



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2024 – 04:50 pm BST

PDB ID : 8RQC
Title : Crystal structure of CRBN-midi in complex with mezigdomide and IKZF1 ZF2
Authors : Furihata, H.; Kroupova, A.; Zollman, D.; Ciulli, A.
Deposited on : 2024-01-17
Resolution : 2.15 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

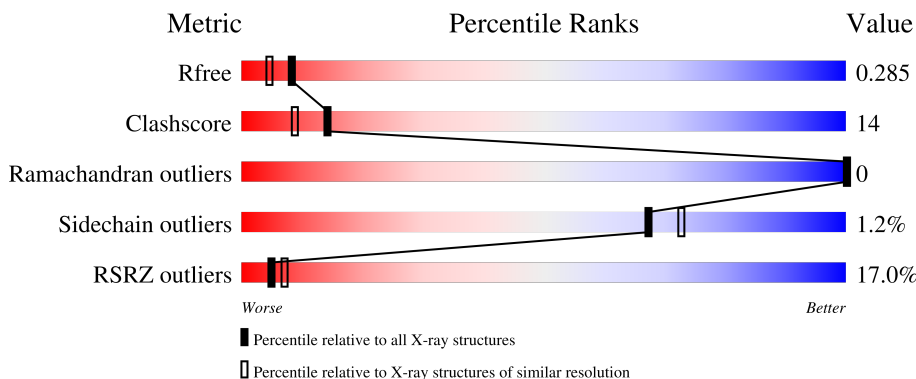
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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	329	 15% 69% 22% 9%
1	D	329	 16% 65% 29% • 5%
2	B	36	 14% 58% 17% 25%
2	E	36	 14% 56% 19% 25%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5303 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 Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	300	2277	1447	385	430	15	0	0	0
1	D	312	2356	1497	401	441	17	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	SER	-	expression tag	UNP Q96SW2
A	78	ILE	CYS	engineered mutation	UNP Q96SW2
A	92	VAL	ILE	engineered mutation	UNP Q96SW2
A	116	ASN	LYS	engineered mutation	UNP Q96SW2
A	134	GLU	GLN	engineered mutation	UNP Q96SW2
A	188	GLY	-	linker	UNP Q96SW2
A	189	SER	-	linker	UNP Q96SW2
A	190	GLY	-	linker	UNP Q96SW2
A	283	TRP	ARG	engineered mutation	UNP Q96SW2
A	287	ASN	CYS	engineered mutation	UNP Q96SW2
A	293	SER	VAL	engineered mutation	UNP Q96SW2
A	302	ASP	GLY	engineered mutation	UNP Q96SW2
A	342	ARG	LEU	engineered mutation	UNP Q96SW2
A	343	GLU	CYS	engineered mutation	UNP Q96SW2
A	359	ILE	THR	engineered mutation	UNP Q96SW2
A	423	ILE	LEU	engineered mutation	UNP Q96SW2
D	40	SER	-	expression tag	UNP Q96SW2
D	78	ILE	CYS	engineered mutation	UNP Q96SW2
D	92	VAL	ILE	engineered mutation	UNP Q96SW2
D	116	ASN	LYS	engineered mutation	UNP Q96SW2
D	134	GLU	GLN	engineered mutation	UNP Q96SW2
D	188	GLY	-	linker	UNP Q96SW2
D	189	SER	-	linker	UNP Q96SW2
D	190	GLY	-	linker	UNP Q96SW2
D	283	TRP	ARG	engineered mutation	UNP Q96SW2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	287	ASN	CYS	engineered mutation	UNP Q96SW2
D	293	SER	VAL	engineered mutation	UNP Q96SW2
D	302	ASP	GLY	engineered mutation	UNP Q96SW2
D	342	ARG	LEU	engineered mutation	UNP Q96SW2
D	343	GLU	CYS	engineered mutation	UNP Q96SW2
D	359	ILE	THR	engineered mutation	UNP Q96SW2
D	423	ILE	LEU	engineered mutation	UNP Q96SW2

- Molecule 2 is a protein called DNA-binding protein Ikaros.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	27	202	125	40	35	2	0	0	0
2	E	27	201	126	40	33	2	0	0	0

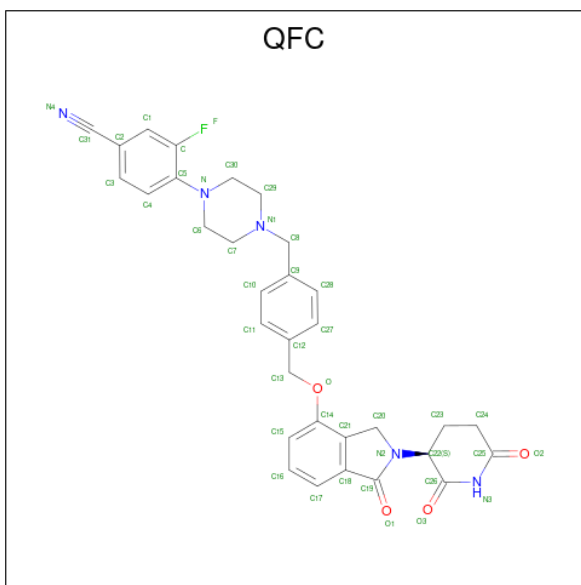
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	139	GLY	-	expression tag	UNP Q13422
B	140	PRO	-	expression tag	UNP Q13422
E	139	GLY	-	expression tag	UNP Q13422
E	140	PRO	-	expression tag	UNP Q13422

