Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 04:12 AM EST

PDB ID	:	3NYN
Title	:	Crystal Structure of G Protein-Coupled Receptor Kinase 6 in Complex with Sangivamycin
Authors	:	Tesmer, J.J.G.; Singh, P.
Deposited on	:	2010-07-15
Resolution	:	2.72 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

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 2.72 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	Percentile Ranks	Value
Rfree		0.224
Clashscore		6
Ramachandran outliers		0.4%
Sidechain outliers		2.3%
RSRZ outliers		4.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
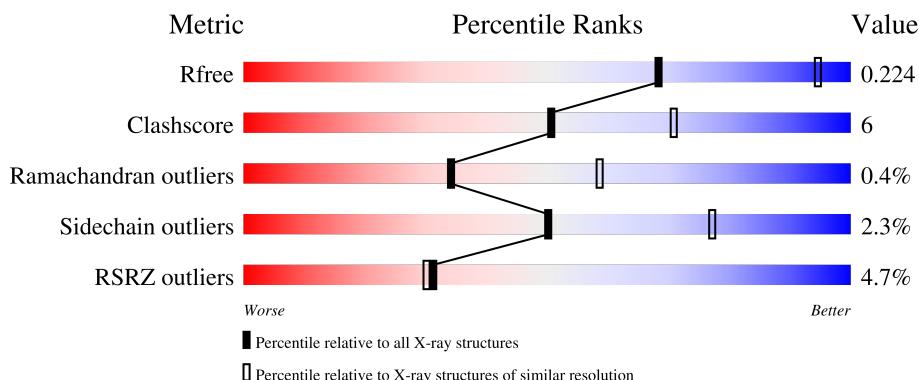
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 <=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	576	4% · 82% · 14% · ·
1	B	576	5% · 81% · 14% · ·
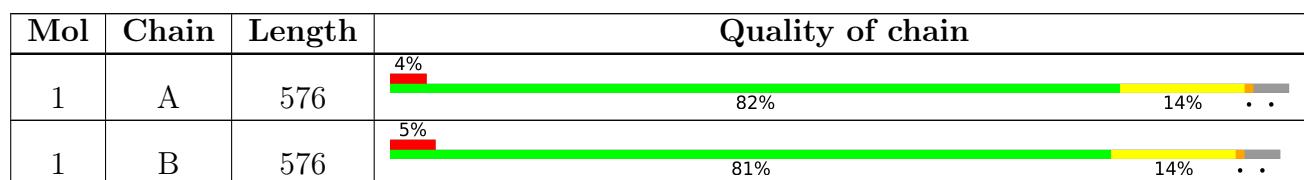
2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 9046 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 G protein-coupled receptor kinase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4454	2834	785	807	28			
1	B	554	Total	C	N	O	S	0	0	0
			4454	2834	785	807	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ACE	-	acetylation	UNP P43250
B	1	ACE	-	acetylation	UNP P43250

- Molecule 2 is SANGIVAMYCIN (three-letter code: SGV) (formula: $C_{12}H_{15}N_5O_5$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			22	12	5	5		

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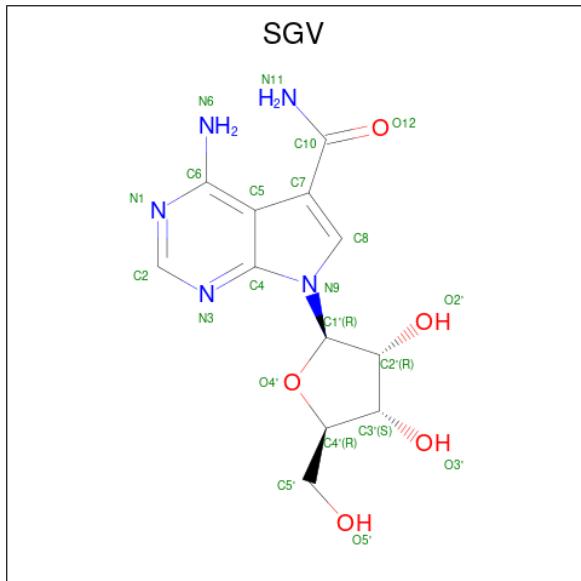
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	22	12	5	5	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
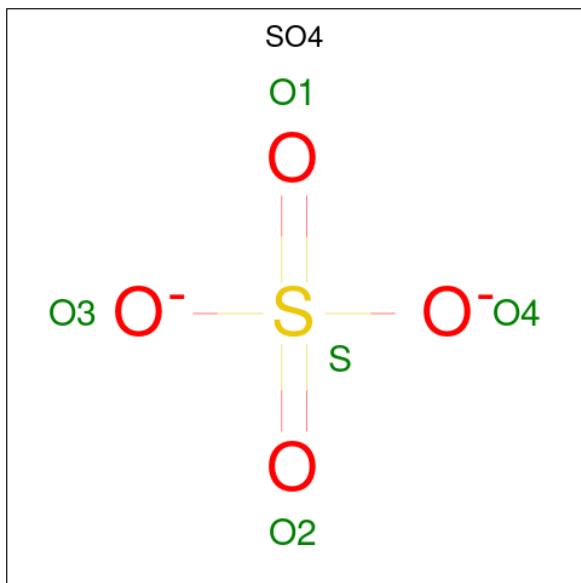
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0

