:OE1	1:B:337:GLN:N	2.38	0.45
1:A:478:TRP:CE2	1:A:485:LYS:HE3	2.51	0.45
1:B:89:PRO:O	1:B:90:LEU:HD23	2.16	0.45
1:C:50:TRP:HB3	1:C:59:LEU:HD22	1.98	0.45
1:C:133:PHE:O	1:C:138:TYR:HB2	2.16	0.45
1:C:447:LEU:HA	1:C:462:LEU:O	2.16	0.45
1:C:102:MET:HE1	1:C:123:ARG:HH22	1.81	0.45
1:C:149:ASP:HB2	1:C:169:VAL:HG11	1.98	0.45
1:A:446:THR:OG1	1:A:466:ASP:OD2	2.29	0.45
1:B:36:TYR:HB3	1:B:241:MET:HG3	1.98	0.45
1:B:233:ASP:HB3	1:B:236:LYS:HG3	1.98	0.45
1:C:68:THR:CG2	1:C:71:LEU:HB2	2.46	0.45
1:B:37:ILE:HG23	1:B:242:ILE:HB	1.99	0.45
1:B:396:ASP:CG	1:B:398:SER:HG	2.23	0.44
1:C:87:ASN:OD1	1:C:370:SER:HB3	2.17	0.44
1:A:489:LEU:HD23	1:A:489:LEU:HA	1.85	0.44
1:B:93:PRO:HA	1:B:109:VAL:HG13	1.99	0.44
1:B:417:ILE:HG23	1:B:438:ARG:CZ	2.47	0.44
1:C:265:TYR:HH	1:C:297:THR:HG1	1.64	0.44
1:C:444:ARG:CZ	1:C:467:LEU:HD23	2.47	0.44
1:B:89:PRO:HD2	1:B:341:ASN:OD1	2.17	0.44
1:A:497:LYS:HE3	1:A:497:LYS:HB2	1.73	0.44
1:C:483:GLN:OE1	1:C:483:GLN:N	2.46	0.44
1:C:219:ASP:OD1	1:C:305:ARG:NH2	2.41	0.44
1:C:326:ASP:OD1	1:C:327:HIS:N	2.50	0.44
1:A:228:GLU:HB3	1:A:229:PHE:CD1	2.53	0.43
1:C:306:LEU:HD23	1:C:306:LEU:HA	1.78	0.43
1:C:478:TRP:CD1	1:C:485:LYS:HB2	2.53	0.43
1:A:435:PRO:HB2	1:A:503:TRP:CD1	2.54	0.43
1:B:413:ALA:HB1	1:B:440:ILE:HD11	2.00	0.43
1:B:209:ILE:HD12	1:B:216:HIS:NE2	2.34	0.43
1:B:94:HIS:CE1	1:B:326:ASP:HA	2.54	0.43
1:B:138:TYR:CE2	1:B:237:PRO:HB2	2.54	0.43
1:B:328:GLY:C	1:B:347:SER:HA	2.43	0.43
1:B:328:GLY:HA3	1:B:347:SER:C	2.43	0.43
1:C:200:TRP:CZ3	1:C:206:ARG:HB2	2.53	0.43
1:C:372:PRO:O	1:C:394:GLY:HA3	2.19	0.43
1:B:454:GLU:HG3	1:B:454:GLU:H	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ASP:OD1	1:B:40:ASP:N	2.50	0.43
1:B:269:THR:HG22	1:B:272:GLU:HG3	2.01	0.43
1:B:373:ASP:C	1:B:376:PRO:HD2	2.44	0.43
