



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:48 PM UTC

PDB ID : 6N8G / pdb_00006n8g
Title : IRAK4 bound to benzoxazole compound
Authors : Larsen, N.A.; Bloudoff, K.; Subramanian, V.; Dobrzanska, M.; Gluza, K.
Deposited on : 2018-11-29
Resolution : 2.00 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

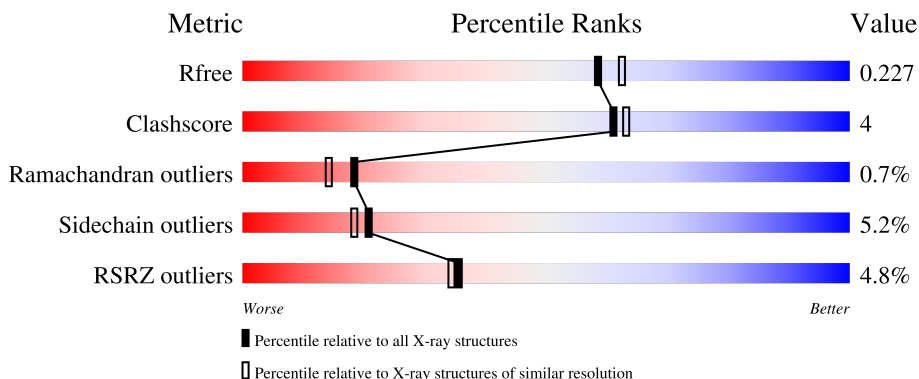
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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.

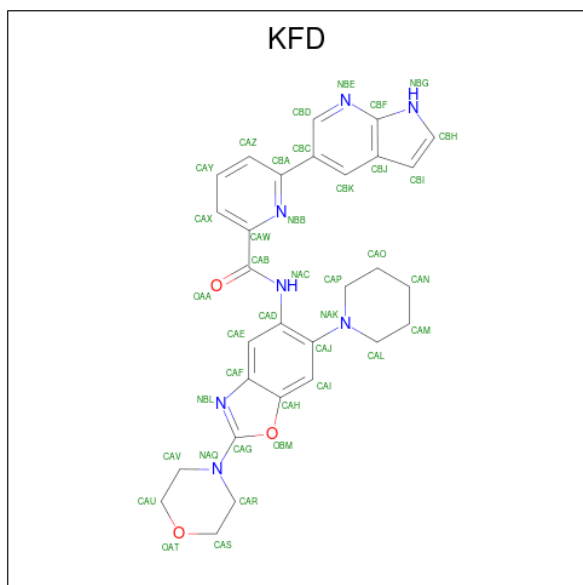
Mol	Chain	Length	Quality of chain
1	A	297	3% 80% 15% • •
1	B	297	6% 81% 14% • •
1	C	297	3% 79% 15% • •
1	D	297	6% 79% 13% • 6%

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	288	Total 2268	C 1420	N 381	O 450	P 3	S 14	0	0	0
1	B	286	Total 2253	C 1409	N 379	O 447	P 3	S 15	0	1	0
1	C	289	Total 2302	C 1444	N 386	O 455	P 3	S 14	0	3	0
1	D	280	Total 2199	C 1375	N 372	O 435	P 3	S 14	0	0	0

- Molecule 2 is N-[2-(morpholin-4-yl)-6-(piperidin-1-yl)-1,3-benzoxazol-5-yl]-6-(1H-pyrrolo[2,3-b]pyridin-5-yl)pyridine-2-carboxamide (CCD ID: KFD) (formula: $C_{29}H_{29}N_7O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 39	C 29	N 7	O 3	0	0
2	B	1	Total 39	C 29	N 7	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			39	29	7	3		
2	D	1	Total	C	N	O	0	0
			39	29	7	3		

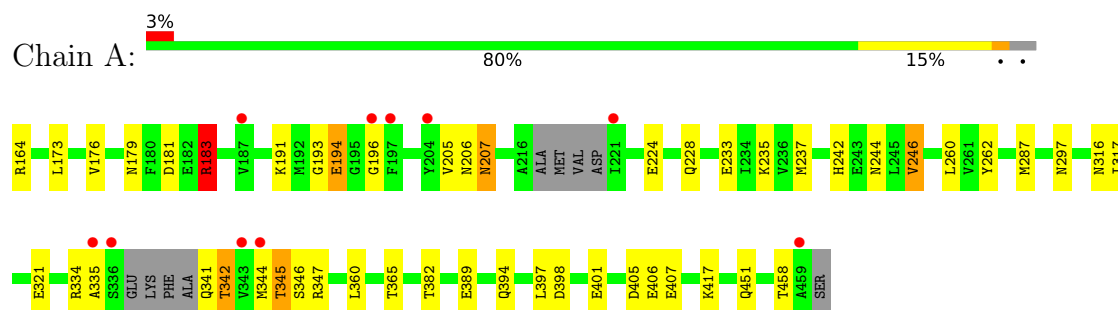
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	144	Total	O	0	0
			144	144		
3	B	95	Total	O	0	0
			95	95		
3	C	161	Total	O	0	0
			161	161		
3	D	96	Total	O	0	0
			96	96		

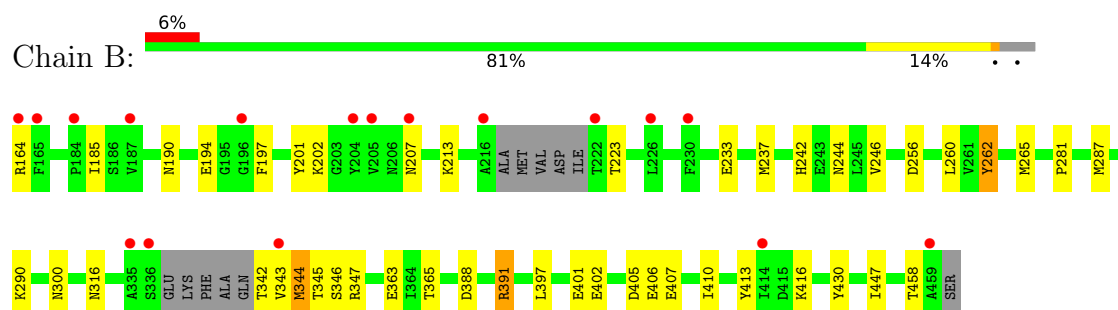
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

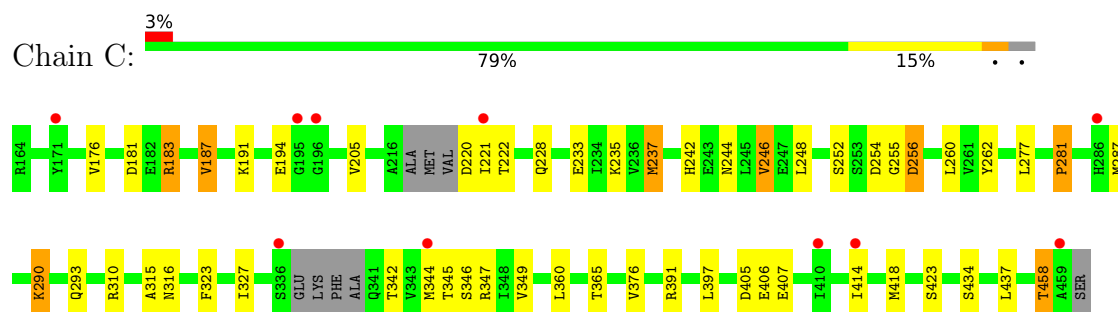
- Molecule 1: Interleukin-1 receptor-associated kinase 4