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

- Molecule 4 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: $C_4H_{10}O_2$).

BU3
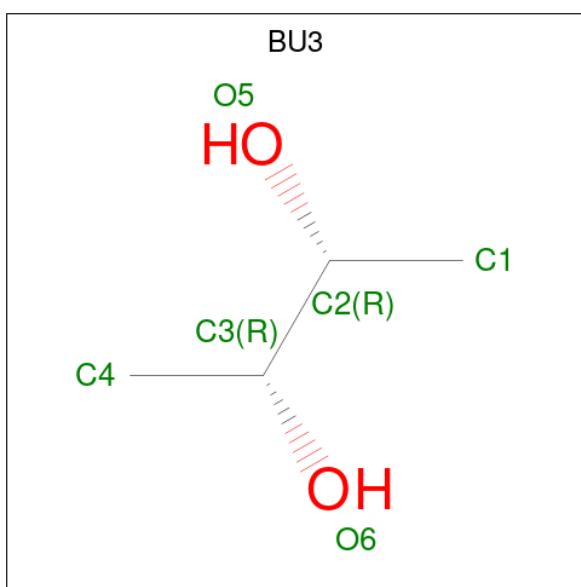
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 4	O 2	0	0
4	B	1	Total 6	C 4	O 2	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total 7	O 7	0	0
5	B	5	Total 5	O 5	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: G protein-coupled receptor kinase 6
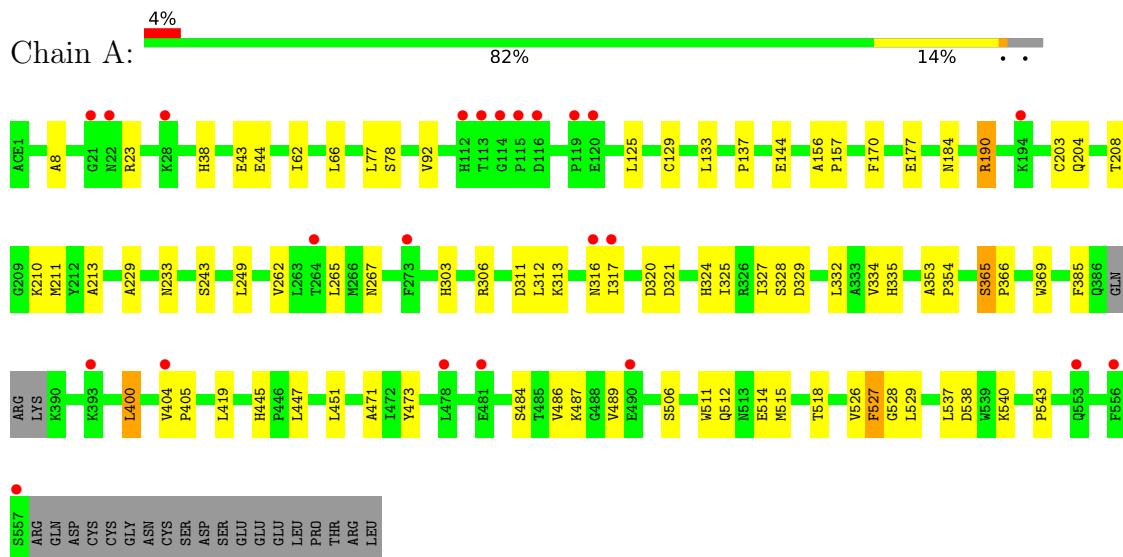
• Molecule 1: G protein-coupled receptor kinase 6
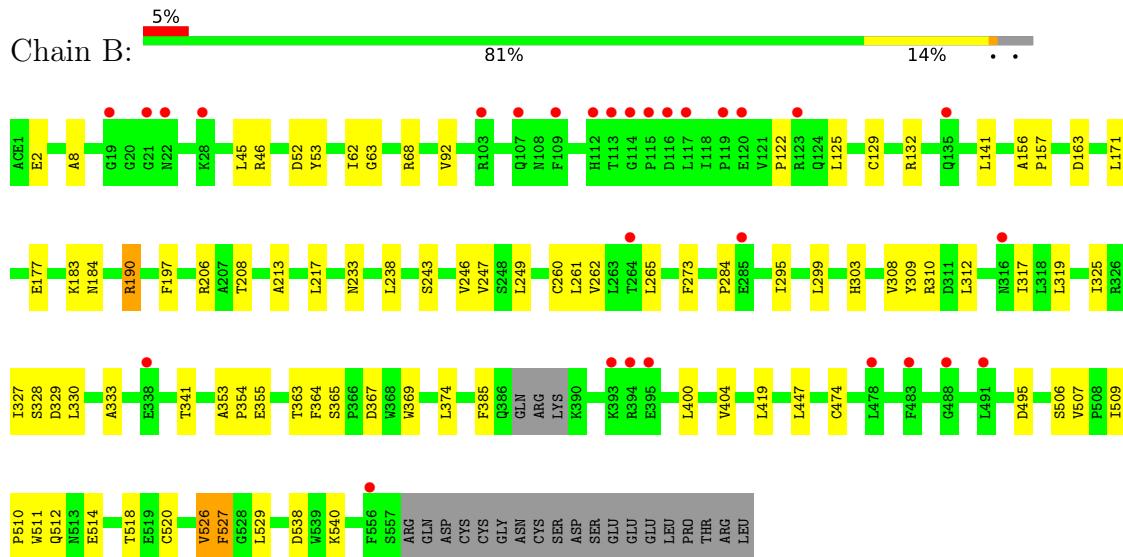
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	154.59Å 154.59Å 207.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.72 36.62 – 2.71	Depositor EDS
% Data completeness (in resolution range)	60.4 (30.00-2.72) 60.4 (36.62-2.71)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.92 (at 2.72Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.227 , 0.238 0.226 , 0.224	Depositor DCC
R_{free} test set	2289 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	62.2	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 44.3	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9046	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SGV, ACE, SO4, BU3