1:B:276:ARG:NE	1:B:346:GLU:OE2	2.41	0.43
1:C:316:SER:O	1:C:357:PRO:HG2	2.18	0.43
1:B:110:PRO:HG3	1:B:433:TYR:CD2	2.53	0.42
1:B:254:PHE:HE2	1:B:287:SER:HB2	1.84	0.42
1:B:258:MET:HE2	1:B:258:MET:HB3	1.82	0.42
1:C:34:ILE:HD12	1:C:133:PHE:CZ	2.54	0.42
1:A:39:PRO:CG	1:A:299:VAL:HG11	2.49	0.42
1:B:209:ILE:HD12	1:B:216:HIS:CE1	2.54	0.42
1:C:244:MET:HE3	1:C:244:MET:HB3	1.81	0.42
1:C:487:GLN:O	1:C:491:GLN:HG3	2.19	0.42
1:A:200:TRP:HA	1:A:205:LYS:O	2.19	0.42
1:A:233:ASP:HB3	1:A:236:LYS:HD3	2.01	0.42
1:B:109:VAL:HG13	1:B:109:VAL:O	2.20	0.42
1:B:283:MET:HE3	1:B:337:GLN:HG3	2.01	0.42
1:B:34:ILE:HD11	1:B:239:PHE:CD1	2.54	0.42
1:B:185:TRP:NE1	1:B:187:SER:HB3	2.35	0.42
1:A:105:HIS:CD2	1:A:106:ARG:HG2	2.55	0.42
1:B:313:LEU:HD12	1:B:313:LEU:HA	1.80	0.42
1:A:114:ASN:OD1	1:A:115:SER:N	2.53	0.42
1:A:469:ASP:CG	1:A:473:MET:H	2.27	0.42
1:B:92:SER:HB2	1:B:93:PRO:HD3	2.02	0.42
1:B:109:VAL:HG22	1:B:111:LEU:O	2.20	0.42
1:A:268:ARG:HE	1:A:272:GLU:HB3	1.85	0.42
1:B:359:ARG:HD3	1:B:402:PHE:CE1	2.49	0.42
1:C:373:ASP:C	1:C:376:PRO:HD2	2.45	0.42
1:B:39:PRO:HD2	1:B:324:SER:O	2.19	0.42
1:B:366:ASP:OD1	1:B:366:ASP:N	2.52	0.42
1:C:417:ILE:HG23	1:C:438:ARG:CZ	2.50	0.42
1:A:248:HIS:CE1	1:A:295:GLN:NE2	2.88	0.41
1:A:326:ASP:OD1	1:A:326:ASP:N	2.50	0.41
1:A:343:PRO:HG3	1:A:416:TYR:CE2	2.54	0.41
1:B:438:ARG:HB2	1:B:503:TRP:CZ3	2.55	0.41
1:C:42:MET:HE3	1:C:296:ILE:HG23	2.02	0.41
1:A:372:PRO:O	1:A:394:GLY:HA3	2.20	0.41
1:B:95:ARG:NH2	2:B:601:SO4:O4	2.53	0.41
1:B:460:GLU:OE1	1:B:462:LEU:HD11	2.20	0.41
1:A:324:SER:OG	1:A:325:SER:N	2.53	0.41
1:A:438:ARG:NE	1:A:501:ASP:OD2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:HIS:HE1	1:B:256:ASP:OD2	2.04	0.41
1:B:344:TYR:HD1	1:B:472:GLN:NE2	2.19	0.41
1:B:420:MET:HE3	1:B:436:VAL:HG21	2.03	0.41
1:C:359:ARG:HH22	1:C:383:ASN:ND2	2.18	0.41
