



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:38 AM UTC

PDB ID : 6VQL / pdb_00006vql
Title : CRYSTAL STRUCTURE OF INTERLEUKIN-1 RECEPTOR-ASSOCIATED KINASE 4 (IRAK4-WT) COMPLEX WITH A NICOTINAMIDE INHIBITOR
Authors : Sack, J.S.
Deposited on : 2020-02-05
Resolution : 2.07 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

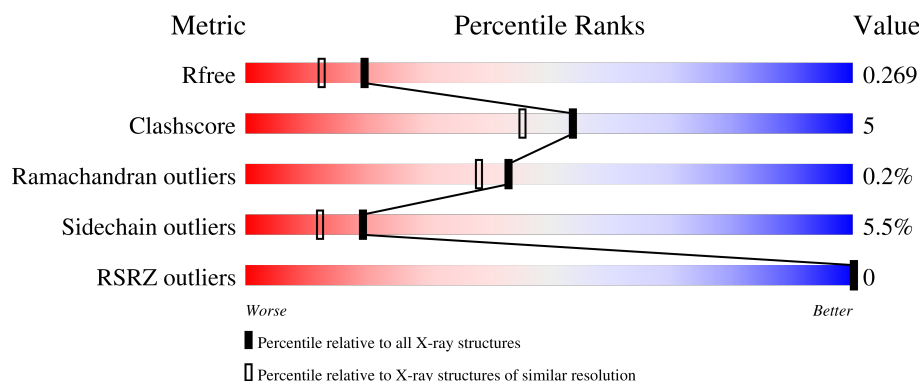
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	305	
1	B	305	
1	C	305	
1	D	305	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8960 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.

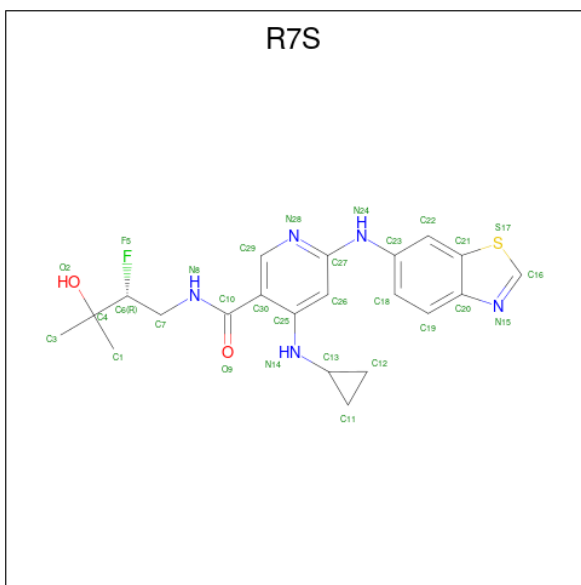
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	P	S	0	0	0
			2170	1359	364	432	2	13			
1	B	286	Total	C	N	O	P	S	0	0	0
			2188	1376	366	430	2	14			
1	C	287	Total	C	N	O	P	S	0	0	0
			2196	1379	369	432	3	13			
1	D	287	Total	C	N	O	P	S	0	0	0
			2184	1369	368	430	3	14			

There are 16 discrepancies between the modelled and reference sequences:

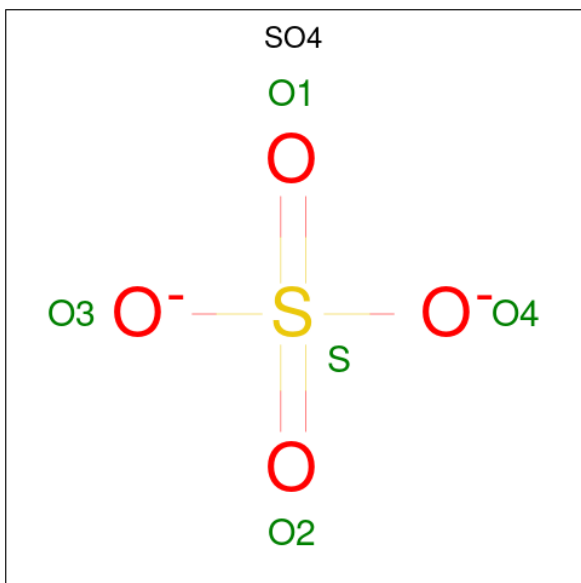
Chain	Residue	Modelled	Actual	Comment	Reference
A	156	GLY	-	expression tag	UNP Q9NWZ3
A	157	ALA	-	expression tag	UNP Q9NWZ3
A	158	MET	-	expression tag	UNP Q9NWZ3
A	159	GLY	-	expression tag	UNP Q9NWZ3
B	156	GLY	-	expression tag	UNP Q9NWZ3
B	157	ALA	-	expression tag	UNP Q9NWZ3
B	158	MET	-	expression tag	UNP Q9NWZ3
B	159	GLY	-	expression tag	UNP Q9NWZ3
C	156	GLY	-	expression tag	UNP Q9NWZ3
C	157	ALA	-	expression tag	UNP Q9NWZ3
C	158	MET	-	expression tag	UNP Q9NWZ3
C	159	GLY	-	expression tag	UNP Q9NWZ3
D	156	GLY	-	expression tag	UNP Q9NWZ3
D	157	ALA	-	expression tag	UNP Q9NWZ3
D	158	MET	-	expression tag	UNP Q9NWZ3
D	159	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is 6-[(1,3-benzothiazol-6-yl)amino]-4-(cyclopropylamino)-N-[(2R)-2-fluoro-3-hydroxy-3-methylbutyl]pyridine-3-carboxamide (CCD ID: R7S) (formula: C₂₁H₂₄FN₅O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			30	21	1	5	2	1		
2	B	1	Total	C	F	N	O	S	0	0
			30	21	1	5	2	1		
2	C	1	Total	C	F	N	O	S	0	0
			30	21	1	5	2	1		
2	D	1	Total	C	F	N	O	S	0	0
			30	21	1	5	2	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is water.

