Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2024 – 12:02 PM EDT

PDB ID	:	3HVL
Title	:	Tethered PXR-LBD/SRC-1p complexed with SR-12813
Authors	:	Lesburg, C.A.; Wang, W.; Prosise, W.W.; Chen, J.; Taremi, S.S.; Le, H.V.; Madison, V.; Cui, X.; Thomas, A.; Cheng, K.C.
Deposited on	:	2009-06-16
Resolution	:	2.10 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:

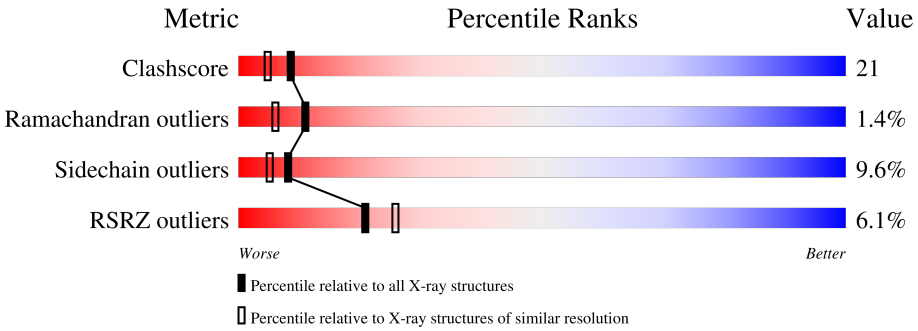
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	344	3% 55% 24% • • 17%
1	B	344	7% 56% 23% 5% 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5056 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 Pregnane X receptor, Linker, Steroid receptor coactivator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	2	0
			2366	1519	409	419	19			
1	B	289	Total	C	N	O	S	0	1	0
			2367	1519	408	421	19			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	MET	-	expression tag	UNP O75469
A	120	LYS	-	expression tag	UNP O75469
A	121	LYS	-	expression tag	UNP O75469
A	122	GLY	-	expression tag	UNP O75469
A	123	HIS	-	expression tag	UNP O75469
A	124	HIS	-	expression tag	UNP O75469
A	125	HIS	-	expression tag	UNP O75469
A	126	HIS	-	expression tag	UNP O75469
A	127	HIS	-	expression tag	UNP O75469
A	128	HIS	-	expression tag	UNP O75469
A	129	GLY	-	expression tag	UNP O75469
A	435	GLY	-	linker	UNP O75469
A	436	GLY	-	linker	UNP O75469
A	437	SER	-	linker	UNP O75469
A	438	GLY	-	linker	UNP O75469
A	439	GLY	-	linker	UNP O75469
B	119	MET	-	expression tag	UNP O75469
B	120	LYS	-	expression tag	UNP O75469
B	121	LYS	-	expression tag	UNP O75469
B	122	GLY	-	expression tag	UNP O75469
B	123	HIS	-	expression tag	UNP O75469
B	124	HIS	-	expression tag	UNP O75469
B	125	HIS	-	expression tag	UNP O75469
B	126	HIS	-	expression tag	UNP O75469
B	127	HIS	-	expression tag	UNP O75469

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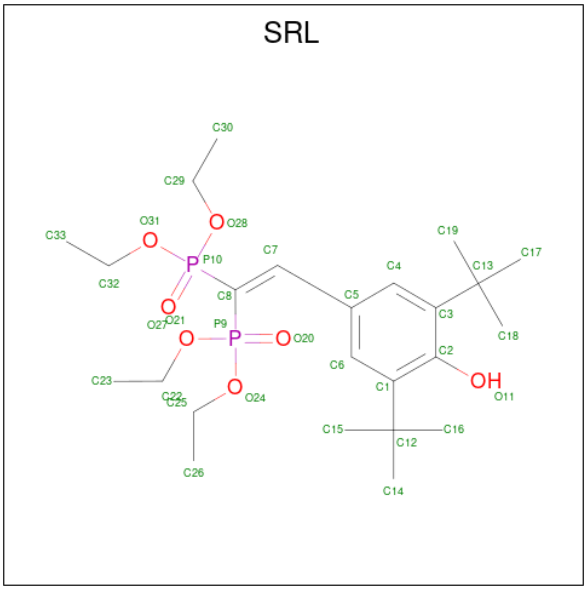
Chain	Residue	Modelled	Actual	Comment	Reference
B	128	HIS	-	expression tag	UNP O75469
B	129	GLY	-	expression tag	UNP O75469
B	435	GLY	-	linker	UNP O75469
B	436	GLY	-	linker	UNP O75469
B	437	SER	-	linker	UNP O75469
B	438	GLY	-	linker	UNP O75469
B	439	GLY	-	linker	UNP O75469

- Molecule 2 is [2-(3,5-DI-TERT-BUTYL-4-HYDROXY-PHENYL)-1-(DIETHOXY-PHOSPHORYL)-VINYL]-PHOSPHONIC ACID DIETHLYL ESTER (three-letter code: SRL) (formula: $C_{24}H_{42}O_7P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			33	24	7	2		
2	B	1	Total	C	O	P	0	0
			33	24	7	2		

- Molecule 3 is water.

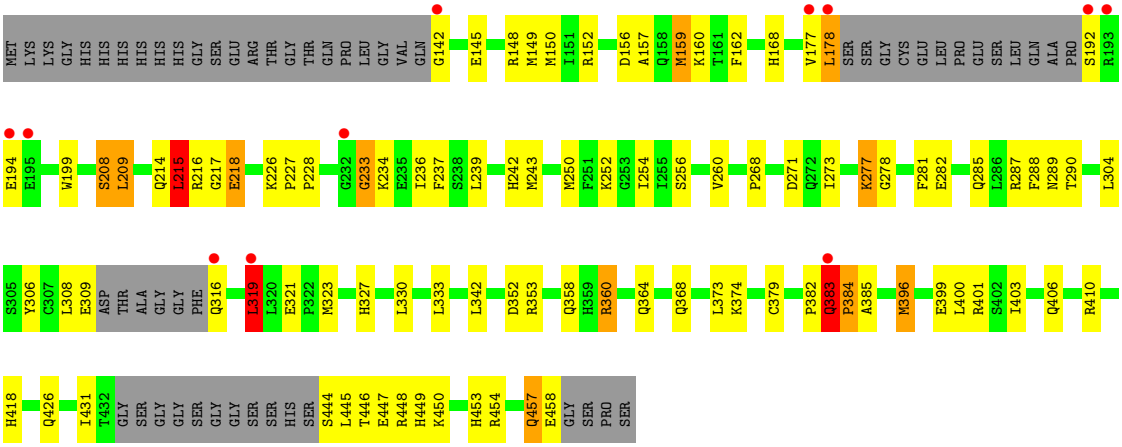
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total	O	0	0
			132	132		
3	B	125	Total	O	0	0
			125	125		

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.