1:C:440:ILE:HD13	1:C:440:ILE:HA	1.84	0.41
1:A:421:ASP:CB	1:A:430:VAL:HG11	2.49	0.41
1:B:140:CYS:HB3	1:B:182:PHE:CD1	2.56	0.41
1:A:208:ASP:OD1	1:A:208:ASP:N	2.54	0.41
1:A:338:ASP:O	1:A:340:LYS:N	2.54	0.41
1:A:440:ILE:HD11	1:A:488:LEU:HD22	2.03	0.41
1:B:225:LEU:HD13	1:B:310:LEU:HD13	2.03	0.41
1:B:246:PRO:HA	1:B:247:PRO:HD3	1.97	0.41
1:B:490:ILE:O	1:B:494:GLN:HG3	2.20	0.41
1:C:43:ARG:HD3	1:C:329:GLU:O	2.21	0.41
1:A:419:ASN:HB3	1:A:433:TYR:HD1	1.85	0.41
1:B:182:PHE:CD2	1:B:185:TRP:HZ3	2.38	0.41
1:B:420:MET:HE3	1:B:420:MET:HB2	1.85	0.41
1:C:208:ASP:C	1:C:209:ILE:HD13	2.46	0.41
1:B:119:PHE:HE2	1:B:433:TYR:HD2	1.68	0.40
1:C:46:ALA:HA	1:C:64:ASP:HB2	2.03	0.40
1:A:330:THR:HB	1:A:333:SER:HB2	2.02	0.40
1:C:91:SER:HB3	1:C:95:ARG:HH22	1.86	0.40
1:C:483:GLN:HG2	1:C:484:LEU:N	2.37	0.40
1:B:263:THR:OG1	1:B:266:LYS:HE2	2.21	0.40
1:C:310:LEU:HD12	1:C:310:LEU:HA	1.89	0.40
1:B:92:SER:HB3	1:B:113:VAL:HG23	2.04	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	434/516 (84%)	412 (95%)	18 (4%)	4 (1%)	14	28
1	B	416/516 (81%)	397 (95%)	17 (4%)	2 (0%)	24	42
1	C	455/516 (88%)	439 (96%)	15 (3%)	1 (0%)	43	62
All	All	1305/1548 (84%)	1248 (96%)	50 (4%)	7 (0%)	24	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ASN
1	A	339	ALA
1	A	456	LYS
1	B	253	SER
1	C	429	LYS
1	B	249	HIS
1	A	406	PRO

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	394/465 (85%)	382 (97%)	12 (3%)	36	61
1	B	380/465 (82%)	360 (95%)	20 (5%)	20	42
1	C	414/465 (89%)	404 (98%)	10 (2%)	43	67
All	All	1188/1395 (85%)	1146 (96%)	42 (4%)	32	57

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	66	VAL
1	A	78	SER
1	A	83	SER
1	A	115	SER
1	A	208	ASP

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Mol	Chain	Res	Type
1	A	256	ASP
1	A	257	CYS