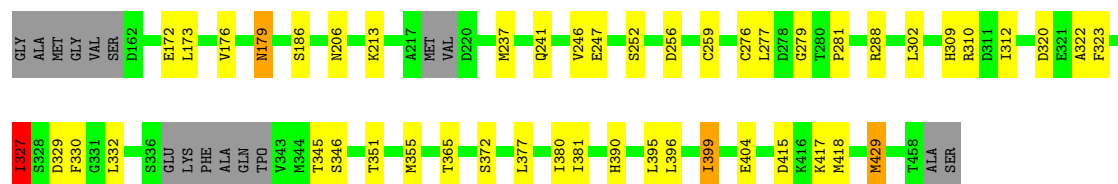
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	11	Total O 11 11	0	0
4	B	16	Total O 16 16	0	0
4	C	9	Total O 9 9	0	0
4	D	16	Total O 16 16	0	0

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.

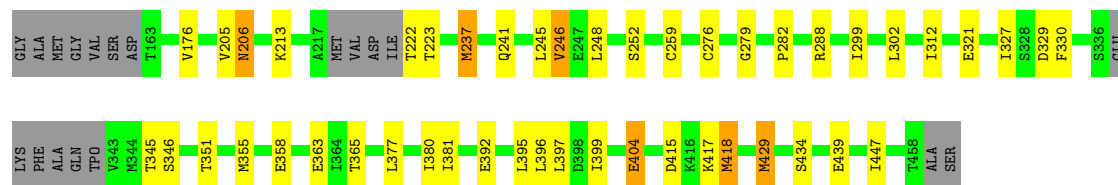
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain A: 



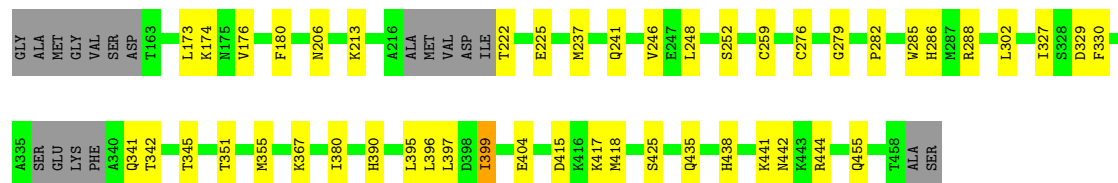
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain B: 



- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain C: 



- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.35Å 140.83Å 86.07Å 90.00° 126.20° 90.00°	Depositor
Resolution (Å)	43.00 – 2.07 43.00 – 2.07	Depositor EDS
% Data completeness (in resolution range)	52.2 (43.00-2.07) 51.7 (43.00-2.07)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.07Å)	Xtriage
Refinement program	BUSTER 2.11.7 (3-OCT-2019)	Depositor
R, R_{free}	0.242 , 0.279 0.249 , 0.269	Depositor DCC
R_{free} test set	2101 reflections (2.65%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8960	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2418e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: TPO, SEP, SO4, R7S

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	0.79	4/2184 (0.2%)	1.11	3/2961 (0.1%)
1	B	0.78	2/2203 (0.1%)	1.12	2/2981 (0.1%)
1	C	0.72	0/2199	1.10	0/2972
1	D	0.77	1/2186 (0.0%)	1.09	2/2957 (0.1%)
All	All	0.77	7/8772 (0.1%)	1.10	7/11871 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	429	MET	SD-CE	-6.56	1.63	1.79
1	A	429	MET	SD-CE	-6.44	1.63	1.79
1	B	429	MET	SD-CE	-6.36	1.63	1.79
1	B	418	MET	SD-CE	-5.65	1.65	1.79
1	A	327	ILE	CA-C	5.65	1.59	1.52
1	A	327	ILE	CG1-CD1	-5.35	1.30	1.51
1	A	327	ILE	CA-CB	5.16	1.60	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	ASP	CA-C-N	6.81	129.40	120.28
1	A	320	ASP	C-N-CA	6.81	129.40	120.28
1	A	206	ASN	CA-CB-CG	6.57	119.17	112.60
1	D	222	THR	CA-C-N	5.57	132.18	121.54
1	D	222	THR	C-N-CA	5.57	132.18	121.54
1	B	396	LEU	CA-C-N	5.03	127.53	120.28
1	B	396	LEU	C-N-CA	5.03	127.53	120.28

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	2170	0	2021	28	0
1	B	2188	0	2096	23	0
1	C	2196	0	2095	25	0
1	D	2184	0	2080	22	0
2	A	30	0	0	1	0
2	B	30	0	0	1	0
2	C	30	0	0	0	0
2	D	30	0	0	0	0
3	A	5	0	0	0	0
3	B	20	0	0	1	0
3	C	15	0	0	0	0
3	D	10	0	0	0	0
4	A	11	0	0	0	0
4	B	16	0	0	0	0
4	C	9	0	0	0	0
4	D	16	0	0	0	0
All	All	8960	0	8292	85	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 5.