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	0.41	0/4553	0.53	0/6140
1	B	0.41	0/4553	0.54	0/6140
All	All	0.41	0/9106	0.53	0/12280

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4454	0	4462	52	0
1	B	4454	0	4462	56	0
2	A	22	0	15	0	0
2	B	22	0	15	0	0
3	A	35	0	0	1	0
3	B	35	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	1	0
5	A	7	0	0	0	0
5	B	5	0	0	0	0
All	All	9046	0	8970	103	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 6.

All (103) 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:B:341:THR:HG22	1:B:363:THR:HG23	1.58	0.84
1:A:62:ILE:HD12	1:A:512:GLN:HG2	1.74	0.69
1:A:312:LEU:HD12	1:A:317:ILE:HD11	1.76	0.66
1:A:325:ILE:C	1:A:325:ILE:HD12	2.19	0.63
1:B:249:LEU:HD12	1:B:262:VAL:O	2.00	0.61
1:A:156:ALA:HB3	1:A:157:PRO:HD3	1.83	0.61
1:A:8:ALA:HB1	1:A:190:ARG:HB3	1.82	0.61
1:A:353:ALA:HB2	1:A:369:TRP:CG	2.37	0.60
1:A:92:VAL:HG12	1:A:92:VAL:O	2.00	0.60
1:A:213:ALA:HB2	1:A:265:LEU:HD12	1.86	0.57
3:A:582:SO4:O2	1:B:540:LYS:NZ	2.39	0.56
1:A:353:ALA:HB1	1:A:354:PRO:HD2	1.88	0.56
1:B:309:TYR:CZ	1:B:327:ILE:HG23	2.41	0.55
1:B:213:ALA:HB2	1:B:265:LEU:HD12	1.89	0.55
1:B:122:PRO:HB2	1:B:125:LEU:HD12	1.88	0.55
1:B:309:TYR:CE2	1:B:327:ILE:HG23	2.42	0.55
1:A:210:LYS:HD3	1:A:514:GLU:HG3	1.89	0.55
1:B:419:LEU:HD23	1:B:447:LEU:HD23	1.88	0.54
1:A:419:LEU:HD13	1:A:445:HIS:CG	2.42	0.54
1:B:92:VAL:O	1:B:92:VAL:HG12	2.06	0.54
1:B:156:ALA:HB3	1:B:157:PRO:HD3	1.91	0.53
1:A:204:GLN:HB2	1:A:211:MET:CE	2.38	0.53
1:A:249:LEU:HD12	1:A:262:VAL:O	2.09	0.53
1:A:385:PHE:HD2	1:A:400:LEU:HD22	1.73	0.53
1:B:184:ASN:O	1:B:206:ARG:HD3	2.09	0.52
1:B:353:ALA:HB2	1:B:369:TRP:CG	2.43	0.52
1:A:204:GLN:HB2	1:A:211:MET:HE3	1.92	0.52
1:A:527:PHE:C	1:A:527:PHE:CD1	2.83	0.51
1:B:400:LEU:HD12	1:B:404:VAL:HG21	1.91	0.51
1:A:208:THR:HG21	1:A:515:MET:HE1	1.92	0.51
1:B:527:PHE:CD1	1:B:527:PHE:C	2.83	0.51
1:B:62:ILE:HD12	1:B:512:GLN:HG2	1.92	0.51
1:B:419:LEU:CD2	1:B:447:LEU:HD23	2.40	0.50
1:A:43:GLU:O	1:A:44:GLU:C	2.50	0.50
1:A:451:LEU:HD12	1:A:451:LEU:N	2.27	0.50
1:B:68:ARG:HG2	4:B:583:BU3:H11	1.94	0.50
1:A:527:PHE:CD2	1:B:527:PHE:CE2	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ALA:HB1	1:B:190:ARG:HB3	1.95	0.49
1:A:527:PHE:HD2	1:B:527:PHE:CE2	2.31	0.48
1:A:38:HIS:HB3	1:B:163:ASP:OD2	2.14	0.47
1:B:238:LEU:HD21	1:B:330:LEU:HD13	1.94	0.47
1:A:125:LEU:HD22	1:A:144:GLU:HG2	1.95	0.47
1:A:316:ASN:O	1:A:317:ILE:HD13	2.15	0.47
1:A:538:ASP:OD1	1:A:538:ASP:C	2.53	0.47
1:B:208:THR:HG22	1:B:520:CYS:SG	2.53	0.47
