



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:46 pm BST

PDB ID : 4IN4
Title : Crystal structure of cpd 15 bound to Keap1 Kelch domain
Authors : Silvian, L.; Marcotte, D.
Deposited on : 2013-01-03
Resolution : 2.59 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 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 : 2.11
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) : 2.11

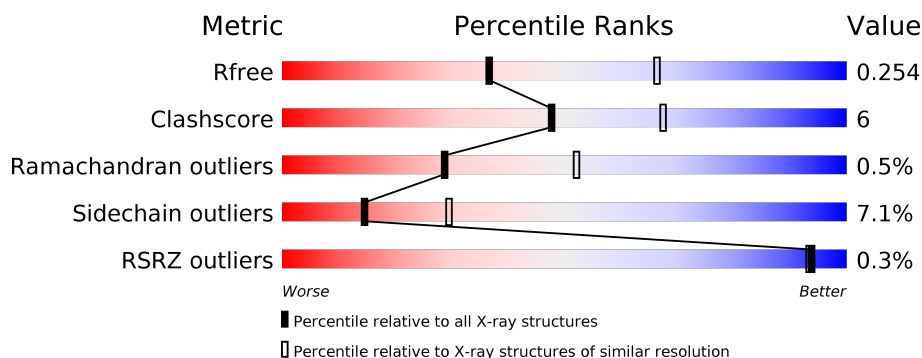
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	299	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 81% 13% • • </div> </div>
1	B	299	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 79% 13% • 5% </div> </div>
1	C	299	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 85% 11% • • </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7007 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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2206	1371	399	421	15			
1	B	284	Total	C	N	O	S	0	0	0
			2185	1358	395	417	15			
1	C	289	Total	C	N	O	S	0	0	0
			2213	1376	400	422	15			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	SER	-	EXPRESSION TAG	UNP Q14145
A	312	GLY	-	EXPRESSION TAG	UNP Q14145
A	313	LEU	-	EXPRESSION TAG	UNP Q14145
A	314	VAL	-	EXPRESSION TAG	UNP Q14145
A	315	PRO	-	EXPRESSION TAG	UNP Q14145
A	316	ARG	-	EXPRESSION TAG	UNP Q14145
A	317	GLY	-	EXPRESSION TAG	UNP Q14145
A	318	SER	-	EXPRESSION TAG	UNP Q14145
A	319	HIS	-	EXPRESSION TAG	UNP Q14145
A	320	MET	-	EXPRESSION TAG	UNP Q14145
B	311	SER	-	EXPRESSION TAG	UNP Q14145
B	312	GLY	-	EXPRESSION TAG	UNP Q14145
B	313	LEU	-	EXPRESSION TAG	UNP Q14145
B	314	VAL	-	EXPRESSION TAG	UNP Q14145
B	315	PRO	-	EXPRESSION TAG	UNP Q14145
B	316	ARG	-	EXPRESSION TAG	UNP Q14145
B	317	GLY	-	EXPRESSION TAG	UNP Q14145
B	318	SER	-	EXPRESSION TAG	UNP Q14145
B	319	HIS	-	EXPRESSION TAG	UNP Q14145
B	320	MET	-	EXPRESSION TAG	UNP Q14145
C	311	SER	-	EXPRESSION TAG	UNP Q14145
C	312	GLY	-	EXPRESSION TAG	UNP Q14145
C	313	LEU	-	EXPRESSION TAG	UNP Q14145

Continued on next page...

Continued from previous page...

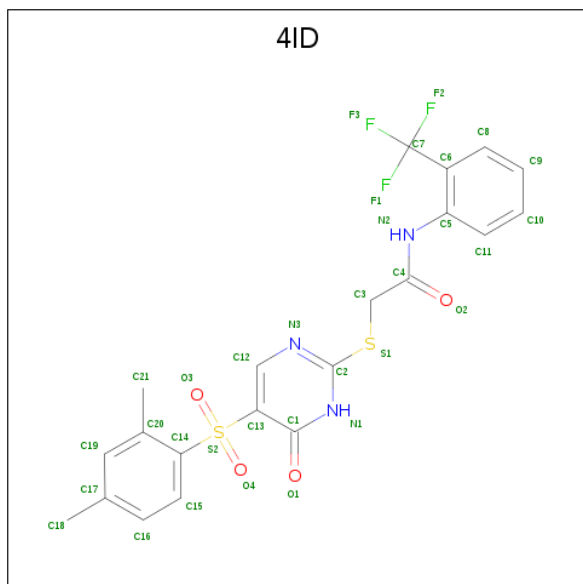
Chain	Residue	Modelled	Actual	Comment	Reference
C	314	VAL	-	EXPRESSION TAG	UNP Q14145
C	315	PRO	-	EXPRESSION TAG	UNP Q14145
C	316	ARG	-	EXPRESSION TAG	UNP Q14145
C	317	GLY	-	EXPRESSION TAG	UNP Q14145
C	318	SER	-	EXPRESSION TAG	UNP Q14145
C	319	HIS	-	EXPRESSION TAG	UNP Q14145
C	320	MET	-	EXPRESSION TAG	UNP Q14145

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 2-({5-[(2,4-dimethylphenyl)sulfonyl]-6-oxo-1,6-dihydropyrimidin-2-yl}sulfanyl)-N-[2-(trifluoromethyl)phenyl]acetamide (three-letter code: 4ID) (formula: $C_{21}H_{18}F_3N_3O_4S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			33	21	3	3	4	2		
3	A	1	Total	C	F	N	O	S	0	0
			33	21	3	3	4	2		
3	B	1	Total	C	F	N	O	S	0	0
			33	21	3	3	4	2		
3	B	1	Total	C	F	N	O	S	0	0
			33	21	3	3	4	2		
3	C	1	Total	C	F	N	O	S	0	0
			33	21	3	3	4	2		
3	C	1	Total	C	F	N	O	S	0	0
			33	21	3	3	4	2		

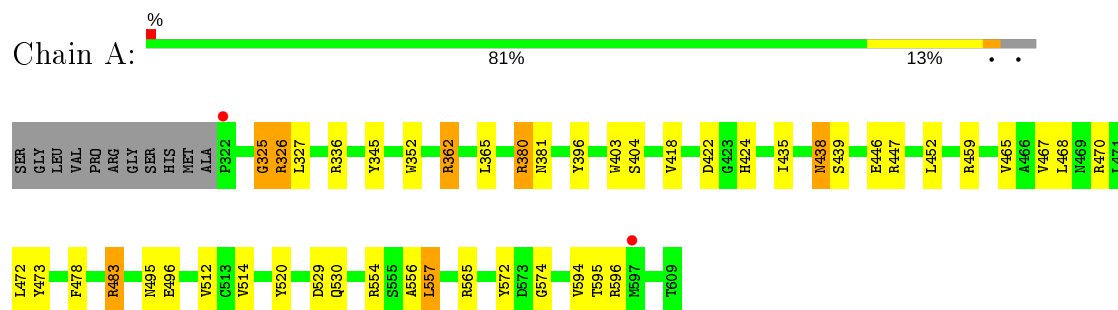
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total	O	0	0
			64	64		
4	B	50	Total	O	0	0
			50	50		
4	C	51	Total	O	0	0
			51	51		

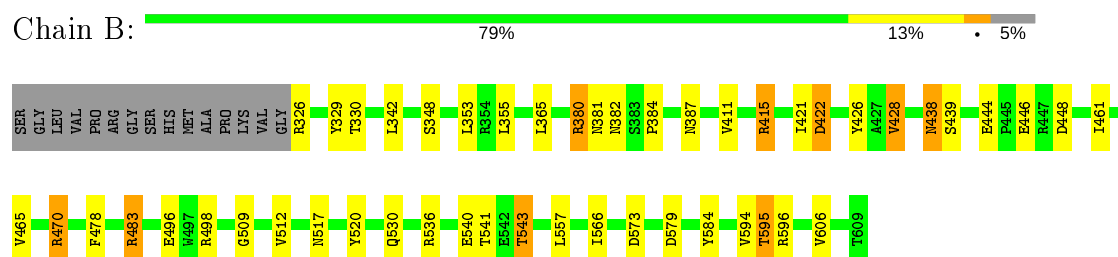
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

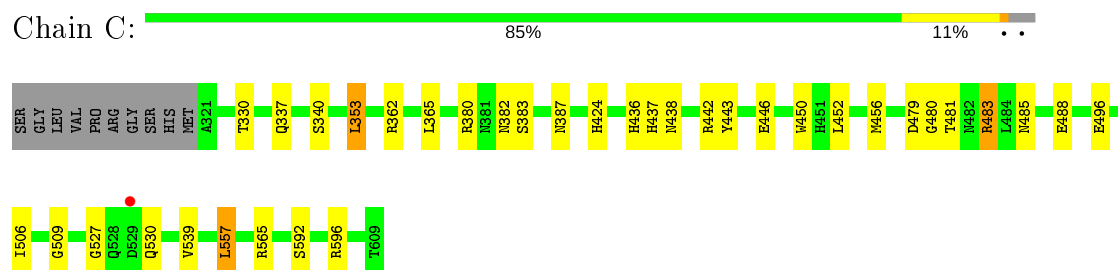
- Molecule 1: Kelch-like ECH-associated protein 1