All (85) 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:C:367:LYS:HZ3	1:C:442:ASN:ND2	1.60	0.99
1:A:281:PRO:HD3	1:B:321:GLU:HG3	1.51	0.92
1:B:237:MET:HG2	1:B:248:LEU:HB2	1.55	0.85
1:A:288:ARG:HB3	1:A:380:ILE:HG23	1.64	0.79
1:D:377:LEU:HD22	1:D:429:MET:HE3	1.65	0.79
1:C:367:LYS:NZ	1:C:442:ASN:ND2	2.30	0.78
1:A:377:LEU:HD22	1:A:429:MET:HE3	1.65	0.77
1:A:186:SER:HB2	1:D:419:ASN:HB2	1.68	0.75
1:B:377:LEU:HD22	1:B:429:MET:HE3	1.67	0.74
1:C:237:MET:HG2	1:C:248:LEU:HB2	1.72	0.72
1:A:309:HIS:CD2	1:A:327:ILE:HD11	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:LYS:HB2	1:D:443:LYS:HD3	1.72	0.69
1:A:246:VAL:HG21	2:A:501:R7S:C19	2.25	0.66
1:A:179:ASN:O	1:A:179:ASN:CG	2.37	0.65
1:B:237:MET:HG2	1:B:248:LEU:CB	2.24	0.65
1:B:415:ASP:HB3	1:B:418:MET:HE2	1.78	0.64
1:D:285:TRP:NE1	1:D:425:SER:OG	2.32	0.62
1:C:285:TRP:NE1	1:C:425:SER:OG	2.35	0.59
1:D:440:LYS:HB2	1:D:443:LYS:CD	2.35	0.57
1:D:173:LEU:HA	1:D:176:VAL:HG22	1.89	0.55
1:C:435:GLN:O	1:C:438:HIS:HD2	1.89	0.55
1:C:367:LYS:NZ	1:C:442:ASN:HD21	2.03	0.54
1:C:237:MET:HG2	1:C:248:LEU:CB	2.37	0.54
1:D:252:SER:HB3	1:D:259:CYS:HB2	1.89	0.54
1:D:237:MET:HE3	1:D:248:LEU:HB2	1.89	0.53
1:A:310:ARG:HD3	1:A:332:LEU:O	2.08	0.53
1:A:237:MET:HE1	1:A:246:VAL:HG13	1.90	0.53
1:A:288:ARG:HB3	1:A:380:ILE:CG2	2.36	0.53
1:D:409:THR:HG22	1:D:412:ASP:OD2	2.09	0.53
1:B:205:VAL:O	1:B:206:ASN:HB2	2.10	0.51
1:C:174:LYS:HG2	1:C:180:PHE:HE2	1.76	0.51
1:D:302:LEU:HD11	1:D:330:PHE:HE1	1.76	0.50
1:A:302:LEU:HD11	1:A:330:PHE:HE1	1.76	0.50
1:C:288:ARG:HB3	1:C:380:ILE:HG23	1.94	0.50
1:C:415:ASP:HB3	1:C:418:MET:HE2	1.94	0.50
1:B:302:LEU:HD11	1:B:330:PHE:HE1	1.77	0.49
1:B:404:GLU:OE2	3:B:502:SO4:O2	2.30	0.48
1:C:173:LEU:HA	1:C:176:VAL:HG22	1.94	0.48
1:A:309:HIS:CD2	1:A:327:ILE:CD1	2.96	0.48
1:C:252:SER:HB3	1:C:259:CYS:HB2	1.95	0.48
1:C:435:GLN:O	1:C:438:HIS:CD2	2.67	0.47
1:A:279:GLY:HA2	1:D:282:PRO:HG2	1.95	0.47
1:A:312:ILE:O	1:A:372:SER:HB3	2.13	0.47
1:B:358:GLU:HB2	1:B:363:GLU:CD	2.39	0.47
1:B:380:ILE:HG21	1:B:429:MET:HE1	1.97	0.47
1:C:302:LEU:HD11	1:C:330:PHE:HE1	1.80	0.47
1:B:245:LEU:HD23	1:B:327:ILE:HB	1.97	0.46
1:B:246:VAL:HG21	2:B:501:R7S:C19	2.45	0.46
1:D:396:LEU:HD12	1:D:399:ILE:HD13	1.98	0.46
1:B:299:ILE:HG22	1:B:447:ILE:HG12	1.98	0.45
1:B:252:SER:HB3	1:B:259:CYS:HB2	1.99	0.45
1:B:288:ARG:HB3	1:B:380:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ASP:HB3	1:A:418:MET:HE2	1.98	0.45
1:D:397:LEU:HD11	1:D:437:LEU:HD22	1.99	0.45
1:A:390:HIS:HB3	1:D:392:GLU:O	2.17	0.44
1:C:396:LEU:HD12	1:C:399:ILE:HD13	1.99	0.44
1:B:417:LYS:HD2	1:C:276:CYS:HB2	1.99	0.44
1:B:381:ILE:HD11	1:B:429:MET:HG2	2.00	0.44
1:C:367:LYS:HD2	1:C:441:LYS:HD2	2.00	0.44
1:D:414:ILE:HG12	1:D:426:VAL:HG11	1.99	0.44
1:A:247:GLU:OE2	1:C:286:HIS:HE1	2.01	0.43
1:A:380:ILE:HG21	1:A:429:MET:HE1	2.00	0.43
1:A:252:SER:HB3	1:A:259:CYS:HB2	2.00	0.43
1:A:381:ILE:HD11	1:A:429:MET:HG2	2.00	0.43
1:B:351:THR:O	1:B:355:MET:HG3	2.18	0.43
1:A:417:LYS:HD2	1:D:276:CYS:HB2	2.01	0.43
1:B:392:GLU:O	1:C:390:HIS:HB3	2.19	0.43
1:D:380:ILE:HG21	1:D:429:MET:HE1	2.01	0.42
1:B:279:GLY:HA2	1:C:282:PRO:HG2	2.01	0.42
1:A:277:LEU:HD12	1:D:416:LYS:HB3	2.02	0.42
1:D:381:ILE:HD11	1:D:429:MET:HG2	2.00	0.42
1:C:222:THR:CB	1:C:225:GLU:CB	2.97	0.42
1:A:276:CYS:HB2	1:D:417:LYS:HD2	2.01	0.42
1:B:282:PRO:HG2	1:C:279:GLY:HA2	2.01	0.42
1:C:438:HIS:HB2	1:C:444:ARG:HG3	2.02	0.42
1:A:172:GLU:O	1:A:176:VAL:HG13	2.20	0.41
1:A:396:LEU:HD12	1:A:399:ILE:HD13	2.01	0.41
1:A:351:THR:O	1:A:355:MET:HG3	2.20	0.41
1:B:380:ILE:CG2	1:B:429:MET:HE1	2.50	0.41
1:C:351:THR:O	1:C:355:MET:HG3	2.21	0.41
1:A:173:LEU:HA	1:A:176:VAL:HG22	2.01	0.41
1:A:322:ALA:O	1:A:323:PHE:HB2	2.21	0.41
1:D:367:LYS:HD2	1:D:441:LYS:HD2	2.02	0.41
1:D:222:THR:CB	1:D:225:GLU:CB	2.99	0.40
1:B:276:CYS:HB2	1:C:417:LYS:HD2	2.02	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	281/305 (92%)	270 (96%)	11 (4%)	0	100	100
1	B	278/305 (91%)	271 (98%)	6 (2%)	1 (0%)	30	23
1	C	278/305 (91%)	269 (97%)	8 (3%)	1 (0%)	30	23
1	D	278/305 (91%)	266 (96%)	12 (4%)	0	100	100
All	All	1115/1220 (91%)	1076 (96%)	37 (3%)	2 (0%)	43	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	206	ASN
1	B	206	ASN

