



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:01 PM UTC

PDB ID : 9PST / pdb_00009pst
Title : IRAK4 in Complex with Compound 5
Authors : Ferrao, R.
Deposited on : 2025-07-26
Resolution : 2.12 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

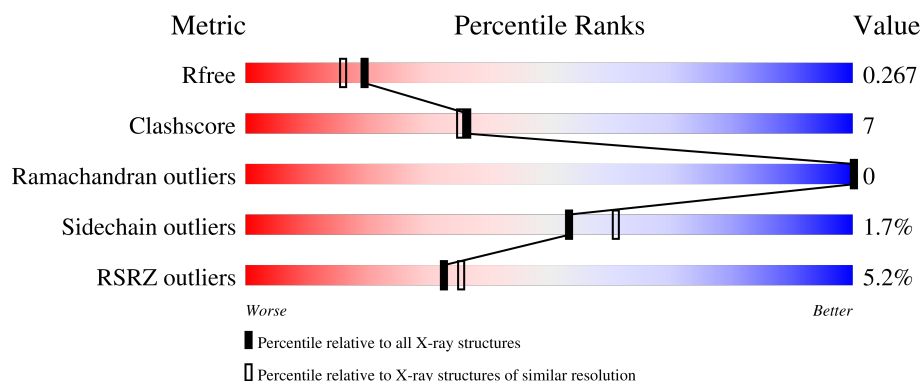
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	304	4% 77% 16% 6%
1	B	304	5% 76% 16% 7%
1	C	304	2% 77% 16% 7%
1	D	304	8% 78% 14% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9616 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.

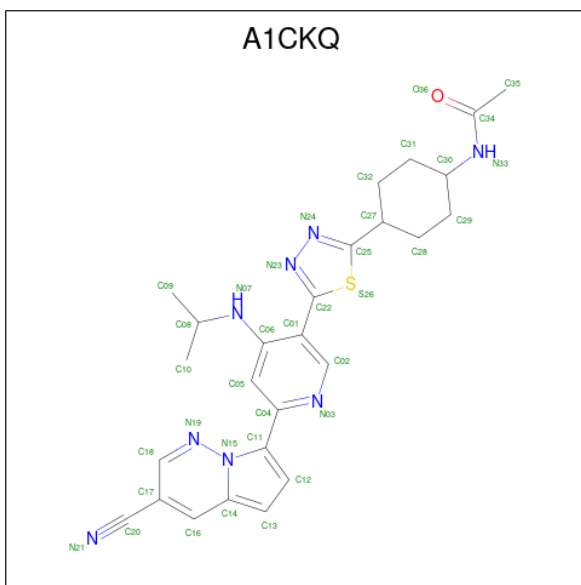
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	P	S	0	0	0
			2244	1409	375	444	2	14			
1	B	282	Total	C	N	O	P	S	0	0	0
			2223	1395	371	440	3	14			
1	C	284	Total	C	N	O	P	S	0	0	0
			2237	1404	375	442	2	14			
1	D	282	Total	C	N	O	P	S	0	0	0
			2229	1397	373	442	3	14			

There are 12 discrepancies between the modelled and reference sequences:

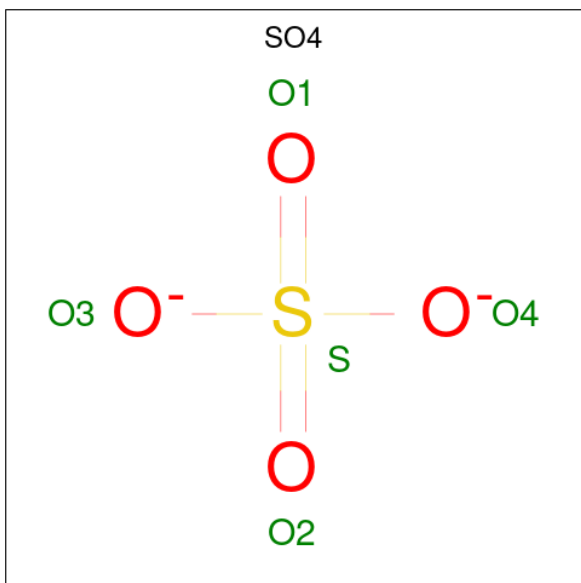
Chain	Residue	Modelled	Actual	Comment	Reference
A	157	GLY	-	expression tag	UNP Q9NWZ3
A	158	ALA	-	expression tag	UNP Q9NWZ3
A	159	MET	-	expression tag	UNP Q9NWZ3
B	157	GLY	-	expression tag	UNP Q9NWZ3
B	158	ALA	-	expression tag	UNP Q9NWZ3
B	159	MET	-	expression tag	UNP Q9NWZ3
C	157	GLY	-	expression tag	UNP Q9NWZ3
C	158	ALA	-	expression tag	UNP Q9NWZ3
C	159	MET	-	expression tag	UNP Q9NWZ3
D	157	GLY	-	expression tag	UNP Q9NWZ3
D	158	ALA	-	expression tag	UNP Q9NWZ3
D	159	MET	-	expression tag	UNP Q9NWZ3

- Molecule 2 is N-[(1R,4r)-4-(5-{(6P)-6-[(8R)-3-cyanopyrrolo[1,2-b]pyridazin-7-yl]-4-[(propan-2-yl)amino]pyridin-3-yl}-1,3,4-thiadiazol-2-yl)cyclohexyl]acetamide (CCD ID: A1CKQ) (formula: C₂₆H₂₈N₈OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 36	C 26	N 8	O 1	S 1	0	0
2	B	1	Total 36	C 26	N 8	O 1	S 1	0	0
2	C	1	Total 36	C 26	N 8	O 1	S 1	0	0
2	D	1	Total 36	C 26	N 8	O 1	S 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

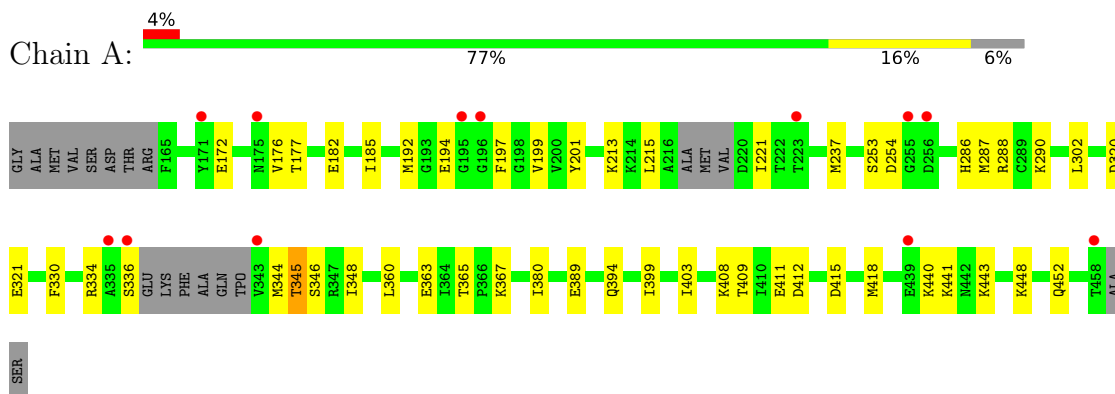
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	145	Total O 145 145	0	0
4	B	121	Total O 121 121	0	0
4	C	138	Total O 138 138	0	0
4	D	115	Total O 115 115	0	0

