Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 03:35 AM EDT

PDB ID	:	5UQE
Title	:	Multidomain structure of human kidney-type glutaminase(KGA/GLS)
Authors	:	Pasquali, C.C.; Dias, S.M.G.; Ambrosio, A.L.B.
Deposited on	:	2017-02-08
Resolution	:	3.60 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 (i) 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 (i)) were used in the production of this report:

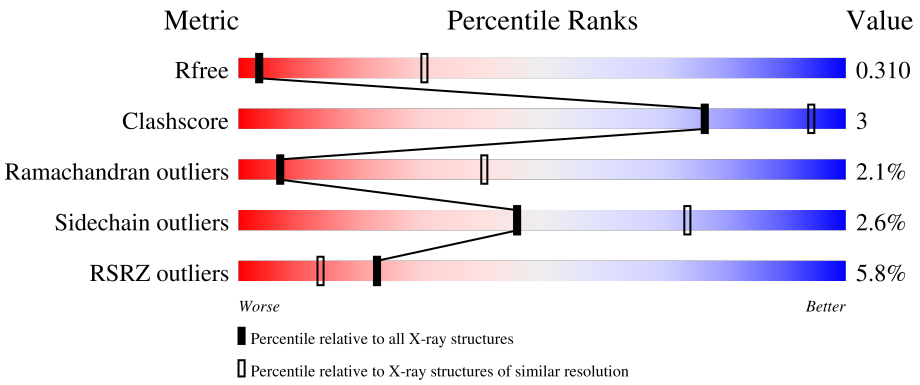
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 <=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	520	8% 85% 9% • 5%
1	B	520	5% 86% 11% • •
1	C	520	7% 83% 9% • 7%
1	D	520	7% 87% 10% • •
1	F	520	70% 7% • 22%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18905 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.

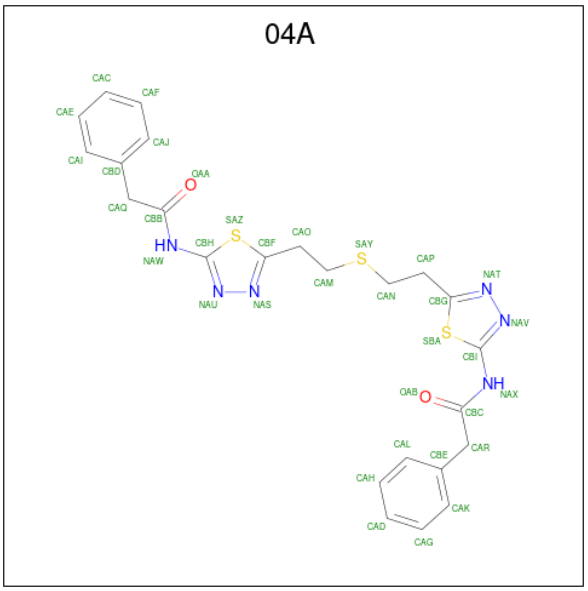
- Molecule 1 is a protein called Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	496	3894	2482	662	718	32	0	0	0
1	B	505	3964	2523	677	732	32	0	0	0
1	C	484	3789	2414	644	699	32	0	0	0
1	D	507	3977	2531	679	735	32	0	0	0
1	F	407	3176	2024	537	587	28	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	LEU	PHE	conflict	UNP O94925
B	219	LEU	PHE	conflict	UNP O94925
C	219	LEU	PHE	conflict	UNP O94925
D	219	LEU	PHE	conflict	UNP O94925
F	219	LEU	PHE	conflict	UNP O94925

- Molecule 2 is N,N'-[sulfanediylbis(ethane-2,1-diyl-1,3,4-thiadiazole-5,2-diyl)]bis(2-phenylacetamide) (three-letter code: 04A) (formula: $C_{24}H_{24}N_6O_2S_3$).



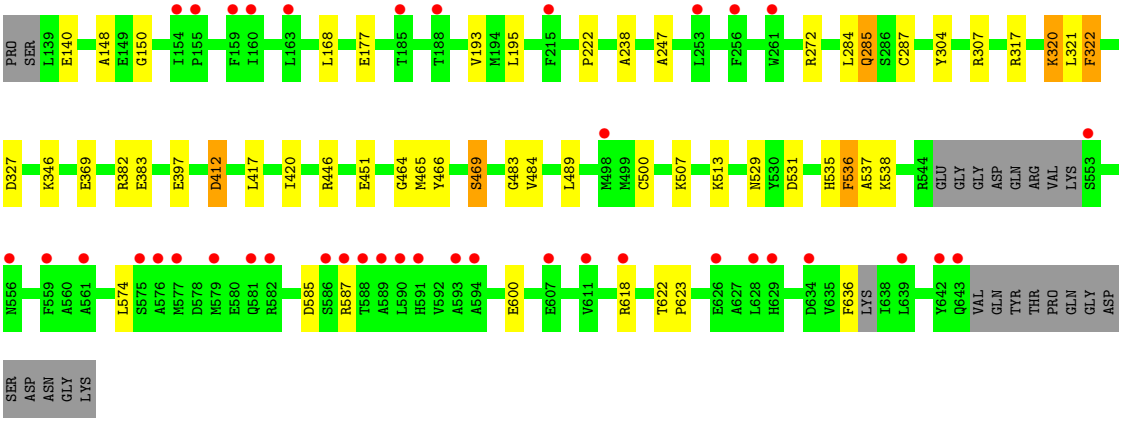
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	35	24	6	2	3	0	0
			Total	C	N	O	S		
2	B	1	35	24	6	2	3	0	0
			Total	C	N	O	S		
2	F	1	35	24	6	2	3	0	0

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.

