



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 01:38 am BST

PDB ID : 6PX9
Title : Crystal structure of procaspase-8 in complex with covalent small molecule inhibitor 63-R
Authors : Xu, J.H.; Wolan, D.W.
Deposited on : 2019-07-25
Resolution : 2.88 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

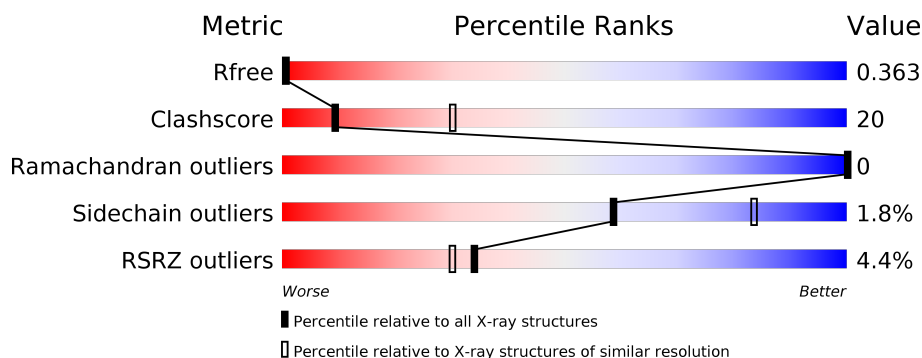
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 on 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	274	<div> <div>3%</div> <div> <div>49%</div> <div>27%</div> <div>•</div> <div>24%</div> </div> </div>
1	B	274	<div> <div>3%</div> <div> <div>49%</div> <div>26%</div> <div>•</div> <div>24%</div> </div> </div>
1	C	274	<div> <div>3%</div> <div> <div>51%</div> <div>24%</div> <div></div> <div>25%</div> </div> </div>
1	D	274	<div> <div>4%</div> <div> <div>53%</div> <div>23%</div> <div></div> <div>23%</div> </div> </div>
1	E	274	<div> <div>4%</div> <div> <div>46%</div> <div>30%</div> <div>•</div> <div>23%</div> </div> </div>
1	F	274	<div> <div>3%</div> <div> <div>53%</div> <div>23%</div> <div></div> <div>24%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9878 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 Caspase-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1643	1049	273	308	13			
1	B	207	Total	C	N	O	S	0	1	0
			1635	1040	272	310	13			
1	C	206	Total	C	N	O	S	0	0	0
			1626	1036	272	305	13			
1	D	210	Total	C	N	O	S	0	1	0
			1646	1046	273	314	13			
1	E	210	Total	C	N	O	S	0	1	0
			1655	1049	276	317	13			
1	F	209	Total	C	N	O	S	0	1	0
			1640	1041	275	311	13			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	374	ALA	ASP	engineered mutation	UNP Q14790
A	384	ALA	ASP	engineered mutation	UNP Q14790
A	409	SER	CYS	engineered mutation	UNP Q14790
A	433	SER	CYS	engineered mutation	UNP Q14790
A	480	ALA	-	expression tag	UNP Q14790
A	481	ALA	-	expression tag	UNP Q14790
A	482	ALA	-	expression tag	UNP Q14790
A	483	LEU	-	expression tag	UNP Q14790
A	484	GLU	-	expression tag	UNP Q14790
A	485	HIS	-	expression tag	UNP Q14790
A	486	HIS	-	expression tag	UNP Q14790
A	487	HIS	-	expression tag	UNP Q14790
A	488	HIS	-	expression tag	UNP Q14790
A	489	HIS	-	expression tag	UNP Q14790
A	490	HIS	-	expression tag	UNP Q14790
B	374	ALA	ASP	engineered mutation	UNP Q14790
B	384	ALA	ASP	engineered mutation	UNP Q14790

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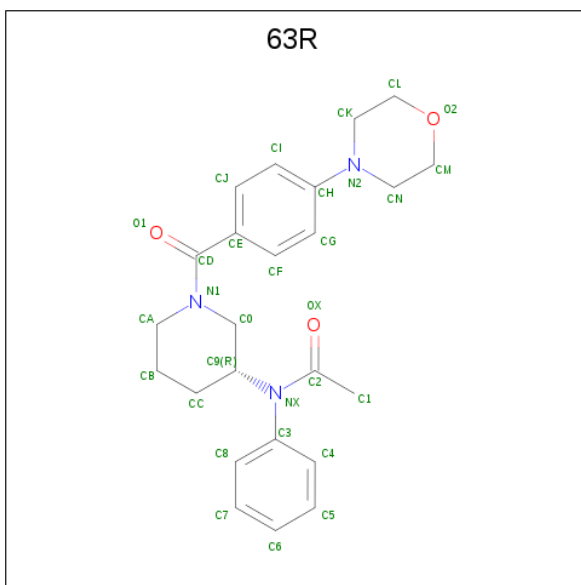
Chain	Residue	Modelled	Actual	Comment	Reference
B	409	SER	CYS	engineered mutation	UNP Q14790
B	433	SER	CYS	engineered mutation	UNP Q14790
B	480	ALA	-	expression tag	UNP Q14790
B	481	ALA	-	expression tag	UNP Q14790
B	482	ALA	-	expression tag	UNP Q14790
B	483	LEU	-	expression tag	UNP Q14790
B	484	GLU	-	expression tag	UNP Q14790
B	485	HIS	-	expression tag	UNP Q14790
B	486	HIS	-	expression tag	UNP Q14790
B	487	HIS	-	expression tag	UNP Q14790
B	488	HIS	-	expression tag	UNP Q14790
B	489	HIS	-	expression tag	UNP Q14790
B	490	HIS	-	expression tag	UNP Q14790
C	374	ALA	ASP	engineered mutation	UNP Q14790
C	384	ALA	ASP	engineered mutation	UNP Q14790
C	409	SER	CYS	engineered mutation	UNP Q14790
C	433	SER	CYS	engineered mutation	UNP Q14790
C	480	ALA	-	expression tag	UNP Q14790
C	481	ALA	-	expression tag	UNP Q14790
C	482	ALA	-	expression tag	UNP Q14790
C	483	LEU	-	expression tag	UNP Q14790
C	484	GLU	-	expression tag	UNP Q14790
C	485	HIS	-	expression tag	UNP Q14790
C	486	HIS	-	expression tag	UNP Q14790
C	487	HIS	-	expression tag	UNP Q14790
C	488	HIS	-	expression tag	UNP Q14790
C	489	HIS	-	expression tag	UNP Q14790
C	490	HIS	-	expression tag	UNP Q14790
D	374	ALA	ASP	engineered mutation	UNP Q14790
D	384	ALA	ASP	engineered mutation	UNP Q14790
D	409	SER	CYS	engineered mutation	UNP Q14790
D	433	SER	CYS	engineered mutation	UNP Q14790
D	480	ALA	-	expression tag	UNP Q14790
D	481	ALA	-	expression tag	UNP Q14790
D	482	ALA	-	expression tag	UNP Q14790
D	483	LEU	-	expression tag	UNP Q14790
D	484	GLU	-	expression tag	UNP Q14790
D	485	HIS	-	expression tag	UNP Q14790
D	486	HIS	-	expression tag	UNP Q14790
D	487	HIS	-	expression tag	UNP Q14790
D	488	HIS	-	expression tag	UNP Q14790
D	489	HIS	-	expression tag	UNP Q14790