- Molecule 1: Kelch-like ECH-associated protein 1



- Molecule 1: Kelch-like ECH-associated protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.60 Å 96.51 Å 142.46 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.51 – 2.59 96.51 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.9 (96.51-2.59) 99.9 (96.51-2.59)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.58 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.191 , 0.250 0.195 , 0.254	Depositor DCC
R_{free} test set	1764 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7007	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4ID, PO4

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	0.78	0/2260	0.93	2/3079 (0.1%)
1	B	0.71	0/2238	0.90	4/3049 (0.1%)
1	C	0.71	0/2267	0.87	0/3090
All	All	0.74	0/6765	0.90	6/9218 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	483	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	415	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	470	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	B	483	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	536	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2206	0	2085	27	0
1	B	2185	0	2070	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2213	0	2096	22	0
2	A	20	0	0	0	0
2	B	15	0	0	0	0
2	C	5	0	0	1	0
3	A	66	0	36	5	0
3	B	66	0	36	4	0
3	C	66	0	36	6	0
4	A	64	0	0	1	0
4	B	50	0	0	0	0
4	C	51	0	0	2	0
All	All	7007	0	6359	81	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (81) 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:557:LEU:HD23	1:A:557:LEU:H	1.53	0.72
1:A:483:ARG:HD3	3:A:706:4ID:O3	1.94	0.68
1:B:557:LEU:H	1:B:557:LEU:HD23	1.62	0.65
1:C:483:ARG:HD2	1:C:527:GLY:HA2	1.82	0.62
1:C:483:ARG:CD	1:C:527:GLY:HA2	2.29	0.62
1:A:438:ASN:HD22	1:A:439:SER:N	2.01	0.59
1:C:483:ARG:HD2	1:C:527:GLY:CA	2.33	0.59
1:C:353:LEU:N	1:C:353:LEU:HD23	2.19	0.58
1:C:485:ASN:HB3	1:C:506:ILE:HG13	1.88	0.56
1:B:365:LEU:HD23	1:B:365:LEU:H	1.69	0.56
1:A:478:PHE:HD1	1:A:483:ARG:HG3	1.69	0.56
1:B:478:PHE:HD1	1:B:483:ARG:HG3	1.70	0.55
1:B:438:ASN:HD22	1:B:438:ASN:C	2.10	0.55
1:A:422:ASP:OD1	1:A:470:ARG:NH1	2.41	0.54
1:A:362:ARG:HB3	4:A:815:HOH:O	2.08	0.54
1:A:438:ASN:HD22	1:A:438:ASN:C	2.10	0.54
1:C:557:LEU:HD23	1:C:557:LEU:H	1.73	0.53
1:B:342:LEU:HD23	1:B:355:LEU:HB2	1.89	0.53
1:B:438:ASN:HD22	1:B:439:SER:N	2.07	0.53
1:C:483:ARG:NH1	3:C:703:4ID:H15	2.24	0.52
1:A:495:ASN:O	1:A:495:ASN:CG	2.48	0.51
1:B:509:GLY:HA2	3:B:704:4ID:H18A	1.93	0.51
1:C:509:GLY:CA	3:C:702:4ID:H18A	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ILE:HD12	1:B:426:TYR:CE1	2.46	0.50
1:A:467:VAL:O	1:A:514:VAL:HG11	2.12	0.50
1:C:424:HIS:HE1	1:C:446:GLU:OE1	1.95	0.49
1:B:329:TYR:O	1:B:606:VAL:HA	2.12	0.49
1:B:478:PHE:CD1	1:B:483:ARG:HG3	2.47	0.49
3:A:706:4ID:O2	3:A:706:4ID:H11	2.13	0.49
1:C:380:ARG:HD3	1:C:382:ASN:OD1	2.12	0.49
1:A:380:ARG:HG2	1:A:381:ASN:N	2.28	0.48
1:A:465:VAL:HG13	1:A:472:LEU:HD21	1.95	0.48
1:A:325:GLY:O	1:A:326:ARG:CB	2.61	0.47
3:C:702:4ID:H11	3:C:702:4ID:O2	2.15	0.47
3:B:705:4ID:O2	3:B:705:4ID:H11	2.15	0.47
1:A:365:LEU:H	1:A:365:LEU:HD23	1.80	0.47
1:A:325:GLY:O	1:A:326:ARG:HB2	2.15	0.47
1:A:572:TYR:CE2	1:A:574:GLY:HA2	2.50	0.47
1:B:382:ASN:OD1	1:B:387:ASN:OD1	2.33	0.47
1:B:573:ASP:C	1:B:573:ASP:OD1	2.53	0.47
1:C:509:GLY:HA3	3:C:702:4ID:H18A	1.95	0.47
1:A:362:ARG:HG3	1:A:365:LEU:HD13	1.97	0.46
1:A:594:VAL:O	1:A:595:THR:HB	2.15	0.46
1:B:509:GLY:CA	3:B:704:4ID:H18A	2.46	0.46
1:C:456:MET:HB3	1:C:488:GLU:OE1	2.16	0.46
1:C:565:ARG:HG3	4:C:815:HOH:O	2.16	0.46
1:A:512:VAL:HA	1:A:520:TYR:O	2.16	0.45
1:C:382:ASN:HA	1:C:387:ASN:HD22	1.80	0.45
1:A:478:PHE:CD1	1:A:483:ARG:HG3	2.50	0.45
1:B:428:VAL:HG13	1:B:465:VAL:HG21	1.98	0.44
1:C:479:ASP:OD1	1:C:479:ASP:C	2.55	0.44
1:A:345:TYR:HB2	1:A:352:TRP:CH2	2.53	0.44
3:A:705:4ID:F1	3:A:705:4ID:N2	2.38	0.43
1:B:380:ARG:HG2	1:B:381:ASN:N	2.32	0.43
1:A:468:LEU:HD13	1:A:514:VAL:HG21	2.01	0.43
1:B:541:THR:OG1	1:B:543:THR:HG23	2.19	0.43
3:C:703:4ID:O2	3:C:703:4ID:H11	2.19	0.43
1:C:436:HIS:CD2	1:C:480:GLY:HA2	2.53	0.43
1:B:594:VAL:O	1:B:595:THR:HG23	2.19	0.42
1:A:396:TYR:HB2	1:A:403:TRP:CE3	2.54	0.42
1:A:472:LEU:HD23	1:A:473:TYR:N	2.35	0.42
1:B:444:GLU:O	1:B:448:ASP:N	2.50	0.42
1:B:579:ASP:OD1	1:B:596:ARG:HD2	2.19	0.42
1:B:422:ASP:OD2	1:B:470:ARG:HD3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ASN:ND2	1:B:438:ASN:C	2.72	0.42
1:C:483:ARG:HB3	1:C:506:ILE:CG2	2.49	0.42
1:B:461:ILE:C	1:B:461:ILE:HD12	2.40	0.41
1:C:437:HIS:HA	2:C:701:PO4:O2	2.20	0.41
1:A:556:ALA:HB2	3:A:705:4ID:C19	2.51	0.41
3:C:702:4ID:C11	3:C:702:4ID:O2	2.67	0.41
3:A:705:4ID:H11	3:A:705:4ID:O2	2.20	0.41
1:A:435:ILE:HD11	1:B:384:PRO:HB3	2.02	0.41
1:B:566:ILE:HB	1:B:584:TYR:HB3	2.01	0.41
1:C:362:ARG:HB3	4:C:835:HOH:O	2.19	0.41
1:B:483:ARG:HD3	3:B:705:4ID:O3	2.20	0.41
1:B:512:VAL:HA	1:B:520:TYR:O	2.21	0.41
1:C:362:ARG:HA	1:C:380:ARG:O	2.21	0.41
1:A:345:TYR:CE1	1:A:595:THR:HG21	2.56	0.41
1:A:424:HIS:HE1	1:A:446:GLU:OE2	2.04	0.40
1:C:443:TYR:HB2	1:C:450:TRP:CE3	2.56	0.40
1:C:382:ASN:HA	1:C:387:ASN:ND2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	286/299 (96%)	274 (96%)	9 (3%)	3 (1%)	15	32
1	B	282/299 (94%)	270 (96%)	11 (4%)	1 (0%)	34	57
1	C	287/299 (96%)	274 (96%)	13 (4%)	0	100	100
All	All	855/897 (95%)	818 (96%)	33 (4%)	4 (0%)	29	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	ARG
1	B	422	ASP
1	A	325	GLY
1	A	336	ARG

