



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:09 PM UTC

PDB ID : 5UQE / pdb_00005uqe
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 ⓘ 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

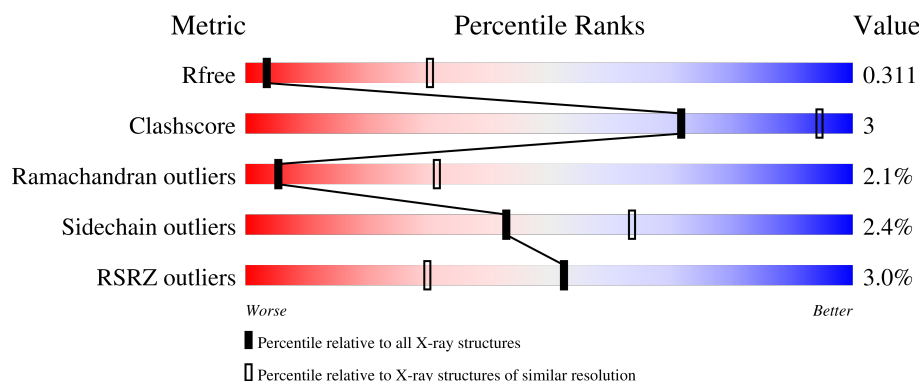
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (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 $\leq 5\%$. 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	520	3% 85% 10% 5%
1	B	520	4% 86% 10% ..
1	C	520	4% 82% 10% 7%
1	D	520	3% 87% 10% ..
1	F	520	% 69% 8% 22%

2 Entry composition

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.

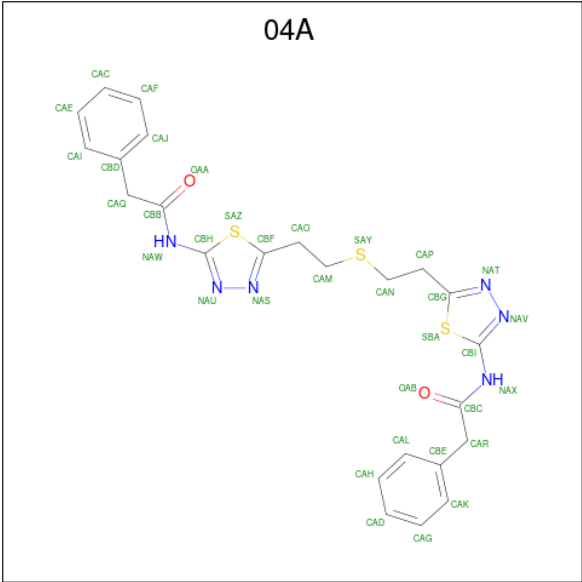
- Molecule 1 is a protein called Glutaminase kidney isoform, mitochondrial.

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

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) (CCD ID: 04A) (formula: C₂₄H₂₄N₆O₂S₃).

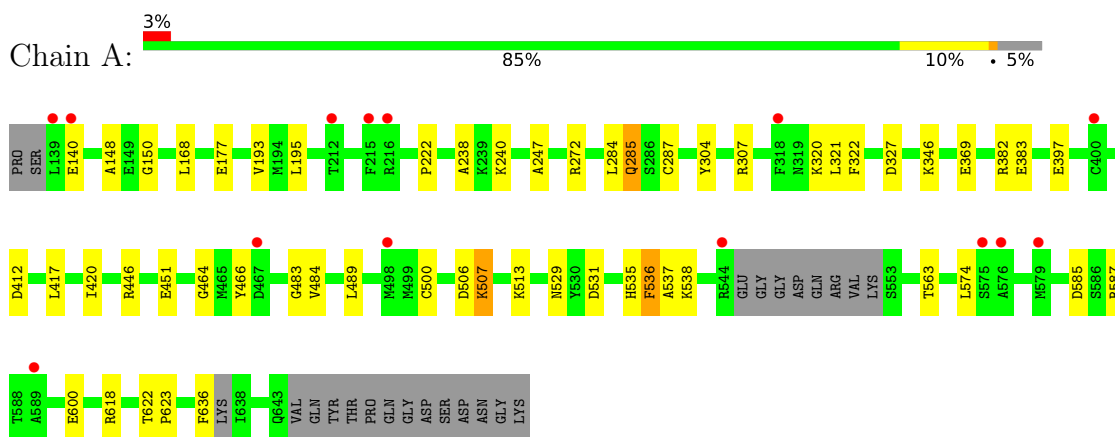


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	24	6	2	3		
2	B	1	Total	C	N	O	S	0	0
			35	24	6	2	3		
2	F	1	Total	C	N	O	S	0	0
			35	24	6	2	3		