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Chain	Residue	Modelled	Actual	Comment	Reference
D	490	HIS	-	expression tag	UNP Q14790
E	374	ALA	ASP	engineered mutation	UNP Q14790
E	384	ALA	ASP	engineered mutation	UNP Q14790
E	409	SER	CYS	engineered mutation	UNP Q14790
E	433	SER	CYS	engineered mutation	UNP Q14790
E	480	ALA	-	expression tag	UNP Q14790
E	481	ALA	-	expression tag	UNP Q14790
E	482	ALA	-	expression tag	UNP Q14790
E	483	LEU	-	expression tag	UNP Q14790
E	484	GLU	-	expression tag	UNP Q14790
E	485	HIS	-	expression tag	UNP Q14790
E	486	HIS	-	expression tag	UNP Q14790
E	487	HIS	-	expression tag	UNP Q14790
E	488	HIS	-	expression tag	UNP Q14790
E	489	HIS	-	expression tag	UNP Q14790
E	490	HIS	-	expression tag	UNP Q14790
F	374	ALA	ASP	engineered mutation	UNP Q14790
F	384	ALA	ASP	engineered mutation	UNP Q14790
F	409	SER	CYS	engineered mutation	UNP Q14790
F	433	SER	CYS	engineered mutation	UNP Q14790
F	480	ALA	-	expression tag	UNP Q14790
F	481	ALA	-	expression tag	UNP Q14790
F	482	ALA	-	expression tag	UNP Q14790
F	483	LEU	-	expression tag	UNP Q14790
F	484	GLU	-	expression tag	UNP Q14790
F	485	HIS	-	expression tag	UNP Q14790
F	486	HIS	-	expression tag	UNP Q14790
F	487	HIS	-	expression tag	UNP Q14790
F	488	HIS	-	expression tag	UNP Q14790
F	489	HIS	-	expression tag	UNP Q14790
F	490	HIS	-	expression tag	UNP Q14790

- Molecule 2 is N-{(3R)-1-[4-(morpholin-4-yl)benzene-1-carbonyl]piperidin-3-yl}-N-phenylacetamide (three-letter code: 63R) (formula: C₂₄H₂₉N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			30	24	3	3		

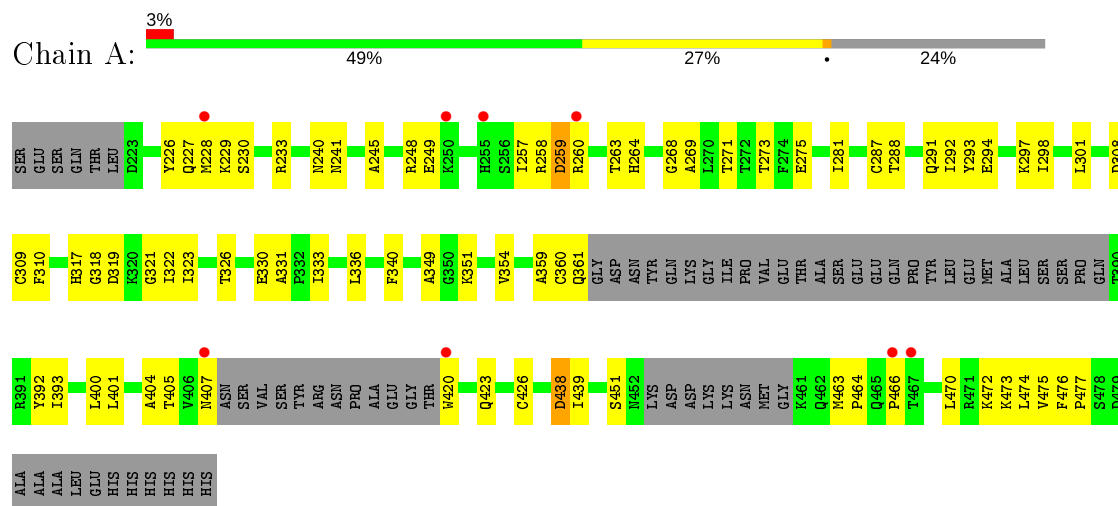
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	B	1	Total O 1 1	0	0

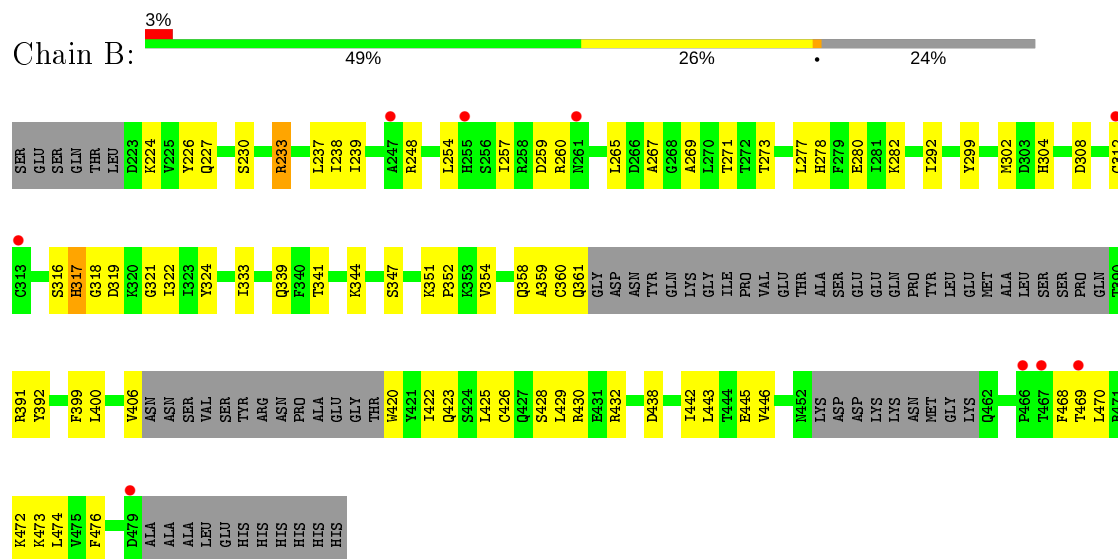
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Caspase-8