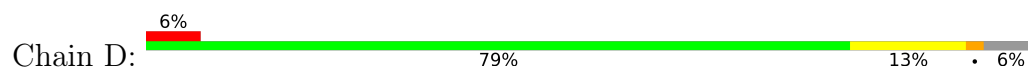
- Molecule 1: Interleukin-1 receptor-associated kinase 4

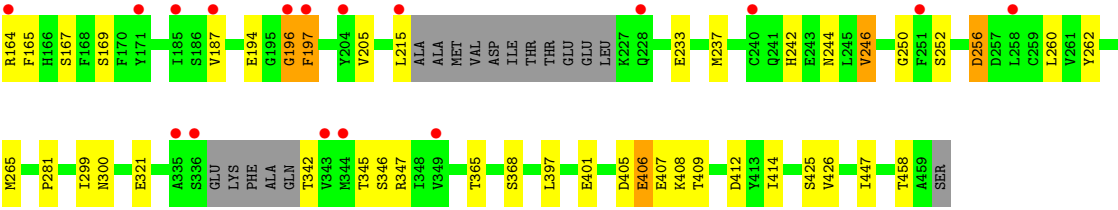


- Molecule 1: Interleukin-1 receptor-associated kinase 4



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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.96Å 141.93Å 88.09Å 90.00° 124.58° 90.00°	Depositor
Resolution (Å)	90.60 – 2.00 90.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (90.60-2.00) 99.8 (90.60-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.174 , 0.220 0.184 , 0.227	Depositor DCC
R_{free} test set	4894 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9674	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.28% 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: KFD, SEP, TPO

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	1.32	9/2271 (0.4%)	1.21	5/3059 (0.2%)
1	B	1.25	7/2259 (0.3%)	1.18	2/3043 (0.1%)
1	C	1.34	8/2316 (0.3%)	1.23	15/3119 (0.5%)
1	D	1.23	3/2202 (0.1%)	1.16	4/2967 (0.1%)
All	All	1.29	27/9048 (0.3%)	1.20	26/12188 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	316	ASN	CA-CB	10.56	1.71	1.53
1	A	183	ARG	CD-NE	-7.24	1.36	1.46
1	C	414	ILE	N-CA	6.83	1.54	1.46
1	D	368	SER	N-CA	-6.71	1.38	1.46
1	C	183	ARG	CD-NE	-6.31	1.37	1.46
1	C	376	VAL	C-O	-6.29	1.17	1.24
1	A	316	ASN	CA-CB	6.22	1.63	1.53
1	A	417	LYS	C-O	-6.17	1.15	1.23
1	A	335	ALA	CA-C	6.09	1.60	1.52
1	D	425	SER	C-O	-5.62	1.16	1.24
1	C	360	LEU	CA-C	5.42	1.60	1.52
1	A	382	THR	CA-C	-5.41	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	281	PRO	CA-C	5.30	1.55	1.52
1	A	360	LEU	CA-C	5.26	1.60	1.52
1	B	316	ASN	CA-CB	5.26	1.62	1.53
1	B	265	MET	N-CA	5.25	1.52	1.46
1	A	193	GLY	CA-C	-5.22	1.46	1.52
1	B	290	LYS	CA-C	5.21	1.59	1.52
1	B	391	ARG	N-CA	5.21	1.52	1.45
1	B	262	TYR	CA-C	-5.20	1.46	1.52
1	A	207	ASN	N-CA	5.17	1.52	1.46
1	D	281	PRO	CA-C	5.16	1.55	1.52
1	A	206	ASN	C-O	5.14	1.29	1.23
1	C	437	LEU	CA-C	5.07	1.60	1.52
1	B	202	LYS	N-CA	-5.04	1.39	1.46
1	C	290	LYS	N-CA	5.04	1.52	1.46
1	C	434	SER	C-O	-5.01	1.18	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	316	ASN	CA-CB-CG	-8.06	104.54	112.60
1	A	183	ARG	NE-CZ-NH2	-7.90	112.09	119.20
1	C	183	ARG	NE-CZ-NH1	7.73	129.23	121.50
1	C	237	MET	CG-SD-CE	-7.36	84.72	100.90
1	B	197	PHE	N-CA-C	-7.35	99.35	109.71
1	D	265	MET	CG-SD-CE	7.04	116.38	100.90
1	C	315	ALA	CA-C-N	6.87	134.14	122.26
1	C	315	ALA	C-N-CA	6.87	134.14	122.26
1	A	183	ARG	NE-CZ-NH1	6.78	128.28	121.50
1	C	281	PRO	CB-CA-C	-6.67	104.90	111.17
1	A	207	ASN	N-CA-C	6.58	121.08	113.38
1	C	183	ARG	NE-CZ-NH2	-6.47	113.37	119.20
1	A	246	VAL	CB-CA-C	5.91	120.95	111.32
1	C	246	VAL	CG1-CB-CG2	5.88	123.74	110.80
1	C	183	ARG	CD-NE-CZ	5.82	132.55	124.40
1	D	169	SER	N-CA-C	-5.64	102.14	110.48
1	C	423	SER	N-CA-C	5.54	118.04	111.33
1	C	316	ASN	CB-CG-ND2	5.52	124.68	116.40
1	C	187	VAL	N-CA-CB	-5.51	104.99	112.16
1	D	196	GLY	N-CA-C	-5.50	102.39	110.97
1	A	317	ILE	N-CA-C	-5.43	99.33	107.37
1	B	316	ASN	CA-CB-CG	-5.34	107.25	112.60
1	D	299	ILE	N-CA-C	-5.34	105.33	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	316	ASN	CB-CG-OD1	-5.32	110.16	120.80
1	C	246	VAL	CA-CB-CG1	5.18	119.20	110.40
1	C	256	ASP	N-CA-C	-5.04	106.64	112.89

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	207	ASN	Peptide
1	C	255	GLY	Peptide

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	2268	0	2220	22	0
1	B	2253	0	2211	17	0
1	C	2302	0	2258	20	0
1	D	2199	0	2150	19	0
2	A	39	0	0	0	0
2	B	39	0	0	1	0
2	C	39	0	0	0	0
2	D	39	0	0	0	0
3	A	144	0	0	4	0
3	B	95	0	0	1	0
3	C	161	0	0	2	0
3	D	96	0	0	3	0
All	All	9674	0	8839	76	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 4.

