



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:37 AM UTC

PDB ID : 4ZOM / pdb_00004zom
Title : RORgamma in complex with inverse agonist 4j.
Authors : Marcotte, D.J.
Deposited on : 2015-05-06
Resolution : 2.27 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

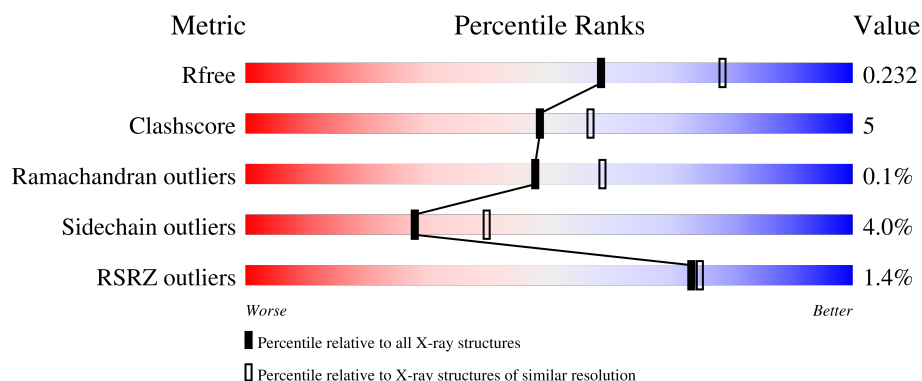
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	225	4% 49% 46% ..
1	B	225	48% 43% 8% .
1	C	225	48% 45% ..
1	D	225	% 54% 35% 7% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7255 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.

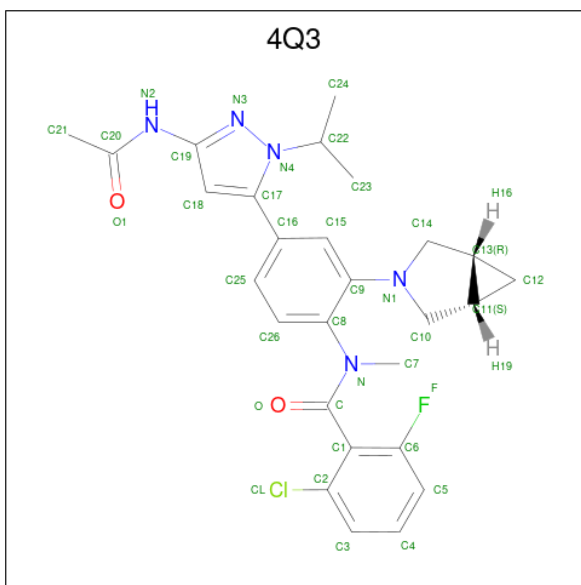
- Molecule 1 is a protein called Nuclear receptor ROR-gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	1	0
			1820	1150	328	328	14			
1	B	222	Total	C	N	O	S	0	0	0
			1786	1132	320	320	14			
1	C	219	Total	C	N	O	S	0	0	0
			1745	1111	308	312	14			
1	D	215	Total	C	N	O	S	0	0	0
			1712	1086	303	309	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	GLY	-	expression tag	UNP P51449
A	264	SER	-	expression tag	UNP P51449
B	263	GLY	-	expression tag	UNP P51449
B	264	SER	-	expression tag	UNP P51449
C	263	GLY	-	expression tag	UNP P51449
C	264	SER	-	expression tag	UNP P51449
D	263	GLY	-	expression tag	UNP P51449
D	264	SER	-	expression tag	UNP P51449

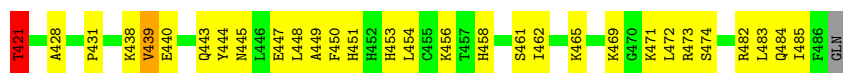
- Molecule 2 is N-{4-[3-(acetylamino)-1-(propan-2-yl)-1H-pyrazol-5-yl]-2-[(1R,5S)-3-azabicyclo[3.1.0]hex-3-yl]phenyl}-2-chloro-6-fluoro-N-methylbenzamide (CCD ID: 4Q3) (formula: C₂₇H₂₉ClFN₅O₂).



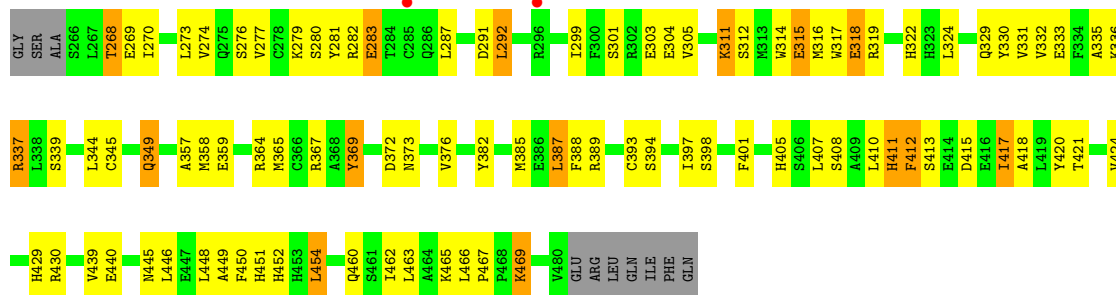
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 36	C 27	Cl 1	F 1	N 5	O 2	0	0
2	B	1	Total 36	C 27	Cl 1	F 1	N 5	O 2	0	0
2	C	1	Total 36	C 27	Cl 1	F 1	N 5	O 2	0	0
2	D	1	Total 36	C 27	Cl 1	F 1	N 5	O 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	37	Total	O	0	0
			37	37		



• Molecule 1: Nuclear receptor ROR-gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	99.42Å 99.42Å 129.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.79 – 2.27 19.79 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.79-2.27) 99.8 (19.79-2.27)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.28Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.200 , 0.240 0.198 , 0.232	Depositor DCC
R_{free} test set	3397 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.339 for -h,-k,l 0.117 for h,-h-k,-l 0.105 for -k,-h,-l	Xtriage
Reported twinning fraction	0.536 for H, K, L 0.464 for -h,-k,l	Depositor
Outliers	0 of 65951 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7255	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: 4Q3