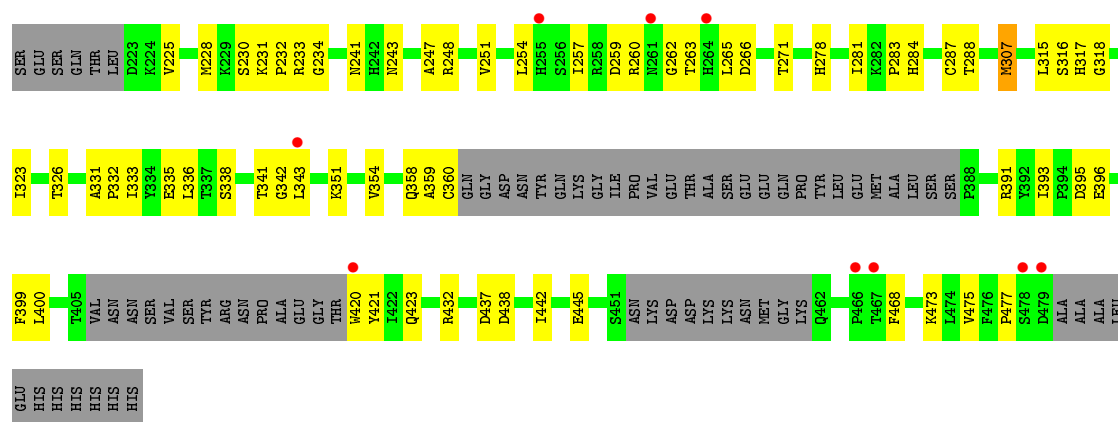


• Molecule 1: Caspase-8

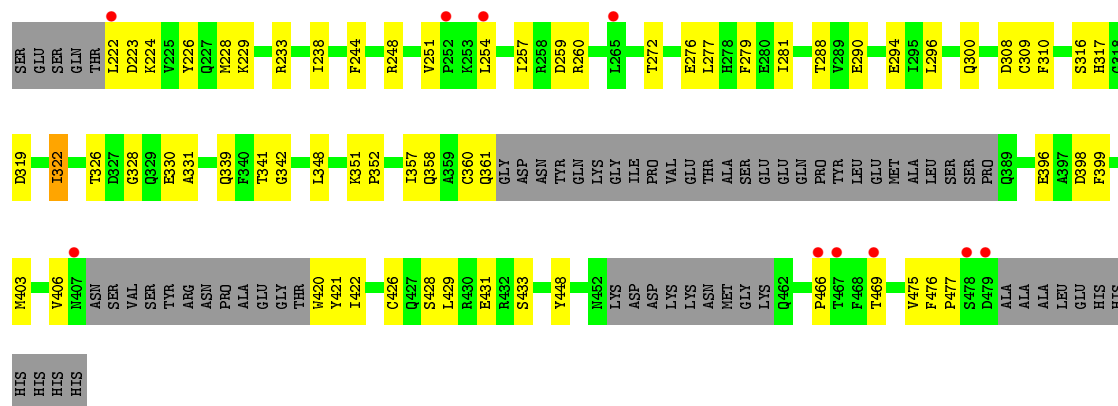


• Molecule 1: Caspase-8

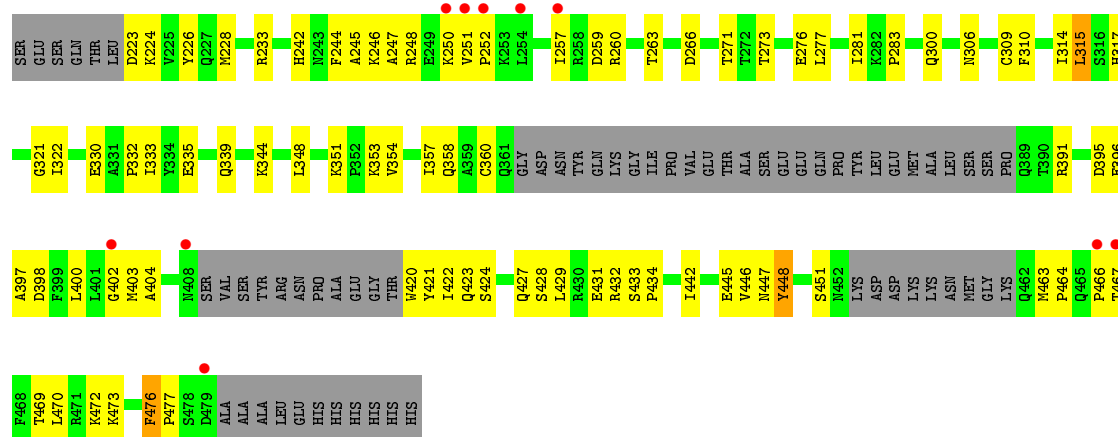




• Molecule 1: Caspase-8

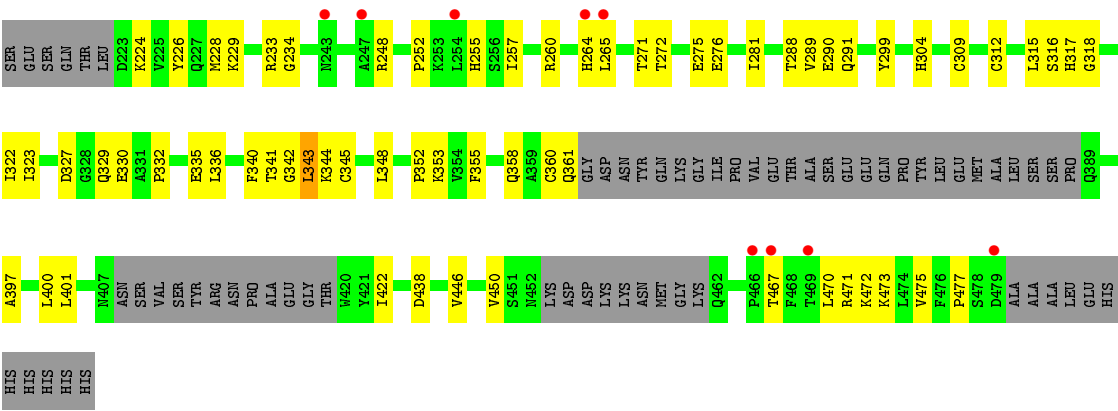


• Molecule 1: Caspase-8



• Molecule 1: Caspase-8





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	101.31Å 101.31Å 175.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.10 – 2.88 48.68 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.10-2.88) 99.4 (48.68-2.88)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.286 , 0.366 0.288 , 0.363	Depositor DCC
R_{free} test set	2260 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 17.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l 0.065 for h,-h-k,-l 0.032 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9878	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8666e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 63R

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	0.39	0/1678	0.53	0/2271
1	B	0.38	0/1677	0.49	0/2272
1	C	0.32	0/1662	0.48	0/2250
1	D	0.39	0/1688	0.53	0/2290
1	E	0.50	1/1697 (0.1%)	0.61	1/2300 (0.0%)
1	F	0.39	0/1680	0.54	0/2278
All	All	0.40	1/10082 (0.0%)	0.53	1/13661 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	477	PRO	N-CD	-9.98	1.33	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	476	PHE	C-N-CD	-8.65	101.58	120.60

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	1643	0	1593	99	0
1	B	1635	0	1570	59	0
1	C	1626	0	1574	46	0
1	D	1646	0	1562	55	0
1	E	1655	0	1577	68	0
1	F	1640	0	1568	61	0
2	B	30	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
All	All	9878	0	9444	381	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 20.