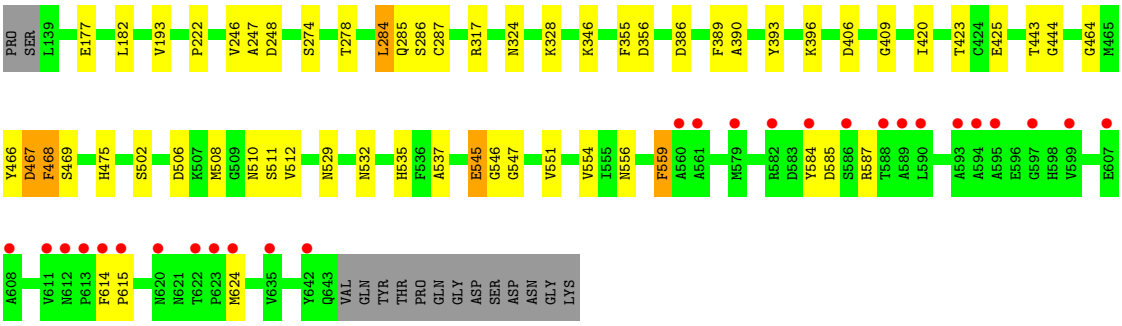
• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain A:



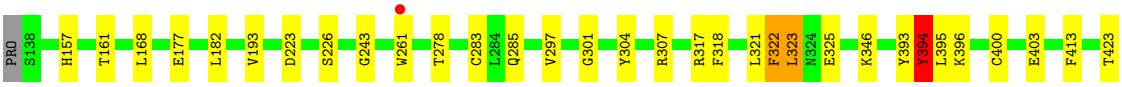
• Molecule 1: Glutaminase kidney isoform, mitochondrial

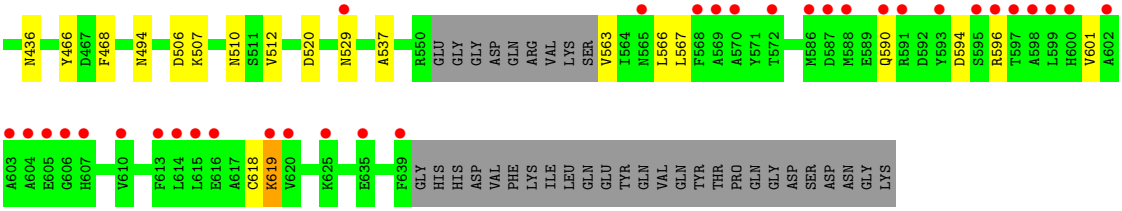
Chain B:



• Molecule 1: Glutaminase kidney isoform, mitochondrial

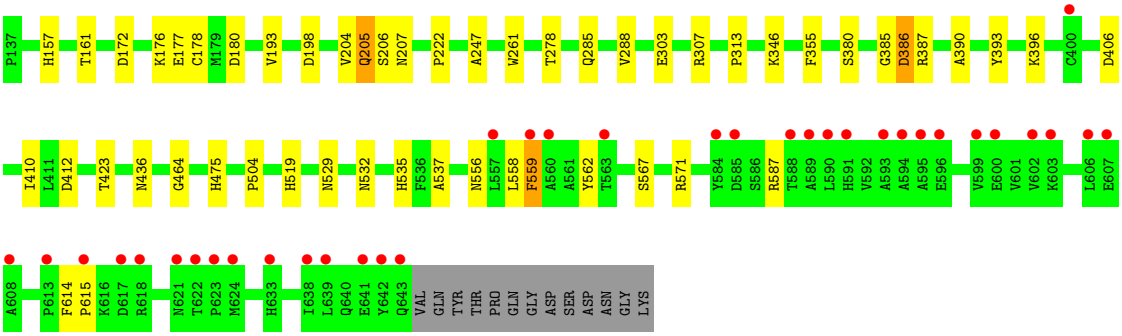
Chain C:





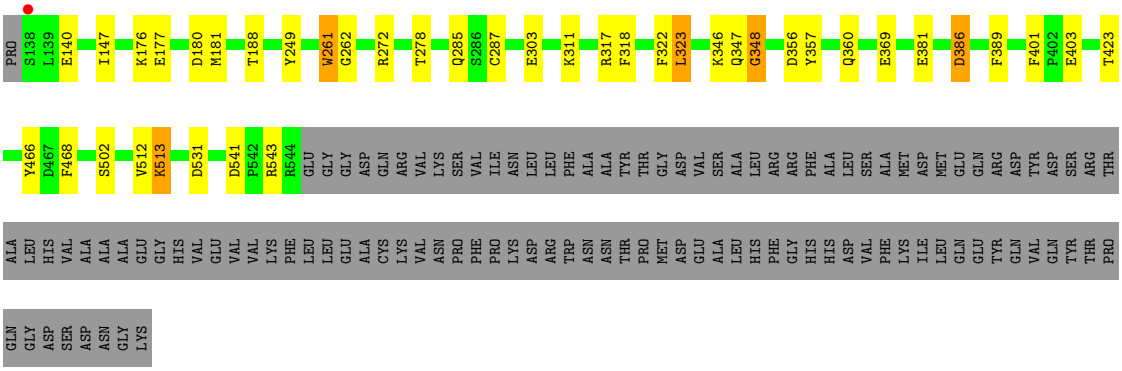
• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain D:



• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	144.42Å 144.42Å 615.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.64 – 3.60 49.64 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.64-3.60) 100.0 (49.64-3.60)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 3.57Å)	Xtriage
Refinement program	PHENIX dev_2733	Depositor
R, R_{free}	0.274 , 0.313 0.275 , 0.310	Depositor DCC
R_{free} test set	3828 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	104.6	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 117.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18905	wwPDB-VP
Average B, all atoms (Å^2)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 04A

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	0.25	0/3981	0.41	0/5377
1	B	0.25	0/4053	0.42	0/5474
1	C	0.26	0/3873	0.42	0/5232
1	D	0.25	0/4067	0.41	0/5493
1	F	0.26	0/3246	0.44	0/4382
All	All	0.25	0/19220	0.42	0/25958

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	3894	0	3847	24	0
1	B	3964	0	3921	28	0
1	C	3789	0	3756	27	0
1	D	3977	0	3934	24	0
1	F	3176	0	3161	22	0
2	A	35	0	24	1	0
2	B	35	0	24	0	0
2	F	35	0	24	0	0
All	All	18905	0	18691	113	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 3.