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	2.33	88/1856 (4.7%)	1.61	17/2496 (0.7%)
1	B	2.41	95/1821 (5.2%)	1.61	19/2454 (0.8%)
1	C	2.45	109/1780 (6.1%)	1.61	16/2400 (0.7%)
1	D	2.44	86/1746 (4.9%)	1.62	16/2352 (0.7%)
All	All	2.41	378/7203 (5.2%)	1.61	68/9702 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (378) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	TRP	N-CA	-12.76	1.31	1.46
1	C	440	GLU	CA-C	-12.74	1.36	1.52
1	A	335	ALA	C-O	11.05	1.37	1.24
1	B	335	ALA	C-O	10.85	1.36	1.24
1	D	376	VAL	C-O	-10.72	1.13	1.24
1	A	399	SER	CA-C	10.42	1.66	1.52
1	C	329	GLN	N-CA	-10.37	1.33	1.46
1	C	461	SER	N-CA	-10.24	1.32	1.46
1	B	399	SER	N-CA	10.24	1.59	1.46
1	D	412	PHE	N-CA	-10.12	1.32	1.46
1	D	336	LYS	C-O	-9.98	1.11	1.24
1	D	467	PRO	CA-C	9.82	1.61	1.52
1	C	272	HIS	N-CA	-9.71	1.34	1.46
1	A	418	ALA	CA-C	-9.55	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	336	LYS	C-O	-9.40	1.12	1.24
1	D	332	VAL	CA-CB	-9.37	1.42	1.54
1	D	382	TYR	CA-C	9.33	1.64	1.52
1	B	280	SER	C-O	-9.30	1.13	1.24
1	A	440	GLU	CA-C	-9.27	1.40	1.52
1	D	274	VAL	C-O	9.27	1.34	1.24
1	A	353	LEU	N-CA	9.26	1.57	1.46
1	C	421	THR	N-CA	-9.25	1.34	1.46
1	D	277	VAL	N-CA	-9.23	1.35	1.46
1	C	350	ILE	CA-CB	9.21	1.65	1.54
1	B	401	PHE	CA-C	9.11	1.64	1.52
1	A	329	GLN	C-O	-9.08	1.13	1.24
1	B	440	GLU	CA-C	-9.04	1.41	1.52
1	D	319	ARG	N-CA	-8.87	1.35	1.46
1	B	377	PHE	C-O	-8.86	1.13	1.23
1	B	311	LYS	CA-C	-8.82	1.41	1.53
1	D	317	TRP	N-CA	-8.79	1.35	1.46
1	D	276	SER	CA-CB	-8.75	1.39	1.53
1	A	311	LYS	CA-C	-8.74	1.41	1.53
1	A	276	SER	CA-CB	-8.64	1.39	1.53
1	D	367	ARG	CA-C	-8.51	1.40	1.52
1	B	313	MET	C-O	8.50	1.34	1.24
1	B	272	HIS	N-CA	-8.40	1.36	1.46
1	B	356	GLY	C-O	8.32	1.35	1.23
1	D	424	VAL	N-CA	-8.32	1.36	1.46
1	B	363	VAL	CA-CB	8.24	1.64	1.54
1	B	418	ALA	CA-C	-8.24	1.42	1.52
1	C	445	ASN	CA-C	-8.24	1.42	1.52
1	D	460	GLN	C-O	-8.19	1.13	1.24
1	D	312	SER	CA-C	8.18	1.63	1.52
1	D	440	GLU	CA-C	-8.18	1.42	1.52
1	B	448	LEU	N-CA	8.15	1.56	1.46
1	A	274	VAL	C-O	8.12	1.33	1.24
1	B	394	SER	CA-C	8.11	1.64	1.52
1	B	447	GLU	N-CA	8.09	1.56	1.46
1	C	418	ALA	CA-C	-8.07	1.42	1.52
1	C	335	ALA	N-CA	-8.06	1.36	1.46
1	A	322	HIS	C-O	-8.01	1.14	1.24
1	D	335	ALA	C-O	7.98	1.33	1.24
1	B	325	THR	C-O	-7.96	1.14	1.24
1	C	360	VAL	N-CA	7.95	1.55	1.46
1	D	330	TYR	C-O	7.93	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	427	ASN	CA-C	7.92	1.61	1.52
1	C	318	GLU	CA-C	7.92	1.63	1.52
1	B	338	LEU	CA-C	-7.89	1.43	1.52
1	D	324	LEU	CA-C	-7.88	1.42	1.52
1	C	416	GLU	C-O	-7.88	1.15	1.24
1	B	316	MET	C-O	-7.88	1.15	1.24
1	B	446	LEU	C-O	7.77	1.33	1.24
1	C	280	SER	C-O	-7.77	1.15	1.24
1	B	350	ILE	CA-CB	7.75	1.63	1.54
1	A	412	PHE	N-CA	-7.73	1.36	1.46
1	A	277	VAL	N-CA	-7.73	1.37	1.46
1	A	312	SER	N-CA	-7.72	1.35	1.45
1	B	375	THR	N-CA	-7.72	1.35	1.45
1	C	444	TYR	CA-C	-7.70	1.43	1.52
1	A	464	ALA	CA-C	7.65	1.63	1.52
1	B	363	VAL	N-CA	7.54	1.55	1.46
1	B	442	LEU	N-CA	7.54	1.55	1.46
1	C	401	PHE	CA-C	7.54	1.62	1.52
1	A	413	SER	CA-C	-7.49	1.43	1.53
1	D	312	SER	N-CA	-7.47	1.36	1.46
1	C	344	LEU	CA-C	-7.47	1.43	1.53
1	D	420	TYR	C-O	-7.43	1.15	1.24
1	A	298	ASN	CA-C	7.41	1.62	1.52
1	A	322	HIS	CA-C	7.41	1.62	1.52
1	A	420	TYR	C-O	-7.36	1.15	1.24
1	C	404	SER	C-O	7.35	1.32	1.24
1	D	282	ARG	N-CA	-7.32	1.37	1.46
1	A	344	LEU	CA-C	-7.32	1.43	1.53
1	B	449	ALA	CA-C	-7.30	1.43	1.52
1	B	277	VAL	CA-C	-7.29	1.43	1.52
1	B	454	LEU	N-CA	7.26	1.55	1.46
1	B	344	LEU	CA-C	-7.19	1.43	1.53
1	A	430	ARG	CA-C	7.18	1.62	1.53
1	A	293	LEU	CA-C	7.18	1.62	1.52
1	B	410	LEU	CA-C	7.18	1.62	1.52
1	D	424	VAL	C-O	7.15	1.32	1.24
1	D	332	VAL	CA-C	7.14	1.61	1.52
1	A	315	GLU	CA-C	7.13	1.62	1.52
1	B	368	ALA	CA-CB	7.13	1.65	1.53
1	A	284	THR	C-O	-7.12	1.14	1.24
1	C	484	GLN	N-CA	-7.12	1.37	1.46
1	D	439	VAL	C-O	-7.12	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	313	MET	N-CA	-7.10	1.37	1.46
1	C	369	TYR	N-CA	-7.10	1.37	1.45
1	D	376	VAL	CA-C	-7.07	1.44	1.52
1	D	408	SER	C-O	-7.05	1.15	1.24
1	D	449	ALA	C-O	-7.04	1.15	1.24
1	A	294	ARG	N-CA	-7.03	1.37	1.46
1	B	443	GLN	N-CA	7.02	1.54	1.46
1	D	304	GLU	C-O	-7.01	1.15	1.24
1	C	465	LYS	C-O	-7.01	1.14	1.24
1	D	301	SER	N-CA	7.01	1.55	1.45
1	B	280	SER	CA-C	7.00	1.62	1.52
1	C	458	HIS	N-CA	7.00	1.57	1.46
1	C	363	VAL	N-CA	6.99	1.54	1.46
1	D	387	LEU	CA-C	6.98	1.62	1.52
1	A	337	ARG	CZ-NH1	6.95	1.42	1.32
1	D	311	LYS	CA-C	-6.95	1.43	1.53
1	B	369	TYR	N-CA	-6.93	1.37	1.45
1	B	304	GLU	C-O	-6.92	1.16	1.24
1	A	450	PHE	C-O	6.90	1.32	1.24
1	D	269	GLU	CA-C	6.90	1.62	1.52
1	C	281	TYR	N-CA	-6.88	1.38	1.46
1	A	353	LEU	CA-CB	-6.88	1.42	1.53
1	C	354	LYS	CA-C	-6.88	1.44	1.52
1	C	395	GLU	CA-C	-6.86	1.44	1.52
1	C	381	LYS	CA-C	-6.85	1.44	1.52
1	B	336	LYS	C-O	-6.84	1.15	1.24
1	B	445	ASN	CA-C	-6.83	1.43	1.52
1	C	313	MET	C-O	6.82	1.32	1.24
1	C	410	LEU	CA-C	6.78	1.62	1.52
1	D	463	LEU	C-O	-6.75	1.16	1.24
1	C	289	LEU	C-O	6.75	1.31	1.24
1	D	418	ALA	CA-C	-6.73	1.44	1.52
1	A	485	ILE	C-O	-6.70	1.16	1.24
1	C	280	SER	CA-C	6.70	1.61	1.52
1	D	279	LYS	C-O	6.70	1.31	1.24
1	A	358	MET	CA-CB	6.68	1.64	1.53
1	D	415	ASP	CB-CG	6.66	1.68	1.52
1	B	402	ASP	C-O	-6.64	1.15	1.24
1	B	467	PRO	CA-C	6.64	1.58	1.52
1	D	274	VAL	CA-CB	-6.63	1.47	1.54
1	A	279	LYS	C-O	6.63	1.31	1.24
1	B	441	GLN	CA-C	-6.62	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	451	HIS	C-O	6.62	1.31	1.24
1	C	448	LEU	C-O	6.58	1.31	1.24
1	A	318	GLU	C-O	-6.58	1.16	1.24
1	B	332	VAL	C-O	-6.55	1.16	1.24
1	C	276	SER	CA-C	6.54	1.61	1.52
1	D	283	GLU	N-CA	-6.53	1.37	1.46
1	C	449	ALA	CA-C	-6.53	1.44	1.52
1	D	460	GLN	CA-CB	6.53	1.65	1.53
1	B	393	CYS	CA-C	6.52	1.61	1.52
1	A	367	ARG	CA-C	-6.51	1.43	1.52
1	B	308	TYR	C-O	-6.51	1.15	1.24
1	C	443	GLN	N-CA	6.51	1.54	1.46
1	C	368	ALA	CA-CB	6.49	1.64	1.53
1	C	350	ILE	CA-C	-6.49	1.44	1.52
1	D	322	HIS	CA-C	6.48	1.61	1.52
1	C	368	ALA	N-CA	-6.46	1.37	1.46
1	C	274	VAL	C-O	6.45	1.31	1.24
1	C	314	TRP	C-O	-6.43	1.16	1.24
1	A	449	ALA	N-CA	-6.41	1.38	1.46
1	A	305	VAL	CA-C	6.41	1.60	1.52
1	C	377	PHE	C-O	-6.39	1.16	1.23
1	B	379	GLU	C-O	6.38	1.31	1.23
1	B	391	LEU	CA-C	-6.38	1.43	1.52
1	B	443	GLN	CA-C	-6.37	1.44	1.52
1	C	308	TYR	N-CA	6.37	1.54	1.46
1	D	315	GLU	N-CA	-6.37	1.38	1.46
1	B	456	LYS	C-O	-6.36	1.16	1.24
1	C	418	ALA	C-O	6.35	1.31	1.24
1	B	353	LEU	CA-C	-6.32	1.44	1.52
1	B	361	VAL	CA-CB	6.31	1.62	1.54
1	D	312	SER	C-O	-6.30	1.16	1.23
1	C	310	ARG	C-O	6.28	1.32	1.24
1	A	376	VAL	C-O	-6.27	1.17	1.24
1	A	451	HIS	CA-C	-6.26	1.44	1.52
1	C	485	ILE	C-O	6.26	1.31	1.24
1	D	318	GLU	C-O	-6.24	1.17	1.24
1	A	408	SER	C-O	-6.23	1.16	1.24
1	B	422	ALA	CA-C	-6.22	1.44	1.52
1	D	349	GLN	N-CA	6.21	1.53	1.46
1	C	375	THR	N-CA	-6.21	1.37	1.45
1	D	329	GLN	C-O	-6.20	1.16	1.24
1	B	358	MET	SD-CE	-6.18	1.64	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	451	HIS	CA-C	-6.18	1.45	1.52