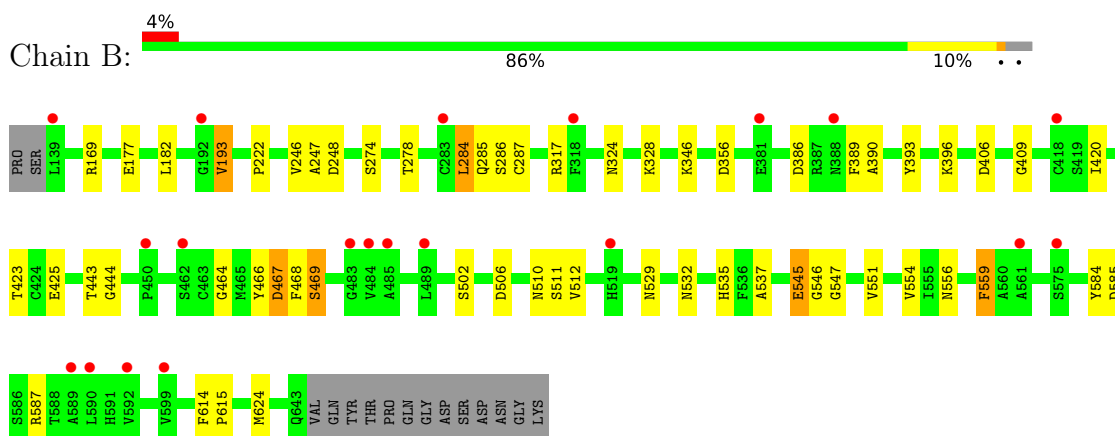
3 Residue-property plots [i](#)

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.

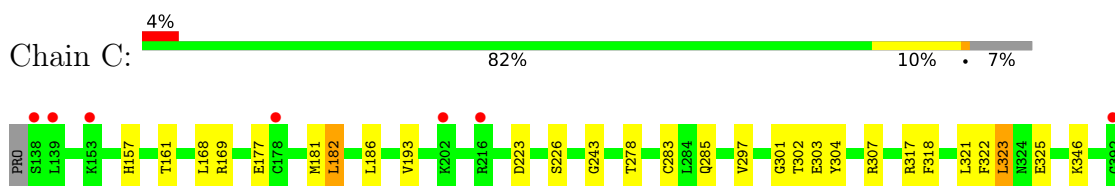
- Molecule 1: Glutaminase kidney isoform, mitochondrial

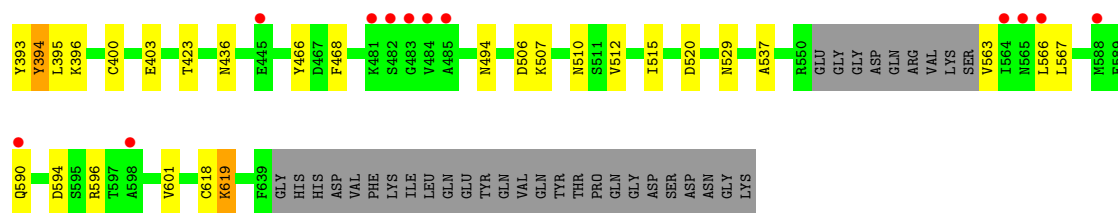


- Molecule 1: Glutaminase kidney isoform, mitochondrial

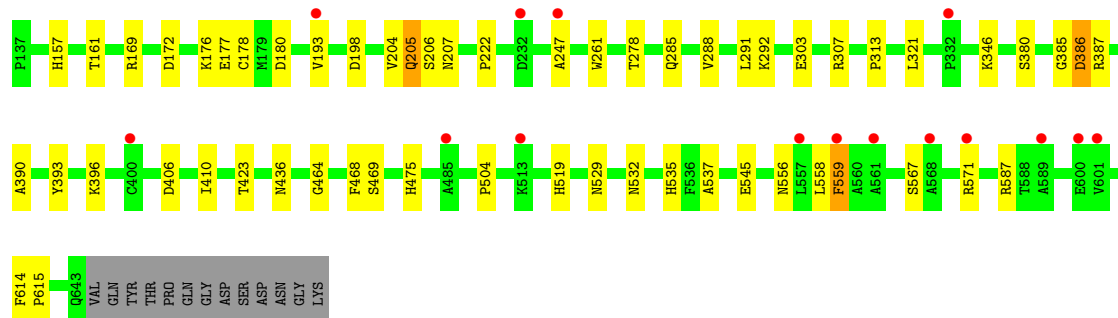
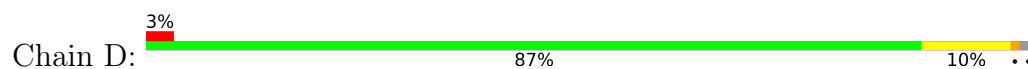


- Molecule 1: Glutaminase kidney isoform, mitochondrial

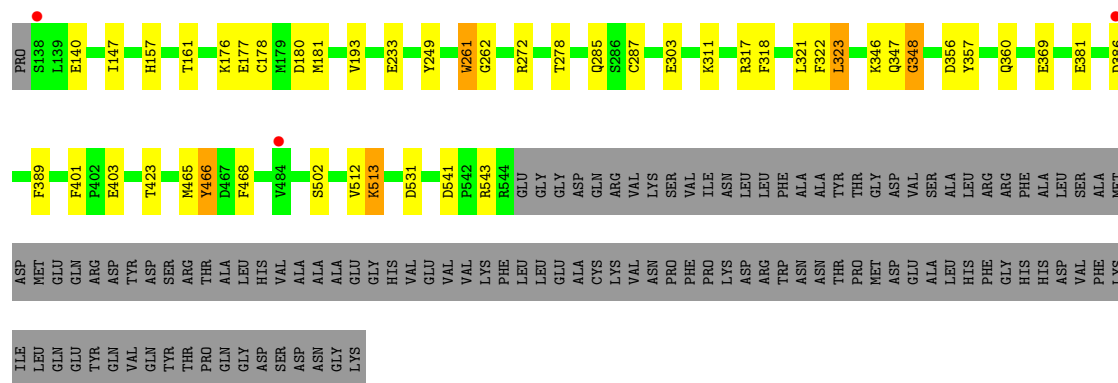




- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Molecule 1: Glutaminase kidney isoform, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 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) 99.9 (49.64-3.60)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.57Å)	Xtriage
Refinement program	PHENIX dev_2733	Depositor
R, R_{free}	0.274 , 0.313 0.275 , 0.311	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)	0.30 , 129.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