All (381) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:MET:HG2	1:A:477:PRO:CD	1.52	1.39
1:A:228:MET:HE3	1:A:476:PHE:CD1	1.74	1.22
1:F:446:VAL:O	1:F:450:VAL:HG12	1.40	1.22
1:A:248:ARG:NH1	1:A:257:ILE:O	1.72	1.21
1:A:226:TYR:CD1	1:A:473:LYS:O	1.95	1.19
1:A:248:ARG:NH2	1:A:259:ASP:OD1	1.78	1.15
1:A:228:MET:CG	1:A:477:PRO:CD	2.25	1.14
1:A:226:TYR:HD1	1:A:473:LYS:O	1.27	1.10
1:A:228:MET:CG	1:A:477:PRO:HD3	1.79	1.10
1:D:322:ILE:HD11	1:D:330:GLU:HB3	1.29	1.10
1:F:318:GLY:O	1:F:361:GLN:HG2	1.50	1.09
1:A:228:MET:CE	1:A:476:PHE:CD1	2.36	1.08
1:A:226:TYR:OH	1:A:470:LEU:HB3	1.55	1.05
1:D:248:ARG:NH1	1:D:259:ASP:OD1	1.90	1.05
1:A:322:ILE:HD12	1:A:330:GLU:HB3	1.38	1.04
1:E:277:LEU:HD23	1:E:476:PHE:HB2	1.38	1.03
1:A:228:MET:CE	1:A:476:PHE:HD1	1.71	1.02
1:A:228:MET:CE	1:A:475:VAL:O	2.07	1.02
1:D:322:ILE:HD11	1:D:330:GLU:CB	1.88	1.02
1:A:360:CYS:C	1:A:361:GLN:OE1	1.99	1.01
1:A:229:LYS:HA	1:A:233:ARG:HH12	1.26	1.00
1:E:339:GLN:OE1	1:E:344:LYS:NZ	1.94	1.00
1:F:264:HIS:CE1	1:F:265:LEU:HD13	1.98	0.98
1:F:264:HIS:CE1	1:F:265:LEU:CD1	2.47	0.97
1:A:229:LYS:HA	1:A:233:ARG:NH1	1.78	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:MET:CG	1:A:477:PRO:HD2	1.92	0.97
1:A:226:TYR:CD1	1:A:473:LYS:C	2.39	0.95
1:A:228:MET:HE2	1:A:475:VAL:O	1.63	0.94
1:C:260:ARG:NH1	1:C:360:CYS:SG	2.41	0.94
1:E:322:ILE:HD13	1:E:330:GLU:HB3	1.49	0.94
1:E:322:ILE:CD1	1:E:330:GLU:HB3	1.98	0.93
1:E:432:ARG:NH1	1:E:445:GLU:OE1	2.03	0.92
1:A:228:MET:HG3	1:A:477:PRO:HD2	1.52	0.92
1:A:294:GLU:O	1:A:298:ILE:HD13	1.70	0.91
1:D:319:ASP:HB3	1:D:361:GLN:HG2	1.53	0.91
1:B:260:ARG:NH1	1:B:360:CYS:SG	2.43	0.90
1:A:226:TYR:HD1	1:A:473:LYS:C	1.73	0.89
1:D:260:ARG:NH1	1:D:360:CYS:SG	2.48	0.87
1:A:293:TYR:O	1:A:297:LYS:NZ	2.09	0.85
1:A:228:MET:HG2	1:A:477:PRO:HD3	0.85	0.84
1:E:351:LYS:O	1:E:353:LYS:NZ	2.15	0.80
1:B:391:ARG:HE	1:B:392:TYR:H	1.28	0.80
1:E:467:THR:HG22	1:F:467:THR:HB	1.64	0.79
1:E:391:ARG:NH1	1:E:395:ASP:OD2	2.16	0.79
1:D:357:ILE:HB	1:D:403:MET:HG3	1.66	0.78
1:A:230:SER:H	1:A:233:ARG:NH1	1.82	0.77
1:D:277:LEU:HD12	1:D:279:PHE:CE2	2.20	0.77
1:E:424:SER:HA	1:E:427:GLN:HG2	1.67	0.77
1:C:432:ARG:NE	1:C:445:GLU:OE1	2.15	0.76
1:E:451:SER:OG	1:F:471:ARG:HD3	1.84	0.75
1:D:319:ASP:HB2	1:D:361:GLN:OE1	1.86	0.75
1:A:360:CYS:O	1:A:361:GLN:OE1	2.04	0.75
1:E:322:ILE:HD11	1:E:330:GLU:CB	2.16	0.74
1:A:271:THR:HG22	1:A:281:ILE:HG21	1.69	0.73
1:D:277:LEU:HD13	1:D:277:LEU:O	1.88	0.73
1:C:420:TRP:HD1	1:C:421:TYR:H	1.37	0.72
1:E:322:ILE:CD1	1:E:330:GLU:CB	2.68	0.71
1:E:400:LEU:HD12	1:E:470:LEU:HD11	1.72	0.71
1:D:277:LEU:CD1	1:D:277:LEU:O	2.39	0.70
1:D:322:ILE:CD1	1:D:330:GLU:HG3	2.21	0.70
1:C:393:ILE:HD11	1:C:399:PHE:HB3	1.72	0.70
1:E:277:LEU:HD23	1:E:476:PHE:CB	2.19	0.70
1:F:248:ARG:NH1	1:F:257:ILE:O	2.25	0.69
1:F:288:THR:H	1:F:291:GLN:HB2	1.57	0.69
1:D:322:ILE:HD11	1:D:330:GLU:CG	2.22	0.69
1:E:250:LYS:N	1:E:250:LYS:HD2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:GLN:N	1:B:351:LYS:HZ2	1.91	0.68
1:E:226:TYR:OH	1:E:398:ASP:OD1	2.10	0.68
1:E:224:LYS:O	1:E:472:LYS:HB3	1.94	0.68
1:C:318:GLY:HA3	1:C:359:ALA:HB1	1.73	0.68
1:F:329:GLN:HG2	1:F:330:GLU:H	1.57	0.68
1:C:243:ASN:O	1:C:326:THR:OG1	2.11	0.67
1:E:245:ALA:HA	1:E:248:ARG:NH1	2.09	0.67
1:E:433:SER:HB3	1:E:476:PHE:O	1.95	0.67
1:A:359:ALA:HB3	1:A:405:THR:HA	1.75	0.67
1:B:438:ASP:OD2	1:B:473:LYS:HG2	1.95	0.67
1:A:226:TYR:HH	1:A:470:LEU:HB3	1.59	0.67
1:B:321:GLY:O	1:B:333:ILE:HD12	1.95	0.66
1:A:228:MET:HE3	1:A:475:VAL:O	1.92	0.66
1:E:322:ILE:HD11	1:E:330:GLU:HB2	1.77	0.66
1:B:319:ASP:HB2	1:B:322:ILE:HG12	1.77	0.66
1:D:254:LEU:CD1	1:D:328:GLY:HA3	2.25	0.66
1:E:246:LYS:O	1:E:250:LYS:HG2	1.96	0.65
1:A:226:TYR:CE1	1:A:473:LYS:C	2.68	0.65
1:E:357:ILE:HB	1:E:403:MET:HG3	1.78	0.65
1:E:271:THR:HG22	1:E:281:ILE:HG21	1.77	0.65
1:B:304:HIS:N	1:B:347:SER:OG	2.30	0.65
1:E:248:ARG:NH2	1:E:259:ASP:OD1	2.30	0.64
1:A:318:GLY:HA3	1:A:359:ALA:HB1	1.78	0.64
1:A:404:ALA:HB2	1:A:464:PRO:HB3	1.78	0.64
1:F:288:THR:O	1:F:289:VAL:C	2.36	0.64
1:B:257:ILE:HD11	1:B:317:HIS:NE2	2.13	0.64
1:E:332:PRO:HD2	1:E:335:GLU:HG3	1.80	0.63
1:F:264:HIS:NE2	1:F:265:LEU:CD1	2.61	0.63
1:A:228:MET:SD	1:A:476:PHE:HA	2.38	0.62
1:B:358:GLN:HE22	1:B:420:TRP:HD1	1.47	0.62
1:E:348:LEU:O	1:E:353:LYS:NZ	2.26	0.62
1:A:240:ASN:OD1	1:A:263:THR:OG1	2.15	0.62
1:C:338:SER:O	1:C:341:THR:OG1	2.17	0.62
1:F:228:MET:O	1:F:233:ARG:NH1	2.33	0.62
1:F:288:THR:HG23	1:F:327:ASP:CG	2.20	0.62
1:C:341:THR:HG22	1:C:396:GLU:OE2	2.00	0.62
1:A:319:ASP:HB3	1:A:322:ILE:HG12	1.82	0.61
1:A:228:MET:HE1	1:A:476:PHE:CD1	2.33	0.61
1:B:339:GLN:OE1	1:B:344:LYS:NZ	2.33	0.61
1:D:254:LEU:HD11	1:D:328:GLY:HA3	1.82	0.61
1:A:294:GLU:O	1:A:298:ILE:CD1	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:THR:HA	1:F:281:ILE:HD13	1.82	0.61
1:B:429:LEU:HD12	1:B:442:ILE:HG21	1.83	0.60
1:B:227:GLN:H	1:B:351:LYS:HZ2	1.47	0.60
1:E:223:ASP:N	1:E:473:LYS:HZ2	1.99	0.60
1:A:322:ILE:CD1	1:A:330:GLU:HB3	2.24	0.60
1:A:230:SER:H	1:A:233:ARG:HH12	1.48	0.60
1:D:319:ASP:HB3	1:D:361:GLN:CG	2.28	0.60
1:A:275:GLU:HG2	1:A:281:ILE:HD13	1.84	0.60
1:D:309:CYS:SG	1:D:310:PHE:N	2.74	0.60
1:A:420:TRP:HB3	1:A:423:GLN:HB2	1.84	0.59
1:E:402:GLY:O	1:E:421:TYR:OH	2.18	0.59
1:B:230:SER:HB2	1:B:308:ASP:OD2	2.02	0.59
1:C:230:SER:OG	1:C:232:PRO:O	2.20	0.59
1:F:438:ASP:OD1	1:F:473:LYS:HG3	2.03	0.59
1:B:233:ARG:HD2	1:B:278:HIS:HB2	1.84	0.59
1:C:323:ILE:HD11	1:C:333:ILE:HG12	1.83	0.59
1:B:341:THR:HB	1:B:344:LYS:H	1.66	0.59
1:A:229:LYS:H	1:A:229:LYS:HD2	1.67	0.59
1:B:239[B]:ILE:HD13	1:B:292:ILE:HG12	1.84	0.59
1:B:316:SER:O	1:B:359:ALA:HA	2.03	0.59
1:B:318:GLY:HA2	1:B:324:TYR:CD2	2.38	0.59
1:B:299:TYR:HA	1:B:302:MET:HG3	1.85	0.58
1:C:228:MET:O	1:C:233:ARG:NH1	2.36	0.58
1:B:248:ARG:NH2	1:B:259:ASP:OD1	2.31	0.58
1:E:260:ARG:HH12	1:E:263:THR:HG21	1.68	0.58
