



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 10:49 am BST

PDB ID : 5JY3
Title : CRYSTAL STRUCTURE OF LXRbeta (NUCLEAR RECEPTOR SUBFAMILY 1, GROUP H, MEMBER 2) COMPLEXED WITH BMS-852927
Authors : Muckelbauer, J.K.
Deposited on : 2016-05-13
Resolution : 2.40 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

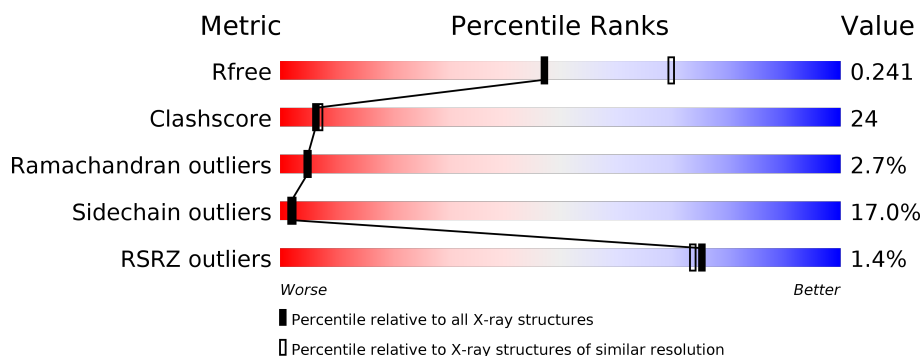
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	264	<div> <div>0%</div> <div> <div>48%</div> <div>27%</div> <div>11%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	264	<div> <div>2%</div> <div> <div>42%</div> <div>35%</div> <div>8%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	264	<div> <div>2%</div> <div> <div>44%</div> <div>32%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	264	<div> <div>40%</div> <div>35%</div> <div>10%</div> <div>•</div> <div>14%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BU1	D	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7798 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 Oxysterols receptor LXR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1862	1192	329	334	7			
1	B	230	Total	C	N	O	S	0	1	0
			1876	1204	329	336	7			
1	C	231	Total	C	N	O	S	0	1	0
			1883	1205	333	338	7			
1	D	227	Total	C	N	O	S	0	0	0
			1855	1187	328	333	7			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	MET	-	initiating methionine	UNP P55055
A	199	HIS	-	expression tag	UNP P55055
A	200	HIS	-	expression tag	UNP P55055
A	201	HIS	-	expression tag	UNP P55055
A	202	HIS	-	expression tag	UNP P55055
A	203	HIS	-	expression tag	UNP P55055
A	204	HIS	-	expression tag	UNP P55055
A	205	GLY	-	expression tag	UNP P55055
A	206	GLU	-	expression tag	UNP P55055
A	207	ASN	-	expression tag	UNP P55055
A	208	LEU	-	expression tag	UNP P55055
A	209	TYR	-	expression tag	UNP P55055
A	210	PHE	-	expression tag	UNP P55055
A	211	GLN	-	expression tag	UNP P55055
A	212	GLY	-	expression tag	UNP P55055
A	213	SER	-	expression tag	UNP P55055
B	198	MET	-	initiating methionine	UNP P55055
B	199	HIS	-	expression tag	UNP P55055
B	200	HIS	-	expression tag	UNP P55055
B	201	HIS	-	expression tag	UNP P55055
B	202	HIS	-	expression tag	UNP P55055

Continued on next page...

Continued from previous page...

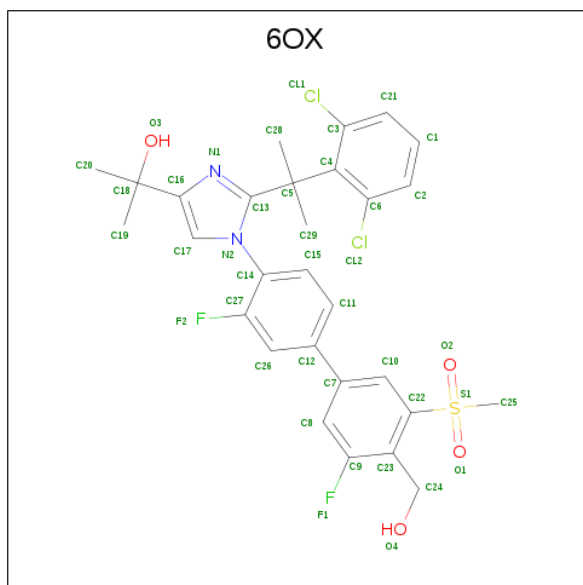
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	HIS	-	expression tag	UNP P55055
B	204	HIS	-	expression tag	UNP P55055
B	205	GLY	-	expression tag	UNP P55055
B	206	GLU	-	expression tag	UNP P55055
B	207	ASN	-	expression tag	UNP P55055
B	208	LEU	-	expression tag	UNP P55055
B	209	TYR	-	expression tag	UNP P55055
B	210	PHE	-	expression tag	UNP P55055
B	211	GLN	-	expression tag	UNP P55055
B	212	GLY	-	expression tag	UNP P55055
B	213	SER	-	expression tag	UNP P55055
C	198	MET	-	initiating methionine	UNP P55055
C	199	HIS	-	expression tag	UNP P55055
C	200	HIS	-	expression tag	UNP P55055
C	201	HIS	-	expression tag	UNP P55055
C	202	HIS	-	expression tag	UNP P55055
C	203	HIS	-	expression tag	UNP P55055
C	204	HIS	-	expression tag	UNP P55055
C	205	GLY	-	expression tag	UNP P55055
C	206	GLU	-	expression tag	UNP P55055
C	207	ASN	-	expression tag	UNP P55055
C	208	LEU	-	expression tag	UNP P55055
C	209	TYR	-	expression tag	UNP P55055
C	210	PHE	-	expression tag	UNP P55055
C	211	GLN	-	expression tag	UNP P55055
C	212	GLY	-	expression tag	UNP P55055
C	213	SER	-	expression tag	UNP P55055
D	198	MET	-	initiating methionine	UNP P55055
D	199	HIS	-	expression tag	UNP P55055
D	200	HIS	-	expression tag	UNP P55055
D	201	HIS	-	expression tag	UNP P55055
D	202	HIS	-	expression tag	UNP P55055
D	203	HIS	-	expression tag	UNP P55055
D	204	HIS	-	expression tag	UNP P55055
D	205	GLY	-	expression tag	UNP P55055
D	206	GLU	-	expression tag	UNP P55055
D	207	ASN	-	expression tag	UNP P55055
D	208	LEU	-	expression tag	UNP P55055
D	209	TYR	-	expression tag	UNP P55055
D	210	PHE	-	expression tag	UNP P55055
D	211	GLN	-	expression tag	UNP P55055
D	212	GLY	-	expression tag	UNP P55055

Continued on next page...

Continued from previous page...

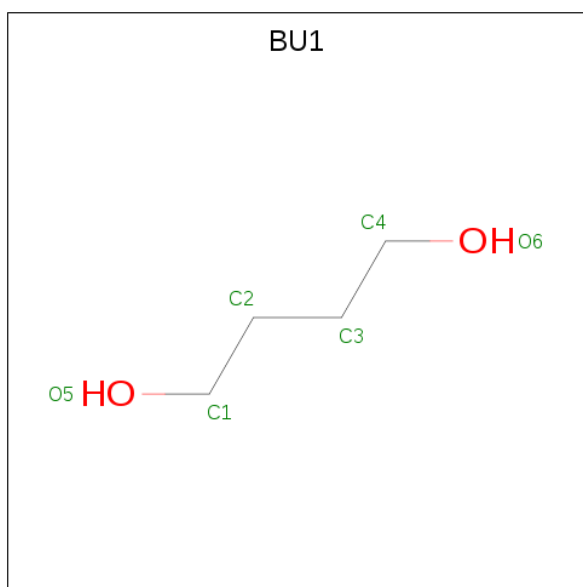
Chain	Residue	Modelled	Actual	Comment	Reference
D	213	SER	-	expression tag	UNP P55055

- Molecule 2 is 2-[2-[2-[2,6-bis(chloranyl)phenyl]propan-2-yl]-1-[2-fluoranyl-4-[3-fluoranyl-4-(hydroxymethyl)-5-methylsulfonyl-phenyl]phenyl]imidazol-4-yl]propan-2-ol (three-letter code: 6OX) (formula: $C_{29}H_{28}Cl_2F_2N_2O_4S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	0
			40	29	2	2	2	4	1		
2	B	1	Total	C	Cl	F	N	O	S	0	0
			40	29	2	2	2	4	1		
2	C	1	Total	C	Cl	F	N	O	S	0	0
			40	29	2	2	2	4	1		
2	D	1	Total	C	Cl	F	N	O	S	0	0
			40	29	2	2	2	4	1		

- Molecule 3 is 1,4-BUTANEDIOL (three-letter code: BU1) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	4	2		
3	D	1	Total	C	O	0	0
			6	4	2		

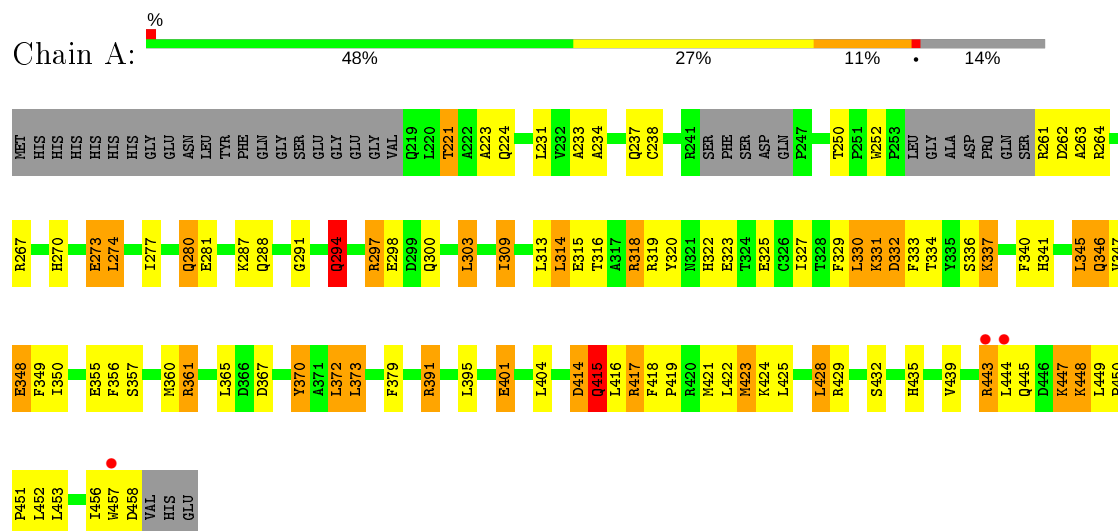
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	37	Total	O	0	0
			37	37		
4	C	37	Total	O	0	0
			37	37		
4	D	41	Total	O	0	0
			41	41		

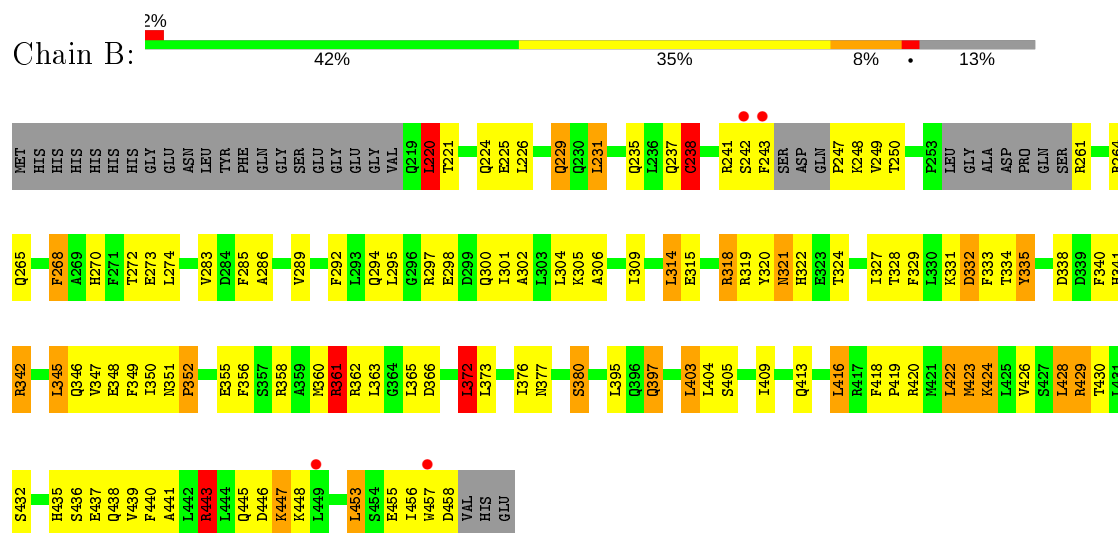
3 Residue-property plots

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.