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

5.1 Standard geometry

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	0.11	0/3981	0.33	0/5377
1	B	0.13	0/4053	0.34	0/5474
1	C	0.13	0/3873	0.36	0/5232
1	D	0.12	0/4067	0.33	0/5493
1	F	0.13	0/3246	0.34	0/4382
All	All	0.12	0/19220	0.34	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

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	29	0
1	D	3977	0	3934	27	0
1	F	3176	0	3161	26	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	122	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 (122) 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:C:393:TYR:O	1:C:394:TYR:C	2.56	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: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: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:506:ASP:O	1:A:507:LYS:C	2.60	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:D:204:VAL:HG23	1:D:205:GLN:N	2.33	0.44
1:D:291:LEU:O	1:D:292:LYS:C	2.61	0.44
1:F:177:GLU:O	1:F:181:MET:N	2.51	0.44
1:F:465:MET:O	1:F:466:TYR:C	2.60	0.43
1:A:238:ALA:HB1	1:A:513:LYS:HG3	2.00	0.43
1:C:181:MET:O	1:C:182:LEU:C	2.62	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:B:467:ASP:C	1:B:469:SER:N	2.76	0.43
1:F:157:HIS:O	1:F:161:THR:OG1	2.30	0.43
1:A:177:GLU:OE1	1:A:177:GLU: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:THR:OG1	1:B:444:GLY:N	2.52	0.42
1:C:567:LEU:HD22	1:C:601:VAL:HG21	2.01	0.42
1:F:177:GLU:O	1:F:178:CYS:C	2.62	0.42
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
1:F:466:TYR:C	1:F:468:PHE:H	2.28	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:C:157:HIS:O	1:C:161:THR:OG1	2.19	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:D:468:PHE:O	1:D:469:SER:C	2.64	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:F:176:LYS:O	1:F:177:GLU:C	2.63	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:302:THR:O	1:C:303:GLU:C	2.63	0.40
1:C:395:LEU:HB3	1:C:400:CYS:HB2	2.03	0.40
1:D:204:VAL:O	1:D:205:GLN:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	5	30
1	B	503/520 (97%)	448 (89%)	44 (9%)	11 (2%)	5	30
1	C	480/520 (92%)	408 (85%)	61 (13%)	11 (2%)	5	30
1	D	505/520 (97%)	442 (88%)	52 (10%)	11 (2%)	5	30
1	F	405/520 (78%)	355 (88%)	45 (11%)	5 (1%)	10	41
All	All	2383/2600 (92%)	2084 (88%)	250 (10%)	49 (2%)	5	31

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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	414 (97%)	14 (3%)	33	58
1	B	435/448 (97%)	426 (98%)	9 (2%)	47	65
1	C	417/448 (93%)	410 (98%)	7 (2%)	53	69
1	D	437/448 (98%)	427 (98%)	10 (2%)	44	64
1	F	353/448 (79%)	343 (97%)	10 (3%)	38	60
All	All	2070/2240 (92%)	2020 (98%)	50 (2%)	43	63

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	LEU
1	A	195	LEU
1	A	240	LYS
1	A	417	LEU
1	A	446	ARG
1	A	451	GLU
1	A	489	LEU
1	A	500	CYS
1	A	531	ASP
1	A	535	HIS
1	A	536	PHE
1	A	563	THR
1	A	574	LEU
1	A	636	PHE
1	B	169	ARG
1	B	182	LEU
1	B	193	VAL
1	B	284	LEU
1	B	356	ASP
1	B	469	SER
1	B	545	GLU
1	B	559	PHE
1	B	624	MET

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Mol	Chain	Res	Type
1	C	168	LEU
1	C	169	ARG
1	C	186	LEU
1	C	283	CYS
1	C	325	GLU
1	C	515	ILE
1	C	520	ASP
1	D	169	ARG
1	D	172	ASP
1	D	198	ASP
1	D	261	TRP
1	D	321	LEU
1	D	380	SER
1	D	475	HIS
1	D	545	GLU
1	D	558	LEU
1	D	559	PHE
1	F	193	VAL
1	F	233	GLU
1	F	261	TRP
1	F	303	GLU
1	F	311	LYS
1	F	321	LEU
1	F	356	ASP
1	F	401	PHE
1	F	513	LYS
1	F	531	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	363	ASN
1	A	416	GLN
1	A	535	HIS
1	A	620	ASN
1	A	632	HIS
1	B	368	ASN
1	B	598	HIS
1	C	207	ASN
1	C	368	ASN
1	C	455	ASN

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Mol	Chain	Res	Type
1	C	516	HIS
1	C	519	HIS
1	D	360	GLN
1	D	368	ASN
1	D	388	ASN
1	D	510	ASN
1	D	535	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	701	-	38,38,38	1.64	9 (23%)	47,49,49	4.14	23 (48%)
2	04A	B	701	-	38,38,38	1.71	8 (21%)	47,49,49	4.44	20 (42%)
2	04A	F	701	-	38,38,38	1.66	8 (21%)	47,49,49	4.30	22 (46%)