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	D	1	1	1	0	0
3	E	1	1	1	0	0

- Molecule 4 is Mezigdomide (three-letter code: QFC) (formula: C₃₂H₃₀FN₅O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	F	N	O	0	0
			42	32	1	5	4		
4	D	1	Total	C	F	N	O	0	0
			42	32	1	5	4		

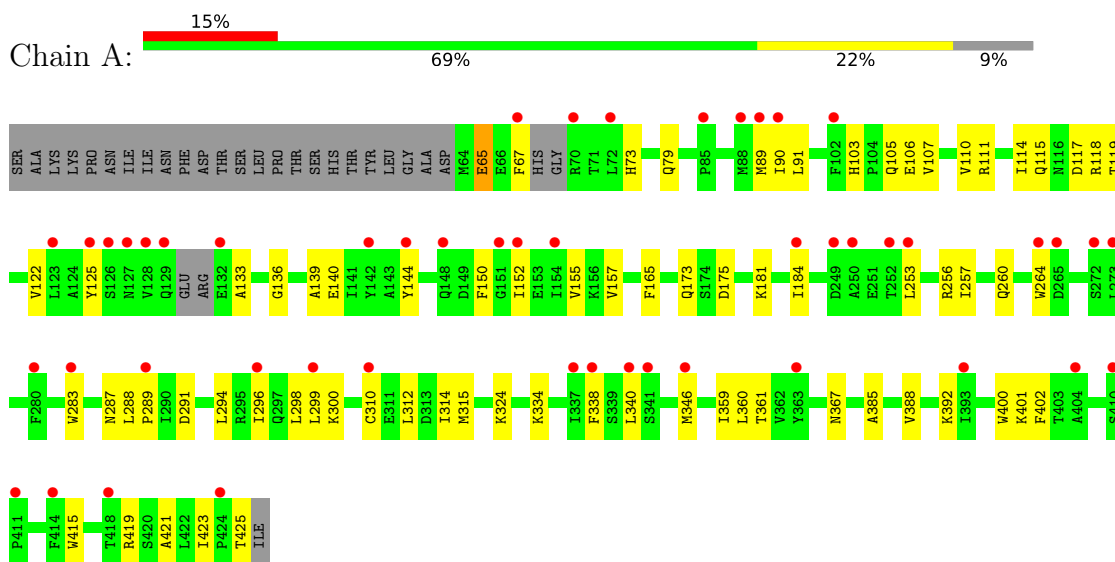
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	75	Total	O	0	0
			75	75		
5	B	11	Total	O	0	0
			11	11		
5	D	83	Total	O	0	0
			83	83		
5	E	10	Total	O	0	0
			10	10		

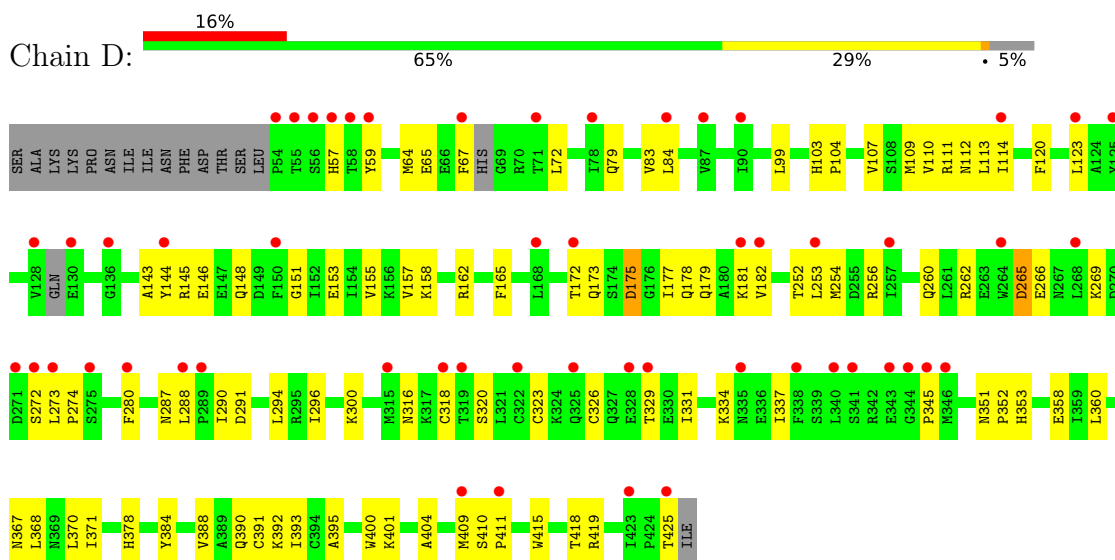
3 Residue-property plots

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: Protein cereblon

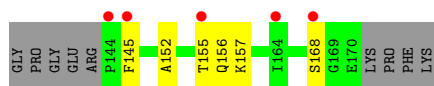


- Molecule 1: Protein cereblon

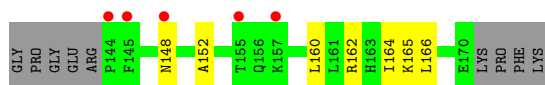


- Molecule 2: DNA-binding protein Ikaros





- Molecule 2: DNA-binding protein Ikaros



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.59Å 142.84Å 56.69Å 90.00° 112.34° 90.00°	Depositor
Resolution (Å)	52.44 – 2.15 52.44 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.5 (52.44-2.15) 97.5 (52.44-2.15)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.14Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.261 , 0.286 0.261 , 0.285	Depositor DCC
R_{free} test set	2021 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtrriage
Anisotropy	0.380	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5303	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: ZN, QFC