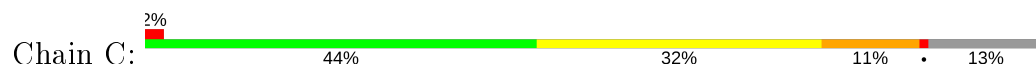
• Molecule 1: Oxysterols receptor LXR-beta

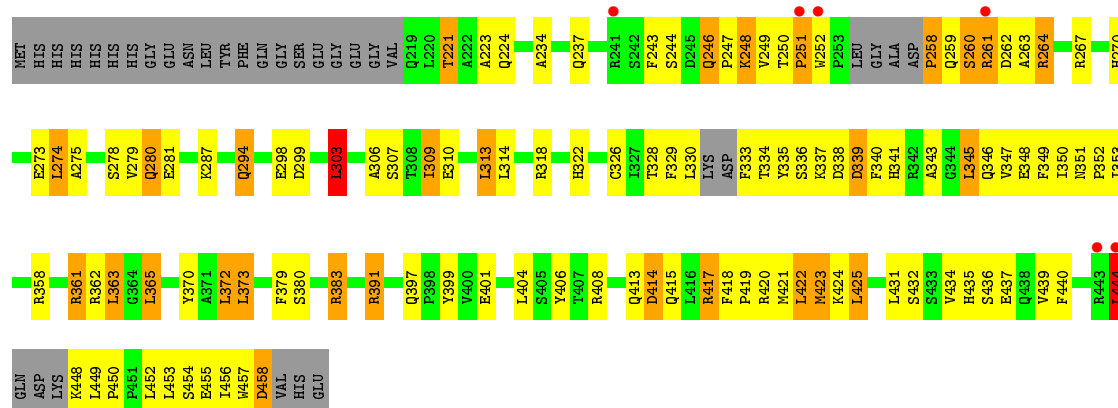


• Molecule 1: Oxysterols receptor LXR-beta



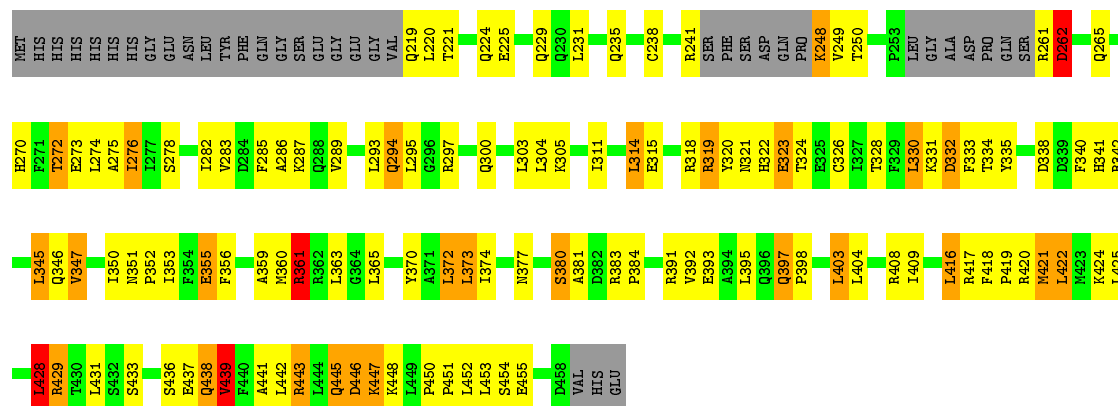
• Molecule 1: Oxysterols receptor LXR-beta





• Molecule 1: Oxysterols receptor LXR-beta

Chain D: 40% 35% 10% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.66Å 120.35Å 55.72Å 90.00° 107.49° 90.00°	Depositor
Resolution (Å)	99.01 – 2.40 33.64 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (99.01-2.40) 97.7 (33.64-2.40)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.268 0.219 , 0.241	Depositor DCC
R_{free} test set	3493 reflections (7.85%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 22.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.479 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7798	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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: BU1, 6OX

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	1.22	8/1897 (0.4%)	1.17	12/2562 (0.5%)
1	B	1.28	6/1915 (0.3%)	1.24	19/2588 (0.7%)
1	C	1.18	3/1921 (0.2%)	1.19	15/2596 (0.6%)
1	D	1.24	4/1889 (0.2%)	1.25	16/2551 (0.6%)
All	All	1.23	21/7622 (0.3%)	1.21	62/10297 (0.6%)

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	D	0	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	CYS	CB-SG	-10.70	1.64	1.82
1	A	401	GLU	CD-OE2	8.00	1.34	1.25
1	A	273	GLU	CG-CD	6.22	1.61	1.51
1	A	355	GLU	CG-CD	6.18	1.61	1.51
1	B	355	GLU	CG-CD	5.85	1.60	1.51
1	B	229	GLN	CG-CD	5.75	1.64	1.51
1	A	379	PHE	CD2-CE2	5.67	1.50	1.39
1	D	397	GLN	CG-CD	5.65	1.64	1.51
1	D	359	ALA	CA-CB	5.62	1.64	1.52
1	A	238	CYS	CB-SG	-5.59	1.72	1.81
1	C	399	TYR	CD2-CE2	-5.46	1.31	1.39
1	A	370	TYR	CD2-CE2	5.44	1.47	1.39
1	B	298	GLU	CG-CD	5.41	1.60	1.51
1	D	355	GLU	CG-CD	5.41	1.60	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	379	PHE	CD2-CE2	5.39	1.50	1.39
1	A	281	GLU	CD-OE2	5.27	1.31	1.25
1	A	355	GLU	CB-CG	5.23	1.62	1.52
1	B	335	TYR	CD2-CE2	-5.15	1.31	1.39
1	B	306	ALA	CA-CB	-5.07	1.41	1.52
1	C	406	TYR	CB-CG	-5.04	1.44	1.51
1	D	370	TYR	CE1-CZ	5.00	1.45	1.38

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	373	LEU	CB-CG-CD2	-8.35	96.80	111.00
1	D	314	LEU	CA-CB-CG	8.02	133.74	115.30
1	C	373	LEU	CB-CG-CD2	-7.97	97.46	111.00
1	A	373	LEU	CB-CG-CD2	-7.83	97.68	111.00
1	D	361	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	D	318	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	C	444	LEU	CA-CB-CG	7.49	132.52	115.30
1	C	420	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	D	365	LEU	CB-CG-CD2	-7.08	98.96	111.00
1	B	372	LEU	CA-CB-CG	6.68	130.66	115.30
1	B	318	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	314	LEU	CA-CB-CG	6.55	130.37	115.30
1	D	397	GLN	C-N-CD	6.54	142.14	128.40
1	B	358	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	B	319	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	B	314	LEU	CA-CB-CG	6.51	130.27	115.30
1	B	361	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	D	319	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	D	443	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	D	318	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	362	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	391	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	420	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	397[A]	GLN	C-N-CD	6.09	141.19	128.40
1	B	397[B]	GLN	C-N-CD	6.09	141.19	128.40
1	C	258	PRO	N-CA-CB	6.03	110.53	103.30
1	A	294	GLN	N-CA-CB	-6.00	99.79	110.60
1	D	372	LEU	CA-CB-CG	5.96	129.01	115.30
1	D	422	LEU	CA-CB-CG	5.87	128.80	115.30
1	B	226	LEU	CB-CG-CD2	-5.86	101.03	111.00
1	C	303	LEU	CB-CG-CD1	5.82	120.90	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	372	LEU	CA-CB-CG	5.69	128.38	115.30
1	B	319	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	367	ASP	CB-CG-OD1	5.58	123.32	118.30
1	D	421	MET	CG-SD-CE	-5.58	91.28	100.20
1	D	428	LEU	CB-CG-CD2	-5.57	101.53	111.00
1	C	363	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	416	LEU	CB-CG-CD1	-5.53	101.60	111.00
1	D	417	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	A	428	LEU	CB-CG-CD2	-5.48	101.69	111.00
1	C	365	LEU	CA-CB-CG	5.48	127.89	115.30
1	D	332	ASP	CB-CG-OD2	5.46	123.22	118.30
1	C	383[A]	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	383[B]	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	391	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	318	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	B	220	LEU	CA-CB-CG	5.37	127.65	115.30
1	B	428	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	367	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	C	372	LEU	CA-CB-CG	5.35	127.61	115.30
1	D	428	LEU	CA-CB-CG	5.28	127.44	115.30
1	D	373	LEU	CB-CG-CD1	5.24	119.91	111.00
1	C	262	ASP	CB-CA-C	-5.21	99.98	110.40
1	B	332	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	372	LEU	CB-CG-CD2	5.18	119.80	111.00
1	C	372	LEU	CB-CG-CD1	5.17	119.79	111.00
1	B	342	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	443	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	303	LEU	CB-CG-CD2	5.07	119.61	111.00
1	A	372	LEU	CB-CG-CD1	5.07	119.61	111.00
1	B	423	MET	CG-SD-CE	-5.01	92.18	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	262	ASP	Peptide

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	1862	0	1895	94	0
1	B	1876	0	1904	101	0
1	C	1883	0	1904	121	0
1	D	1855	0	1887	100	0
2	A	40	0	0	4	0
2	B	40	0	0	5	0
2	C	40	0	0	4	0
2	D	40	0	0	4	0
3	B	6	0	10	1	0
3	D	6	0	10	5	0
4	A	35	0	0	1	0
4	B	37	0	0	1	0
4	C	37	0	0	3	0
4	D	41	0	0	1	0
All	All	7798	0	7610	368	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 24.