5.3.2 Protein sidechains [i](#)

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	220/260 (85%)	210 (96%)	10 (4%)	24	18
1	B	230/260 (88%)	214 (93%)	16 (7%)	14	7
1	C	227/260 (87%)	216 (95%)	11 (5%)	23	16
1	D	226/260 (87%)	213 (94%)	13 (6%)	18	11
All	All	903/1040 (87%)	853 (94%)	50 (6%)	19	12

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	213	LYS
1	A	241	GLN
1	A	256	ASP
1	A	327	ILE
1	A	329	ASP
1	A	365	THR
1	A	395	LEU
1	A	399	ILE
1	A	404	GLU
1	B	176	VAL
1	B	213	LYS
1	B	222	THR
1	B	223	THR
1	B	237	MET
1	B	241	GLN
1	B	246	VAL
1	B	312	ILE
1	B	329	ASP
1	B	365	THR
1	B	395	LEU
1	B	397	LEU
1	B	399	ILE
1	B	404	GLU
1	B	434	SER
1	B	439	GLU
1	C	213	LYS
1	C	241	GLN
1	C	246	VAL
1	C	327	ILE
1	C	329	ASP
1	C	341	GLN
1	C	395	LEU
1	C	397	LEU
1	C	399	ILE
1	C	404	GLU
1	C	455	GLN
1	D	169	SER
1	D	213	LYS
1	D	223	THR
1	D	241	GLN
1	D	246	VAL
1	D	258	LEU

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Mol	Chain	Res	Type
1	D	329	ASP
1	D	341	GLN
1	D	365	THR
1	D	395	LEU
1	D	397	LEU
1	D	399	ILE
1	D	439	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	A	244	ASN
1	B	229	GLN
1	B	394	GLN
1	B	452	GLN
1	C	286	HIS
1	C	394	GLN
1	C	438	HIS
1	C	442	ASN
1	D	286	HIS
1	D	394	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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
1	SEP	A	346	1	8,9,10	1.03	1 (12%)	7,12,14	3.36	1 (14%)
1	SEP	D	346	1	8,9,10	1.08	0	7,12,14	2.43	1 (14%)
1	SEP	B	346	1	8,9,10	0.82	0	7,12,14	3.65	2 (28%)
1	TPO	A	345	1	8,10,11	1.21	0	10,14,16	1.10	1 (10%)
1	TPO	C	342	1	8,10,11	1.07	0	10,14,16	1.29	1 (10%)
1	TPO	D	345	1	8,10,11	1.34	2 (25%)	10,14,16	1.40	2 (20%)
1	SEP	C	346	1	8,9,10	0.67	0	7,12,14	0.63	0
1	TPO	B	345	1	8,10,11	1.07	0	10,14,16	1.17	2 (20%)
1	TPO	D	342	1	8,10,11	1.06	1 (12%)	10,14,16	1.77	2 (20%)
1	TPO	C	345	1	8,10,11	1.03	1 (12%)	10,14,16	0.96	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
1	SEP	A	346	1	-	2/6/8/10	-
1	SEP	D	346	1	-	2/6/8/10	-
1	SEP	B	346	1	-	4/6/8/10	-
1	TPO	A	345	1	-	4/9/11/13	-
1	TPO	C	342	1	-	2/9/11/13	-
1	TPO	D	345	1	-	3/9/11/13	-
1	SEP	C	346	1	-	2/6/8/10	-
1	TPO	B	345	1	-	4/9/11/13	-
1	TPO	D	342	1	-	2/9/11/13	-
1	TPO	C	345	1	-	2/9/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	345	TPO	P-OG1	-2.53	1.55	1.59
1	D	345	TPO	P-OG1	-2.28	1.55	1.59
1	D	345	TPO	CB-CA	2.20	1.58	1.53
1	A	346	SEP	CB-CA	2.16	1.58	1.52
1	D	342	TPO	P-OG1	-2.06	1.55	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	SEP	OG-CB-CA	9.02	116.92	108.14
1	A	346	SEP	OG-CB-CA	8.28	116.21	108.14
1	D	346	SEP	OG-CB-CA	5.98	113.96	108.14
1	D	342	TPO	P-OG1-CB	-3.72	113.21	123.33
1	B	346	SEP	O3P-P-OG	2.95	114.36	106.67
1	D	342	TPO	O2P-P-OG1	2.65	116.16	105.85
1	D	345	TPO	P-OG1-CB	-2.42	116.74	123.33
1	C	342	TPO	O2P-P-OG1	2.34	114.98	105.85
1	A	345	TPO	P-OG1-CB	-2.23	117.27	123.33
1	B	345	TPO	O2P-P-OG1	2.12	114.11	105.85
1	B	345	TPO	P-OG1-CB	-2.05	117.75	123.33
1	D	345	TPO	O2P-P-O1P	-2.02	102.98	110.83

