



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 12:54 PM EDT

PDB ID : 3OSA  
Title : Estrogen Receptor  
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Deposited on : 2010-09-08  
Resolution : 2.30 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](mailto: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.

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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 : 2.23.2  
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) : 2.23.2

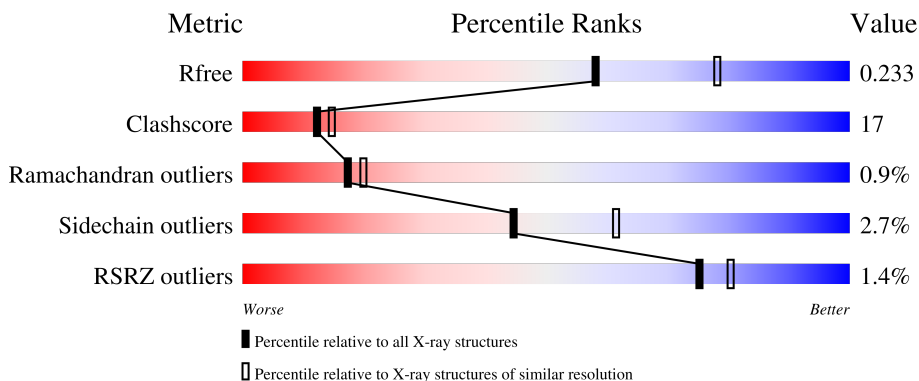
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	258	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">2%      67%      21%      5%      7%</p>
1	B	258	<div style="display: flex; align-items: center;"> <div style="width: 67%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">67%      22%      • 7%</p>
1	C	258	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">2%      67%      19%      • 11%</p>
1	D	258	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 12%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">2%      64%      22%      • 12%</p>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7770 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.

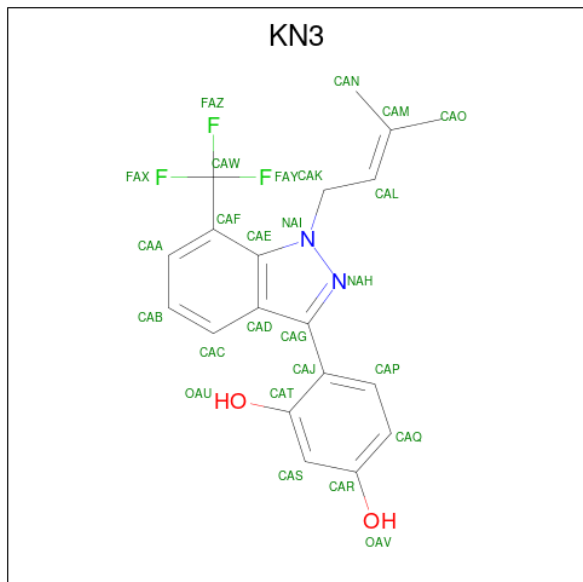
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	239	1890	1210	324	338	18	0	2	0
1	B	239	1882	1206	320	339	17	0	1	0
1	C	230	1814	1159	309	328	18	0	1	0
1	D	226	1769	1131	300	320	18	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	SER	-	expression tag	UNP P03372
A	297	ASN	-	expression tag	UNP P03372
A	298	ALA	-	expression tag	UNP P03372
A	372	ARG	LEU	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	UNP P03372
B	296	SER	-	expression tag	UNP P03372
B	297	ASN	-	expression tag	UNP P03372
B	298	ALA	-	expression tag	UNP P03372
B	372	ARG	LEU	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372
C	296	SER	-	expression tag	UNP P03372
C	297	ASN	-	expression tag	UNP P03372
C	298	ALA	-	expression tag	UNP P03372
C	372	ARG	LEU	engineered mutation	UNP P03372
C	536	SER	LEU	engineered mutation	UNP P03372
D	296	SER	-	expression tag	UNP P03372
D	297	ASN	-	expression tag	UNP P03372
D	298	ALA	-	expression tag	UNP P03372
D	372	ARG	LEU	engineered mutation	UNP P03372
D	536	SER	LEU	engineered mutation	UNP P03372

- Molecule 2 is 4-[1-(3-methylbut-2-en-1-yl)-7-(trifluoromethyl)-1H-indazol-3-yl]benzene-1,3-diol (three-letter code: KN3) (formula: C<sub>19</sub>H<sub>17</sub>F<sub>3</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	F	N			O
2	A	1	Total	C	F	N	O	0	0
			26	19	3	2	2		
2	B	1	Total	C	F	N	O	0	0
			26	19	3	2	2		
2	C	1	Total	C	F	N	O	0	0
			26	19	3	2	2		
2	D	1	Total	C	F	N	O	0	0
			26	19	3	2	2		

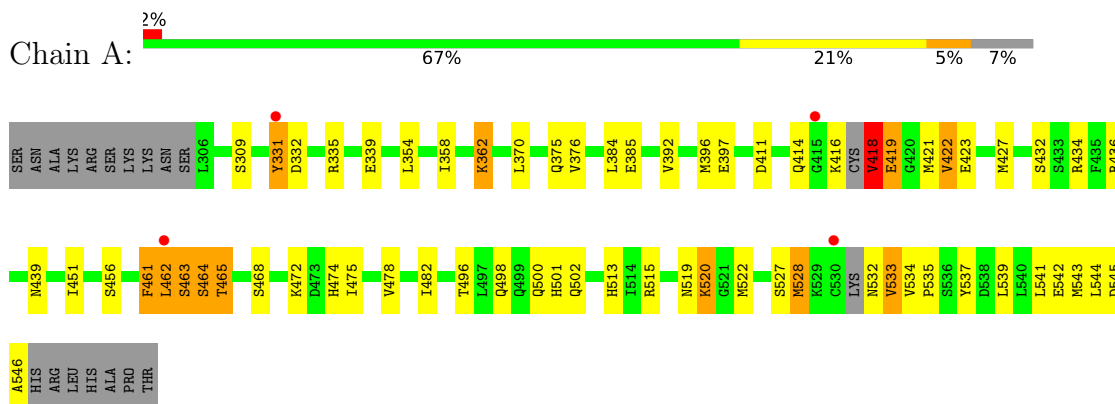
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	84	Total	O	0	0
			84	84		
3	C	74	Total	O	0	0
			74	74		
3	D	85	Total	O	0	0
			85	85		

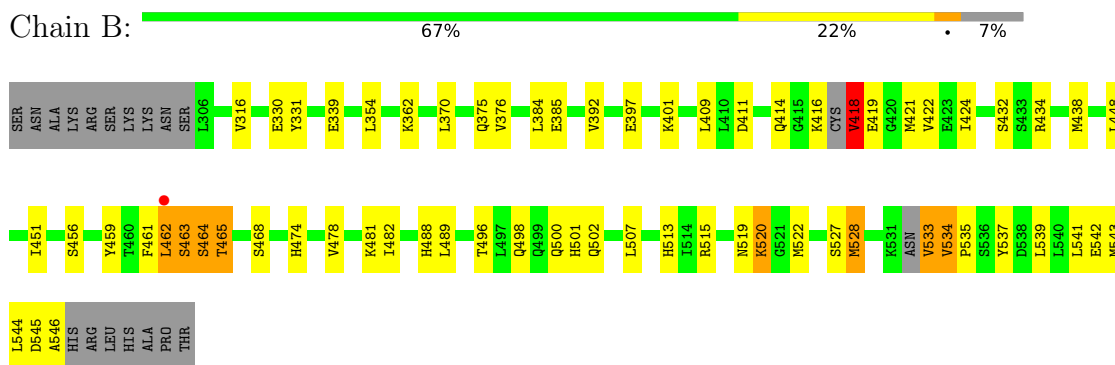
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

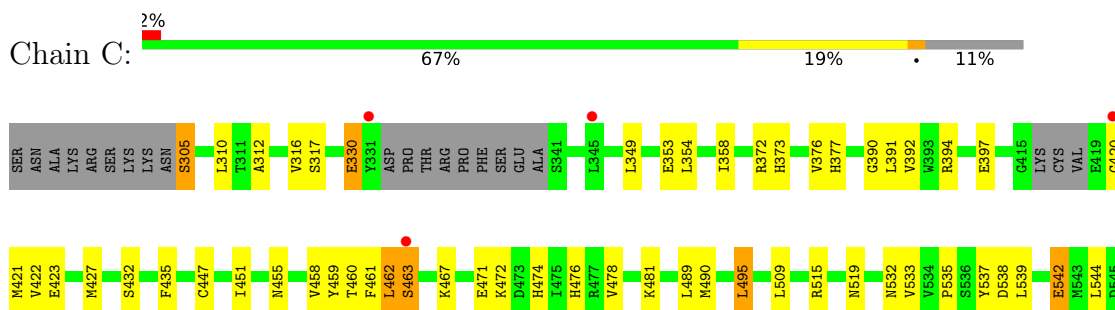
- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor



