



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:00 PM UTC

PDB ID : 4LA0 / pdb_00004la0
Title : X-ray study of human serum albumin complexed with bicalutamide
Authors : Wang, Z.; Ho, J.X.; Ruble, J.; Rose, J.P.; Carter, D.C.
Deposited on : 2013-06-18
Resolution : 2.40 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

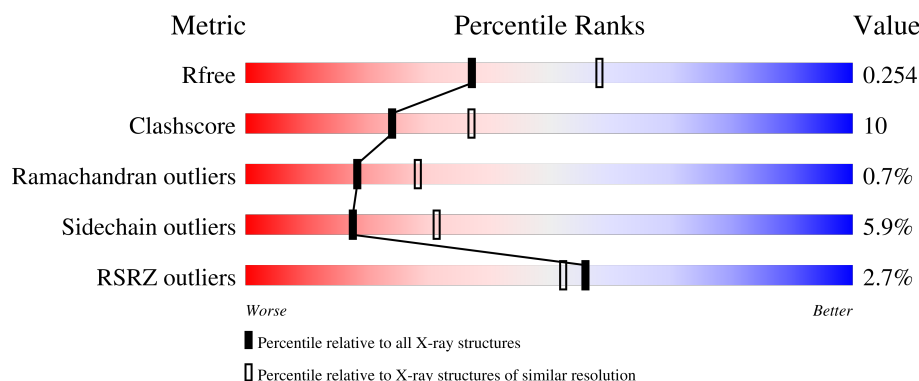
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	585	% 72% 24% ..
1	B	585	4% 77% 20% ..

2 Entry composition [i](#)

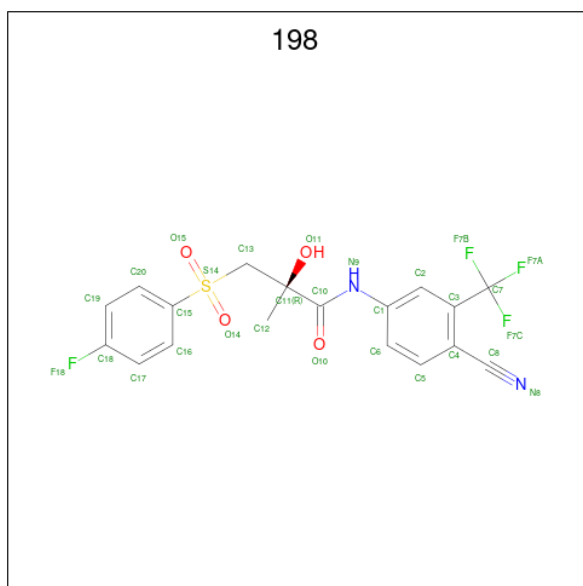
There are 3 unique types of molecules in this entry. The entry contains 9482 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERUM ALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4623	2918	782	882	41			
1	B	580	Total	C	N	O	S	0	0	0
			4618	2915	781	881	41			

- Molecule 2 is R-BICALUTAMIDE (CCD ID: 198) (formula: C₁₈H₁₄F₄N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0
			29	18	4	2	4	1	
2	B	1	Total	C	F	N	O	S	0
			29	18	4	2	4	1	

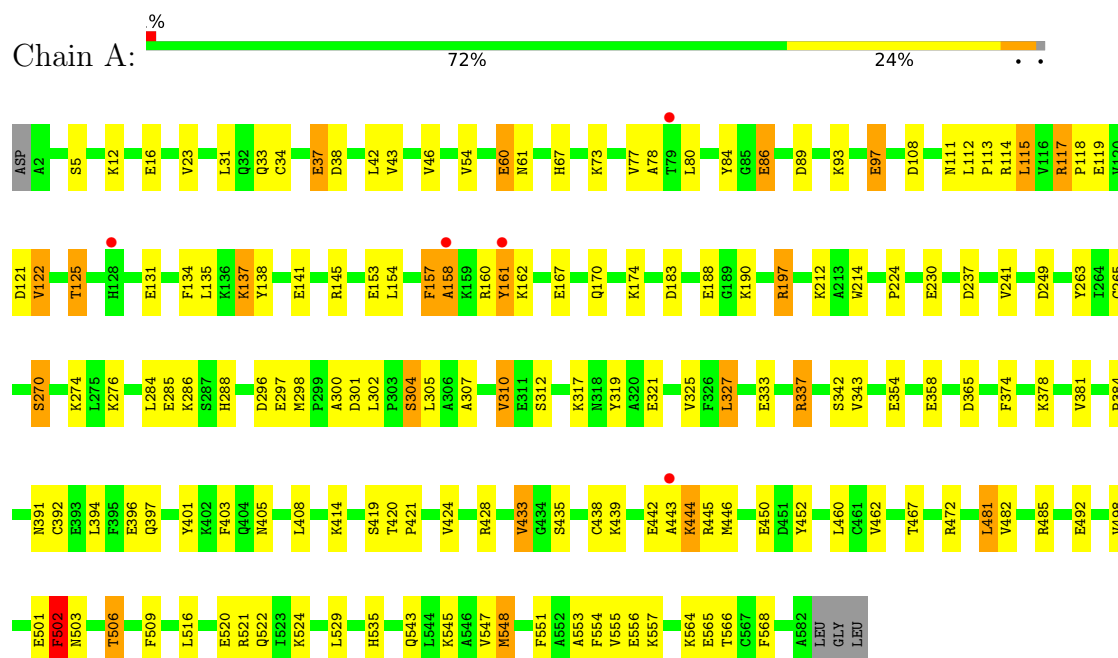
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total 123	O 123	0	0
3	B	60	Total 60	O 60	0	0