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	231/242 (96%)	216 (94%)	15 (6%)	17	34
1	B	230/242 (95%)	213 (93%)	17 (7%)	13	28
1	C	232/242 (96%)	215 (93%)	17 (7%)	14	28
All	All	693/726 (96%)	644 (93%)	49 (7%)	14	29

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	327	LEU
1	A	362	ARG
1	A	380	ARG
1	A	404	SER
1	A	418	VAL
1	A	438	ASN
1	A	447	ARG
1	A	452	LEU
1	A	496	GLU
1	A	529	ASP
1	A	530	GLN
1	A	554	ARG
1	A	557	LEU
1	A	565	ARG
1	A	596	ARG
1	B	326	ARG
1	B	330	THR
1	B	348	SER
1	B	353	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	380	ARG
1	B	411	VAL
1	B	415	ARG
1	B	428	VAL
1	B	438	ASN
1	B	446	GLU
1	B	496	GLU
1	B	498	ARG
1	B	517	ASN
1	B	530	GLN
1	B	540	GLU
1	B	543	THR
1	B	595	THR
1	C	330	THR
1	C	337	GLN
1	C	340	SER
1	C	353	LEU
1	C	365	LEU
1	C	383	SER
1	C	438	ASN
1	C	442	ARG
1	C	452	LEU
1	C	481	THR
1	C	483	ARG
1	C	496	GLU
1	C	530	GLN
1	C	539	VAL
1	C	557	LEU
1	C	592	SER
1	C	596	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	ASN
1	A	424	HIS
1	A	438	ASN
1	B	382	ASN
1	B	432	HIS
1	B	438	ASN
1	C	359	GLN
1	C	387	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	424	HIS
1	C	438	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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$
2	PO4	A	702	-	4,4,4	1.35	1 (25%)	6,6,6	0.63	0
3	4ID	A	706	-	34,35,35	3.36	4 (11%)	48,52,52	2.97	21 (43%)
3	4ID	B	704	-	34,35,35	3.84	4 (11%)	48,52,52	2.92	25 (52%)
2	PO4	C	701	-	4,4,4	1.15	0	6,6,6	0.65	0
3	4ID	C	702	-	34,35,35	3.94	5 (14%)	48,52,52	2.88	24 (50%)
2	PO4	B	701	-	4,4,4	0.78	0	6,6,6	0.74	0
3	4ID	B	705	-	34,35,35	3.80	6 (17%)	48,52,52	2.76	18 (37%)
2	PO4	A	701	-	4,4,4	0.73	0	6,6,6	0.70	0
2	PO4	A	704	-	4,4,4	0.86	0	6,6,6	1.47	1 (16%)
2	PO4	B	702	-	4,4,4	0.72	0	6,6,6	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	A	703	-	4,4,4	0.87	0	6,6,6	0.73	0
2	PO4	B	703	-	4,4,4	0.76	0	6,6,6	0.59	0
3	4ID	C	703	-	34,35,35	3.33	4 (11%)	48,52,52	2.80	20 (41%)
3	4ID	A	705	-	34,35,35	3.89	4 (11%)	48,52,52	2.72	22 (45%)

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
3	4ID	C	702	-	-	2/27/27/27	0/3/3/3
3	4ID	A	706	-	-	2/27/27/27	0/3/3/3
3	4ID	B	704	-	-	3/27/27/27	0/3/3/3
3	4ID	B	705	-	-	2/27/27/27	0/3/3/3
3	4ID	C	703	-	-	4/27/27/27	0/3/3/3
3	4ID	A	705	-	-	4/27/27/27	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	704	4ID	C13-S2	-17.25	1.54	1.78
3	A	705	4ID	C13-S2	-16.22	1.56	1.78
3	C	702	4ID	C14-S2	-15.44	1.57	1.78
3	C	702	4ID	C13-S2	-15.43	1.57	1.78
3	B	705	4ID	C14-S2	-14.96	1.58	1.78
3	B	705	4ID	C13-S2	-14.67	1.58	1.78
3	A	705	4ID	C14-S2	-14.62	1.58	1.78
3	C	703	4ID	C14-S2	-14.35	1.58	1.78
3	A	706	4ID	C14-S2	-13.34	1.60	1.78
3	A	706	4ID	C13-S2	-12.86	1.60	1.78
3	B	704	4ID	C14-S2	-12.60	1.61	1.78
3	C	703	4ID	C13-S2	-12.02	1.61	1.78
3	C	702	4ID	C3-C4	4.33	1.56	1.51
3	B	704	4ID	C2-S1	-4.04	1.68	1.75
3	A	706	4ID	C2-S1	-4.01	1.68	1.75
3	B	705	4ID	C3-C4	3.99	1.56	1.51
3	B	705	4ID	C2-S1	-3.57	1.68	1.75
3	C	702	4ID	C2-S1	-3.46	1.69	1.75
3	A	705	4ID	C5-N2	-3.38	1.35	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	705	4ID	C2-S1	-3.26	1.69	1.75
3	A	706	4ID	C3-C4	3.23	1.55	1.51
3	C	703	4ID	C2-S1	-2.81	1.70	1.75
3	B	705	4ID	C5-N2	-2.62	1.36	1.41
3	B	704	4ID	C5-N2	-2.51	1.37	1.41
3	C	702	4ID	C5-N2	-2.51	1.37	1.41
3	C	703	4ID	C5-N2	-2.49	1.37	1.41
3	B	705	4ID	C12-C13	-2.11	1.36	1.39
2	A	702	PO4	P-O4	-2.04	1.48	1.54