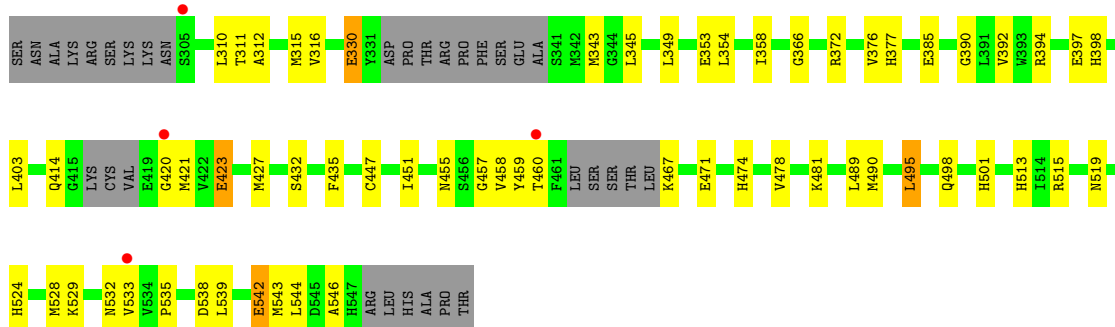
- Molecule 1: Estrogen receptor



A546  
HIS  
ARG  
LEU  
HIS  
ALA  
PRO  
THR

• Molecule 1: Estrogen receptor

Chain D: 2% 64% 22% 12%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.56Å 58.48Å 93.32Å 85.88° 74.75° 62.76°	Depositor
Resolution (Å)	38.15 – 2.30 38.15 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.8 (38.15-2.30) 91.6 (38.15-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.196 , 0.240 0.193 , 0.233	Depositor DCC
$R_{free}$ test set	1991 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.9	Xtrriage
Anisotropy	0.726	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.176 for h,h-k,h-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7770	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: KN3

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	0.91	11/1926 (0.6%)	0.90	4/2606 (0.2%)
1	B	0.93	12/1917 (0.6%)	0.90	6/2595 (0.2%)
1	C	0.57	0/1845	0.74	0/2491
1	D	0.55	0/1798	0.73	0/2428
All	All	0.76	23/7486 (0.3%)	0.82	10/10120 (0.1%)

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	C	0	1
1	D	0	1
All	All	0	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	533	VAL	CB-CG1	-12.81	1.25	1.52
1	A	331	TYR	CE1-CZ	-11.94	1.23	1.38
1	B	533	VAL	CB-CG2	-11.63	1.28	1.52
1	A	533	VAL	CB-CG2	-11.61	1.28	1.52
1	B	331	TYR	CE1-CZ	-11.45	1.23	1.38
1	B	331	TYR	CE2-CZ	-10.85	1.24	1.38
1	A	331	TYR	CE2-CZ	-10.75	1.24	1.38
1	B	331	TYR	CG-CD2	-10.14	1.25	1.39
1	A	331	TYR	CG-CD1	-10.08	1.26	1.39
1	B	461	PHE	CE2-CZ	-9.96	1.18	1.37
1	A	461	PHE	CE2-CZ	-9.91	1.18	1.37
1	A	331	TYR	CG-CD2	-9.71	1.26	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	461	PHE	CE1-CZ	-9.32	1.19	1.37
1	B	331	TYR	CG-CD1	-9.25	1.27	1.39
1	A	461	PHE	CG-CD1	-8.94	1.25	1.38
1	B	461	PHE	CG-CD1	-8.92	1.25	1.38
1	A	418	VAL	CB-CG2	-8.67	1.34	1.52
1	B	461	PHE	CE1-CZ	-8.65	1.21	1.37
1	B	418	VAL	CB-CG1	-8.06	1.35	1.52
1	A	461	PHE	CG-CD2	-7.71	1.27	1.38
1	B	461	PHE	CG-CD2	-7.23	1.27	1.38
1	A	533	VAL	CB-CG1	-6.28	1.39	1.52
1	B	419	GLU	CB-CG	-5.44	1.41	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	533	VAL	CG1-CB-CG2	-19.67	79.43	110.90
1	B	533	VAL	CG1-CB-CG2	-17.43	83.02	110.90
1	A	362	LYS	CD-CE-NZ	-8.51	92.12	111.70
1	B	462	LEU	CB-CG-CD1	7.15	123.15	111.00
1	B	462	LEU	CA-CB-CG	-6.34	100.72	115.30
1	B	461	PHE	CB-CG-CD2	5.83	124.88	120.80
1	B	362	LYS	CD-CE-NZ	-5.60	98.83	111.70
1	B	528	MET	CB-CG-SD	5.39	128.57	112.40
1	A	419	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	A	418	VAL	CB-CA-C	-5.15	101.62	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	330	GLU	Peptide
1	D	330	GLU	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	1890	0	1893	71	0
1	B	1882	0	1886	68	0
1	C	1814	0	1834	59	0
1	D	1769	0	1777	79	0
2	A	26	0	15	3	0
2	B	26	0	15	8	0
2	C	26	0	16	6	0
2	D	26	0	16	7	0
3	A	68	0	0	7	0
3	B	84	0	0	8	0
3	C	74	0	0	4	0
3	D	85	0	0	24	0
All	All	7770	0	7452	253	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 17.