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	0.52	0/2325	0.70	0/3170
1	D	0.51	0/2409	0.70	0/3284
2	B	0.51	0/206	0.69	0/275
2	E	0.57	0/205	0.75	0/273
All	All	0.52	0/5145	0.70	0/7002

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2277	0	2132	61	0
1	D	2356	0	2195	70	0
2	B	202	0	188	3	0
2	E	201	0	190	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	42	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	42	0	0	1	0
5	A	75	0	0	4	0
5	B	11	0	0	0	0
5	D	83	0	0	1	0
5	E	10	0	0	1	0
All	All	5303	0	4705	138	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 14.

All (138) 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:D:410:SER:HB2	1:D:411:PRO:HD3	1.51	0.89
1:A:65:GLU:HG2	1:A:144:TYR:O	1.86	0.76
1:D:290:ILE:HD12	1:D:294:LEU:HD23	1.70	0.73
1:D:262:ARG:HA	1:D:266:GLU:CB	2.21	0.71
1:D:265:ASP:O	1:D:265:ASP:OD1	2.10	0.70
1:A:257:ILE:HD13	1:A:312:LEU:HD13	1.73	0.69
1:D:111:ARG:HA	1:D:114:ILE:HD12	1.74	0.69
1:D:266:GLU:HA	1:D:269:LYS:CB	2.23	0.69
1:A:346:MET:CE	1:A:419:ARG:HD3	2.23	0.68
1:A:125:TYR:HA	1:A:133:ALA:HB2	1.77	0.67
1:D:252:THR:HG22	1:D:256:ARG:HD2	1.77	0.65
1:D:178:GLN:NE2	5:D:702:HOH:O	2.30	0.63
1:D:83:VAL:HG13	1:D:123:LEU:HD13	1.81	0.62
1:A:338:PHE:HE2	1:A:340:LEU:HD13	1.63	0.62
1:A:367:ASN:HA	1:A:392:LYS:HD2	1.82	0.62
1:A:89:MET:HG2	1:A:90:ILE:N	2.15	0.61
1:A:264:TRP:CE2	1:A:334:LYS:HD2	2.36	0.61
1:D:99:LEU:HB2	1:D:157:VAL:HG22	1.81	0.61
1:A:346:MET:HE1	1:A:419:ARG:HD3	1.83	0.60
1:A:119:THR:HG22	1:A:140:GLU:HG3	1.82	0.60
1:A:89:MET:HE3	1:A:91:LEU:HB2	1.83	0.60
1:A:103:HIS:HB2	1:A:106:GLU:HG3	1.84	0.60
1:D:290:ILE:CG2	1:D:294:LEU:HB3	2.32	0.59
2:E:148:ASN:HB2	5:E:307:HOH:O	2.03	0.59
1:D:351:ASN:HB2	1:D:352:PRO:HD2	1.86	0.58
1:D:326:CYS:SG	1:D:329:THR:HG22	2.42	0.58
1:D:337:ILE:HG23	1:D:345:PRO:HB3	1.86	0.58
1:A:298:LEU:O	1:A:299:LEU:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ASP:OD1	1:D:177:ILE:HG23	2.05	0.57
1:A:289:PRO:HB3	1:A:360:LEU:HD22	1.87	0.56
1:A:89:MET:CE	1:A:91:LEU:HD13	2.36	0.55
1:A:296:ILE:O	1:A:300:LYS:HG3	2.07	0.55
1:D:290:ILE:HG23	1:D:294:LEU:HB3	1.88	0.55
1:D:404:ALA:HB1	1:D:409:MET:HG3	1.89	0.55
1:A:324:LYS:HG2	1:A:423:ILE:HG23	1.88	0.55
1:A:73:HIS:HB2	1:A:184:ILE:HG13	1.88	0.54
1:A:111:ARG:O	1:A:115:GLN:HG3	2.08	0.54
1:D:329:THR:HB	1:D:393:ILE:HD13	1.91	0.53
1:A:91:LEU:CB	1:A:122:VAL:HG21	2.39	0.53
1:A:173:GLN:HB2	1:A:175:ASP:OD1	2.10	0.52
1:D:111:ARG:NH2	1:D:146:GLU:OE2	2.39	0.52
1:D:287:ASN:HB3	1:D:345:PRO:HD2	1.92	0.51
1:A:119:THR:HG21	5:A:703:HOH:O	2.11	0.51
1:D:103:HIS:O	1:D:107:VAL:HG13	2.10	0.51
1:A:346:MET:SD	1:A:419:ARG:HD3	2.50	0.50
1:D:104:PRO:O	1:D:107:VAL:HG22	2.12	0.50
1:D:57:HIS:HD2	1:D:59:TYR:OH	1.94	0.50
1:A:425:THR:C	5:A:712:HOH:O	2.50	0.50
1:D:367:ASN:HA	1:D:392:LYS:HD2	1.94	0.50
1:A:89:MET:HE1	1:A:91:LEU:HD13	1.93	0.49
1:A:89:MET:CG	1:A:90:ILE:N	2.75	0.49
1:A:119:THR:HA	1:A:139:ALA:O	2.13	0.49
1:D:329:THR:HG21	1:D:391:CYS:SG	2.52	0.49
1:D:395:ALA:O	2:E:166:LEU:HD13	2.12	0.49
1:D:370:LEU:HD21	1:D:401:LYS:HD3	1.94	0.49
1:D:291:ASP:OD1	1:D:291:ASP:N	2.41	0.48
1:A:105:GLN:HG2	1:A:106:GLU:N	2.28	0.48
2:B:145:PHE:CE1	2:B:157:LYS:HB2	2.48	0.48
1:A:110:VAL:O	1:A:114:ILE:HG12	2.14	0.48
2:E:162:ARG:HA	2:E:165:LYS:HD3	1.96	0.47
1:A:421:ALA:O	5:A:701:HOH:O	2.20	0.47
1:A:257:ILE:HD11	1:A:312:LEU:HB2	1.96	0.47
1:D:148:GLN:HG3	1:D:153:GLU:HA	1.96	0.47
1:D:352:PRO:HD3	1:D:378:HIS:ND1	2.30	0.47
1:A:118:ARG:NH2	1:A:140:GLU:OE2	2.48	0.46
1:A:260:GLN:HE21	1:A:260:GLN:HB3	1.59	0.46
1:D:64:MET:HG2	1:D:145:ARG:HB2	1.97	0.46
1:A:107:VAL:O	1:A:111:ARG:HG3	2.16	0.46