All (113) 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:B:466:TYR:O	1:B:468:PHE:N	2.01	0.94
1:D:204:VAL:O	1:D:206:SER:N	2.16	0.78
1:C:403:GLU:N	1:C:403:GLU:OE1	2.17	0.77
1:F:176:LYS:NZ	1:F:180:ASP:OD2	2.23	0.72
1:B:545:GLU:OE1	1:B:546:GLY:N	2.26	0.68
1:F:278:THR:O	1:F:423:THR:OG1	2.10	0.67
1:A:587:ARG:NH1	1:B:584:TYR:OH	2.28	0.67
1:D:176:LYS:NZ	1:D:180:ASP:OD2	2.28	0.66
1:C:566:LEU:HD22	1:C:590:GLN:HB2	1.79	0.64
1:A:140:GLU:N	1:A:140:GLU:OE1	2.31	0.63
1:D:278:THR:O	1:D:423:THR:OG1	2.16	0.63
1:A:529:ASN:OD1	1:B:529:ASN:ND2	2.33	0.61
1:C:466:TYR:O	1:C:468:PHE:N	2.34	0.60
1:B:324:ASN:N	1:B:328:LYS:O	2.35	0.60
1:D:177:GLU:OE1	1:D:177:GLU:N	2.34	0.59
1:B:532:ASN:OD1	1:B:535:HIS:N	2.35	0.58
1:A:284:LEU:N	1:A:420:ILE:O	2.30	0.57
1:C:594:ASP:OD1	1:D:587:ARG:NH1	2.38	0.57
1:D:303:GLU:OE1	1:D:307:ARG:NH1	2.37	0.57
1:A:287:CYS:SG	1:A:483:GLY:N	2.79	0.56
1:A:585:ASP:OD1	1:A:618:ARG:NH1	2.38	0.56
1:C:177:GLU:N	1:C:177:GLU:OE1	2.38	0.55
1:C:506:ASP:OD1	1:C:507:LYS:N	2.39	0.55
1:B:278:THR:O	1:B:423:THR:OG1	2.24	0.55
1:B:506:ASP:N	1:B:510:ASN:O	2.34	0.55
1:A:320:LYS:O	1:A:322:PHE:N	2.40	0.55
1:D:567:SER:OG	1:D:571:ARG:NH2	2.40	0.55
1:C:436:ASN:O	1:C:436:ASN:ND2	2.40	0.54
1:F:272:ARG:NH2	1:F:369:GLU:OE2	2.38	0.54
1:F:386:ASP:O	1:F:389:PHE:N	2.39	0.53
1:D:387:ARG:O	1:D:390:ALA:N	2.42	0.53
1:D:157:HIS:O	1:D:161:THR:OG1	2.27	0.52
1:D:436:ASN:O	1:D:436:ASN:ND2	2.43	0.52
1:F:403:GLU:N	1:F:403:GLU:OE1	2.41	0.51
1:A:382:ARG:NH2	1:A:412:ASP:OD2	2.41	0.51
1:C:618:CYS:O	1:C:619:LYS:HB2	2.11	0.50
1:A:585:ASP:OD2	1:B:587:ARG:NH1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ASP:OD2	1:C:226:SER:OG	2.30	0.49
1:C:594:ASP:OD2	1:C:596:ARG:NH1	2.45	0.49
1:C:393:TYR:O	1:C:396:LYS:N	2.38	0.49
1:D:178:CYS:N	1:D:207:ASN:OD1	2.46	0.49
1:F:147:ILE:O	1:F:147:ILE:HG22	2.13	0.48
1:A:397:GLU:OE1	1:D:387:ARG:N	2.45	0.48
1:A:272:ARG:NH2	1:A:369:GLU:OE2	2.47	0.48
1:B:406:ASP:OD2	1:B:409:GLY:N	2.43	0.48
1:B:274:SER:OG	1:B:425:GLU:OE2	2.29	0.47
1:B:545:GLU:OE1	1:B:547:GLY:N	2.46	0.47
1:F:261:TRP:CE3	1:F:513:LYS:CE	2.98	0.47
1:D:393:TYR:O	1:D:396:LYS:HB3	2.15	0.46
1:B:285:GLN:O	1:B:287:CYS:N	2.49	0.46
1:C:157:HIS:O	1:C:161:THR:OG1	2.19	0.46
1:F:541:ASP:O	1:F:543:ARG:N	2.40	0.46
1:A:383:GLU:N	1:A:383:GLU:OE1	2.49	0.45
1:F:188:THR:O	1:F:188:THR:OG1	2.31	0.45
1:F:261:TRP:CD2	1:F:513:LYS:HE2	2.51	0.45
1:D:532:ASN:OD1	1:D:535:HIS:N	2.44	0.45
1:F:140:GLU:OE1	1:F:140:GLU:N	2.43	0.45
1:C:618:CYS:O	1:C:619:LYS:CB	2.65	0.45
1:A:465:MET:O	1:A:469:SER:OG	2.30	0.44
1:B:284:LEU:N	1:B:420:ILE:O	2.42	0.44
1:C:278:THR:O	1:C:423:THR:OG1	2.35	0.44
1:C:322:PHE:O	1:C:323:LEU:HG	2.17	0.44
1:B:467:ASP:HB2	1:B:508:MET:HE1	1.99	0.44
1:D:204:VAL:HG23	1:D:205:GLN:N	2.33	0.44
1:F:177:GLU:O	1:F:181:MET:N	2.51	0.44
1:A:238:ALA:HB1	1:A:513:LYS:HG3	2.00	0.43
1:C:393:TYR:O	1:C:394:TYR:C	2.56	0.43
1:F:322:PHE:O	1:F:323:LEU:HG	2.17	0.43
1:C:297:VAL:O	1:C:301:GLY:N	2.45	0.43
1:A:177:GLU:OE1	1:A:177:GLU:N	2.52	0.43
1:B:443:THR:OG1	1:B:444:GLY:N	2.52	0.43
1:D:614:PHE:N	1:D:615:PRO:HD3	2.33	0.42
1:A:285:GLN:HG2	1:A:484:VAL:HG22	2.01	0.42
1:B:177:GLU:OE1	1:B:177:GLU:N	2.41	0.42
1:C:304:TYR:HA	1:C:307:ARG:HD3	2.00	0.42
1:C:529:ASN:OD1	1:D:529:ASN:ND2	2.48	0.42
1:A:304:TYR:HA	1:A:307:ARG:HD3	2.02	0.42
1:C:567:LEU:HD22	1:C:601:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:TRP:CE3	1:F:513:LYS:HE2	2.54	0.42
1:A:397:GLU:HB2	1:D:386:ASP:HB3	2.02	0.42
2:A:701:04A:HAD	1:B:317:ARG:HH22	1.85	0.42
1:B:393:TYR:O	1:B:396:LYS:HB3	2.19	0.42
1:A:587:ARG:NH1	1:B:585:ASP:OD2	2.35	0.42
1:B:386:ASP:CB	1:C:393:TYR:OH	2.68	0.42
1:C:494:ASN:OD1	1:D:532:ASN:ND2	2.53	0.42
1:F:317:ARG:O	1:F:318:PHE:CB	2.68	0.42
1:B:556:ASN:HA	1:B:559:PHE:CE2	2.55	0.42
1:D:285:GLN:O	1:D:288:VAL:HG22	2.20	0.42
1:A:536:PHE:O	1:A:538:LYS:N	2.52	0.41
1:D:519:HIS:O	1:D:519:HIS:ND1	2.47	0.41
1:F:261:TRP:HE3	1:F:262:GLY:N	2.17	0.41
1:F:346:LYS:O	1:F:348:GLY:N	2.53	0.41
1:B:246:VAL:O	1:B:248:ASP:N	2.53	0.41
1:C:506:ASP:N	1:C:510:ASN:O	2.36	0.41
1:F:249:TYR:OH	1:F:381:GLU:OE2	2.26	0.41
1:D:556:ASN:HA	1:D:559:PHE:CE2	2.55	0.41
1:A:600:GLU:OE1	1:A:600:GLU:N	2.46	0.41
1:B:551:VAL:HA	1:B:554:VAL:HB	2.01	0.41
1:A:529:ASN:ND2	1:B:529:ASN:OD1	2.42	0.41
1:B:386:ASP:O	1:B:389:PHE:HB3	2.21	0.41
1:C:563:VAL:HG12	1:C:590:GLN:HB3	2.02	0.41
1:A:148:ALA:O	1:A:150:GLY:N	2.50	0.41
1:B:390:ALA:HB2	1:C:393:TYR:HD2	1.86	0.41
1:C:317:ARG:O	1:C:318:PHE:HB3	2.21	0.41
1:F:285:GLN:O	1:F:287:CYS:N	2.48	0.41
1:F:386:ASP:O	1:F:389:PHE:HB2	2.21	0.41
1:B:502:SER:HB2	1:B:511:SER:OG	2.20	0.40
1:C:395:LEU:HB3	1:C:400:CYS:HB2	2.03	0.40
1:F:357:TYR:O	1:F:360:GLN:HB2	2.20	0.40
1:D:406:ASP:O	1:D:410:ILE:HG12	2.21	0.40
1:A:622:THR:HB	1:A:623:PRO:HD2	2.03	0.40
1:D:614:PHE:N	1:D:615:PRO:CD	2.84	0.40
1:F:502:SER:HB2	1:F:513:LYS:CE	2.51	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	490/520 (94%)	431 (88%)	48 (10%)	11 (2%)	6 39
1	B	503/520 (97%)	448 (89%)	44 (9%)	11 (2%)	6 39
1	C	480/520 (92%)	408 (85%)	61 (13%)	11 (2%)	6 38
1	D	505/520 (97%)	442 (88%)	52 (10%)	11 (2%)	6 39
1	F	405/520 (78%)	355 (88%)	45 (11%)	5 (1%)	13 51
All	All	2383/2600 (92%)	2084 (88%)	250 (10%)	49 (2%)	7 40