1:B:514:GLU:O	1:B:518:THR:HG23	2.14	0.47
1:A:471:ALA:HB3	1:A:473:TYR:CE1	2.50	0.47
1:B:92:VAL:O	1:B:92:VAL:CG1	2.62	0.47
1:B:325:ILE:HD12	1:B:325:ILE:C	2.35	0.47
1:B:273:PHE:CE1	1:B:474:CYS:HA	2.50	0.47
1:B:538:ASP:OD1	1:B:538:ASP:C	2.54	0.47
1:A:320:ASP:OD1	1:A:324:HIS:N	2.44	0.46
1:B:132:ARG:HG3	1:B:141:LEU:HD13	1.97	0.46
1:B:303:HIS:CE1	1:B:364:PHE:HB3	2.51	0.46
1:B:353:ALA:HB1	1:B:354:PRO:HD2	1.98	0.46
1:A:92:VAL:O	1:A:92:VAL:CG1	2.64	0.46
1:B:327:ILE:HG22	1:B:328:SER:N	2.31	0.46
1:B:295:ILE:HD13	1:B:374:LEU:HD23	1.99	0.45
1:A:486:VAL:HG12	1:A:487:LYS:O	2.16	0.45
1:B:355:GLU:OE2	1:B:355:GLU:N	2.36	0.45
1:A:311:ASP:CG	1:A:332:LEU:HD12	2.37	0.45
1:B:507:VAL:HG12	1:B:510:PRO:HD2	1.99	0.45
1:A:177:GLU:HB3	1:A:511:TRP:CE3	2.52	0.45
1:A:353:ALA:HB1	1:A:354:PRO:CD	2.48	0.44
1:A:419:LEU:CD2	1:A:447:LEU:HD23	2.47	0.44
1:A:133:LEU:HD12	1:A:137:PRO:HB3	1.99	0.44
1:B:46:ARG:HG3	1:B:171:LEU:HD11	2.00	0.44
1:A:203:CYS:O	1:A:211:MET:HE1	2.18	0.44
1:B:62:ILE:O	1:B:63:GLY:C	2.55	0.44
1:A:66:LEU:HD13	1:A:170:PHE:HB2	2.00	0.44
1:A:303:HIS:O	1:A:306:ARG:N	2.50	0.44
1:A:334:VAL:HG22	1:A:335:HIS:N	2.33	0.43
1:B:52:ASP:O	1:B:53:TYR:C	2.57	0.43
1:A:365:SER:N	1:A:366:PRO:CD	2.81	0.43
1:A:529:LEU:HD11	1:B:529:LEU:HD11	2.01	0.43
1:B:509:ILE:HB	1:B:510:PRO:HD3	2.00	0.43
1:A:404:VAL:HG12	1:A:405:PRO:O	2.19	0.43
1:B:299:LEU:HD22	1:B:367:ASP:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ASP:OD1	1:A:540:LYS:HG2	2.20	0.42
1:B:197:PHE:HB2	1:B:217:LEU:HD22	2.02	0.42
1:B:308:VAL:HG13	1:B:310:ARG:HG3	2.01	0.42
1:B:246:VAL:HG12	1:B:247:VAL:O	2.19	0.42
1:A:267:ASN:ND2	1:A:321:ASP:OD1	2.53	0.42
1:B:385:PHE:HA	1:B:400:LEU:HD23	2.00	0.42
1:B:509:ILE:N	1:B:510:PRO:CD	2.83	0.42
1:B:177:GLU:HB3	1:B:511:TRP:CE3	2.56	0.41
1:A:77:LEU:O	1:A:78:SER:C	2.58	0.41
1:A:316:ASN:C	1:A:317:ILE:HD13	2.41	0.41
1:A:484:SER:O	1:A:486:VAL:HG23	2.20	0.41
1:B:312:LEU:HD12	1:B:317:ILE:HD11	2.01	0.41
1:B:246:VAL:HG12	1:B:247:VAL:N	2.36	0.41
1:B:249:LEU:HD11	1:B:261:LEU:HB3	2.02	0.41
1:A:327:ILE:HG22	1:A:328:SER:N	2.35	0.41
1:A:537:LEU:HD23	1:A:543:PRO:N	2.35	0.41
1:B:511:TRP:O	1:B:514:GLU:HB3	2.21	0.41
1:B:171:LEU:HD23	1:B:171:LEU:HA	1.84	0.41
1:A:514:GLU:O	1:A:518:THR:HG23	2.20	0.41
1:A:177:GLU:HB3	1:A:511:TRP:CZ3	2.56	0.40
1:A:229:ALA:O	1:A:233:ASN:HB2	2.21	0.40
1:A:528:GLY:HA3	1:B:526:VAL:HG23	2.03	0.40
1:B:319:LEU:CD2	1:B:325:ILE:HG22	2.51	0.40
1:B:233:ASN:ND2	1:B:333:ALA:O	2.54	0.40
1:B:2:GLU:O	1:B:2:GLU:CG	2.69	0.40