1:D:83:VAL:CG1	1:D:123:LEU:HD13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:PRO:HG2	1:D:280:PHE:HA	1.97	0.46
1:D:253:LEU:HA	1:D:256:ARG:HD3	1.98	0.45
1:D:114:ILE:HD13	1:D:144:TYR:CZ	2.51	0.45
1:D:165:PHE:HB2	1:D:182:VAL:HB	1.99	0.45
1:A:150:PHE:C	1:A:152:ILE:H	2.18	0.45
4:D:602:QFC:C6	4:D:602:QFC:F	2.54	0.45
1:A:264:TRP:NE1	1:A:334:LYS:HD2	2.32	0.45
1:D:358:GLU:OE1	1:D:419:ARG:HD3	2.17	0.45
1:D:79:GLN:O	1:D:182:VAL:N	2.46	0.44
1:D:331:ILE:HD12	1:D:368:LEU:HD21	1.99	0.44
1:D:79:GLN:O	1:D:181:LYS:HA	2.18	0.44
1:D:172:THR:HG22	1:D:178:GLN:HB2	2.00	0.44
1:D:384:TYR:OH	1:D:411:PRO:HD2	2.17	0.44
1:A:385:ALA:O	1:A:402:PHE:HA	2.17	0.44
1:D:320:SER:O	1:D:425:THR:N	2.46	0.44
1:A:91:LEU:HB2	1:A:122:VAL:HG21	1.98	0.44
1:D:143:ALA:HB3	1:D:158:LYS:HB2	2.00	0.44
1:D:173:GLN:OE1	1:D:179:GLN:HG3	2.18	0.44
1:D:113:LEU:HD21	1:D:120:PHE:HB3	2.00	0.44
1:D:67:PHE:CZ	1:D:144:TYR:HB3	2.53	0.44
1:D:260:GLN:NE2	1:D:316:ASN:OD1	2.35	0.44
1:A:359:ILE:HD11	1:A:400:TRP:HZ3	1.81	0.44
1:D:334:LYS:HA	1:D:337:ILE:HD12	1.99	0.44
1:A:253:LEU:O	1:A:257:ILE:HG12	2.18	0.43
1:A:89:MET:HE3	1:A:91:LEU:CB	2.47	0.43
1:D:84:LEU:HA	1:D:84:LEU:HD23	1.75	0.43
1:D:65:GLU:O	1:D:143:ALA:HA	2.19	0.43
1:D:371:ILE:HD11	1:D:390:GLN:OE1	2.19	0.43
1:A:256:ARG:NE	1:A:260:GLN:OE1	2.50	0.43
1:A:155:VAL:HG12	1:A:157:VAL:HG12	2.01	0.43
4:A:602:QFC:F	4:A:602:QFC:C30	2.57	0.43
1:D:401:LYS:HD2	1:D:415:TRP:CZ2	2.54	0.43
1:A:312:LEU:HD12	1:A:312:LEU:HA	1.81	0.42
1:D:109:MET:HE3	1:D:113:LEU:HD22	2.01	0.42
1:A:136:GLY:HA3	1:A:165:PHE:CZ	2.54	0.42
1:D:272:SER:C	1:D:273:LEU:HD12	2.40	0.42
1:A:361:THR:HA	1:A:415:TRP:O	2.19	0.42
1:D:353:HIS:CE1	2:E:148:ASN:OD1	2.73	0.42
1:D:103:HIS:ND1	1:D:104:PRO:HD2	2.35	0.42
2:E:160:LEU:HD11	2:E:164:ILE:HD11	2.02	0.42
1:A:401:LYS:HB2	1:A:415:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ALA:HB1	5:A:701:HOH:O	2.20	0.41
1:D:337:ILE:HG12	1:D:360:LEU:HD11	2.02	0.41
1:D:72:LEU:HD21	1:D:162:ARG:HD2	2.02	0.41
1:D:296:ILE:O	1:D:300:LYS:HG3	2.20	0.41
1:A:67:PHE:HE1	1:A:144:TYR:HB3	1.85	0.41
1:D:67:PHE:CE2	1:D:144:TYR:HB3	2.55	0.41
1:D:388:VAL:HG21	2:E:152:ALA:HB2	2.01	0.41
1:A:89:MET:HE3	1:A:91:LEU:HD13	2.01	0.41
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.87	0.41
1:A:256:ARG:NH2	1:D:151:GLY:O	2.53	0.41
1:D:109:MET:O	1:D:112:ASN:HB2	2.20	0.41
1:D:400:TRP:CZ3	1:D:418:THR:HG22	2.55	0.41
1:D:401:LYS:HD2	1:D:415:TRP:CH2	2.56	0.41
1:A:283:TRP:CE2	1:A:287:ASN:ND2	2.89	0.41
1:A:291:ASP:H	1:A:294:LEU:HD12	1.85	0.41
1:D:110:VAL:HG21	1:D:155:VAL:HG11	2.03	0.41
1:D:288:LEU:HD12	1:D:288:LEU:HA	1.97	0.41
1:D:290:ILE:HD13	1:D:290:ILE:HA	1.91	0.41
1:A:310:CYS:O	1:A:314:ILE:HG12	2.21	0.41
1:A:103:HIS:HB2	1:A:106:GLU:CG	2.50	0.40
1:A:150:PHE:C	1:A:152:ILE:N	2.74	0.40
2:B:155:THR:HG22	2:B:156:GLN:HG3	2.03	0.40
2:E:160:LEU:O	2:E:164:ILE:HG12	2.22	0.40
1:A:79:GLN:O	1:A:181:LYS:HA	2.22	0.40
1:D:254:MET:HE3	1:D:254:MET:HB3	1.95	0.40
1:A:117:ASP:O	1:A:119:THR:HG23	2.21	0.40
1:A:257:ILE:HG23	1:A:315:MET:HE1	2.04	0.40
1:A:388:VAL:HG21	2:B:152:ALA:HB2	2.03	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	294/329 (89%)	279 (95%)	15 (5%)	0	100	100
1	D	307/329 (93%)	298 (97%)	9 (3%)	0	100	100
2	B	25/36 (69%)	25 (100%)	0	0	100	100
2	E	25/36 (69%)	25 (100%)	0	0	100	100
All	All	651/730 (89%)	627 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	232/293 (79%)	231 (100%)	1 (0%)	89	92
1	D	236/293 (80%)	231 (98%)	5 (2%)	48	53
2	B	21/30 (70%)	20 (95%)	1 (5%)	21	19
2	E	20/30 (67%)	20 (100%)	0	100	100
All	All	509/646 (79%)	502 (99%)	7 (1%)	67	68