All (368) 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)
2:B:501:6OX:CL2	2:B:501:6OX:C28	2.11	1.35
2:D:501:6OX:C28	2:D:501:6OX:CL2	2.17	1.29
1:D:341:HIS:CE1	1:D:347:VAL:HG23	1.79	1.18
1:C:408:ARG:HH22	1:D:408:ARG:NH2	1.43	1.14
1:A:261:ARG:NH2	4:A:601:HOH:O	1.83	1.11
1:C:457:TRP:HZ2	1:D:300:GLN:NE2	1.51	1.08
1:C:221:THR:HG22	1:C:224:GLN:H	1.15	1.07
1:D:341:HIS:HE1	1:D:347:VAL:HG23	1.08	1.01
1:C:246:GLN:OE1	4:C:601:HOH:O	1.77	1.00
1:A:457:TRP:HZ2	1:B:300:GLN:HE21	1.05	0.95
1:A:457:TRP:HZ2	1:B:300:GLN:NE2	1.64	0.94
1:B:242:SER:O	1:B:243:PHE:CD1	2.20	0.94
1:C:457:TRP:CZ2	1:D:300:GLN:NE2	2.36	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:PHE:HB3	2:C:501:6OX:C25	1.97	0.93
1:C:383[B]:ARG:HD2	4:C:617:HOH:O	1.67	0.92
1:C:347:VAL:HG13	1:C:348:GLU:OE2	1.71	0.91
1:C:274:LEU:HG	2:C:501:6OX:C25	2.02	0.89
1:A:221:THR:HG22	1:A:224:GLN:H	1.34	0.89
1:C:326:CYS:HB3	1:C:334:THR:HG23	1.54	0.88
1:A:273:GLU:HG2	1:C:444:LEU:HD23	1.56	0.88
1:C:246:GLN:HB2	1:C:330:LEU:HD13	1.55	0.88
1:B:438:GLN:HG3	1:B:441:ALA:HB3	1.56	0.87
1:C:259:GLN:O	1:C:260:SER:OG	1.92	0.87
1:D:360:MET:SD	1:D:424:LYS:HG2	2.14	0.87
2:D:501:6OX:CL1	2:D:501:6OX:C29	2.60	0.86
1:C:457:TRP:HZ2	1:D:300:GLN:HE22	1.19	0.86
1:A:329:PHE:HB3	2:A:501:6OX:C25	2.06	0.85
1:C:408:ARG:HH22	1:D:408:ARG:HH22	1.26	0.84
1:C:408:ARG:NH2	1:D:408:ARG:NH2	2.26	0.84
1:D:219:GLN:HA	1:D:409:ILE:HD11	1.59	0.83
1:D:283:VAL:HG22	1:D:304:LEU:HD21	1.59	0.83
1:C:246:GLN:CB	1:C:330:LEU:HD13	2.09	0.82
1:A:274:LEU:HG	2:A:501:6OX:C25	2.10	0.82
1:B:261:ARG:O	1:B:265:GLN:HG3	1.79	0.82
2:A:501:6OX:CL2	2:A:501:6OX:C28	2.65	0.81
2:C:501:6OX:CL1	2:C:501:6OX:C29	2.66	0.81
1:B:446:ASP:HB3	1:C:287:LYS:NZ	1.96	0.81
1:A:414:ASP:O	1:A:415:GLN:HB2	1.80	0.80
1:B:345:LEU:HB3	1:B:350:ILE:CD1	2.11	0.79
1:D:341:HIS:HE1	1:D:347:VAL:CG2	1.93	0.79
1:A:457:TRP:CZ2	1:B:300:GLN:NE2	2.45	0.79
1:C:221:THR:HG22	1:C:224:GLN:N	1.97	0.79
1:D:321:ASN:HD21	1:D:324:THR:HG23	1.49	0.78
1:C:345:LEU:HB3	1:C:350:ILE:HD11	1.65	0.77
1:C:261:ARG:HE	1:C:263:ALA:HB2	1.48	0.77
1:C:347:VAL:CG1	1:C:348:GLU:OE2	2.31	0.77
1:B:286:ALA:HA	1:B:289:VAL:HG13	1.67	0.77
1:B:274:LEU:HG	2:B:501:6OX:C25	2.14	0.77
1:D:438:GLN:HG3	1:D:441:ALA:HB3	1.66	0.77
1:C:221:THR:CG2	1:C:224:GLN:HG3	2.14	0.76
1:D:452:LEU:O	1:D:455:GLU:HB3	1.84	0.76
1:A:331:LYS:O	1:A:332:ASP:HB2	1.85	0.76
1:A:264:ARG:HH11	1:C:347:VAL:HG11	1.50	0.75
1:C:260:SER:O	1:C:261:ARG:HG2	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:HIS:HE1	1:B:347:VAL:HG22	1.51	0.74
1:C:258:PRO:O	4:C:602:HOH:O	2.05	0.74
1:B:361:ARG:HH11	1:B:361:ARG:HG3	1.53	0.73
1:D:286:ALA:HA	1:D:289:VAL:HG13	1.68	0.73
1:D:221:THR:H	1:D:224:GLN:HE21	1.37	0.73
1:D:361:ARG:HH11	1:D:361:ARG:HG3	1.53	0.72
1:B:351:ASN:HB2	1:B:352:PRO:HD3	1.72	0.72
1:D:274:LEU:HG	2:D:501:6OX:C25	2.19	0.72
1:A:450:PRO:HG3	1:B:305:LYS:HD2	1.72	0.71
1:D:235:GLN:HG3	3:D:502:BU1:H21	1.73	0.70
1:A:264:ARG:NH1	1:C:347:VAL:HG11	2.06	0.70
1:D:283:VAL:HG22	1:D:304:LEU:CD2	2.22	0.70
1:C:347:VAL:HG22	1:C:351:ASN:HD22	1.55	0.70
1:D:361:ARG:HH11	1:D:361:ARG:CG	2.05	0.69
1:A:252:TRP:CH2	1:A:267:ARG:HD2	2.27	0.69
1:D:320:TYR:OH	1:D:322:HIS:HD2	1.75	0.69
1:B:345:LEU:HB3	1:B:350:ILE:HD12	1.75	0.69
1:B:345:LEU:HB3	1:B:350:ILE:HD11	1.73	0.68
1:B:361:ARG:HH11	1:B:361:ARG:CG	2.06	0.68
1:D:374:ILE:CD1	3:D:502:BU1:H11	2.23	0.68
1:B:320:TYR:OH	1:B:322:HIS:CD2	2.47	0.68
1:D:272:THR:HG23	1:D:450:PRO:HG2	1.75	0.68
1:B:320:TYR:OH	1:B:322:HIS:HD2	1.76	0.68
1:A:291:GLY:O	1:A:294:GLN:HB3	1.93	0.68
1:C:260:SER:O	1:C:261:ARG:CG	2.42	0.68
1:C:221:THR:HG22	1:C:224:GLN:HG3	1.76	0.68
1:A:439:VAL:O	1:A:439:VAL:HG12	1.93	0.68
1:C:309:ILE:HD13	1:C:313:LEU:HD22	1.75	0.68
1:C:328:THR:HA	1:C:333:PHE:O	1.94	0.68
1:C:261:ARG:HG3	1:C:263:ALA:H	1.58	0.68
1:C:345:LEU:CB	1:C:350:ILE:HD11	2.23	0.68
1:D:235:GLN:NE2	3:D:502:BU1:O5	2.23	0.67
1:D:438:GLN:O	1:D:438:GLN:HG2	1.94	0.67
1:A:297:ARG:HH11	1:A:300:GLN:HE22	1.43	0.67
1:A:423:MET:HE2	1:A:423:MET:HA	1.77	0.66
1:B:446:ASP:HB3	1:C:287:LYS:HZ1	1.61	0.66
1:A:439:VAL:CG2	1:C:435:HIS:HE1	2.09	0.66
1:C:440:PHE:O	1:D:439:VAL:HG21	1.95	0.66
1:D:276:ILE:HG13	1:D:453:LEU:HD13	1.78	0.66
1:B:238:CYS:SG	1:B:285:PHE:HB2	2.36	0.66
1:A:458:ASP:OD1	1:B:297:ARG:NH2	2.27	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:6OX:CL1	2:B:501:6OX:C29	2.82	0.65
1:C:246:GLN:HB2	1:C:330:LEU:CD1	2.26	0.65
1:C:326:CYS:CB	1:C:334:THR:HG23	2.27	0.65
1:D:361:ARG:NH1	1:D:361:ARG:HG3	2.09	0.65
1:B:341:HIS:HE1	1:B:347:VAL:CG2	2.09	0.65
1:B:360:MET:SD	1:B:424:LYS:HG2	2.36	0.65
1:B:445:GLN:HB3	1:B:447:LYS:HD3	1.79	0.65
1:A:439:VAL:HG23	1:C:435:HIS:HE1	1.61	0.65
1:A:341:HIS:CE1	1:A:347:VAL:HG13	2.32	0.64
1:C:221:THR:CG2	1:C:224:GLN:H	2.01	0.64
1:B:328:THR:HA	1:B:333:PHE:O	1.99	0.63
1:D:221:THR:H	1:D:224:GLN:NE2	1.96	0.63
1:A:280:GLN:HE22	1:D:443:ARG:HB3	1.63	0.63
1:D:351:ASN:HB2	1:D:352:PRO:HD3	1.78	0.63
1:D:270:HIS:HE1	1:D:335:TYR:OH	1.81	0.63
1:C:431:LEU:O	1:C:434:VAL:HG12	1.99	0.63
1:A:221:THR:HG22	1:A:224:GLN:N	2.12	0.62
1:C:423:MET:HE1	1:D:425:LEU:HD12	1.81	0.62
1:D:451:PRO:HA	1:D:454:SER:HB3	1.80	0.62
1:B:447:LYS:NZ	1:B:447:LYS:HB2	2.14	0.62
1:B:270:HIS:HE1	1:B:335:TYR:OH	1.82	0.62
1:B:423:MET:O	1:B:426:VAL:HB	2.00	0.62
1:A:267:ARG:O	1:A:270:HIS:HB3	2.00	0.62
1:B:321:ASN:HD21	1:B:324:THR:CG2	2.12	0.62
1:A:457:TRP:CE3	1:B:283:VAL:HG13	2.35	0.61
1:B:361:ARG:HG3	1:B:361:ARG:NH1	2.14	0.61
1:C:414:ASP:O	1:C:415:GLN:HB2	2.00	0.61
1:A:457:TRP:CZ3	1:B:283:VAL:HG13	2.35	0.61
1:D:321:ASN:HD21	1:D:324:THR:CG2	2.14	0.61
1:C:306:ALA:HB3	1:C:383[B]:ARG:HD3	1.81	0.61
1:A:298:GLU:HG3	1:D:346:GLN:HE22	1.64	0.61
1:B:221:THR:H	1:B:224:GLN:NE2	1.99	0.61
1:D:324:THR:OG1	1:D:326:CYS:HB2	2.01	0.60
1:D:320:TYR:OH	1:D:322:HIS:CD2	2.54	0.60
1:A:322:HIS:CD2	1:A:322:HIS:O	2.55	0.60
1:B:320:TYR:CE2	1:B:322:HIS:HD2	2.19	0.60
1:C:458:ASP:OD1	1:D:297:ARG:NH2	2.30	0.60
1:D:418:PHE:HB3	1:D:419:PRO:HD3	1.84	0.60
1:D:374:ILE:HD12	3:D:502:BU1:H11	1.84	0.60
1:D:438:GLN:O	1:D:438:GLN:CG	2.50	0.60
1:D:250:THR:HG23	1:D:273:GLU:OE1	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:MET:CE	1:A:423:MET:HA	2.31	0.59
1:C:450:PRO:O	1:C:454:SER:HB2	2.02	0.59
2:D:501:6OX:CL1	2:D:501:6OX:C13	2.87	0.59
1:B:345:LEU:CB	1:B:350:ILE:HD11	2.31	0.59
1:C:341:HIS:HE1	1:C:347:VAL:HA	1.66	0.59
1:B:321:ASN:ND2	1:B:324:THR:OG1	2.35	0.59
1:B:320:TYR:CZ	1:B:322:HIS:HD2	2.21	0.59
1:C:306:ALA:CB	1:C:383[B]:ARG:HD3	2.33	0.58
1:D:328:THR:HA	1:D:333:PHE:O	2.04	0.58
1:B:351:ASN:CB	1:B:352:PRO:HD3	2.33	0.58
1:D:315:GLU:O	1:D:319:ARG:HG3	2.03	0.58
1:A:340:PHE:O	1:A:345:LEU:HB2	2.04	0.58
1:A:234:ALA:HA	1:A:237:GLN:CD	2.22	0.58
1:B:446:ASP:CB	1:C:287:LYS:NZ	2.65	0.58
1:B:345:LEU:CB	1:B:350:ILE:CD1	2.81	0.57
1:D:275:ALA:HB3	1:D:453:LEU:HD21	1.84	0.57
1:C:419:PRO:HG3	1:D:418:PHE:HE2	1.69	0.57
1:C:401:GLU:HG2	1:D:416:LEU:HD11	1.86	0.57
1:A:261:ARG:HG3	1:A:262:ASP:N	2.20	0.57
1:C:260:SER:O	1:C:261:ARG:CB	2.52	0.57
1:D:381:ALA:HB2	1:D:392:VAL:HG22	1.87	0.56
1:D:338:ASP:HB3	1:D:342:ARG:HH21	1.69	0.56
1:A:360:MET:SD	1:A:424:LYS:HG2	2.44	0.56
1:B:446:ASP:HB3	1:C:287:LYS:HZ3	1.71	0.56
1:C:347:VAL:HG22	1:C:351:ASN:ND2	2.20	0.56
1:B:237:GLN:HG2	1:B:241:ARG:NH2	2.20	0.56
1:D:351:ASN:CB	1:D:352:PRO:HD3	2.34	0.56
1:A:439:VAL:CG2	1:C:435:HIS:CE1	2.88	0.56
1:C:365:LEU:HD22	1:C:421:MET:CE	2.35	0.56
1:A:356:PHE:CZ	1:A:428:LEU:HD13	2.40	0.56
1:C:339:ASP:N	1:C:339:ASP:OD1	2.39	0.56
1:C:322:HIS:HB3	1:C:361:ARG:HE	1.71	0.56
2:A:501:6OX:C13	2:A:501:6OX:CL1	2.92	0.55
1:A:443:ARG:HE	1:B:458:ASP:HA	1.71	0.55
1:A:414:ASP:O	1:A:415:GLN:CB	2.54	0.55
1:B:340:PHE:HB3	1:B:350:ILE:HD13	1.88	0.55
1:B:309:ILE:HG22	4:B:606:HOH:O	2.06	0.54
1:B:231:LEU:HD23	1:B:372:LEU:HD13	1.90	0.54
1:D:438:GLN:CG	1:D:441:ALA:HB3	2.35	0.54
1:B:321:ASN:HD21	1:B:324:THR:HG23	1.71	0.54
1:D:436:SER:O	1:D:439:VAL:HG22	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:THR:CG2	1:D:450:PRO:HG2	2.37	0.54
1:A:221:THR:CG2	1:A:224:GLN:H	2.15	0.54
1:B:341:HIS:CE1	1:B:347:VAL:HG22	2.38	0.54
1:C:278:SER:O	1:C:281:GLU:HB2	2.08	0.54
1:D:238:CYS:SG	1:D:285:PHE:HB2	2.48	0.54
1:D:262:ASP:HA	1:D:265:GLN:HG3	1.89	0.54
1:D:319:ARG:HD3	1:D:328:THR:O	2.07	0.54
1:A:347:VAL:HG21	1:C:264:ARG:HH11	1.73	0.53