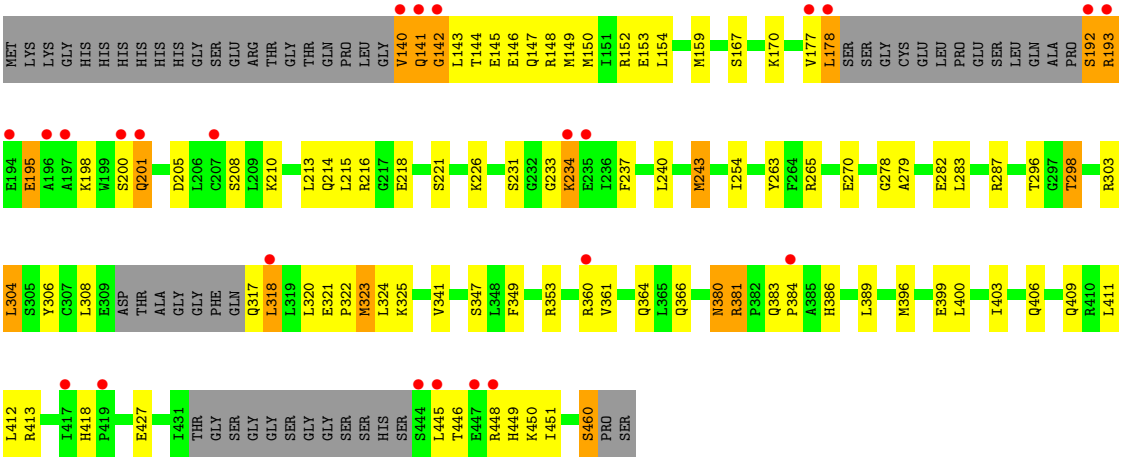
• Molecule 1: Pregnane X receptor, Linker, Steroid receptor coactivator 1

Chain A:



• Molecule 1: Pregnane X receptor, Linker, Steroid receptor coactivator 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.44Å 88.84Å 105.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.42 – 2.10 42.72 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (67.42-2.10) 95.5 (42.72-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.10Å)	Xtriage
Refinement program	BUSTER-TNT 1.3.1	Depositor
R, R_{free}	0.220 , 0.265 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	49.1	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 63.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.002 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5056	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 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: SRL

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	0.66	0/2415	0.74	2/3247 (0.1%)
1	B	0.63	0/2416	0.73	0/3249
All	All	0.64	0/4831	0.74	2/6496 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	159	MET	CG-SD-CE	-8.04	87.34	100.20
1	A	215	LEU	CA-CB-CG	5.25	127.37	115.30

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	2366	0	2388	107	0
1	B	2367	0	2384	96	0
2	A	33	0	41	5	0
2	B	33	0	41	5	0
3	A	132	0	0	8	0
3	B	125	0	0	15	0
All	All	5056	0	4854	200	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 21.