There are no symmetry-related clashes.

5.3   Torsion angles   ⓘ

5.3.1   Protein backbone   ⓘ

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	550/576 (96%)	502 (91%)	46 (8%)	2 (0%)	34	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	550/576 (96%)	494 (90%)	54 (10%)	2 (0%)	34	58
All	All	1100/1152 (96%)	996 (90%)	100 (9%)	4 (0%)	34	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	VAL
1	A	329	ASP
1	B	183	LYS
1	B	284	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	481/502 (96%)	470 (98%)	11 (2%)	50	77
1	B	481/502 (96%)	470 (98%)	11 (2%)	50	77
All	All	962/1004 (96%)	940 (98%)	22 (2%)	50	77

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	129	CYS
1	A	184	ASN
1	A	190	ARG
1	A	243	SER
1	A	313	LYS
1	A	365	SER
1	A	400	LEU
1	A	506	SER
1	A	526	VAL
1	A	527	PHE
1	B	45	LEU

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Mol	Chain	Res	Type
1	B	129	CYS
1	B	190	ARG
1	B	243	SER
1	B	260	CYS
1	B	329	ASP
1	B	365	SER
1	B	495	ASP
1	B	506	SER
1	B	526	VAL
1	B	527	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	B	108	ASN
1	B	179	GLN
1	B	359	ASN