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	LEU
1	A	507	LYS
1	B	467	ASP
1	C	537	ALA
1	D	205	GLN
1	D	537	ALA
1	A	285	GLN
1	A	464	GLY
1	B	193	VAL
1	B	247	ALA
1	B	464	GLY
1	C	193	VAL
1	C	619	LYS
1	D	247	ALA
1	D	464	GLY
1	F	323	LEU
1	F	348	GLY
1	F	512	VAL
1	A	537	ALA
1	B	286	SER
1	B	537	ALA

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Mol	Chain	Res	Type
1	C	182	LEU
1	C	323	LEU
1	D	385	GLY
1	D	386	ASP
1	A	247	ALA
1	A	327	ASP
1	A	346	LYS
1	A	466	TYR
1	B	222	PRO
1	B	346	LYS
1	C	285	GLN
1	C	321	LEU
1	C	512	VAL
1	D	222	PRO
1	D	346	LYS
1	F	347	GLN
1	F	466	TYR
1	A	222	PRO
1	B	512	VAL
1	D	504	PRO
1	C	243	GLY
1	C	346	LYS
1	C	394	TYR
1	D	193	VAL
1	A	193	VAL
1	D	313	PRO
1	B	614	PHE
1	B	615	PRO

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	428/448 (96%)	411 (96%)	17 (4%)	31	65
1	B	435/448 (97%)	425 (98%)	10 (2%)	50	76
1	C	417/448 (93%)	409 (98%)	8 (2%)	57	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	437/448 (98%)	427 (98%)	10 (2%)	50	76
1	F	353/448 (79%)	344 (98%)	9 (2%)	47	75
All	All	2070/2240 (92%)	2016 (97%)	54 (3%)	46	74

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	LEU
1	A	195	LEU
1	A	317	ARG
1	A	320	LYS
1	A	322	PHE
1	A	412	ASP
1	A	417	LEU
1	A	446	ARG
1	A	451	GLU
1	A	469	SER
1	A	489	LEU
1	A	500	CYS
1	A	531	ASP
1	A	535	HIS
1	A	536	PHE
1	A	574	LEU
1	A	636	PHE
1	B	182	LEU
1	B	284	LEU
1	B	355	PHE
1	B	356	ASP
1	B	468	PHE
1	B	469	SER
1	B	475	HIS
1	B	545	GLU
1	B	559	PHE
1	B	624	MET
1	C	168	LEU
1	C	261	TRP
1	C	283	CYS
1	C	322	PHE
1	C	325	GLU
1	C	394	TYR
1	C	413	PHE

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Mol	Chain	Res	Type
1	C	520	ASP
1	D	172	ASP
1	D	198	ASP
1	D	261	TRP
1	D	355	PHE
1	D	380	SER
1	D	412	ASP
1	D	475	HIS
1	D	558	LEU
1	D	559	PHE
1	D	562	TYR
1	F	261	TRP
1	F	303	GLU
1	F	311	LYS
1	F	356	ASP
1	F	386	ASP
1	F	401	PHE
1	F	468	PHE
1	F	513	LYS
1	F	531	ASP