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	A	701	-	-	12/24/24/24	0/4/4/4
2	04A	B	701	-	-	8/24/24/24	0/4/4/4
2	04A	F	701	-	-	12/24/24/24	0/4/4/4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	04A	CBF-NAS	4.42	1.35	1.29
2	F	701	04A	CBF-NAS	4.23	1.35	1.29
2	B	701	04A	CBG-NAT	4.18	1.35	1.29
2	F	701	04A	CBG-NAT	4.08	1.34	1.29
2	A	701	04A	CBG-NAT	4.05	1.34	1.29
2	A	701	04A	CBF-NAS	4.04	1.34	1.29
2	A	701	04A	CBB-NAW	3.38	1.43	1.37
2	B	701	04A	CBH-NAW	3.21	1.43	1.38
2	B	701	04A	CBB-NAW	3.16	1.42	1.37
2	F	701	04A	CBB-NAW	3.14	1.42	1.37
2	B	701	04A	CBI-NAX	3.06	1.42	1.38
2	A	701	04A	CBH-NAW	3.03	1.42	1.38
2	F	701	04A	CBH-NAW	3.00	1.42	1.38
2	B	701	04A	CBC-NAX	2.90	1.42	1.37
2	B	701	04A	CBH-NAU	2.85	1.35	1.31
2	F	701	04A	CBC-NAX	2.81	1.42	1.37
2	F	701	04A	CBI-NAX	2.79	1.42	1.38
2	A	701	04A	CBC-NAX	2.69	1.42	1.37
2	F	701	04A	CBH-NAU	2.67	1.35	1.31
2	A	701	04A	CBI-NAX	2.65	1.42	1.38
2	B	701	04A	CBI-NAV	2.64	1.35	1.31
2	F	701	04A	CBI-NAV	2.57	1.35	1.31
2	A	701	04A	CBH-NAU	2.53	1.35	1.31
2	A	701	04A	CBI-NAV	2.43	1.34	1.31
2	A	701	04A	NAV-NAT	-2.01	1.35	1.39

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	04A	CBH-SAZ-CBF	11.29	96.53	87.07
2	F	701	04A	CBH-SAZ-CBF	10.99	96.28	87.07
2	B	701	04A	CBI-SBA-CBG	10.77	96.09	87.07
2	A	701	04A	CBH-SAZ-CBF	10.57	95.92	87.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	04A	SBA-CBG-NAT	-10.53	105.31	113.98
2	B	701	04A	NAW-CBH-NAU	10.20	129.92	120.81
2	F	701	04A	SAZ-CBF-NAS	-10.14	105.64	113.98
2	F	701	04A	CBI-SBA-CBG	10.13	95.55	87.07
2	B	701	04A	SAZ-CBF-NAS	-10.09	105.67	113.98
2	A	701	04A	CBI-SBA-CBG	9.95	95.40	87.07
2	A	701	04A	SAZ-CBF-NAS	-9.87	105.86	113.98
2	F	701	04A	NAW-CBH-NAU	9.72	129.49	120.81
2	F	701	04A	SBA-CBG-NAT	-9.60	106.08	113.98
2	A	701	04A	SBA-CBG-NAT	-9.53	106.14	113.98
2	B	701	04A	SAZ-CBH-NAU	-8.33	105.22	114.52
2	A	701	04A	SAZ-CBH-NAU	-8.09	105.49	114.52
2	F	701	04A	SAZ-CBH-NAU	-8.07	105.51	114.52
2	A	701	04A	NAW-CBH-NAU	8.03	127.98	120.81
2	B	701	04A	NAX-CBI-NAV	7.81	127.79	120.81
2	B	701	04A	SBA-CBI-NAV	-7.66	105.96	114.52
2	F	701	04A	SBA-CBI-NAV	-7.36	106.30	114.52
2	A	701	04A	SBA-CBI-NAV	-7.29	106.38	114.52
2	A	701	04A	CAQ-CBB-NAW	7.18	123.15	114.40
2	F	701	04A	CAQ-CBB-NAW	7.01	122.95	114.40
2	B	701	04A	CAQ-CBB-NAW	6.91	122.83	114.40
2	F	701	04A	NAX-CBI-NAV	6.78	126.87	120.81
2	A	701	04A	NAX-CBI-NAV	6.22	126.37	120.81
2	F	701	04A	CAR-CBC-NAX	5.35	120.92	114.40
2	B	701	04A	CAP-CBG-SBA	4.07	127.94	120.63
2	B	701	04A	CAR-CBC-NAX	3.95	119.22	114.40
2	A	701	04A	CAR-CBC-NAX	3.87	119.12	114.40
2	A	701	04A	CAO-CBF-SAZ	3.79	127.43	120.63
2	B	701	04A	CBG-NAT-NAV	3.71	116.89	113.03
2	B	701	04A	CBH-NAU-NAS	3.62	116.63	112.02
2	A	701	04A	CBH-NAU-NAS	3.62	116.62	112.02
2	F	701	04A	CAP-CBG-SBA	3.56	127.02	120.63
2	A	701	04A	CAP-CBG-SBA	3.44	126.81	120.63
2	B	701	04A	CAO-CBF-NAS	3.42	128.51	123.57
2	F	701	04A	CBH-NAU-NAS	3.40	116.34	112.02
2	F	701	04A	CAO-CBF-SAZ	3.28	126.51	120.63
2	F	701	04A	CBF-NAS-NAU	3.09	116.24	113.03
2	A	701	04A	CBI-NAV-NAT	3.05	115.90	112.02
2	F	701	04A	CBG-NAT-NAV	3.04	116.19	113.03
2	A	701	04A	CBG-NAT-NAV	3.04	116.18	113.03
2	F	701	04A	CBI-NAV-NAT	3.03	115.88	112.02
2	A	701	04A	CBF-NAS-NAU	2.97	116.11	113.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	701	04A	CAO-CBF-NAS	2.96	127.85	123.57
2	B	701	04A	CBI-NAV-NAT	2.94	115.75	112.02
2	B	701	04A	CAO-CBF-SAZ	2.89	125.81	120.63
2	B	701	04A	CBF-NAS-NAU	2.81	115.95	113.03
2	B	701	04A	CAN-SAY-CAM	2.66	110.24	101.87
2	A	701	04A	SBA-CBI-NAX	2.64	127.25	123.72
2	F	701	04A	CAN-SAY-CAM	2.62	110.12	101.87
2	A	701	04A	OAA-CBB-NAW	-2.51	117.69	122.44
2	F	701	04A	OAA-CBB-NAW	-2.48	117.74	122.44
2	A	701	04A	CAP-CBG-NAT	2.41	127.05	123.57
2	F	701	04A	CBC-NAX-CBI	-2.35	119.67	123.69
2	F	701	04A	SBA-CBI-NAX	2.32	126.83	123.72
2	F	701	04A	CAP-CBG-NAT	2.30	126.90	123.57
2	A	701	04A	CBC-NAX-CBI	-2.21	119.92	123.69
2	B	701	04A	CAP-CBG-NAT	2.20	126.75	123.57
2	A	701	04A	CAN-SAY-CAM	2.18	108.72	101.87
2	A	701	04A	CAO-CBF-NAS	2.17	126.71	123.57
2	A	701	04A	SAZ-CBH-NAW	2.10	126.53	123.72
2	B	701	04A	OAA-CBB-NAW	-2.07	118.51	122.44