All (76) 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:179:ASN:HB3	3:A:696:HOH:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:HIS:HD2	1:C:244:ASN:H	1.24	0.82
1:D:405:ASP:O	1:D:407:GLU:N	2.17	0.77
1:C:181:ASP:OD1	1:C:183:ARG:HD3	1.90	0.72
1:C:233:GLU:HG2	1:C:260:LEU:HD13	1.73	0.71
1:C:242:HIS:CD2	1:C:244:ASN:H	2.09	0.69
1:A:242:HIS:CD2	1:A:244:ASN:H	2.10	0.69
1:D:242:HIS:CD2	1:D:244:ASN:H	2.13	0.67
1:B:242:HIS:CD2	1:B:244:ASN:H	2.13	0.66
1:A:242:HIS:HD2	1:A:244:ASN:H	1.43	0.65
1:A:397:LEU:C	1:A:397:LEU:HD12	2.23	0.64
1:A:181:ASP:OD1	1:A:183:ARG:HD3	1.99	0.62
1:A:321:GLU:HG2	1:C:281:PRO:HD3	1.82	0.62
1:D:242:HIS:HD2	1:D:244:ASN:H	1.48	0.61
1:C:237:MET:HE3	1:C:248:LEU:HB2	1.83	0.60
1:A:181:ASP:OD1	1:A:183:ARG:CD	2.49	0.60
1:C:287:MET:HE1	1:C:290:LYS:HD3	1.82	0.60
1:D:215:LEU:C	3:D:653:HOH:O	2.45	0.59
1:D:397:LEU:C	1:D:397:LEU:HD12	2.28	0.59
1:D:409:THR:HG22	1:D:412:ASP:OD2	2.04	0.58
1:C:405:ASP:O	1:C:407:GLU:N	2.37	0.58
1:C:397:LEU:HD12	1:C:397:LEU:C	2.30	0.56
1:C:327:ILE:HG23	3:C:658:HOH:O	2.06	0.56
1:D:407:GLU:O	1:D:408:LYS:HG2	2.07	0.55
1:D:197:PHE:HA	3:D:637:HOH:O	2.07	0.54
1:C:391:ARG:HD3	3:C:686:HOH:O	2.08	0.53
1:B:237:MET:CE	1:B:262:TYR:HE2	2.22	0.53
1:A:233:GLU:HG2	1:A:260:LEU:HD13	1.90	0.52
1:B:405:ASP:O	1:B:407:GLU:N	2.43	0.51
1:D:237:MET:HE1	1:D:246:VAL:HG12	1.92	0.50
1:D:300:ASN:HA	1:D:447:ILE:HG21	1.94	0.50
1:A:207:ASN:O	3:A:601:HOH:O	2.19	0.50
1:C:287:MET:HA	1:C:287:MET:HE3	1.93	0.50
1:A:233:GLU:OE2	3:A:602:HOH:O	2.19	0.50
1:A:228:GLN:CB	3:A:736:HOH:O	2.59	0.49
1:A:297:ASN:ND2	1:A:451:GLN:OE1	2.45	0.49
1:D:405:ASP:C	1:D:407:GLU:H	2.21	0.49
1:D:164:ARG:HD2	3:D:673:HOH:O	2.13	0.48
1:B:287[B]:MET:HE3	1:B:287[B]:MET:CA	2.44	0.48
1:A:191:LYS:NZ	1:A:194:GLU:OE2	2.34	0.48
1:A:237:MET:CE	1:A:262:TYR:HE2	2.27	0.47
1:B:410:ILE:HD13	1:B:430:TYR:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:LEU:C	1:B:397:LEU:HD12	2.39	0.47
1:C:287:MET:HE2	1:C:323:PHE:HB2	1.97	0.47
1:D:165:PHE:HB3	1:D:250:GLY:HA2	1.97	0.46
1:D:256:ASP:N	1:D:256:ASP:OD1	2.48	0.46
1:C:287:MET:HE2	1:C:323:PHE:CB	2.45	0.46
1:B:242:HIS:HD2	1:B:244:ASN:H	1.62	0.46
1:C:233:GLU:HG2	1:C:260:LEU:CD1	2.45	0.46
1:C:191:LYS:NZ	1:C:194:GLU:OE1	2.39	0.45
1:A:181:ASP:OD1	1:A:183:ARG:HD2	2.17	0.45
1:B:416:LYS:HB3	1:C:277:LEU:HD12	1.99	0.45
1:B:233:GLU:HG2	1:B:260:LEU:HD13	1.97	0.45
1:A:287:MET:HA	1:A:287:MET:HE2	1.99	0.45
1:A:405:ASP:O	1:A:407:GLU:N	2.50	0.45
1:D:233:GLU:HG2	1:D:260:LEU:HD13	1.98	0.45
1:B:190:ASN:O	1:B:201:TYR:HA	2.18	0.44
1:D:196:GLY:O	1:D:197:PHE:C	2.60	0.44
1:B:287[B]:MET:HE3	1:B:287[B]:MET:HA	1.99	0.43
1:B:300:ASN:HA	1:B:447:ILE:HG21	2.00	0.43
1:B:213:LYS:NZ	2:B:501:KFD:NBE	2.66	0.43
1:C:237:MET:HE1	1:C:262:TYR:HE2	1.84	0.43
1:A:334:ARG:NH2	1:A:345:TPO:O3P	2.36	0.43
1:D:405:ASP:C	1:D:407:GLU:N	2.77	0.43
1:A:397:LEU:HD12	1:A:398:ASP:N	2.34	0.42
1:A:341:GLN:O	1:A:342:TPO:C	2.68	0.42
1:B:344:MET:HE2	1:B:363:GLU:HG3	2.02	0.42
1:D:414:ILE:CD1	1:D:426:VAL:HG11	2.50	0.42
1:D:237:MET:CE	1:D:262:TYR:HE2	2.33	0.41
1:A:173:LEU:HA	1:A:176:VAL:HG22	2.02	0.41
1:C:310:ARG:NH1	1:C:349:VAL:HG22	2.35	0.41
1:B:402:GLU:OE1	1:B:413:TYR:OH	2.34	0.41
1:C:293:GLN:HE22	1:C:458:THR:HG21	1.86	0.41
1:B:401:GLU:HG3	3:B:605:HOH:O	2.19	0.41
1:A:389:GLU:HA	1:A:394:GLN:HE21	1.86	0.41
1:B:388:ASP:HB3	1:B:391:ARG:HB3	2.03	0.41

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	279/297 (94%)	266 (95%)	11 (4%)	2 (1%)	18	14
1	B	279/297 (94%)	271 (97%)	7 (2%)	1 (0%)	30	27
1	C	283/297 (95%)	270 (95%)	11 (4%)	2 (1%)	18	14
1	D	272/297 (92%)	261 (96%)	8 (3%)	3 (1%)	11	7
All	All	1113/1188 (94%)	1068 (96%)	37 (3%)	8 (1%)	18	14

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	254	ASP
1	C	406	GLU
1	D	197	PHE
1	D	406	GLU
1	A	406	GLU
1	B	406	GLU
1	A	196	GLY
1	D	187	VAL

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	246/255 (96%)	234 (95%)	12 (5%)	22	20
1	B	245/255 (96%)	234 (96%)	11 (4%)	24	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	251/255 (98%)	235 (94%)	16 (6%)	16	12
1	D	238/255 (93%)	226 (95%)	12 (5%)	22	20
All	All	980/1020 (96%)	929 (95%)	51 (5%)	21	18

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
1	A	183	ARG
1	A	194	GLU
1	A	205	VAL
1	A	224	GLU
1	A	235	LYS
1	A	246	VAL
1	A	344	MET
1	A	347	ARG
1	A	365	THR
1	A	401	GLU
1	A	458	THR
1	B	164	ARG
1	B	185	ILE
1	B	194	GLU
1	B	223	THR
1	B	246	VAL
1	B	256	ASP
1	B	343	VAL
1	B	344	MET
1	B	347	ARG
1	B	365	THR
1	B	458	THR
1	C	176	VAL
1	C	187	VAL
1	C	205	VAL
1	C	220	ASP
1	C	221	ILE
1	C	222	THR
1	C	228	GLN
1	C	235	LYS
1	C	246	VAL
1	C	252	SER
1	C	256	ASP