All (200) 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:270:GLU:HB3	1:B:445:LEU:HD12	1.42	1.01
1:B:323:MET:HE3	1:B:403:ILE:HG21	1.40	1.00
1:B:214:GLN:HE21	1:B:216:ARG:HH11	0.98	0.97
1:B:214:GLN:HE21	1:B:216:ARG:NH1	1.66	0.92
1:B:323:MET:CE	1:B:403:ILE:HG21	1.99	0.92
1:A:316:GLN:HA	1:A:319:LEU:HD23	1.56	0.88
1:A:215:LEU:HD22	1:A:304:LEU:CD2	2.09	0.81
1:B:323:MET:CE	1:B:323:MET:HA	2.10	0.81
1:A:177:VAL:HG13	3:A:528:HOH:O	1.81	0.80
1:A:273:ILE:O	1:A:277:LYS:HG3	1.82	0.78
1:A:319:LEU:HD22	1:A:319:LEU:H	1.48	0.78
1:B:360:ARG:O	1:B:364:GLN:HG2	1.83	0.78
1:B:150[B]:MET:HE2	1:B:154:LEU:HG	1.64	0.78
1:B:323:MET:HE3	1:B:323:MET:HA	1.67	0.76
1:B:254:ILE:HD11	1:B:287:ARG:HD2	1.65	0.75
1:A:406[A]:GLN:NE2	1:A:410:ARG:HH21	1.86	0.74
1:A:214:GLN:HE21	1:A:216:ARG:HH11	1.34	0.74
1:B:215:LEU:HD23	1:B:304:LEU:HD22	1.69	0.74
1:B:270:GLU:HB3	1:B:445:LEU:CD1	2.17	0.73
1:B:427:GLU:OE2	1:B:451:ILE:HG13	1.88	0.73
1:A:215:LEU:HD22	1:A:304:LEU:HD21	1.71	0.72
1:A:234:LYS:NZ	1:A:418:HIS:HD2	1.88	0.72
1:A:447:GLU:O	1:A:450:LYS:HE2	1.88	0.71
1:B:150[B]:MET:SD	1:B:263:TYR:HE1	2.14	0.70
1:A:242:HIS:HD2	1:A:243[A]:MET:CE	2.05	0.70
1:A:215:LEU:HD22	1:A:304:LEU:HD23	1.74	0.69
1:B:323:MET:CE	1:B:403:ILE:HD13	2.22	0.69
1:B:361:VAL:HG23	3:B:487:HOH:O	1.93	0.69
1:A:360:ARG:O	1:A:364:GLN:HG3	1.93	0.67
1:A:243[B]:MET:CE	2:A:1:SRL:H302	2.25	0.66
1:A:254:ILE:HD11	1:A:287:ARG:HD2	1.77	0.66
1:B:149:MET:HG3	1:B:152:ARG:NH2	2.11	0.66
1:B:150[B]:MET:HE3	1:B:153:GLU:HB3	1.75	0.66
1:A:243[B]:MET:HE1	2:A:1:SRL:H302	1.78	0.66
1:B:233:GLY:O	1:B:234:LYS:HB3	1.96	0.65
1:B:386:HIS:ND1	3:B:477:HOH:O	2.29	0.65
1:B:409:GLN:NE2	3:B:529:HOH:O	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:HIS:HD2	1:A:243[A]:MET:HE2	1.63	0.64
1:B:141:GLN:HE21	1:B:148:ARG:HG2	1.62	0.64
1:A:157:ALA:HB2	1:A:260:VAL:CG2	2.27	0.64
1:B:144:THR:HG23	1:B:147:GLN:H	1.63	0.64
1:A:360:ARG:HG3	1:A:364:GLN:NE2	2.14	0.63
1:B:380:ASN:HD22	1:B:380:ASN:H	1.45	0.63
1:B:214:GLN:NE2	1:B:216:ARG:NH1	2.45	0.63
1:B:304:LEU:HD23	1:B:304:LEU:N	2.14	0.63
1:B:296:THR:OG1	1:B:298:THR:HG23	1.98	0.62
1:A:316:GLN:CA	1:A:319:LEU:HD23	2.27	0.62
1:B:150[B]:MET:SD	1:B:263:TYR:CE1	2.92	0.62
1:A:256:SER:O	1:A:260:VAL:HG13	2.00	0.62
1:B:149:MET:HE3	3:B:505:HOH:O	1.98	0.62
1:A:157:ALA:HB2	1:A:260:VAL:HG22	1.82	0.61
1:A:333:LEU:HD11	1:A:396:MET:HE2	1.82	0.61
1:B:144:THR:CG2	1:B:147:GLN:HG3	2.31	0.61
1:B:141:GLN:O	1:B:141:GLN:HG3	2.00	0.61
1:A:209:LEU:CD1	1:A:321:GLU:HG2	2.31	0.60
1:A:217:GLY:HA2	1:B:178:LEU:O	2.00	0.60
1:A:445:LEU:HD12	1:A:448:ARG:NH2	2.17	0.60
1:B:460:SER:HB3	3:B:465:HOH:O	2.01	0.59
1:B:201:GLN:HA	1:B:201:GLN:OE1	2.01	0.59
1:B:141:GLN:O	1:B:143:LEU:N	2.32	0.59
1:A:382:PRO:O	1:A:383:GLN:O	2.19	0.59
1:B:403:ILE:HA	1:B:406:GLN:HG3	1.85	0.59
1:B:226:LYS:HG2	3:B:78:HOH:O	2.03	0.59
1:A:444:SER:HA	1:A:447:GLU:OE1	2.04	0.58
1:B:412:LEU:HD12	3:B:529:HOH:O	2.04	0.58
1:B:144:THR:HG22	1:B:147:GLN:CG	2.34	0.58
1:A:157:ALA:CB	1:A:260:VAL:HG22	2.33	0.58
1:A:360:ARG:HG3	1:A:364:GLN:HE21	1.69	0.57
1:B:323:MET:HE3	1:B:403:ILE:HD13	1.86	0.57
1:B:380:ASN:H	1:B:380:ASN:ND2	2.03	0.57
1:A:281:PHE:CE2	1:A:323:MET:HE3	2.40	0.57
1:B:213:LEU:HD23	1:B:213:LEU:C	2.24	0.57
1:B:403:ILE:HA	1:B:406:GLN:CG	2.34	0.57
1:A:360:ARG:CD	1:A:364:GLN:HE21	2.17	0.56
1:B:279:ALA:HB1	1:B:283:LEU:HD13	1.87	0.56
1:A:399:GLU:O	1:A:403:ILE:HG13	2.06	0.56
1:A:168:HIS:HD2	3:A:525:HOH:O	1.89	0.56
1:A:233:GLY:O	1:A:236:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:N	1:A:178:LEU:HD23	2.22	0.55
1:A:157:ALA:CB	1:A:260:VAL:CG2	2.85	0.55
1:A:383:GLN:CG	1:A:384:PRO:HD3	2.37	0.54
1:B:141:GLN:O	3:B:532:HOH:O	2.18	0.54
1:B:144:THR:HG22	1:B:147:GLN:CD	2.27	0.54
1:A:281:PHE:CE2	1:A:323:MET:CE	2.91	0.54
1:B:298:THR:HG21	3:B:507:HOH:O	2.06	0.54
1:A:157:ALA:HA	1:A:260:VAL:HG21	1.90	0.53
1:A:226:LYS:HG3	1:A:227:PRO:HD2	1.90	0.53
1:A:383:GLN:CB	1:A:384:PRO:CD	2.86	0.53
1:A:418:HIS:HE1	3:A:90:HOH:O	1.90	0.53
1:A:215:LEU:CD2	1:A:304:LEU:HD21	2.39	0.53
1:A:383:GLN:O	1:A:385:ALA:N	2.42	0.53
1:A:150:MET:HE1	1:A:368:GLN:HB3	1.91	0.52
1:B:192:SER:HA	3:B:521:HOH:O	2.09	0.52
1:B:195:GLU:O	1:B:195:GLU:OE1	2.28	0.52
1:B:214:GLN:NE2	1:B:216:ARG:HH11	1.84	0.52
1:B:380:ASN:ND2	1:B:380:ASN:N	2.57	0.52
1:B:216:ARG:HH11	1:B:216:ARG:HG3	1.75	0.52
1:A:277:LYS:HD2	1:A:449:HIS:CE1	2.45	0.51
1:B:323:MET:HE3	1:B:323:MET:CA	2.37	0.51
1:A:278:GLY:HA3	1:A:353:ARG:HD2	1.91	0.51
1:B:306:TYR:CG	2:B:2:SRL:H181	2.46	0.51
1:A:289:ASN:HD22	1:A:327:HIS:HD1	1.58	0.51
1:A:383:GLN:CB	1:A:384:PRO:HD3	2.40	0.51