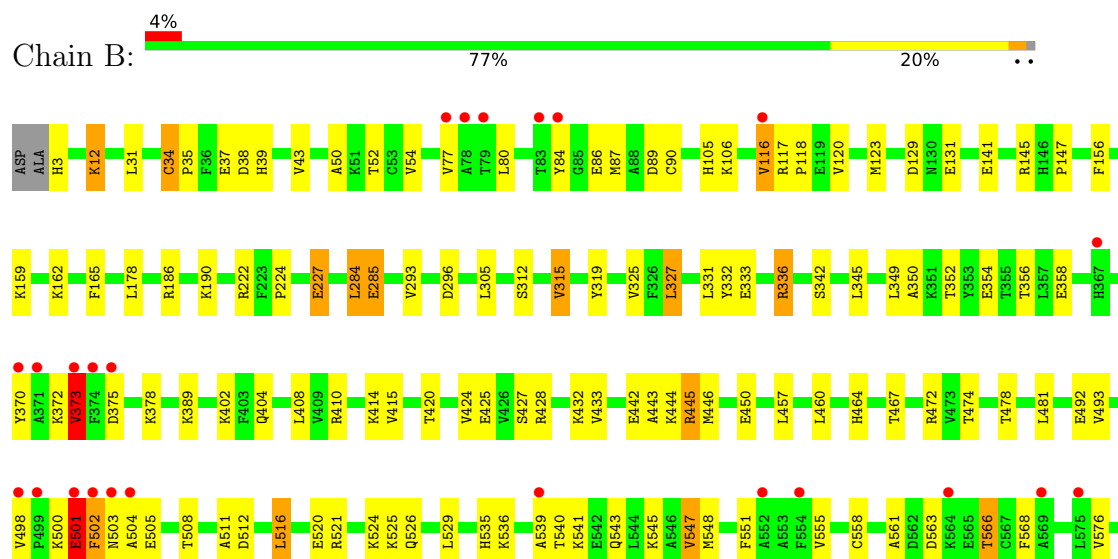
3 Residue-property plots

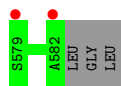
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: SERUM ALBUMIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.44Å 59.57Å 95.96Å 73.22° 83.93° 74.17°	Depositor
Resolution (Å)	29.86 – 2.40 29.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.3 (29.86-2.40) 87.2 (29.86-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.199 , 0.254 0.203 , 0.254	Depositor DCC
R_{free} test set	1877 reflections (4.17%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9482	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 198

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	0.65	3/4713 (0.1%)	1.05	26/6357 (0.4%)
1	B	0.56	0/4708	0.96	11/6350 (0.2%)
All	All	0.61	3/9421 (0.0%)	1.01	37/12707 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	TYR	N-CA	6.93	1.54	1.46
1	A	157	PHE	C-N	5.19	1.40	1.33
1	A	160	ARG	CA-C	5.02	1.59	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ARG	N-CA-C	12.17	124.62	111.36
1	A	157	PHE	CA-C-O	-12.10	107.73	120.55
1	A	161	TYR	N-CA-C	-11.39	98.94	111.36
1	A	160	ARG	CA-C-N	9.19	133.34	120.29
1	A	160	ARG	C-N-CA	9.19	133.34	120.29
1	A	157	PHE	N-CA-C	-8.73	101.77	111.28
1	A	481	LEU	N-CA-C	-8.13	103.31	113.55
1	A	300	ALA	N-CA-C	8.04	119.95	111.03
1	A	158	ALA	N-CA-CB	7.94	124.76	110.32
1	B	498	VAL	CA-C-N	7.43	127.87	119.92
1	B	498	VAL	C-N-CA	7.43	127.87	119.92
1	A	117	ARG	CA-C-N	6.31	127.73	119.84
1	A	117	ARG	C-N-CA	6.31	127.73	119.84
1	A	378	LYS	CA-C-N	-6.17	113.33	119.56
1	A	378	LYS	C-N-CA	-6.17	113.33	119.56
1	B	481	LEU	N-CA-C	-6.16	105.79	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	501	GLU	CA-C-N	-6.08	114.22	122.86
1	B	501	GLU	C-N-CA	-6.08	114.22	122.86
1	B	373	VAL	CB-CA-C	-6.00	104.03	111.70
1	A	157	PHE	N-CA-CB	5.89	118.79	110.12
1	A	555	VAL	N-CA-C	-5.70	105.17	110.53
1	B	378	LYS	CA-C-N	-5.56	113.94	119.56
1	B	378	LYS	C-N-CA	-5.56	113.94	119.56
1	B	336	ARG	CB-CA-C	-5.52	101.30	110.68
1	B	502	PHE	N-CA-C	5.36	117.56	108.02
1	B	501	GLU	N-CA-C	5.26	122.00	110.80
1	A	16	GLU	N-CA-C	5.25	117.42	111.11
1	A	391	ASN	N-CA-C	5.25	117.00	111.28
1	A	485	ARG	CA-C-N	-5.20	113.68	119.19
1	A	485	ARG	C-N-CA	-5.20	113.68	119.19
1	A	450	GLU	N-CA-C	5.15	116.89	111.28
1	A	365	ASP	CA-C-N	5.15	125.19	119.32
1	A	365	ASP	C-N-CA	5.15	125.19	119.32
1	A	502	PHE	N-CA-CB	5.14	119.17	110.49
1	A	365	ASP	CB-CA-C	5.13	115.86	110.17
1	A	501	GLU	N-CA-C	5.07	117.70	111.82
1	A	158	ALA	N-CA-C	5.06	118.94	112.87