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Mol	Chain	Res	Type
1	C	344	MET
1	C	347	ARG
1	C	365	THR
1	C	418	MET
1	C	458	THR
1	D	167	SER
1	D	194	GLU
1	D	205	VAL
1	D	246	VAL
1	D	252	SER
1	D	256	ASP
1	D	321	GLU
1	D	347	ARG
1	D	365	THR
1	D	401	GLU
1	D	406	GLU
1	D	458	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	206	ASN
1	A	242	HIS
1	A	297	ASN
1	A	307	HIS
1	A	394	GLN
1	A	442	ASN
1	A	451	GLN
1	B	206	ASN
1	B	207	ASN
1	B	242	HIS
1	B	293	GLN
1	B	297	ASN
1	B	307	HIS
1	B	394	GLN
1	B	451	GLN
1	C	242	HIS
1	C	293	GLN
1	C	297	ASN
1	C	394	GLN
1	C	442	ASN

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Mol	Chain	Res	Type
1	C	451	GLN
1	C	455	GLN
1	D	190	ASN
1	D	242	HIS
1	D	297	ASN
1	D	451	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TPO	B	345	1	8,10,11	1.21	1 (12%)	10,14,16	1.62	1 (10%)
1	SEP	A	346	1	8,9,10	0.69	0	7,12,14	1.54	1 (14%)
1	SEP	D	346	1	8,9,10	0.82	0	7,12,14	1.36	1 (14%)
1	TPO	A	345	1	8,10,11	1.28	1 (12%)	10,14,16	1.41	1 (10%)
1	TPO	A	342	1	8,10,11	1.48	1 (12%)	10,14,16	1.21	0
1	SEP	C	346	1	8,9,10	0.62	0	7,12,14	1.58	2 (28%)
1	TPO	D	342	1	8,10,11	1.02	0	10,14,16	1.35	1 (10%)
1	TPO	D	345	1	8,10,11	1.17	1 (12%)	10,14,16	1.41	2 (20%)
1	TPO	B	342	1	8,10,11	1.23	1 (12%)	10,14,16	1.18	2 (20%)
1	SEP	B	346	1	8,9,10	0.74	0	7,12,14	1.57	1 (14%)
1	TPO	C	345	1	8,10,11	1.30	1 (12%)	10,14,16	1.09	1 (10%)
1	TPO	C	342	1	8,10,11	1.06	1 (12%)	10,14,16	1.02	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	B	345	1	-	3/9/11/13	-
1	SEP	A	346	1	-	2/6/8/10	-
1	SEP	D	346	1	-	5/6/8/10	-
1	TPO	A	345	1	-	3/9/11/13	-
1	TPO	A	342	1	-	1/9/11/13	-
1	SEP	C	346	1	-	2/6/8/10	-
1	TPO	D	342	1	-	1/9/11/13	-
1	TPO	D	345	1	-	4/9/11/13	-
1	TPO	B	342	1	-	4/9/11/13	-
1	SEP	B	346	1	-	2/6/8/10	-
1	TPO	C	345	1	-	4/9/11/13	-
1	TPO	C	342	1	-	4/9/11/13	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	342	TPO	P-OG1	3.01	1.64	1.59
1	B	342	TPO	P-OG1	2.56	1.64	1.59
1	C	345	TPO	P-OG1	2.44	1.63	1.59
1	D	345	TPO	P-OG1	2.42	1.63	1.59
1	A	345	TPO	P-OG1	2.30	1.63	1.59
1	C	342	TPO	P-OG1	2.18	1.63	1.59
1	B	345	TPO	P-OG1	2.14	1.63	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	TPO	P-OG1-CB	-3.93	112.65	123.33
1	D	342	TPO	P-OG1-CB	-3.56	113.64	123.33
1	C	346	SEP	OG-CB-CA	3.08	111.15	108.14
1	A	345	TPO	P-OG1-CB	-3.04	115.07	123.33
1	A	346	SEP	OG-CB-CA	3.01	111.07	108.14
1	D	345	TPO	P-OG1-CB	-2.83	115.65	123.33
1	B	346	SEP	O3P-P-OG	-2.81	99.33	106.67
1	D	346	SEP	OG-CB-CA	2.58	110.65	108.14
1	B	342	TPO	P-OG1-CB	-2.46	116.65	123.33
1	C	345	TPO	P-OG1-CB	-2.44	116.68	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	TPO	CG2-CB-CA	2.11	117.38	113.26
1	D	345	TPO	O2P-P-OG1	2.08	113.95	105.85
1	C	346	SEP	O3P-P-O2P	2.02	115.39	107.80

There are no chirality outliers.

All (35) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
1	B	342	TPO	N-CA-CB-CG2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	345	TPO	1	0
1	A	342	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	KFD	B	501	-	45,45,45	2.47	19 (42%)	61,64,64	2.93	24 (39%)
2	KFD	A	501	-	45,45,45	2.15	15 (33%)	61,64,64	2.58	23 (37%)
2	KFD	D	501	-	45,45,45	2.87	21 (46%)	61,64,64	2.75	22 (36%)
2	KFD	C	501	-	45,45,45	2.26	18 (40%)	61,64,64	2.69	27 (44%)

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	KFD	B	501	-	-	3/20/36/36	0/7/7/7
2	KFD	A	501	-	-	3/20/36/36	0/7/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KFD	D	501	-	-	3/20/36/36	0/7/7/7
2	KFD	C	501	-	-	3/20/36/36	0/7/7/7