1	C	276	SER	C-O	6.18	1.31	1.24
1	C	327	ALA	CA-CB	-6.16	1.43	1.53
1	B	415	ASP	CB-CG	6.16	1.67	1.52
1	B	334	PHE	CA-CB	-6.16	1.43	1.53
1	B	418	ALA	CA-CB	6.14	1.62	1.53
1	A	376	VAL	CA-C	-6.13	1.45	1.52
1	D	393	CYS	CA-CB	6.12	1.61	1.53
1	B	369	TYR	CA-C	6.10	1.60	1.52
1	D	299	ILE	N-CA	-6.10	1.39	1.46
1	B	309	GLN	N-CA	6.09	1.54	1.46
1	B	460	GLN	C-O	-6.08	1.16	1.24
1	D	322	HIS	N-CA	-6.08	1.39	1.46
1	B	382	TYR	C-O	-6.06	1.16	1.24
1	A	312	SER	CA-C	6.05	1.60	1.52
1	C	456	LYS	C-O	-6.04	1.17	1.24
1	C	389	ARG	CZ-NH2	6.03	1.41	1.33
1	C	331	VAL	CA-CB	-6.01	1.47	1.54
1	C	353	LEU	N-CA	6.00	1.53	1.46
1	A	463	LEU	C-O	-5.98	1.17	1.24
1	C	456	LYS	N-CA	5.98	1.53	1.46
1	C	363	VAL	C-O	-5.96	1.17	1.24
1	B	386	GLU	C-O	-5.94	1.16	1.24
1	D	339	SER	C-O	-5.93	1.16	1.23
1	A	315	GLU	N-CA	-5.91	1.38	1.46
1	C	400	ILE	N-CA	5.89	1.53	1.46
1	C	471	LYS	CA-C	-5.89	1.45	1.52
1	C	420	TYR	N-CA	5.88	1.53	1.46
1	D	281	TYR	CA-C	5.88	1.60	1.52
1	C	421	THR	CB-CG2	-5.88	1.33	1.52
1	C	308	TYR	CA-C	-5.87	1.45	1.52
1	A	355	ALA	CA-C	5.87	1.60	1.52
1	D	430	ARG	CA-C	5.86	1.59	1.52
1	D	339	SER	CA-C	-5.86	1.45	1.52
1	A	331	VAL	CA-C	-5.85	1.44	1.52
1	B	371	ALA	CA-C	5.84	1.60	1.52
1	A	418	ALA	CA-CB	5.82	1.62	1.53
1	B	416	GLU	CD-OE1	5.82	1.36	1.25
1	B	303	GLU	C-O	-5.82	1.17	1.24
1	C	269	GLU	CA-C	5.81	1.60	1.52
1	D	344	LEU	CA-C	-5.80	1.45	1.52
1	C	376	VAL	CA-C	-5.78	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	465	LYS	C-O	-5.78	1.16	1.24
1	A	269	GLU	CA-C	5.77	1.60	1.52
1	A	353	LEU	CA-C	-5.77	1.45	1.52
1	B	360	VAL	N-CA	5.76	1.53	1.46
1	B	321	ALA	N-CA	-5.75	1.38	1.46
1	D	333	GLU	CA-C	-5.73	1.45	1.52
1	A	329	GLN	C-N	-5.72	1.26	1.33
1	A	353	LEU	C-O	5.71	1.30	1.24
1	D	319	ARG	CA-C	5.69	1.60	1.52
1	A	381	LYS	C-O	-5.69	1.16	1.24
1	C	450	PHE	CG-CD1	-5.68	1.26	1.38
1	A	381	LYS	CA-C	-5.67	1.45	1.52
1	C	325	THR	C-O	-5.66	1.17	1.24
1	B	357	ALA	C-O	5.66	1.30	1.24
1	B	375	THR	CA-C	5.65	1.59	1.52
1	D	357	ALA	C-O	5.65	1.30	1.24
1	B	414	GLU	C-O	5.64	1.30	1.24
1	A	429	HIS	CA-CB	5.62	1.63	1.53
1	B	350	ILE	CA-C	-5.62	1.46	1.52
1	C	315	GLU	CD-OE2	5.62	1.36	1.25
1	B	457	THR	CA-C	5.62	1.61	1.52
1	D	446	LEU	CA-CB	5.61	1.62	1.53
1	A	305	VAL	N-CA	-5.61	1.40	1.46
1	B	428	ALA	CA-CB	-5.60	1.44	1.53
1	D	280	SER	C-O	-5.59	1.17	1.24
1	A	282	ARG	C-O	-5.59	1.17	1.24
1	C	311	LYS	C-O	-5.59	1.16	1.23
1	D	417	ILE	CA-C	-5.59	1.46	1.52
1	D	305	VAL	CA-C	5.58	1.59	1.52
1	B	411	HIS	C-O	-5.58	1.16	1.23
1	C	281	TYR	CB-CG	-5.57	1.39	1.51
1	A	369	TYR	CA-CB	-5.55	1.44	1.53
1	D	358	MET	CA-CB	5.55	1.62	1.53
1	D	373	ASN	CA-C	5.55	1.59	1.52
1	C	402	ASP	CA-CB	5.54	1.62	1.53
1	D	359	GLU	CA-C	5.54	1.60	1.52
1	B	464	ALA	CA-C	5.53	1.60	1.52
1	C	453	HIS	C-O	5.53	1.31	1.24
1	B	466	LEU	CA-C	-5.53	1.46	1.53
1	D	369	TYR	CA-CB	-5.52	1.45	1.53
1	A	333	GLU	C-O	-5.52	1.17	1.24
1	C	360	VAL	C-O	5.51	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	371	ALA	N-CA	-5.51	1.39	1.46
1	C	431	PRO	N-CA	5.50	1.53	1.47
1	D	287	LEU	CA-C	5.50	1.59	1.52
1	A	316	MET	C-O	-5.49	1.17	1.24
1	A	352	LEU	N-CA	5.49	1.52	1.46
1	C	407	LEU	CA-C	-5.47	1.45	1.52
1	B	360	VAL	C-O	5.45	1.30	1.24
1	C	302	ARG	N-CA	5.45	1.53	1.46
1	A	280	SER	N-CA	5.45	1.53	1.46
1	C	319	ARG	CA-C	5.45	1.59	1.52
1	C	323	HIS	N-CA	5.45	1.52	1.46
1	A	310	ARG	CA-C	-5.43	1.45	1.52
1	C	278	CYS	CA-CB	-5.43	1.44	1.53
1	B	298	ASN	CA-C	5.42	1.59	1.52
1	C	447	GLU	C-N	-5.42	1.27	1.33
1	C	414	GLU	CA-C	-5.41	1.45	1.52
1	B	311	LYS	C-O	-5.40	1.16	1.23
1	B	448	LEU	CA-C	-5.39	1.45	1.52
1	C	291	ASP	C-O	-5.39	1.18	1.24
1	A	383	GLY	N-CA	5.38	1.53	1.45
1	C	439	VAL	C-O	5.38	1.30	1.24
1	B	333	GLU	CA-CB	5.38	1.61	1.53
1	B	354	LYS	CA-C	-5.37	1.45	1.52
1	B	387	LEU	CA-CB	-5.37	1.44	1.53
1	A	452	HIS	CA-CB	-5.36	1.44	1.53
1	C	284	THR	C-O	-5.35	1.16	1.24
1	D	292	LEU	N-CA	-5.35	1.40	1.46
1	D	279	LYS	N-CA	-5.35	1.40	1.46
1	A	282	ARG	N-CA	-5.34	1.39	1.46
1	B	337	ARG	CZ-NH1	5.33	1.40	1.32
1	C	406	SER	C-O	-5.32	1.17	1.24
1	D	364	ARG	C-O	-5.32	1.17	1.24
1	B	322	HIS	CA-C	5.31	1.59	1.52
1	D	450	PHE	C-O	5.30	1.30	1.24
1	A	274	VAL	CA-CB	-5.30	1.48	1.54
1	A	433	LEU	CA-C	-5.30	1.46	1.52
1	B	480	VAL	C-O	-5.30	1.17	1.24
1	C	403	PHE	C-O	5.30	1.30	1.24
1	C	307	GLY	C-N	-5.29	1.26	1.33
1	C	483	LEU	N-CA	-5.28	1.39	1.46
1	A	331	VAL	C-O	-5.26	1.17	1.24
1	B	435	GLU	C-O	5.26	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	268	THR	CA-CB	5.26	1.61	1.53
1	B	274	VAL	CA-CB	-5.26	1.48	1.54
1	B	436	LYS	C-O	5.26	1.30	1.24
1	C	358	MET	SD-CE	-5.26	1.66	1.79
1	B	426	ILE	CA-CB	-5.25	1.47	1.54
1	B	431	PRO	CA-CB	-5.25	1.46	1.53
1	B	307	GLY	CA-C	5.25	1.59	1.51
1	A	280	SER	C-O	-5.25	1.18	1.24
1	A	472	LEU	CA-C	5.25	1.59	1.52
1	A	349	GLN	N-CA	5.24	1.52	1.46
1	C	473	ARG	CA-C	-5.24	1.46	1.52
1	B	420	TYR	N-CA	5.24	1.52	1.46
1	C	337	ARG	CZ-NH1	5.24	1.40	1.32
1	A	402	ASP	N-CA	5.24	1.52	1.46
1	C	391	LEU	C-O	-5.23	1.17	1.24
1	D	452	HIS	CA-CB	-5.23	1.45	1.53
1	C	279	LYS	N-CA	-5.22	1.40	1.46
1	D	331	VAL	CA-C	-5.20	1.46	1.52
1	C	324	LEU	CA-CB	-5.19	1.45	1.53
1	C	447	GLU	N-CA	5.19	1.52	1.46
1	C	451	HIS	C-O	-5.19	1.18	1.24
1	A	278	CYS	CA-CB	-5.18	1.45	1.53
1	C	277	VAL	N-CA	-5.18	1.40	1.46
1	A	424	VAL	CA-C	5.18	1.59	1.52
1	A	357	ALA	C-O	5.17	1.30	1.24
1	C	416	GLU	CD-OE1	5.17	1.35	1.25
1	D	385	MET	N-CA	-5.17	1.40	1.46
1	A	435	GLU	CD-OE1	5.16	1.35	1.25
1	A	445	ASN	CA-CB	-5.16	1.45	1.53
1	D	299	ILE	C-N	5.16	1.40	1.33
1	D	421	THR	N-CA	-5.16	1.40	1.46
1	B	454	LEU	CA-C	-5.15	1.45	1.52
1	C	420	TYR	C-O	-5.15	1.18	1.24
1	D	319	ARG	C-O	-5.15	1.18	1.24
1	D	430	ARG	NE-CZ	-5.14	1.27	1.33
1	A	391	LEU	CA-C	-5.13	1.45	1.52
1	A	467	PRO	C-O	-5.13	1.18	1.24
1	A	388	PHE	CA-CB	5.12	1.60	1.53
1	C	316	MET	C-O	-5.11	1.18	1.24
1	C	280	SER	CA-CB	-5.11	1.45	1.53
1	A	350	ILE	CA-C	-5.11	1.46	1.52
1	A	417	ILE	CA-C	-5.11	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	404	SER	CA-C	5.11	1.59	1.52
1	C	444	TYR	N-CA	5.10	1.52	1.46
1	D	465	LYS	C-O	-5.09	1.17	1.23
1	B	403	PHE	C-O	5.09	1.30	1.24
1	A	365	MET	N-CA	5.08	1.52	1.46
1	D	445	ASN	CA-CB	-5.08	1.45	1.53
1	A	368	ALA	CA-C	5.08	1.59	1.52
1	D	411	HIS	N-CA	-5.08	1.39	1.46
1	B	353	LEU	N-CA	5.07	1.52	1.46
1	C	311	LYS	CA-C	-5.06	1.46	1.53
1	C	325	THR	CA-CB	5.06	1.61	1.53
1	D	413	SER	CA-C	-5.06	1.46	1.53
1	C	271	GLU	C-O	5.05	1.30	1.24
1	C	472	LEU	N-CA	-5.05	1.40	1.46
1	C	401	PHE	CA-CB	5.05	1.61	1.53
1	C	272	HIS	CA-CB	5.04	1.61	1.53
1	C	277	VAL	C-O	-5.04	1.18	1.24
1	C	360	VAL	CA-CB	-5.04	1.48	1.54
1	B	450	PHE	CG-CD1	-5.04	1.28	1.38
1	A	332	VAL	CA-CB	-5.03	1.47	1.54
1	D	407	LEU	CA-C	-5.03	1.46	1.52
1	C	386	GLU	CD-OE1	5.03	1.34	1.25
1	A	319	ARG	CD-NE	-5.02	1.39	1.46
1	C	272	HIS	CA-C	5.02	1.59	1.52
1	A	269	GLU	N-CA	-5.02	1.39	1.46
1	A	334	PHE	CA-C	-5.02	1.46	1.52
1	D	429	HIS	CA-CB	5.01	1.62	1.53
1	B	404	SER	C-O	5.01	1.29	1.24