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	GLU
2	B	168	SER
1	D	175	ASP
1	D	265	ASP
1	D	318[A]	CYS
1	D	318[B]	CYS
1	D	323	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	79	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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
4	QFC	D	602	-	47,47,47	3.61	17 (36%)	65,67,67	3.85	26 (40%)
4	QFC	A	602	-	47,47,47	3.91	21 (44%)	65,67,67	3.68	19 (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
4	QFC	D	602	-	-	4/19/54/54	0/6/6/6
4	QFC	A	602	-	-	2/19/54/54	0/6/6/6

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	QFC	C8-N1	10.07	1.67	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	QFC	C19-N2	9.73	1.45	1.36
4	D	602	QFC	C8-N1	9.63	1.66	1.47
4	D	602	QFC	C19-N2	9.40	1.45	1.36
4	A	602	QFC	C13-C12	8.20	1.70	1.50
4	A	602	QFC	C18-C19	8.20	1.62	1.48
4	D	602	QFC	C13-C12	8.11	1.69	1.50
4	A	602	QFC	C22-N2	7.70	1.55	1.46
4	D	602	QFC	C18-C19	7.69	1.61	1.48
4	D	602	QFC	C22-N2	7.42	1.55	1.46
4	A	602	QFC	C20-C21	7.13	1.59	1.50
4	A	602	QFC	C20-N2	7.02	1.52	1.46
4	D	602	QFC	C20-C21	6.47	1.58	1.50
4	A	602	QFC	C26-N3	6.00	1.47	1.37
4	D	602	QFC	C20-N2	5.93	1.51	1.46
4	A	602	QFC	C25-N3	5.47	1.46	1.37
4	D	602	QFC	C26-N3	5.42	1.46	1.37
4	D	602	QFC	C25-N3	4.77	1.45	1.37
4	A	602	QFC	C14-C21	4.67	1.46	1.40
4	A	602	QFC	C5-N	4.34	1.50	1.41
4	A	602	QFC	C1-C	4.06	1.44	1.37
4	A	602	QFC	C2-C31	3.97	1.53	1.44
4	D	602	QFC	C5-N	3.86	1.49	1.41
4	D	602	QFC	C2-C31	3.82	1.53	1.44
4	D	602	QFC	C1-C	3.72	1.44	1.37
4	D	602	QFC	C14-C21	3.72	1.45	1.40
4	A	602	QFC	C17-C18	2.64	1.44	1.39
4	A	602	QFC	C30-N	2.62	1.50	1.46
4	A	602	QFC	C22-C26	2.47	1.56	1.51
4	D	602	QFC	C11-C12	2.45	1.44	1.38
4	A	602	QFC	C11-C12	2.45	1.44	1.38
4	A	602	QFC	C6-N	2.41	1.50	1.46
4	A	602	QFC	O-C14	2.41	1.42	1.37
4	A	602	QFC	C5-C	2.41	1.45	1.40
4	D	602	QFC	C17-C18	2.39	1.43	1.39
4	D	602	QFC	C22-C26	2.39	1.56	1.51
4	A	602	QFC	C1-C2	2.31	1.43	1.39
4	D	602	QFC	C1-C2	2.13	1.43	1.39