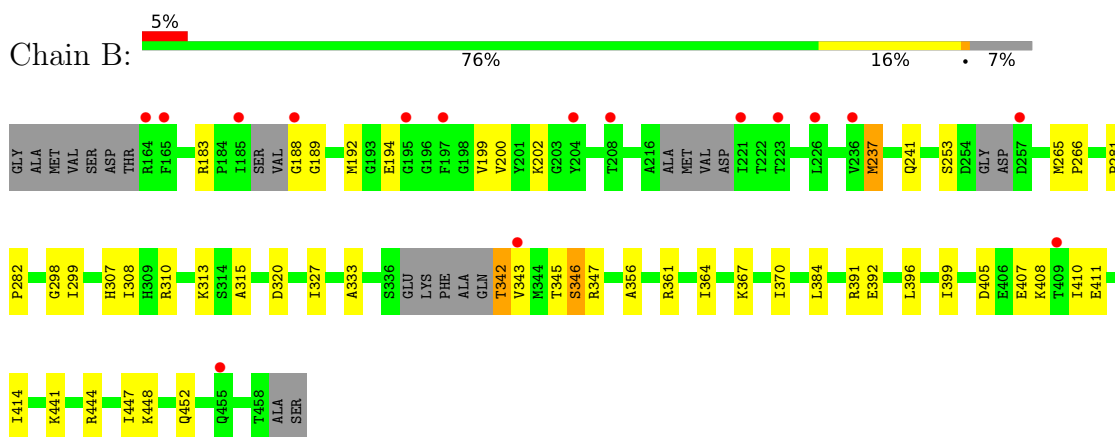
3 Residue-property plots [i](#)

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.

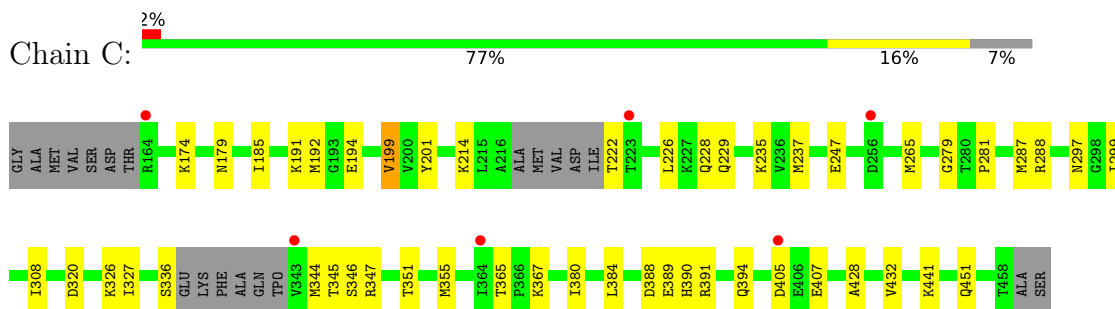
- Molecule 1: Interleukin-1 receptor-associated kinase 4



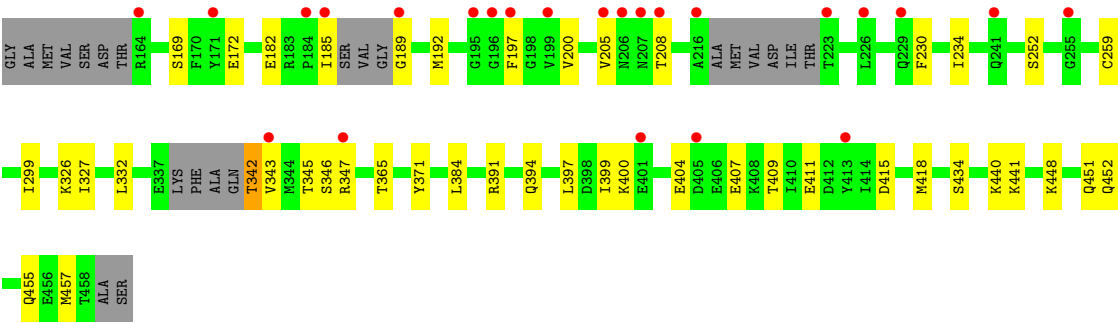
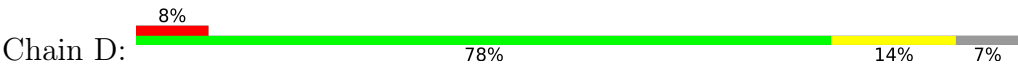
- Molecule 1: Interleukin-1 receptor-associated kinase 4



- 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	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.22Å 140.96Å 110.12Å 90.00° 93.22° 90.00°	Depositor
Resolution (Å)	30.97 – 2.12 30.97 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.97-2.12) 89.4 (30.97-2.12)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.86 (at 2.12Å)	Xtrriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.210 , 0.269 0.214 , 0.267	Depositor DCC
R_{free} test set	3690 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtrriage
Anisotropy	0.424	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9616	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1038e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: A1CKQ, SO4, 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	0.34	0/2259	0.51	0/3044
1	B	0.31	0/2225	0.47	0/2996
1	C	0.33	0/2252	0.49	0/3034
1	D	0.32	0/2232	0.50	0/3005
All	All	0.33	0/8968	0.49	0/12079

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	2244	0	2203	33	0
1	B	2223	0	2175	34	0
1	C	2237	0	2196	35	0
1	D	2229	0	2181	30	0
2	A	36	0	0	0	0
2	B	36	0	0	0	0
2	C	36	0	0	0	0
2	D	36	0	0	0	0
3	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	10	0	0	1	0
4	A	145	0	0	4	0
4	B	121	0	0	9	0
4	C	138	0	0	5	0
4	D	115	0	0	5	0
All	All	9616	0	8755	128	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 7.