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	4623	0	4543	97	0
1	B	4618	0	4538	85	1
2	A	29	0	14	4	0
2	B	29	0	14	1	0
3	A	123	0	0	10	0
3	B	60	0	0	7	0
All	All	9482	0	9109	184	1

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 10.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:NH2	3:A:725:HOH:O	1.82	1.08
1:A:135:LEU:HG	1:A:161:TYR:CE1	2.05	0.90
1:B:89:ASP:OD2	3:B:754:HOH:O	1.88	0.90
1:A:333:GLU:OE1	1:A:337:ARG:NH2	2.08	0.85
1:B:501:GLU:O	1:B:535:HIS:NE2	2.10	0.85
1:A:158:ALA:HA	1:A:161:TYR:HE2	1.40	0.84
2:B:601:198:F7A	3:B:745:HOH:O	1.86	0.82
1:B:34:CYS:HG	1:B:84:TYR:HH	0.84	0.82
1:B:80:LEU:HD11	1:B:84:TYR:CE2	2.19	0.76
1:B:414:LYS:O	1:B:472:ARG:NH1	2.16	0.76
1:B:500:LYS:O	1:B:502:PHE:N	2.18	0.76
1:A:31:LEU:HD11	1:A:78:ALA:HB2	1.67	0.75
1:A:158:ALA:HA	1:A:161:TYR:CE2	2.25	0.71
1:A:405:ASN:HA	1:A:408:LEU:HD12	1.72	0.71
1:A:522:GLN:OE1	3:A:742:HOH:O	2.09	0.69
1:A:135:LEU:HG	1:A:161:TYR:HE1	1.57	0.68
1:A:428:ARG:NH2	3:A:742:HOH:O	2.27	0.66
1:A:270:SER:O	3:A:733:HOH:O	2.14	0.66
1:B:80:LEU:HD11	1:B:84:TYR:CD2	2.31	0.66
1:A:119:GLU:HB2	1:A:122:VAL:HG22	1.76	0.66
1:B:159:LYS:NZ	1:B:285:GLU:OE1	2.28	0.66
1:A:230:GLU:OE1	3:A:766:HOH:O	2.15	0.65
1:B:186:ARG:NH2	3:B:729:HOH:O	1.88	0.65
1:B:87:MET:HG2	1:B:105:HIS:CD2	2.31	0.65
1:A:435:SER:O	1:A:439:LYS:HE3	1.96	0.65
1:A:157:PHE:HZ	1:A:188:GLU:HG2	1.62	0.63
1:B:12:LYS:HE2	1:B:54:VAL:HG13	1.81	0.63
1:B:116:VAL:N	3:B:720:HOH:O	2.30	0.63
1:A:298:MET:HE3	1:A:302:LEU:HD12	1.80	0.63
1:A:12:LYS:HD3	1:A:54:VAL:HG13	1.81	0.62
1:A:114:ARG:HH22	1:A:520:GLU:CD	2.08	0.62
1:B:370:TYR:O	1:B:373:VAL:HG22	2.00	0.61
1:A:114:ARG:NH2	1:A:520:GLU:OE2	2.28	0.60
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.36	0.60
1:A:135:LEU:HD21	1:A:162:LYS:HB2	1.84	0.60
1:A:419:SER:OG	1:A:421:PRO:HD2	2.02	0.59
1:A:424:VAL:O	1:A:428:ARG:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:O	1:A:170:GLN:HG2	2.04	0.58
1:A:502:PHE:HB2	1:A:535:HIS:CE1	2.39	0.58
1:A:46:VAL:HG23	1:A:73:LYS:HG2	1.85	0.58
1:A:154:LEU:O	1:A:158:ALA:N	2.36	0.57
1:B:558:CYS:HA	1:B:561:ALA:HB2	1.87	0.57
1:B:467:THR:O	1:B:467:THR:OG1	2.19	0.57
1:B:123:MET:HE2	1:B:165:PHE:HZ	1.69	0.56
1:B:80:LEU:HD12	1:B:80:LEU:O	2.05	0.56
1:B:327:LEU:HD21	1:B:354:GLU:HB2	1.87	0.56
1:A:153:GLU:OE2	1:A:288:HIS:ND1	2.35	0.56
1:B:332:TYR:O	1:B:336:ARG:HG3	2.06	0.56
1:B:525:LYS:HG2	1:B:551:PHE:CE1	2.41	0.56
1:A:212:LYS:NZ	3:A:789:HOH:O	2.39	0.56
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.88	0.55
1:A:516:LEU:O	1:A:521:ARG:NH2	2.39	0.55
1:B:516:LEU:HB3	1:B:520:GLU:HB2	1.89	0.55
1:B:543:GLN:O	1:B:547:VAL:HG12	2.07	0.54
1:A:138:TYR:CD2	1:A:161:TYR:CE2	2.96	0.54
1:A:414:LYS:O	1:A:472:ARG:NH2	2.41	0.54
1:B:408:LEU:HD13	1:B:427:SER:HB2	1.91	0.54