1:A:309:ILE:O	1:A:309:ILE:HD13	2.07	0.53
1:B:443:ARG:HD2	1:C:280:GLN:HE21	1.74	0.53
1:A:429:ARG:HD2	1:B:430:THR:OG1	2.08	0.53
1:A:453:LEU:HB2	1:B:456:ILE:HD11	1.91	0.53
1:A:221:THR:HG23	1:A:223:ALA:H	1.74	0.53
1:A:450:PRO:HB2	1:B:455:GLU:OE2	2.08	0.53
1:C:418:PHE:HB3	1:C:419:PRO:HD3	1.91	0.53
1:C:275:ALA:O	1:C:279:VAL:HG23	2.09	0.53
1:B:446:ASP:CB	1:C:287:LYS:HZ3	2.22	0.52
1:C:294:GLN:O	1:C:391:ARG:NH2	2.41	0.52
1:B:249:VAL:HG22	1:B:270:HIS:CD2	2.44	0.52
1:A:445:GLN:HA	1:A:445:GLN:NE2	2.25	0.52
1:C:244:SER:O	1:C:247:PRO:HD2	2.10	0.52
1:A:347:VAL:HG11	1:C:264:ARG:HH11	1.73	0.52
1:D:219:GLN:HA	1:D:409:ILE:CD1	2.37	0.52
1:A:233:ALA:C	1:A:237:GLN:OE1	2.48	0.52
1:C:318:ARG:HG3	1:C:370:TYR:CD2	2.44	0.52
1:D:315:GLU:OE1	3:D:502:BU1:H12	2.10	0.52
1:C:397:GLN:O	1:C:401:GLU:HG3	2.09	0.51
1:B:315:GLU:OE1	1:B:318:ARG:HD3	2.11	0.51
1:A:234:ALA:N	1:A:237:GLN:OE1	2.43	0.51
1:A:347:VAL:HB	1:A:348:GLU:OE2	2.11	0.51
1:D:340:PHE:O	1:D:345:LEU:HB2	2.10	0.51
1:D:250:THR:O	1:D:270:HIS:HD2	1.94	0.51
2:B:501:6OX:C13	2:B:501:6OX:CL1	2.97	0.50
1:C:418:PHE:HB3	1:C:419:PRO:CD	2.41	0.50
1:B:360:MET:O	1:B:363:LEU:HB2	2.10	0.50
1:A:234:ALA:HA	1:A:237:GLN:OE1	2.12	0.50
1:B:220:LEU:HD13	1:B:405:SER:HB2	1.93	0.50
1:C:450:PRO:HG3	1:D:305:LYS:HD2	1.93	0.50
1:B:235:GLN:HG3	3:B:502:BU1:C4	2.41	0.50
1:D:321:ASN:ND2	1:D:324:THR:OG1	2.45	0.50
1:D:311:ILE:HG12	1:D:374:ILE:HG23	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:ASN:O	1:D:380:SER:OG	2.29	0.50
1:A:439:VAL:O	1:A:439:VAL:CG1	2.59	0.50
1:B:225:GLU:O	1:B:229:GLN:HG3	2.11	0.50
1:A:435:HIS:CE1	1:C:439:VAL:CG2	2.95	0.50
1:D:338:ASP:CB	1:D:342:ARG:HH21	2.25	0.50
1:A:318:ARG:HG2	1:A:370:TYR:CD2	2.47	0.50
1:D:321:ASN:OD1	1:D:323:GLU:HB2	2.12	0.50
1:A:331:LYS:O	1:A:332:ASP:CB	2.58	0.49
1:B:250:THR:O	1:B:270:HIS:HD2	1.94	0.49
1:C:349:PHE:CZ	1:C:435:HIS:HB2	2.47	0.49
1:D:446:ASP:C	1:D:446:ASP:OD1	2.49	0.49
1:B:356:PHE:CZ	1:B:428:LEU:HD13	2.47	0.49
1:D:250:THR:HG23	1:D:273:GLU:CD	2.32	0.49
1:C:261:ARG:HG3	1:C:263:ALA:N	2.28	0.49
1:C:365:LEU:HD22	1:C:421:MET:HE1	1.94	0.49
1:D:380:SER:O	1:D:383:ARG:HG2	2.13	0.49
1:C:457:TRP:CH2	1:D:287:LYS:HG2	2.47	0.49
1:A:336:SER:O	1:A:337:LYS:C	2.51	0.49
1:B:329:PHE:HB3	2:B:501:6OX:C25	2.43	0.49
1:D:439:VAL:HG12	1:D:443:ARG:HE	1.78	0.49
1:C:252:TRP:HE3	1:C:270:HIS:CD2	2.31	0.49
1:C:453:LEU:HD11	1:D:304:LEU:HD23	1.94	0.49
1:A:263:ALA:O	1:A:267:ARG:HG3	2.12	0.48
1:D:248:LYS:HA	1:D:248:LYS:HE2	1.95	0.48
1:D:250:THR:N	1:D:273:GLU:OE1	2.43	0.48
1:D:363:LEU:HD21	1:D:420:ARG:HG2	1.94	0.48
1:C:221:THR:CG2	1:C:223:ALA:HB3	2.43	0.48
1:C:246:GLN:HB3	1:C:330:LEU:HD13	1.95	0.48
1:A:234:ALA:HA	1:A:237:GLN:HG2	1.95	0.48
1:C:309:ILE:CD1	1:C:313:LEU:HD22	2.43	0.48
1:B:346:GLN:HE22	1:C:298:GLU:HG3	1.79	0.48
1:C:322:HIS:HB2	1:C:361:ARG:HG3	1.96	0.48
1:C:313:LEU:HD13	2:C:501:6OX:C1	2.43	0.48
1:C:326:CYS:HB3	1:C:334:THR:CG2	2.35	0.48
1:A:273:GLU:O	1:A:277:ILE:HD12	2.14	0.48
1:A:418:PHE:HB3	1:A:419:PRO:HD3	1.96	0.48
1:B:438:GLN:CG	1:B:438:GLN:O	2.60	0.48
1:C:307:SER:HB3	1:C:383[B]:ARG:NH1	2.28	0.48
1:B:304:LEU:HA	1:B:304:LEU:HD12	1.74	0.48
1:B:447:LYS:HB2	1:B:447:LYS:HZ3	1.77	0.48
1:C:243:PHE:O	1:C:246:GLN:HG2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:LEU:CD1	1:B:405:SER:HB2	2.44	0.47
1:D:350:ILE:O	1:D:353:ILE:HB	2.14	0.47
1:A:424:LYS:O	1:A:428:LEU:HB2	2.15	0.47
1:D:286:ALA:CA	1:D:289:VAL:HG13	2.41	0.47
1:A:322:HIS:ND1	1:A:361:ARG:NE	2.53	0.47
1:C:221:THR:HG21	1:C:224:GLN:HG3	1.96	0.47
1:C:340:PHE:O	1:C:345:LEU:HB2	2.14	0.47
1:A:274:LEU:HD12	1:A:274:LEU:HA	1.81	0.47
1:A:280:GLN:HB2	1:D:443:ARG:HH11	1.78	0.47
1:A:457:TRP:CE3	1:B:283:VAL:CG1	2.98	0.47
1:B:237:GLN:HG2	1:B:241:ARG:CZ	2.45	0.47
1:B:377:ASN:O	1:B:380:SER:OG	2.30	0.47
1:C:246:GLN:O	1:C:249:VAL:HG22	2.15	0.47
1:C:422:LEU:O	1:C:425:LEU:HB2	2.15	0.47
1:A:439:VAL:HG23	1:C:435:HIS:CE1	2.47	0.47
1:B:453:LEU:O	1:B:457:TRP:HB2	2.15	0.47
1:A:346:GLN:HG3	1:A:349:PHE:H	1.80	0.47
1:C:380:SER:O	1:C:383[B]:ARG:HG3	2.13	0.47
1:D:286:ALA:HA	1:D:289:VAL:CG1	2.40	0.46
1:D:384:PRO:HD3	4:D:613:HOH:O	2.15	0.46
1:B:426:VAL:O	1:B:429:ARG:HB2	2.16	0.46
1:B:361:ARG:CG	1:B:361:ARG:NH1	2.73	0.46
1:B:363:LEU:HD21	1:B:420:ARG:HB3	1.97	0.46
1:A:234:ALA:HA	1:A:237:GLN:CG	2.45	0.46
1:D:278:SER:O	1:D:282:ILE:HG13	2.16	0.46
1:A:443:ARG:NH1	1:B:436:SER:HB2	2.31	0.46
1:C:299:ASP:O	1:C:303:LEU:HB2	2.16	0.46
1:D:397:GLN:O	1:D:398:PRO:C	2.54	0.46
1:B:418:PHE:HB3	1:B:419:PRO:HD3	1.98	0.45
1:C:309:ILE:HD13	1:C:309:ILE:O	2.16	0.45
1:C:326:CYS:SG	1:C:336:SER:HB3	2.56	0.45
1:C:457:TRP:CE3	1:C:457:TRP:HA	2.51	0.45
1:B:366:ASP:C	1:B:366:ASP:OD1	2.55	0.45
1:C:252:TRP:CE3	1:C:270:HIS:CD2	3.05	0.45
1:D:429:ARG:HD3	1:D:429:ARG:HA	1.73	0.45
1:D:445:GLN:HB3	1:D:447:LYS:HE2	1.99	0.45
1:A:449:LEU:O	1:A:451:PRO:HD3	2.16	0.45
1:C:322:HIS:CB	1:C:361:ARG:HE	2.30	0.45
1:B:372:LEU:O	1:B:376:ILE:HG13	2.16	0.45
1:A:297:ARG:NH1	1:A:300:GLN:HE22	2.11	0.45
1:A:330:LEU:O	1:A:331:LYS:C	2.55	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:GLN:O	1:B:238:CYS:HB2	2.17	0.45
1:B:429:ARG:HD3	1:B:429:ARG:HA	1.48	0.44
1:A:435:HIS:HE1	1:C:439:VAL:CG2	2.30	0.44
1:B:349:PHE:CE2	1:B:435:HIS:HD2	2.35	0.44
1:D:303:LEU:HA	1:D:303:LEU:HD23	1.80	0.44
1:D:356:PHE:CZ	1:D:428:LEU:HD13	2.52	0.44
1:A:419:PRO:HB3	1:B:422:LEU:HD21	1.99	0.44
1:A:401:GLU:HG2	1:B:416:LEU:HD11	1.98	0.44
1:D:294:GLN:O	1:D:391:ARG:NH2	2.37	0.44
1:B:242:SER:O	1:B:243:PHE:HD1	1.89	0.44
1:A:221:THR:CG2	1:A:224:GLN:HG3	2.48	0.44
1:C:274:LEU:HD12	1:C:274:LEU:HA	1.84	0.44
1:C:246:GLN:N	1:C:247:PRO:CD	2.81	0.44
1:C:252:TRP:CH2	1:C:267:ARG:HD2	2.52	0.44
1:C:358:ARG:O	1:C:362:ARG:HG3	2.18	0.44
1:B:456:ILE:HG22	1:B:457:TRP:CD1	2.53	0.44
1:C:234:ALA:HA	1:C:237:GLN:HG2	2.00	0.44
1:C:457:TRP:CZ3	1:D:283:VAL:HG13	2.52	0.44
1:B:376:ILE:CD1	1:B:403:LEU:HD12	2.47	0.43
1:A:417:ARG:O	1:A:421:MET:HG3	2.18	0.43
1:B:363:LEU:HB3	1:B:365:LEU:CD1	2.48	0.43
1:A:391:ARG:O	1:A:395:LEU:HG	2.19	0.43
1:C:439:VAL:O	1:C:439:VAL:HG12	2.19	0.43
1:A:287:LYS:HZ3	1:D:446:ASP:HB2	1.83	0.43
1:A:347:VAL:HG21	1:C:264:ARG:NH1	2.34	0.43
1:B:320:TYR:CE2	1:B:322:HIS:CD2	3.03	0.43
1:B:439:VAL:O	1:B:440:PHE:C	2.57	0.43
1:A:323:GLU:C	1:A:325:GLU:H	2.20	0.43
1:C:248:LYS:HA	1:C:248:LYS:HD2	1.60	0.43
1:C:250:THR:HA	1:C:251:PRO:HD2	1.84	0.43
1:C:333:PHE:HB3	1:C:335:TYR:CE2	2.54	0.43
1:A:418:PHE:HE2	1:B:419:PRO:HG3	1.84	0.43
1:C:267:ARG:HB3	1:C:343:ALA:HB2	2.01	0.43
1:A:447:LYS:HB2	1:A:447:LYS:HE3	1.66	0.43
1:C:417:ARG:O	1:C:421:MET:HG3	2.19	0.42
1:D:438:GLN:HG3	1:D:441:ALA:CB	2.43	0.42
1:D:330:LEU:HA	1:D:330:LEU:HD23	1.71	0.42
1:B:224:GLN:HE21	1:B:224:GLN:HB2	1.66	0.42
1:B:340:PHE:HB3	1:B:350:ILE:CD1	2.49	0.42
1:D:351:ASN:O	1:D:355:GLU:HG3	2.20	0.42
1:C:267:ARG:O	1:C:270:HIS:HB3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:HIS:CD2	1:C:335:TYR:HH	2.37	0.42
1:A:320:TYR:CG	1:A:357:SER:HB3	2.55	0.41
1:A:457:TRP:CH2	1:B:292:PHE:HE2	2.38	0.41
1:B:403:LEU:HB3	1:B:418:PHE:CE1	2.55	0.41
1:C:352:PRO:O	1:C:353:ILE:C	2.58	0.41
1:C:349:PHE:O	1:C:353:ILE:HG13	2.20	0.41
1:C:310:GLU:CD	1:C:383[A]:ARG:HH22	2.23	0.41
1:A:237:GLN:NE2	1:A:288:GLN:HE22	2.17	0.41
1:A:333:PHE:CD2	1:A:333:PHE:N	2.87	0.41
1:D:403:LEU:HD11	1:D:421:MET:HE2	2.03	0.41
1:A:297:ARG:HD3	1:A:300:GLN:NE2	2.35	0.41
1:A:457:TRP:HE3	1:B:283:VAL:CG1	2.33	0.41
1:C:457:TRP:CE3	1:D:283:VAL:HG13	2.55	0.41
1:C:252:TRP:CZ2	1:C:267:ARG:HD2	2.56	0.41
1:A:315:GLU:O	1:A:319:ARG:CD	2.68	0.41
1:B:327:ILE:HG21	1:B:329:PHE:CZ	2.55	0.41
1:D:437:GLU:C	1:D:439:VAL:H	2.24	0.41
1:A:448:LYS:HA	1:A:448:LYS:HD3	1.81	0.41
1:B:247:PRO:HB2	1:B:249:VAL:HG12	2.03	0.41
1:B:439:VAL:HB	1:B:443:ARG:HG3	2.03	0.41
1:A:316:THR:HG23	1:A:327:ILE:HG21	2.02	0.40
1:B:268:PHE:C	1:B:268:PHE:CD2	2.94	0.40
1:B:301:ILE:O	1:B:302:ALA:C	2.59	0.40
1:A:221:THR:CG2	1:A:223:ALA:HB3	2.51	0.40
1:A:309:ILE:O	1:A:313:LEU:HG	2.22	0.40
1:D:225:GLU:O	1:D:229:GLN:HG3	2.21	0.40
1:D:421:MET:O	1:D:424:LYS:HB2	2.22	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	222/264 (84%)	197 (89%)	17 (8%)	8 (4%)	3	3
1	B	225/264 (85%)	209 (93%)	14 (6%)	2 (1%)	17	25
1	C	224/264 (85%)	202 (90%)	15 (7%)	7 (3%)	4	3
1	D	221/264 (84%)	202 (91%)	12 (5%)	7 (3%)	4	3
All	All	892/1056 (84%)	810 (91%)	58 (6%)	24 (3%)	5	5