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	KFD	OBM-CAH	-8.93	1.24	1.38
2	D	501	KFD	CBJ-CBF	-6.73	1.32	1.42
2	A	501	KFD	CBC-CBA	-5.96	1.39	1.49
2	B	501	KFD	CBC-CBA	-5.91	1.39	1.49
2	C	501	KFD	CBJ-CBF	-5.85	1.33	1.42
2	B	501	KFD	CBJ-CBF	-5.43	1.34	1.42
2	D	501	KFD	CBC-CBA	-5.25	1.40	1.49
2	C	501	KFD	OBM-CAG	-5.12	1.27	1.37
2	D	501	KFD	CAE-CAF	-5.08	1.32	1.40
2	B	501	KFD	CBK-CBJ	-4.60	1.33	1.40
2	D	501	KFD	CAD-NAC	-4.57	1.32	1.41
2	A	501	KFD	CBJ-CBF	-4.56	1.35	1.42
2	D	501	KFD	CBK-CBJ	-4.48	1.33	1.40
2	B	501	KFD	CAG-NBL	4.43	1.38	1.30
2	A	501	KFD	CAE-CAF	-4.36	1.33	1.40
2	B	501	KFD	CAI-CAH	-4.29	1.31	1.38
2	C	501	KFD	CBC-CBA	-4.25	1.42	1.49
2	A	501	KFD	CAF-NBL	-4.17	1.31	1.39
2	A	501	KFD	CBD-NBE	4.03	1.42	1.34
2	A	501	KFD	CBK-CBJ	-3.91	1.34	1.40
2	D	501	KFD	CAJ-NAK	-3.73	1.33	1.41
2	C	501	KFD	CBK-CBJ	-3.72	1.34	1.40
2	C	501	KFD	CBD-NBE	3.68	1.41	1.34
2	B	501	KFD	CAE-CAD	-3.68	1.33	1.39
2	D	501	KFD	CAG-NBL	3.53	1.36	1.30
2	D	501	KFD	CAR-NAQ	3.41	1.53	1.47
2	D	501	KFD	CBJ-CBI	-3.36	1.34	1.43
2	B	501	KFD	CAF-NBL	-3.32	1.33	1.39
2	D	501	KFD	CAI-CAH	-3.31	1.33	1.38
2	D	501	KFD	CAH-CAF	-3.30	1.34	1.38
2	C	501	KFD	CAN-CAM	3.27	1.63	1.51
2	B	501	KFD	CAI-CAJ	3.20	1.44	1.39
2	B	501	KFD	CAW-CAB	-3.19	1.41	1.50
2	C	501	KFD	CAD-NAC	-3.16	1.35	1.41
2	B	501	KFD	CAJ-NAK	-3.11	1.34	1.41
2	D	501	KFD	CAW-CAB	-3.05	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	KFD	OAT-CAS	3.01	1.54	1.42
2	B	501	KFD	CAH-CAF	-3.00	1.34	1.38
2	C	501	KFD	CBH-NBG	-2.98	1.32	1.38
2	A	501	KFD	CBH-NBG	-2.95	1.32	1.38
2	B	501	KFD	OBM-CAG	-2.89	1.31	1.37
2	C	501	KFD	CAR-NAQ	2.87	1.52	1.47
2	C	501	KFD	CAE-CAF	-2.84	1.35	1.40
2	A	501	KFD	CAV-NAQ	2.83	1.52	1.47
2	C	501	KFD	CAJ-NAK	-2.81	1.35	1.41
2	B	501	KFD	CBJ-CBI	-2.76	1.35	1.43
2	D	501	KFD	CBD-NBE	2.69	1.39	1.34
2	B	501	KFD	CAE-CAF	-2.68	1.35	1.40
2	D	501	KFD	CBH-NBG	-2.65	1.33	1.38
2	D	501	KFD	CAD-CAJ	2.65	1.43	1.40
2	A	501	KFD	CBJ-CBI	-2.61	1.36	1.43
2	B	501	KFD	CAR-CAS	2.60	1.60	1.50
2	D	501	KFD	CAF-NBL	-2.59	1.34	1.39
2	C	501	KFD	CAP-NAK	2.57	1.51	1.46
2	A	501	KFD	CAW-CAB	-2.55	1.43	1.50
2	C	501	KFD	CAH-CAF	-2.53	1.35	1.38
2	A	501	KFD	CAD-CAJ	2.52	1.43	1.40
2	D	501	KFD	CAE-CAD	-2.52	1.35	1.39
2	C	501	KFD	CAI-CAJ	2.50	1.43	1.39
2	C	501	KFD	CBF-NBE	-2.46	1.31	1.35
2	D	501	KFD	CAV-NAQ	2.45	1.51	1.47
2	B	501	KFD	CAV-CAU	2.43	1.59	1.50
2	B	501	KFD	CAO-CAN	-2.42	1.42	1.51
2	B	501	KFD	OAT-CAU	2.35	1.51	1.42
2	A	501	KFD	CAR-CAS	2.23	1.58	1.50
2	C	501	KFD	CAV-CAU	2.21	1.58	1.50
2	A	501	KFD	CAG-NBL	2.19	1.34	1.30
2	A	501	KFD	CAI-CAH	-2.17	1.35	1.38
2	D	501	KFD	CBF-NBG	-2.15	1.33	1.36
2	C	501	KFD	CBJ-CBI	-2.12	1.37	1.43
2	C	501	KFD	CAG-NBL	2.11	1.34	1.30
2	D	501	KFD	CAV-CAU	2.10	1.58	1.50
2	A	501	KFD	CAJ-NAK	-2.01	1.37	1.41