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	04A	SAY-CAM-CAO-CBF
2	A	701	04A	SAY-CAN-CAP-CBG
2	A	701	04A	CAM-CAO-CBF-NAS
2	A	701	04A	OAA-CBB-NAW-CBH
2	A	701	04A	CAQ-CBB-NAW-CBH
2	A	701	04A	NAU-CBH-NAW-CBB
2	A	701	04A	SAZ-CBH-NAW-CBB
2	A	701	04A	NAV-CBI-NAX-CBC
2	A	701	04A	SBA-CBI-NAX-CBC
2	B	701	04A	SAY-CAM-CAO-CBF
2	B	701	04A	SAY-CAN-CAP-CBG
2	B	701	04A	OAA-CBB-NAW-CBH
2	B	701	04A	CAQ-CBB-NAW-CBH
2	B	701	04A	NAU-CBH-NAW-CBB
2	B	701	04A	SAZ-CBH-NAW-CBB
2	B	701	04A	NAV-CBI-NAX-CBC
2	B	701	04A	SBA-CBI-NAX-CBC
2	F	701	04A	SAY-CAM-CAO-CBF

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Mol	Chain	Res	Type	Atoms
2	F	701	04A	OAA-CBB-NAW-CBH
2	F	701	04A	CAQ-CBB-NAW-CBH
2	F	701	04A	NAU-CBH-NAW-CBB
2	F	701	04A	SAZ-CBH-NAW-CBB
2	F	701	04A	NAV-CBI-NAX-CBC
2	F	701	04A	SBA-CBI-NAX-CBC
2	A	701	04A	CAN-CAP-CBG-SBA
2	F	701	04A	CBE-CAR-CBC-OAB
2	F	701	04A	CBC-CAR-CBE-CAL
2	A	701	04A	CAM-CAO-CBF-SAZ
2	F	701	04A	CBC-CAR-CBE-CAK
2	F	701	04A	CBE-CAR-CBC-NAX
2	F	701	04A	CAP-CAN-SAY-CAM
2	A	701	04A	CAN-CAP-CBG-NAT