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

Mol	Chain	Res	Type
1	B	598	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	04A	F	701	-	32,38,38	1.47	6 (18%)	29,49,49	1.61	7 (24%)
2	04A	A	701	-	32,38,38	1.44	6 (18%)	29,49,49	1.59	7 (24%)
2	04A	B	701	-	32,38,38	1.58	6 (18%)	29,49,49	1.47	6 (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
2	04A	F	701	-	-	8/18/24/24	0/4/4/4
2	04A	A	701	-	-	3/18/24/24	0/4/4/4
2	04A	B	701	-	-	3/18/24/24	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	04A	CAO-CBF	3.90	1.51	1.49
2	B	701	04A	CAP-CBG	3.65	1.51	1.49
2	B	701	04A	CBH-NAW	3.56	1.43	1.36
2	F	701	04A	CAO-CBF	3.49	1.51	1.49
2	A	701	04A	CBB-NAW	3.48	1.43	1.35
2	B	701	04A	CBI-NAX	3.43	1.42	1.36
2	A	701	04A	CBH-NAW	3.40	1.42	1.36
2	F	701	04A	CBH-NAW	3.38	1.42	1.36
2	B	701	04A	CBB-NAW	3.30	1.42	1.35
2	F	701	04A	CBB-NAW	3.27	1.42	1.35
2	F	701	04A	CBI-NAX	3.20	1.42	1.36
2	A	701	04A	CAO-CBF	3.16	1.51	1.49
2	A	701	04A	CBI-NAX	3.07	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	04A	CBC-NAX	3.07	1.42	1.35
2	F	701	04A	CAP-CBG	3.00	1.51	1.49
2	F	701	04A	CBC-NAX	2.99	1.42	1.35
2	A	701	04A	CBC-NAX	2.90	1.42	1.35
2	A	701	04A	CAP-CBG	2.52	1.51	1.49

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	04A	CAQ-CBB-NAW	4.06	123.15	114.77
2	F	701	04A	CAQ-CBB-NAW	3.96	122.95	114.77
2	B	701	04A	CAQ-CBB-NAW	3.90	122.83	114.77
2	F	701	04A	CBI-NAX-CBC	-3.66	119.67	129.54
2	A	701	04A	CBI-NAX-CBC	-3.56	119.92	129.54
2	A	701	04A	OAA-CBB-NAW	-3.25	117.69	123.63
2	F	701	04A	OAA-CBB-NAW	-3.23	117.74	123.63
2	B	701	04A	CBI-NAX-CBC	-3.03	121.36	129.54
2	F	701	04A	CAR-CBC-NAX	2.98	120.92	114.77
2	B	701	04A	OAA-CBB-NAW	-2.81	118.51	123.63
2	B	701	04A	CAN-SAY-CAM	2.76	110.24	101.87
2	F	701	04A	CAN-SAY-CAM	2.72	110.12	101.87
2	A	701	04A	CAN-SAY-CAM	2.26	108.72	101.87
2	F	701	04A	OAB-CBC-NAX	-2.15	119.70	123.63
2	B	701	04A	CAR-CBC-NAX	2.15	119.22	114.77
2	A	701	04A	CBH-NAW-CBB	-2.12	123.82	129.54
2	A	701	04A	CAR-CBC-NAX	2.10	119.12	114.77
2	B	701	04A	CBH-NAW-CBB	-2.04	124.04	129.54
2	A	701	04A	CAP-CAN-SAY	-2.03	108.53	113.84
2	F	701	04A	CBH-NAW-CBB	-2.02	124.08	129.54

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	04A	SAY-CAN-CAP-CBG
2	B	701	04A	SAY-CAM-CAO-CBF
2	F	701	04A	SAY-CAM-CAO-CBF
2	F	701	04A	CBC-CAR-CBE-CAK
2	F	701	04A	CBC-CAR-CBE-CAL
2	F	701	04A	CBE-CAR-CBC-OAB
2	F	701	04A	CBE-CAR-CBC-NAX
2	F	701	04A	CAP-CAN-SAY-CAM

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Mol	Chain	Res	Type	Atoms
2	A	701	04A	CAQ-CBB-NAW-CBH
2	B	701	04A	CAQ-CBB-NAW-CBH
2	F	701	04A	CAQ-CBB-NAW-CBH
2	A	701	04A	OAA-CBB-NAW-CBH
2	B	701	04A	OAA-CBB-NAW-CBH
2	F	701	04A	OAA-CBB-NAW-CBH

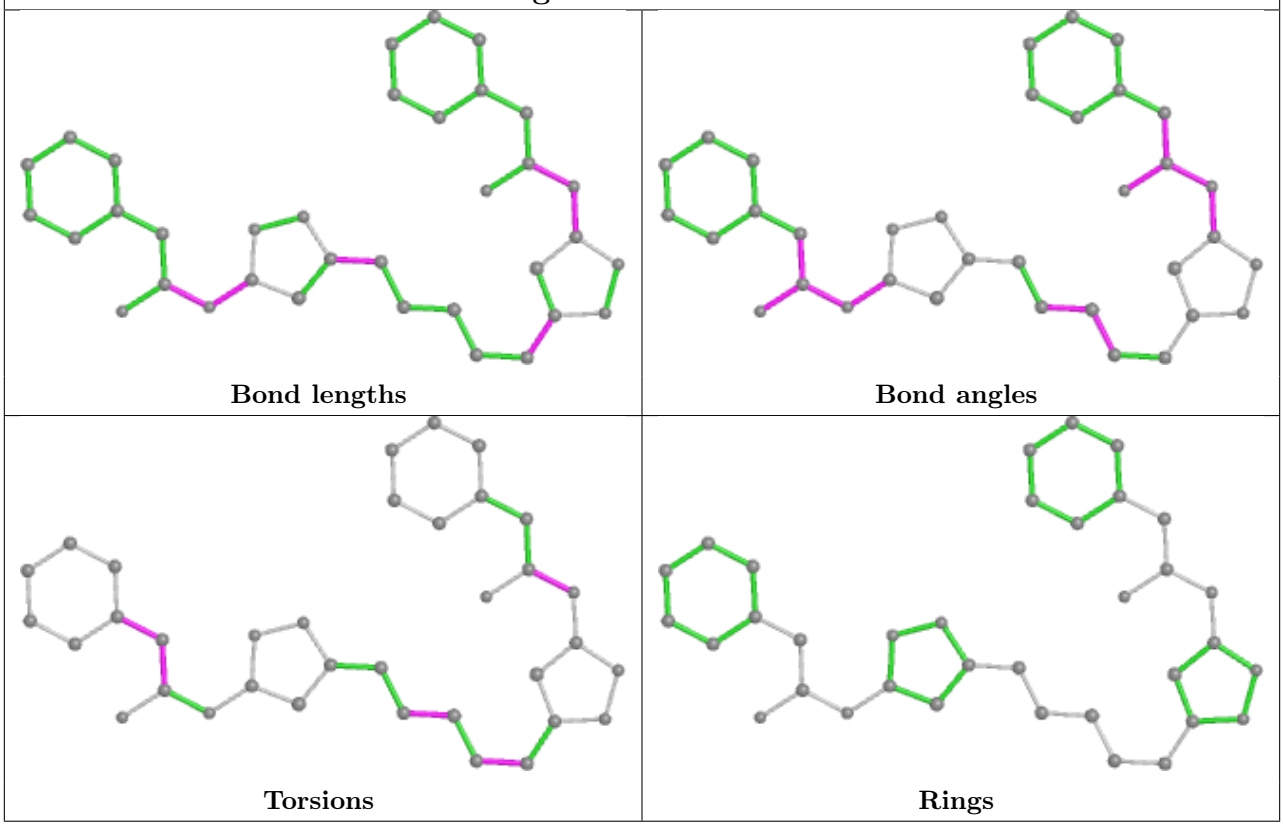
There are no ring outliers.