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	346	SEP	N-CA-CB-OG
1	A	346	SEP	C-CA-CB-OG
1	B	345	TPO	N-CA-CB-OG1
1	B	346	SEP	CB-OG-P-O2P
1	B	346	SEP	CB-OG-P-O3P
1	C	345	TPO	N-CA-CB-OG1
1	C	345	TPO	O-C-CA-CB
1	C	346	SEP	N-CA-CB-OG
1	D	345	TPO	N-CA-CB-OG1
1	D	346	SEP	N-CA-CB-OG
1	D	346	SEP	C-CA-CB-OG
1	B	346	SEP	CB-OG-P-O1P
1	B	346	SEP	CA-CB-OG-P
1	C	342	TPO	C-CA-CB-CG2
1	D	345	TPO	CB-OG1-P-O2P
1	A	345	TPO	CB-OG1-P-O1P
1	D	342	TPO	CB-OG1-P-O3P
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	O-C-CA-CB
1	C	342	TPO	O-C-CA-CB
1	C	346	SEP	C-CA-CB-OG
1	D	342	TPO	O-C-CA-CB
1	D	345	TPO	O-C-CA-CB
1	B	345	TPO	CB-OG1-P-O1P
1	A	345	TPO	CG2-CB-OG1-P

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Mol	Chain	Res	Type	Atoms
1	B	345	TPO	CG2-CB-OG1-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	C	502	-	4,4,4	0.37	0	6,6,6	0.28	0
3	SO4	B	503	-	4,4,4	0.29	0	6,6,6	0.10	0
3	SO4	C	503	-	4,4,4	0.29	0	6,6,6	0.11	0
3	SO4	B	502	-	4,4,4	0.22	0	6,6,6	0.06	0
3	SO4	B	504	-	4,4,4	0.25	0	6,6,6	0.08	0
2	R7S	B	501	-	31,33,33	0.32	0	40,48,48	0.66	0
3	SO4	C	504	-	4,4,4	0.27	0	6,6,6	0.11	0
3	SO4	D	502	-	4,4,4	0.26	0	6,6,6	0.29	0
3	SO4	B	505	-	4,4,4	0.28	0	6,6,6	0.07	0
2	R7S	A	501	-	31,33,33	0.33	0	40,48,48	0.64	0
2	R7S	D	501	-	31,33,33	0.30	0	40,48,48	0.61	0
3	SO4	A	502	-	4,4,4	0.27	0	6,6,6	0.12	0
2	R7S	C	501	-	31,33,33	0.28	0	40,48,48	0.65	0
3	SO4	D	503	-	4,4,4	0.32	0	6,6,6	0.12	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	R7S	B	501	-	-	2/20/25/25	0/4/4/4
2	R7S	D	501	-	-	2/20/25/25	0/4/4/4
2	R7S	C	501	-	-	0/20/25/25	0/4/4/4
2	R7S	A	501	-	-	3/20/25/25	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	R7S	O9-C10-C30-C29
2	D	501	R7S	O9-C10-C30-C29
2	A	501	R7S	O9-C10-C30-C29
2	A	501	R7S	N8-C10-C30-C29
2	B	501	R7S	N8-C10-C30-C29
2	D	501	R7S	N8-C10-C30-C29
2	A	501	R7S	C12-C13-N14-C25

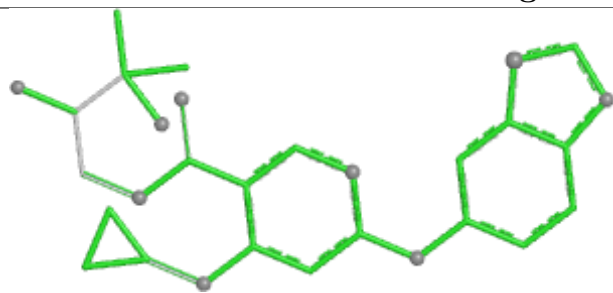
There are no ring outliers.

