



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:10 AM UTC

PDB ID : 8FA0 / pdb\_00008fa0  
Title : Crystal structure of clade A/E 93TH057 HIV-1 gp120 core in complex with NBD-14208, an HIV-1 gp120 antagonist  
Authors : Kwon, Y.D.; Kwong, P.D.  
Deposited on : 2022-11-25  
Resolution : 2.09 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

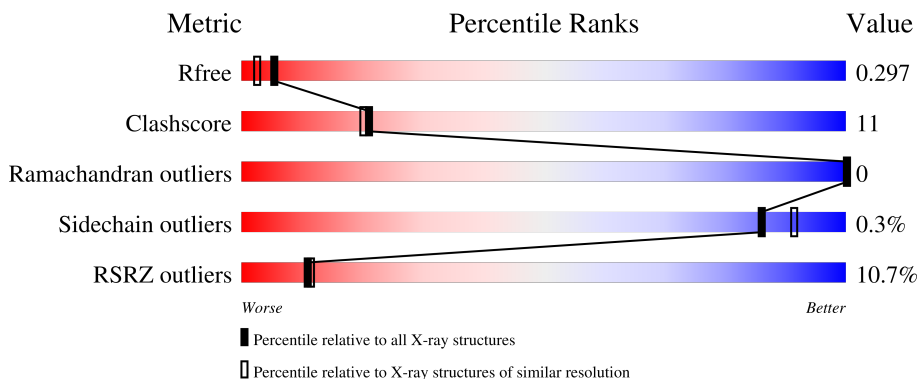
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	353	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2907 atoms, of which 34 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.

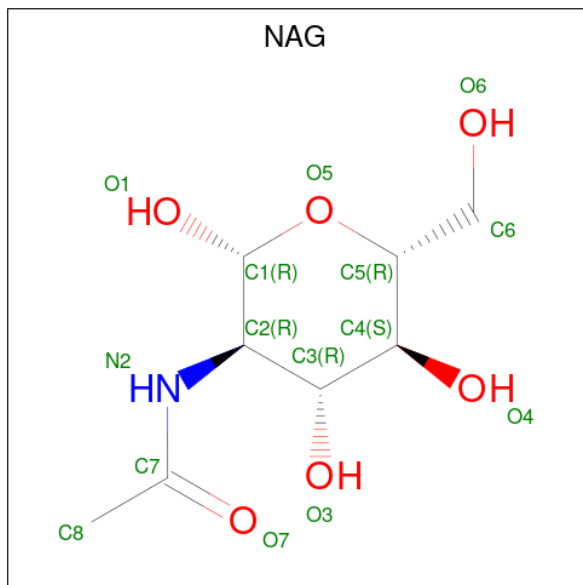
- Molecule 1 is a protein called HIV-1 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	336	2639	1658	457	503	21	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	375	SER	HIS	engineered mutation	UNP A0A0M3KKW8

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



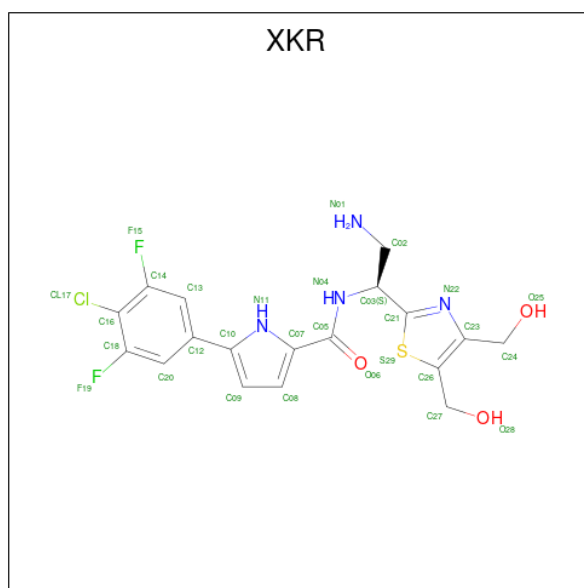
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is N-((1S)-2-amino-1-[4,5-bis(hydroxymethyl)-1,3-thiazol-2-yl]ethyl)-5-(4-chloro-3,5-difluorophenyl)-1H-pyrrole-2-carboxamide (CCD ID: XKR) (formula: C<sub>18</sub>H<sub>17</sub>ClF<sub>2</sub>N<sub>4</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	
3	A	1	Total	C	Cl	F	H	N	O	S	0	0
			46	18	1	2	17	4	3	1		
3	A	1	Total	C	Cl	F	H	N	O	S	0	0
			46	18	1	2	17	4	3	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	15	8	2	4	1	0	0