1:A:454:ARG:O	1:A:458:GLU:HG2	2.11	0.51
1:B:237:PHE:CD1	1:B:418:HIS:CD2	2.99	0.51
1:A:239:LEU:O	1:A:243[B]:MET:HG3	2.10	0.50
1:A:281:PHE:CZ	1:A:323:MET:CE	2.94	0.50
1:B:150[B]:MET:HE2	1:B:154:LEU:CG	2.40	0.50
1:A:243[B]:MET:HE2	2:A:1:SRL:H292	1.94	0.50
1:A:383:GLN:HB2	1:A:384:PRO:HD3	1.94	0.50
1:A:234:LYS:HZ1	1:A:418:HIS:HD2	1.58	0.50
1:A:360:ARG:CG	1:A:364:GLN:HE21	2.23	0.49
1:B:231:SER:O	1:B:231:SER:OG	2.28	0.49
1:B:282:GLU:HG2	1:B:400:LEU:HG	1.95	0.49
1:A:156:ASP:OD1	1:A:160:LYS:HE2	2.12	0.48
1:A:445:LEU:O	1:A:449:HIS:HD2	1.97	0.48
1:B:213:LEU:HD21	1:B:215:LEU:CD1	2.43	0.48
1:A:282:GLU:OE2	1:A:401:ARG:HA	2.14	0.48
1:A:282:GLU:HG2	1:A:400:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243[B]:MET:CE	2:A:1:SRL:C30	2.92	0.48
1:A:268:PRO:HG2	1:A:271:ASP:OD1	2.14	0.47
1:A:454:ARG:HD3	3:A:501:HOH:O	2.14	0.47
1:A:281:PHE:CZ	1:A:323:MET:HE2	2.48	0.47
1:A:281:PHE:HZ	1:A:323:MET:HE2	1.79	0.47
1:A:360:ARG:CG	1:A:364:GLN:NE2	2.77	0.47
1:A:306:TYR:CG	2:A:1:SRL:H181	2.49	0.47
1:A:150:MET:CE	1:A:368:GLN:NE2	2.77	0.47
1:A:142:GLY:N	1:A:379:CYS:HG	2.13	0.47
1:A:374:LYS:HE3	3:A:515:HOH:O	2.15	0.47
1:B:243:MET:HB3	2:B:2:SRL:H231	1.97	0.46
1:A:453:HIS:CE1	1:A:457:GLN:HE22	2.33	0.46
1:A:342:LEU:HD13	1:A:373:LEU:HA	1.97	0.46
1:A:148:ARG:HD3	3:A:508:HOH:O	2.15	0.46
1:A:227:PRO:HD2	1:A:309:GLU:OE1	2.15	0.46
1:A:285:GLN:HG3	1:A:323:MET:HE3	1.98	0.46
1:B:296:THR:O	1:B:298:THR:HG22	2.16	0.46
1:B:205:ASP:OD2	1:B:413:ARG:HD2	2.16	0.45
1:B:323:MET:HE1	1:B:403:ILE:HG21	1.91	0.45
1:B:147:GLN:O	1:B:150[A]:MET:HB3	2.16	0.45
1:A:290:THR:HG21	3:A:499:HOH:O	2.16	0.45
1:A:321:GLU:OE2	1:A:410:ARG:NH2	2.49	0.45
1:B:317:GLN:HB3	1:B:318:LEU:H	1.56	0.45
1:B:411:LEU:HD22	2:B:2:SRL:H252	1.98	0.45
1:A:316:GLN:CA	1:A:319:LEU:CD2	2.94	0.45
1:B:399:GLU:HA	1:B:399:GLU:OE1	2.17	0.45
1:B:140:VAL:O	1:B:142:GLY:N	2.50	0.45
1:A:319:LEU:H	1:A:319:LEU:CD2	2.25	0.45
1:A:333:LEU:HD11	1:A:396:MET:CE	2.46	0.45
1:A:352:ASP:OD1	1:A:401:ARG:NH1	2.41	0.45
1:A:330:LEU:HA	1:A:396:MET:HE1	1.99	0.45
1:A:199:TRP:CH2	1:A:237:PHE:HE1	2.36	0.44
1:B:383:GLN:HB3	1:B:384:PRO:HD2	1.98	0.44
1:A:406[A]:GLN:O	1:A:410:ARG:HG3	2.17	0.44
1:B:381:ARG:NH2	3:B:473:HOH:O	2.42	0.44
1:A:242:HIS:CD2	1:A:243[A]:MET:CE	2.95	0.44
1:A:242:HIS:CD2	1:A:243[A]:MET:HE1	2.52	0.44
1:A:277:LYS:HE3	1:A:277:LYS:HB3	1.41	0.44
1:A:383:GLN:O	1:A:384:PRO:C	2.56	0.44
1:B:381:ARG:HD3	1:B:389:LEU:HD23	2.00	0.43
1:A:218:GLU:HB2	1:B:178:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LEU:CD1	1:A:396:MET:CE	2.96	0.43
1:B:216:ARG:O	1:B:303:ARG:HD2	2.18	0.43
1:A:218:GLU:H	1:B:178:LEU:HB3	1.84	0.43
1:B:323:MET:CE	1:B:403:ILE:CD1	2.95	0.43
1:A:323:MET:CE	1:A:403:ILE:HG21	2.48	0.43
1:A:145:GLU:O	1:A:149:MET:HG2	2.18	0.43
1:B:216:ARG:NH1	1:B:216:ARG:HG3	2.33	0.43
1:B:150[B]:MET:HE2	1:B:154:LEU:CD2	2.49	0.43
1:B:213:LEU:HD23	1:B:214:GLN:N	2.34	0.43
1:B:349:PHE:O	1:B:366:GLN:HB2	2.19	0.42
1:B:213:LEU:HD21	1:B:215:LEU:HD11	2.01	0.42
1:B:278:GLY:HA3	1:B:353:ARG:HD2	2.00	0.42
2:B:2:SRL:H303	3:B:503:HOH:O	2.20	0.42
1:A:383:GLN:CG	1:A:384:PRO:CD	2.97	0.42
1:A:406[B]:GLN:O	1:A:410:ARG:HG3	2.19	0.42
1:B:303:ARG:HG2	3:B:466:HOH:O	2.19	0.42
1:A:208:SER:HB2	1:A:321:GLU:OE1	2.20	0.42
1:A:242:HIS:HD2	1:A:243[A]:MET:HE1	1.78	0.42
1:B:360:ARG:HD3	1:B:360:ARG:HA	1.82	0.42
1:A:150:MET:HE3	1:A:368:GLN:NE2	2.34	0.42
1:A:250:MET:HG3	1:A:288:PHE:CZ	2.55	0.42
1:B:144:THR:CG2	1:B:147:GLN:CG	2.95	0.41
1:B:360:ARG:NE	3:B:496:HOH:O	2.53	0.41
1:B:141:GLN:NE2	1:B:148:ARG:HG2	2.32	0.41
1:B:218:GLU:H	1:B:218:GLU:HG3	1.57	0.41
1:A:316:GLN:HA	1:A:319:LEU:CD2	2.37	0.41
1:B:325:LYS:HD2	3:B:490:HOH:O	2.19	0.41
1:A:383:GLN:HG3	1:A:384:PRO:CD	2.51	0.41
1:B:321:GLU:OE2	1:B:322:PRO:HD2	2.20	0.41
1:B:411:LEU:HB2	2:B:2:SRL:H332	2.03	0.41
1:A:228:PRO:HD3	1:B:221:SER:HB3	2.03	0.40
1:A:446:THR:HG23	3:A:493:HOH:O	2.20	0.40
1:A:426:GLN:HA	1:A:431:ILE:HB	2.02	0.40
1:B:192:SER:O	1:B:193:ARG:O	2.39	0.40
1:B:218:GLU:HA	1:B:303:ARG:CZ	2.51	0.40
1:B:240:LEU:HA	1:B:240:LEU:HD23	1.77	0.40
1:B:445:LEU:O	1:B:449:HIS:ND1	2.50	0.40
1:A:358:GLN:HE21	1:A:358:GLN:HA	1.86	0.40
1:A:252:LYS:HB3	1:A:252:LYS:HE3	1.99	0.40
1:B:318:LEU:H	1:B:318:LEU:HG	1.76	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	281/344 (82%)	270 (96%)	7 (2%)	4 (1%)	11 6
1	B	282/344 (82%)	271 (96%)	7 (2%)	4 (1%)	11 6
All	All	563/688 (82%)	541 (96%)	14 (2%)	8 (1%)	11 6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	GLN
1	A	384	PRO
1	B	141	GLN
1	B	193	ARG
1	B	142	GLY
1	B	234	LYS
1	A	319	LEU
1	A	233	GLY