All (253) 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:C:310:LEU:O	1:C:481:LYS:NZ	1.62	1.30
1:D:310:LEU:O	1:D:481:LYS:NZ	1.62	1.29
1:A:513[A]:HIS:NE2	1:C:459:TYR:HE1	1.45	1.14
1:B:513[A]:HIS:NE2	1:D:459:TYR:HE1	1.50	1.10
1:B:513[A]:HIS:CD2	1:D:459:TYR:CE1	2.42	1.08
1:A:513[A]:HIS:CD2	1:C:459:TYR:CE1	2.43	1.06
1:A:513[A]:HIS:NE2	1:C:459:TYR:CE1	2.23	1.05
1:B:513[A]:HIS:NE2	1:D:459:TYR:CE1	2.28	1.01
1:C:305:SER:N	3:C:202:HOH:O	1.98	0.96
1:D:311:THR:O	3:D:275:HOH:O	1.88	0.91
1:A:513[A]:HIS:CE1	1:C:459:TYR:CD1	2.59	0.91
1:B:519:ASN:HD22	1:D:519:ASN:HD22	1.20	0.90
1:B:513[A]:HIS:CD2	1:D:459:TYR:HE1	1.86	0.90
1:D:533:VAL:HG11	2:D:1:KN3:HANA	1.54	0.89
1:A:519:ASN:HD22	1:C:519:ASN:HD22	1.22	0.88
1:A:513[A]:HIS:CE1	1:C:459:TYR:HD1	1.91	0.86
1:D:315:MET:N	3:D:275:HOH:O	2.10	0.85
1:A:532:ASN:CB	1:A:533:VAL:HA	2.07	0.84
1:A:513[A]:HIS:CD2	1:C:459:TYR:HE1	1.90	0.83
1:B:513[A]:HIS:CE1	1:D:459:TYR:CD1	2.67	0.83
1:D:330:GLU:OE1	3:D:53:HOH:O	1.94	0.83
1:A:498:GLN:O	1:A:502:GLN:HG3	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:VAL:HG11	2:D:1:KN3:CAN	2.10	0.81
1:A:331:TYR:CE2	1:A:332:ASP:HB2	2.17	0.80
1:B:513[A]:HIS:CE1	1:D:459:TYR:HD1	1.98	0.80
1:B:513[A]:HIS:CE1	1:D:455:ASN:O	2.37	0.78
1:D:397:GLU:HB3	3:D:190:HOH:O	1.83	0.78
1:A:397:GLU:HG2	3:A:207:HOH:O	1.84	0.77
1:B:498:GLN:O	1:B:502:GLN:HG3	1.85	0.77
1:A:385:GLU:OE1	3:A:11:HOH:O	2.01	0.76
1:D:315:MET:HB2	3:D:275:HOH:O	1.86	0.75
2:B:1:KN3:HAC	2:B:1:KN3:HAP	1.69	0.75
1:B:456:SER:HA	1:B:515:ARG:NH2	2.03	0.73
1:C:533:VAL:HG11	2:C:1:KN3:HAN	1.71	0.73
1:C:373:HIS:HD2	1:C:537:TYR:OH	1.70	0.73
1:D:397:GLU:CB	3:D:190:HOH:O	2.36	0.72
1:B:385:GLU:OE1	3:B:137:HOH:O	2.08	0.72
1:A:331:TYR:CD2	1:A:332:ASP:HB2	2.25	0.71
1:B:513[A]:HIS:HE1	1:D:455:ASN:O	1.73	0.71
1:C:330:GLU:OE1	3:C:176:HOH:O	2.08	0.71
1:C:353:GLU:OE1	2:C:1:KN3:OAV	2.08	0.70
1:C:538:ASP:O	1:C:542:GLU:HG2	1.91	0.70
1:A:462:LEU:O	1:A:463:SER:CB	2.40	0.70
1:A:456:SER:HA	1:A:515:ARG:NH2	2.05	0.69
1:D:385:GLU:OE1	3:D:146:HOH:O	2.09	0.69
1:A:513[A]:HIS:CE1	1:C:459:TYR:CE1	2.79	0.69
1:D:421:MET:N	3:D:227:HOH:O	2.13	0.69
1:B:513[B]:HIS:NE2	3:B:153:HOH:O	2.25	0.68
1:D:474:HIS:NE2	3:D:52:HOH:O	2.26	0.68
1:D:310:LEU:HB3	3:D:275:HOH:O	1.92	0.68
1:D:474:HIS:CD2	3:D:52:HOH:O	2.45	0.68
1:B:513[B]:HIS:CD2	3:B:153:HOH:O	2.47	0.67
1:B:456:SER:O	3:B:168:HOH:O	2.11	0.67
1:C:459:TYR:OH	3:C:44:HOH:O	2.08	0.67
1:A:513[A]:HIS:CE1	1:C:455:ASN:O	2.49	0.66
1:D:538:ASP:O	1:D:542:GLU:CG	2.44	0.66
1:B:418:VAL:HG12	1:B:421:MET:HG2	1.79	0.64
1:A:335:ARG:NH2	3:A:62:HOH:O	2.29	0.64
1:A:468:SER:OG	3:A:557:HOH:O	2.15	0.64
1:A:532:ASN:CB	1:A:533:VAL:CA	2.76	0.64
1:D:394:ARG:O	3:D:277:HOH:O	2.15	0.64
1:D:354:LEU:O	1:D:358:ILE:HD13	1.97	0.63
1:A:461:PHE:HB3	3:A:557:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:SER:O	1:A:464:SER:OG	2.17	0.63
1:D:538:ASP:O	1:D:542:GLU:HG2	1.99	0.63
1:A:513[A]:HIS:HE1	1:C:455:ASN:O	1.83	0.62
1:C:538:ASP:O	1:C:542:GLU:CG	2.48	0.62
1:D:533:VAL:CG1	2:D:1:KN3:HANA	2.27	0.62
1:A:513[B]:HIS:HD2	1:C:515:ARG:NH2	1.97	0.62
1:B:513[A]:HIS:CE1	1:D:459:TYR:CE1	2.86	0.62
1:C:354:LEU:O	1:C:358:ILE:HD13	2.00	0.61
1:D:366:GLY:O	3:D:52:HOH:O	2.16	0.61
1:B:519:ASN:ND2	1:D:519:ASN:HD22	1.94	0.61
2:D:1:KN3:OAU	2:D:1:KN3:HAC	2.01	0.61
1:D:392:VAL:HG13	1:D:432:SER:HA	1.83	0.60
2:B:1:KN3:FAZ	2:B:1:KN3:HAKA	1.92	0.60
1:C:392:VAL:HG13	1:C:432:SER:HA	1.83	0.60
1:A:419:GLU:HA	1:A:422:VAL:HG13	1.83	0.60
1:A:461:PHE:HD1	1:A:472:LYS:HG2	1.67	0.59
1:D:390:GLY:O	1:D:394:ARG:HG3	2.03	0.58
1:D:315:MET:CB	3:D:275:HOH:O	2.44	0.58
1:A:528:MET:CE	1:A:533:VAL:HG21	2.34	0.58
1:B:418:VAL:HG12	1:B:421:MET:CG	2.33	0.58
1:C:376:VAL:HG22	1:C:544:LEU:HD12	1.86	0.58
1:D:315:MET:CA	3:D:275:HOH:O	2.52	0.58
1:C:373:HIS:CD2	1:C:537:TYR:OH	2.56	0.57
1:A:519:ASN:ND2	1:C:519:ASN:HD22	1.98	0.57
1:D:312:ALA:O	1:D:316:VAL:HG23	2.04	0.57
1:A:461:PHE:HE1	1:A:475:ILE:HD12	1.70	0.56
1:C:420:GLY:O	1:C:421:MET:HG3	2.05	0.56
1:A:513[A]:HIS:CG	1:C:459:TYR:CD1	2.93	0.56
1:D:392:VAL:HG12	1:D:435:PHE:CD2	2.41	0.56
1:C:312:ALA:O	1:C:316:VAL:HG23	2.05	0.56
1:A:384:LEU:HD23	1:A:522:MET:HE2	1.87	0.56
1:B:513[A]:HIS:CG	1:D:459:TYR:CD1	2.93	0.56
1:B:519:ASN:HD22	1:D:519:ASN:ND2	1.97	0.56
1:C:390:GLY:O	1:C:394:ARG:HG3	2.06	0.56
1:D:420:GLY:O	1:D:421:MET:HG3	2.06	0.56
1:C:461:PHE:HB2	1:C:472:LYS:NZ	2.22	0.55
1:B:513[B]:HIS:HD2	1:D:515:ARG:NH2	2.05	0.55
1:B:384:LEU:HD23	1:B:522:MET:HE2	1.88	0.55
1:B:513[A]:HIS:CD2	1:D:459:TYR:CD1	2.93	0.55
1:A:513[A]:HIS:CD2	1:C:459:TYR:CD1	2.94	0.55
1:D:312:ALA:HB3	3:D:145:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513[A]:HIS:ND1	1:D:459:TYR:HD1	2.06	0.54
1:B:528:MET:CE	1:B:533:VAL:HG21	2.37	0.54
1:C:461:PHE:O	1:C:462:LEU:CB	2.55	0.54
1:C:392:VAL:HG12	1:C:435:PHE:CD2	2.43	0.54
1:D:376:VAL:HG22	1:D:544:LEU:HD12	1.88	0.54
1:A:474:HIS:O	1:A:478:VAL:HG23	2.08	0.54
1:B:370:LEU:O	1:B:375:GLN:NE2	2.41	0.54
2:A:1:KN3:HAC	2:A:1:KN3:HAP	1.90	0.53
1:A:513[A]:HIS:ND1	1:C:459:TYR:CD1	2.75	0.53
1:A:513[A]:HIS:ND1	1:C:459:TYR:HD1	2.05	0.53
1:A:534:VAL:CG1	1:A:534:VAL:O	2.56	0.53
1:A:528:MET:HE1	1:A:533:VAL:HG21	1.91	0.53
1:B:534:VAL:O	1:B:534:VAL:CG1	2.56	0.53
1:A:461:PHE:CD1	1:A:472:LYS:HG2	2.43	0.53
1:C:474:HIS:O	1:C:478:VAL:HG23	2.09	0.53
1:D:524:HIS:O	1:D:528:MET:HG2	2.09	0.53
1:A:519:ASN:HD22	1:C:519:ASN:ND2	2.00	0.52
1:B:339:GLU:HA	1:B:416:LYS:O	2.10	0.52
1:D:330:GLU:O	1:D:330:GLU:HG3	2.10	0.52
1:D:529:LYS:O	1:D:529:LYS:HG2	2.10	0.52
1:C:330:GLU:O	1:C:330:GLU:HG3	2.10	0.52
1:A:461:PHE:O	1:A:462:LEU:CB	2.58	0.51
2:C:1:KN3:OAU	2:C:1:KN3:HAC	2.11	0.51
1:D:403:LEU:HD13	3:D:277:HOH:O	2.10	0.51
1:A:309:SER:O	3:A:56:HOH:O	2.18	0.51
1:B:501:HIS:HE1	3:D:187:HOH:O	1.93	0.51
1:B:528:MET:HE2	1:B:533:VAL:HG21	1.92	0.51
1:D:533:VAL:HG12	1:D:533:VAL:O	2.11	0.51
1:A:392:VAL:HG13	1:A:432:SER:HA	1.93	0.51