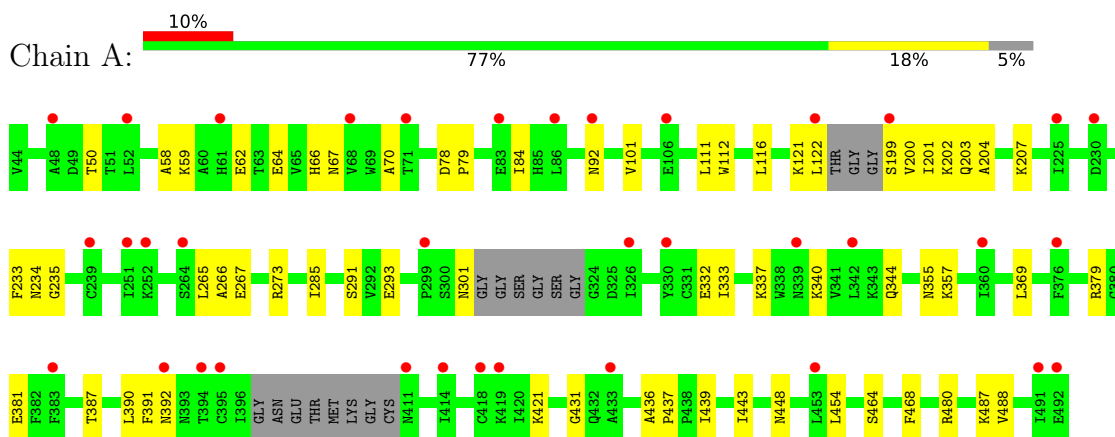
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	49	Total	O	0	0
			49	49		

### 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: HIV-1 gp120 core



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.21Å 66.97Å 90.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.35 – 2.09 36.35 – 2.09	Depositor EDS
% Data completeness (in resolution range)	94.2 (36.35-2.09) 94.3 (36.35-2.09)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.08Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.243 , 0.298 0.243 , 0.297	Depositor DCC
$R_{free}$ test set	1071 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.5	Xtrriage
Anisotropy	0.251	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 29.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2907	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% 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: NAG, XKR, EPE

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	0.33	0/2693	0.43	0/3655

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2639	0	2578	61	2
2	A	112	0	104	1	0
3	A	58	34	0	1	0
4	A	15	0	17	2	0
5	A	49	0	0	16	0
All	All	2873	34	2699	61	2

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 11.