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	KFD	CBJ-CBF-NBE	-11.25	119.99	126.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	KFD	OBM-CAG-NBL	-10.13	107.12	116.47
2	B	501	KFD	CBJ-CBF-NBE	-9.65	120.93	126.66
2	D	501	KFD	CAI-CAJ-NAK	-8.98	109.50	122.59
2	D	501	KFD	CBJ-CBF-NBE	-8.83	121.42	126.66
2	D	501	KFD	OBM-CAG-NBL	-8.40	108.72	116.47
2	A	501	KFD	CBJ-CBF-NBE	-7.20	122.39	126.66
2	B	501	KFD	CAF-NBL-CAG	6.69	108.69	103.42
2	A	501	KFD	CAF-NBL-CAG	6.49	108.54	103.42
2	C	501	KFD	OBM-CAG-NBL	-6.16	110.79	116.47
2	C	501	KFD	CAI-CAJ-NAK	-6.08	113.74	122.59
2	A	501	KFD	OBM-CAG-NBL	-5.99	110.95	116.47
2	A	501	KFD	CAI-CAJ-NAK	-5.92	113.96	122.59
2	A	501	KFD	CBK-CBJ-CBF	5.68	122.75	118.20
2	D	501	KFD	CAX-CAW-NBB	-5.34	116.69	122.92
2	B	501	KFD	CAE-CAD-CAJ	-4.94	114.39	119.80
2	A	501	KFD	CAU-OAT-CAS	4.91	125.77	109.88
2	B	501	KFD	CAI-CAH-CAF	-4.81	119.49	124.45
2	D	501	KFD	CBC-CBA-NBB	4.81	122.99	116.04
2	B	501	KFD	CAE-CAF-CAH	4.69	124.36	120.27
2	C	501	KFD	CAX-CAW-NBB	-4.62	117.53	122.92
2	D	501	KFD	CBK-CBJ-CBF	4.56	121.86	118.20
2	A	501	KFD	CBC-CBA-NBB	4.44	122.45	116.04
2	B	501	KFD	CAS-CAR-NAQ	-4.18	101.02	109.82
2	B	501	KFD	OBM-CAH-CAI	4.15	133.68	124.95
2	A	501	KFD	CAV-NAQ-CAR	4.13	121.10	112.68
2	B	501	KFD	CAI-CAJ-NAK	-4.08	116.64	122.59
2	B	501	KFD	CAU-OAT-CAS	3.96	122.69	109.88
2	C	501	KFD	CBK-CBJ-CBF	3.88	121.31	118.20
2	A	501	KFD	CAX-CAW-NBB	-3.74	118.55	122.92
2	C	501	KFD	OBM-CAH-CAF	-3.71	105.27	107.80
2	B	501	KFD	CBK-CBJ-CBF	3.67	121.14	118.20
2	C	501	KFD	OBM-CAH-CAI	3.66	132.65	124.95
2	C	501	KFD	CAV-NAQ-CAR	3.55	119.93	112.68
2	D	501	KFD	CBA-NBB-CAW	3.54	124.36	118.22
2	D	501	KFD	CAH-OBM-CAG	3.52	109.80	103.96
2	D	501	KFD	CAN-CAM-CAL	-3.49	104.74	111.19
2	A	501	KFD	OBM-CAH-CAI	3.43	132.16	124.95
2	C	501	KFD	OAT-CAS-CAR	-3.39	104.47	111.77
2	D	501	KFD	CAH-CAF-NBL	3.33	111.69	108.60
2	D	501	KFD	CAV-NAQ-CAR	3.30	119.42	112.68
2	D	501	KFD	CAB-CAW-NBB	3.29	122.63	117.43
2	B	501	KFD	OAT-CAS-CAR	3.25	118.77	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	KFD	CAI-CAH-CAF	-3.24	121.11	124.45
2	B	501	KFD	CBC-CBA-NBB	3.24	120.72	116.04
2	C	501	KFD	CAY-CAX-CAW	3.19	122.44	118.63
2	C	501	KFD	CBJ-CBF-NBG	3.17	110.04	108.24
2	A	501	KFD	CAY-CAX-CAW	3.14	122.38	118.63
2	A	501	KFD	CAP-NAK-CAL	3.10	118.55	111.57
2	C	501	KFD	CAF-NBL-CAG	3.09	105.86	103.42
2	C	501	KFD	CAH-OBM-CAG	3.07	109.05	103.96
2	B	501	KFD	CAX-CAW-NBB	-2.99	119.43	122.92
2	B	501	KFD	CAH-OBM-CAG	2.96	108.87	103.96
2	B	501	KFD	CBC-CBD-NBE	-2.91	119.65	124.28
2	B	501	KFD	CAP-NAK-CAL	2.85	117.97	111.57
2	A	501	KFD	OAT-CAS-CAR	2.84	117.90	111.77
2	D	501	KFD	CAP-NAK-CAJ	2.74	122.70	116.19
2	D	501	KFD	CAW-CAB-NAC	-2.69	107.24	113.99
2	A	501	KFD	CAE-CAF-CAH	2.68	122.61	120.27
2	C	501	KFD	CBF-CBJ-CBI	-2.66	104.98	106.48
2	C	501	KFD	CBD-NBE-CBF	2.65	121.39	116.19
2	B	501	KFD	CAE-CAD-NAC	2.56	128.66	121.95
2	B	501	KFD	CBA-NBB-CAW	2.56	122.66	118.22
2	D	501	KFD	OAA-CAB-NAC	2.53	130.17	123.75
2	C	501	KFD	CBA-NBB-CAW	2.52	122.59	118.22
2	D	501	KFD	CAZ-CBA-NBB	-2.48	118.70	121.97
2	A	501	KFD	CBI-CBH-NBG	-2.48	107.39	110.25
2	C	501	KFD	CAJ-CAD-NAC	-2.47	114.05	118.61
2	C	501	KFD	CBI-CBH-NBG	-2.47	107.40	110.25
2	C	501	KFD	CBC-CBD-NBE	-2.45	120.39	124.28
2	C	501	KFD	CBK-CBC-CBD	-2.44	114.48	117.10
2	B	501	KFD	CBD-NBE-CBF	2.42	120.92	116.19
2	B	501	KFD	CBF-NBG-CBH	-2.40	106.73	108.11
2	A	501	KFD	CBA-NBB-CAW	2.40	122.39	118.22
2	D	501	KFD	CAU-OAT-CAS	2.39	117.62	109.88
2	A	501	KFD	CAZ-CAY-CAX	-2.33	117.25	120.24
2	C	501	KFD	CAI-CAH-CAF	-2.30	122.08	124.45
2	B	501	KFD	CBF-CBJ-CBI	2.29	107.77	106.48
2	D	501	KFD	CBC-CBD-NBE	-2.26	120.69	124.28
2	A	501	KFD	CBC-CBD-NBE	-2.25	120.71	124.28
2	A	501	KFD	CAN-CAM-CAL	-2.22	107.09	111.19
2	C	501	KFD	CAZ-CAY-CAX	-2.22	117.40	120.24
2	A	501	KFD	CAB-CAW-NBB	2.20	120.91	117.43
2	A	501	KFD	CBF-NBG-CBH	2.18	109.37	108.11
2	D	501	KFD	CAY-CAX-CAW	2.17	121.22	118.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	KFD	CBJ-CBF-NBG	2.17	109.47	108.24
2	C	501	KFD	CAN-CAO-CAP	-2.14	107.23	111.19
2	B	501	KFD	CAI-CAJ-CAD	2.14	122.93	119.95
2	D	501	KFD	CAS-CAR-NAQ	-2.12	105.34	109.82
2	D	501	KFD	OBM-CAH-CAI	2.09	129.35	124.95
2	A	501	KFD	CAZ-CBA-CBC	-2.07	118.14	121.97
2	C	501	KFD	CAB-CAW-NBB	2.06	120.68	117.43
2	C	501	KFD	OAT-CAU-CAV	-2.05	107.36	111.77
2	D	501	KFD	CBI-CBH-NBG	-2.05	107.89	110.25
2	C	501	KFD	CAO-CAP-NAK	2.04	114.91	111.06
2	C	501	KFD	NBG-CBF-NBE	2.01	129.94	126.69

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	KFD	CAI-CAJ-NAK-CAP
2	A	501	KFD	CAI-CAJ-NAK-CAL
2	C	501	KFD	CAI-CAJ-NAK-CAP
2	D	501	KFD	CAI-CAJ-NAK-CAP
2	C	501	KFD	CAI-CAJ-NAK-CAL
2	A	501	KFD	CAI-CAJ-NAK-CAP
2	B	501	KFD	CAI-CAJ-NAK-CAL
2	D	501	KFD	CAI-CAJ-NAK-CAL
2	D	501	KFD	CAD-CAJ-NAK-CAP
2	A	501	KFD	CAD-CAJ-NAK-CAL
2	B	501	KFD	CAD-CAJ-NAK-CAP
2	C	501	KFD	CAD-CAJ-NAK-CAP

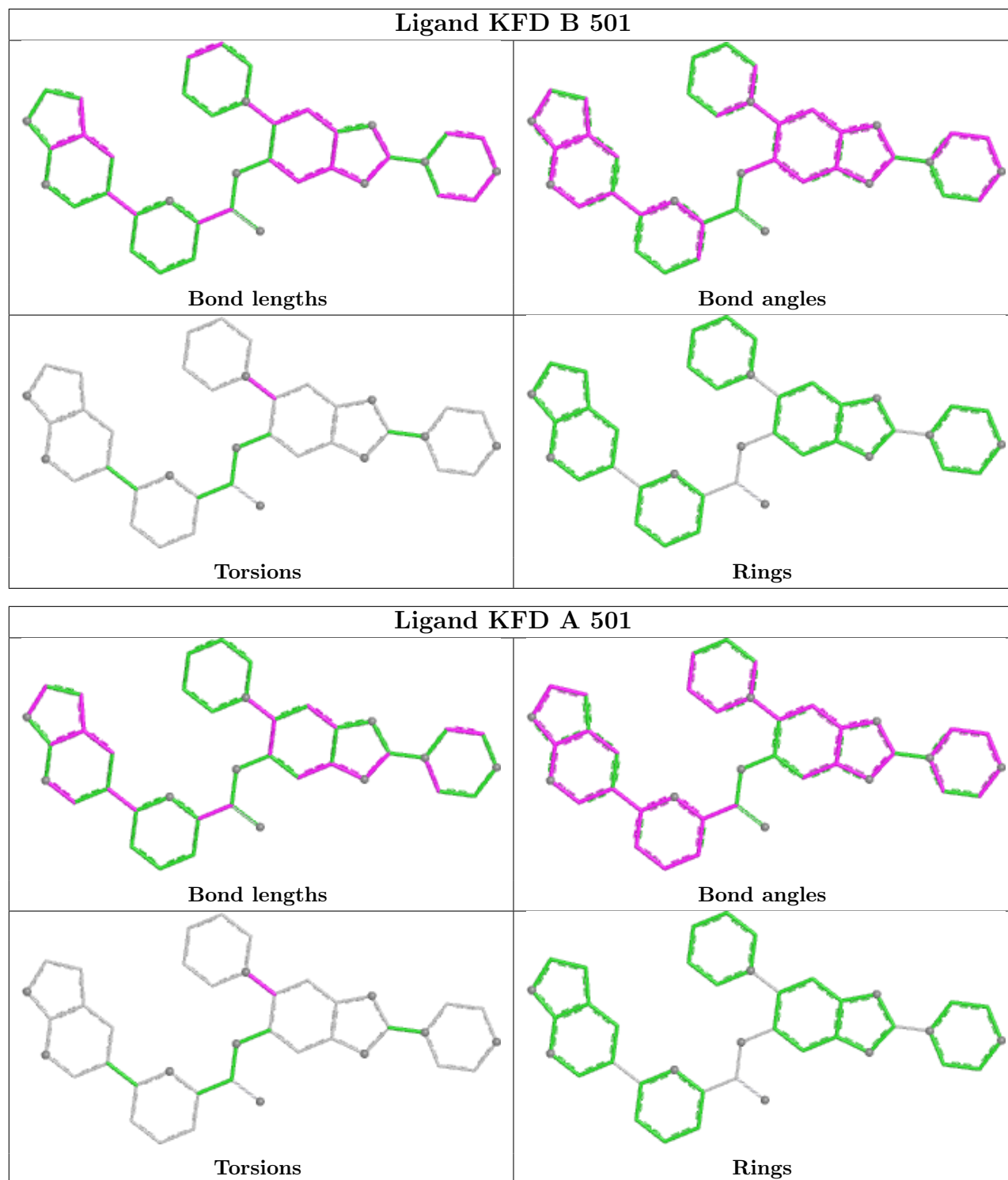
There are no ring outliers.