1 monomer is involved in 1 short contact:

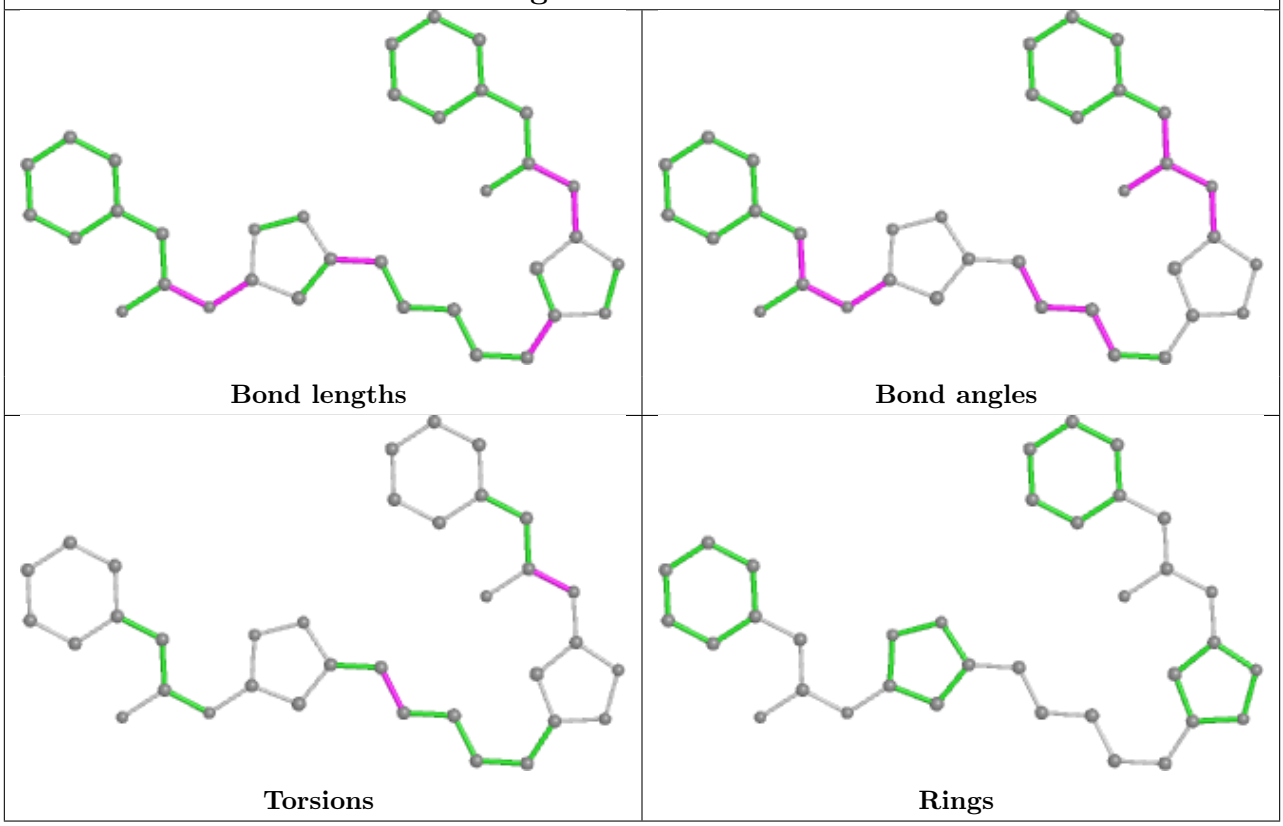
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	04A	1	0

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 then 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.