1:E:257:ILE:HD11	1:E:317:HIS:ND1	2.17	0.58
1:A:331:ALA:HB1	1:A:336:LEU:HD21	1.86	0.58
1:B:239[A]:ILE:HD13	1:B:292:ILE:HG12	1.84	0.58
1:E:433:SER:N	1:E:434:PRO:CD	2.66	0.58
1:F:341:THR:HB	1:F:344:LYS:HB2	1.86	0.58
1:B:400:LEU:HD12	1:B:470:LEU:HD11	1.85	0.57
1:D:322:ILE:HD11	1:D:330:GLU:HG3	1.84	0.57
1:F:446:VAL:O	1:F:450:VAL:CG1	2.32	0.57
1:A:393:ILE:HD11	1:A:401:LEU:HB2	1.87	0.56
1:D:288:THR:HA	1:D:326:THR:H	1.70	0.56
1:E:260:ARG:HH12	1:E:263:THR:CG2	2.18	0.56
1:E:317:HIS:HD2	1:E:360:CYS:HB2	1.70	0.56
1:A:361:GLN:OE1	1:A:361:GLN:N	2.40	0.55
1:F:450:VAL:O	1:F:450:VAL:HG22	2.06	0.55
1:F:341:THR:O	1:F:345:CYS:N	2.39	0.55
1:E:335:GLU:O	1:E:339:GLN:NE2	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:315:LEU:HD21	1:F:422:ILE:HD12	1.89	0.55
1:F:340:PHE:N	1:F:340:PHE:CD1	2.73	0.55
1:A:226:TYR:CE2	1:A:472:LYS:HG3	2.41	0.55
1:C:266:ASP:OD1	1:C:423:GLN:NE2	2.38	0.55
1:E:260:ARG:O	1:E:263:THR:OG1	2.23	0.55
1:A:298:ILE:N	1:A:298:ILE:HD12	2.21	0.55
1:A:228:MET:HE3	1:A:475:VAL:C	2.27	0.55
1:F:252:PRO:O	1:F:255:HIS:N	2.39	0.55
1:A:228:MET:SD	1:A:476:PHE:HD1	2.29	0.55
1:F:224:LYS:HE3	1:F:472:LYS:NZ	2.22	0.55
1:B:432:ARG:NH1	1:B:445:GLU:OE1	2.41	0.54
1:D:358:GLN:CD	1:D:422:ILE:HG13	2.26	0.54
1:A:228:MET:O	1:A:233:ARG:NH1	2.40	0.54
1:A:264:HIS:CD2	1:A:264:HIS:H	2.25	0.54
1:A:340:PHE:N	1:A:340:PHE:CD1	2.76	0.54
1:B:391:ARG:HE	1:B:392:TYR:N	2.04	0.54
1:F:288:THR:O	1:F:291:GLN:N	2.40	0.54
1:F:341:THR:HG22	1:F:342:GLY:N	2.23	0.54
1:C:432:ARG:HB3	1:C:437:ASP:HB2	1.89	0.53
1:D:322:ILE:HG12	1:D:331:ALA:H	1.74	0.53
1:F:348:LEU:HB3	1:F:353:LYS:HE2	1.89	0.53
1:C:354:VAL:HG22	1:C:400:LEU:HD23	1.90	0.53
1:E:447:ASN:HB3	1:E:463:MET:HE1	1.90	0.53
1:B:425:LEU:O	1:B:429:LEU:HB2	2.09	0.53
1:D:319:ASP:CB	1:D:361:GLN:OE1	2.55	0.53
1:F:271:THR:HG22	1:F:281:ILE:HG21	1.90	0.52
1:A:241:ASN:HD22	1:A:326:THR:HG23	1.74	0.52
1:B:227:GLN:H	1:B:351:LYS:NZ	2.06	0.52
1:D:257:ILE:HG23	1:D:257:ILE:O	2.10	0.52
1:F:329:GLN:HG2	1:F:330:GLU:N	2.25	0.52
1:D:319:ASP:O	1:D:322:ILE:HG22	2.10	0.52
1:A:245:ALA:O	1:A:249:GLU:HG3	2.10	0.52
1:A:273:THR:HG21	1:A:426:CYS:HB3	1.91	0.52
1:F:318:GLY:O	1:F:361:GLN:CG	2.39	0.52
1:C:331:ALA:HB1	1:C:336:LEU:HD21	1.92	0.52
1:C:271:THR:HG22	1:C:281:ILE:HG21	1.91	0.51
1:F:260:ARG:NH1	1:F:360:CYS:SG	2.84	0.51
1:C:468:PHE:O	1:D:466:PRO:HD2	2.10	0.51
1:D:254:LEU:HD12	1:D:328:GLY:HA3	1.93	0.51
1:E:442:ILE:O	1:E:446:VAL:HG23	2.11	0.51
1:A:400:LEU:HB2	1:A:470:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:TRP:CZ2	1:B:423:GLN:HG3	2.46	0.51
1:B:267:ALA:O	1:B:271:THR:HG23	2.10	0.50
1:E:403:MET:HG2	1:E:404:ALA:N	2.27	0.50
1:E:429:LEU:HD23	1:E:442:ILE:HD13	1.93	0.50
1:C:358:GLN:HE22	1:C:420:TRP:HE1	1.59	0.50
1:A:228:MET:CE	1:A:476:PHE:CE1	2.94	0.50
1:C:262:GLY:HA2	1:C:265:LEU:HD23	1.94	0.50
1:F:316:SER:OG	1:F:317:HIS:N	2.40	0.50
1:F:288:THR:HG22	1:F:289:VAL:N	2.25	0.50
1:E:448:TYR:CD1	1:F:471:ARG:HD2	2.46	0.50
1:C:247:ALA:O	1:C:251:VAL:HG12	2.11	0.50
1:C:281:ILE:HG22	1:C:283:PRO:HD3	1.94	0.50
1:E:404:ALA:HB2	1:E:464:PRO:HB3	1.92	0.50
1:A:271:THR:O	1:A:275:GLU:HG3	2.11	0.50
1:B:425:LEU:HA	1:B:446:VAL:HG11	1.94	0.50
1:E:321:GLY:O	1:E:333:ILE:HG23	2.12	0.50
1:A:228:MET:CG	1:A:475:VAL:O	2.61	0.49
1:C:432:ARG:HD2	1:C:437:ASP:OD2	2.12	0.49
1:B:438:ASP:O	1:B:442:ILE:HG12	2.12	0.49
1:A:228:MET:HG2	1:A:475:VAL:O	2.13	0.49
1:F:358:GLN:HB2	1:F:422:ILE:HG13	1.95	0.49
1:F:226:TYR:HE2	1:F:470:LEU:HB3	1.76	0.49
1:B:351:LYS:HG3	1:B:352:PRO:HD2	1.95	0.49
1:F:312:CYS:O	1:F:355:PHE:HA	2.12	0.49
1:A:228:MET:HE1	1:A:476:PHE:CE1	2.48	0.49
1:E:309:CYS:SG	1:E:310:PHE:N	2.86	0.49
1:F:400:LEU:HD23	1:F:401:LEU:N	2.27	0.49
1:F:288:THR:HG22	1:F:290:GLU:H	1.78	0.49
1:A:287:CYS:HB3	1:A:292:ILE:HG13	1.95	0.48
1:A:258:ARG:O	1:A:317:HIS:HE1	1.96	0.48
1:C:438:ASP:HB2	1:C:473:LYS:HE2	1.94	0.48
1:D:399:PHE:H	1:D:469:THR:HG23	1.78	0.48
1:B:317:HIS:HB2	1:B:360:CYS:O	2.13	0.48
1:E:427:GLN:HG3	1:E:428:SER:N	2.28	0.48
1:B:391:ARG:NE	1:B:392:TYR:H	2.05	0.48
1:B:248:ARG:NH1	1:B:257:ILE:O	2.47	0.48
1:C:254:LEU:HD23	1:C:257:ILE:HD13	1.94	0.48
1:A:298:ILE:CD1	1:A:298:ILE:N	2.76	0.48
1:A:226:TYR:OH	1:A:472:LYS:N	2.47	0.48
1:D:421:TYR:CD1	1:D:421:TYR:C	2.85	0.48
1:B:238:ILE:HD12	1:B:271:THR:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:GLN:HE22	1:D:420:TRP:HD1	1.62	0.48
1:C:251:VAL:HG11	1:C:254:LEU:HD13	1.96	0.48
1:D:316:SER:OG	1:D:317:HIS:N	2.46	0.48
1:F:299:TYR:O	1:F:304:HIS:NE2	2.39	0.47
1:A:298:ILE:CD1	1:A:298:ILE:H	2.27	0.47
1:F:400:LEU:HD12	1:F:470:LEU:HD11	1.97	0.47
1:F:471:ARG:HH11	1:F:471:ARG:CB	2.27	0.47
1:A:451:SER:HB3	1:A:463:MET:CE	2.44	0.47
1:C:438:ASP:O	1:C:442:ILE:HG12	2.15	0.47
1:E:420:TRP:CE3	1:E:423:GLN:HG3	2.50	0.47
1:F:224:LYS:HD2	1:F:224:LYS:HA	1.63	0.47
1:B:226:TYR:CD1	1:B:352:PRO:HD3	2.50	0.47
1:D:296:LEU:O	1:D:300:GLN:N	2.40	0.47
1:D:330:GLU:OE1	1:D:330:GLU:N	2.46	0.47
1:C:225:VAL:HG22	1:C:473:LYS:HG2	1.96	0.47
1:F:228:MET:HE3	1:F:233:ARG:HD3	1.97	0.47
1:B:317:HIS:O	1:B:324:TYR:HB2	2.15	0.47
1:B:399:PHE:HB2	1:B:469:THR:HG22	1.97	0.47
1:D:422:ILE:O	1:D:422:ILE:HG22	2.14	0.46
1:F:322:ILE:CG2	1:F:323:ILE:N	2.78	0.46
1:D:426:CYS:HA	1:D:429:LEU:HB2	1.98	0.46
1:B:280:GLU:OE2	1:B:282:LYS:HD3	2.14	0.46
1:C:288:THR:HG22	1:C:326:THR:HG22	1.98	0.46
1:C:251:VAL:CG1	1:C:254:LEU:HB2	2.46	0.46
1:B:399:PHE:HB2	1:B:469:THR:CG2	2.46	0.46
1:F:309:CYS:HB2	1:F:352:PRO:HG2	1.97	0.46
1:A:354:VAL:HG13	1:A:400:LEU:HD23	1.97	0.46
1:F:341:THR:HG22	1:F:343:LEU:H	1.81	0.46
1:A:288:THR:HB	1:A:291:GLN:H	1.81	0.46
1:A:321:GLY:HA2	1:A:392:TYR:HE2	1.81	0.46
1:D:428:SER:HA	1:D:431:GLU:HB3	1.97	0.46
1:D:341:THR:HB	1:D:396:GLU:OE2	2.16	0.45
1:A:309:CYS:SG	1:A:310:PHE:N	2.89	0.45
1:F:332:PRO:O	1:F:336:LEU:HG	2.16	0.45
1:A:271:THR:HA	1:A:281:ILE:HG12	1.97	0.45