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	QFC	C21-C20-N2	21.30	108.61	101.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	602	QFC	C21-C20-N2	20.38	108.31	101.79
4	D	602	QFC	C20-N2-C19	-15.20	106.87	113.12
4	A	602	QFC	C20-N2-C19	-14.76	107.05	113.12
4	D	602	QFC	C1-C-C5	-5.72	118.62	123.34
4	D	602	QFC	C18-C19-N2	4.59	109.15	106.44
4	D	602	QFC	C23-C22-N2	4.26	118.71	114.11
4	D	602	QFC	C8-N1-C29	-4.26	101.58	111.06
4	A	602	QFC	C1-C-C5	-4.26	119.82	123.34
4	D	602	QFC	C22-N2-C19	4.20	128.50	121.81
4	A	602	QFC	C22-N2-C19	4.11	128.35	121.81
4	A	602	QFC	C18-C19-N2	3.99	108.80	106.44
4	D	602	QFC	C24-C25-N3	-3.96	112.20	116.65
4	A	602	QFC	C20-C21-C18	-3.83	107.51	109.88
4	D	602	QFC	C2-C1-C	3.64	123.50	118.72
4	D	602	QFC	C30-N-C6	-3.63	103.50	111.52
4	A	602	QFC	C24-C25-N3	-3.47	112.75	116.65
4	D	602	QFC	C8-N1-C7	-3.40	103.50	111.06
4	D	602	QFC	C24-C23-C22	3.36	116.08	109.77
4	D	602	QFC	C6-C7-N1	3.33	117.47	110.64
4	D	602	QFC	C9-C8-N1	-3.21	106.89	113.12
4	D	602	QFC	C30-C29-N1	3.16	117.12	110.64
4	A	602	QFC	C2-C1-C	3.09	122.78	118.72
4	A	602	QFC	O-C14-C21	3.03	120.08	115.71
4	D	602	QFC	O2-C25-N3	2.86	124.81	120.28
4	A	602	QFC	C3-C2-C1	-2.82	115.78	119.76
4	D	602	QFC	C20-C21-C18	-2.68	108.22	109.88
4	A	602	QFC	C8-N1-C29	-2.68	105.10	111.06
4	A	602	QFC	C18-C21-C14	2.61	121.53	120.19
4	D	602	QFC	C3-C2-C1	-2.60	116.08	119.76
4	D	602	QFC	C18-C21-C14	2.59	121.51	120.19
4	D	602	QFC	C29-N1-C7	2.52	114.50	108.83
4	D	602	QFC	C17-C18-C19	2.45	133.62	129.63
4	A	602	QFC	O2-C25-N3	2.41	124.10	120.28
4	D	602	QFC	C-C5-N	-2.36	117.67	120.47
4	A	602	QFC	C17-C18-C19	2.21	133.24	129.63
4	D	602	QFC	O-C14-C21	2.21	118.89	115.71
4	D	602	QFC	C23-C22-C26	2.21	115.40	111.61
4	A	602	QFC	C1-C2-C31	2.14	122.38	119.54
4	A	602	QFC	C29-C30-N	2.09	114.77	110.70
4	D	602	QFC	C8-C9-C28	-2.08	116.87	120.77
4	A	602	QFC	C8-N1-C7	-2.06	106.48	111.06
4	A	602	QFC	C9-C8-N1	-2.03	109.19	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	QFC	C24-C23-C22	2.01	113.54	109.77
4	D	602	QFC	C1-C2-C31	2.00	122.20	119.54

There are no chirality outliers.

All (6) torsion outliers are listed below:

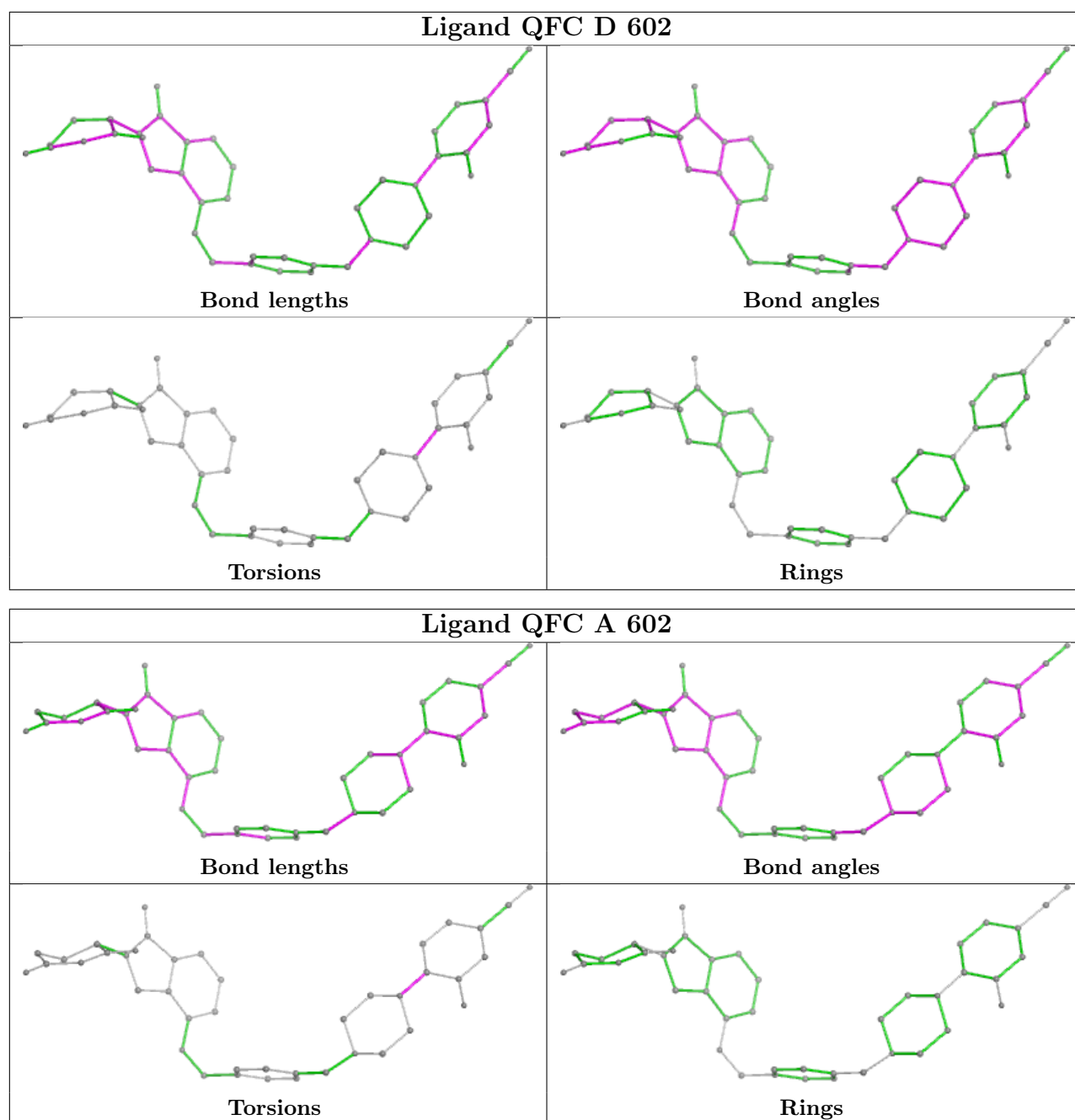
Mol	Chain	Res	Type	Atoms
4	D	602	QFC	C-C5-N-C30
4	D	602	QFC	C-C5-N-C6
4	D	602	QFC	C4-C5-N-C6
4	A	602	QFC	C-C5-N-C30
4	A	602	QFC	C4-C5-N-C30
4	D	602	QFC	C4-C5-N-C30

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	602	QFC	1	0
4	A	602	QFC	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	300/329 (91%)	1.20	49 (16%) 5 7	42, 59, 101, 129	0
1	D	312/329 (94%)	1.12	54 (17%) 5 7	39, 60, 97, 152	1 (0%)
2	B	27/36 (75%)	0.88	5 (18%) 4 6	46, 58, 79, 85	0
2	E	27/36 (75%)	0.86	5 (18%) 4 6	44, 55, 71, 75	0
All	All	666/730 (91%)	1.14	113 (16%) 5 7	39, 59, 98, 152	1 (0%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	LEU	5.0
1	A	264	TRP	4.5
1	A	363	TYR	4.4
1	D	182	VAL	4.4
1	A	289	PRO	4.2
1	A	299	LEU	4.2
1	A	129	GLN	4.1
1	A	410	SER	3.8
1	A	128	VAL	3.8
1	A	250	ALA	3.7
1	A	102	PHE	3.7
1	A	340	LEU	3.7
1	D	58	THR	3.7
1	D	423	ILE	3.5
1	D	341	SER	3.5
1	D	55	THR	3.5
1	A	154	ILE	3.5
1	D	328	GLU	3.4
1	D	264	TRP	3.4
1	A	127	ASN	3.3
1	A	125	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	89	MET	3.2
1	D	344	GLY	3.1
1	D	87	VAL	3.1
1	A	310	CYS	3.0
1	D	150	PHE	3.0
1	A	132	GLU	2.9
1	A	144	TYR	2.9
1	A	414	PHE	2.9
1	A	265	ASP	2.9
1	D	67	PHE	2.9
1	D	318[A]	CYS	2.9
1	D	322	CYS	2.9
1	A	273	LEU	2.8
1	D	273	LEU	2.8
1	D	125	TYR	2.8
1	A	152	ILE	2.8
1	A	411	PRO	2.8
1	A	272	SER	2.8
1	D	271	ASP	2.8
1	A	346	MET	2.7
1	A	418	THR	2.7
1	D	325	GLN	2.7
1	A	424	PRO	2.7
1	D	84	LEU	2.7
1	D	409	MET	2.7
1	A	67	PHE	2.7
1	A	338	PHE	2.7
1	D	289	PRO	2.7
1	A	283	TRP	2.7
1	D	172	THR	2.7
1	D	253	LEU	2.6
1	D	272	SER	2.6
1	D	340	LEU	2.6
1	A	70	ARG	2.6
1	D	128	VAL	2.6
1	D	346	MET	2.6
1	D	345	PRO	2.6
1	D	90	ILE	2.6
1	A	151	GLY	2.5
1	A	296	ILE	2.5
1	D	54	PRO	2.5
1	D	56	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	268	LEU	2.5
1	D	144	TYR	2.5
1	D	329	THR	2.5
1	A	88	MET	2.4
1	D	319	THR	2.4
1	D	78	ILE	2.4
2	B	168	SER	2.4
1	A	90	ILE	2.4
1	D	114	ILE	2.4
1	D	257	ILE	2.4
1	A	123	LEU	2.4
1	D	130	GLU	2.4
1	A	85	PRO	2.4
2	B	144	PRO	2.4
1	A	72	LEU	2.3
2	E	157	LYS	2.3
1	D	315	MET	2.3
1	D	123	LEU	2.3
1	A	341	SER	2.3
1	A	337	ILE	2.3
1	D	71	THR	2.3
2	B	155	THR	2.3
1	D	411	PRO	2.2
2	E	145	PHE	2.2
1	A	184	ILE	2.2
1	D	288	LEU	2.2
1	A	249	ASP	2.2
1	D	136	GLY	2.2
1	D	335	ASN	2.2
1	D	425	THR	2.2
1	D	275	SER	2.2
1	D	343	GLU	2.2
1	A	393	ILE	2.1
1	A	252	THR	2.1
1	A	148	GLN	2.1
1	D	181	LYS	2.1
1	A	280	PHE	2.1
1	D	280	PHE	2.1
2	B	164	ILE	2.1
2	E	155	THR	2.1
1	A	126	SER	2.1
1	D	57	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	168	LEU	2.1
1	A	404	ALA	2.0
1	D	338	PHE	2.0
2	B	145	PHE	2.0
2	E	148	ASN	2.0
2	E	144	PRO	2.0
1	A	142	TYR	2.0
1	D	59	TYR	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](#)