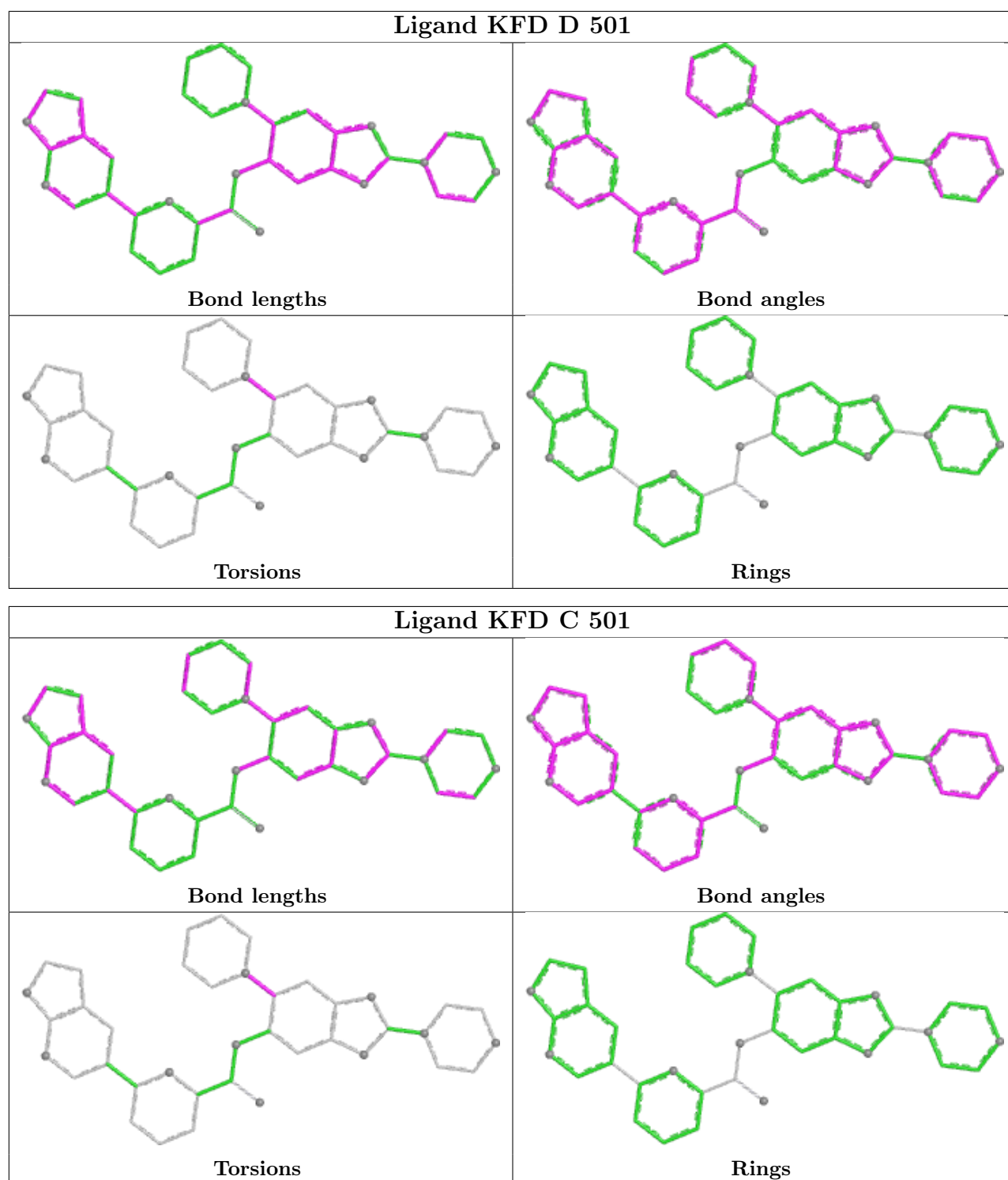
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	KFD	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 ⓘ

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	285/297 (95%)	0.12	10 (3%)	47 46	29, 43, 80, 107	0
1	B	283/297 (95%)	0.29	17 (6%)	27 26	20, 50, 94, 114	1 (0%)
1	C	286/297 (96%)	0.12	10 (3%)	47 46	23, 43, 79, 103	3 (1%)
1	D	277/297 (93%)	0.28	17 (6%)	27 26	30, 49, 93, 114	0
All	All	1131/1188 (95%)	0.20	54 (4%)	35 34	20, 45, 88, 114	4 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	ILE	5.1
1	D	185	ILE	4.8
1	D	187	VAL	4.1
1	C	171[A]	TYR	3.5
1	D	196	GLY	3.4
1	C	195	GLY	3.3
1	B	187	VAL	3.2
1	B	335	ALA	3.1
1	A	196	GLY	3.0
1	D	197	PHE	3.0
1	A	343	VAL	3.0
1	D	336	SER	2.9
1	D	204	TYR	2.7
1	B	196	GLY	2.7
1	A	335	ALA	2.7
1	C	459	ALA	2.7
1	A	336	SER	2.6
1	B	205	VAL	2.6
1	D	343	VAL	2.6
1	D	240	CYS	2.6
1	D	215	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	187	VAL	2.6
1	D	171	TYR	2.5
1	A	344	MET	2.5
1	B	216	ALA	2.5
1	B	204	TYR	2.5
1	D	251	PHE	2.5
1	B	222	THR	2.4
1	B	336	SER	2.4
1	C	221	ILE	2.4
1	A	204	TYR	2.4
1	C	336	SER	2.4
1	B	184	PRO	2.4
1	A	459	ALA	2.4
1	D	344	MET	2.4
1	B	226	LEU	2.4
1	B	164	ARG	2.4
1	B	414	ILE	2.3
1	C	196	GLY	2.3
1	C	414	ILE	2.3
1	B	207	ASN	2.2
1	B	230	PHE	2.2
1	C	410	ILE	2.2
1	C	286[A]	HIS	2.2
1	D	258	LEU	2.2
1	A	197	PHE	2.1
1	D	228	GLN	2.1
1	C	344	MET	2.1
1	B	165	PHE	2.1
1	D	335	ALA	2.1
1	B	343	VAL	2.1
1	D	349	VAL	2.0
1	B	459	ALA	2.0
1	D	164	ARG	2.0