All (128) 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:C:287:MET:SD	4:C:710:HOH:O	2.40	0.79
1:D:326:LYS:NZ	4:D:601:HOH:O	2.21	0.73
1:A:440:LYS:HE2	1:A:443:LYS:HD3	1.74	0.70
1:C:389:GLU:H	1:C:389:GLU:CD	2.00	0.70
1:B:407:GLU:HB3	1:B:408:LYS:HE3	1.74	0.69
1:A:334:ARG:NH2	1:A:345:TPO:O1P	2.22	0.68
1:A:321:GLU:HG3	1:C:281:PRO:HD3	1.75	0.67
1:A:440:LYS:HB2	1:A:443:LYS:HG3	1.76	0.67
1:C:214:LYS:NZ	4:C:603:HOH:O	2.26	0.67
1:A:367:LYS:NZ	1:A:441:LYS:O	2.25	0.66
1:C:297:ASN:OD1	1:C:451:GLN:NE2	2.25	0.64
1:A:415:ASP:HB3	1:A:418:MET:HE2	1.78	0.64
1:C:191:LYS:NZ	1:C:194:GLU:OE2	2.26	0.63
1:D:185:ILE:HG13	1:D:192:MET:HG2	1.80	0.62
1:D:326:LYS:NZ	4:D:607:HOH:O	2.32	0.62
1:D:384:LEU:HB3	1:D:391:ARG:NH1	2.13	0.62
1:D:299:ILE:HG13	1:D:327:ILE:CD1	2.31	0.61
1:C:388:ASP:HB3	1:C:391:ARG:HB3	1.83	0.61
1:B:405:ASP:HB2	1:B:407:GLU:OE1	2.01	0.60
1:C:229:GLN:HE21	1:C:347:ARG:HH12	1.51	0.59
1:A:389:GLU:HA	1:A:394:GLN:HG2	1.84	0.59
1:C:174:LYS:HD2	1:C:179:ASN:OD1	2.02	0.58
1:B:347:ARG:NH1	4:B:609:HOH:O	2.37	0.57
1:C:194:GLU:HG2	1:C:199:VAL:HB	1.88	0.56
1:A:197:PHE:HE1	1:A:221:ILE:HG12	1.71	0.55
1:B:361:ARG:NH1	4:B:614:HOH:O	2.41	0.54
1:D:452:GLN:NE2	4:D:615:HOH:O	2.41	0.53
1:C:288:ARG:HB3	1:C:380:ILE:HG23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:LYS:HD3	1:B:441:LYS:HB2	1.90	0.53
1:C:367:LYS:HD2	1:C:441:LYS:HB2	1.91	0.53
1:A:448:LYS:NZ	4:A:612:HOH:O	2.42	0.53
1:A:182:GLU:OE2	1:A:201:TYR:OH	2.26	0.53
1:C:229:GLN:NE2	1:C:347:ARG:HH12	2.07	0.52
1:D:342:TPO:HG23	1:D:343:VAL:H	1.74	0.52
1:B:202:LYS:NZ	4:B:616:HOH:O	2.41	0.52
1:B:448:LYS:O	1:B:452:GLN:HG2	2.09	0.51
1:D:342:TPO:HG21	1:D:365:THR:HB	1.92	0.51
1:A:194:GLU:HG3	1:A:199:VAL:HG22	1.93	0.51
1:B:370:ILE:HD11	1:B:447:ILE:HB	1.93	0.50
1:B:343:VAL:HG23	1:B:364:ILE:HB	1.93	0.50
1:C:320:ASP:OD2	4:C:601:HOH:O	2.20	0.50
1:D:252:SER:HB3	1:D:259:CYS:HB2	1.94	0.49
1:B:265:MET:HE2	4:B:650:HOH:O	2.11	0.49
1:A:448:LYS:O	1:A:452:GLN:HG3	2.13	0.49
1:C:308:ILE:HD11	1:C:336:SER:HB3	1.94	0.49
1:A:213:LYS:HE3	1:A:215:LEU:HD21	1.94	0.49
1:C:199:VAL:HG13	1:C:201:TYR:CE1	2.49	0.48
1:B:282:PRO:HG2	1:C:279:GLY:HA2	1.95	0.48
1:B:299:ILE:HG13	1:B:327:ILE:HD11	1.95	0.48
1:D:299:ILE:HG13	1:D:327:ILE:HD11	1.96	0.47
1:B:192:MET:HE3	1:B:200:VAL:HG12	1.96	0.47
1:D:407:GLU:O	1:D:407:GLU:HG2	2.13	0.47
1:A:344:MET:SD	1:A:363:GLU:HG2	2.54	0.47
1:C:405:ASP:HB2	1:C:407:GLU:OE1	2.15	0.47
1:B:307:HIS:ND1	4:B:607:HOH:O	2.33	0.47
1:A:409:THR:HG22	1:A:412:ASP:CG	2.40	0.47
1:B:241:GLN:O	4:B:601:HOH:O	2.20	0.47
1:A:320:ASP:OD2	4:A:601:HOH:O	2.21	0.46
1:B:310:ARG:HD2	4:B:701:HOH:O	2.15	0.46
1:D:397:LEU:HD23	1:D:397:LEU:HA	1.70	0.46
1:A:408:LYS:NZ	4:A:616:HOH:O	2.47	0.46
1:B:384:LEU:HB3	1:B:391:ARG:NH1	2.30	0.46
1:C:185:ILE:HD13	1:C:192:MET:HG2	1.97	0.46
1:D:448:LYS:O	1:D:452:GLN:HG3	2.16	0.46
1:B:281:PRO:HD3	4:B:666:HOH:O	2.16	0.46
1:D:409:THR:HG23	1:D:411:GLU:N	2.31	0.46
1:B:299:ILE:HG13	1:B:327:ILE:CD1	2.46	0.46
1:A:176:VAL:HG23	1:A:177:THR:HG23	1.97	0.45
1:D:192:MET:HE3	1:D:200:VAL:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ILE:O	1:A:403:ILE:HG13	2.16	0.45
1:D:400:LYS:O	1:D:404:GLU:HG3	2.15	0.45
1:A:286:HIS:NE2	1:A:290:LYS:HE2	2.30	0.45
1:B:396:LEU:O	1:B:399:ILE:HG12	2.15	0.45
1:B:308:ILE:O	1:B:333:ALA:HA	2.16	0.45
1:C:389:GLU:CD	1:C:389:GLU:N	2.73	0.45
1:D:342:TPO:O1P	1:D:441:LYS:NZ	2.33	0.45
1:A:197:PHE:CE1	1:A:221:ILE:HG12	2.52	0.45
1:D:371:TYR:OH	1:D:397:LEU:HD11	2.17	0.45
1:C:235:LYS:HG3	4:C:607:HOH:O	2.17	0.45
1:C:320:ASP:OD1	1:C:320:ASP:C	2.60	0.45
1:D:394:GLN:NE2	4:D:620:HOH:O	2.48	0.45
1:D:205:VAL:O	1:D:208:THR:HB	2.17	0.44
1:D:440:LYS:N	3:D:503:SO4:O4	2.44	0.44
1:B:392:GLU:N	1:C:390:HIS:O	2.41	0.44
1:B:266:PRO:HD2	1:B:320:ASP:HA	2.00	0.44
1:A:172:GLU:O	1:A:176:VAL:HG13	2.18	0.43
1:A:288:ARG:HB3	1:A:380:ILE:HG23	1.99	0.43
1:C:299:ILE:HG13	1:C:327:ILE:HD11	1.99	0.43
1:C:384:LEU:HB3	1:C:391:ARG:NH1	2.32	0.43
1:D:451:GLN:O	1:D:455:GLN:HG2	2.17	0.43
1:B:194:GLU:HG3	1:B:199:VAL:HG22	2.00	0.43
1:D:457:MET:O	4:D:602:HOH:O	2.21	0.43
1:B:356:ALA:HB1	1:B:444:ARG:HH22	1.83	0.43
1:B:411:GLU:HA	1:B:414:ILE:HG13	2.01	0.43
1:A:334:ARG:HD3	1:A:334:ARG:HA	1.84	0.43
1:D:415:ASP:HB3	1:D:418:MET:HE2	2.01	0.43
1:C:428:ALA:O	1:C:432:VAL:HG23	2.19	0.43
1:C:247:GLU:OE2	4:C:602:HOH:O	2.20	0.42
1:D:342:TPO:HG23	1:D:343:VAL:N	2.34	0.42
1:B:346:SEP:O1P	1:B:346:SEP:N	2.53	0.42
1:C:226:LEU:HD23	1:C:226:LEU:HA	1.85	0.42
1:D:230:PHE:O	1:D:234:ILE:HG13	2.19	0.42
1:C:389:GLU:O	1:C:394:GLN:NE2	2.52	0.42
1:A:254:ASP:N	1:A:254:ASP:OD1	2.50	0.41
1:B:188:GLY:N	4:B:623:HOH:O	2.52	0.41
1:B:370:ILE:HD13	1:B:370:ILE:HA	1.84	0.41
1:B:298:GLY:HA3	1:B:327:ILE:HD12	2.02	0.41
1:C:288:ARG:HB3	1:C:380:ILE:CG2	2.51	0.41
1:C:351:THR:O	1:C:355:MET:HG3	2.21	0.41
1:C:265:MET:SD	1:C:326:LYS:HD2	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:MET:HE3	1:C:344:MET:HB3	1.94	0.41
1:D:169:SER:OG	1:D:172:GLU:HG3	2.20	0.41
1:D:197:PHE:HE2	1:D:332:LEU:HD21	1.86	0.41
1:A:321:GLU:CG	1:C:281:PRO:HD3	2.47	0.41
1:B:237:MET:HA	1:B:237:MET:HE2	2.00	0.41
1:C:191:LYS:HE3	1:C:194:GLU:HG3	2.03	0.41
1:A:185:ILE:HG21	1:A:192:MET:HG2	2.03	0.41
1:A:302:LEU:HD11	1:A:330:PHE:HE1	1.85	0.41
1:A:348:ILE:HD13	1:A:360:LEU:O	2.21	0.41
1:A:409:THR:HG23	1:A:411:GLU:N	2.36	0.41
1:D:185:ILE:HD13	1:D:189:GLY:O	2.22	0.40
1:A:287:MET:HE3	1:A:290:LYS:HB2	2.03	0.40
1:B:313:LYS:HE3	1:B:315:ALA:HB3	2.04	0.40
1:D:409:THR:HG23	1:D:411:GLU:H	1.86	0.40
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.84	0.40
1:B:183:ARG:HB2	1:B:189:GLY:HA3	2.03	0.40
1:A:320:ASP:OD2	4:A:602:HOH:O	2.22	0.40
1:B:342:TPO:O3P	1:B:441:LYS:NZ	2.46	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	277/304 (91%)	273 (99%)	4 (1%)	0	100	100
1	B	270/304 (89%)	264 (98%)	6 (2%)	0	100	100
1	C	276/304 (91%)	271 (98%)	5 (2%)	0	100	100
1	D	272/304 (90%)	267 (98%)	5 (2%)	0	100	100
All	All	1095/1216 (90%)	1075 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	241/260 (93%)	237 (98%)	4 (2%)	53	61
1	B	241/260 (93%)	238 (99%)	3 (1%)	63	71
1	C	245/260 (94%)	240 (98%)	5 (2%)	48	55
1	D	242/260 (93%)	238 (98%)	4 (2%)	53	61
All	All	969/1040 (93%)	953 (98%)	16 (2%)	53	61