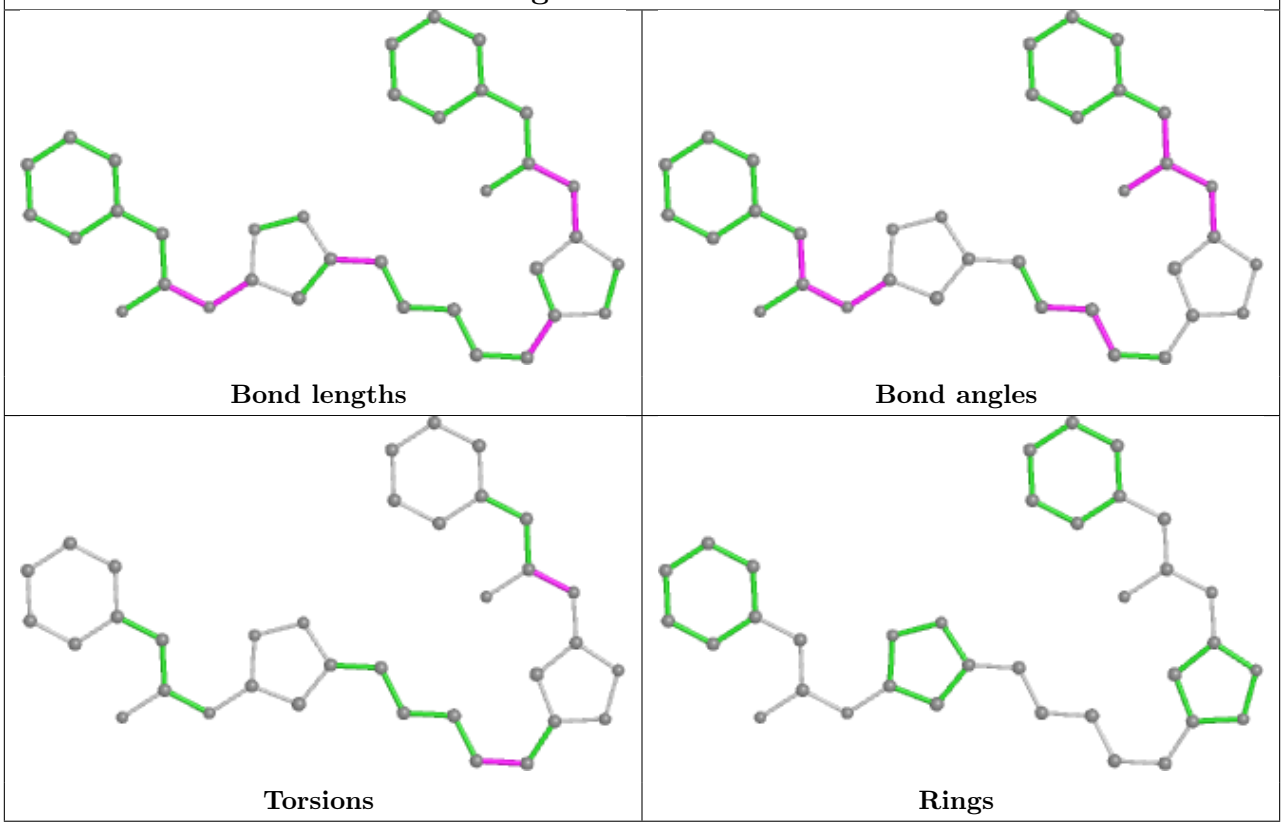
Ligand 04A F 701



Ligand 04A A 701



Ligand 04A B 701



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	496/520 (95%)	0.30	40 (8%)	12	7	83, 162, 254, 284	0
1	B	505/520 (97%)	0.06	27 (5%)	26	16	61, 118, 258, 301	2 (0%)
1	C	484/520 (93%)	0.20	35 (7%)	15	9	55, 113, 277, 307	1 (0%)
1	D	507/520 (97%)	0.22	36 (7%)	16	9	57, 117, 266, 321	2 (0%)
1	F	407/520 (78%)	-0.33	1 (0%)	95	91	37, 97, 143, 170	0
All	All	2399/2600 (92%)	0.10	139 (5%)	23	13	37, 120, 259, 321	5 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	588	MET	8.4
1	C	590	GLN	7.5
1	B	589	ALA	7.4
1	C	565	ASN	6.6
1	D	594	ALA	6.2
1	B	594	ALA	6.1
1	A	579	MET	5.6
1	A	607	GLU	5.6
1	A	590	LEU	5.5
1	A	591	HIS	5.2
1	B	593	ALA	5.2
1	C	620	VAL	5.1
1	A	582	ARG	4.8
1	A	581	GLN	4.8
1	A	559	PHE	4.6
1	B	613	PRO	4.6
1	B	614	PHE	4.5
1	B	599	VAL	4.5
1	A	611	VAL	4.5
1	B	588	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	616	GLU	4.2
1	D	638	ILE	4.2
1	C	606	GLY	4.1
1	C	570	ALA	4.0
1	C	569	ALA	4.0
1	C	598	ALA	4.0
1	B	615	PRO	4.0
1	D	588	THR	3.8
1	D	589	ALA	3.7
1	A	577	MET	3.7
1	B	612	ASN	3.7
1	C	619	LYS	3.6
1	D	639	LEU	3.6
1	A	575	SER	3.6
1	D	623	PRO	3.5
1	C	599	LEU	3.5
1	B	590	LEU	3.5
1	A	593	ALA	3.5
1	C	591	ARG	3.5
1	D	563	THR	3.4
1	A	618	ARG	3.4
1	D	618	ARG	3.3
1	A	589	ALA	3.3
1	F	138	SER	3.3
1	A	634	ASP	3.2
1	D	560	ALA	3.2
1	C	596	ARG	3.1
1	B	622	THR	3.1
1	C	635	GLU	3.1
1	B	624	MET	3.1
1	C	602	ALA	3.1
1	D	642	TYR	3.0
1	A	628	LEU	3.0
1	D	595	ALA	3.0
1	C	600	HIS	3.0
1	B	579	MET	3.0
1	C	639	PHE	2.9
1	D	633	HIS	2.9
1	A	155	PRO	2.9
1	D	599	VAL	2.9
1	D	584	TYR	2.9
1	A	556	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	643	GLN	2.9
1	B	623	PRO	2.8
1	A	188	THR	2.8
1	A	594	ALA	2.8
1	D	608	ALA	2.7
1	D	600	GLU	2.7
1	D	596	GLU	2.7
1	C	572	THR	2.7
1	A	586	SER	2.7
1	C	568	PHE	2.7
1	D	615	PRO	2.7
1	C	586	MET	2.6
1	D	559	PHE	2.6
1	D	585	ASP	2.6
1	B	595	ALA	2.6
1	B	620	ASN	2.6
1	B	561	ALA	2.6
1	A	561	ALA	2.6
1	A	256	PHE	2.5
1	C	625	LYS	2.5
1	C	607	HIS	2.5
1	A	163	LEU	2.5
1	D	613	PRO	2.5
1	C	614	LEU	2.5
1	B	584	TYR	2.5
1	A	576	ALA	2.5
1	D	400	CYS	2.5
1	D	607	GLU	2.5
1	A	185	THR	2.4
1	C	613	PHE	2.4
1	A	160	ILE	2.4
1	C	529	ASN	2.4
1	D	617	ASP	2.4
1	A	553	SER	2.4
1	A	159	PHE	2.4
1	C	615	LEU	2.4
1	A	626	GLU	2.3
1	A	154	ILE	2.3
1	A	261	TRP	2.3
1	A	643	GLN	2.3
1	B	607	GLU	2.3
1	B	611	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	624	MET	2.3
1	B	582	ARG	2.3
1	C	605	GLU	2.3
1	D	603	LYS	2.3
1	A	587	ARG	2.3
1	B	635	VAL	2.3
1	B	642	TYR	2.3
1	C	593	TYR	2.3
1	D	641	GLU	2.3
1	C	595	SER	2.2
1	B	608	ALA	2.2
1	B	560	ALA	2.2
1	C	261	TRP	2.2
1	B	597	GLY	2.2
1	C	604	ALA	2.2
1	D	557	LEU	2.2
1	A	642	TYR	2.1
1	D	621	ASN	2.1
1	D	593	ALA	2.1
1	C	610	VAL	2.1
1	D	606	LEU	2.1
1	D	590	LEU	2.1
1	A	588	THR	2.1
1	B	586	SER	2.1
1	D	591	HIS	2.1
1	C	597	THR	2.1
1	C	587	ASP	2.1
1	A	253	LEU	2.1
1	A	629	HIS	2.1
1	D	622	THR	2.1
1	D	602	VAL	2.1
1	A	639	LEU	2.0
1	C	603	ALA	2.0
1	A	498	MET	2.0
1	A	215	PHE	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)