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

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
1	SEP	D	346	10/11	0.53	0.12	81,99,131,140	0
1	TPO	A	342	11/12	0.64	0.23	64,84,92,99	0
1	TPO	D	342	11/12	0.65	0.18	88,103,115,128	0
1	TPO	B	342	11/12	0.66	0.21	83,91,122,122	0
1	SEP	B	346	10/11	0.73	0.10	68,88,123,128	0
1	TPO	C	342	11/12	0.75	0.21	88,114,117,119	0
1	SEP	A	346	10/11	0.77	0.11	76,82,111,122	0
1	SEP	C	346	10/11	0.77	0.11	65,84,104,112	0
1	TPO	D	345	11/12	0.89	0.12	57,68,84,101	0
1	TPO	A	345	11/12	0.90	0.12	61,66,84,88	0
1	TPO	B	345	11/12	0.93	0.10	56,61,76,80	0
1	TPO	C	345	11/12	0.93	0.11	55,61,75,76	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

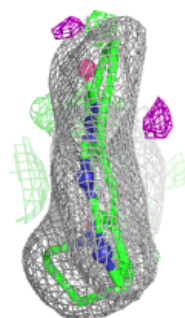
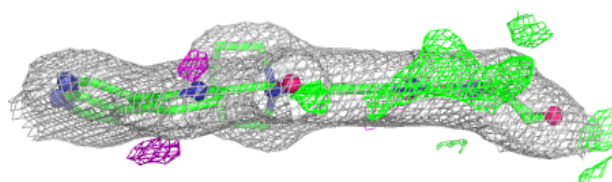
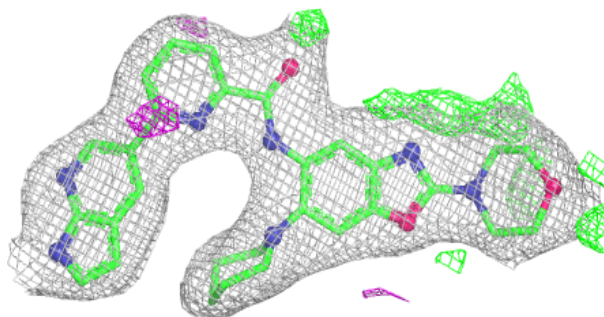
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	KFD	D	501	39/39	0.93	0.10	34,47,63,69	0
2	KFD	B	501	39/39	0.94	0.09	30,38,55,60	0
2	KFD	C	501	39/39	0.97	0.06	28,32,46,50	0
2	KFD	A	501	39/39	0.97	0.06	27,35,47,52	0

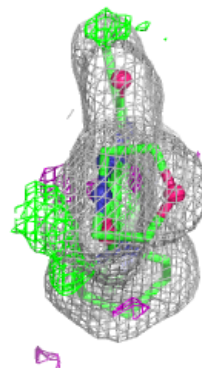
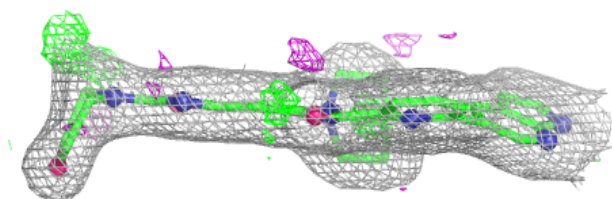
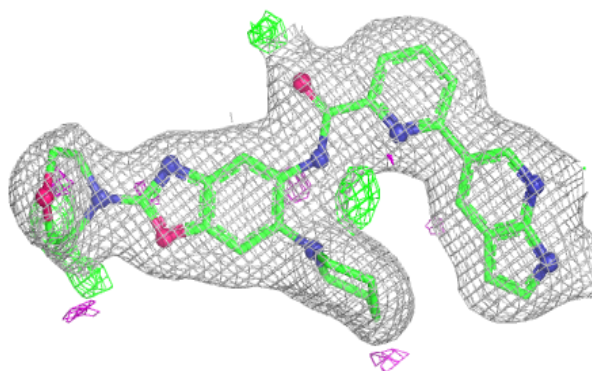
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KFD D 501:

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

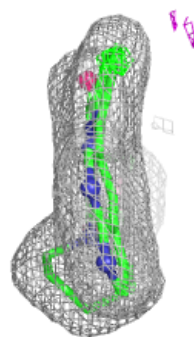
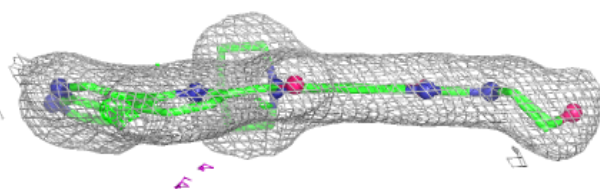
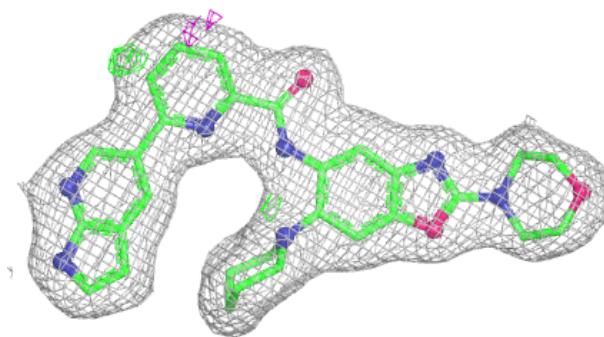
**Electron density around KFD B 501:**

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

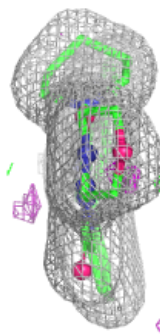
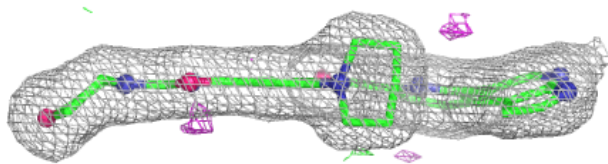
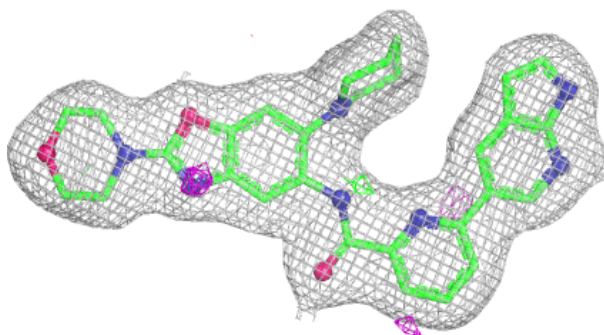


Electron density around KFD C 501:

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

**Electron density around KFD A 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.