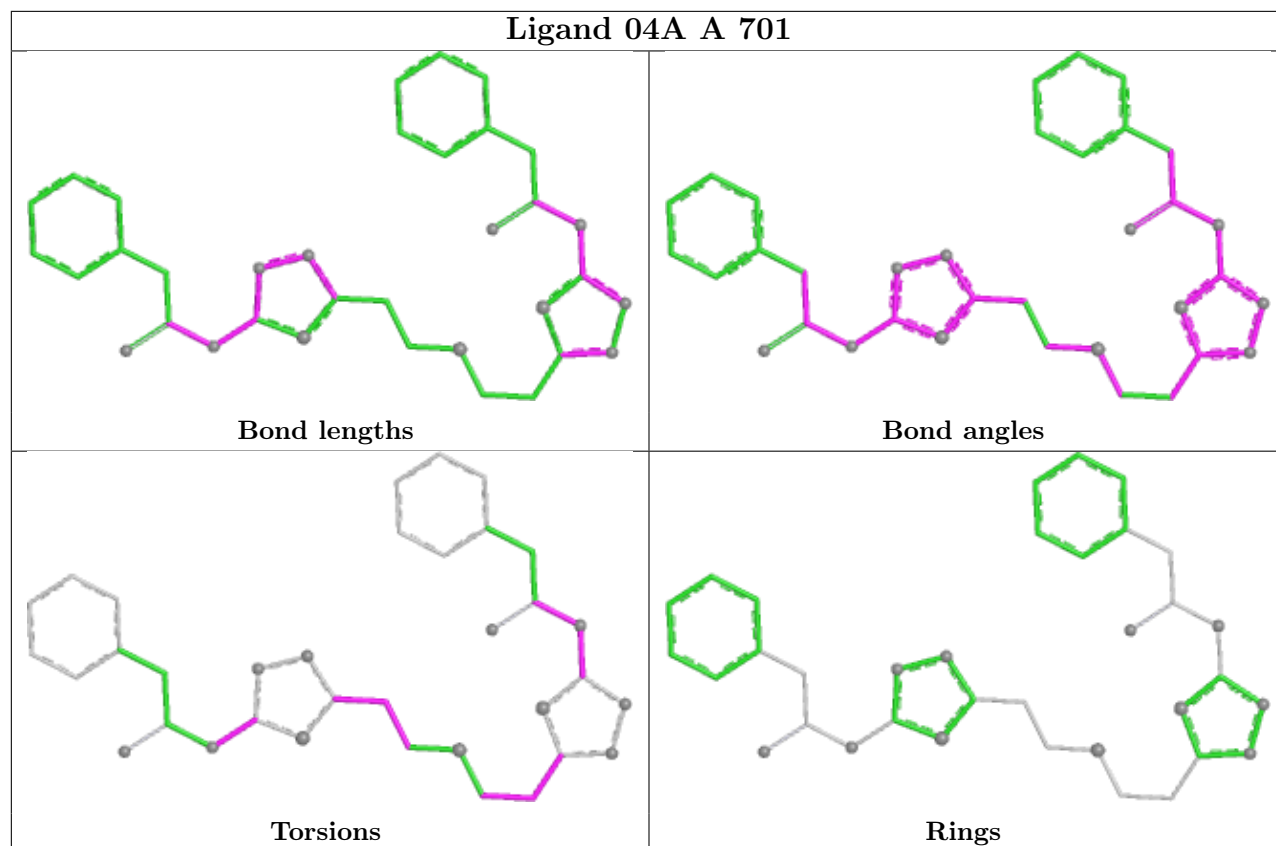
There are no ring outliers.

1 monomer is involved in 1 short contact:

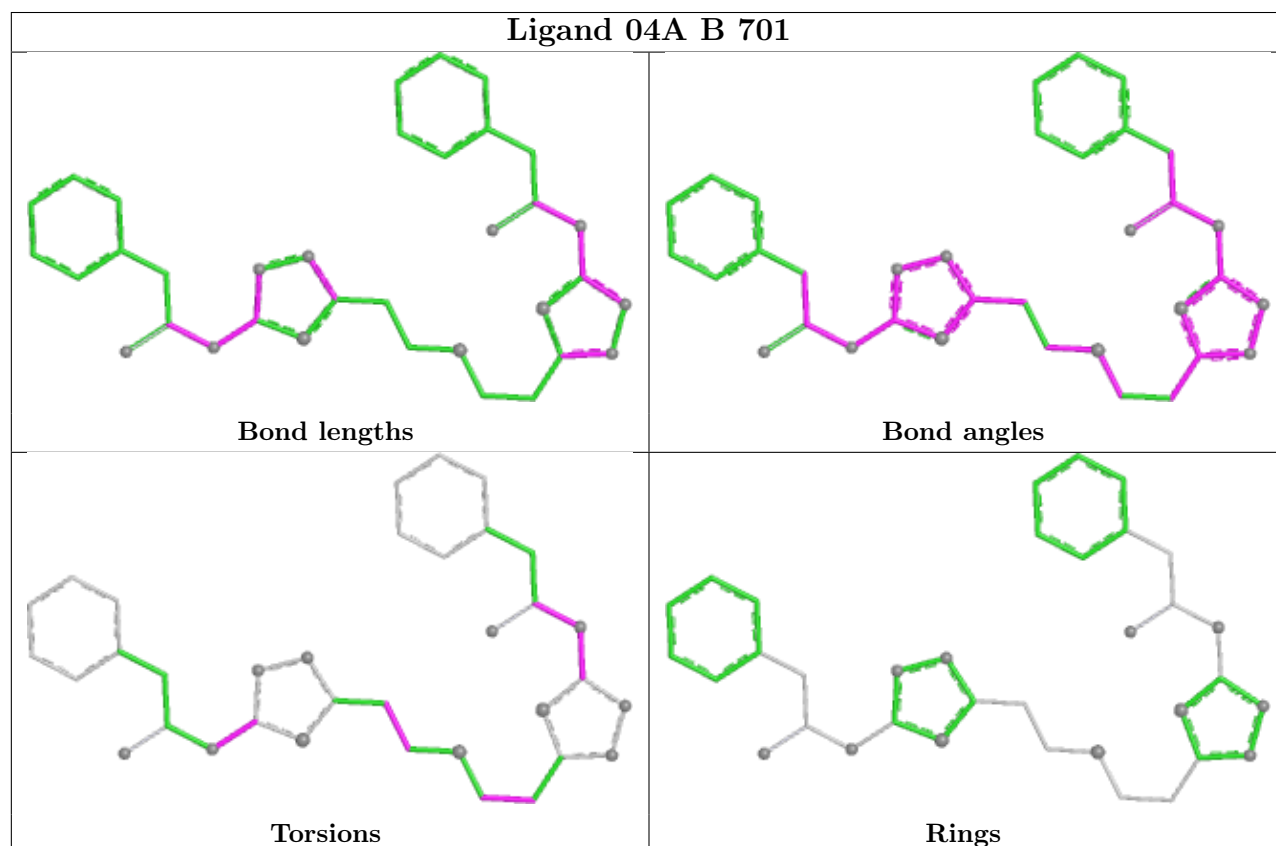
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	04A	1	0