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	412	PHE	CB-CA-C	-8.01	99.95	109.80
1	D	454	LEU	N-CA-C	7.79	119.77	111.28
1	C	397	ILE	CB-CA-C	-7.64	102.03	112.04
1	D	469	LYS	CA-C-N	7.63	128.62	119.99
1	D	469	LYS	C-N-CA	7.63	128.62	119.99
1	B	407	LEU	N-CA-C	7.58	119.54	111.28
1	B	358	MET	CG-SD-CE	7.44	117.27	100.90
1	B	277	VAL	N-CA-C	-7.41	103.24	110.72
1	B	334	PHE	N-CA-C	-7.00	103.64	111.28
1	C	469	LYS	N-CA-C	-6.90	100.09	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	266	SER	N-CA-C	6.74	119.22	110.53
1	B	408	SER	CA-C-N	6.72	129.83	120.29
1	B	408	SER	C-N-CA	6.72	129.83	120.29
1	B	455	CYS	CB-CA-C	-6.71	99.45	110.85
1	B	461	SER	N-CA-C	6.62	120.81	112.87
1	C	445	ASN	N-CA-C	6.50	118.37	111.28
1	A	266	SER	N-CA-C	6.49	119.53	109.60
1	A	268	THR	N-CA-C	-6.25	104.52	111.71
1	B	455	CYS	N-CA-C	6.24	118.16	111.36
1	A	380	GLY	N-CA-C	-6.20	106.86	114.92
1	C	421	THR	N-CA-C	-6.20	104.07	111.69
1	A	381	LYS	CA-C-O	-6.18	114.54	121.40
1	A	374	ARG	N-CA-C	6.14	119.65	111.30
1	B	278	CYS	N-CA-C	6.09	118.71	111.71
1	A	454	LEU	N-CA-C	6.07	118.67	111.33
1	C	289	LEU	O-C-N	6.05	128.38	122.09
1	B	299	ILE	CB-CA-C	6.04	119.15	110.33
1	C	271	GLU	O-C-N	6.01	129.66	122.27
1	A	372	ASP	N-CA-C	-5.96	104.69	111.07
1	C	352	LEU	N-CA-C	5.84	117.64	111.28
1	B	289	LEU	N-CA-C	5.82	117.30	111.07
1	A	281	TYR	N-CA-C	-5.81	104.86	111.14
1	B	316	MET	CA-C-O	-5.78	114.75	120.82
1	C	440	GLU	O-C-N	5.76	128.08	122.09
1	D	273	LEU	CB-CA-C	5.66	120.47	110.85
1	A	365	MET	N-CA-C	5.58	118.90	111.75
1	C	328	ILE	N-CA-C	-5.54	105.10	110.42
1	D	365	MET	CB-CA-C	-5.47	100.51	110.63
1	B	271	GLU	O-C-N	5.45	128.37	122.15
1	C	428	ALA	N-CA-C	5.45	119.55	113.01
1	C	317	TRP	N-CA-C	5.44	117.64	111.11
1	D	389	ARG	N-CA-C	5.42	117.19	111.28
1	D	466	LEU	CA-C-N	-5.39	114.83	120.38
1	D	466	LEU	C-N-CA	-5.39	114.83	120.38
1	D	276	SER	N-CA-C	5.38	116.83	111.07
1	B	454	LEU	N-CA-C	5.38	117.84	111.33
1	D	337	ARG	N-CA-C	5.37	119.46	113.01
1	A	389	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	C	291	ASP	N-CA-C	5.34	116.78	111.07
1	A	453	HIS	N-CA-C	5.32	117.07	111.28
1	B	449	ALA	N-CA-C	5.28	116.84	111.14
1	A	393	CYS	CA-C-N	5.27	127.60	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	CYS	C-N-CA	5.27	127.60	120.38
1	B	410	LEU	N-CA-C	5.24	119.16	112.87
1	D	393	CYS	CA-C-N	5.21	127.58	120.54
1	D	393	CYS	C-N-CA	5.21	127.58	120.54
1	B	383	GLY	N-CA-C	-5.19	102.96	110.90
1	A	303	GLU	N-CA-C	5.17	117.00	111.36
1	A	361	VAL	N-CA-C	-5.17	105.46	110.42
1	C	361	VAL	CB-CA-C	-5.16	105.09	112.22
1	A	297	SER	N-CA-C	-5.08	105.92	111.82
1	A	317	TRP	N-CA-C	5.08	116.51	111.07
1	D	314	TRP	CA-C-N	5.08	127.35	120.44
1	D	314	TRP	C-N-CA	5.08	127.35	120.44
1	C	324	LEU	N-CA-CB	5.08	117.58	110.12
1	C	355	ALA	N-CA-C	5.03	116.76	111.28
1	D	299	ILE	N-CA-C	-5.02	102.27	108.89
1	D	382	TYR	N-CA-C	5.01	117.41	109.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	482	ARG	Peptide
1	A	483	LEU	Peptide