1:B:141:GLU:OE1	1:B:145:ARG:NH1	2.37	0.53
1:A:442:GLU:O	1:A:444:LYS:N	2.41	0.53
1:B:37:GLU:H	1:B:37:GLU:CD	2.15	0.53
1:A:302:LEU:HB3	1:A:337:ARG:NH1	2.23	0.53
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.90	0.53
1:B:561:ALA:O	1:B:563:ASP:N	2.35	0.52
1:A:108:ASP:OD1	1:A:197:ARG:HD2	2.08	0.52
1:B:227:GLU:HB2	3:B:724:HOH:O	2.10	0.52
1:B:402:LYS:HG2	1:B:545:LYS:HZ1	1.74	0.52
1:B:516:LEU:O	1:B:521:ARG:NH2	2.42	0.52
1:A:230:GLU:OE2	1:A:263:TYR:OH	2.18	0.51
1:B:50:ALA:O	1:B:54:VAL:HG23	2.10	0.51
1:A:77:VAL:O	1:A:80:LEU:HD12	2.09	0.51
1:B:39:HIS:O	1:B:43:VAL:HG23	2.10	0.51
1:A:118:PRO:HG2	2:A:601:198:H121	1.92	0.51
1:A:274:LYS:NZ	1:A:297:GLU:OE2	2.28	0.51
1:B:428:ARG:NH1	1:B:526:GLN:OE1	2.42	0.51
1:B:410:ARG:HG2	1:B:414:LYS:HE2	1.93	0.50
1:A:135:LEU:HG	1:A:161:TYR:CZ	2.46	0.50
1:A:237:ASP:O	1:A:241:VAL:HG23	2.11	0.50
1:A:553:ALA:O	1:A:556:GLU:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:LEU:HD13	1:B:350:ALA:HB2	1.93	0.50
1:A:381:VAL:O	1:A:384:PRO:HD2	2.12	0.50
1:A:317:LYS:HE2	1:A:321:GLU:OE2	2.12	0.49
1:A:60:GLU:HG2	1:A:61:ASN:ND2	2.26	0.49
1:A:503:ASN:HB3	1:A:506:THR:HG23	1.93	0.49
1:B:89:ASP:OD1	1:B:90:CYS:N	2.45	0.49
1:B:3:HIS:CD2	1:B:3:HIS:O	2.66	0.49
1:A:564:LYS:C	1:A:566:THR:H	2.20	0.49
1:B:501:GLU:O	1:B:535:HIS:CE1	2.66	0.48
1:A:117:ARG:NH2	1:A:183:ASP:OD1	2.46	0.48
1:A:438:CYS:O	1:A:445:ARG:NH2	2.46	0.48
1:A:37:GLU:H	1:A:37:GLU:CD	2.22	0.47
1:A:433:VAL:HG23	1:A:452:TYR:CD2	2.49	0.47
1:B:305:LEU:HD21	1:B:333:GLU:HB3	1.96	0.47
1:B:536:LYS:O	1:B:540:THR:OG1	2.30	0.47
1:A:89:ASP:OD2	3:A:778:HOH:O	2.20	0.47
1:A:115:LEU:HD21	1:A:141:GLU:HB3	1.95	0.47
1:B:319:TYR:OH	1:B:358:GLU:OE2	2.26	0.47
1:A:119:GLU:OE2	3:A:757:HOH:O	2.20	0.47
1:A:310:VAL:HG13	1:A:374:PHE:HE2	1.79	0.47
1:B:349:LEU:HA	1:B:352:THR:HG22	1.97	0.47
1:A:134:PHE:CE1	2:A:601:198:H131	2.50	0.47
1:A:420:THR:O	1:A:424:VAL:HG23	2.15	0.47
1:B:420:THR:O	1:B:424:VAL:HG23	2.14	0.47
1:A:342:SER:HB3	1:A:446:MET:HG2	1.96	0.47
1:A:60:GLU:OE1	1:A:61:ASN:N	2.44	0.47
1:B:535:HIS:C	1:B:535:HIS:HD1	2.23	0.46
1:B:561:ALA:HB1	1:B:563:ASP:OD1	2.16	0.46
1:B:156:PHE:CD1	1:B:284:LEU:HB3	2.51	0.46
1:A:33:GLN:NE2	3:A:822:HOH:O	1.98	0.46
1:A:516:LEU:HB3	1:A:520:GLU:HB2	1.96	0.46
1:B:511:ALA:HA	1:B:568:PHE:CE2	2.51	0.46
1:B:561:ALA:C	1:B:563:ASP:H	2.22	0.46
1:B:186:ARG:O	1:B:190:LYS:HG2	2.16	0.46
1:B:80:LEU:CD1	1:B:84:TYR:CD2	2.97	0.46
1:A:327:LEU:HD21	1:A:354:GLU:HG3	1.98	0.45
1:A:154:LEU:HA	1:A:157:PHE:HB2	1.98	0.45
1:B:131:GLU:OE2	1:B:162:LYS:HE3	2.17	0.45
1:B:356:THR:HG21	1:B:373:VAL:HA	1.99	0.45
1:B:464:HIS:HE1	1:B:474:THR:OG1	2.00	0.45
1:B:31:LEU:HB2	1:B:39:HIS:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:LYS:HB2	1:B:375:ASP:HB2	1.99	0.45
1:A:115:LEU:HD22	1:A:145:ARG:CZ	2.47	0.45