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 ⓘ

18 ligands are 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	$\#|Z| > 2$
3	SO4	A	581	-	4,4,4	0.16	0	6,6,6	0.10	0
3	SO4	A	585	-	4,4,4	0.14	0	6,6,6	0.10	0
4	BU3	B	583	-	4,5,5	5.05	4 (100%)	6,6,6	0.51	0
3	SO4	B	582	-	4,4,4	0.18	0	6,6,6	0.42	0
3	SO4	A	578	-	4,4,4	0.17	0	6,6,6	0.27	0
3	SO4	A	582	-	4,4,4	0.17	0	6,6,6	0.33	0
3	SO4	B	580	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	B	581	-	4,4,4	0.14	0	6,6,6	0.11	0
3	SO4	B	585	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	A	584	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SGV	A	577	-	22,24,24	1.34	2 (9%)	23,36,36	1.80	3 (13%)
3	SO4	B	584	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SGV	B	577	-	22,24,24	1.31	2 (9%)	23,36,36	1.93	5 (21%)
4	BU3	A	583	-	4,5,5	4.95	4 (100%)	6,6,6	0.66	0
3	SO4	B	578	-	4,4,4	0.13	0	6,6,6	0.22	0
3	SO4	B	579	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	A	579	-	4,4,4	0.15	0	6,6,6	0.10	0
3	SO4	A	580	-	4,4,4	0.14	0	6,6,6	0.17	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SGV	B	577	-	-	2/3/26/26	0/3/3/3
4	BU3	B	583	-	-	0/4/4/4	-
4	BU3	A	583	-	-	0/4/4/4	-
2	SGV	A	577	-	-	2/3/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	583	BU3	C4-C3	-6.41	1.32	1.51
4	B	583	BU3	C1-C2	-6.40	1.32	1.51
4	B	583	BU3	C4-C3	-6.34	1.33	1.51
4	A	583	BU3	C1-C2	-6.10	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	577	SGV	C7-C5	4.44	1.48	1.42
2	A	577	SGV	C7-C5	4.24	1.47	1.42
4	B	583	BU3	O6-C3	-3.40	1.33	1.43
4	A	583	BU3	O6-C3	-3.30	1.34	1.43
4	B	583	BU3	O5-C2	-3.07	1.34	1.43
4	A	583	BU3	O5-C2	-2.97	1.35	1.43
2	B	577	SGV	C8-N9	-2.16	1.34	1.38
2	A	577	SGV	C2-N3	2.11	1.35	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	577	SGV	C7-C5-C4	-6.31	102.50	107.54
2	B	577	SGV	C7-C5-C4	-6.19	102.60	107.54
2	B	577	SGV	N3-C2-N1	-3.96	122.49	128.68
2	B	577	SGV	C5-C7-C10	-3.44	119.84	127.13
2	A	577	SGV	N3-C2-N1	-3.42	123.34	128.68
2	A	577	SGV	C5-C7-C10	-3.14	120.48	127.13
2	B	577	SGV	C8-N9-C1'	-2.11	123.61	125.48
2	B	577	SGV	C2-N1-C6	2.04	122.25	118.75

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	577	SGV	O4'-C4'-C5'-O5'
2	A	577	SGV	C3'-C4'-C5'-O5'
2	B	577	SGV	O4'-C4'-C5'-O5'
2	B	577	SGV	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	583	BU3	1	0
3	A	582	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 then 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.