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	ASP
1	A	444	LEU
1	A	447	LYS
1	C	260	SER
1	C	261	ARG
1	C	456	ILE
1	A	330	LEU
1	A	331	LYS
1	A	415	GLN
1	C	414	ASP
1	D	332	ASP
1	D	438	GLN
1	A	346	GLN
1	A	414	ASP
1	B	332	ASP
1	C	455	GLU
1	D	293	LEU
1	B	437	GLU
1	C	251	PRO
1	C	346	GLN
1	D	262	ASP
1	D	323	GLU
1	D	439	VAL
1	D	330	LEU

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	202/233 (87%)	172 (85%)	30 (15%)	3	3
1	B	203/233 (87%)	165 (81%)	38 (19%)	1	2
1	C	204/233 (88%)	169 (83%)	35 (17%)	2	2
1	D	201/233 (86%)	166 (83%)	35 (17%)	2	2
All	All	810/932 (87%)	672 (83%)	138 (17%)	2	2

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	THR
1	A	231	LEU
1	A	250	THR
1	A	274	LEU
1	A	280	GLN
1	A	294	GLN
1	A	303	LEU
1	A	309	ILE
1	A	314	LEU
1	A	318	ARG
1	A	334	THR
1	A	337	LYS
1	A	345	LEU
1	A	348	GLU
1	A	350	ILE
1	A	361	ARG
1	A	365	LEU
1	A	372	LEU
1	A	373	LEU
1	A	404	LEU
1	A	415	GLN
1	A	417	ARG
1	A	422	LEU
1	A	423	MET
1	A	425	LEU
1	A	432	SER
1	A	443	ARG
1	A	448	LYS
1	A	452	LEU
1	A	456	ILE
1	B	220	LEU
1	B	231	LEU
1	B	238	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	248	LYS
1	B	264	ARG
1	B	268	PHE
1	B	272	THR
1	B	273	GLU
1	B	294	GLN
1	B	295	LEU
1	B	314	LEU
1	B	321	ASN
1	B	331	LYS
1	B	334	THR
1	B	338	ASP
1	B	342	ARG
1	B	345	LEU
1	B	348	GLU
1	B	352	PRO
1	B	361	ARG
1	B	372	LEU
1	B	380	SER
1	B	395	LEU
1	B	397[A]	GLN
1	B	397[B]	GLN
1	B	403	LEU
1	B	404	LEU
1	B	409	ILE
1	B	413	GLN
1	B	416	LEU
1	B	422	LEU
1	B	424	LYS
1	B	429	ARG
1	B	432	SER
1	B	443	ARG
1	B	447	LYS
1	B	448	LYS
1	B	453	LEU
1	C	221	THR
1	C	246	GLN
1	C	248	LYS
1	C	264	ARG
1	C	273	GLU
1	C	274	LEU
1	C	280	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	294	GLN
1	C	303	LEU
1	C	309	ILE
1	C	313	LEU
1	C	314	LEU
1	C	337	LYS
1	C	338	ASP
1	C	339	ASP
1	C	345	LEU
1	C	361	ARG
1	C	363	LEU
1	C	372	LEU
1	C	373	LEU
1	C	404	LEU
1	C	413	GLN
1	C	417	ARG
1	C	422	LEU
1	C	423	MET
1	C	424	LYS
1	C	425	LEU
1	C	432	SER
1	C	436	SER
1	C	437	GLU
1	C	444	LEU
1	C	448	LYS
1	C	449	LEU
1	C	452	LEU
1	C	458	ASP
1	D	220	LEU
1	D	231	LEU
1	D	241	ARG
1	D	248	LYS
1	D	249	VAL
1	D	261	ARG
1	D	272	THR
1	D	276	ILE
1	D	294	GLN
1	D	295	LEU
1	D	314	LEU
1	D	331	LYS
1	D	334	THR
1	D	345	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	347	VAL
1	D	361	ARG
1	D	372	LEU
1	D	373	LEU
1	D	380	SER
1	D	393	GLU
1	D	395	LEU
1	D	403	LEU
1	D	404	LEU
1	D	416	LEU
1	D	422	LEU
1	D	428	LEU
1	D	429	ARG
1	D	431	LEU
1	D	433	SER
1	D	439	VAL
1	D	442	LEU
1	D	445	GLN
1	D	446	ASP
1	D	447	LYS
1	D	448	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	GLN
1	A	230	GLN
1	A	280	GLN
1	A	288	GLN
1	A	300	GLN
1	A	341	HIS
1	A	387	GLN
1	A	435	HIS
1	A	445	GLN
1	B	224	GLN
1	B	230	GLN
1	B	270	HIS
1	B	300	GLN
1	B	321	ASN
1	B	322	HIS
1	B	341	HIS
1	B	346	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	435	HIS
1	B	445	GLN
1	C	239	ASN
1	C	280	GLN
1	C	288	GLN
1	C	300	GLN
1	C	341	HIS
1	C	435	HIS
1	D	224	GLN
1	D	270	HIS
1	D	300	GLN
1	D	321	ASN
1	D	322	HIS
1	D	341	HIS
1	D	346	GLN
1	D	415	GLN
1	D	435	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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
3	BU1	B	502	-	5,5,5	0.61	0	4,4,4	0.55	0
3	BU1	D	502	-	5,5,5	0.30	0	4,4,4	1.31	0
2	6OX	A	501	-	39,43,43	1.94	8 (20%)	55,68,68	2.55	19 (34%)
2	6OX	B	501	-	39,43,43	1.65	6 (15%)	55,68,68	2.90	26 (47%)
2	6OX	C	501	-	39,43,43	1.71	8 (20%)	55,68,68	2.10	14 (25%)
2	6OX	D	501	-	39,43,43	1.82	8 (20%)	55,68,68	2.68	22 (40%)