1:A:554:PHE:HA	1:A:557:LYS:HB3	1.98	0.44
1:B:521:ARG:HD3	1:B:555:VAL:HG11	1.98	0.44
1:B:389:LYS:HA	1:B:445:ARG:HH12	1.83	0.44
1:B:408:LEU:HD21	1:B:526:GLN:HB3	1.98	0.44
1:A:34:CYS:HG	1:A:84:TYR:HH	1.63	0.44
1:A:23:VAL:HG12	1:A:43:VAL:HG22	2.00	0.44
1:A:121:ASP:O	1:A:125:THR:OG1	2.35	0.44
1:A:298:MET:CE	1:A:302:LEU:HD12	2.46	0.44
1:B:120:VAL:HG13	1:B:178:LEU:HD23	1.99	0.44
2:A:601:198:O10	2:A:601:198:H2	2.18	0.44
1:B:35:PRO:HG2	1:B:38:ASP:OD2	2.18	0.44
1:B:80:LEU:HD11	1:B:84:TYR:HE2	1.74	0.44
1:A:93:LYS:HD2	1:A:97:GLU:HB2	1.99	0.43
1:B:404:GLN:O	1:B:408:LEU:HB2	2.18	0.43
1:B:117:ARG:HA	1:B:118:PRO:HD3	1.85	0.43
1:A:38:ASP:O	1:A:42:LEU:HG	2.18	0.43
1:A:131:GLU:OE2	1:A:162:LYS:HE3	2.18	0.43
1:A:111:ASN:OD1	3:A:808:HOH:O	2.21	0.43
1:A:433:VAL:HG23	1:A:452:TYR:HD2	1.83	0.43
1:B:504:ALA:O	1:B:508:THR:HG23	2.19	0.43
1:A:401:TYR:CE1	1:A:522:GLN:HG2	2.54	0.43
1:B:408:LEU:HD23	1:B:529:LEU:HD23	1.99	0.43
1:A:117:ARG:HA	1:A:118:PRO:HD3	1.75	0.43
1:A:67:HIS:NE2	1:A:249:ASP:OD1	2.52	0.43
1:B:331:LEU:HD12	1:B:331:LEU:HA	1.83	0.43
1:B:415:VAL:HA	1:B:472:ARG:HH22	1.83	0.43
1:B:512:ASP:O	1:B:516:LEU:HD13	2.19	0.43
1:A:60:GLU:OE1	1:A:60:GLU:N	2.52	0.42
1:A:564:LYS:C	1:A:566:THR:N	2.76	0.42
1:B:457:LEU:HD23	1:B:457:LEU:HA	1.86	0.42
1:A:34:CYS:SG	1:A:84:TYR:OH	2.72	0.42
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.58	0.42
1:B:222:ARG:HD2	1:B:293:VAL:CG1	2.50	0.42
1:B:284:LEU:HD12	1:B:284:LEU:HA	1.90	0.42
1:B:222:ARG:HD2	1:B:293:VAL:HG13	2.01	0.42
1:A:137:LYS:HD3	2:A:601:198:O15	2.20	0.42
1:A:197:ARG:HD3	1:A:462:VAL:HG21	2.02	0.42
1:A:394:LEU:HD23	1:A:403:PHE:HE1	1.83	0.42
1:A:529:LEU:HB2	1:A:548:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLU:H	1:A:86:GLU:CD	2.28	0.42
1:B:87:MET:HE2	1:B:87:MET:HB3	1.92	0.42
1:A:392:CYS:O	1:A:396:GLU:HG2	2.19	0.41
1:B:545:LYS:HA	1:B:545:LYS:HD2	1.85	0.41
1:A:112:LEU:HA	1:A:113:PRO:HD2	1.84	0.41
1:B:345:LEU:O	1:B:349:LEU:HG	2.20	0.41
1:B:442:GLU:O	1:B:444:LYS:N	2.53	0.41
1:A:174:LYS:NZ	3:B:703:HOH:O	2.47	0.41
1:A:307:ALA:O	1:A:312:SER:HB2	2.20	0.41
1:B:410:ARG:O	1:B:414:LYS:HG3	2.21	0.41
1:A:304:SER:O	1:A:305:LEU:CB	2.69	0.41
1:A:319:TYR:OH	1:A:358:GLU:OE2	2.27	0.41
1:B:342:SER:HB3	1:B:446:MET:HG2	2.03	0.41
1:B:503:ASN:OD1	1:B:505:GLU:N	2.53	0.41
1:B:106:LYS:HD3	1:B:147:PRO:HB2	2.03	0.41
1:A:394:LEU:HD12	1:A:397:GLN:HE21	1.86	0.40
1:A:509:PHE:O	1:A:568:PHE:HB3	2.21	0.40
1:A:481:LEU:HD12	1:A:481:LEU:HA	1.74	0.40
1:B:116:VAL:HG12	3:B:720:HOH:O	2.20	0.40
1:B:428:ARG:O	1:B:432:LYS:HG3	2.22	0.40
1:B:31:LEU:HB2	1:B:39:HIS:CE1	2.56	0.40
1:B:563:ASP:O	1:B:566:THR:HG23	2.21	0.40
1:B:312:SER:O	1:B:315:VAL:HG12	2.22	0.40
1:A:97:GLU:CD	1:A:97:GLU:H	2.29	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ASP:OD1	1:B:541:LYS:NZ[1_455]	2.08	0.12