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	705	4ID	C13-C1-N1	-7.81	115.98	125.56
3	C	703	4ID	C12-N3-C2	7.65	121.69	115.44
3	B	704	4ID	C13-C12-N3	-7.48	117.14	123.60
3	C	702	4ID	C13-C1-N1	-7.22	116.70	125.56
3	A	706	4ID	C12-N3-C2	6.89	121.06	115.44
3	B	705	4ID	C13-C1-N1	-6.75	117.28	125.56
3	C	703	4ID	C3-S1-C2	6.74	110.32	101.63
3	A	706	4ID	C13-C1-N1	-6.66	117.38	125.56
3	B	705	4ID	C12-N3-C2	6.56	120.80	115.44
3	A	706	4ID	F1-C7-C6	-6.56	101.28	112.70
3	A	706	4ID	O4-S2-O3	-6.52	106.78	119.23
3	C	703	4ID	O4-S2-O3	-6.51	106.81	119.23
3	C	702	4ID	C12-N3-C2	6.48	120.73	115.44
3	B	704	4ID	C12-N3-C2	6.42	120.68	115.44
3	B	704	4ID	C13-C1-N1	-6.18	117.98	125.56
3	C	703	4ID	C1-N1-C2	6.08	122.75	115.79
3	C	702	4ID	F3-C7-C6	-5.85	102.51	112.70
3	A	706	4ID	C3-C4-N2	5.72	122.26	114.41
3	C	703	4ID	C13-C1-N1	-5.72	118.54	125.56
3	C	702	4ID	C13-C12-N3	-5.67	118.70	123.60
3	C	702	4ID	C1-N1-C2	5.57	122.18	115.79
3	B	704	4ID	O4-S2-O3	-5.48	108.75	119.23
3	A	705	4ID	C12-N3-C2	5.47	119.91	115.44
3	C	703	4ID	N3-C2-N1	-5.45	120.81	127.57
3	B	705	4ID	C1-N1-C2	5.14	121.69	115.79
3	B	705	4ID	F1-C7-C6	-5.10	103.82	112.70
3	A	705	4ID	C1-N1-C2	5.07	121.61	115.79
3	C	702	4ID	C3-C4-N2	4.93	121.16	114.41
3	A	705	4ID	C16-C17-C19	4.86	125.26	117.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	705	4ID	C3-C4-N2	4.86	121.07	114.41
3	B	705	4ID	C4-C3-S1	4.69	125.49	112.84
3	A	705	4ID	C20-C19-C17	-4.61	117.44	122.17
3	B	705	4ID	N3-C2-N1	-4.61	121.86	127.57
3	A	706	4ID	C3-S1-C2	4.56	107.51	101.63
3	A	706	4ID	C4-C3-S1	4.53	125.04	112.84
3	B	704	4ID	C3-C4-N2	4.47	120.54	114.41
3	B	705	4ID	C3-S1-C2	4.43	107.35	101.63
3	A	705	4ID	F1-C7-C6	-4.33	105.17	112.70
3	A	705	4ID	C13-C12-N3	-4.30	119.89	123.60
3	A	706	4ID	C13-C12-N3	-4.25	119.93	123.60
3	B	704	4ID	C1-N1-C2	4.19	120.60	115.79
3	A	706	4ID	C1-N1-C2	4.19	120.59	115.79
3	B	704	4ID	C19-C20-C14	4.09	119.81	116.94
3	C	702	4ID	C20-C19-C17	-4.09	117.97	122.17
3	C	702	4ID	N3-C2-N1	-4.01	122.59	127.57
3	B	704	4ID	C20-C19-C17	-3.98	118.08	122.17
3	B	704	4ID	F2-C7-C6	-3.95	105.83	112.70
3	B	705	4ID	C7-C6-C5	-3.94	117.82	120.72
3	C	702	4ID	C4-C3-S1	3.89	123.33	112.84
3	A	706	4ID	C8-C6-C5	3.84	123.11	118.33
3	A	705	4ID	N3-C2-N1	-3.80	122.85	127.57
3	C	703	4ID	C19-C20-C14	3.77	119.58	116.94
3	A	705	4ID	C3-C4-N2	3.71	119.50	114.41
3	C	702	4ID	C16-C17-C19	3.68	123.49	117.95
3	B	705	4ID	C15-C16-C17	-3.66	116.47	121.38
3	B	704	4ID	C16-C17-C19	3.65	123.43	117.95
3	B	705	4ID	C16-C17-C19	3.57	123.31	117.95
3	B	704	4ID	C15-C16-C17	-3.56	116.62	121.38
3	A	706	4ID	O4-S2-C14	3.54	113.86	107.96
3	A	705	4ID	C8-C6-C5	3.51	122.70	118.33
3	B	704	4ID	N3-C2-N1	-3.49	123.23	127.57
3	B	705	4ID	O3-S2-C13	3.49	113.77	107.96
3	B	705	4ID	C13-C12-N3	-3.42	120.65	123.60
3	C	702	4ID	O4-S2-C13	-3.40	102.30	107.96
3	A	706	4ID	N3-C2-N1	-3.37	123.39	127.57
3	B	704	4ID	O2-C4-C3	-3.34	115.81	121.58
3	C	702	4ID	C8-C6-C5	3.34	122.49	118.33
3	B	704	4ID	C12-C13-C1	3.33	120.36	114.79
3	A	705	4ID	C18-C17-C16	-3.31	110.58	120.94
3	A	705	4ID	C7-C6-C5	-3.27	118.31	120.72
3	A	705	4ID	C15-C16-C17	-3.21	117.08	121.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	704	4ID	O4-S2-C14	3.21	113.31	107.96
3	C	702	4ID	C3-S1-C2	3.16	105.70	101.63
3	C	703	4ID	C13-C12-N3	-3.16	120.87	123.60
3	A	706	4ID	C7-C6-C5	-3.15	118.40	120.72
3	C	703	4ID	C20-C19-C17	-3.10	118.98	122.17
3	A	705	4ID	O3-S2-C14	-3.06	102.85	107.96
3	C	702	4ID	C19-C20-C14	3.04	119.07	116.94
3	B	705	4ID	C8-C6-C5	3.03	122.10	118.33
3	A	706	4ID	C11-C5-C6	-3.01	116.91	119.88
3	A	705	4ID	C12-C13-C1	2.96	119.75	114.79
3	C	703	4ID	F3-C7-C6	-2.94	107.57	112.70
3	C	703	4ID	C21-C20-C14	-2.94	121.28	124.16
3	A	706	4ID	C16-C17-C19	2.93	122.36	117.95
3	C	702	4ID	O2-C4-C3	-2.90	116.58	121.58
3	C	703	4ID	O3-S2-C14	2.88	112.76	107.96
2	A	704	PO4	O4-P-O2	2.87	117.20	107.97
3	A	706	4ID	C15-C16-C17	-2.87	117.54	121.38
3	B	704	4ID	C1-C13-S2	-2.85	116.59	121.14
3	A	706	4ID	C19-C20-C14	2.76	118.87	116.94
3	A	705	4ID	O2-C4-C3	-2.74	116.84	121.58
3	B	704	4ID	C8-C6-C5	2.70	121.70	118.33
3	C	702	4ID	C15-C14-S2	-2.64	112.42	116.40
3	A	706	4ID	C20-C19-C17	-2.64	119.46	122.17
3	B	705	4ID	O4-S2-O3	-2.63	114.20	119.23
3	A	705	4ID	C3-S1-C2	2.60	104.99	101.63
3	C	703	4ID	C3-C4-N2	2.59	117.96	114.41
3	C	702	4ID	C12-C13-C1	2.56	119.08	114.79
3	B	704	4ID	C18-C17-C16	-2.56	112.94	120.94
3	B	704	4ID	C15-C14-C20	-2.56	118.81	121.17
3	B	705	4ID	C6-C5-N2	-2.56	118.01	120.54
3	B	704	4ID	C4-C3-S1	2.53	119.67	112.84
3	A	705	4ID	O3-S2-C13	2.52	112.16	107.96
3	C	703	4ID	O4-S2-C14	2.52	112.15	107.96
3	C	702	4ID	O4-S2-C14	2.51	112.14	107.96
3	C	703	4ID	C8-C6-C5	2.50	121.45	118.33
3	C	702	4ID	C11-C5-C6	-2.46	117.46	119.88
3	B	704	4ID	C6-C5-N2	-2.45	118.12	120.54
3	B	705	4ID	C11-C5-C6	-2.41	117.51	119.88
3	C	703	4ID	O3-S2-C13	2.41	111.97	107.96
3	C	703	4ID	O2-C4-C3	-2.37	117.49	121.58
3	A	706	4ID	O2-C4-C3	-2.35	117.52	121.58
3	A	705	4ID	C11-C5-C6	-2.30	117.61	119.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	704	4ID	C3-S1-C2	2.30	104.60	101.63
3	A	706	4ID	C15-C14-C20	-2.30	119.05	121.17
3	B	705	4ID	O2-C4-N2	-2.22	119.58	123.63
3	A	705	4ID	F2-C7-C6	-2.20	108.86	112.70
3	B	704	4ID	F2-C7-F1	2.20	113.80	105.72
3	C	702	4ID	C1-C13-S2	-2.20	117.64	121.14
3	C	702	4ID	C18-C17-C16	-2.19	114.08	120.94
3	C	703	4ID	C15-C16-C17	-2.19	118.45	121.38
3	A	705	4ID	C18-C17-C19	2.17	124.15	120.94
3	A	705	4ID	O4-S2-O3	-2.15	115.12	119.23
3	C	702	4ID	F3-C7-F1	2.10	113.44	105.72
3	B	704	4ID	C16-C15-C14	2.10	123.23	120.03
3	C	703	4ID	C1-C13-S2	2.09	124.47	121.14
3	C	703	4ID	C16-C17-C19	2.08	121.07	117.95
3	B	704	4ID	C11-C5-C6	-2.07	117.84	119.88
3	C	702	4ID	C21-C20-C19	-2.04	115.72	119.49
3	C	702	4ID	C15-C16-C17	-2.02	118.67	121.38
3	A	706	4ID	F3-C7-F1	2.00	113.07	105.72

There are no chirality outliers.

All (17) torsion outliers are listed below:

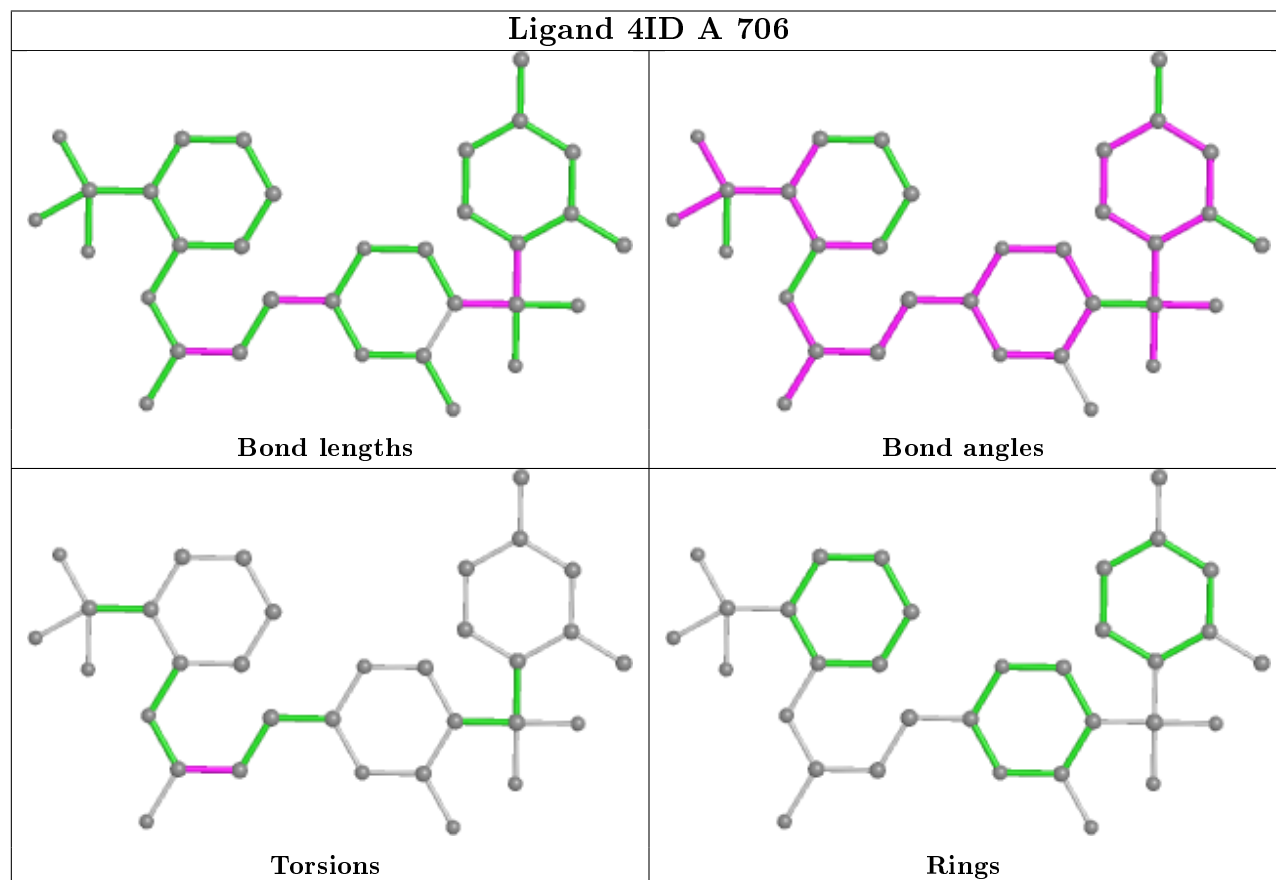
Mol	Chain	Res	Type	Atoms
3	C	702	4ID	S1-C3-C4-N2
3	A	705	4ID	S1-C3-C4-N2
3	A	705	4ID	N3-C2-S1-C3
3	C	703	4ID	C1-C13-S2-O3
3	C	702	4ID	S1-C3-C4-O2
3	C	703	4ID	S1-C3-C4-O2
3	A	705	4ID	N1-C2-S1-C3
3	B	704	4ID	S1-C3-C4-N2
3	B	704	4ID	C1-C13-S2-O4
3	B	704	4ID	S1-C3-C4-O2
3	A	705	4ID	S1-C3-C4-O2
3	A	706	4ID	S1-C3-C4-N2
3	B	705	4ID	S1-C3-C4-N2
3	C	703	4ID	S1-C3-C4-N2
3	A	706	4ID	S1-C3-C4-O2
3	B	705	4ID	S1-C3-C4-O2
3	C	703	4ID	C12-C13-S2-O3

There are no ring outliers.

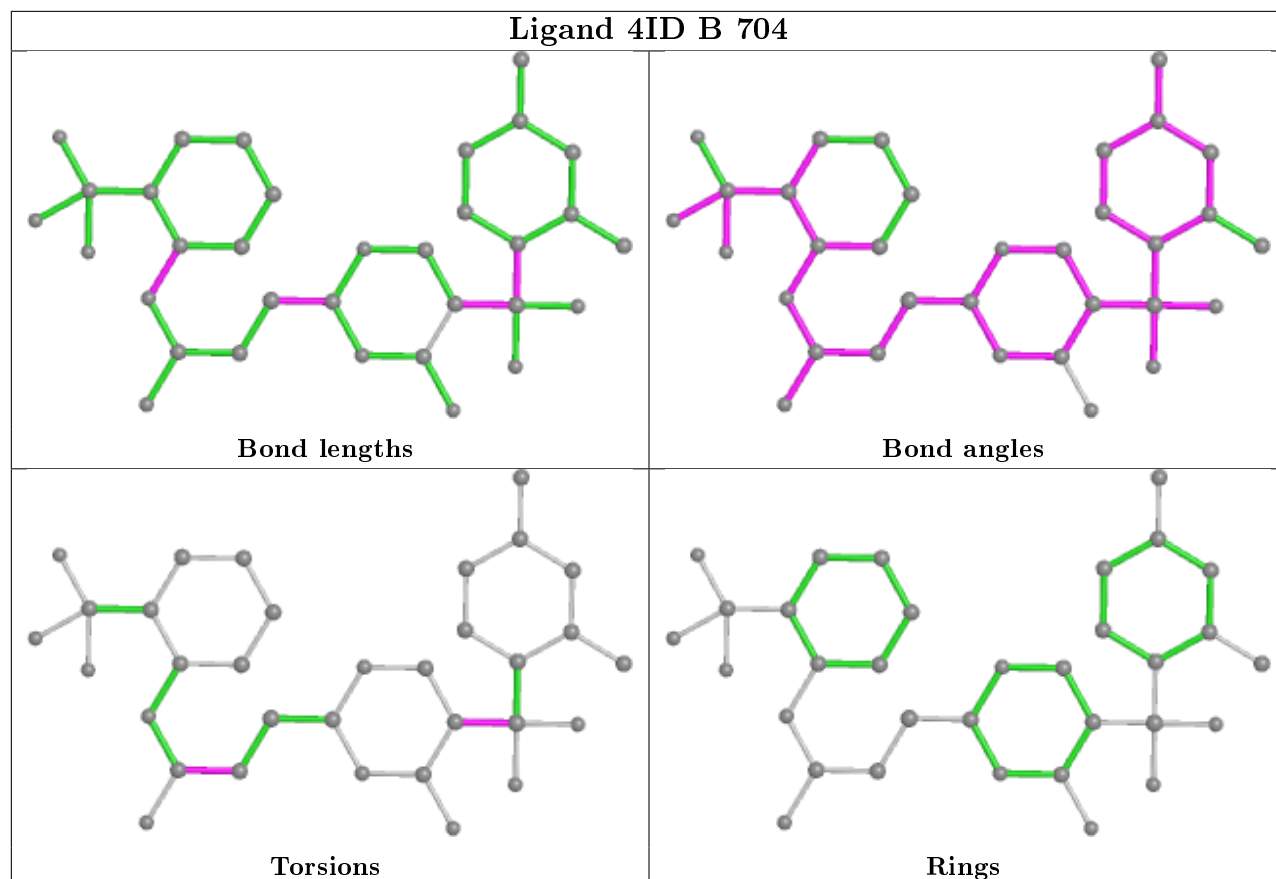
7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	706	4ID	2	0
3	B	704	4ID	2	0
2	C	701	PO4	1	0
3	C	702	4ID	4	0
3	B	705	4ID	2	0
3	C	703	4ID	2	0
3	A	705	4ID	3	0

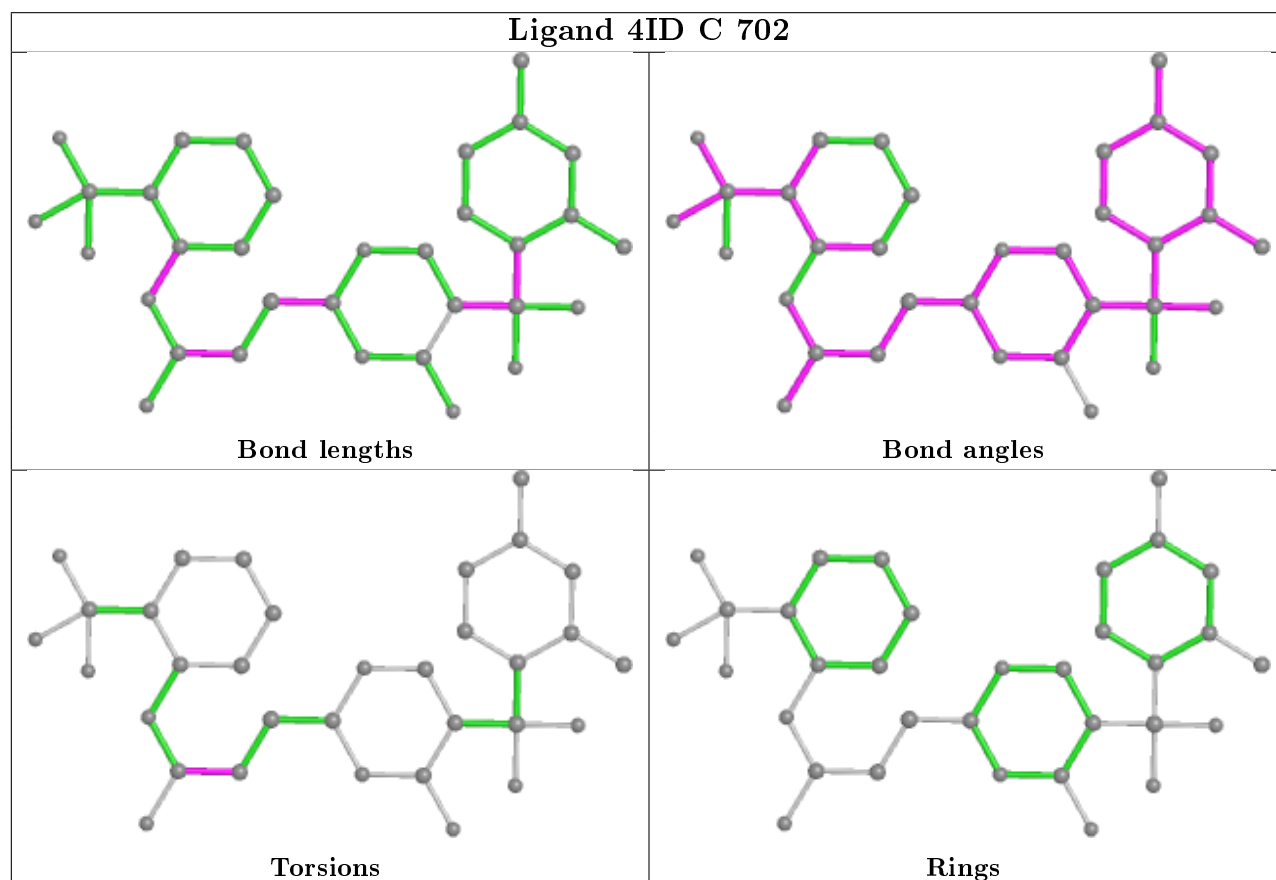
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