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	MET
1	A	253	SER
1	A	336	SER
1	A	365	THR
1	B	237	MET
1	B	253	SER
1	B	410	ILE
1	C	199	VAL
1	C	222	THR
1	C	228	GLN
1	C	237	MET
1	C	365	THR
1	D	182	GLU
1	D	347	ARG
1	D	399	ILE
1	D	434	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	190	ASN
1	A	306	HIS

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Mol	Chain	Res	Type
1	A	452	GLN
1	A	455	GLN
1	B	179	ASN
1	B	207	ASN
1	B	306	HIS
1	B	442	ASN
1	C	166	HIS
1	C	175	ASN
1	C	229	GLN
1	C	244	ASN
1	C	297	ASN
1	C	307	HIS
1	C	451	GLN
1	C	452	GLN
1	C	455	GLN
1	D	178	ASN
1	D	229	GLN
1	D	435	GLN
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 ⓘ

10 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	A	345	1	8,10,11	2.75	1 (12%)	10,14,16	1.23	1 (10%)
1	TPO	D	342	1	8,10,11	3.19	1 (12%)	10,14,16	1.31	1 (10%)
1	SEP	C	346	1	8,9,10	1.66	1 (12%)	7,12,14	1.20	1 (14%)
1	SEP	A	346	1	8,9,10	1.67	1 (12%)	7,12,14	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	B	342	1	8,10,11	2.82	1 (12%)	10,14,16	1.25	0
1	TPO	C	345	1	8,10,11	2.53	1 (12%)	10,14,16	1.42	1 (10%)
1	SEP	D	346	1	8,9,10	1.66	1 (12%)	7,12,14	1.54	1 (14%)
1	SEP	B	346	1	8,9,10	1.65	1 (12%)	7,12,14	1.60	1 (14%)
1	TPO	D	345	1	8,10,11	2.71	1 (12%)	10,14,16	1.13	1 (10%)
1	TPO	B	345	1	8,10,11	2.53	1 (12%)	10,14,16	1.40	2 (20%)

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	A	345	1	-	2/9/11/13	-
1	TPO	D	342	1	-	3/9/11/13	-
1	SEP	C	346	1	-	3/6/8/10	-
1	SEP	A	346	1	-	0/6/8/10	-
1	TPO	B	342	1	-	4/9/11/13	-
1	TPO	C	345	1	-	4/9/11/13	-
1	SEP	D	346	1	-	3/6/8/10	-
1	SEP	B	346	1	-	1/6/8/10	-
1	TPO	D	345	1	-	2/9/11/13	-
1	TPO	B	345	1	-	2/9/11/13	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	342	TPO	P-OG1	8.69	1.74	1.59
1	B	342	TPO	P-OG1	7.63	1.72	1.59
1	A	345	TPO	P-OG1	7.53	1.72	1.59
1	D	345	TPO	P-OG1	7.35	1.72	1.59
1	C	345	TPO	P-OG1	6.88	1.71	1.59
1	B	345	TPO	P-OG1	6.79	1.71	1.59
1	A	346	SEP	P-O1P	3.72	1.62	1.50
1	C	346	SEP	P-O1P	3.68	1.61	1.50
1	D	346	SEP	P-O1P	3.57	1.61	1.50
1	B	346	SEP	P-O1P	3.55	1.61	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	SEP	OG-CB-CA	3.71	111.75	108.14
1	D	346	SEP	OG-CB-CA	3.51	111.56	108.14
1	D	342	TPO	OG1-P-O1P	-2.92	98.91	109.33
1	C	346	SEP	OG-CB-CA	2.58	110.65	108.14
1	B	345	TPO	OG1-P-O1P	-2.47	100.53	109.33
1	B	345	TPO	P-OG1-CB	-2.33	116.98	123.33
1	A	345	TPO	OG1-P-O1P	-2.23	101.39	109.33
1	C	345	TPO	P-OG1-CB	-2.19	117.38	123.33
1	D	345	TPO	OG1-P-O1P	-2.14	101.71	109.33

There are no chirality outliers.