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
3	BU1	B	502	-	-	2/3/3/3	-
3	BU1	D	502	-	-	3/3/3/3	-
2	6OX	A	501	-	-	12/28/34/34	0/4/4/4
2	6OX	B	501	-	-	10/28/34/34	0/4/4/4
2	6OX	C	501	-	-	11/28/34/34	0/4/4/4
2	6OX	D	501	-	-	9/28/34/34	0/4/4/4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	6OX	C22-S1	-6.67	1.68	1.77
2	C	501	6OX	C5-C4	4.77	1.60	1.54
2	B	501	6OX	C7-C12	-4.44	1.38	1.49
2	A	501	6OX	C7-C12	-4.36	1.38	1.49
2	D	501	6OX	C5-C4	4.34	1.59	1.54
2	B	501	6OX	C17-N2	-4.25	1.34	1.39
2	D	501	6OX	C17-N2	-4.19	1.34	1.39
2	C	501	6OX	C7-C12	-4.02	1.39	1.49
2	D	501	6OX	C7-C12	-3.97	1.39	1.49
2	A	501	6OX	C24-C23	3.83	1.55	1.51
2	C	501	6OX	C17-N2	-3.74	1.35	1.39
2	A	501	6OX	C17-N2	-3.70	1.35	1.39
2	A	501	6OX	O2-S1	3.69	1.54	1.44
2	D	501	6OX	O3-C18	-3.67	1.39	1.44
2	C	501	6OX	O2-S1	3.34	1.53	1.44
2	B	501	6OX	O2-S1	3.15	1.52	1.44
2	C	501	6OX	C17-C16	-3.05	1.31	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	6OX	C22-S1	2.95	1.82	1.77
2	D	501	6OX	O2-S1	2.82	1.51	1.44
2	C	501	6OX	C13-N2	-2.81	1.32	1.37
2	A	501	6OX	C5-C4	2.75	1.57	1.54
2	B	501	6OX	C28-C5	2.56	1.58	1.54
2	C	501	6OX	C13-N1	-2.54	1.30	1.34
2	B	501	6OX	C19-C18	-2.45	1.50	1.52
2	D	501	6OX	C26-C27	2.39	1.41	1.37
2	A	501	6OX	F1-C9	-2.31	1.29	1.35
2	D	501	6OX	C24-C23	2.26	1.54	1.51
2	C	501	6OX	C22-S1	-2.14	1.74	1.77
2	D	501	6OX	O4-C24	2.13	1.50	1.41
2	A	501	6OX	C23-C22	2.13	1.43	1.41

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	6OX	C24-C23-C9	-8.77	116.34	122.53
2	B	501	6OX	C29-C5-C4	-7.38	97.61	111.32
2	A	501	6OX	C24-C23-C22	7.32	129.07	122.52
2	D	501	6OX	C5-C13-N1	-7.30	116.27	122.93
2	B	501	6OX	C27-C14-N2	6.26	127.42	119.92
2	B	501	6OX	C5-C13-N1	-6.24	117.24	122.93
2	D	501	6OX	C27-C14-N2	5.93	127.03	119.92
2	B	501	6OX	C29-C5-C28	5.82	114.75	107.58
2	B	501	6OX	C28-C5-C13	-5.69	100.85	110.57
2	A	501	6OX	O2-S1-O1	-5.55	108.35	117.92
2	B	501	6OX	O2-S1-O1	-5.46	108.51	117.92
2	D	501	6OX	O2-S1-O1	-5.45	108.53	117.92
2	C	501	6OX	O2-S1-O1	-5.42	108.59	117.92
2	D	501	6OX	C4-C3-CL1	-5.22	109.67	122.26
2	C	501	6OX	F2-C27-C14	-4.99	117.19	121.04
2	D	501	6OX	C4-C6-CL2	-4.83	110.61	122.26
2	C	501	6OX	C13-N1-C16	4.80	107.73	101.33
2	C	501	6OX	C29-C5-C13	-4.80	102.37	110.57
2	B	501	6OX	C4-C6-CL2	-4.79	110.71	122.26
2	A	501	6OX	C5-C13-N1	-4.67	118.67	122.93
2	D	501	6OX	C21-C3-CL1	4.65	127.73	118.41
2	D	501	6OX	C10-C22-C23	-4.62	118.72	121.80
2	B	501	6OX	C8-C9-C23	-4.58	121.37	124.59
2	C	501	6OX	O1-S1-C22	4.35	113.34	108.27
2	B	501	6OX	C25-S1-C22	4.13	111.23	105.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	6OX	O3-C18-C19	4.08	115.28	107.08
2	D	501	6OX	C28-C5-C13	-4.05	103.64	110.57
2	A	501	6OX	F1-C9-C23	-4.04	112.82	117.63
2	B	501	6OX	C2-C6-CL2	4.02	126.48	118.41
2	D	501	6OX	C2-C6-CL2	4.00	126.43	118.41
2	D	501	6OX	C29-C5-C28	3.85	112.33	107.58
2	A	501	6OX	C13-N1-C16	3.79	106.38	101.33
2	D	501	6OX	C24-C23-C9	-3.77	119.87	122.53
2	D	501	6OX	C29-C5-C13	-3.72	104.21	110.57
2	C	501	6OX	C29-C5-C4	3.54	117.90	111.32
2	B	501	6OX	C6-C4-C3	3.53	121.00	115.78
2	A	501	6OX	O3-C18-C16	-3.46	102.74	108.93
2	D	501	6OX	C25-S1-C22	3.36	110.09	105.11
2	C	501	6OX	C2-C6-CL2	-3.35	111.68	118.41
2	A	501	6OX	C29-C5-C4	-3.30	105.18	111.32
2	B	501	6OX	C10-C22-S1	3.30	121.73	116.26
2	A	501	6OX	C27-C14-N2	3.24	123.80	119.92
2	B	501	6OX	C10-C22-C23	-3.24	119.64	121.80
2	A	501	6OX	O2-S1-C22	3.22	112.02	108.27
2	A	501	6OX	C28-C5-C4	3.17	117.22	111.32
2	B	501	6OX	C21-C3-CL1	3.16	124.75	118.41
2	D	501	6OX	C20-C18-C19	3.03	114.19	110.49
2	D	501	6OX	C13-N1-C16	3.00	105.33	101.33
2	A	501	6OX	C28-C5-C13	-2.98	105.48	110.57
2	C	501	6OX	C27-C14-N2	-2.97	116.35	119.92
2	B	501	6OX	C20-C18-C19	2.97	114.12	110.49
2	D	501	6OX	O3-C18-C20	2.81	112.72	107.08
2	D	501	6OX	C26-C27-C14	2.80	123.69	121.44
2	C	501	6OX	C28-C5-C4	-2.72	106.26	111.32
2	C	501	6OX	C8-C9-C23	-2.72	122.68	124.59
2	B	501	6OX	C28-C5-C4	2.71	116.36	111.32
2	C	501	6OX	C29-C5-C28	2.70	110.90	107.58
2	B	501	6OX	C21-C3-C4	-2.68	119.07	121.56
2	B	501	6OX	C9-C23-C22	2.65	118.38	114.58
2	B	501	6OX	C21-C1-C2	2.63	123.98	120.25
2	B	501	6OX	C13-N1-C16	2.59	104.78	101.33
2	B	501	6OX	C24-C23-C9	-2.56	120.73	122.53
2	B	501	6OX	C4-C3-CL1	-2.53	116.16	122.26
2	B	501	6OX	C1-C2-C6	-2.51	115.60	119.39
2	B	501	6OX	F2-C27-C14	2.50	122.97	121.04
2	B	501	6OX	F2-C27-C26	-2.30	114.02	118.61
2	D	501	6OX	O1-S1-C22	2.29	110.94	108.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	6OX	C10-C22-S1	2.26	120.02	116.26
2	C	501	6OX	C11-C12-C7	-2.26	117.45	121.36
2	A	501	6OX	C21-C3-C4	-2.24	119.48	121.56
2	A	501	6OX	O1-S1-C25	2.18	111.63	108.49
2	A	501	6OX	C11-C12-C7	-2.14	117.64	121.36
2	A	501	6OX	C20-C18-C19	2.13	113.09	110.49
2	A	501	6OX	C25-S1-C22	2.11	108.24	105.11
2	A	501	6OX	O1-S1-C22	2.11	110.72	108.27
2	D	501	6OX	C9-C23-C22	2.10	117.59	114.58
2	D	501	6OX	C29-C5-C4	-2.09	107.44	111.32
2	D	501	6OX	C10-C22-S1	2.07	119.70	116.26
2	D	501	6OX	C12-C26-C27	-2.06	117.83	119.59
2	C	501	6OX	O3-C18-C20	2.06	111.22	107.08
2	B	501	6OX	C10-C7-C12	-2.03	117.51	120.86

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	6OX	C6-C4-C5-C28
2	A	501	6OX	C17-C16-C18-C19
2	A	501	6OX	C17-C16-C18-C20
2	A	501	6OX	C10-C22-S1-C25
2	A	501	6OX	C23-C22-S1-C25
2	A	501	6OX	C10-C22-S1-O2
2	A	501	6OX	C23-C22-S1-O2
2	B	501	6OX	C6-C4-C5-C28
2	B	501	6OX	C10-C22-S1-C25
2	B	501	6OX	C23-C22-S1-C25
2	C	501	6OX	C3-C4-C5-C29
2	C	501	6OX	C9-C23-C24-O4
2	C	501	6OX	C10-C22-S1-C25
2	C	501	6OX	C23-C22-S1-C25
2	C	501	6OX	C10-C22-S1-O2
2	C	501	6OX	C23-C22-S1-O2
2	D	501	6OX	C6-C4-C5-C28
2	D	501	6OX	C10-C22-S1-C25
2	D	501	6OX	C23-C22-S1-C25
2	A	501	6OX	C6-C4-C5-C13
2	B	501	6OX	C6-C4-C5-C13
2	C	501	6OX	C3-C4-C5-C13
2	D	501	6OX	C6-C4-C5-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	501	6OX	N1-C13-C5-C29
2	B	501	6OX	N1-C13-C5-C28
2	D	501	6OX	N1-C13-C5-C29
2	D	501	6OX	C10-C22-S1-O2
2	B	501	6OX	C23-C22-S1-O2
2	D	501	6OX	C23-C22-S1-O2
2	B	501	6OX	C17-C16-C18-C19
2	B	501	6OX	C17-C16-C18-C20
2	C	501	6OX	C17-C16-C18-C20
3	B	502	BU1	O5-C1-C2-C3
3	D	502	BU1	O5-C1-C2-C3
3	D	502	BU1	C2-C3-C4-O6
2	A	501	6OX	N1-C13-C5-C28
2	D	501	6OX	N1-C13-C5-C28
2	B	501	6OX	N1-C13-C5-C29
3	B	502	BU1	C1-C2-C3-C4
2	B	501	6OX	C10-C22-S1-O2
3	D	502	BU1	C1-C2-C3-C4
2	C	501	6OX	C22-C23-C24-O4
2	A	501	6OX	C11-C12-C7-C10
2	C	501	6OX	C17-C16-C18-C19
2	D	501	6OX	C17-C16-C18-C20
2	A	501	6OX	C11-C12-C7-C8
2	C	501	6OX	N2-C13-C5-C29