1:B:254:LEU:HD22	1:B:257:ILE:HD12	1.98	0.45
1:E:314:ILE:HB	1:E:357:ILE:HG12	1.99	0.45
1:E:448:TYR:O	1:E:451:SER:O	2.33	0.45
1:A:230:SER:N	1:A:233:ARG:NH1	2.59	0.45
1:E:396:GLU:O	1:E:469:THR:HG21	2.17	0.45
1:D:272:THR:O	1:D:276:GLU:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ALA:C	1:A:351:LYS:H	2.19	0.45
1:A:228:MET:SD	1:A:233:ARG:HD3	2.57	0.45
1:B:237:LEU:HD11	1:B:299:TYR:CE1	2.52	0.45
1:E:273:THR:O	1:E:276:GLU:HB2	2.16	0.45
1:E:354:VAL:HG13	1:E:400:LEU:HD22	1.97	0.45
1:B:344:LYS:HB3	1:B:344:LYS:HE2	1.76	0.45
1:A:466:PRO:HB2	1:B:468:PHE:CE1	2.52	0.45
1:B:269:ALA:O	1:B:273:THR:OG1	2.19	0.45
1:E:463:MET:HB3	1:E:463:MET:HE2	1.90	0.45
1:D:308:ASP:O	1:D:352:PRO:HD2	2.17	0.44
1:D:228:MET:HG3	1:D:475:VAL:O	2.17	0.44
1:E:281:ILE:HG22	1:E:283:PRO:HD3	1.99	0.44
1:A:260:ARG:HG3	1:A:317:HIS:CE1	2.53	0.44
1:E:244:PHE:HB3	1:E:247:ALA:HB3	1.99	0.44
1:C:307:MET:O	1:C:351:LYS:NZ	2.31	0.44
1:E:433:SER:N	1:E:434:PRO:HD2	2.32	0.44
1:D:254:LEU:HD11	1:D:328:GLY:CA	2.46	0.44
1:A:226:TYR:HD1	1:A:474:LEU:N	2.16	0.44
1:A:273:THR:HG21	1:A:426:CYS:CB	2.48	0.44
1:F:264:HIS:CE1	1:F:265:LEU:HD12	2.47	0.44
1:C:332:PRO:HB2	1:C:335:GLU:HG3	2.00	0.44
1:B:224:LYS:HB2	1:B:472:LYS:HB3	2.00	0.44
1:D:251:VAL:HG12	1:D:254:LEU:H	1.83	0.44
1:E:427:GLN:O	1:E:431:GLU:HB2	2.18	0.44
1:C:254:LEU:HD23	1:C:257:ILE:HG21	1.99	0.43
1:C:233:ARG:HG3	1:C:278:HIS:HB2	2.00	0.43
1:A:227:GLN:HG2	1:A:308:ASP:OD2	2.18	0.43
1:D:421:TYR:CD1	1:D:421:TYR:O	2.70	0.43
1:A:360:CYS:O	1:A:361:GLN:CD	2.57	0.43
1:B:354:VAL:HG13	1:B:400:LEU:HB3	2.01	0.43
1:C:475:VAL:O	1:C:477:PRO:HD3	2.18	0.43
1:D:290:GLU:O	1:D:294:GLU:HG3	2.17	0.43
1:C:241:ASN:HB2	1:C:316:SER:HB2	1.99	0.43
1:E:250:LYS:N	1:E:250:LYS:CD	2.72	0.43
1:A:226:TYR:CD1	1:A:474:LEU:N	2.85	0.43
1:A:439:ILE:HG21	1:A:474:LEU:HD23	2.00	0.43
1:C:284:HIS:HB3	1:C:287:CYS:SG	2.59	0.43
1:D:248:ARG:HG2	1:D:257:ILE:HG22	1.99	0.43
1:E:266:ASP:HB3	1:E:422:ILE:HG21	2.01	0.43
1:E:344:LYS:HE2	1:E:344:LYS:HB3	1.74	0.43
1:B:400:LEU:HD21	1:B:443:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:GLN:H	1:B:406:VAL:C	2.22	0.43
1:D:222:LEU:HD23	1:D:224:LYS:NZ	2.33	0.43
1:F:322:ILE:HG22	1:F:323:ILE:N	2.33	0.43
1:B:273:THR:O	1:B:277:LEU:HG	2.19	0.42
1:C:251:VAL:HG13	1:C:254:LEU:HB2	2.01	0.42
1:D:300:GLN:HG3	1:D:339:GLN:O	2.19	0.42
1:D:433:SER:OG	1:D:476:PHE:O	2.37	0.42
1:A:226:TYR:CD2	1:A:472:LYS:HG3	2.54	0.42
1:A:438:ASP:HA	1:A:475:VAL:HG22	2.00	0.42
1:D:226:TYR:OH	1:D:398:ASP:OD1	2.24	0.42
1:E:306:ASN:OD1	1:E:306:ASN:N	2.51	0.42
1:F:272:THR:O	1:F:276:GLU:HG3	2.19	0.42
1:F:332:PRO:HD2	1:F:335:GLU:HB2	2.00	0.42
1:A:323:ILE:HG12	1:A:333:ILE:HD11	2.01	0.42
1:B:422:ILE:O	1:B:422:ILE:HG22	2.19	0.42
1:C:248:ARG:NH2	1:C:259:ASP:OD1	2.53	0.42
1:E:463:MET:HE3	1:E:464:PRO:HD2	2.01	0.42
1:A:230:SER:N	1:A:233:ARG:HH12	2.16	0.42
1:A:241:ASN:ND2	1:A:326:THR:HG23	2.34	0.42
1:C:234:GLY:HA2	1:C:307:MET:HG2	2.02	0.42
1:E:348:LEU:HA	1:E:351:LYS:HD2	2.02	0.42
1:E:300:GLN:HG3	1:E:339:GLN:O	2.20	0.42
1:F:271:THR:O	1:F:275:GLU:HB2	2.19	0.42
1:F:345:CYS:SG	1:F:348:LEU:HD12	2.60	0.42
1:A:226:TYR:CD1	1:A:474:LEU:CA	3.02	0.42
1:C:391:ARG:NH2	1:C:395:ASP:OD2	2.53	0.42
1:F:397:ALA:HB1	1:F:471:ARG:HG3	2.01	0.42
1:D:229:LYS:N	1:D:308:ASP:OD2	2.53	0.42
1:F:322:ILE:HD12	1:F:330:GLU:HB3	2.01	0.42
1:A:463:MET:SD	1:B:469:THR:OG1	2.78	0.42
1:B:474:LEU:HD21	1:B:476:PHE:CZ	2.54	0.42
1:D:348:LEU:HA	1:D:351:LYS:HD2	2.02	0.42
1:A:241:ASN:ND2	1:A:287:CYS:O	2.47	0.41
1:C:260:ARG:HH21	1:C:315:LEU:HB3	1.85	0.41
1:C:263:THR:HA	1:C:266:ASP:HB2	2.02	0.41
1:E:396:GLU:HG2	1:E:397:ALA:H	1.85	0.41
1:F:234:GLY:HA3	1:F:309:CYS:O	2.19	0.41
1:D:277:LEU:HD12	1:D:279:PHE:HE2	1.76	0.41
1:E:315:LEU:HD23	1:E:358:GLN:HG2	2.02	0.41
1:C:342:GLY:H	1:C:396:GLU:CD	2.23	0.41
1:E:464:PRO:O	1:E:466:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:LEU:HD13	1:B:282:LYS:HB2	2.02	0.41
1:F:475:VAL:O	1:F:477:PRO:HD3	2.20	0.41
1:A:226:TYR:HD1	1:A:474:LEU:CA	2.32	0.41
1:B:428:SER:HB3	1:B:445:GLU:OE1	2.20	0.41
1:D:254:LEU:CD1	1:D:328:GLY:CA	2.97	0.41
1:F:229:LYS:HA	1:F:233:ARG:HH12	1.85	0.41
1:A:466:PRO:HD2	1:B:468:PHE:O	2.20	0.41
1:E:224:LYS:C	1:E:472:LYS:HB3	2.39	0.41
1:F:450:VAL:O	1:F:450:VAL:CG2	2.69	0.41
1:C:230:SER:OG	1:C:231:LYS:N	2.54	0.41
1:D:238:ILE:HD13	1:D:281:ILE:HG23	2.02	0.41
1:A:226:TYR:CZ	1:A:472:LYS:N	2.86	0.41
1:A:268:GLY:O	1:A:271:THR:OG1	2.27	0.41
1:F:345:CYS:SG	1:F:345:CYS:O	2.78	0.41
1:E:251:VAL:HA	1:E:252:PRO:HD2	1.84	0.40
1:A:269:ALA:O	1:A:273:THR:HG23	2.21	0.40
1:B:273:THR:HG23	1:B:430:ARG:HG2	2.03	0.40
1:B:426:CYS:O	1:B:430:ARG:HG3	2.21	0.40
1:D:244:PHE:O	1:D:248:ARG:HG3	2.21	0.40
1:D:475:VAL:O	1:D:477:PRO:HD3	2.21	0.40
1:A:260:ARG:NH1	1:A:260:ARG:HB3	2.36	0.40
1:B:237:LEU:HB2	1:B:312:CYS:HA	2.03	0.40
1:C:254:LEU:CD2	1:C:257:ILE:HD13	2.51	0.40
1:D:342:GLY:N	1:D:396:GLU:OE1	2.54	0.40
1:F:229:LYS:CA	1:F:233:ARG:HH12	2.34	0.40
1:C:266:ASP:HA	1:C:423:GLN:HE22	1.86	0.40
1:A:297:LYS:O	1:A:301:LEU:HD12	2.22	0.40
1:E:233:ARG:HG2	1:E:233:ARG:HH11	1.87	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	201/274 (73%)	179 (89%)	22 (11%)	0	100	100
1	B	200/274 (73%)	176 (88%)	24 (12%)	0	100	100
1	C	198/274 (72%)	183 (92%)	15 (8%)	0	100	100
1	D	203/274 (74%)	181 (89%)	22 (11%)	0	100	100
1	E	203/274 (74%)	186 (92%)	17 (8%)	0	100	100
1	F	202/274 (74%)	172 (85%)	30 (15%)	0	100	100
All	All	1207/1644 (73%)	1077 (89%)	130 (11%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	180/244 (74%)	177 (98%)	3 (2%)	60	84
1	B	181/244 (74%)	178 (98%)	3 (2%)	60	84
1	C	179/244 (73%)	176 (98%)	3 (2%)	60	84
1	D	180/244 (74%)	175 (97%)	5 (3%)	43	75
1	E	183/244 (75%)	179 (98%)	4 (2%)	52	80
1	F	180/244 (74%)	179 (99%)	1 (1%)	86	95
All	All	1083/1464 (74%)	1064 (98%)	19 (2%)	59	83