All (24) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	345	TPO	1	0
1	D	342	TPO	4	0
1	B	342	TPO	1	0
1	B	346	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	A1CKQ	D	501	-	39,40,40	1.18	2 (5%)	50,57,57	1.60	10 (20%)
3	SO4	B	503	-	4,4,4	0.74	0	6,6,6	0.32	0
2	A1CKQ	C	501	-	39,40,40	1.37	3 (7%)	50,57,57	1.82	12 (24%)
3	SO4	D	503	-	4,4,4	0.69	0	6,6,6	0.10	0
3	SO4	D	502	-	4,4,4	0.67	0	6,6,6	0.18	0
2	A1CKQ	A	501	-	39,40,40	1.33	3 (7%)	50,57,57	1.67	9 (18%)
2	A1CKQ	B	501	-	39,40,40	1.25	2 (5%)	50,57,57	1.34	8 (16%)
3	SO4	B	502	-	4,4,4	0.62	0	6,6,6	0.23	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
2	A1CKQ	C	501	-	-	4/20/32/32	0/5/5/5
2	A1CKQ	A	501	-	-	3/20/32/32	0/5/5/5
2	A1CKQ	B	501	-	-	3/20/32/32	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1CKQ	D	501	-	-	3/20/32/32	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A1CKQ	C18-N19	5.26	1.36	1.29
2	B	501	A1CKQ	C18-N19	4.86	1.35	1.29
2	C	501	A1CKQ	C18-N19	4.85	1.35	1.29
2	D	501	A1CKQ	C18-N19	4.71	1.35	1.29
2	C	501	A1CKQ	C18-C17	-3.58	1.38	1.42
2	B	501	A1CKQ	C18-C17	-2.68	1.39	1.42
2	A	501	A1CKQ	C18-C17	-2.53	1.39	1.42
2	D	501	A1CKQ	C18-C17	-2.50	1.39	1.42
2	A	501	A1CKQ	C01-C22	2.14	1.50	1.47
2	C	501	A1CKQ	N15-N19	-2.11	1.35	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A1CKQ	C32-C27-C25	-6.96	103.72	112.23
2	C	501	A1CKQ	C28-C27-C25	6.33	119.97	112.23
2	C	501	A1CKQ	C32-C27-C25	-5.70	105.26	112.23
2	D	501	A1CKQ	C28-C27-C25	5.58	119.06	112.23
2	A	501	A1CKQ	C28-C27-C25	3.95	117.06	112.23
2	B	501	A1CKQ	C32-C27-C25	-3.56	107.88	112.23
2	D	501	A1CKQ	C13-C12-C11	3.54	111.12	107.48
2	D	501	A1CKQ	C32-C27-C25	-3.52	107.94	112.23
2	C	501	A1CKQ	C13-C12-C11	3.41	110.99	107.48
2	B	501	A1CKQ	C13-C12-C11	3.33	110.91	107.48
2	A	501	A1CKQ	C13-C12-C11	3.11	110.67	107.48
2	B	501	A1CKQ	C05-C04-C11	-2.81	118.52	122.82
2	D	501	A1CKQ	C32-C31-C30	-2.74	108.49	111.49
2	B	501	A1CKQ	C13-C14-C16	2.64	136.13	126.76
2	B	501	A1CKQ	C28-C27-C25	2.64	115.46	112.23
2	C	501	A1CKQ	C13-C14-C16	2.59	135.94	126.76
2	A	501	A1CKQ	C13-C14-C16	2.59	135.93	126.76
2	D	501	A1CKQ	C31-C30-N33	2.58	115.72	110.57
2	C	501	A1CKQ	C32-C31-C30	-2.56	108.69	111.49
2	D	501	A1CKQ	C13-C14-C16	2.51	135.67	126.76
2	B	501	A1CKQ	C16-C14-N15	-2.51	116.12	118.66
2	B	501	A1CKQ	C31-C30-N33	2.49	115.54	110.57
2	A	501	A1CKQ	C05-C04-C11	-2.42	119.12	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	A1CKQ	C16-C14-N15	-2.40	116.23	118.66
2	C	501	A1CKQ	C06-C01-C22	2.40	124.06	122.30
2	C	501	A1CKQ	C31-C30-N33	2.36	115.29	110.57
2	A	501	A1CKQ	C16-C14-N15	-2.35	116.28	118.66
2	C	501	A1CKQ	C16-C14-N15	-2.28	116.35	118.66
2	D	501	A1CKQ	C05-C04-C11	-2.27	119.34	122.82
2	A	501	A1CKQ	C32-C27-C28	2.24	114.72	110.00
2	C	501	A1CKQ	C17-C18-N19	-2.17	122.60	125.76
2	A	501	A1CKQ	C04-C11-N15	2.12	128.90	125.25
2	A	501	A1CKQ	C17-C18-N19	-2.12	122.68	125.76
2	C	501	A1CKQ	C31-C32-C27	2.08	114.83	111.18
2	D	501	A1CKQ	C17-C18-N19	-2.06	122.76	125.76
2	C	501	A1CKQ	C01-C22-N23	2.05	126.79	122.23
2	C	501	A1CKQ	C32-C27-C28	2.04	114.29	110.00
2	D	501	A1CKQ	C06-N07-C08	-2.02	121.79	124.66
2	B	501	A1CKQ	C29-C28-C27	-2.01	107.64	111.18

There are no chirality outliers.

All (13) torsion outliers are listed below:

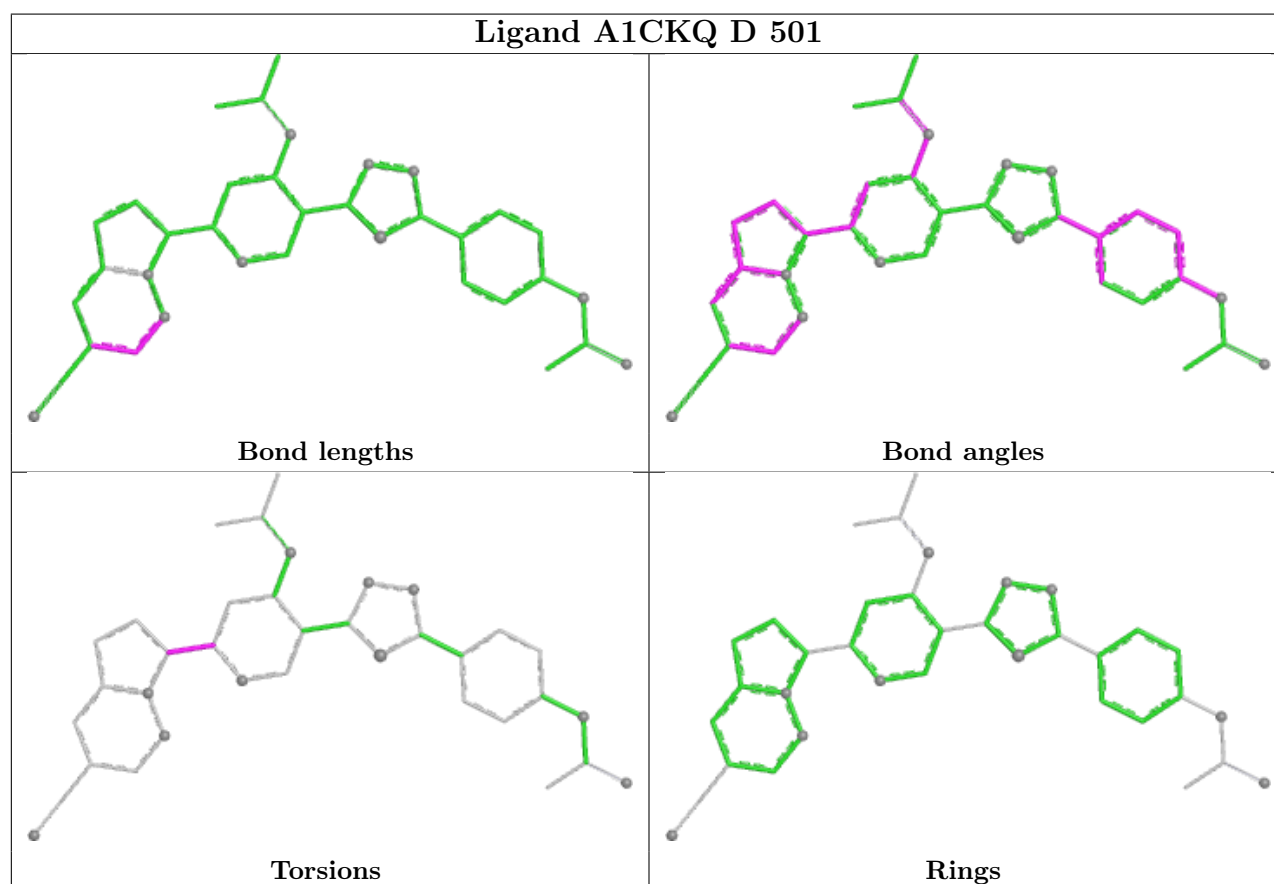
Mol	Chain	Res	Type	Atoms
2	C	501	A1CKQ	S26-C25-C27-C32
2	A	501	A1CKQ	C05-C04-C11-N15
2	A	501	A1CKQ	N03-C04-C11-N15
2	B	501	A1CKQ	C05-C04-C11-N15
2	B	501	A1CKQ	N03-C04-C11-N15
2	C	501	A1CKQ	C05-C04-C11-N15
2	C	501	A1CKQ	N03-C04-C11-N15
2	D	501	A1CKQ	C05-C04-C11-N15
2	D	501	A1CKQ	N03-C04-C11-N15
2	C	501	A1CKQ	C05-C04-C11-C12
2	D	501	A1CKQ	C05-C04-C11-C12
2	A	501	A1CKQ	S26-C25-C27-C32
2	B	501	A1CKQ	N24-C25-C27-C32

There are no ring outliers.

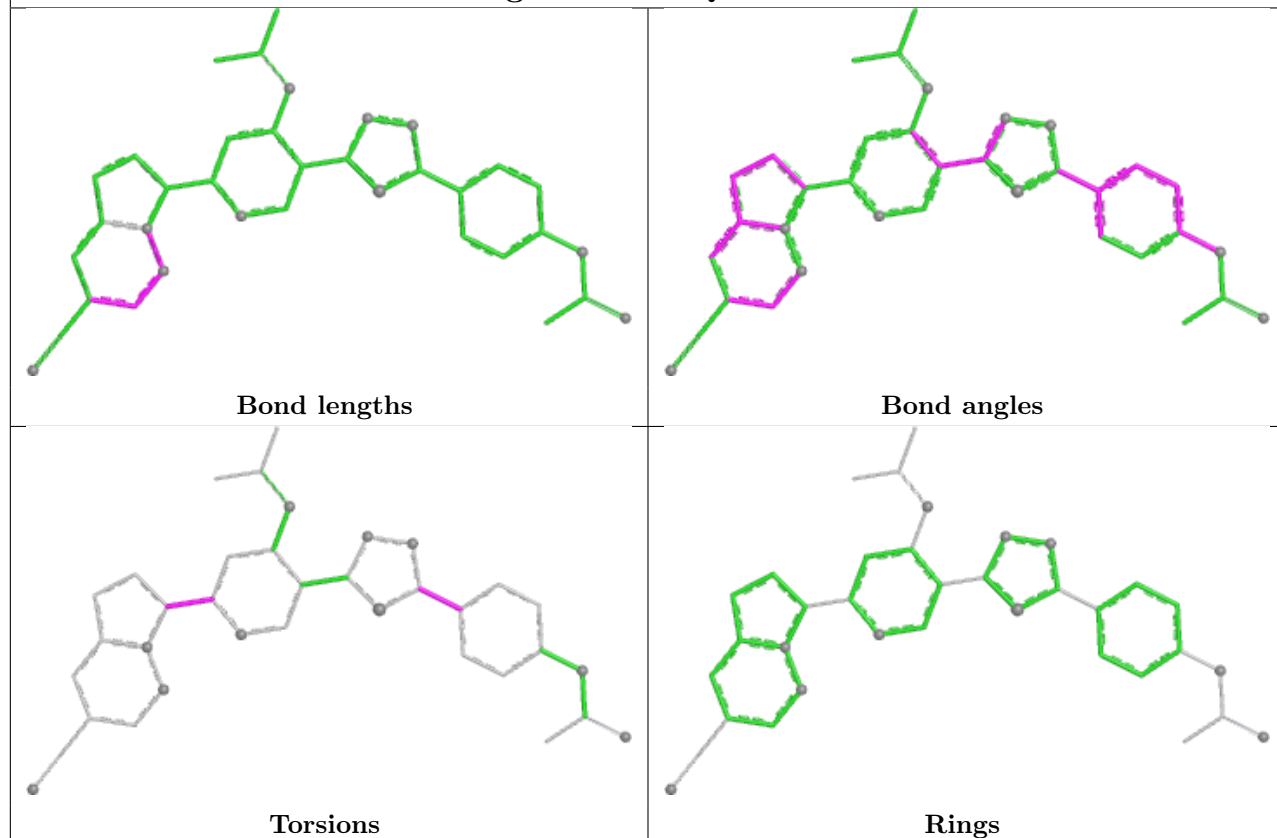
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	503	SO4	1	0