1:A:339:GLU:HA	1:A:416:LYS:O	2.11	0.50
1:B:465:THR:HG23	1:B:468:SER:CB	2.41	0.50
1:B:397:GLU:OE2	3:B:554:HOH:O	2.18	0.50
1:B:411:ASP:CG	1:B:414:GLN:HG3	2.30	0.50
1:B:501:HIS:HD2	3:D:191:HOH:O	1.93	0.50
1:D:474:HIS:O	1:D:478:VAL:HG23	2.11	0.50
1:D:457:GLY:HA2	3:D:14:HOH:O	2.12	0.50
1:B:513[A]:HIS:ND1	1:D:459:TYR:CD1	2.78	0.50
2:B:1:KN3:HAP	2:B:1:KN3:CAC	2.34	0.50
1:A:539:LEU:HG	1:A:543:MET:CE	2.42	0.49
1:B:464:SER:O	1:B:465:THR:O	2.28	0.49
1:B:541:LEU:O	1:B:544:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:GLU:O	1:C:427:MET:HG3	2.12	0.49
1:B:462:LEU:O	1:B:463:SER:CB	2.59	0.49
1:C:495:LEU:N	1:C:495:LEU:HD23	2.27	0.49
1:D:535:PRO:HA	1:D:539:LEU:HD23	1.94	0.49
1:B:392:VAL:HG13	1:B:432:SER:HA	1.94	0.49
1:D:538:ASP:O	1:D:542:GLU:HG3	2.12	0.49
1:A:331:TYR:CD2	1:A:332:ASP:CB	2.95	0.49
1:B:330:GLU:HG3	3:B:8:HOH:O	2.11	0.49
1:B:534:VAL:O	1:B:534:VAL:HG12	2.12	0.49
1:A:411:ASP:CG	1:A:414:GLN:HG3	2.32	0.49
1:A:370:LEU:O	1:A:375:GLN:NE2	2.45	0.48
1:C:467:LYS:O	1:C:471:GLU:HG2	2.14	0.48
1:D:423:GLU:O	1:D:427:MET:HG3	2.14	0.48
2:B:1:KN3:NAH	2:B:1:KN3:OAU	2.45	0.48
1:C:376:VAL:HG22	1:C:544:LEU:CD1	2.43	0.48
2:B:1:KN3:HAKA	2:B:1:KN3:CAW	2.44	0.48
1:B:474:HIS:O	1:B:478:VAL:HG23	2.14	0.47
1:A:520:LYS:HD2	1:A:520:LYS:HA	1.57	0.47
1:D:397:GLU:HA	3:D:190:HOH:O	2.15	0.47
1:A:545:ASP:O	1:A:546:ALA:C	2.53	0.47
2:B:1:KN3:HAC	2:B:1:KN3:CAP	2.42	0.47
1:D:458:VAL:HG22	1:D:458:VAL:O	2.15	0.47
1:A:358:ILE:O	1:A:362:LYS:HG3	2.14	0.47
1:D:316:VAL:HG21	1:D:489:LEU:HD21	1.97	0.47
1:A:513[B]:HIS:HD2	1:C:515:ARG:HH22	1.59	0.47
1:A:541:LEU:O	1:A:544:LEU:HB2	2.15	0.47
1:C:462:LEU:O	1:C:463:SER:C	2.51	0.46
1:D:377:HIS:CE1	1:D:460:THR:O	2.68	0.46
1:B:434:ARG:HD3	1:D:459:TYR:HE2	1.79	0.46
1:B:496:THR:O	1:B:500:GLN:HG3	2.15	0.46
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.50	0.46
1:D:467:LYS:O	1:D:471:GLU:HG2	2.16	0.46
1:A:376:VAL:HG11	1:A:537:TYR:CD2	2.50	0.46
1:C:458:VAL:O	1:C:458:VAL:HG22	2.16	0.46
1:C:421:MET:N	3:C:259:HOH:O	2.09	0.46
1:A:528:MET:HE2	1:A:533:VAL:HG21	1.98	0.46
2:A:1:KN3:FAX	2:A:1:KN3:HAKA	2.05	0.46
1:A:498:GLN:HA	1:A:501[A]:HIS:CE1	2.50	0.45
1:B:418:VAL:O	1:B:422:VAL:HG23	2.16	0.45
1:B:354:LEU:HD21	1:B:535:PRO:HB3	1.98	0.45
1:D:414:GLN:NE2	3:D:212:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:LEU:HG	1:B:543:MET:CE	2.46	0.45
1:A:354:LEU:HD21	1:A:535:PRO:HB3	1.98	0.45
1:B:434:ARG:O	1:B:438:MET:HG3	2.15	0.45
1:C:533:VAL:HG11	2:C:1:KN3:CAN	2.43	0.45
1:D:533:VAL:HG11	2:D:1:KN3:HAN	1.93	0.45
1:C:447:CYS:O	1:C:451:ILE:HG13	2.16	0.45
1:B:545:ASP:O	1:B:546:ALA:C	2.55	0.45
1:D:376:VAL:HG22	1:D:544:LEU:CD1	2.47	0.45
1:B:481:LYS:HE2	1:B:481:LYS:HB2	1.76	0.44
1:B:463:SER:O	1:B:464:SER:OG	2.32	0.44
1:C:535:PRO:HA	1:C:539:LEU:HD23	1.99	0.44
2:A:1:KN3:OAU	2:A:1:KN3:NAH	2.48	0.44
1:C:372:ARG:O	1:C:376:VAL:HG23	2.17	0.44
1:C:397:GLU:OE2	1:C:397:GLU:N	2.37	0.44
1:D:349:LEU:HG	1:D:353:GLU:OE1	2.18	0.44
1:A:396:MET:HE2	1:A:436:ARG:HA	2.00	0.44
1:A:534:VAL:O	1:A:534:VAL:HG13	2.17	0.44
1:D:495:LEU:N	1:D:495:LEU:HD23	2.32	0.44
1:C:533:VAL:HG12	1:C:533:VAL:O	2.18	0.44
1:B:451:ILE:HG13	1:B:482:ILE:HG21	1.99	0.44
1:A:461:PHE:HE1	1:A:475:ILE:CD1	2.30	0.44
1:C:349:LEU:HG	1:C:353:GLU:OE1	2.18	0.43
1:A:542:GLU:C	1:A:544:LEU:N	2.72	0.43
1:B:488:HIS:CD2	3:B:206:HOH:O	2.71	0.43
1:B:542:GLU:C	1:B:544:LEU:N	2.72	0.43
1:A:464:SER:O	1:A:465:THR:O	2.35	0.43
1:C:377:HIS:CE1	1:C:460:THR:O	2.72	0.43
1:A:451:ILE:HG13	1:A:482:ILE:HG21	2.01	0.43
1:A:434:ARG:HD3	1:C:459:TYR:HE2	1.83	0.43
1:B:459:TYR:CD1	1:D:513:HIS:HB2	2.54	0.43
1:A:418:VAL:O	1:A:421:MET:HB2	2.20	0.42
1:B:520:LYS:HD2	1:B:520:LYS:HA	1.55	0.42
1:D:447:CYS:O	1:D:451:ILE:HG13	2.18	0.42
1:B:376:VAL:HG11	1:B:537:TYR:CD2	2.54	0.42
1:B:411:ASP:OD2	1:B:414:GLN:HG3	2.19	0.42
1:D:345:LEU:HD23	1:D:345:LEU:HA	1.82	0.42
1:A:439:ASN:HA	3:A:261:HOH:O	2.18	0.42
1:D:539:LEU:HG	1:D:543:MET:HE1	2.02	0.42
2:B:1:KN3:CAC	2:B:1:KN3:CAP	2.97	0.42
1:D:372:ARG:O	1:D:376:VAL:HG23	2.19	0.42
1:B:488:HIS:HD2	3:B:206:HOH:O	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:490:MET:HB3	1:D:495:LEU:HG	2.02	0.42
1:B:418:VAL:O	1:B:421:MET:HB2	2.20	0.42
1:B:448:LEU:HD21	1:B:507:LEU:HB3	2.02	0.42
1:C:316:VAL:HG21	1:C:489:LEU:HD21	2.02	0.42
1:A:331:TYR:CD2	1:A:331:TYR:C	2.94	0.41
2:D:1:KN3:OAU	2:D:1:KN3:CAC	2.66	0.41
1:D:397:GLU:CA	3:D:190:HOH:O	2.66	0.41
1:D:398:HIS:CD2	1:D:403:LEU:HD12	2.55	0.41
1:A:542:GLU:C	1:A:544:LEU:H	2.24	0.41
1:A:418:VAL:HG12	1:A:419:GLU:H	1.85	0.41
1:B:401:LYS:HB3	1:B:409:LEU:HD11	2.02	0.41
1:B:542:GLU:C	1:B:544:LEU:H	2.24	0.41
1:A:496:THR:O	1:A:500:GLN:HG3	2.20	0.41
1:B:316:VAL:HG21	1:B:489:LEU:HD21	2.03	0.41
2:C:1:KN3:HAOB	2:C:1:KN3:HAK	1.72	0.41
1:D:397:GLU:OE2	1:D:397:GLU:N	2.42	0.41
1:B:424:ILE:HB	2:B:1:KN3:HAOA	2.02	0.41
1:C:391:LEU:HD22	2:C:1:KN3:OAU	2.21	0.41
1:C:490:MET:HB3	1:C:495:LEU:HG	2.03	0.41
1:A:418:VAL:HG23	1:A:421:MET:HG3	2.03	0.40
1:B:542:GLU:O	1:B:544:LEU:N	2.55	0.40
1:C:509:LEU:HD23	1:C:509:LEU:HA	1.83	0.40
1:D:414:GLN:OE1	3:D:212:HOH:O	2.22	0.40
1:B:528:MET:HE1	1:B:533:VAL:HG21	2.03	0.40
1:A:423:GLU:O	1:A:427:MET:HG3	2.22	0.40
1:D:343:MET:HE1	2:D:1:KN3:HAOB	2.03	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	235/258 (91%)	222 (94%)	10 (4%)	3 (1%)	12	12
1	B	234/258 (91%)	223 (95%)	9 (4%)	2 (1%)	17	20
1	C	225/258 (87%)	216 (96%)	7 (3%)	2 (1%)	17	20
1	D	218/258 (84%)	212 (97%)	5 (2%)	1 (0%)	29	35
All	All	912/1032 (88%)	873 (96%)	31 (3%)	8 (1%)	17	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	LEU
1	A	463	SER
1	A	465	THR
1	B	463	SER
1	B	465	THR
1	C	462	LEU
1	D	546	ALA
1	C	463	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/232 (89%)	201 (97%)	6 (3%)	42	58
1	B	206/232 (89%)	201 (98%)	5 (2%)	49	66
1	C	201/232 (87%)	193 (96%)	8 (4%)	31	44
1	D	194/232 (84%)	190 (98%)	4 (2%)	53	70
All	All	808/928 (87%)	785 (97%)	23 (3%)	44	60