1	A	316	SER
1	A	407	ASP
1	A	421	ASP
1	A	442	THR
1	B	37	ILE
1	B	40	ASP
1	B	57	SER
1	B	83	SER
1	B	91	SER
1	B	121	THR
1	B	134	SER
1	B	215	SER
1	B	256	ASP
1	B	286	SER
1	B	288	SER
1	B	311	ASP
1	B	313	LEU
1	B	329	GLU
1	B	350	VAL
1	B	370	SER
1	B	386	GLN
1	B	392	VAL
1	B	430	VAL
1	B	478	TRP
1	C	78	SER
1	C	152	THR
1	C	213	SER
1	C	215	SER
1	C	271	SER
1	C	275	VAL
1	C	284	GLU
1	C	286	SER
1	C	340	LYS
1	C	427	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	147	HIS

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Mol	Chain	Res	Type
1	A	248	HIS
1	A	295	GLN
1	A	327	HIS
1	A	349	ASN
1	A	358	GLN
1	A	487	GLN
1	A	494	GLN
1	B	44	ASN
1	B	60	GLN
1	B	112	ASN
1	B	207	HIS
1	B	334	HIS
1	B	349	ASN
1	B	390	HIS
1	B	443	HIS
1	B	457	GLN
1	C	94	HIS
1	C	136	ASN
1	C	165	ASN
1	C	245	ASN
1	C	264	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	601	-	4,4,4	0.23	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

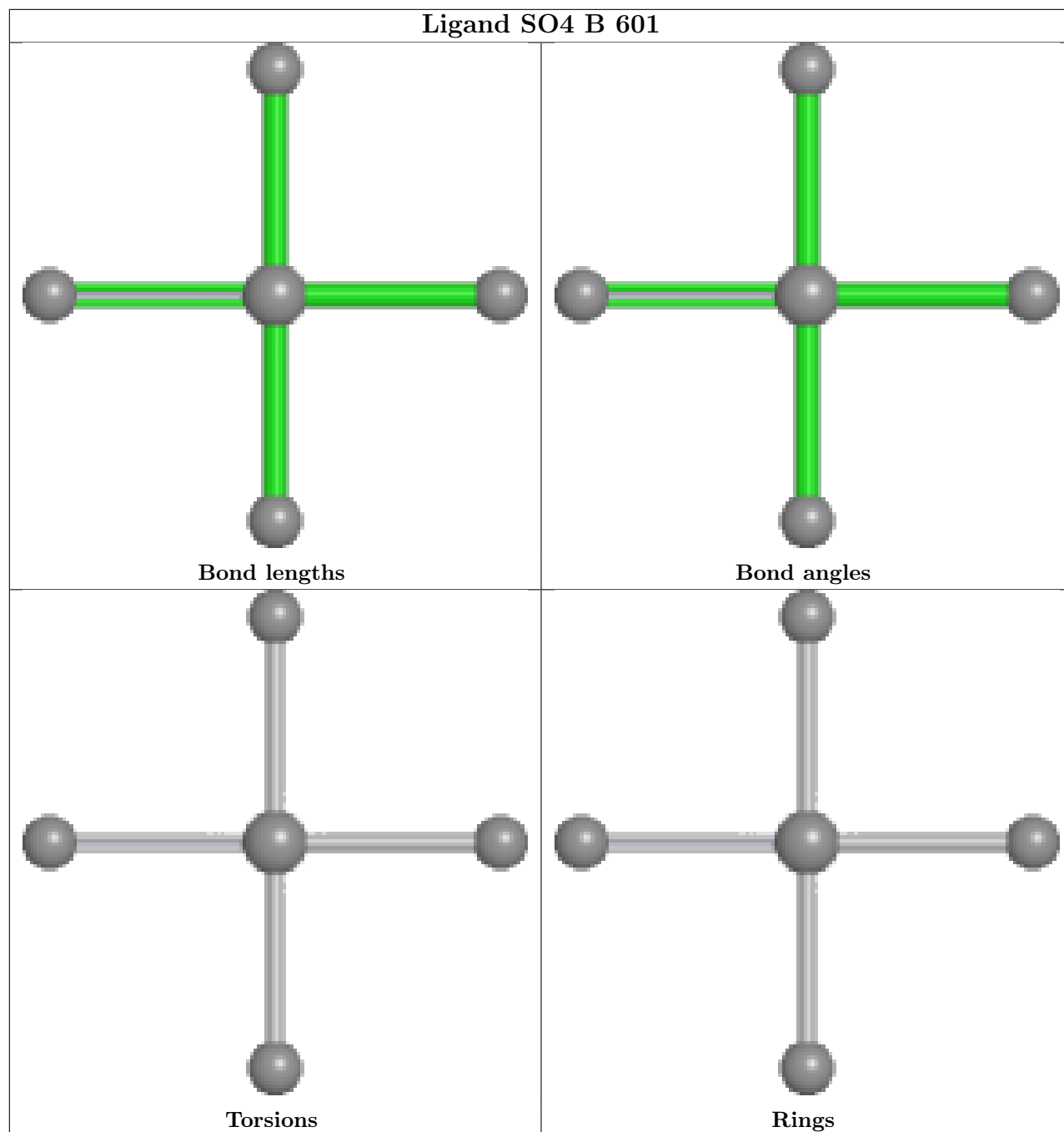
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	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	442/516 (85%)	0.53	31 (7%) 22 16	47, 67, 106, 142	0
1	B	426/516 (82%)	0.92	53 (12%) 8 6	54, 80, 110, 135	0
1	C	463/516 (89%)	0.36	20 (4%) 40 31	42, 61, 89, 144	0
All	All	1331/1548 (85%)	0.59	104 (7%) 19 14	42, 69, 107, 144	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	504	TYR	5.4
1	B	283	MET	5.0
1	A	422	GLY	4.7
1	A	511	ASP	4.5
1	B	328	GLY	4.4
1	B	251	TYR	4.2
1	C	409	PRO	4.0
1	B	503	TRP	3.9
1	A	248	HIS	3.9
1	A	251	TYR	3.8
1	A	338	ASP	3.7
1	C	255	ASN	3.6
1	B	250	PRO	3.6
1	B	31	ARG	3.4
1	C	429	LYS	3.4
1	C	512	LEU	3.4
1	C	478	TRP	3.4
1	B	339	ALA	3.3
1	A	188	TYR	3.3
1	B	433	TYR	3.3
1	C	337	GLN	3.3
1	C	430	VAL	3.3
1	A	249	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	428	GLY	3.0