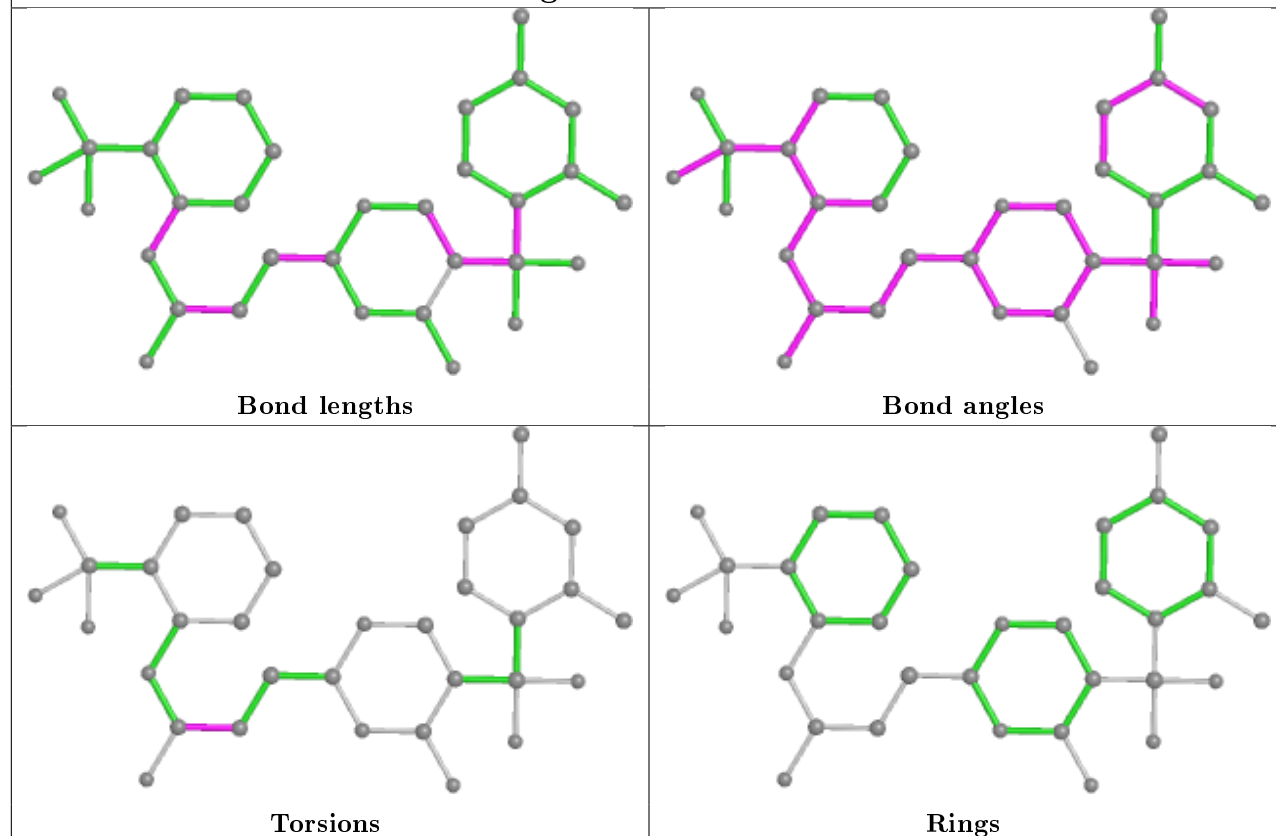
Ligand 4ID B 704



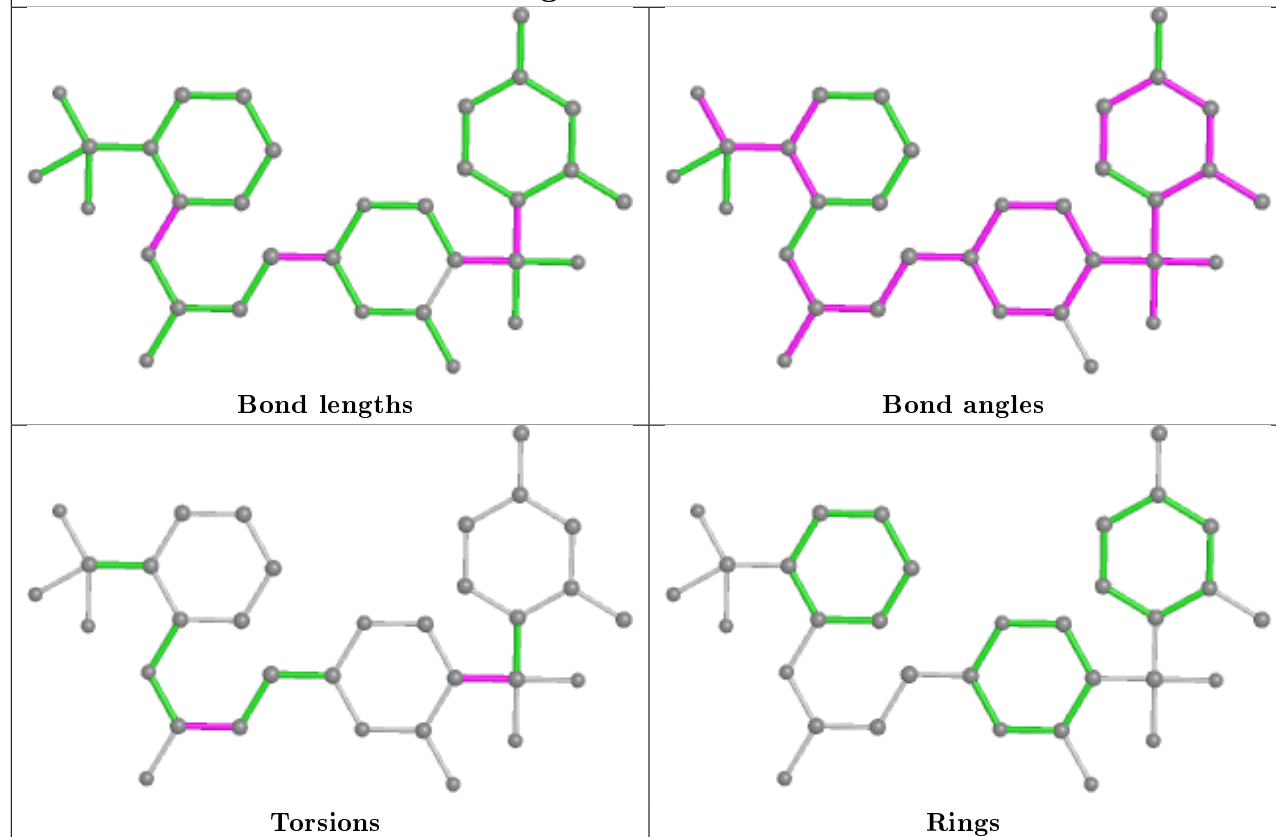
Ligand 4ID C 702

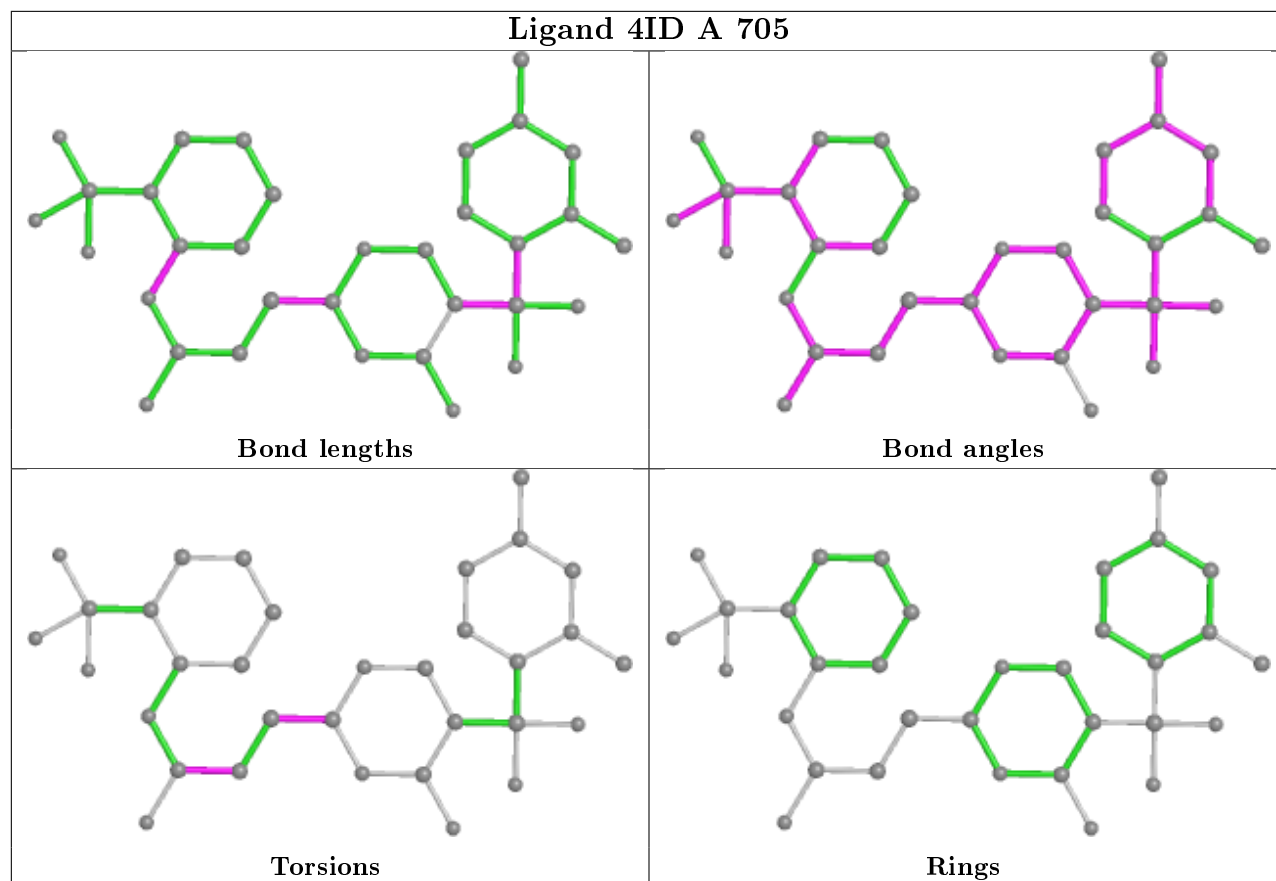


Ligand 4ID B 705



Ligand 4ID C 703





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	288/299 (96%)	-0.19	2 (0%) 87 86	9, 16, 35, 84	25 (8%)
1	B	284/299 (94%)	-0.12	0 100 100	11, 21, 40, 64	25 (8%)
1	C	289/299 (96%)	-0.11	1 (0%) 94 93	10, 22, 44, 61	25 (8%)
All	All	861/897 (95%)	-0.14	3 (0%) 94 93	9, 20, 40, 84	75 (8%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	322	PRO	2.4
1	C	529	ASP	2.1
1	A	597	MET	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 carbohydrates 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(Å ²)	Q<0.9
2	PO4	B	702	5/5	0.87	0.24	67,70,76,79	0

Continued on next page...

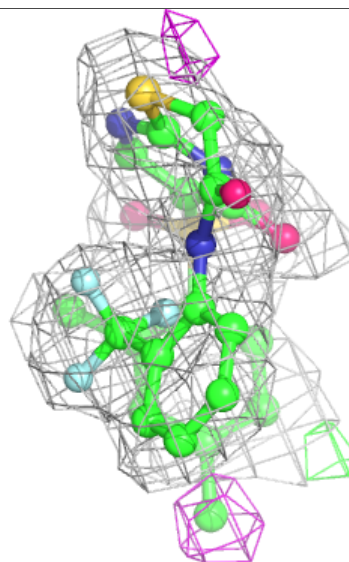
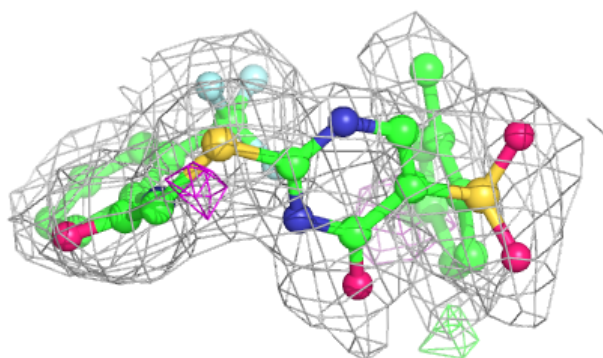