Ligand SGV A 577

Bond lengths

Bond angles

Torsions

Rings

Ligand SGV B 577

Bond lengths

Bond angles

Torsions

Rings
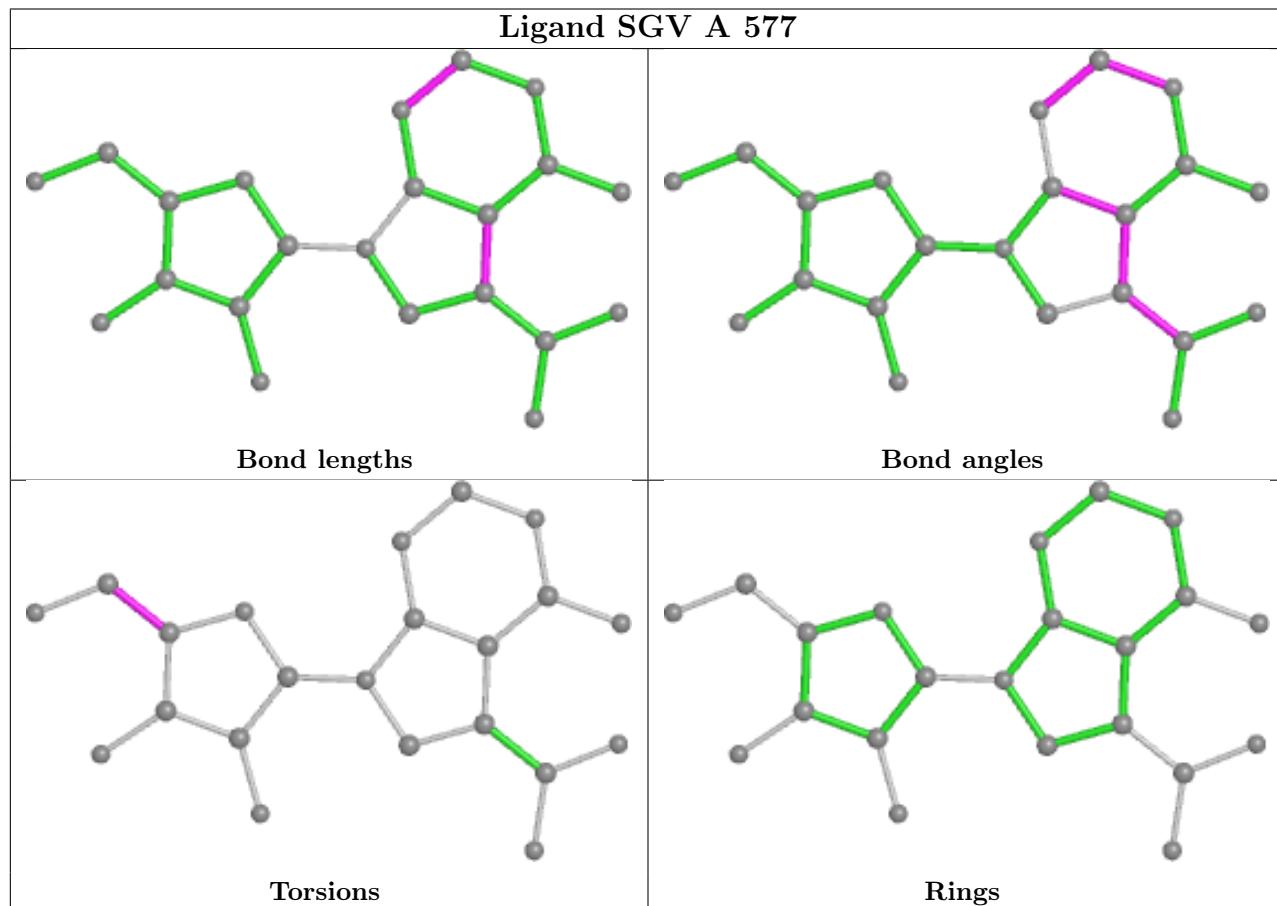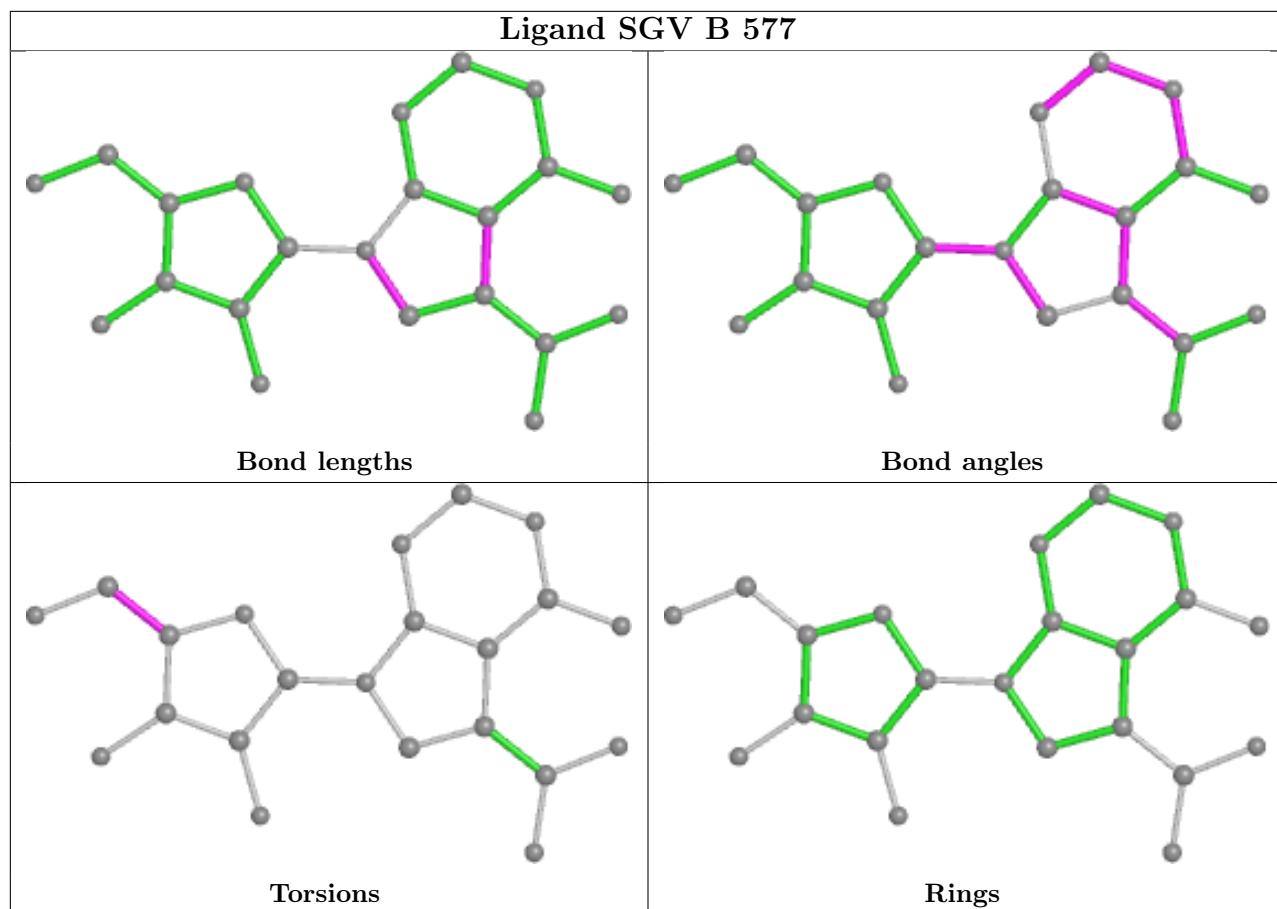
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	553/576 (96%)	0.18	23 (4%)	36	35	49, 99, 220, 248	0
1	B	553/576 (96%)	0.20	29 (5%)	27	26	47, 109, 231, 260	0
All	All	1106/1152 (96%)	0.19	52 (4%)	31	30	47, 102, 227, 260	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	113	THR	6.3
1	B	112	HIS	4.8
1	B	113	THR	4.8
1	A	114	GLY	4.7
1	A	22	ASN	4.7
1	A	120	GLU	4.2
1	A	557	SER	4.1
1	B	28	LYS	3.9
1	A	556	PHE	3.8
1	B	22	ASN	3.7
1	B	19	GLY	3.6
1	B	135	GLN	3.6
1	B	488	GLY	3.4
1	B	491	LEU	3.4
1	A	119	PRO	3.4
1	B	114	GLY	3.4
1	B	483	PHE	3.2
1	B	478	LEU	3.2
1	B	123	ARG	3.0
1	B	395	GLU	3.0
1	B	393	LYS	3.0
1	B	116	ASP	3.0
1	B	556	PHE	3.0
1	A	553	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	21	GLY	2.9
1	B	109	PHE	2.9
1	A	28	LYS	2.8
1	A	393	LYS	2.8
1	B	107	GLN	2.8
1	B	120	GLU	2.6
1	B	285	GLU	2.6
1	B	117	LEU	2.6
1	B	115	PRO	2.6
1	B	103	ARG	2.6
1	A	264	THR	2.5
1	B	264	THR	2.5
1	A	273	PHE	2.5
1	A	404	VAL	2.4
1	B	119	PRO	2.4
1	A	478	LEU	2.3
1	B	316	ASN	2.2
1	A	481	GLU	2.2