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	261/302 (86%)	244 (94%)	17 (6%)	17 14
1	B	261/302 (86%)	228 (87%)	33 (13%)	4 2
All	All	522/604 (86%)	472 (90%)	50 (10%)	8 5

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

Mol	Chain	Res	Type
1	A	152	ARG
1	A	159	MET
1	A	162	PHE
1	A	178	LEU
1	A	192	SER
1	A	194	GLU
1	A	208	SER
1	A	209	LEU
1	A	215	LEU
1	A	218	GLU
1	A	277	LYS
1	A	308	LEU
1	A	319	LEU
1	A	360	ARG
1	A	383	GLN
1	A	396	MET
1	A	457	GLN
1	B	140	VAL
1	B	145	GLU
1	B	146	GLU
1	B	159	MET
1	B	167	SER
1	B	170	LYS
1	B	177	VAL
1	B	178	LEU
1	B	192	SER
1	B	195	GLU
1	B	198	LYS
1	B	200	SER
1	B	201	GLN
1	B	208	SER
1	B	210	LYS
1	B	243	MET
1	B	265	ARG
1	B	298	THR
1	B	304	LEU
1	B	308	LEU
1	B	318	LEU
1	B	320	LEU
1	B	323	MET
1	B	324	LEU
1	B	341	VAL
1	B	347	SER

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Mol	Chain	Res	Type
1	B	380	ASN
1	B	381	ARG
1	B	396	MET
1	B	446	THR
1	B	448	ARG
1	B	450	LYS
1	B	460	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	214	GLN
1	A	272	GLN
1	A	285	GLN
1	A	358	GLN
1	A	364	GLN
1	A	368	GLN
1	A	383	GLN
1	A	418	HIS
1	A	449	HIS
1	A	453	HIS
1	A	457	GLN
1	B	141	GLN
1	B	214	GLN
1	B	224	ASN
1	B	272	GLN
1	B	380	ASN
1	B	386	HIS
1	B	418	HIS
1	B	453	HIS
1	B	457	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
2	SRL	B	2	-	30,33,33	2.01	11 (36%)	47,50,50	2.30	15 (31%)
2	SRL	A	1	-	30,33,33	1.84	9 (30%)	47,50,50	1.99	14 (29%)