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	ASP
1	A	407	ASN
1	A	438	ASP
1	B	233	ARG
1	B	265	LEU
1	B	317	HIS
1	C	307	MET

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Mol	Chain	Res	Type
1	C	317	HIS
1	C	343	LEU
1	D	223	ASP
1	D	233	ARG
1	D	322	ILE
1	D	406	VAL
1	D	448	TYR
1	E	228	MET
1	E	242	HIS
1	E	315	LEU
1	E	448	TYR
1	F	343	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	HIS
1	A	317	HIS
1	D	407	ASN
1	E	462	GLN
1	F	452	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	63R	B	600	1	33,33,33	2.23	6 (18%)	44,45,45	1.23	6 (13%)

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	63R	B	600	1	-	0/24/42/42	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	63R	CD-N1	6.56	1.49	1.34
2	B	600	63R	C2-NX	5.34	1.47	1.37
2	B	600	63R	C3-NX	5.07	1.51	1.43
2	B	600	63R	CE-CD	4.76	1.57	1.50
2	B	600	63R	CH-N2	3.62	1.48	1.38
2	B	600	63R	C0-N1	2.34	1.49	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	63R	C0-C9-NX	-3.77	108.77	116.59
2	B	600	63R	CC-CB-CA	2.81	114.78	110.85
2	B	600	63R	CM-CN-N2	2.25	114.17	110.02
2	B	600	63R	C9-C0-N1	-2.18	106.63	109.57
2	B	600	63R	C1-C2-NX	2.06	120.83	117.86
2	B	600	63R	CL-CK-N2	2.05	113.81	110.02