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	418	VAL
1	A	422	VAL
1	A	464	SER

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Mol	Chain	Res	Type
1	A	520	LYS
1	A	527	SER
1	A	528	MET
1	B	418	VAL
1	B	464	SER
1	B	520	LYS
1	B	527	SER
1	B	534	VAL
1	C	305	SER
1	C	317	SER
1	C	422	VAL
1	C	476[A]	HIS
1	C	476[B]	HIS
1	C	495	LEU
1	C	532	ASN
1	C	542	GLU
1	D	423	GLU
1	D	495	LEU
1	D	532	ASN
1	D	542	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	519	ASN
1	B	501	HIS
1	B	519	ASN
1	C	373	HIS
1	C	377	HIS
1	C	488	HIS
1	C	502	GLN
1	C	513	HIS
1	D	377	HIS
1	D	502	GLN
1	D	513	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	KN3	A	1	-	25,28,28	3.25	6 (24%)	32,42,42	2.76	6 (18%)
2	KN3	B	1	-	25,28,28	3.71	7 (28%)	32,42,42	1.80	8 (25%)
2	KN3	C	1	-	25,28,28	3.95	7 (28%)	32,42,42	2.17	12 (37%)
2	KN3	D	1	-	25,28,28	3.67	6 (24%)	32,42,42	1.83	8 (25%)

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	KN3	A	1	-	-	2/11/15/15	0/3/3/3
2	KN3	B	1	-	-	1/11/15/15	0/3/3/3
2	KN3	C	1	-	-	1/11/15/15	0/3/3/3
2	KN3	D	1	-	-	6/11/15/15	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	KN3	NAH-NAI	-13.46	1.22	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	KN3	NAH-NAI	-13.38	1.22	1.37
2	C	1	KN3	NAH-NAI	-12.35	1.23	1.37
2	A	1	KN3	NAH-NAI	-12.23	1.24	1.37
2	B	1	KN3	CAJ-CAG	-9.48	1.37	1.49
2	D	1	KN3	CAJ-CAG	-8.67	1.38	1.49
2	A	1	KN3	CAJ-CAG	-8.28	1.39	1.49
2	C	1	KN3	CAK-CAL	-7.67	1.30	1.49
2	C	1	KN3	CAN-CAM	-7.05	1.31	1.50
2	C	1	KN3	CAJ-CAG	-6.66	1.41	1.49
2	C	1	KN3	CAW-CAF	6.16	1.57	1.50
2	C	1	KN3	CAO-CAM	5.43	1.65	1.50
2	D	1	KN3	CAK-CAL	-5.02	1.36	1.49
2	D	1	KN3	CAW-CAF	4.83	1.56	1.50
2	B	1	KN3	CAW-CAF	4.30	1.55	1.50
2	A	1	KN3	CAK-CAL	-4.12	1.39	1.49
2	B	1	KN3	CAG-NAH	-3.95	1.32	1.35
2	D	1	KN3	CAG-NAH	-3.81	1.32	1.35
2	B	1	KN3	CAK-CAL	-3.50	1.40	1.49
2	A	1	KN3	CAL-CAM	2.80	1.40	1.32
2	A	1	KN3	CAO-CAM	2.75	1.57	1.50
2	B	1	KN3	CAL-CAM	2.53	1.39	1.32
2	D	1	KN3	CAA-CAF	2.31	1.40	1.37
2	A	1	KN3	CAG-NAH	-2.27	1.33	1.35
2	C	1	KN3	CAG-NAH	-2.24	1.33	1.35
2	B	1	KN3	CAA-CAF	2.03	1.40	1.37

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	KN3	FAY-CAW-CAF	-11.31	100.59	112.32
2	C	1	KN3	CAO-CAM-CAL	-5.41	107.00	122.65
2	A	1	KN3	CAT-CAJ-CAG	-5.22	116.13	121.28
2	D	1	KN3	CAW-CAF-CAE	5.02	122.67	119.46
2	A	1	KN3	CAW-CAF-CAE	4.90	122.59	119.46
2	C	1	KN3	CAW-CAF-CAE	4.80	122.53	119.46
2	A	1	KN3	CAK-CAL-CAM	4.69	135.33	127.14
2	B	1	KN3	CAT-CAJ-CAG	-4.64	116.70	121.28
2	D	1	KN3	FAX-CAW-CAF	-4.29	107.87	112.32
2	C	1	KN3	CAT-CAJ-CAG	4.17	125.40	121.28
2	B	1	KN3	FAZ-CAW-CAF	-3.82	108.36	112.32
2	B	1	KN3	CAJ-CAG-NAH	3.52	126.81	120.78
2	A	1	KN3	CAJ-CAG-NAH	3.13	126.14	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	KN3	FAY-CAW-CAF	-3.11	109.10	112.32
2	A	1	KN3	CAP-CAJ-CAG	3.09	123.98	120.14
2	C	1	KN3	CAO-CAM-CAN	3.08	121.40	114.60
2	B	1	KN3	CAK-CAL-CAM	3.02	132.41	127.14
2	D	1	KN3	CAT-CAJ-CAG	2.93	124.17	121.28
2	C	1	KN3	CAN-CAM-CAL	2.90	131.04	122.65
2	B	1	KN3	CAC-CAD-CAE	2.85	122.06	116.73
2	C	1	KN3	CAP-CAJ-CAG	-2.77	116.71	120.14
2	D	1	KN3	CAO-CAM-CAL	-2.76	114.67	122.65
2	D	1	KN3	CAP-CAJ-CAG	-2.75	116.73	120.14
2	C	1	KN3	CAK-NAI-NAH	2.73	125.71	117.98
2	D	1	KN3	CAO-CAM-CAN	2.67	120.49	114.60
2	B	1	KN3	CAO-CAM-CAN	2.64	120.43	114.60
2	C	1	KN3	FAX-CAW-CAF	-2.55	109.67	112.32
2	B	1	KN3	CAN-CAM-CAL	-2.43	115.62	122.65
2	C	1	KN3	FAY-CAW-CAF	-2.35	109.89	112.32
2	C	1	KN3	CAB-CAC-CAD	-2.32	117.68	120.89
2	C	1	KN3	CAK-CAL-CAM	-2.28	123.15	127.14
2	B	1	KN3	CAP-CAJ-CAT	2.11	121.39	117.45
2	D	1	KN3	CAC-CAD-CAE	2.09	120.63	116.73
2	C	1	KN3	FAZ-CAW-CAF	2.08	114.48	112.32