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	SRL	B	2	-	-	4/34/44/44	0/1/1/1
2	SRL	A	1	-	-	5/34/44/44	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	SRL	C4-C3	4.62	1.46	1.39
2	B	2	SRL	P9-O20	4.38	1.51	1.46
2	B	2	SRL	C2-C1	4.14	1.46	1.41
2	B	2	SRL	C4-C3	3.98	1.45	1.39
2	A	1	SRL	P10-O28	2.99	1.64	1.57
2	B	2	SRL	C6-C1	2.85	1.43	1.39
2	A	1	SRL	C2-C1	2.83	1.45	1.41
2	A	1	SRL	P9-O20	2.79	1.49	1.46
2	B	2	SRL	C2-C3	2.73	1.44	1.41
2	A	1	SRL	C6-C1	2.58	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	SRL	C13-C3	2.52	1.58	1.54
2	A	1	SRL	P10-O31	2.49	1.63	1.57
2	A	1	SRL	O11-C2	-2.32	1.31	1.37
2	A	1	SRL	C2-C3	2.20	1.44	1.41
2	B	2	SRL	P9-O21	2.18	1.62	1.57
2	B	2	SRL	O11-C2	-2.15	1.32	1.37
2	B	2	SRL	P10-O31	2.13	1.62	1.57
2	B	2	SRL	C19-C13	2.06	1.60	1.53
2	B	2	SRL	C12-C1	2.05	1.58	1.54
2	A	1	SRL	C16-C12	2.01	1.60	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	SRL	C13-C3-C2	7.45	129.83	121.96
2	A	1	SRL	C3-C2-C1	5.41	127.85	122.64
2	B	2	SRL	C3-C2-C1	5.31	127.76	122.64
2	B	2	SRL	C4-C3-C2	-5.23	111.92	116.85
2	A	1	SRL	C13-C3-C2	4.81	127.04	121.96
2	B	2	SRL	O24-P9-O21	4.07	113.45	101.89
2	A	1	SRL	O24-P9-O21	3.96	113.16	101.89
2	A	1	SRL	C4-C3-C2	-3.94	113.14	116.85
2	A	1	SRL	C6-C1-C2	-3.72	113.35	116.85
2	B	2	SRL	C5-C7-C8	-3.67	123.99	130.93
2	B	2	SRL	C6-C1-C2	-3.65	113.42	116.85
2	B	2	SRL	O20-P9-C8	-3.62	106.01	113.03
2	B	2	SRL	P10-O28-C29	-3.26	111.17	121.87
2	A	1	SRL	O20-P9-C8	-3.05	107.12	113.03
2	A	1	SRL	O21-P9-O20	-3.05	106.95	115.03
2	B	2	SRL	O21-P9-O20	-3.04	106.96	115.03
2	B	2	SRL	C12-C1-C2	2.92	125.04	121.96
2	A	1	SRL	O24-P9-C8	2.89	114.39	104.76
2	A	1	SRL	C5-C7-C8	-2.75	125.72	130.93
2	B	2	SRL	O24-P9-C8	2.75	113.92	104.76
2	A	1	SRL	O28-P10-O27	-2.72	107.81	115.03
2	A	1	SRL	P10-O31-C32	-2.69	113.01	121.87
2	A	1	SRL	P10-O28-C29	-2.56	113.47	121.87
2	B	2	SRL	C18-C13-C3	2.42	115.47	110.86
2	B	2	SRL	P10-O31-C32	-2.38	114.06	121.87
2	B	2	SRL	O27-P10-C8	2.37	117.61	113.03
2	B	2	SRL	O28-P10-O27	-2.16	109.30	115.03
2	A	1	SRL	O28-P10-C8	2.06	111.63	104.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	SRL	O24-P9-O20	-2.03	109.66	115.03

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	SRL	C29-O28-P10-O27
2	A	1	SRL	C29-O28-P10-O27
2	B	2	SRL	C29-O28-P10-O31
2	A	1	SRL	C32-O31-P10-C8
2	A	1	SRL	C32-O31-P10-O28
2	B	2	SRL	C32-O31-P10-O28
2	A	1	SRL	C29-O28-P10-O31
2	A	1	SRL	C7-C8-P10-O28
2	B	2	SRL	C7-C8-P10-O28

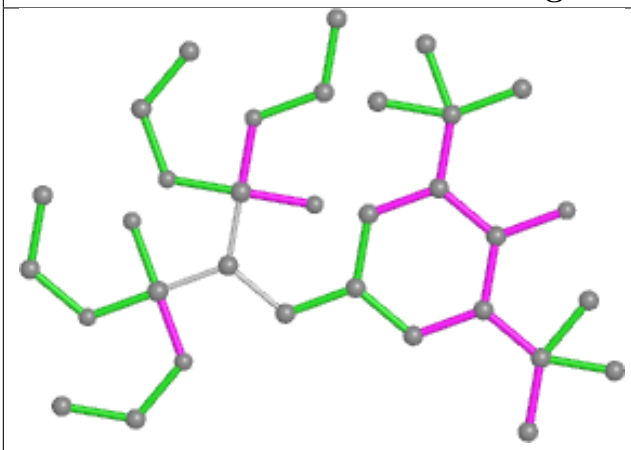
There are no ring outliers.

2 monomers are involved in 10 short contacts:

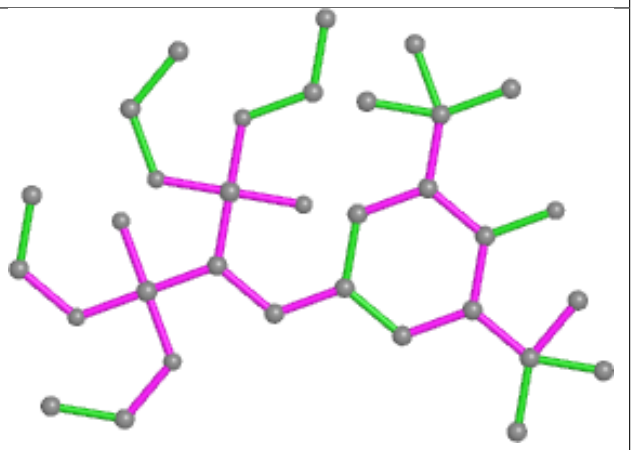
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	SRL	5	0
2	A	1	SRL	5	0

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.