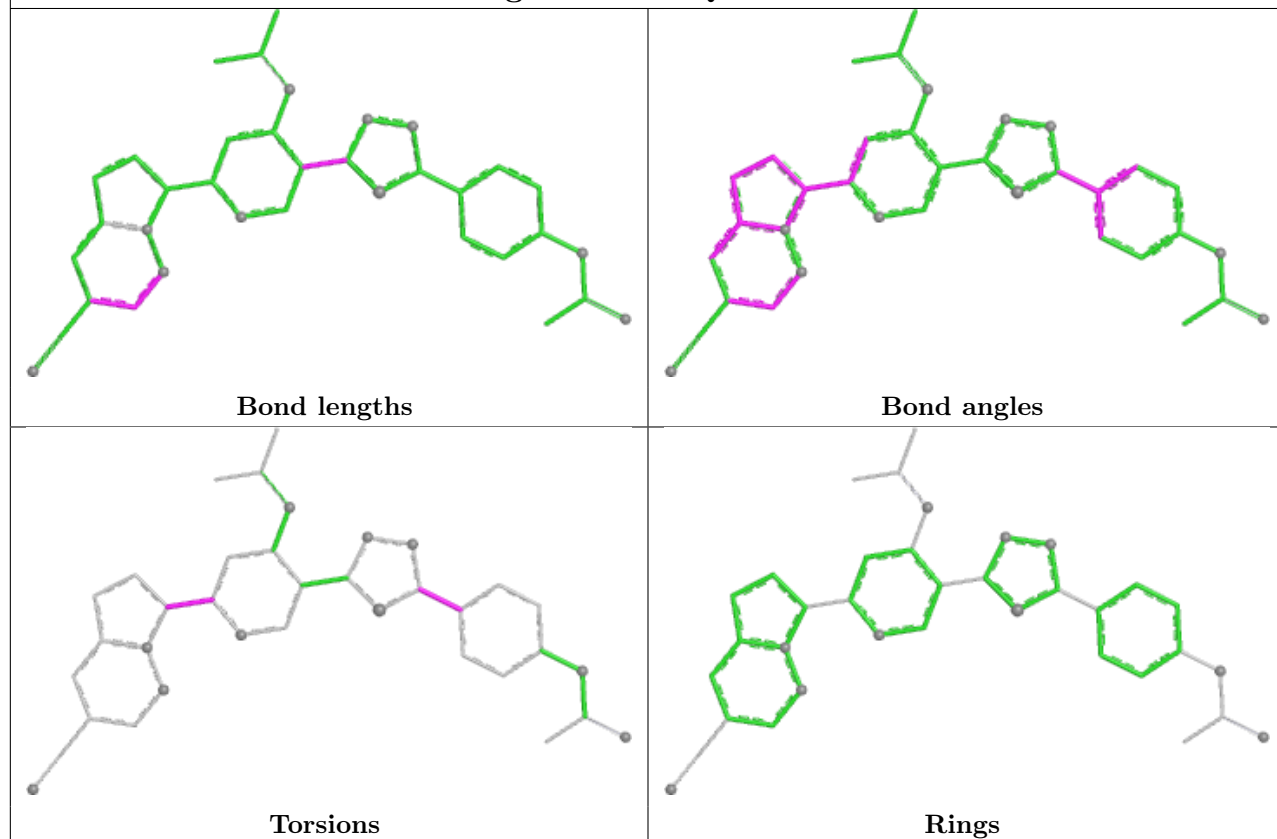
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