1	A	116	ASP	2.2
1	A	112	HIS	2.1
1	A	21	GLY	2.1
1	A	115	PRO	2.1
1	A	490	GLU	2.1
1	A	194	LYS	2.1
1	B	338	GLU	2.1
1	A	316	ASN	2.1
1	B	394	ARG	2.0
1	A	317	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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	A	584	5/5	0.71	0.20	219,219,220,220	0
3	SO4	B	584	5/5	0.82	0.22	225,226,226,227	0
3	SO4	B	579	5/5	0.86	0.18	183,184,184,185	0
3	SO4	B	585	5/5	0.89	0.43	164,165,165,166	0
3	SO4	A	585	5/5	0.92	0.18	157,158,158,158	0
3	SO4	A	579	5/5	0.92	0.08	169,169,169,170	0
3	SO4	A	580	5/5	0.95	0.11	106,107,107,107	0
4	BU3	A	583	6/6	0.95	0.24	66,67,68,68	0
2	SGV	A	577	22/22	0.96	0.29	84,86,89,89	0
2	SGV	B	577	22/22	0.96	0.24	90,92,95,95	0
3	SO4	B	578	5/5	0.97	0.06	85,86,88,89	0
3	SO4	A	581	5/5	0.97	0.20	118,118,119,119	0
3	SO4	B	580	5/5	0.97	0.09	109,110,111,111	0
4	BU3	B	583	6/6	0.97	0.20	66,68,69,69	0
3	SO4	B	581	5/5	0.98	0.14	123,123,124,125	0
3	SO4	B	582	5/5	0.98	0.08	66,67,68,70	0
3	SO4	A	578	5/5	0.98	0.07	80,81,81,83	0
3	SO4	A	582	5/5	0.99	0.10	60,61,62,62	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 SGV A 577:

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 SGV B 577:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.