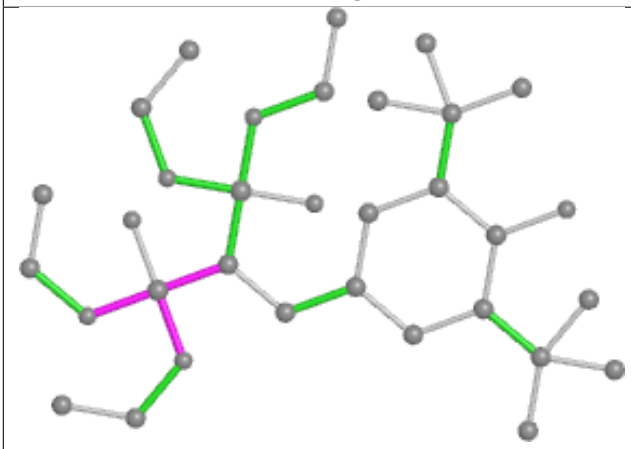
Ligand SRL B 2



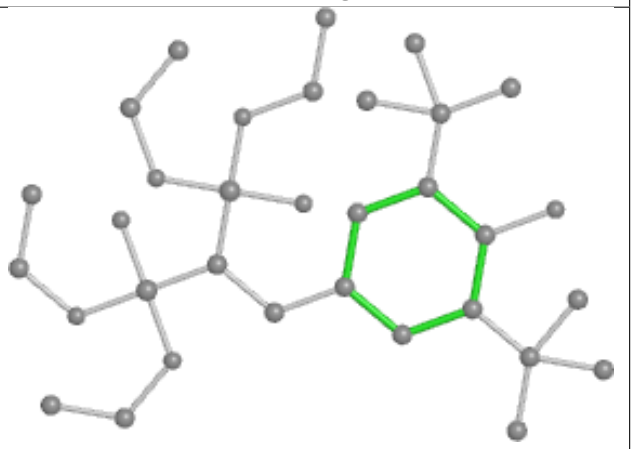
Bond lengths



Bond angles

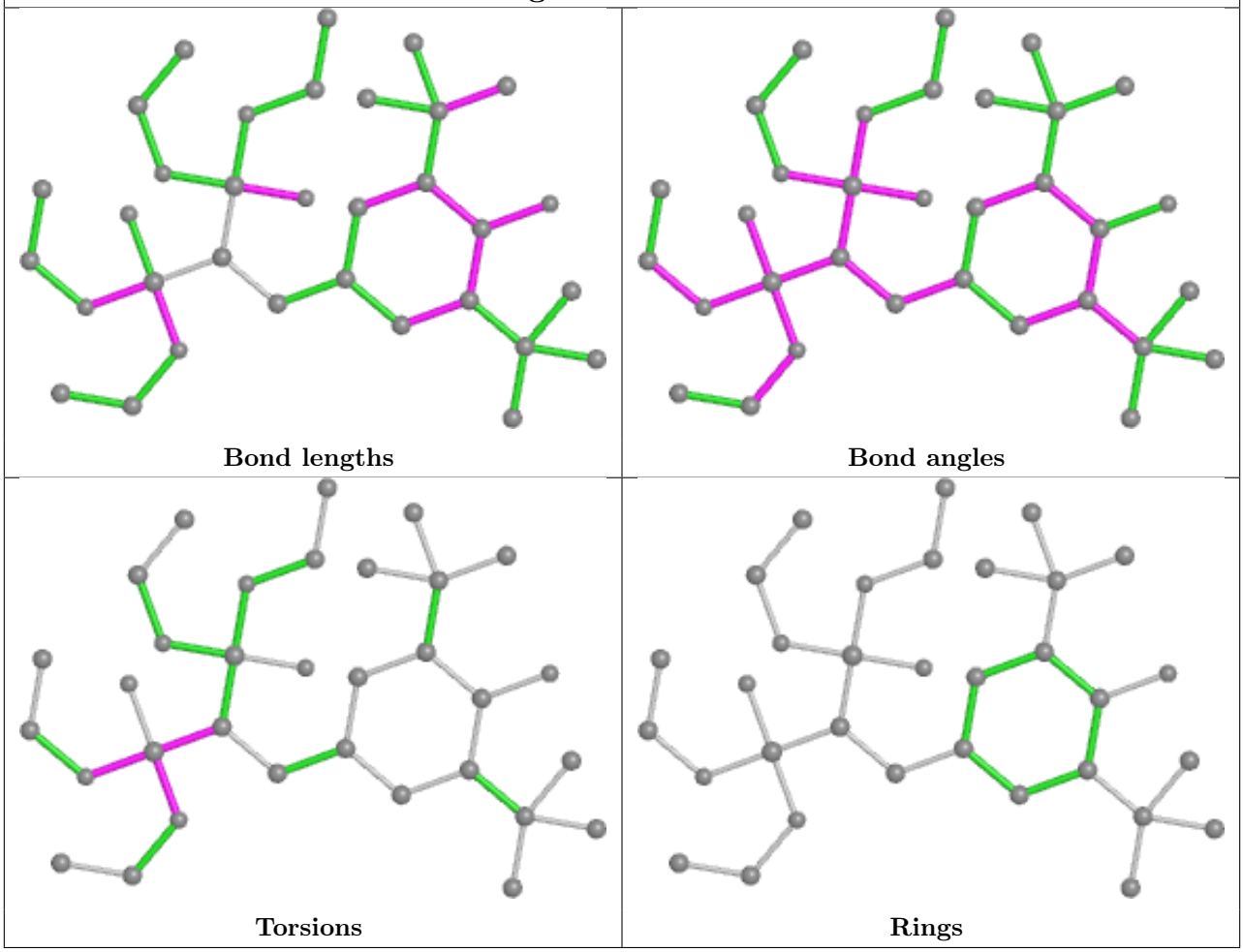


Torsions



Rings

Ligand SRL A 1



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, 95^{th} 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	287/344 (83%)	0.15	11 (3%)	40	46	37, 55, 89, 122	0
1	B	289/344 (84%)	0.44	24 (8%)	11	14	41, 58, 99, 149	0
All	All	576/688 (83%)	0.30	35 (6%)	21	26	37, 57, 98, 149	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	ALA	7.5
1	B	197	ALA	6.1
1	B	192	SER	5.8
1	A	383	GLN	5.6
1	B	140	VAL	5.4
1	B	194	GLU	5.3
1	A	177	VAL	5.3
1	B	178	LEU	5.2
1	B	193	ARG	4.9
1	A	178	LEU	4.0
1	B	200	SER	3.8
1	A	316	GLN	3.8
1	A	232	GLY	3.8
1	B	445	LEU	3.8
1	A	192	SER	3.3
1	B	234	LYS	3.2
1	B	417	ILE	3.1
1	B	360	ARG	3.1
1	B	318	LEU	2.9
1	B	141	GLN	2.7
1	A	142	GLY	2.7
1	B	201	GLN	2.6
1	B	207	CYS	2.6
1	A	195	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	177	VAL	2.5
1	B	384	PRO	2.5
1	B	444	SER	2.4
1	B	419	PRO	2.3
1	B	448	ARG	2.2
1	A	194	GLU	2.2
1	B	447	GLU	2.2
1	A	319	LEU	2.2
1	B	142	GLY	2.1
1	B	235	GLU	2.1
1	A	193	ARG	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)

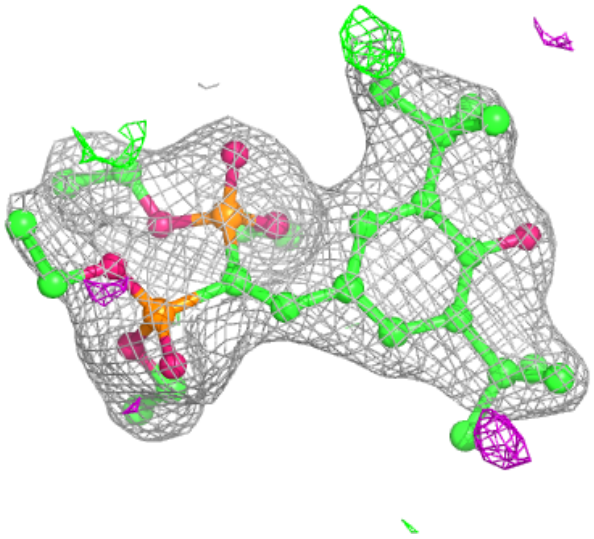
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