3 monomers are involved in 3 short contacts:

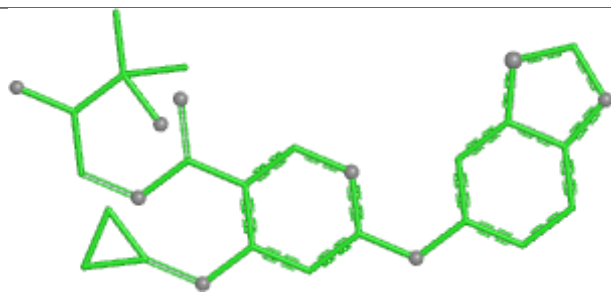
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	SO4	1	0
2	B	501	R7S	1	0
2	A	501	R7S	1	0

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.

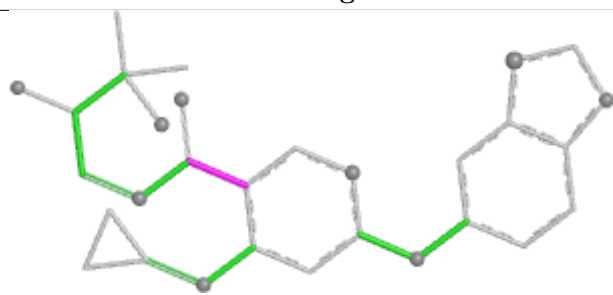
Ligand R7S B 501



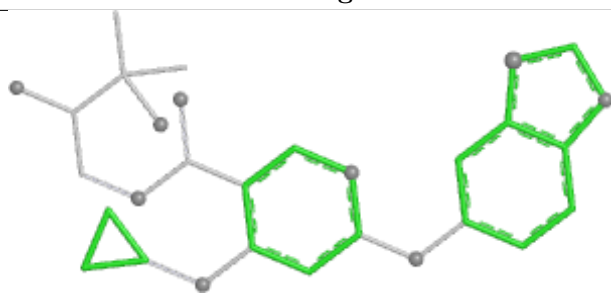
Bond lengths



Bond angles

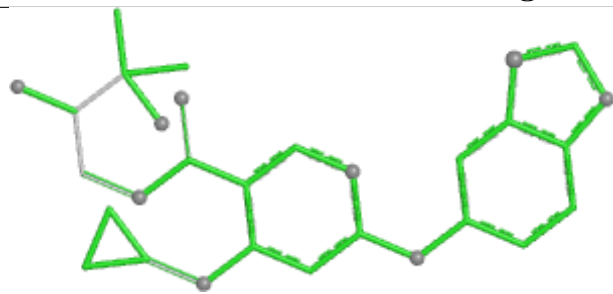


Torsions

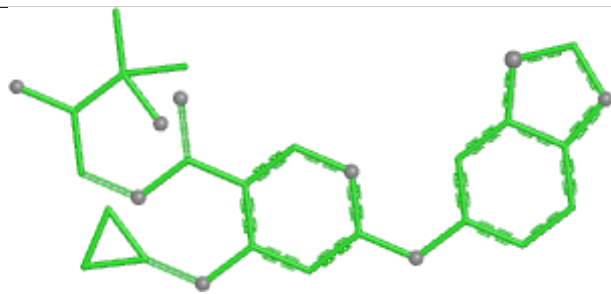


Rings

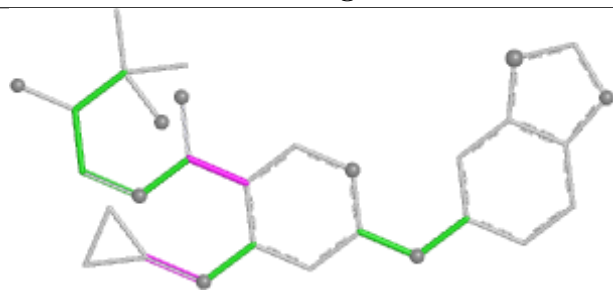
Ligand R7S A 501



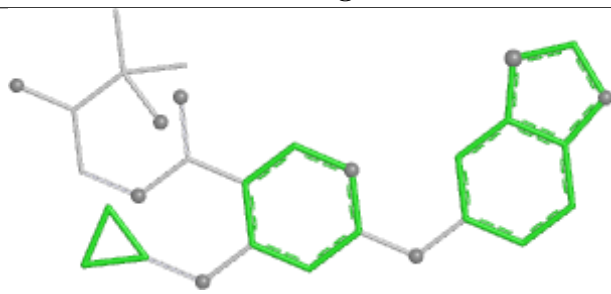
Bond lengths



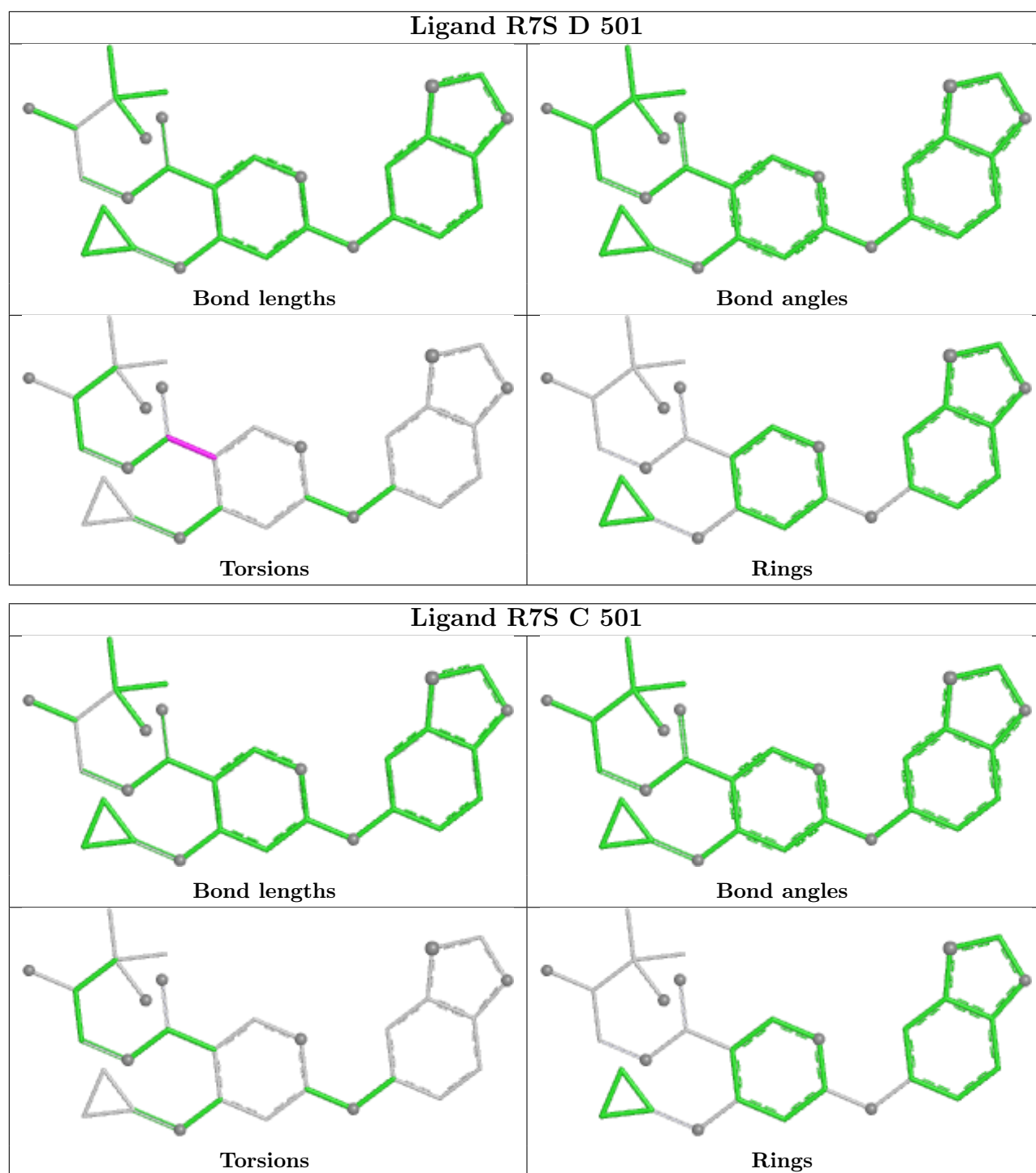
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	287/305 (94%)	-1.19	0 100 100	12, 43, 65, 76	0
1	B	284/305 (93%)	-1.23	0 100 100	10, 37, 56, 65	0
1	C	284/305 (93%)	-1.18	0 100 100	16, 40, 61, 89	0
1	D	284/305 (93%)	-1.23	0 100 100	13, 42, 59, 70	0
All	All	1139/1220 (93%)	-1.21	0 100 100	10, 40, 61, 89	0

There are no RSRZ outliers to report.

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	C	346	10/11	0.96	0.06	82,86,119,120	0
1	SEP	D	346	10/11	0.96	0.04	49,55,94,97	0