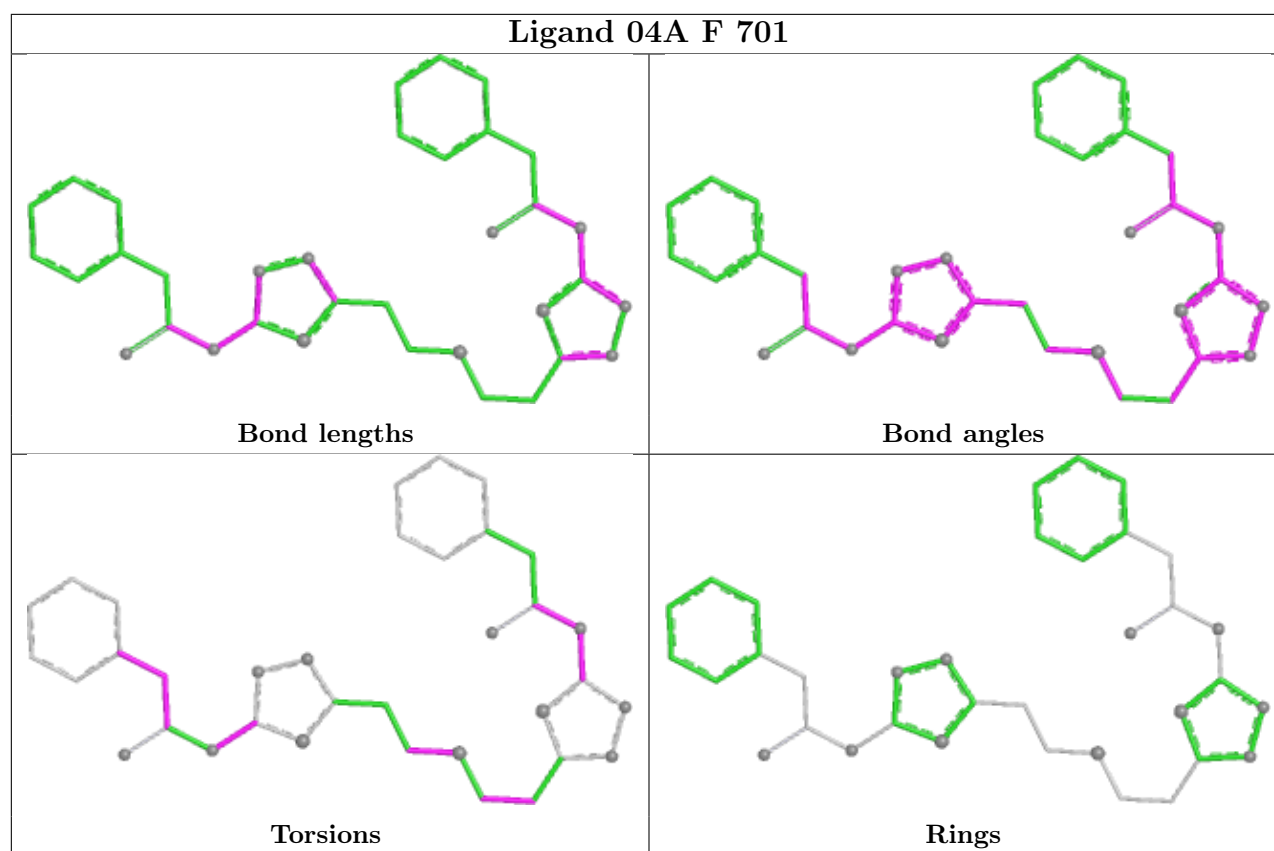
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	496/520 (95%)	0.36	14 (2%)	55	31	83, 162, 254, 284	0
1	B	505/520 (97%)	0.30	20 (3%)	42	24	61, 118, 258, 301	2 (0%)
1	C	484/520 (93%)	0.46	19 (3%)	43	24	55, 113, 277, 307	1 (0%)
1	D	507/520 (97%)	0.48	15 (2%)	52	30	57, 117, 266, 321	2 (0%)
1	F	407/520 (78%)	-0.02	3 (0%)	84	61	37, 97, 143, 170	0
All	All	2399/2600 (92%)	0.33	71 (2%)	52	30	37, 120, 259, 321	5 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	589	ALA	5.2
1	C	590	GLN	4.8
1	D	559	PHE	4.6
1	A	212	THR	4.4
1	B	318	PHE	4.2
1	C	483	GLY	3.7
1	C	566	LEU	3.6
1	A	139	LEU	3.4
1	D	400	CYS	3.2
1	B	388	ASN	3.2
1	B	599	VAL	3.1
1	C	484	VAL	3.0
1	C	598	ALA	3.0
1	D	193	VAL	2.9
1	B	590	LEU	2.9
1	A	589	ALA	2.9
1	A	498	MET	2.9
1	D	332	PRO	2.8
1	B	381	GLU	2.8
1	B	450	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	485	ALA	2.8
1	A	216	ARG	2.7
1	A	400	CYS	2.7
1	A	318	PHE	2.7
1	D	557	LEU	2.7
1	C	139	LEU	2.7
1	A	575	SER	2.7
1	D	561	ALA	2.6
1	B	418	CYS	2.5
1	C	178	CYS	2.5
1	D	485	ALA	2.5
1	C	588	MET	2.4
1	A	467	ASP	2.4
1	C	202	LYS	2.4
1	D	601	VAL	2.4
1	A	544	ARG	2.4
1	C	392	GLY	2.3
1	B	575	SER	2.3
1	C	138	SER	2.3
1	F	138	SER	2.3
1	D	513	LYS	2.3
1	D	589	ALA	2.3
1	C	565	ASN	2.3
1	D	600	GLU	2.3
1	B	283	CYS	2.2
1	B	139	LEU	2.2
1	B	561	ALA	2.2
1	D	247	ALA	2.2
1	B	462	SER	2.2
1	D	571	ARG	2.2
1	A	579	MET	2.2
1	F	386	ASP	2.1
1	F	484	VAL	2.1
1	A	215	PHE	2.1
1	B	519	HIS	2.1
1	C	153	LYS	2.1
1	C	481	LYS	2.1
1	C	216	ARG	2.1
1	D	568	ALA	2.1
1	B	483	GLY	2.1
1	A	576	ALA	2.1
1	C	445	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	564	ILE	2.1
1	C	485	ALA	2.1
1	B	489	LEU	2.1
1	C	482	SER	2.0
1	B	484	VAL	2.0
1	B	592	VAL	2.0
1	B	192	GLY	2.0
1	A	140	GLU	2.0
1	D	232	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