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	1820	0	1799	21	0
1	B	1786	0	1759	28	0
1	C	1745	0	1711	10	0
1	D	1712	0	1681	14	0
2	A	36	0	29	0	0
2	B	36	0	29	2	0
2	C	36	0	29	2	0
2	D	36	0	29	5	0
3	A	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	37	0	0	3	0
All	All	7255	0	7066	78	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 5.

All (78) 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:473:ARG:HG2	1:B:473:ARG:HH11	1.27	0.98
1:A:412:PHE:HZ	1:A:466:LEU:HD21	1.37	0.86
1:C:417:ILE:O	1:C:421:THR:HB	1.78	0.83
1:A:321:ALA:O	1:A:325:THR:HG23	1.84	0.77
1:B:358:MET:HE3	1:B:361:VAL:HB	1.70	0.71
1:A:412:PHE:CZ	1:A:466:LEU:HD21	2.26	0.70
2:D:501:4Q3:H15	2:D:501:4Q3:H26	1.73	0.70
1:B:473:ARG:HG2	1:B:473:ARG:NH1	1.95	0.69
1:B:285:CYS:O	1:B:286:GLN:HB3	1.92	0.68
1:A:362:LEU:HD21	1:A:475:LEU:HD23	1.76	0.67
1:D:369:TYR:OH	1:D:405:HIS:HD2	1.79	0.65
2:D:501:4Q3:H15	2:D:501:4Q3:C7	2.32	0.59
1:D:369:TYR:OH	1:D:405:HIS:CD2	2.58	0.57
1:C:347:ASN:O	1:C:351:VAL:HG23	2.06	0.56
1:C:454:LEU:HD21	1:C:462:ILE:HD11	1.88	0.55
1:A:410:LEU:HD23	1:A:412:PHE:CE1	2.41	0.55
1:B:473:ARG:HH11	1:B:473:ARG:CG	2.07	0.55
2:C:501:4Q3:H26	2:C:501:4Q3:H15	1.89	0.54
1:D:394:SER:O	1:D:398:SER:HB2	2.08	0.54
1:D:454:LEU:HD21	1:D:462:ILE:HD11	1.90	0.54
1:C:270:ILE:C	1:C:270:ILE:HD12	2.33	0.54
1:B:358:MET:HE3	1:B:361:VAL:CB	2.38	0.54
1:C:280:SER:O	1:C:281:TYR:C	2.50	0.53
1:A:359:GLU:HB3	1:A:472:LEU:HD21	1.90	0.53
1:D:283:GLU:OE1	1:D:337:ARG:NH1	2.40	0.53
1:D:311:LYS:HD3	1:D:315:GLU:HG3	1.90	0.53
1:C:323:HIS:HE1	1:C:379:GLU:OE2	1.92	0.52
1:A:412:PHE:CE1	1:A:462:ILE:HD12	2.45	0.52
1:A:412:PHE:CZ	1:A:466:LEU:CD2	2.93	0.51
1:A:308:TYR:OH	1:A:379:GLU:OE1	2.25	0.51
1:B:444:TYR:CZ	1:B:448:LEU:HD21	2.45	0.51
1:B:387:LEU:HD23	1:B:387:LEU:C	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:TYR:CE1	1:B:466:LEU:HD13	2.46	0.51
1:D:270:ILE:HG21	1:D:448:LEU:HD12	1.93	0.50
1:B:324:LEU:HD22	1:B:358:MET:HE1	1.94	0.50
1:B:358:MET:O	1:B:362:LEU:HG	2.12	0.50
1:B:400:ILE:HG21	2:B:501:4Q3:H16	1.94	0.49
1:A:282:ARG:NH2	1:D:318:GLU:OE2	2.45	0.49
1:B:347:ASN:O	1:B:351:VAL:HG23	2.12	0.49
1:A:393:CYS:O	1:A:397:ILE:HG12	2.12	0.48
1:B:376:VAL:O	1:B:382:TYR:HA	2.14	0.48
1:B:396:LEU:HD21	1:B:479:HIS:HD2	1.77	0.48
1:D:345:CYS:O	1:D:349:GLN:HG3	2.13	0.48
1:C:270:ILE:HD12	1:C:271:GLU:N	2.29	0.48
1:A:270:ILE:HD13	1:A:449:ALA:HA	1.95	0.47
1:B:387:LEU:HD23	1:B:387:LEU:O	2.13	0.47
1:D:401:PHE:HE1	2:D:501:4Q3:H17	1.79	0.47
1:A:266:SER:OG	1:A:267:LEU:N	2.47	0.47
1:B:473:ARG:NH2	3:B:601:HOH:O	2.29	0.46
1:A:412:PHE:HZ	1:A:466:LEU:CD2	2.16	0.46
1:B:273:LEU:O	1:B:274:VAL:C	2.56	0.46
1:B:364:ARG:NH1	3:B:604:HOH:O	2.46	0.46
1:A:323:HIS:HE1	1:A:379:GLU:OE2	1.99	0.46
1:B:336:LYS:O	1:B:342:MET:HE2	2.16	0.46
1:B:454:LEU:HD21	1:B:462:ILE:HD11	1.97	0.45
1:C:410:LEU:O	1:C:411:HIS:C	2.59	0.45
1:B:410:LEU:O	1:B:411:HIS:C	2.60	0.44
2:C:501:4Q3:H15	2:C:501:4Q3:C7	2.48	0.44
1:B:444:TYR:OH	1:B:448:LEU:HD21	2.18	0.44
1:D:291:ASP:O	1:D:292:LEU:C	2.57	0.44
1:B:401:PHE:HE1	2:B:501:4Q3:H17	1.84	0.43
1:D:388:PHE:HB2	1:D:397:ILE:HD13	2.01	0.43
1:A:285:CYS:O	1:A:287:LEU:N	2.49	0.43
2:D:501:4Q3:H26	2:D:501:4Q3:C14	2.46	0.42
1:B:479:HIS:CE1	1:B:483:LEU:HD11	2.54	0.42
1:D:410:LEU:O	1:D:411:HIS:C	2.61	0.42
1:A:332:VAL:HG22	1:A:353:LEU:HD22	2.01	0.42
1:B:308:TYR:OH	1:B:379:GLU:OE1	2.24	0.42
1:A:266:SER:O	1:A:270:ILE:HG23	2.20	0.42
1:B:453:HIS:HE1	3:B:605:HOH:O	2.03	0.42
1:A:314:TRP:HH2	1:A:487:GLN:HB2	1.86	0.41
1:C:482:ARG:HA	1:C:482:ARG:HD3	1.74	0.41
1:A:288:ARG:NH2	1:A:291:ASP:OD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:GLU:O	1:D:316:MET:C	2.61	0.41
1:B:458:HIS:HA	1:B:460:GLN:HE22	1.86	0.41
2:D:501:4Q3:C14	2:D:501:4Q3:N	2.84	0.41
1:C:278:CYS:HB3	1:C:415:ASP:OD1	2.21	0.41
1:A:306:THR:O	1:A:307:GLY:C	2.64	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	222/225 (99%)	215 (97%)	6 (3%)	1 (0%)	24	29
1	B	220/225 (98%)	213 (97%)	7 (3%)	0	100	100
1	C	217/225 (96%)	207 (95%)	10 (5%)	0	100	100
1	D	213/225 (95%)	204 (96%)	9 (4%)	0	100	100
All	All	872/900 (97%)	839 (96%)	32 (4%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	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	197/200 (98%)	191 (97%)	6 (3%)	36	51
1	B	191/200 (96%)	184 (96%)	7 (4%)	30	43
1	C	185/200 (92%)	175 (95%)	10 (5%)	20	27
1	D	183/200 (92%)	176 (96%)	7 (4%)	29	42
All	All	756/800 (94%)	726 (96%)	30 (4%)	28	40

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	271	GLU
1	A	303	GLU
1	A	336	LYS
1	A	412	PHE
1	A	476	CYS
1	A	481	GLU
1	B	298	ASN
1	B	303	GLU
1	B	328	ILE
1	B	329	GLN
1	B	412	PHE
1	B	473	ARG
1	B	482	ARG
1	C	268	THR
1	C	303	GLU
1	C	374	ARG
1	C	387	LEU
1	C	394	SER
1	C	412	PHE
1	C	421	THR
1	C	438	LYS
1	C	439	VAL
1	C	474	SER
1	D	268	THR
1	D	303	GLU
1	D	372	ASP
1	D	387	LEU
1	D	412	PHE
1	D	417	ILE
1	D	469	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	ASN
1	A	405	HIS
1	A	451	HIS
1	A	452	HIS
1	B	298	ASN
1	B	405	HIS
1	B	429	HIS
1	B	441	GLN
1	B	451	HIS
1	B	453	HIS
1	B	460	GLN
1	B	479	HIS
1	C	323	HIS
1	C	347	ASN
1	C	411	HIS
1	C	427	ASN
1	D	405	HIS
1	D	434	GLN
1	D	452	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	4Q3	D	501	-	40,40,40	2.25	15 (37%)	52,60,60	2.34	18 (34%)
2	4Q3	B	501	-	40,40,40	2.53	18 (45%)	52,60,60	2.77	21 (40%)
2	4Q3	C	501	-	40,40,40	2.53	14 (35%)	52,60,60	2.40	21 (40%)
2	4Q3	A	501	-	40,40,40	2.50	15 (37%)	52,60,60	2.09	15 (28%)

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	4Q3	D	501	-	-	5/28/41/41	0/5/5/5
2	4Q3	B	501	-	-	5/28/41/41	0/5/5/5
2	4Q3	C	501	-	-	10/28/41/41	0/5/5/5
2	4Q3	A	501	-	-	9/28/41/41	0/5/5/5

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	4Q3	C8-N	-7.10	1.35	1.44
2	C	501	4Q3	C17-N4	-6.29	1.28	1.36
2	B	501	4Q3	C1-C2	6.10	1.48	1.39
2	A	501	4Q3	C17-N4	-5.83	1.29	1.36
2	B	501	4Q3	C17-N4	-5.58	1.29	1.36
2	D	501	4Q3	C1-C6	5.57	1.48	1.39
2	A	501	4Q3	C1-C6	5.49	1.48	1.39
2	B	501	4Q3	C8-N	-5.47	1.37	1.44
2	B	501	4Q3	C8-C9	5.00	1.49	1.41
2	C	501	4Q3	C14-N1	4.92	1.54	1.46
2	C	501	4Q3	C1-C2	4.91	1.47	1.39
2	C	501	4Q3	C1-C6	4.77	1.47	1.39
2	D	501	4Q3	C18-C17	-4.62	1.30	1.38
2	D	501	4Q3	C17-N4	-4.55	1.31	1.36
2	D	501	4Q3	C14-C13	4.49	1.59	1.53
2	C	501	4Q3	C8-C9	4.46	1.48	1.41
2	B	501	4Q3	C14-N1	4.40	1.53	1.46
2	A	501	4Q3	C15-C16	-4.22	1.33	1.39
2	C	501	4Q3	C9-N1	-4.21	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	4Q3	C14-C13	4.07	1.58	1.53
2	C	501	4Q3	C25-C16	4.04	1.45	1.39
2	A	501	4Q3	C14-C13	3.83	1.58	1.53
2	D	501	4Q3	C9-N1	-3.53	1.33	1.41
2	D	501	4Q3	C8-C9	3.51	1.47	1.41
2	B	501	4Q3	C16-C17	-3.37	1.43	1.48
2	B	501	4Q3	C-N	-3.30	1.30	1.36
2	C	501	4Q3	C1-C	3.20	1.55	1.51
2	C	501	4Q3	F-C6	3.20	1.44	1.35
2	B	501	4Q3	O-C	3.17	1.28	1.22
2	B	501	4Q3	C26-C8	3.13	1.44	1.39
2	C	501	4Q3	C16-C17	-3.12	1.43	1.48
2	D	501	4Q3	C8-N	-3.08	1.40	1.44
2	B	501	4Q3	C9-N1	-3.05	1.34	1.41
2	A	501	4Q3	C-N	-3.05	1.30	1.36
2	D	501	4Q3	C1-C2	3.02	1.44	1.39
2	A	501	4Q3	C18-C17	-3.00	1.33	1.38
2	D	501	4Q3	C10-N1	2.96	1.51	1.46
2	A	501	4Q3	C21-C20	2.92	1.56	1.50
2	A	501	4Q3	C24-C22	-2.87	1.44	1.52
2	A	501	4Q3	C16-C17	2.81	1.52	1.48
2	B	501	4Q3	C12-C13	2.79	1.57	1.49
2	D	501	4Q3	C21-C20	2.79	1.56	1.50
2	D	501	4Q3	C1-C	2.65	1.54	1.51
2	B	501	4Q3	C20-N2	-2.55	1.31	1.37
2	A	501	4Q3	C18-C19	-2.53	1.36	1.40
2	D	501	4Q3	N4-N3	2.48	1.43	1.38
2	A	501	4Q3	C9-N1	-2.37	1.36	1.41
2	A	501	4Q3	C8-C9	2.37	1.45	1.41
2	D	501	4Q3	C22-N4	-2.36	1.43	1.48
2	A	501	4Q3	C10-N1	2.34	1.50	1.46
2	D	501	4Q3	C-N	-2.31	1.31	1.36
2	B	501	4Q3	C25-C16	2.30	1.42	1.39
2	C	501	4Q3	C8-N	-2.27	1.41	1.44
2	C	501	4Q3	C-N	-2.23	1.32	1.36
2	D	501	4Q3	C18-C19	-2.23	1.36	1.40
2	B	501	4Q3	C4-C3	-2.09	1.35	1.38
2	B	501	4Q3	C18-C17	-2.07	1.34	1.38
2	A	501	4Q3	C14-N1	2.03	1.49	1.46
2	B	501	4Q3	C2-CL	2.01	1.78	1.73
2	C	501	4Q3	O1-C20	2.01	1.27	1.23
2	B	501	4Q3	C19-N3	-2.01	1.31	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	4Q3	C10-C11	2.00	1.55	1.53