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	579/585 (99%)	553 (96%)	21 (4%)	5 (1%)	14	22
1	B	578/585 (99%)	549 (95%)	26 (4%)	3 (0%)	24	37
All	All	1157/1170 (99%)	1102 (95%)	47 (4%)	8 (1%)	18	28

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	444	LYS
1	B	501	GLU
1	A	502	PHE
1	B	443	ALA
1	B	539	ALA
1	A	443	ALA
1	A	5	SER
1	A	565	GLU

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	508/511 (99%)	475 (94%)	33 (6%)	15	27
1	B	508/511 (99%)	481 (95%)	27 (5%)	20	36
All	All	1016/1022 (99%)	956 (94%)	60 (6%)	18	31

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	60	GLU
1	A	86	GLU
1	A	97	GLU
1	A	115	LEU
1	A	122	VAL

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Mol	Chain	Res	Type
1	A	125	THR
1	A	137	LYS
1	A	190	LYS
1	A	197	ARG
1	A	270	SER
1	A	276	LYS
1	A	284	LEU
1	A	285	GLU
1	A	301	ASP
1	A	304	SER
1	A	310	VAL
1	A	325	VAL
1	A	327	LEU
1	A	337	ARG
1	A	433	VAL
1	A	460	LEU
1	A	467	THR
1	A	482	VAL
1	A	492	GLU
1	A	498	VAL
1	A	506	THR
1	A	524	LYS
1	A	543	GLN
1	A	545	LYS
1	A	547	VAL
1	A	548	MET
1	A	551	PHE
1	B	12	LYS
1	B	34	CYS
1	B	52	THR
1	B	77	VAL
1	B	86	GLU
1	B	116	VAL
1	B	227	GLU
1	B	284	LEU
1	B	285	GLU
1	B	315	VAL
1	B	325	VAL
1	B	327	LEU
1	B	373	VAL
1	B	425	GLU
1	B	433	VAL

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Mol	Chain	Res	Type
1	B	445	ARG
1	B	450	GLU
1	B	460	LEU
1	B	478	THR
1	B	492	GLU
1	B	493	VAL
1	B	516	LEU
1	B	524	LYS
1	B	547	VAL
1	B	548	MET
1	B	566	THR
1	B	576	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	385	GLN
1	A	459	GLN
1	B	3	HIS
1	B	105	HIS
1	B	267	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	198	A	601	-	30,30,30	1.46	4 (13%)	44,46,46	2.87	7 (15%)
2	198	B	601	-	30,30,30	1.43	3 (10%)	44,46,46	2.64	5 (11%)

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	198	A	601	-	-	1/30/30/30	0/2/2/2
2	198	B	601	-	-	3/30/30/30	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	198	C4-C8	5.46	1.52	1.44
2	B	601	198	C4-C8	5.27	1.52	1.44
2	B	601	198	C10-N9	3.42	1.43	1.35
2	A	601	198	C10-N9	2.97	1.42	1.35
2	A	601	198	C11-C10	-2.37	1.51	1.54
2	A	601	198	C15-S14	2.18	1.80	1.76
2	B	601	198	C7-C3	2.10	1.55	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	198	O15-S14-O14	-16.07	101.22	118.45
2	B	601	198	O15-S14-O14	-15.01	102.36	118.45
2	A	601	198	O14-S14-C15	5.75	113.84	108.33
2	B	601	198	C11-C10-N9	4.21	119.15	114.66
2	B	601	198	O15-S14-C15	3.63	111.80	108.33
2	A	601	198	F7C-C7-C3	-2.98	107.36	112.65
2	A	601	198	O15-S14-C15	2.71	110.92	108.33
2	B	601	198	O14-S14-C15	2.56	110.79	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	198	F7A-C7-C3	-2.52	108.18	112.65
2	B	601	198	C12-C11-C10	2.47	111.62	107.98
2	A	601	198	O14-S14-C13	2.10	112.82	107.97
2	A	601	198	F7A-C7-F7B	2.02	113.06	105.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