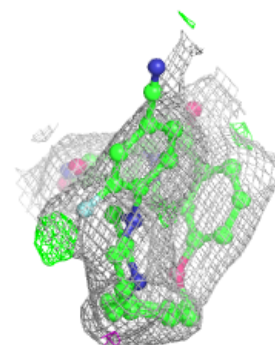
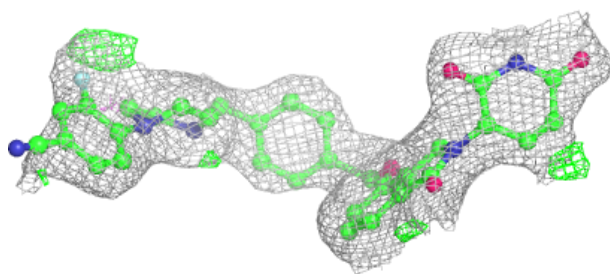
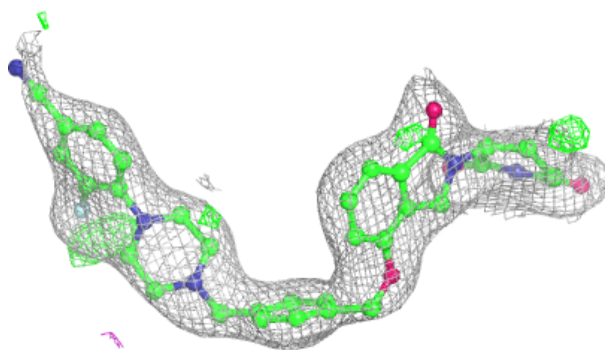
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	QFC	D	602	42/42	0.88	0.12	38,50,62,70	0
4	QFC	A	602	42/42	0.89	0.14	39,52,81,93	0
3	ZN	D	601	1/1	0.96	0.05	69,69,69,69	0
3	ZN	E	201	1/1	0.98	0.04	44,44,44,44	0
3	ZN	A	601	1/1	0.99	0.04	52,52,52,52	0
3	ZN	B	201	1/1	0.99	0.03	45,45,45,45	0

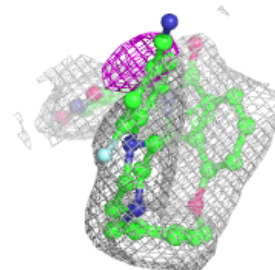
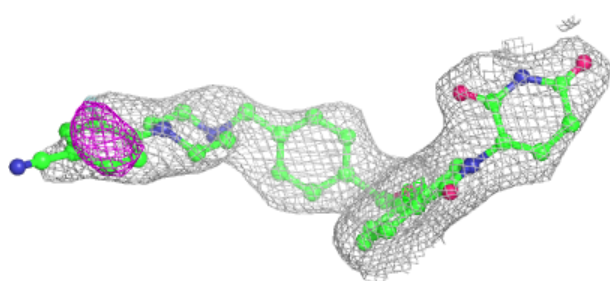
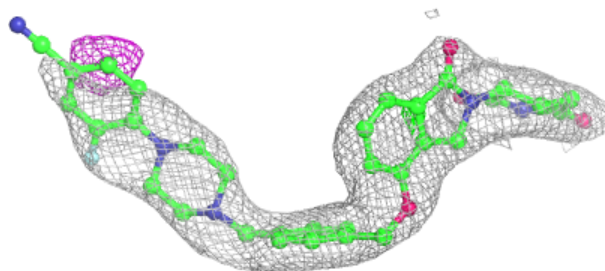
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QFC D 602:

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

**Electron density around QFC A 602:**

$2mF_o-DF_c$ (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.