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	4Q3	C18-C17-N4	8.88	110.42	105.77
2	D	501	4Q3	C12-C13-C14	-8.14	102.91	116.13
2	B	501	4Q3	C9-C8-N	7.04	129.56	122.29
2	C	501	4Q3	C15-C9-N1	-6.56	113.03	122.59
2	A	501	4Q3	C1-C2-CL	-5.92	111.99	119.62
2	D	501	4Q3	C19-N3-N4	-5.81	99.11	103.78
2	C	501	4Q3	C18-C19-N3	-5.62	108.31	112.34
2	C	501	4Q3	C9-C8-N	5.10	127.56	122.29
2	C	501	4Q3	C12-C13-C14	-5.07	107.88	116.13
2	B	501	4Q3	C25-C16-C15	5.07	125.11	119.25
2	B	501	4Q3	C15-C9-N1	-4.95	115.38	122.59
2	A	501	4Q3	C19-N3-N4	-4.95	99.80	103.78
2	B	501	4Q3	C26-C25-C16	-4.47	116.03	120.80
2	A	501	4Q3	C24-C22-N4	-4.42	102.15	109.98
2	D	501	4Q3	C9-C8-N	4.28	126.71	122.29
2	C	501	4Q3	C23-C22-C24	4.27	124.05	112.46
2	B	501	4Q3	C24-C22-N4	-4.17	102.59	109.98
2	B	501	4Q3	C10-N1-C14	4.07	117.55	111.64
2	A	501	4Q3	O1-C20-C21	-4.04	114.86	122.05
2	B	501	4Q3	C17-N4-N3	-3.96	109.02	112.66
2	B	501	4Q3	C16-C17-N4	-3.95	119.91	124.15
2	D	501	4Q3	C15-C9-N1	-3.90	116.91	122.59
2	D	501	4Q3	C25-C16-C17	-3.88	113.31	120.67
2	D	501	4Q3	C24-C22-N4	-3.75	103.32	109.98
2	A	501	4Q3	C7-N-C	3.48	125.89	118.72
2	C	501	4Q3	C3-C2-C1	3.46	126.50	121.86
2	B	501	4Q3	C12-C13-C14	-3.35	110.68	116.13
2	C	501	4Q3	C4-C5-C6	3.33	123.66	118.49
2	D	501	4Q3	C1-C2-CL	-3.30	115.37	119.62
2	A	501	4Q3	C12-C13-C14	-3.23	110.88	116.13
2	A	501	4Q3	O1-C20-N2	3.22	126.97	121.90
2	C	501	4Q3	C26-C25-C16	-3.21	117.36	120.80
2	D	501	4Q3	C10-N1-C14	3.18	116.25	111.64
2	B	501	4Q3	O-C-C1	3.16	125.52	119.49
2	B	501	4Q3	C26-C8-N	-3.14	114.07	118.73
2	B	501	4Q3	C25-C16-C17	-3.10	114.81	120.67
2	D	501	4Q3	C25-C16-C15	3.08	122.81	119.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	4Q3	C18-C19-N2	3.04	137.11	129.35
2	B	501	4Q3	C18-C19-N2	3.04	137.10	129.35
2	B	501	4Q3	C18-C19-N3	-3.03	110.17	112.34
2	A	501	4Q3	C15-C9-N1	-2.96	118.27	122.59
2	C	501	4Q3	O-C-C1	2.96	125.15	119.49
2	B	501	4Q3	C12-C11-C13	2.92	63.49	59.53
2	B	501	4Q3	C4-C5-C6	2.91	123.01	118.49
2	D	501	4Q3	C7-N-C8	-2.90	112.67	116.74
2	B	501	4Q3	C7-N-C8	2.89	120.81	116.74
2	C	501	4Q3	F-C6-C1	2.84	123.12	118.15
2	A	501	4Q3	C3-C2-CL	2.83	124.00	118.42
2	C	501	4Q3	C8-C9-N1	2.80	124.93	119.91
2	C	501	4Q3	C18-C17-N4	2.80	107.24	105.77
2	C	501	4Q3	C25-C16-C15	2.78	122.46	119.25
2	A	501	4Q3	C16-C15-C9	2.77	123.99	118.69
2	D	501	4Q3	C23-C22-N4	-2.76	105.08	109.98
2	D	501	4Q3	C7-N-C	2.76	124.41	118.72
2	A	501	4Q3	C26-C25-C16	-2.75	117.86	120.80
2	A	501	4Q3	C8-C9-N1	2.59	124.55	119.91
2	D	501	4Q3	C18-C17-N4	2.57	107.12	105.77
2	D	501	4Q3	C26-C8-N	-2.53	114.97	118.73
2	C	501	4Q3	C1-C2-CL	-2.48	116.42	119.62
2	A	501	4Q3	C25-C16-C15	2.45	122.08	119.25
2	C	501	4Q3	C2-C1-C6	-2.41	112.88	116.72
2	C	501	4Q3	C10-N1-C14	2.41	115.13	111.64
2	D	501	4Q3	O1-C20-N2	2.37	125.63	121.90
2	D	501	4Q3	C12-C13-C11	2.34	62.70	59.53
2	B	501	4Q3	C8-C9-N1	2.31	124.06	119.91
2	C	501	4Q3	C5-C6-C1	-2.28	119.29	123.48
2	A	501	4Q3	C15-C9-C8	-2.20	116.69	120.06
2	D	501	4Q3	C6-C1-C	2.19	124.86	121.54
2	C	501	4Q3	C26-C8-N	-2.17	115.52	118.73
2	D	501	4Q3	C2-C1-C6	-2.08	113.41	116.72
2	A	501	4Q3	C6-C1-C	2.05	124.64	121.54
2	C	501	4Q3	C25-C26-C8	2.04	123.19	119.10
2	B	501	4Q3	C19-N3-N4	2.04	105.42	103.78
2	C	501	4Q3	C19-N3-N4	2.04	105.42	103.78
2	B	501	4Q3	C25-C26-C8	2.02	123.16	119.10

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	4Q3	C9-C8-N-C
2	C	501	4Q3	O-C-N-C8
2	C	501	4Q3	C9-C8-N-C7
2	B	501	4Q3	C25-C16-C17-C18
2	C	501	4Q3	C25-C16-C17-C18
2	B	501	4Q3	C15-C16-C17-C18
2	A	501	4Q3	C1-C-N-C8
2	D	501	4Q3	C25-C16-C17-C18
2	C	501	4Q3	C26-C8-N-C7
2	A	501	4Q3	C15-C16-C17-C18
2	C	501	4Q3	C15-C16-C17-C18
2	A	501	4Q3	C25-C16-C17-C18
2	D	501	4Q3	C15-C16-C17-C18
2	A	501	4Q3	O-C-N-C8
2	C	501	4Q3	C1-C-N-C8
2	A	501	4Q3	C9-C8-N-C7
2	B	501	4Q3	C15-C16-C17-N4
2	D	501	4Q3	O-C-N-C8
2	A	501	4Q3	C15-C16-C17-N4
2	B	501	4Q3	C25-C16-C17-N4
2	A	501	4Q3	C25-C16-C17-N4
2	A	501	4Q3	C9-C8-N-C
2	B	501	4Q3	C9-C8-N-C
2	D	501	4Q3	C9-C8-N-C
2	C	501	4Q3	C25-C16-C17-N4
2	D	501	4Q3	C15-C16-C17-N4
2	A	501	4Q3	C1-C-N-C7
2	C	501	4Q3	O-C-N-C7
2	C	501	4Q3	C15-C16-C17-N4

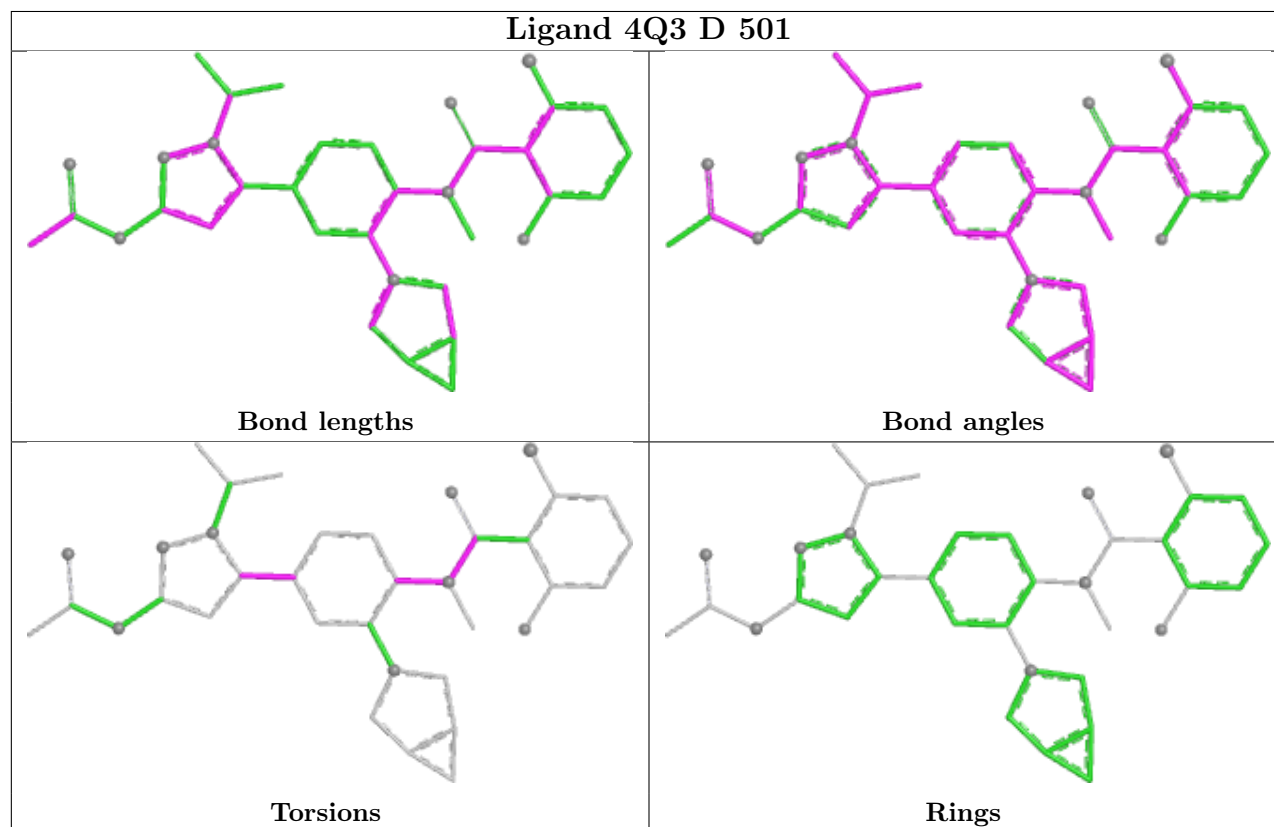
There are no ring outliers.