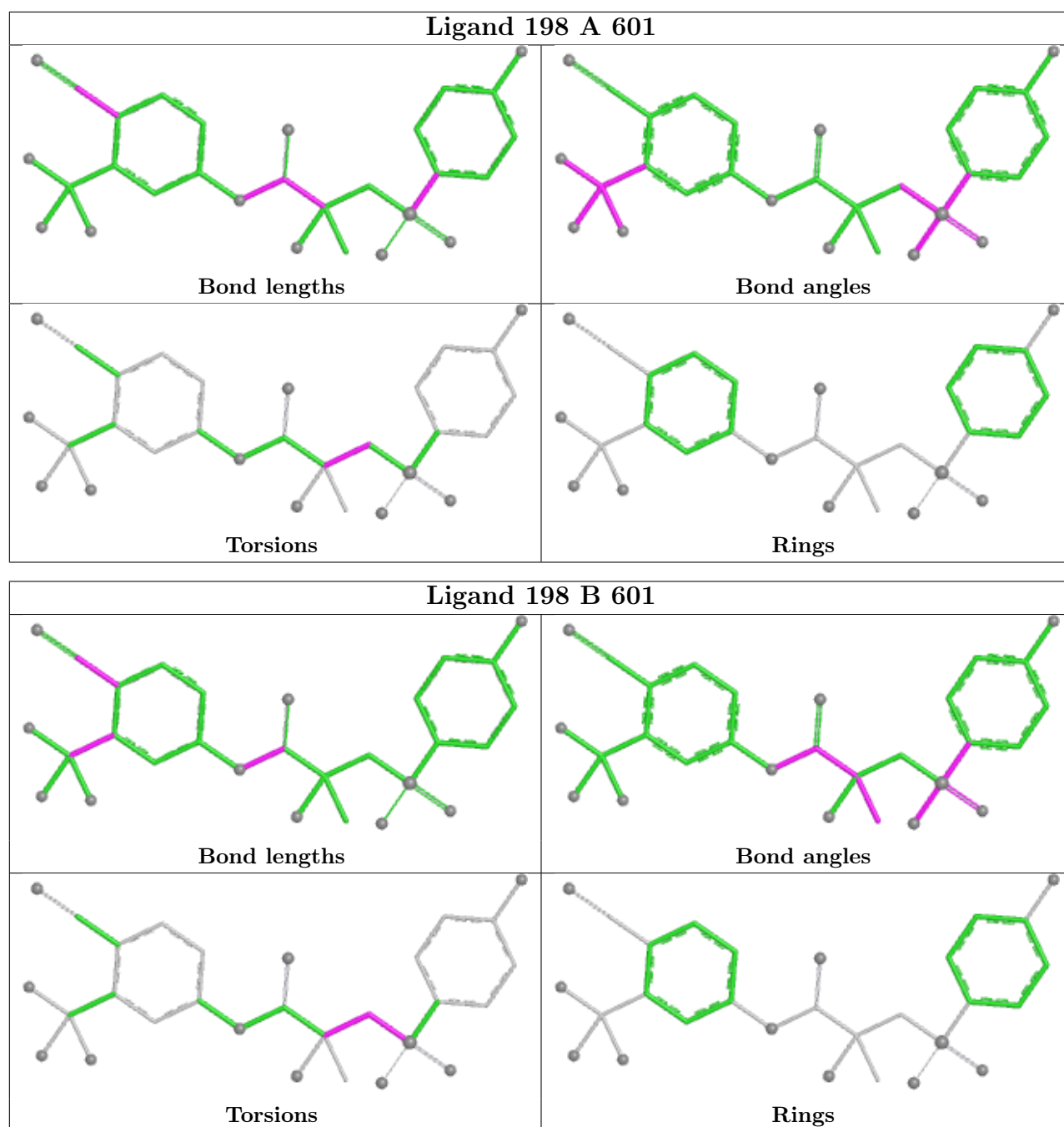
Mol	Chain	Res	Type	Atoms
2	A	601	198	C12-C11-C13-S14
2	B	601	198	C11-C13-S14-C15
2	B	601	198	C12-C11-C13-S14
2	B	601	198	C11-C13-S14-O15