There are no chirality outliers.

All (10) torsion outliers are listed below:

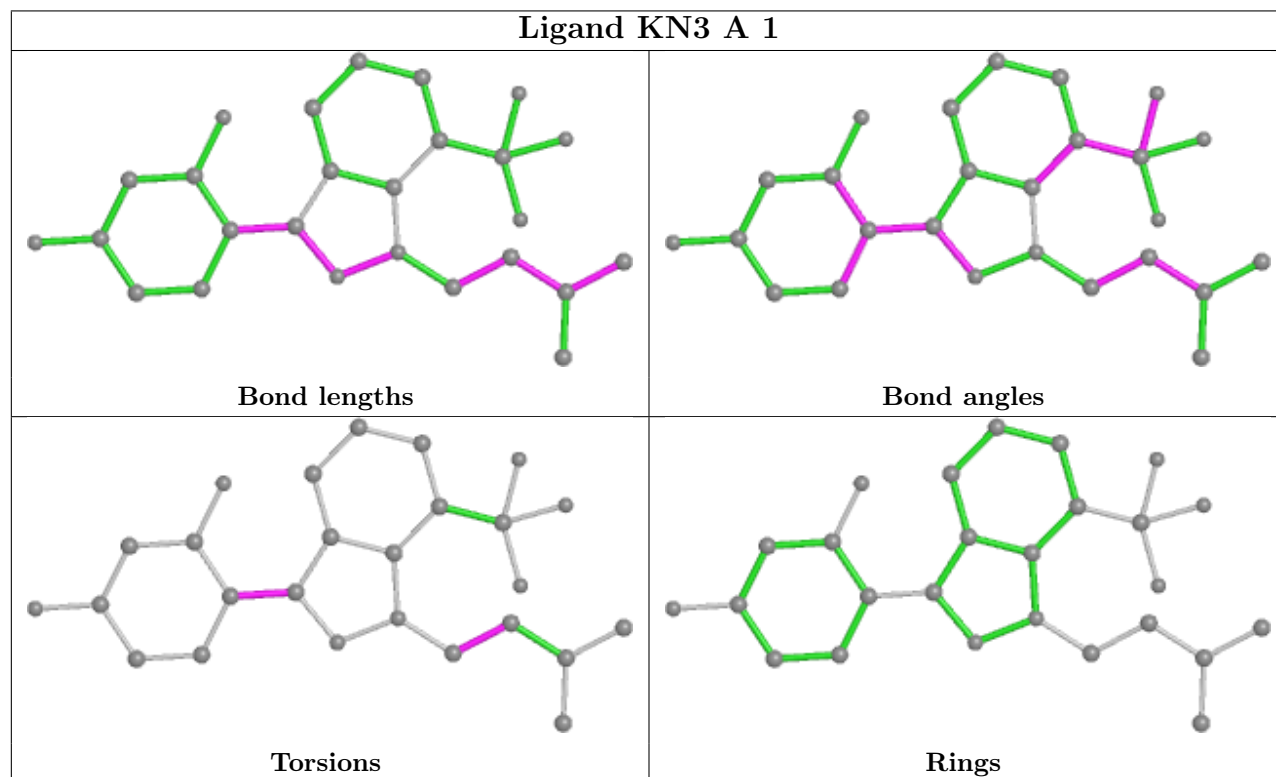
Mol	Chain	Res	Type	Atoms
2	A	1	KN3	NAH-CAG-CAJ-CAP
2	D	1	KN3	CAE-CAF-CAW-FAX
2	D	1	KN3	CAE-CAF-CAW-FAZ
2	D	1	KN3	CAE-CAF-CAW-FAY
2	A	1	KN3	NAI-CAK-CAL-CAM
2	B	1	KN3	NAH-CAG-CAJ-CAP
2	D	1	KN3	CAA-CAF-CAW-FAZ
2	D	1	KN3	CAA-CAF-CAW-FAX
2	C	1	KN3	NAH-CAG-CAJ-CAP
2	D	1	KN3	NAH-CAG-CAJ-CAP