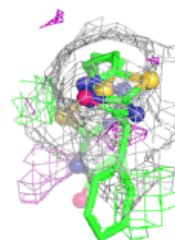
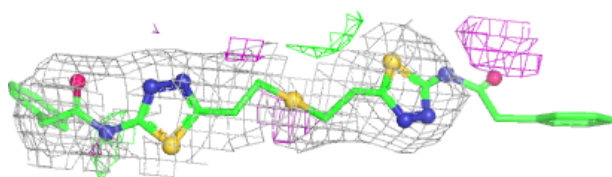
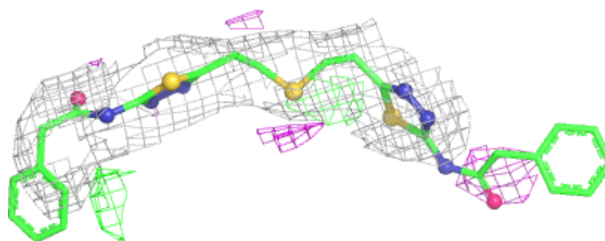
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	04A	A	701	35/35	0.88	0.17	59,118,192,198	0
2	04A	B	701	35/35	0.92	0.14	24,127,195,200	0
2	04A	F	701	35/35	0.94	0.13	68,94,131,144	35

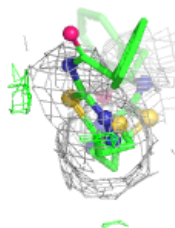
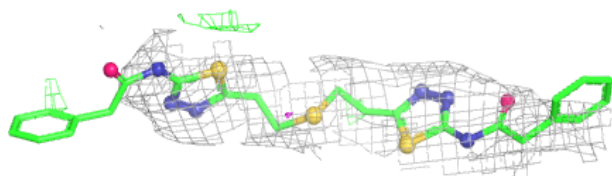
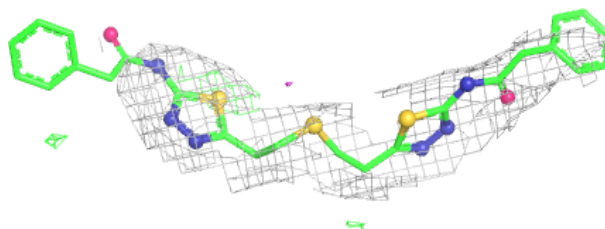
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

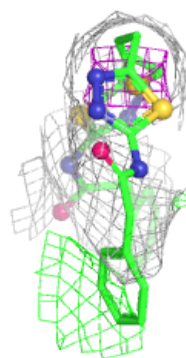
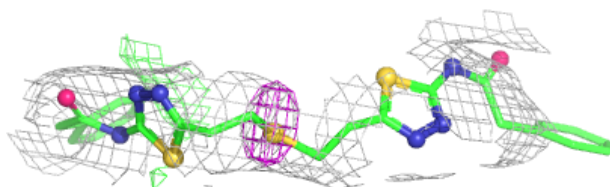
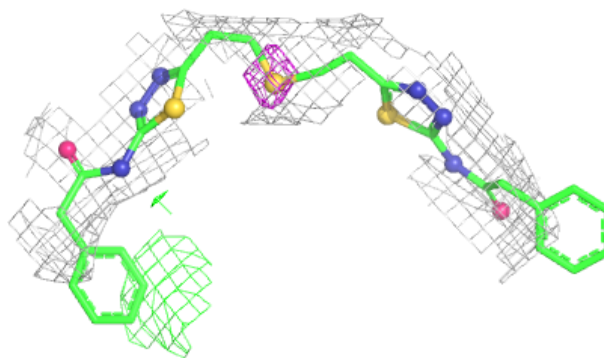
**Electron density around 04A B 701:**

$2mF_o-DF_c$ (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.