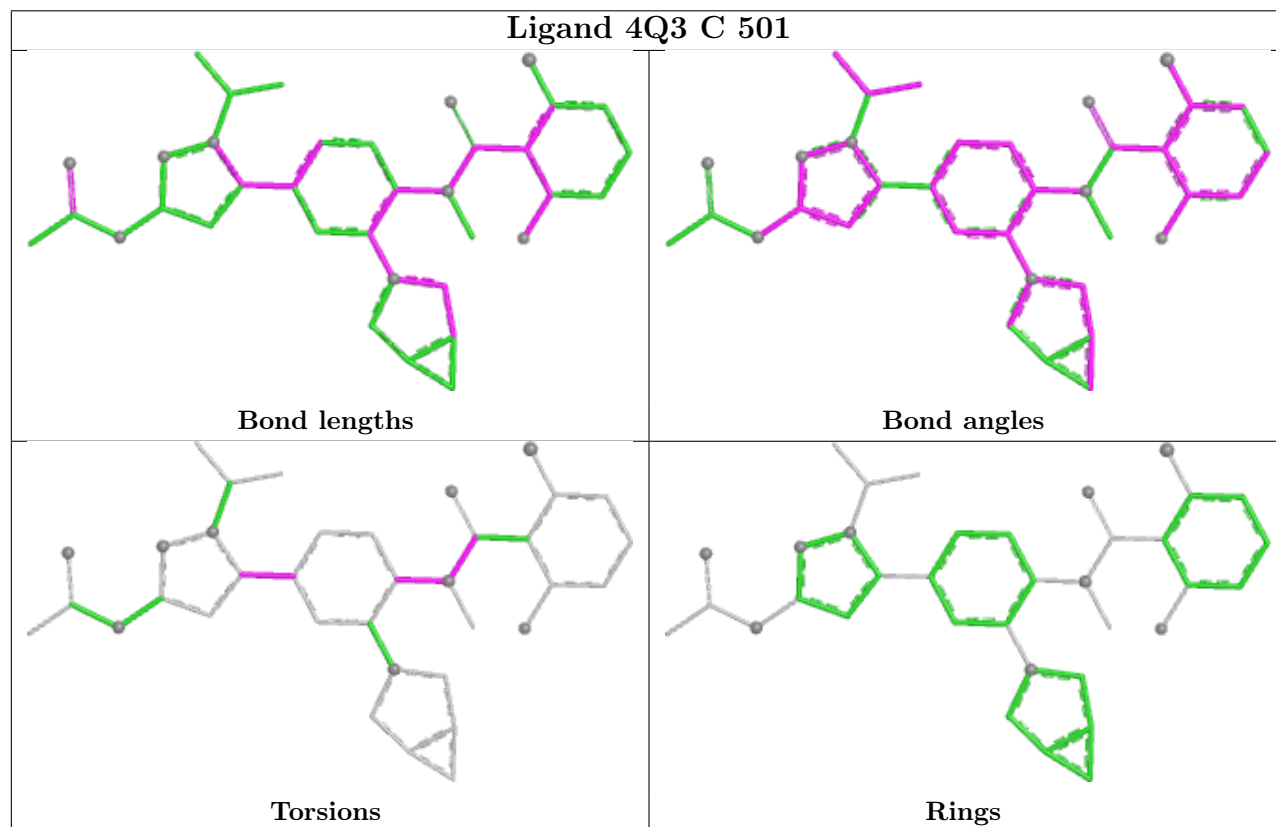
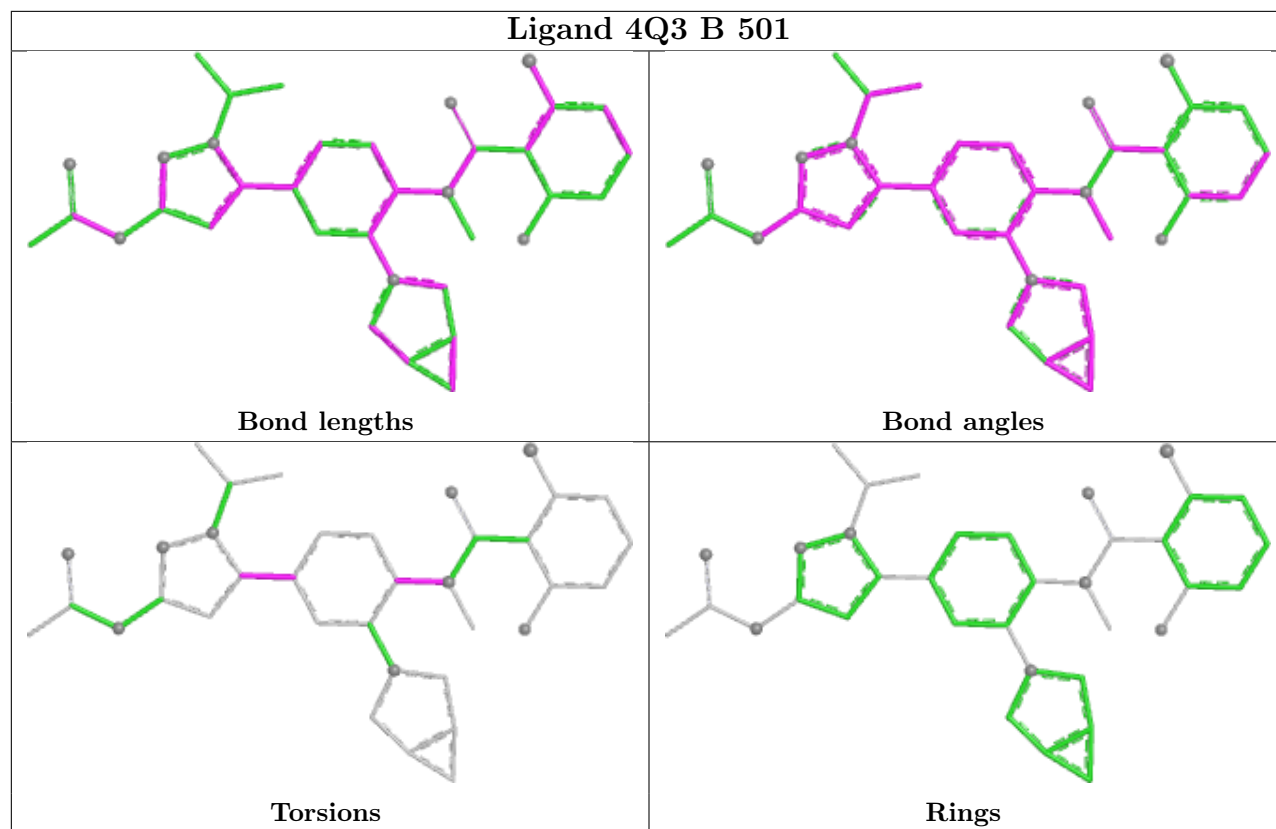
3 monomers are involved in 9 short contacts:

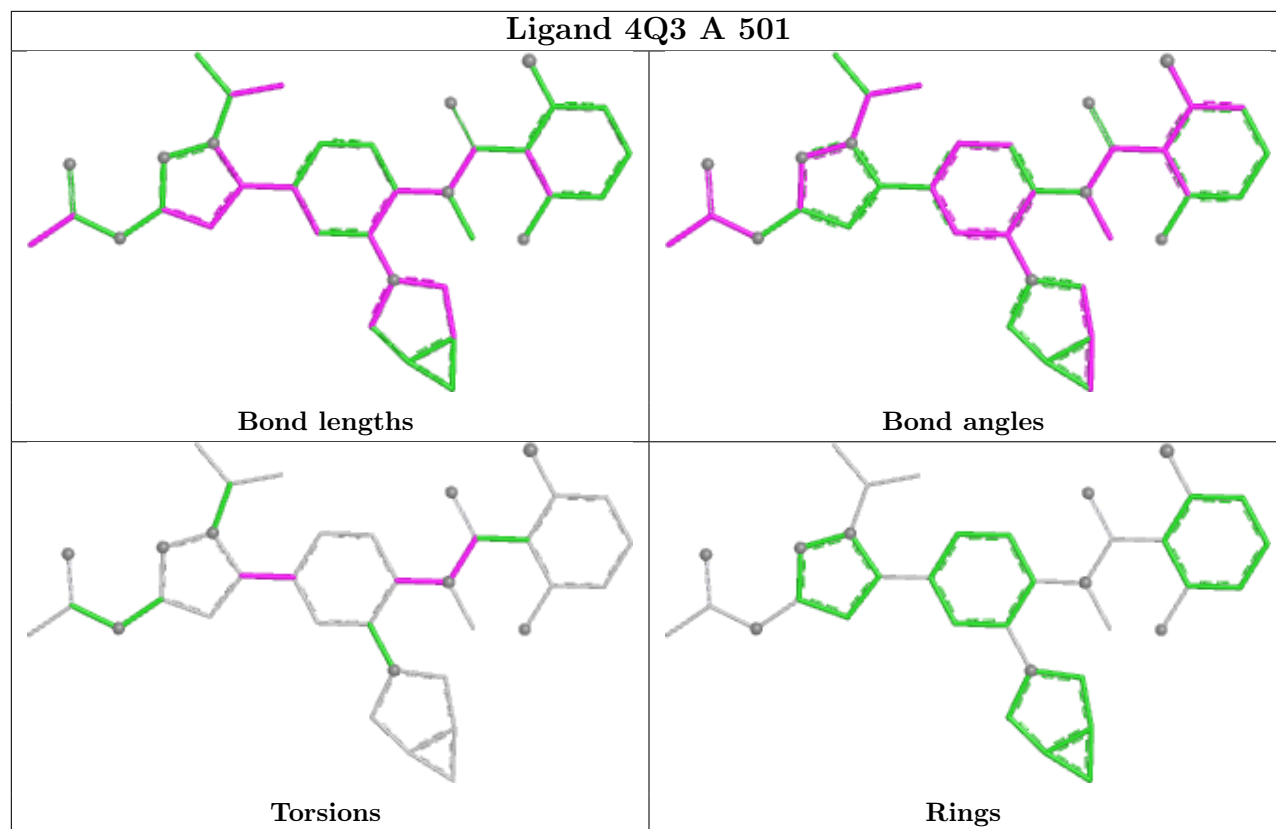
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	4Q3	5	0
2	B	501	4Q3	2	0
2	C	501	4Q3	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	223/225 (99%)	0.03	8 (3%)	46	48	19, 39, 65, 87	5 (2%)
1	B	222/225 (98%)	-0.04	1 (0%)	87	88	20, 39, 64, 70	3 (1%)
1	C	219/225 (97%)	-0.06	1 (0%)	87	88	21, 38, 61, 79	5 (2%)
1	D	215/225 (95%)	-0.08	2 (0%)	81	82	20, 38, 61, 81	5 (2%)
All	All	879/900 (97%)	-0.04	12 (1%)	73	75	19, 38, 64, 87	18 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	ALA	3.0
1	A	484	GLN	3.0
1	B	268	THR	2.7
1	A	482	ARG	2.6
1	C	285	CYS	2.5
1	A	486	PHE	2.5
1	A	412	PHE	2.5
1	A	483	LEU	2.4
1	D	285	CYS	2.2
1	A	481	GLU	2.1
1	A	272[A]	HIS	2.1
1	D	296	ARG	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](#)

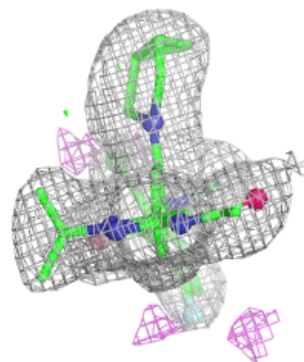
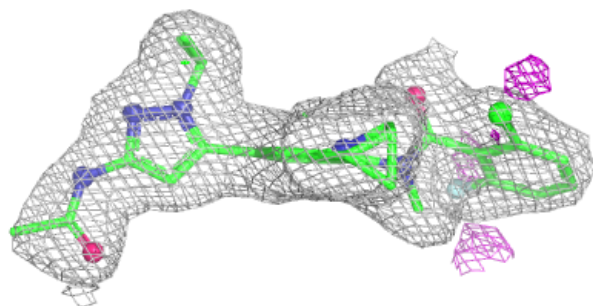
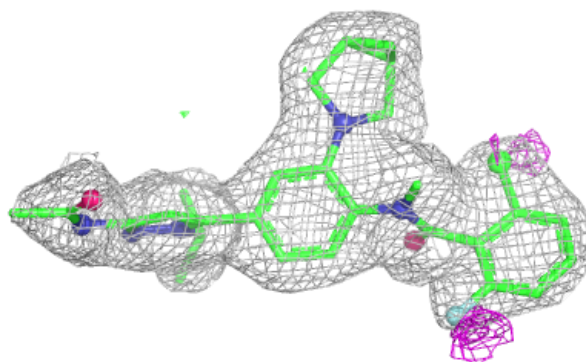
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	4Q3	A	501	36/36	0.92	0.09	29,42,55,85	0
2	4Q3	B	501	36/36	0.93	0.09	28,35,48,73	0
2	4Q3	C	501	36/36	0.93	0.08	28,34,52,72	0
2	4Q3	D	501	36/36	0.93	0.08	30,38,50,78	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.

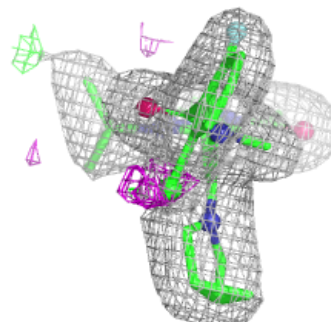
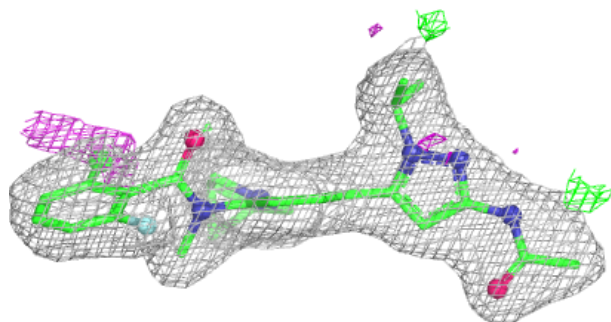
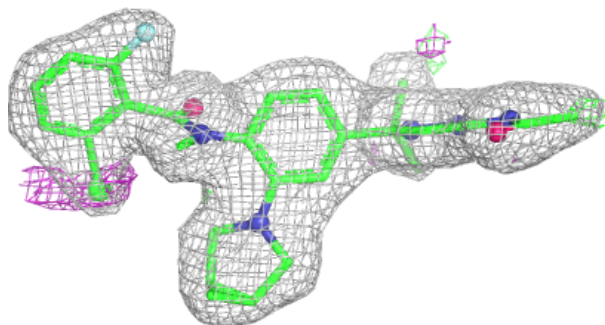
Electron density around 4Q3 A 501:

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

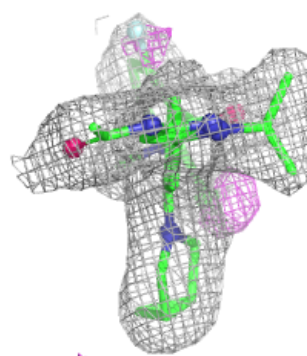
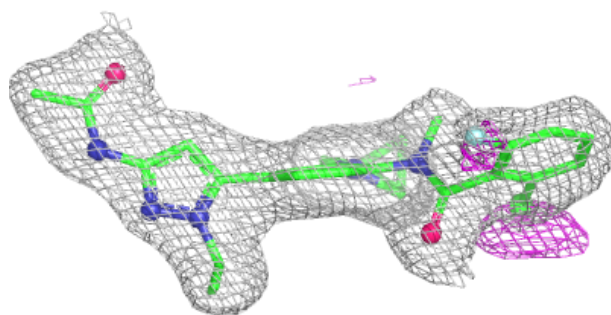
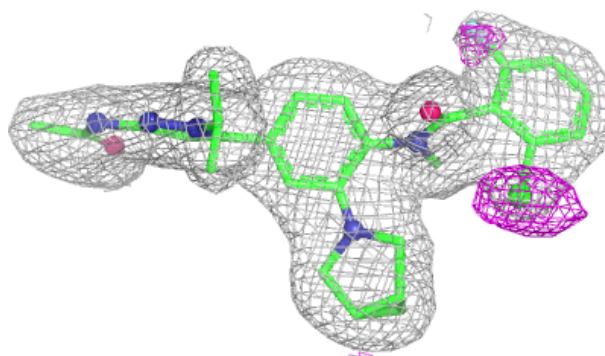


Electron density around 4Q3 B 501:

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

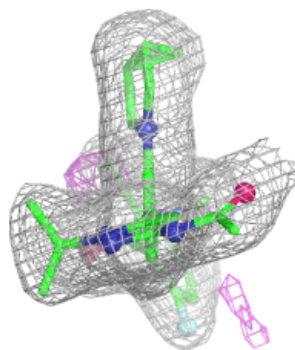
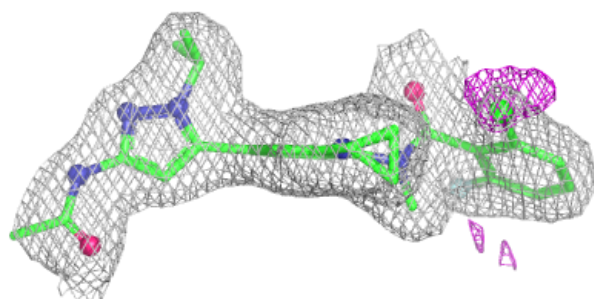
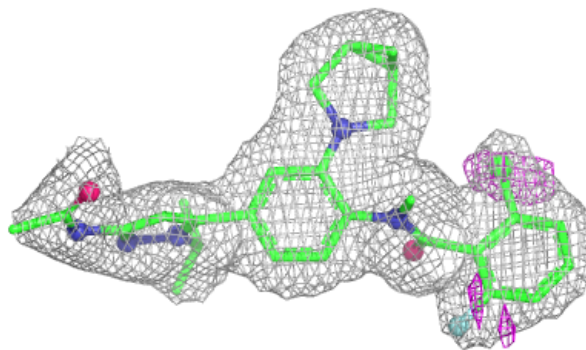
**Electron density around 4Q3 C 501:**

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



Electron density around 4Q3 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.