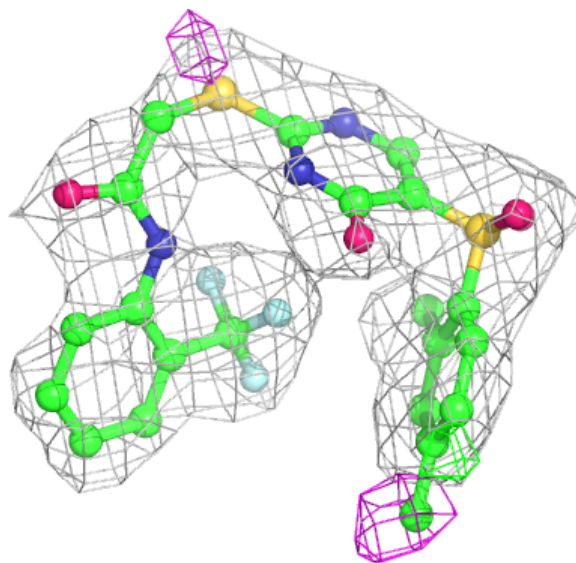
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	A	701	5/5	0.88	0.24	62,64,69,73	0
2	PO4	A	703	5/5	0.88	0.24	60,67,70,74	0
2	PO4	A	704	5/5	0.89	0.30	46,50,53,57	0
2	PO4	B	703	5/5	0.95	0.28	41,41,43,44	0
3	4ID	B	705	33/33	0.96	0.17	19,24,27,31	0
3	4ID	A	706	33/33	0.96	0.17	18,22,31,32	0
3	4ID	C	703	33/33	0.96	0.18	20,25,30,35	0
2	PO4	B	701	5/5	0.97	0.15	27,30,31,33	0
3	4ID	B	704	33/33	0.97	0.18	18,24,27,28	0
2	PO4	C	701	5/5	0.97	0.12	29,30,33,37	0
3	4ID	C	702	33/33	0.97	0.16	19,21,25,29	0
3	4ID	A	705	33/33	0.97	0.18	18,22,31,36	0
2	PO4	A	702	5/5	0.99	0.13	23,25,27,28	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.

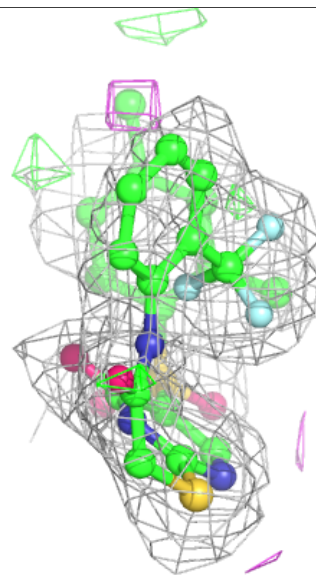
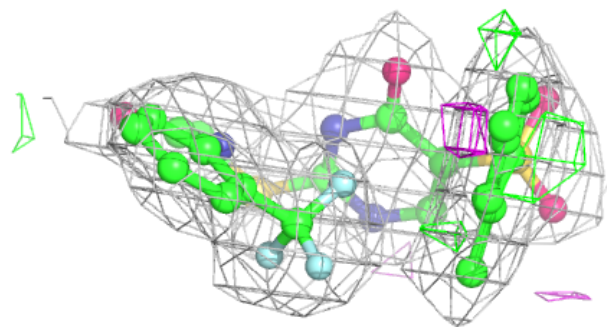
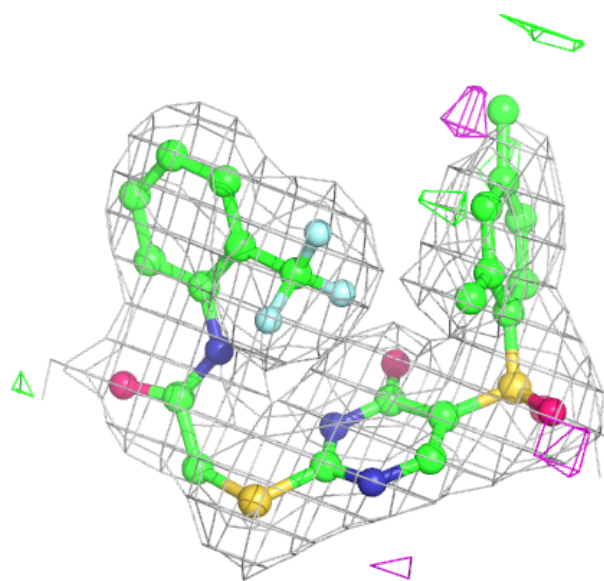
Electron density around 4ID B 705:

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



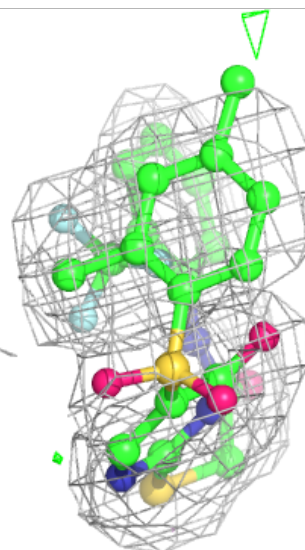
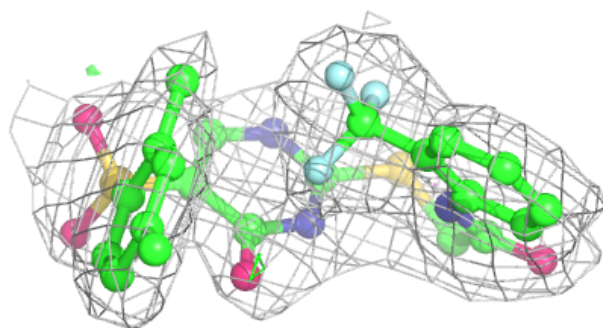
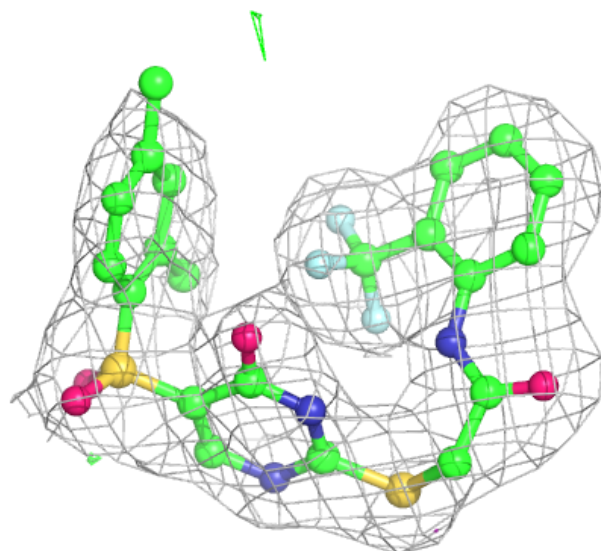
Electron density around 4ID A 706:

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



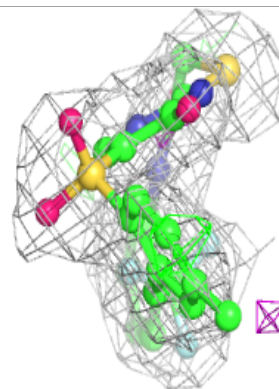
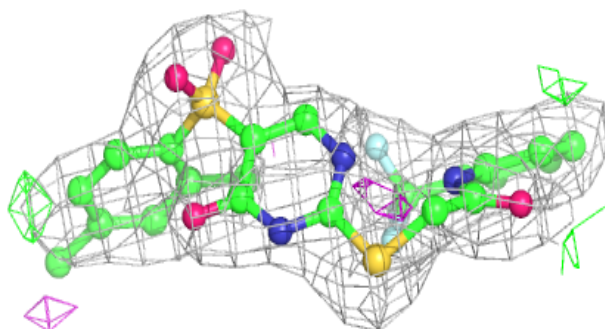
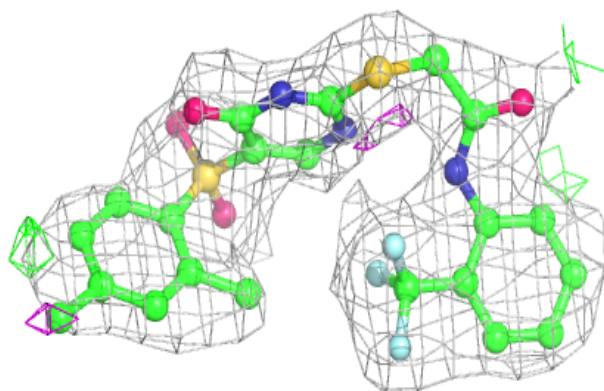
Electron density around 4ID C 703:

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

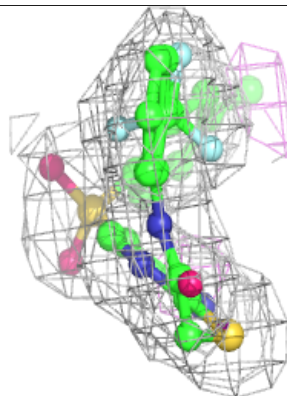
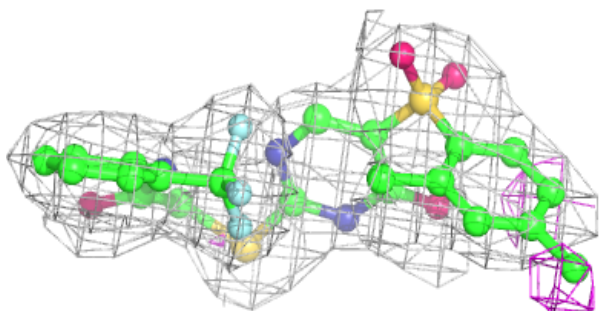
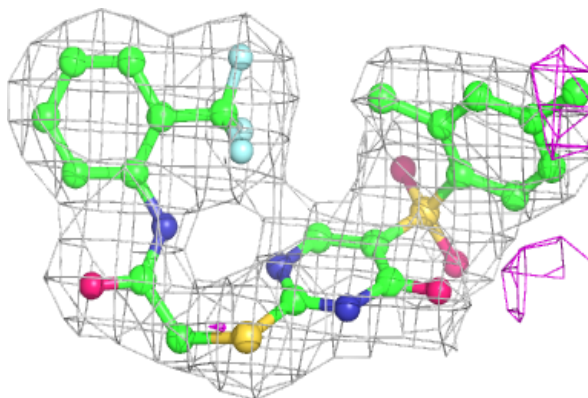


Electron density around 4ID B 704:

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

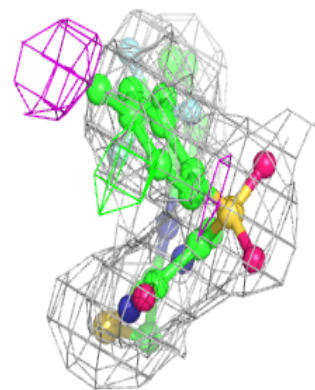
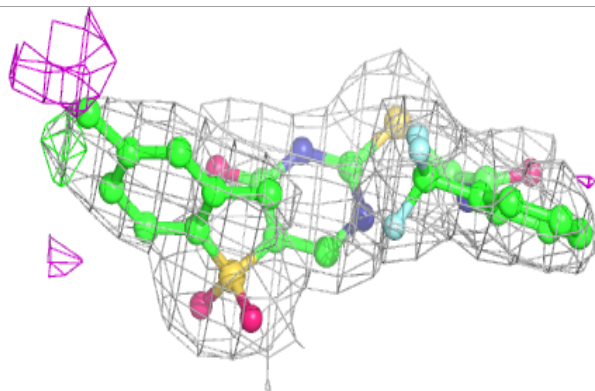
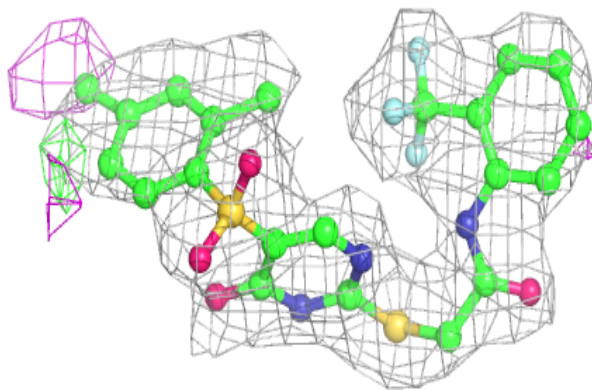
**Electron density around 4ID C 702:**

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



Electron density around 4ID A 705:

$2mF_o-DF_c$ (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.