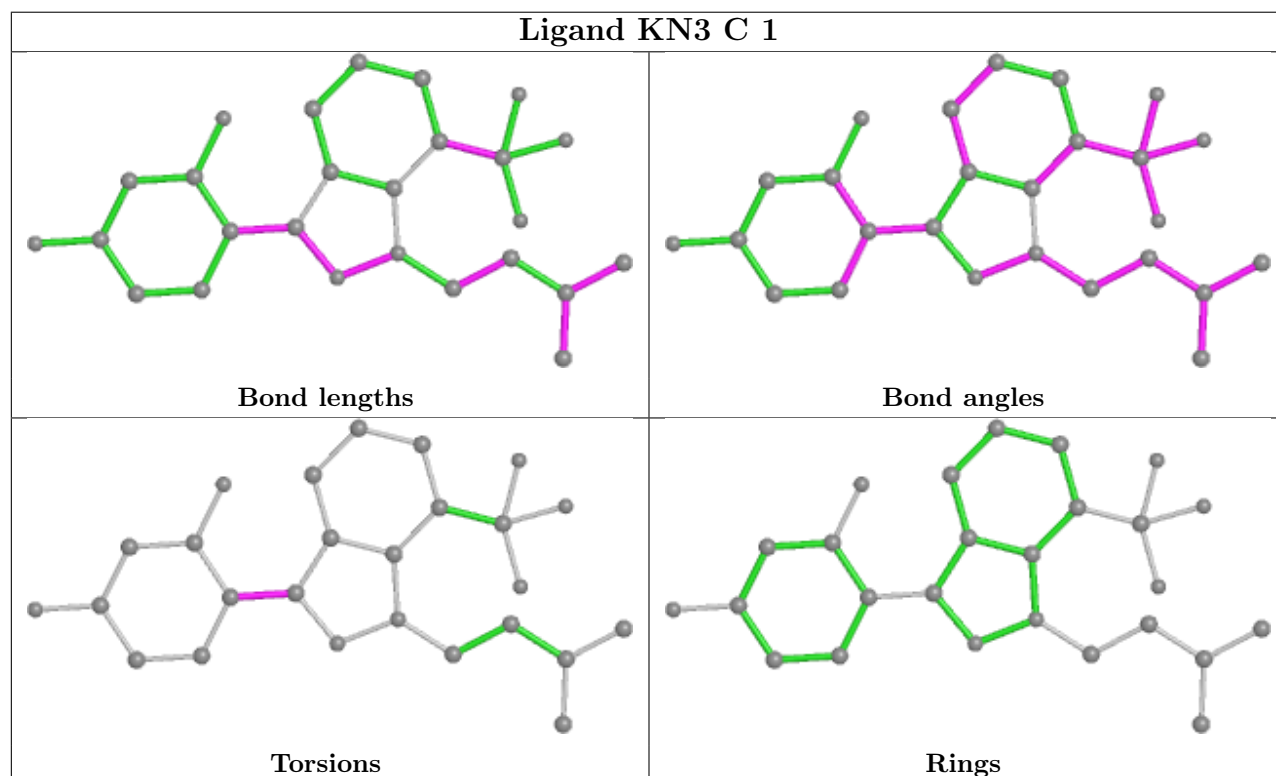
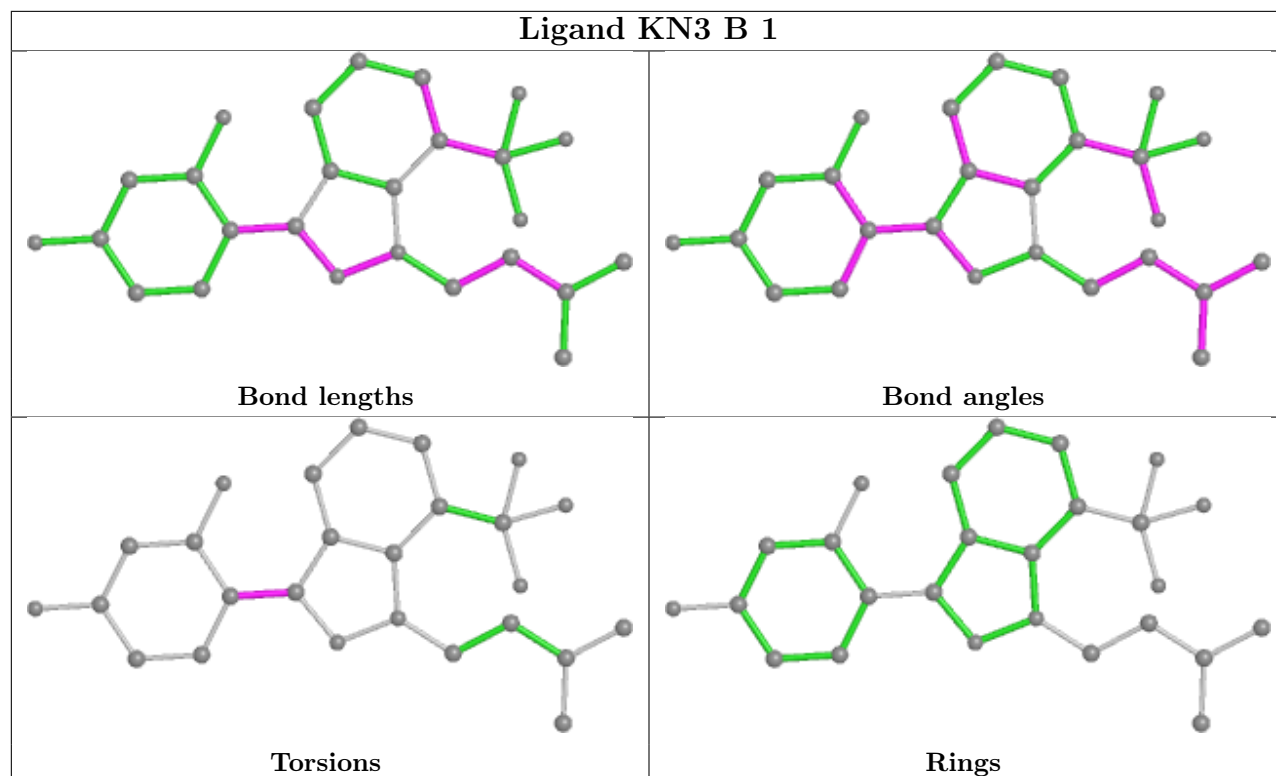
There are no ring outliers.

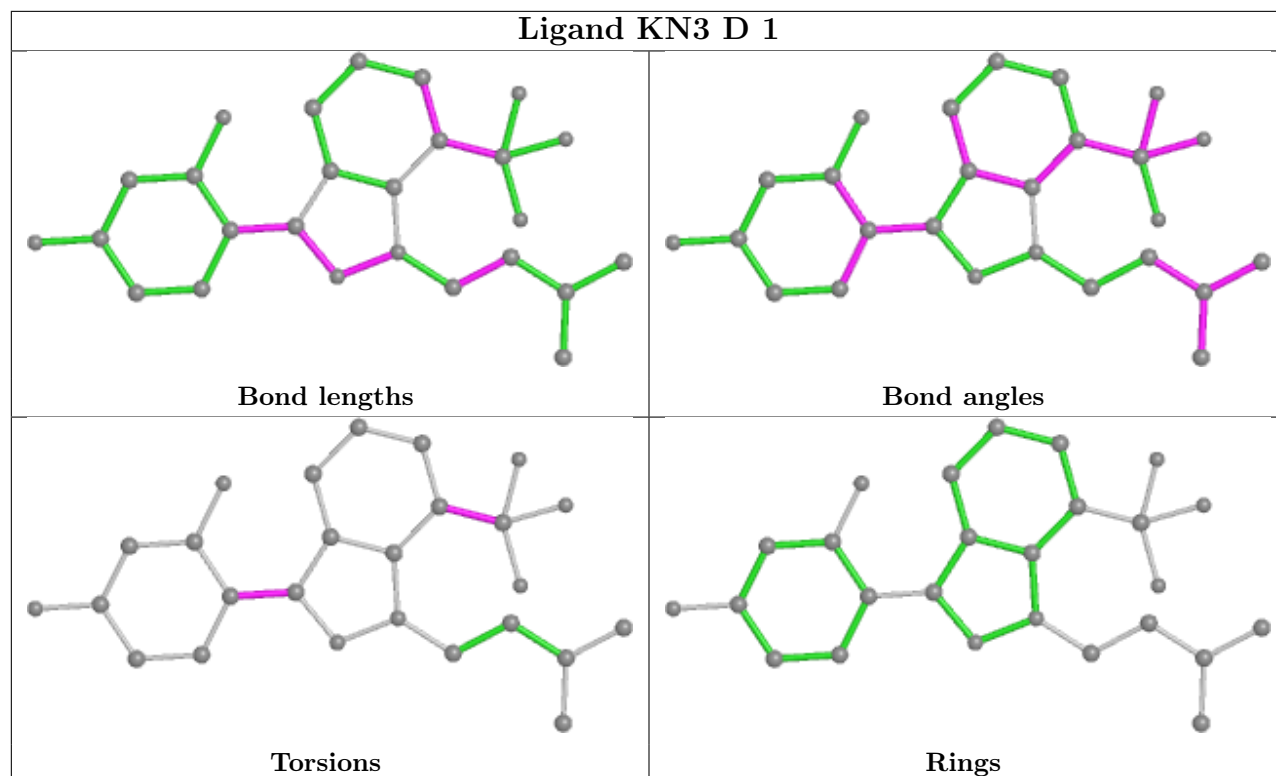
4 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	KN3	3	0
2	B	1	KN3	8	0
2	C	1	KN3	6	0
2	D	1	KN3	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	239/258 (92%)	-0.40	4 (1%) 70 76	14, 36, 84, 116	0
1	B	239/258 (92%)	-0.39	1 (0%) 92 95	15, 35, 84, 115	0
1	C	230/258 (89%)	-0.40	4 (1%) 70 76	18, 35, 90, 112	0
1	D	226/258 (87%)	-0.38	4 (1%) 68 74	19, 35, 85, 109	0
All	All	934/1032 (90%)	-0.39	13 (1%) 75 80	14, 35, 87, 116	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	462	LEU	5.3
1	A	462	LEU	3.0
1	D	533	VAL	2.6
1	A	530	CYS	2.6
1	A	331	TYR	2.4
1	D	305	SER	2.4
1	D	460	THR	2.4
1	C	331	TYR	2.3
1	C	420	GLY	2.2
1	A	415	GLY	2.1
1	C	463	SER	2.1
1	D	420	GLY	2.1
1	C	345	LEU	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