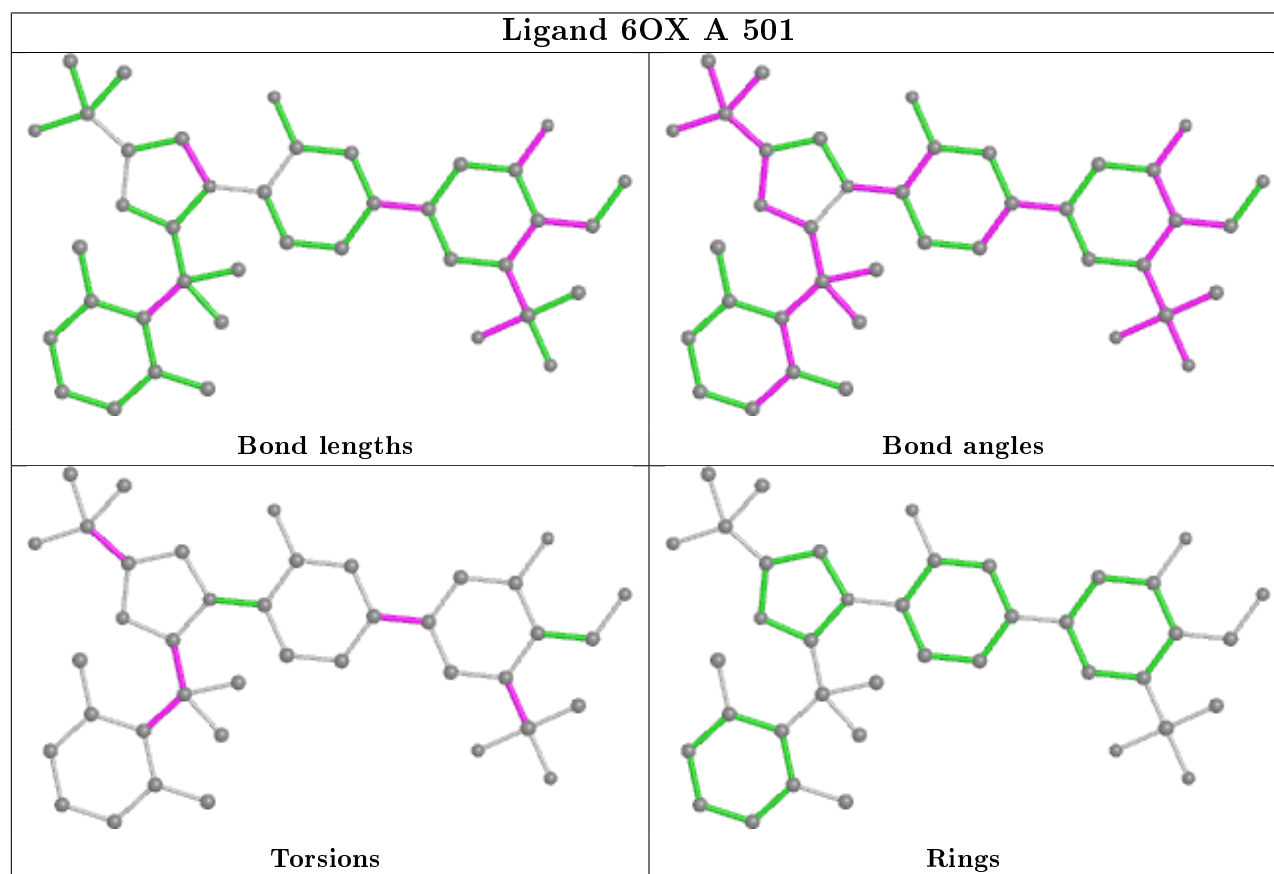
There are no ring outliers.

6 monomers are involved in 23 short contacts:

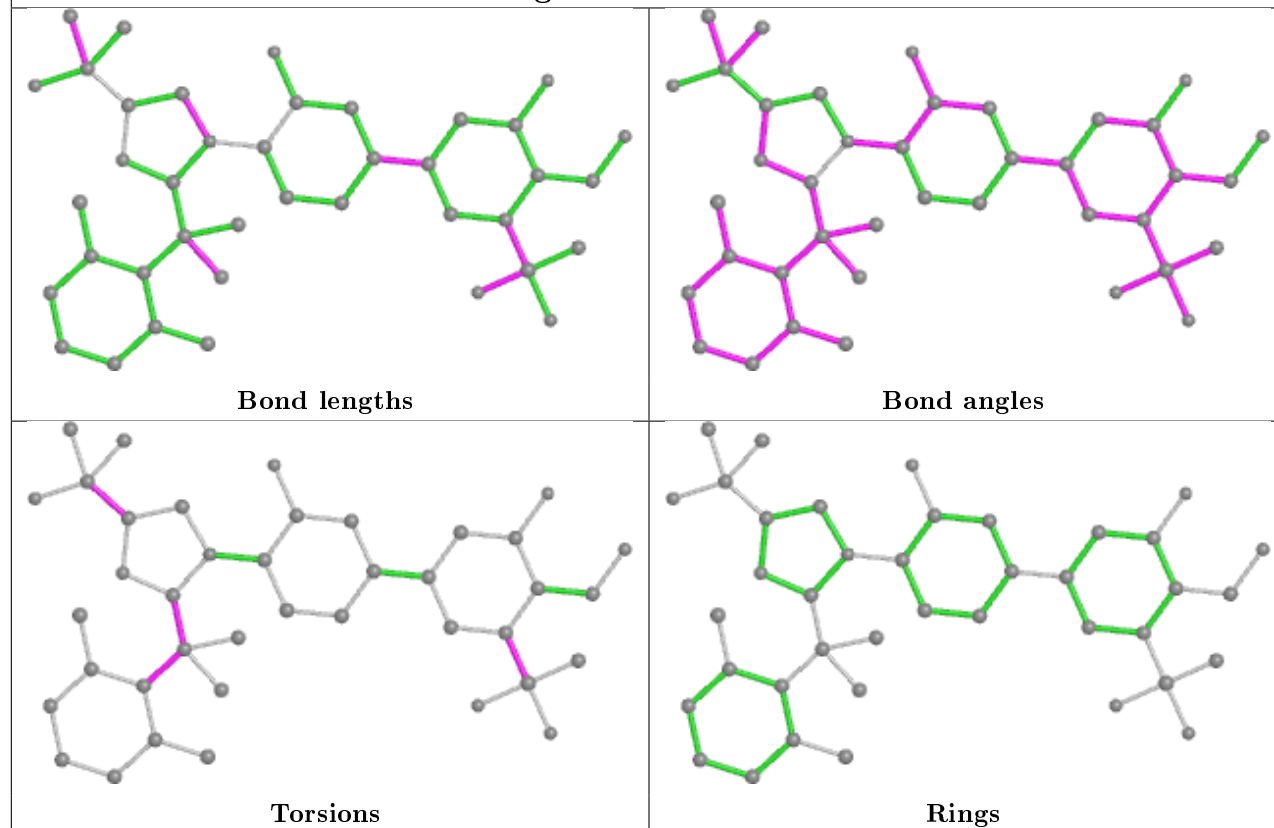
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	BU1	1	0
3	D	502	BU1	5	0
2	A	501	6OX	4	0
2	B	501	6OX	5	0
2	C	501	6OX	4	0
2	D	501	6OX	4	0

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

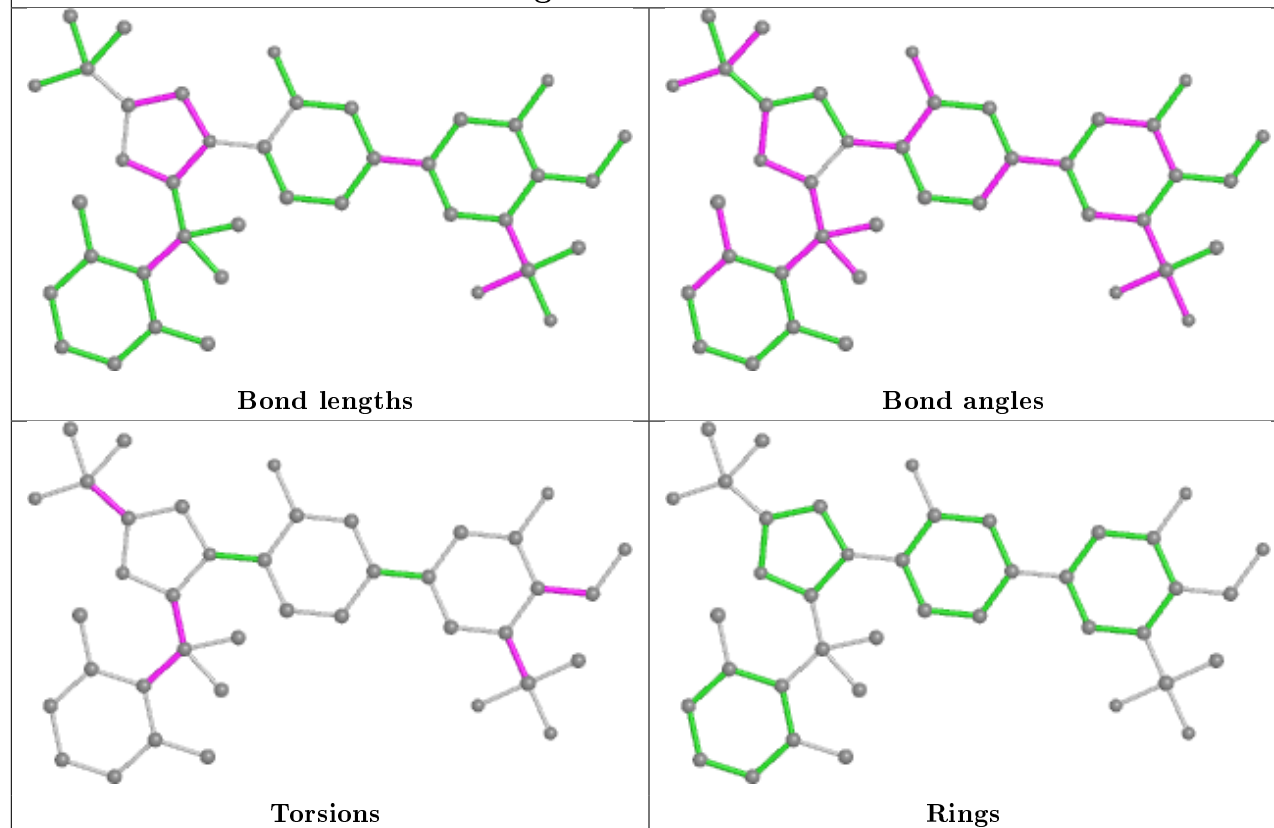
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