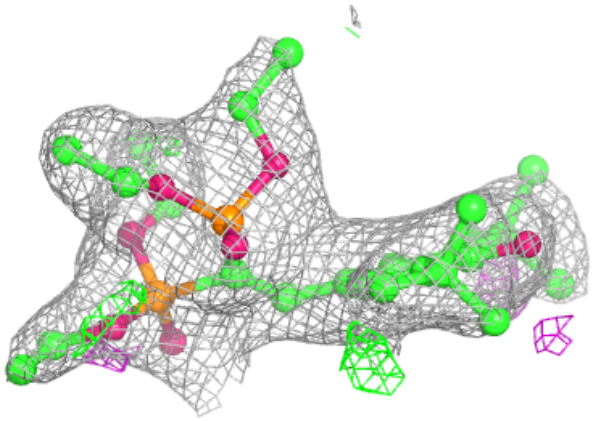
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SRL	B	2	33/33	0.94	0.14	55,66,77,79	0
2	SRL	A	1	33/33	0.96	0.13	45,59,68,69	0

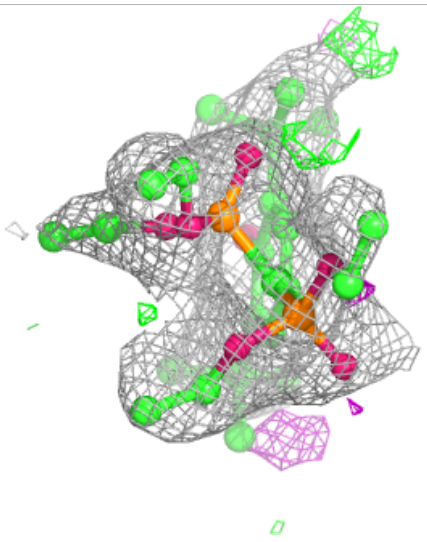
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SRL B 2:

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

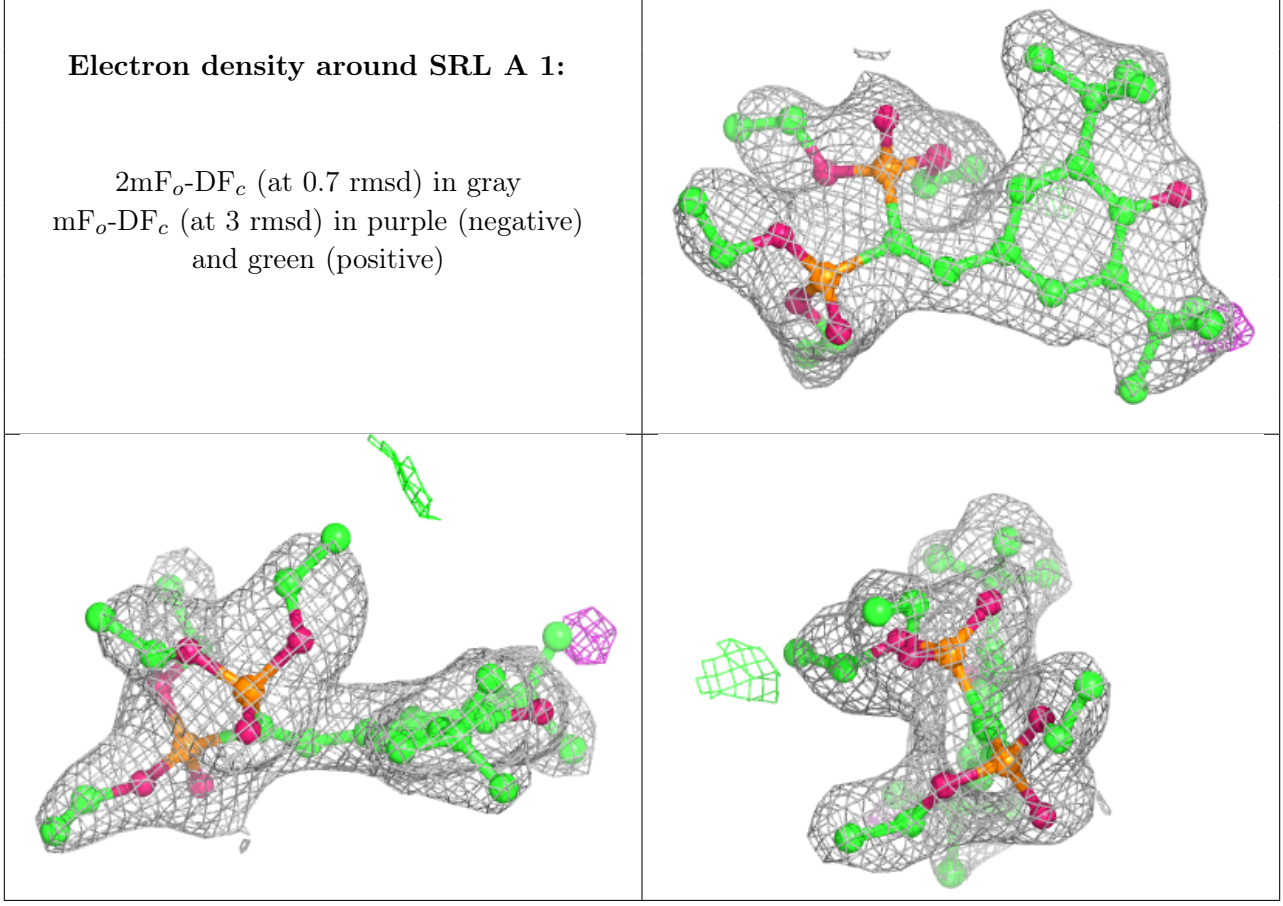






Electron density around SRL A 1:

$2mF_o$-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.