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	198	4	0
2	B	601	198	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	581/585 (99%)	-0.18	5 (0%) 81 78	20, 38, 67, 94	0
1	B	580/585 (99%)	0.22	26 (4%) 38 34	30, 53, 87, 101	0
All	All	1161/1170 (99%)	0.02	31 (2%) 56 52	20, 45, 82, 101	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	TYR	6.4
1	A	158	ALA	5.3
1	B	579	SER	3.7
1	B	79	THR	3.6
1	A	79	THR	3.6
1	B	371	ALA	3.1
1	B	370	TYR	3.1
1	B	84	TYR	2.9
1	A	443	ALA	2.8
1	B	116	VAL	2.8
1	B	539	ALA	2.7
1	B	502	PHE	2.7
1	B	374	PHE	2.6
1	B	582	ALA	2.6
1	B	373	VAL	2.6
1	B	499	PRO	2.5
1	B	78	ALA	2.5
1	B	77	VAL	2.4
1	B	564	LYS	2.4
1	B	367	HIS	2.3
1	B	498	VAL	2.2
1	B	501	GLU	2.2
1	B	375	ASP	2.2
1	B	554	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	569	ALA	2.1
1	B	503	ASN	2.1
1	B	575	LEU	2.1
1	B	83	THR	2.1
1	B	552	ALA	2.1
1	A	128	HIS	2.1
1	B	504	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

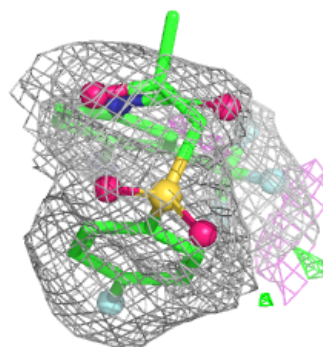
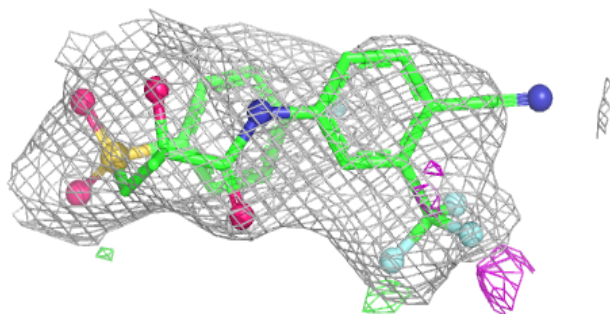
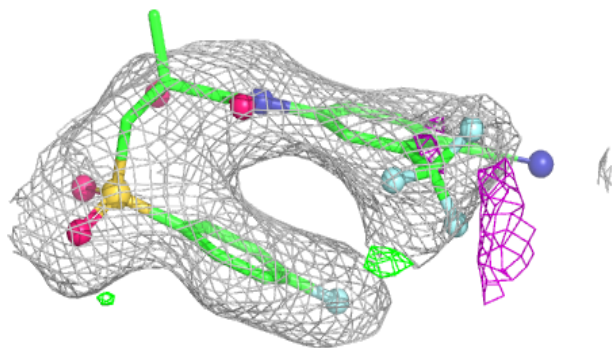
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	198	A	601	29/29	0.87	0.10	42,60,72,77	0
2	198	B	601	29/29	0.87	0.09	49,58,68,75	0

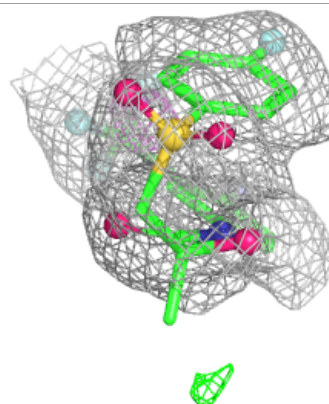
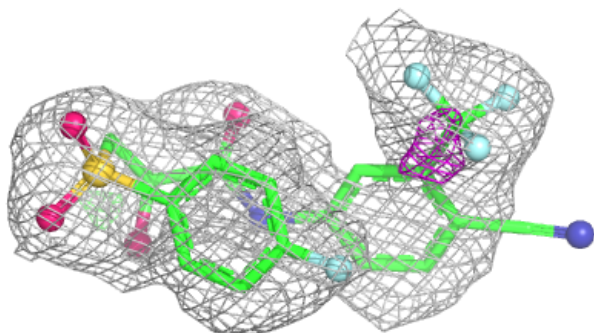
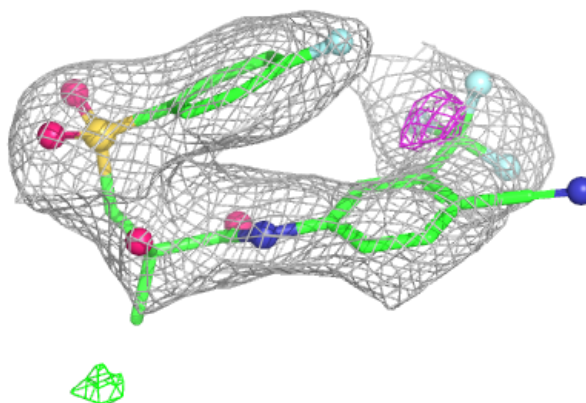
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 198 A 601:

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

**Electron density around 198 B 601:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.