1	SEP	B	346	10/11	0.97	0.05	61,64,98,100	0
1	TPO	A	345	11/12	0.98	0.04	67,70,91,94	0
1	TPO	C	342	11/12	0.98	0.06	82,83,96,97	4
1	SEP	A	346	10/11	0.98	0.03	67,72,104,104	0
1	TPO	D	342	11/12	0.98	0.05	61,63,77,79	4
1	TPO	B	345	11/12	0.98	0.04	61,63,85,85	0
1	TPO	D	345	11/12	0.99	0.04	43,49,61,63	0
1	TPO	C	345	11/12	0.99	0.05	79,81,83,83	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

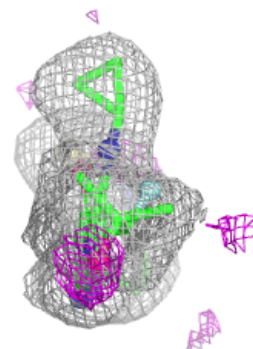
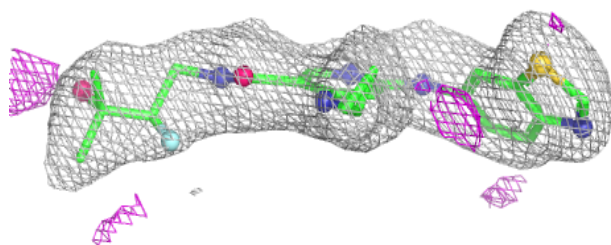
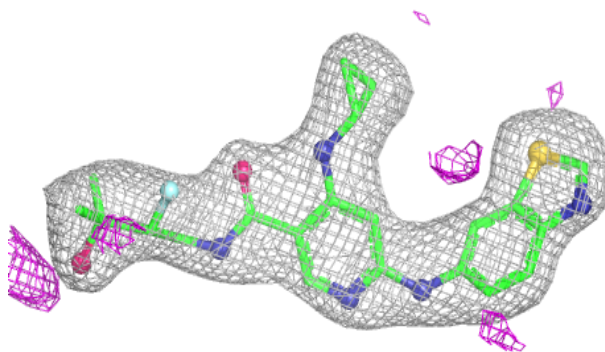
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	504	5/5	0.94	0.10	142,142,142,142	0
3	SO4	B	505	5/5	0.95	0.07	140,140,140,140	0
3	SO4	B	503	5/5	0.97	0.06	131,131,131,131	0
3	SO4	B	504	5/5	0.97	0.04	116,116,116,116	0
3	SO4	A	502	5/5	0.97	0.05	142,142,142,142	0
3	SO4	B	502	5/5	0.97	0.05	129,129,129,129	0
3	SO4	D	502	5/5	0.98	0.04	71,71,71,72	0
3	SO4	D	503	5/5	0.98	0.04	85,85,85,85	0
2	R7S	A	501	30/30	0.99	0.03	22,24,28,29	0
3	SO4	C	502	5/5	0.99	0.07	54,54,54,54	0
3	SO4	C	503	5/5	0.99	0.05	87,88,88,88	0
2	R7S	B	501	30/30	0.99	0.03	16,21,22,23	0
2	R7S	C	501	30/30	0.99	0.03	21,24,27,28	0
2	R7S	D	501	30/30	0.99	0.03	24,27,28,28	0