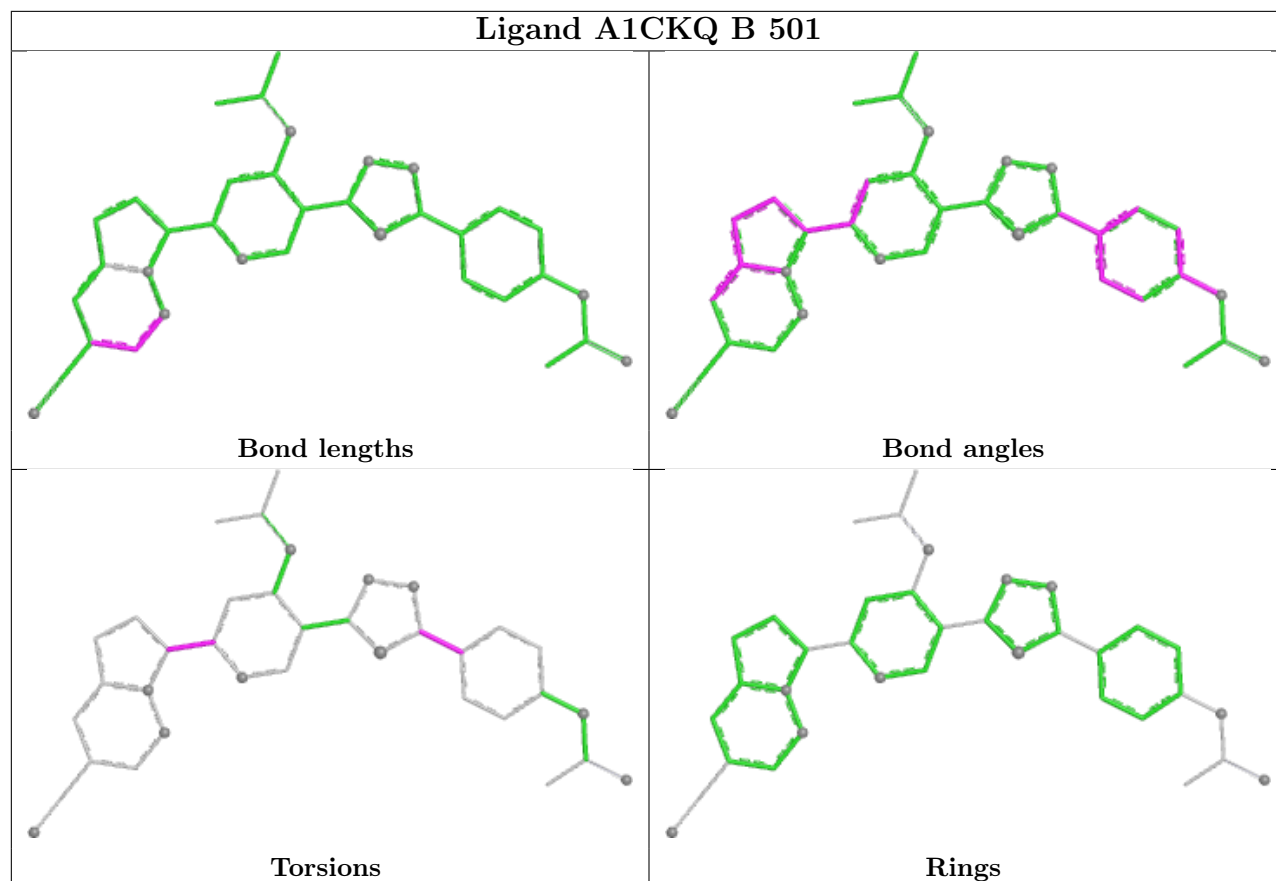


Ligand A1CKQ C 501



Ligand A1CKQ A 501





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	283/304 (93%)	0.39	12 (4%)	40 43	20, 35, 57, 75	0
1	B	279/304 (91%)	0.64	16 (5%)	29 32	20, 39, 62, 76	0
1	C	282/304 (92%)	0.40	6 (2%)	63 66	20, 34, 55, 72	0
1	D	279/304 (91%)	0.55	24 (8%)	16 17	21, 38, 65, 83	0
All	All	1123/1216 (92%)	0.49	58 (5%)	33 35	20, 36, 59, 83	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	439	GLU	4.6
1	B	223	THR	4.3
1	D	255	GLY	4.0
1	B	226	LEU	3.9
1	A	343	VAL	3.7
1	D	207	ASN	3.7
1	D	223	THR	3.7
1	A	256	ASP	3.6
1	D	164	ARG	3.6
1	D	205	VAL	3.5
1	A	196	GLY	3.4
1	C	256	ASP	3.1
1	A	171	TYR	3.1
1	D	195	GLY	3.1
1	B	197	PHE	3.1
1	D	226	LEU	3.0
1	B	257	ASP	2.9
1	A	336	SER	2.9
1	C	343	VAL	2.9
1	D	208	THR	2.9
1	D	196	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	185	ILE	2.9
1	A	335	ALA	2.8
1	D	185	ILE	2.8
1	B	164	ARG	2.7
1	D	347	ARG	2.7
1	A	195	GLY	2.6
1	B	195	GLY	2.6
1	B	221	ILE	2.6
1	A	458	THR	2.5
1	D	241	GLN	2.5
1	A	175	ASN	2.5
1	D	189	GLY	2.4
1	C	405	ASP	2.4
1	C	164	ARG	2.4
1	B	204	TYR	2.4
1	D	206	ASN	2.4
1	B	165	PHE	2.4
1	B	343	VAL	2.4
1	D	343	VAL	2.4
1	A	255	GLY	2.3
1	B	188	GLY	2.3
1	B	409	THR	2.3
1	D	216	ALA	2.3
1	B	236	VAL	2.3
1	D	199	VAL	2.3
1	D	197	PHE	2.2
1	C	223	THR	2.2
1	D	171	TYR	2.1
1	D	405	ASP	2.1
1	D	413	TYR	2.1
1	D	401	GLU	2.0
1	B	455	GLN	2.0
1	B	208	THR	2.0
1	D	184	PRO	2.0
1	C	364	ILE	2.0
1	D	229	GLN	2.0
1	A	223	THR	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(Å ²)	Q<0.9
1	SEP	A	346	10/11	0.75	0.14	49,57,75,79	0
1	TPO	D	342	11/12	0.76	0.18	52,57,64,65	0
1	SEP	C	346	10/11	0.77	0.11	49,59,80,82	0
1	SEP	D	346	10/11	0.77	0.15	55,64,76,80	0
1	TPO	B	342	11/12	0.82	0.15	53,58,64,67	0
1	SEP	B	346	10/11	0.84	0.13	47,58,67,71	0
1	TPO	D	345	11/12	0.89	0.13	46,56,59,61	0
1	TPO	A	345	11/12	0.90	0.10	37,45,51,58	0
1	TPO	C	345	11/12	0.92	0.11	40,47,55,58	0
1	TPO	B	345	11/12	0.93	0.09	42,46,50,59	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

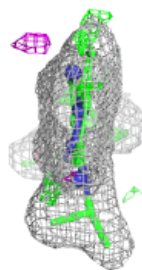
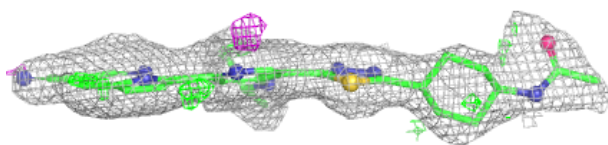
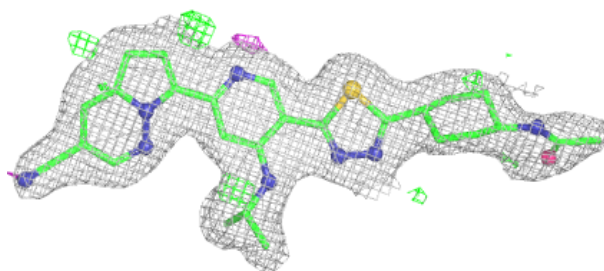
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	503	5/5	0.80	0.25	56,59,66,67	0
3	SO4	D	503	5/5	0.90	0.18	53,55,59,62	0
3	SO4	D	502	5/5	0.92	0.12	51,52,55,58	0
2	A1CKQ	C	501	36/36	0.93	0.10	20,27,38,41	0
2	A1CKQ	A	501	36/36	0.94	0.08	18,25,35,36	0
2	A1CKQ	B	501	36/36	0.94	0.10	25,32,48,51	0
2	A1CKQ	D	501	36/36	0.95	0.09	21,30,43,46	0
3	SO4	B	502	5/5	0.96	0.09	42,44,48,51	0

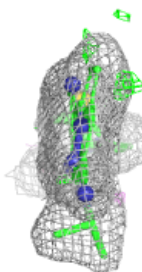
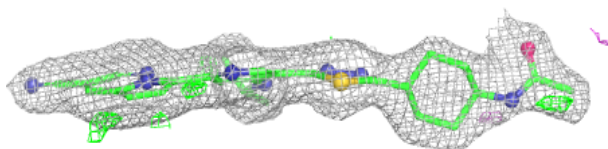
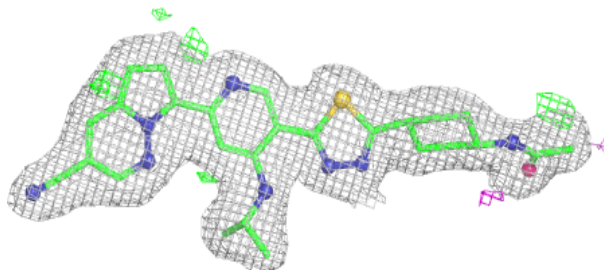
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1CKQ 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)

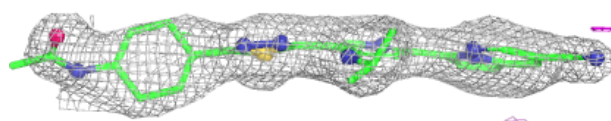
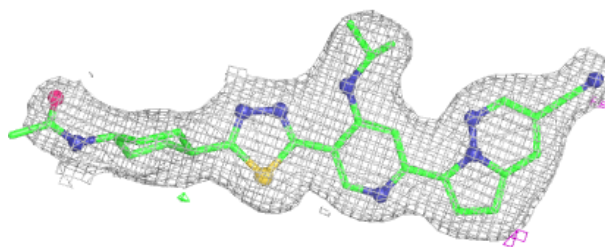
**Electron density around A1CKQ A 501:**

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

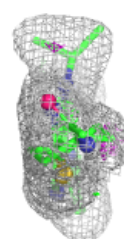
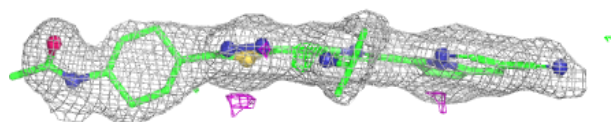
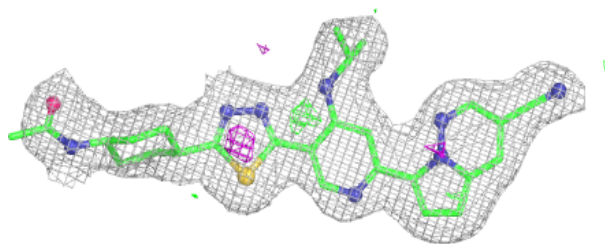


Electron density around A1CKQ B 501:

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

**Electron density around A1CKQ 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.