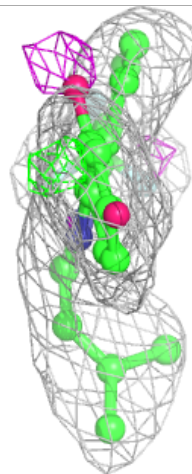
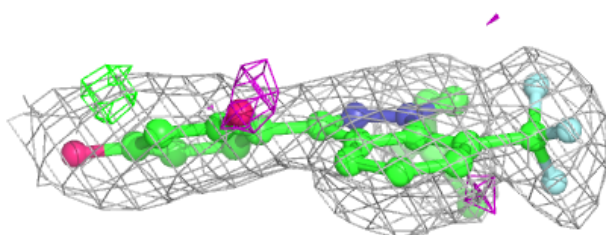
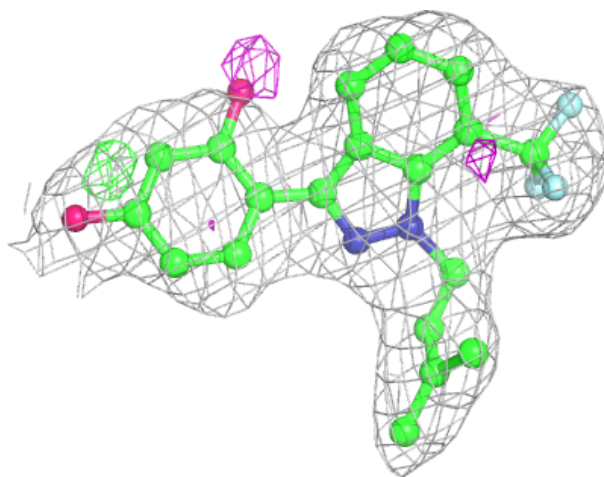
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	KN3	D	1	26/26	0.90	0.15	32,42,55,61	0
2	KN3	C	1	26/26	0.93	0.18	32,43,54,56	0
2	KN3	B	1	26/26	0.95	0.12	26,34,47,52	0
2	KN3	A	1	26/26	0.96	0.10	18,38,49,55	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.

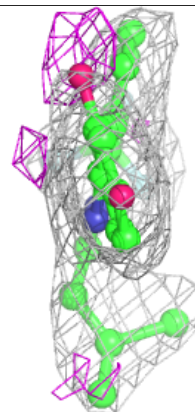
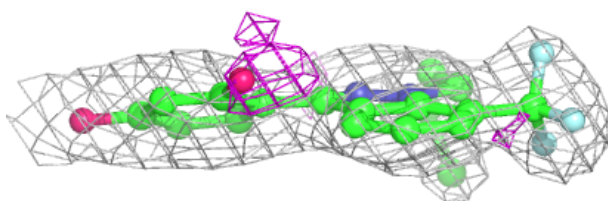
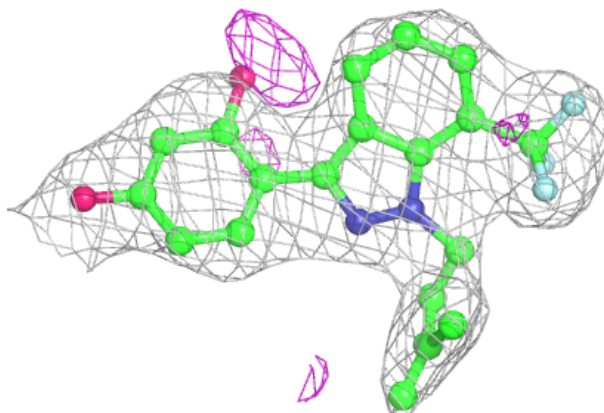
**Electron density around KN3 D 1:**

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

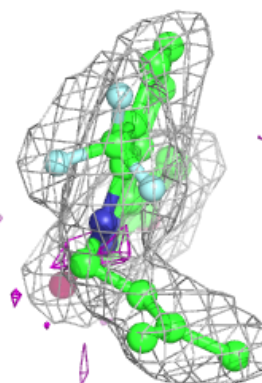
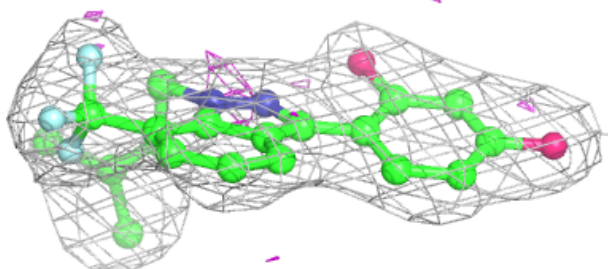
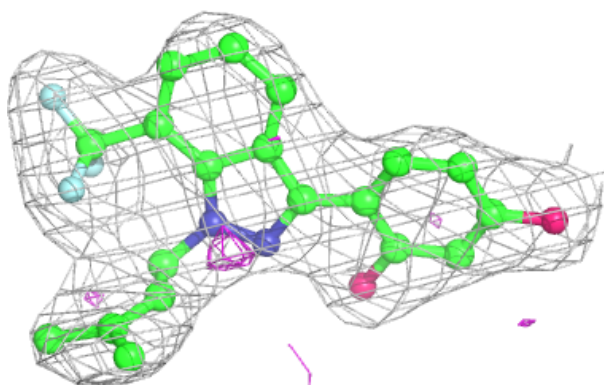


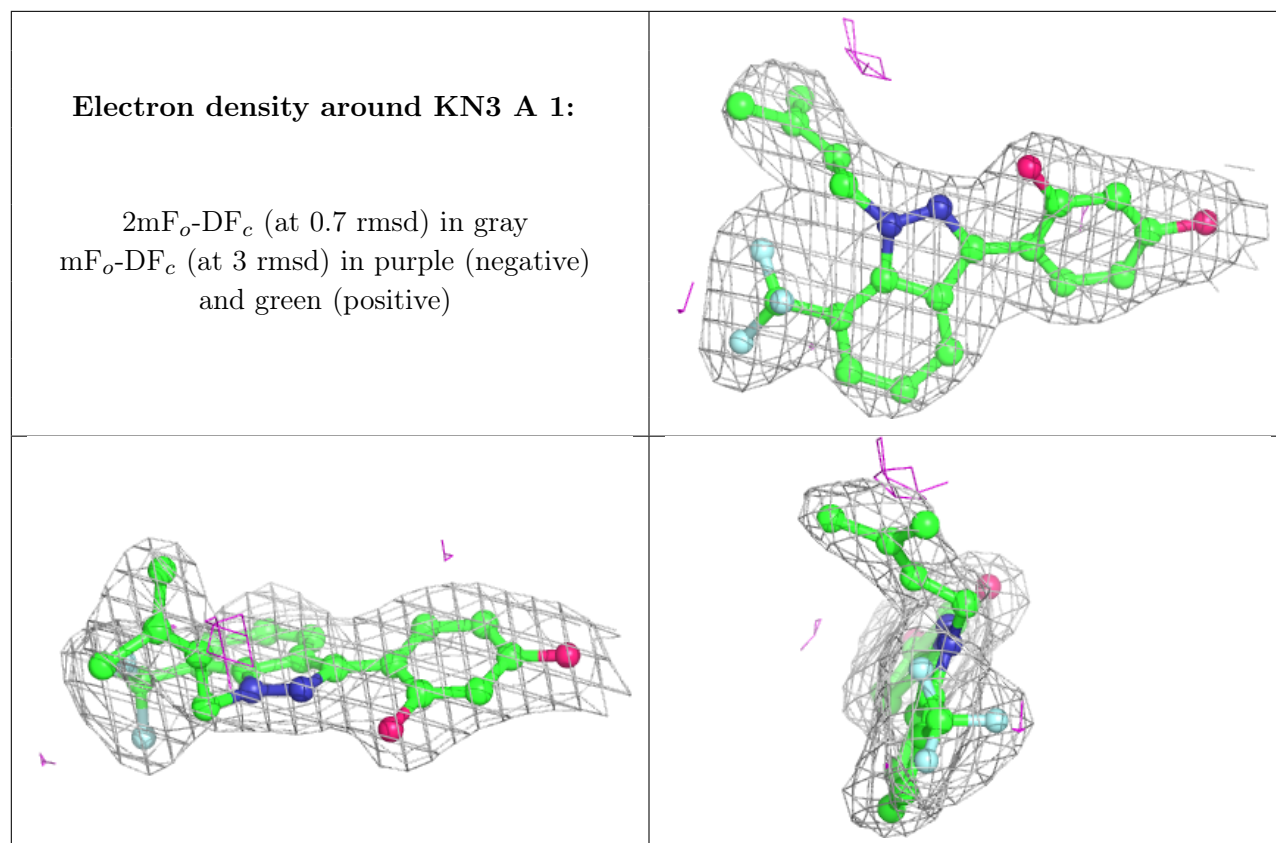
**Electron density around KN3 C 1:**

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

**Electron density around KN3 B 1:**

$2mF_o-DF_c$  (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.