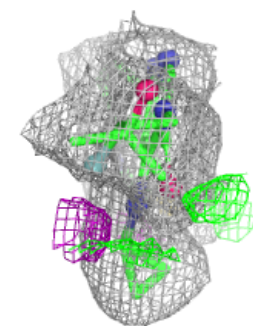
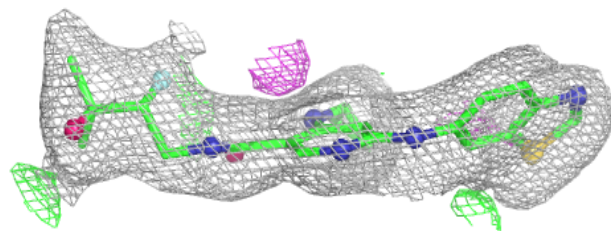
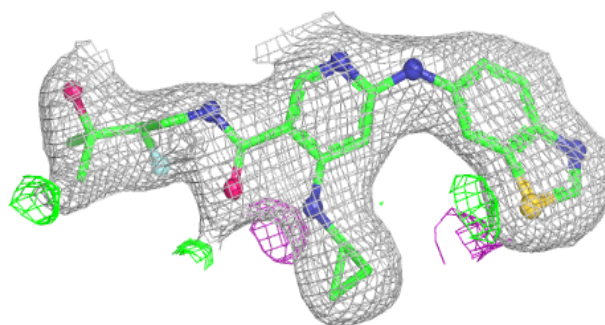
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around R7S 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)

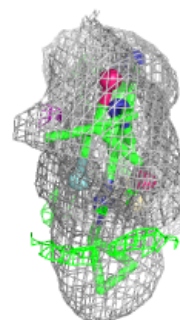
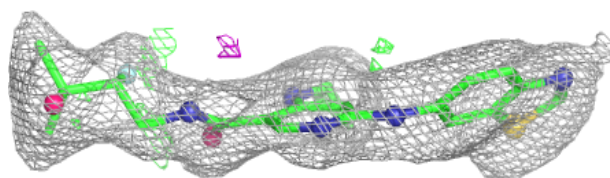
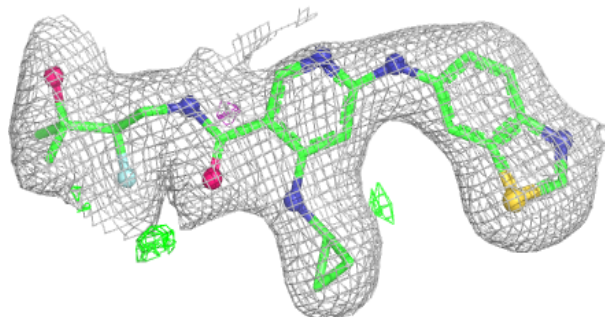
**Electron density around R7S B 501:**

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

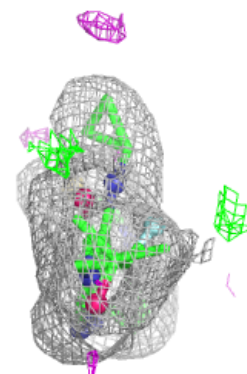
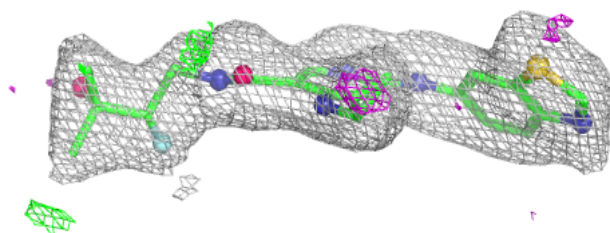
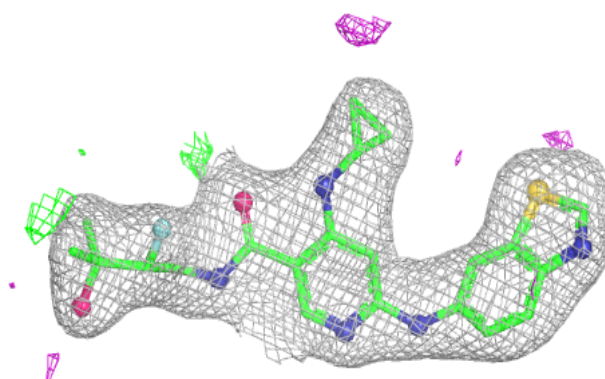


Electron density around R7S C 501:

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

**Electron density around R7S 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.