1	B	447	LEU	3.0
1	B	478	TRP	2.9
1	A	201	ASP	2.9
1	A	339	ALA	2.9
1	A	209	ILE	2.9
1	B	253	SER	2.9
1	B	483	GLN	2.8
1	C	254	PHE	2.8
1	B	197	PRO	2.8
1	B	84	ALA	2.8
1	B	413	ALA	2.7
1	B	206	ARG	2.7
1	A	119	PHE	2.7
1	A	336	LEU	2.7
1	A	147	HIS	2.7
1	B	445	TYR	2.7
1	B	382	SER	2.7
1	B	285	LYS	2.7
1	A	504	TYR	2.7
1	B	368	LEU	2.6
1	A	337	GLN	2.6
1	B	54	ALA	2.6
1	B	448	SER	2.6
1	B	116	ARG	2.6
1	B	252	ASN	2.6
1	C	358	GLN	2.5
1	B	461	ILE	2.5
1	A	409	PRO	2.4
1	C	318	ASN	2.4
1	B	501	ASP	2.4
1	C	197	PRO	2.4
1	B	436	VAL	2.3
1	A	314	GLY	2.3
1	B	83	SER	2.3
1	B	444	ARG	2.3
1	B	284	GLU	2.3
1	B	488	LEU	2.3
1	C	152	THR	2.3
1	A	340	LYS	2.3
1	B	109	VAL	2.3
1	A	255	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	341	ASN	2.3
1	C	427	ASP	2.3
1	A	31	ARG	2.3
1	A	254	PHE	2.3
1	A	510	LYS	2.3
1	B	429	LYS	2.3
1	A	198	HIS	2.3
1	B	490	ILE	2.3
1	B	123	ARG	2.3
1	B	282	THR	2.2
1	B	480	THR	2.2
1	B	87	ASN	2.2
1	B	497	LYS	2.2
1	C	249	HIS	2.2
1	B	449	LEU	2.2
1	B	451	VAL	2.2
1	C	257	CYS	2.2
1	B	98	LEU	2.2
1	B	458	LEU	2.2
1	B	443	HIS	2.1
1	B	201	ASP	2.1
1	B	415	LEU	2.1
1	C	248	HIS	2.1
1	A	250	PRO	2.1
1	C	250	PRO	2.1
1	B	381	LEU	2.1
1	A	120	SER	2.1
1	B	327	HIS	2.1
1	A	430	VAL	2.1
1	B	402	PHE	2.1
1	A	330	THR	2.1
1	A	432	THR	2.1
1	C	425	ASP	2.1
1	B	496	LEU	2.0
1	B	366	ASP	2.0
1	B	185	TRP	2.0
1	A	197	PRO	2.0
1	A	285	LYS	2.0
1	A	433	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

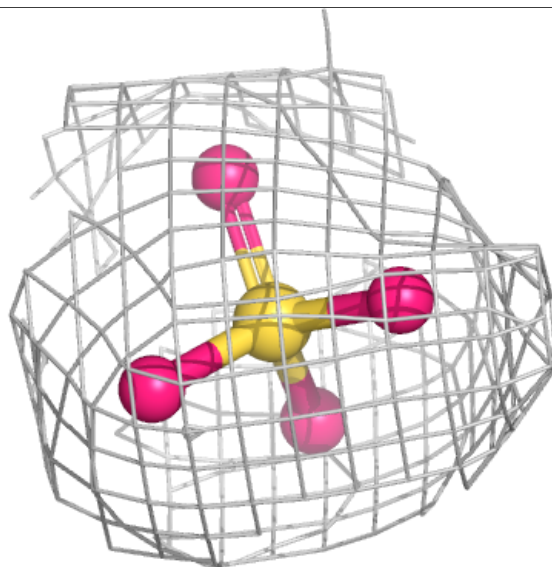
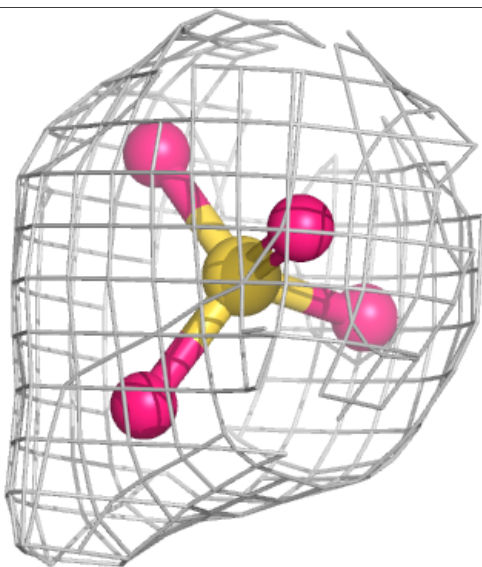
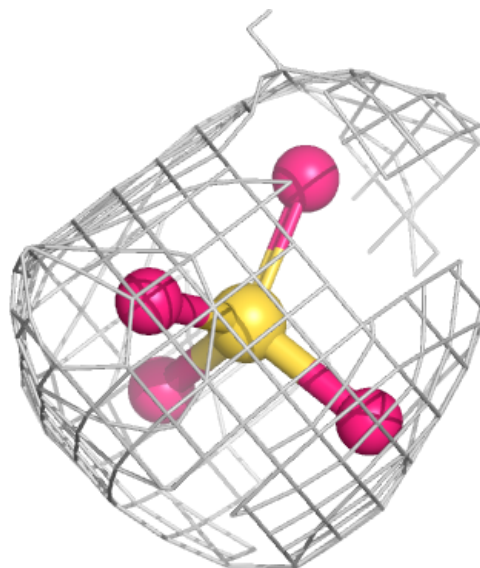
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	601	5/5	0.90	0.10	84,88,92,102	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 B 601:

$2mF_o - DF_c$ (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.