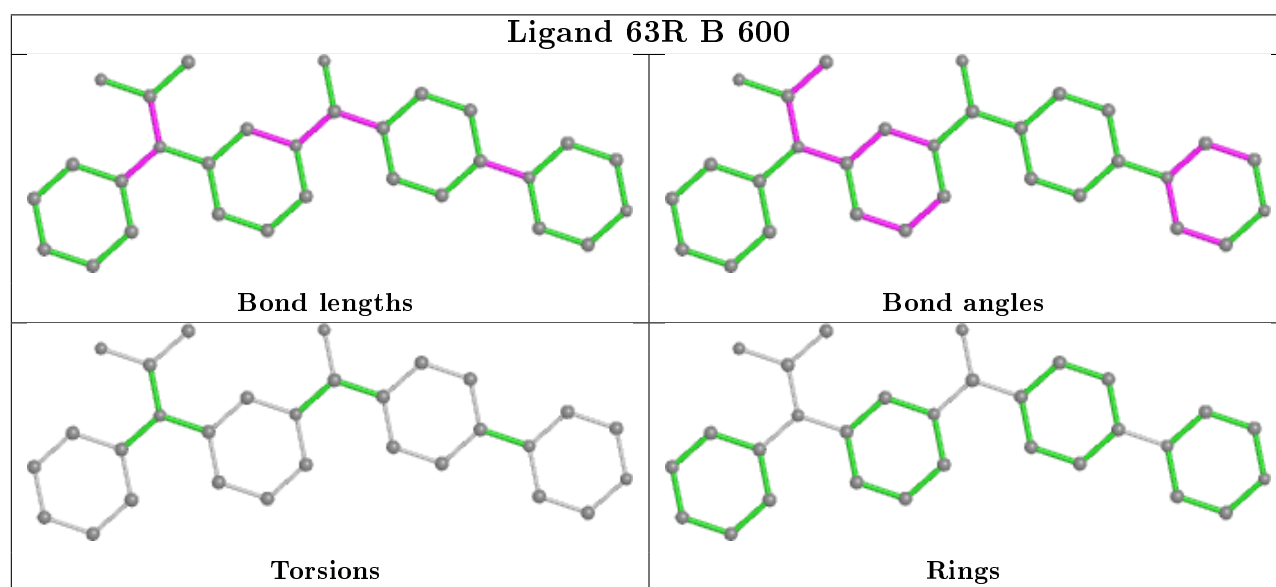
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	209/274 (76%)	0.42	8 (3%)	40 36	39, 42, 45, 46	0
1	B	207/274 (75%)	0.31	9 (4%)	35 31	37, 40, 43, 46	0
1	C	206/274 (75%)	0.42	9 (4%)	34 30	43, 45, 47, 49	0
1	D	210/274 (76%)	0.37	10 (4%)	30 26	44, 47, 49, 51	0
1	E	210/274 (76%)	0.39	10 (4%)	30 26	42, 44, 47, 50	0
1	F	209/274 (76%)	0.51	9 (4%)	35 31	43, 46, 48, 49	0
All	All	1251/1644 (76%)	0.40	55 (4%)	34 30	37, 44, 48, 51	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	222	LEU	3.5
1	D	479	ASP	3.5
1	A	228	MET	3.5
1	C	478	SER	3.2
1	E	250	LYS	3.2
1	E	479	ASP	3.1
1	F	467	THR	3.1
1	E	254	LEU	3.0
1	A	467	THR	2.9
1	C	467	THR	2.9
1	C	420	TRP	2.9
1	B	479	ASP	2.8
1	C	255	HIS	2.8
1	C	466	PRO	2.7
1	E	252	PRO	2.7
1	A	250	LYS	2.6
1	D	478	SER	2.6
1	F	466	PRO	2.5
1	A	407	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	466	PRO	2.5
1	F	265	LEU	2.5
1	D	265	LEU	2.5
1	F	264	HIS	2.5
1	C	264	HIS	2.5
1	E	466	PRO	2.4
1	F	469	THR	2.3
1	A	255	HIS	2.3
1	B	469	THR	2.3
1	D	254	LEU	2.3
1	E	251	VAL	2.3
1	E	408	ASN	2.3
1	A	420	TRP	2.3
1	C	479	ASP	2.3
1	D	252	PRO	2.3
1	B	312	CYS	2.3
1	D	469	THR	2.3
1	B	261	ASN	2.2
1	E	257	ILE	2.2
1	D	466	PRO	2.2
1	D	407	ASN	2.2
1	F	254	LEU	2.2
1	B	467	THR	2.2
1	B	466	PRO	2.1
1	F	479	ASP	2.1
1	D	467	THR	2.1
1	B	313	CYS	2.1
1	B	247	ALA	2.1
1	E	402	GLY	2.1
1	C	343	LEU	2.0
1	A	260	ARG	2.0
1	F	247	ALA	2.0
1	C	261	ASN	2.0
1	B	255	HIS	2.0
1	E	467	THR	2.0
1	F	243	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

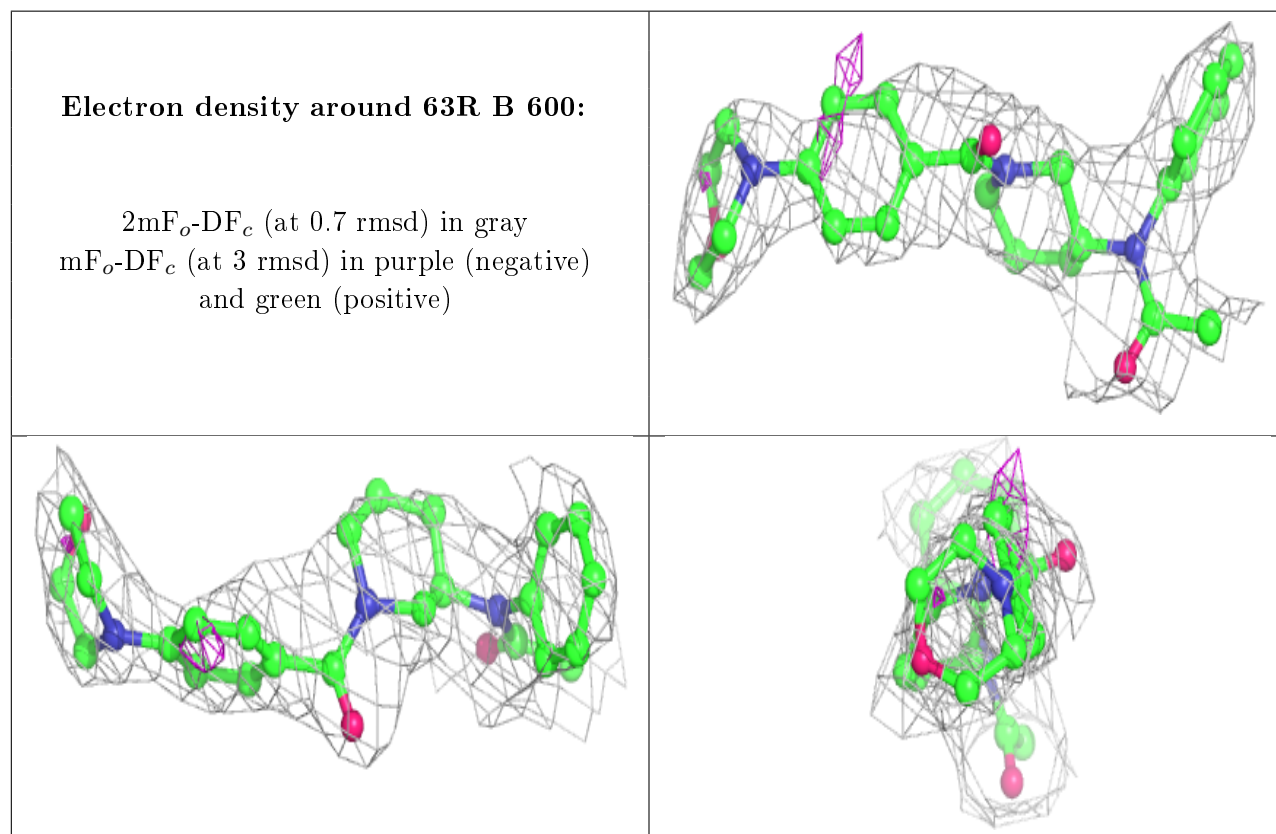
There are no carbohydrates in this entry.

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(\AA^2)	Q<0.9
2	63R	B	600	30/30	0.86	0.38	42,42,42,42	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.