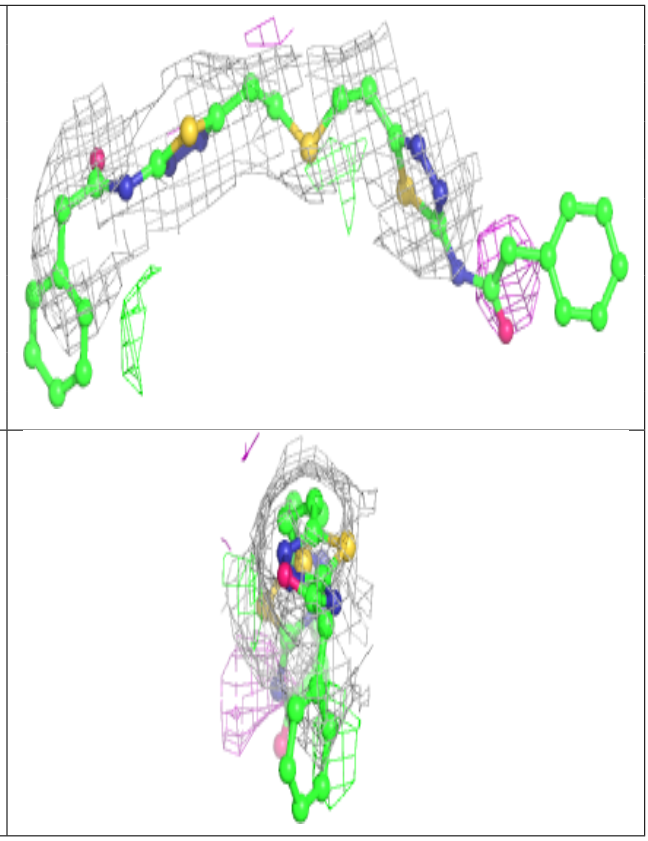
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	04A	A	701	35/35	0.88	0.34	59,118,192,198	0
2	04A	B	701	35/35	0.91	0.28	24,127,195,200	0
2	04A	F	701	35/35	0.96	0.21	68,94,131,144	35

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.

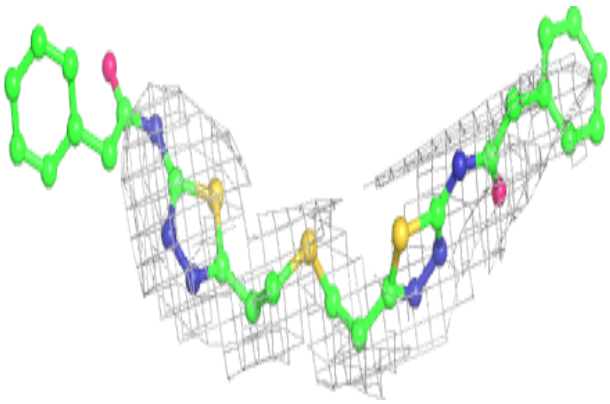
Electron density around 04A A 701:

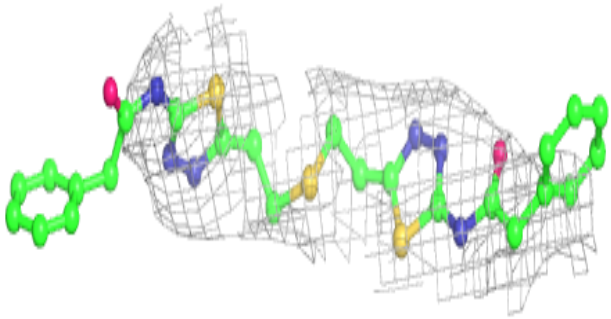
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 04A B 701:

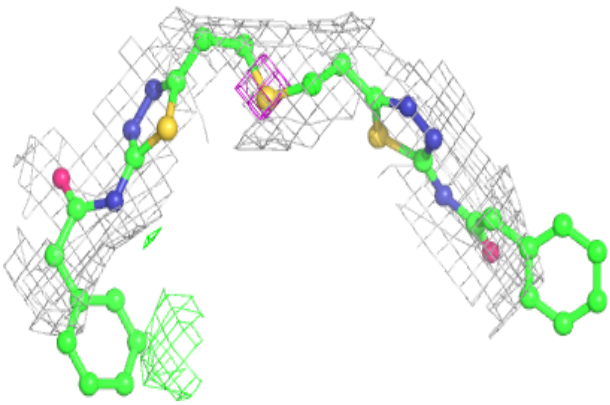
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

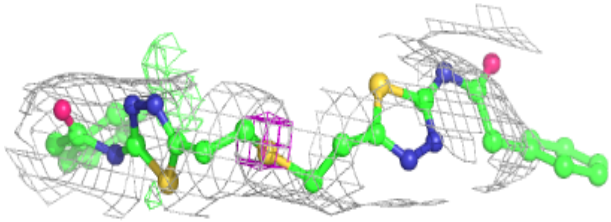


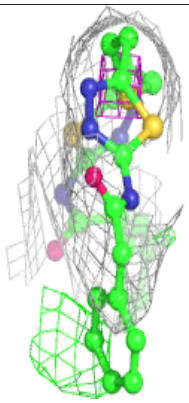


Electron density around 04A F 701:

$2mF_o$-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.