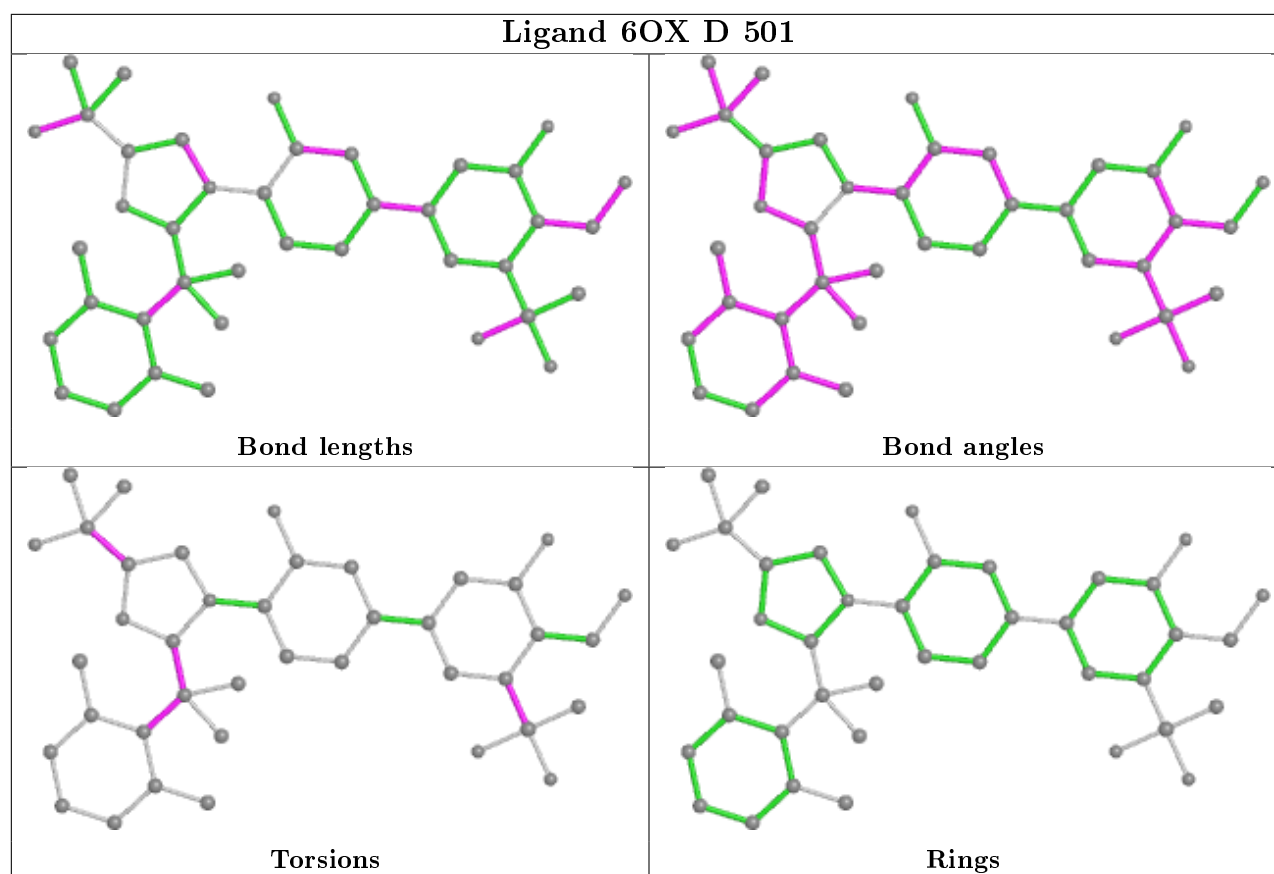


Ligand 6OX B 501



Ligand 6OX C 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	228/264 (86%)	-0.07	3 (1%) 77 75	28, 47, 83, 95	0
1	B	230/264 (87%)	-0.17	4 (1%) 70 68	30, 46, 75, 85	0
1	C	231/264 (87%)	-0.04	6 (2%) 56 54	27, 47, 86, 99	0
1	D	227/264 (85%)	-0.14	0 100 100	29, 46, 70, 83	0
All	All	916/1056 (86%)	-0.10	13 (1%) 75 73	27, 47, 79, 99	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	444	LEU	4.7
1	A	444	LEU	3.7
1	C	443	ARG	3.4
1	C	241	ARG	3.0
1	C	252	TRP	3.0
1	B	242	SER	2.6
1	B	243	PHE	2.5
1	C	251	PRO	2.4
1	C	261	ARG	2.4
1	B	449	LEU	2.3
1	A	443	ARG	2.2
1	A	457	TRP	2.1
1	B	457	TRP	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

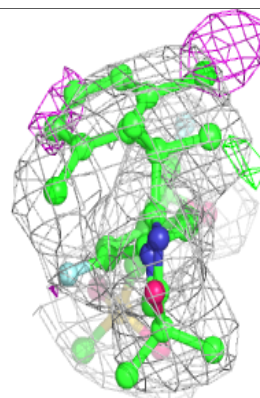
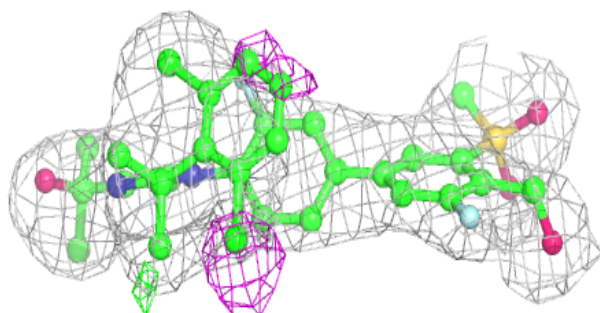
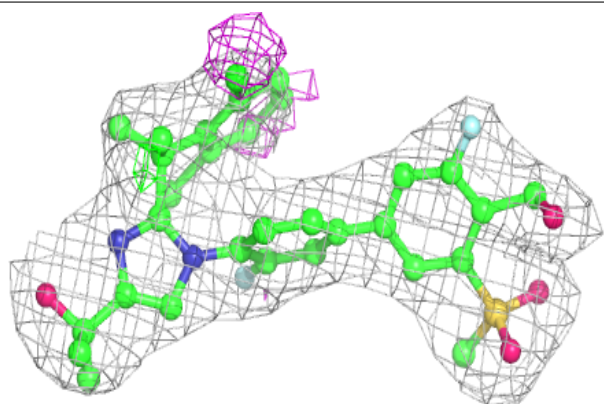
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	6OX	A	501	40/40	0.92	0.18	36,56,76,78	0
3	BU1	B	502	6/6	0.93	0.21	46,49,58,62	0
3	BU1	D	502	6/6	0.95	0.19	44,46,50,55	0
2	6OX	D	501	40/40	0.95	0.15	35,48,60,64	0
2	6OX	C	501	40/40	0.96	0.14	44,58,69,72	0
2	6OX	B	501	40/40	0.97	0.15	40,47,65,68	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.

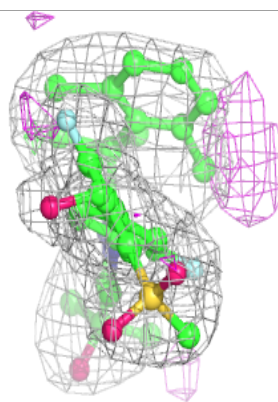
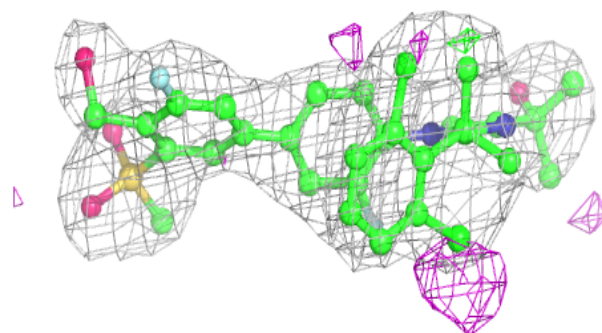
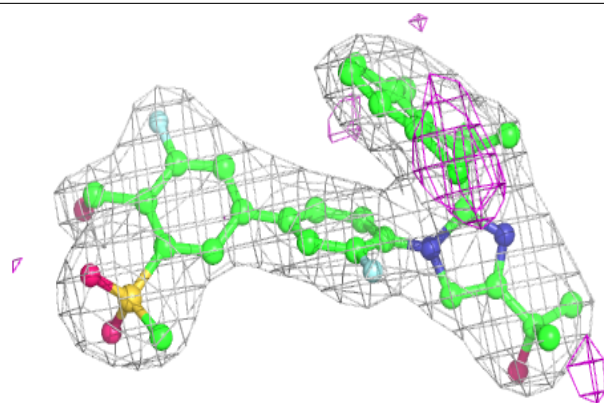
Electron density around 6OX A 501:

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

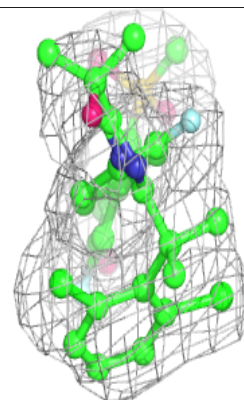
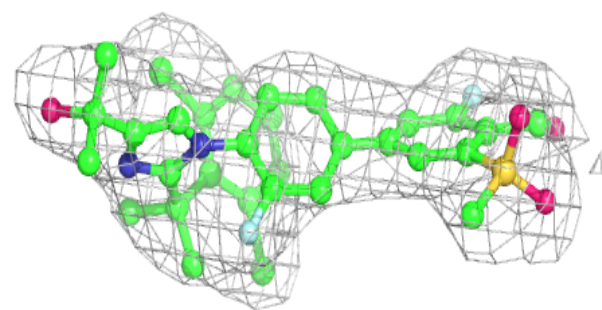
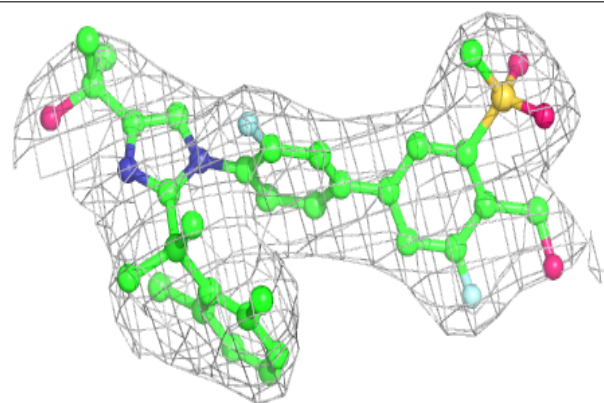


Electron density around 6OX D 501:

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

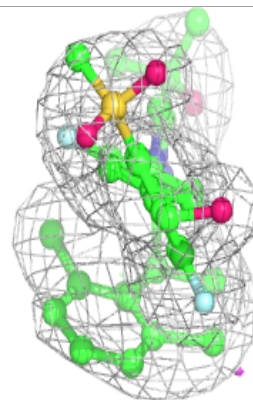
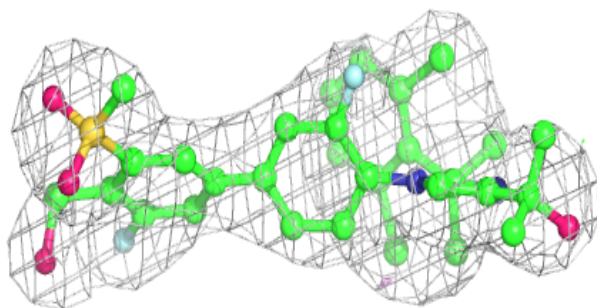
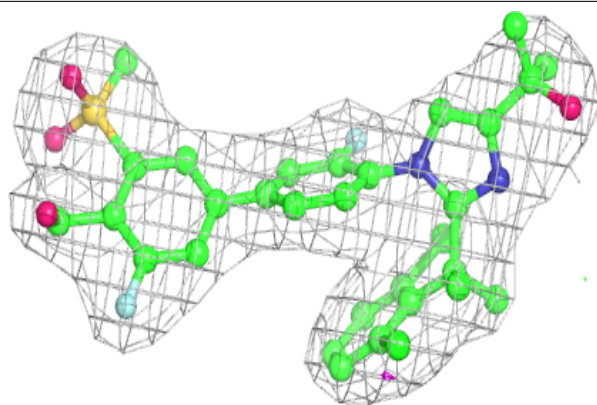
**Electron density around 6OX C 501:**

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



Electron density around 6OX 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.