All (61) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HD12	1:A:201:ILE:CG1	1.74	1.18
1:A:202:LYS:NZ	5:A:601:HOH:O	1.82	1.11
1:A:122:LEU:HD12	1:A:201:ILE:HG12	1.39	1.04
1:A:122:LEU:HD12	1:A:201:ILE:HG13	1.41	0.98
1:A:200:VAL:HG21	4:A:511:EPE:H62	1.44	0.97
1:A:293:GLU:OE1	5:A:602:HOH:O	1.96	0.82
1:A:200:VAL:CG2	4:A:511:EPE:H62	2.09	0.81
1:A:387:THR:HG23	1:A:390:LEU:HD12	1.62	0.80
1:A:448:ASN:OD1	5:A:603:HOH:O	1.99	0.79
1:A:121:LYS:HG2	1:A:122:LEU:H	1.48	0.79
1:A:101:VAL:HG21	1:A:480:ARG:HG2	1.64	0.78
1:A:122:LEU:CD1	1:A:201:ILE:HG13	2.13	0.78
1:A:202:LYS:CE	5:A:601:HOH:O	2.28	0.77
1:A:379:ARG:NE	5:A:605:HOH:O	2.24	0.69
1:A:202:LYS:HE2	5:A:601:HOH:O	1.91	0.67
1:A:355:ASN:ND2	5:A:607:HOH:O	2.30	0.65
1:A:207:LYS:HD2	1:A:439:ILE:HG23	1.79	0.65
1:A:387:THR:O	1:A:387:THR:HG22	1.98	0.64
1:A:92:ASN:O	1:A:487:LYS:NZ	2.25	0.64
1:A:387:THR:HG22	1:A:390:LEU:HB2	1.81	0.63
1:A:431:GLY:HA2	3:A:510:XKR:N22	2.15	0.62
1:A:355:ASN:ND2	5:A:609:HOH:O	2.35	0.60
1:A:454:LEU:HD22	1:A:468:PHE:HB3	1.82	0.59
1:A:121:LYS:CG	1:A:122:LEU:H	2.16	0.58
1:A:112:TRP:CE3	1:A:116:LEU:HD22	2.40	0.56
1:A:344:GLN:NE2	5:A:606:HOH:O	2.27	0.55
1:A:122:LEU:HB2	1:A:199:SER:O	2.06	0.55
1:A:357:LYS:HE3	1:A:464:SER:HA	1.89	0.55
1:A:50:THR:HG22	1:A:488:VAL:HG11	1.90	0.52
1:A:207:LYS:HE3	1:A:437:PRO:O	2.09	0.52
1:A:265:LEU:HD11	1:A:291:SER:OG	2.09	0.52
1:A:58:ALA:HB2	1:A:70:ALA:HB3	1.92	0.51
1:A:337:LYS:HG3	2:A:507:NAG:O5	2.10	0.51
1:A:387:THR:CG2	1:A:390:LEU:HB2	2.40	0.51
1:A:267:GLU:HG3	5:A:629:HOH:O	2.11	0.50
1:A:387:THR:HG23	1:A:390:LEU:CD1	2.38	0.50
1:A:392:ASN:ND2	5:A:612:HOH:O	2.45	0.49
1:A:381:GLU:HG3	1:A:443:ILE:HD13	1.94	0.49
1:A:387:THR:HG21	1:A:391:PHE:HE2	1.78	0.48
1:A:64:GLU:OE1	1:A:66:HIS:HB2	2.15	0.47
1:A:301:ASN:ND2	5:A:613:HOH:O	2.47	0.47
1:A:64:GLU:HB3	1:A:67:ASN:HD22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LYS:HG2	1:A:122:LEU:N	2.23	0.46
1:A:203:GLN:HG3	1:A:204:ALA:N	2.31	0.46
1:A:78:ASP:OD1	1:A:79:PRO:HD2	2.16	0.45
1:A:207:LYS:HE2	1:A:436:ALA:HB3	1.98	0.45
1:A:122:LEU:CB	1:A:199:SER:O	2.65	0.45
1:A:379:ARG:HG3	5:A:605:HOH:O	2.15	0.45
1:A:111:LEU:C	1:A:111:LEU:HD23	2.43	0.44
1:A:293:GLU:CD	5:A:602:HOH:O	2.51	0.44
1:A:59:LYS:HB2	1:A:62:GLU:HG3	2.00	0.44
1:A:387:THR:CG2	1:A:390:LEU:HD12	2.40	0.44
1:A:122:LEU:CD1	1:A:201:ILE:CG1	2.66	0.43
1:A:439:ILE:HG21	5:A:631:HOH:O	2.18	0.43
1:A:233:PHE:CE2	1:A:235:GLY:HA2	2.54	0.43
1:A:369:LEU:HD12	1:A:421:LYS:HE3	2.00	0.42
1:A:340:LYS:O	1:A:344:GLN:HG3	2.19	0.42
1:A:332:GLU:C	1:A:333:ILE:HG13	2.44	0.42
1:A:234:ASN:OD1	1:A:234:ASN:C	2.63	0.41
1:A:266:ALA:HB1	5:A:618:HOH:O	2.19	0.41
1:A:273:ARG:HB2	1:A:285:ILE:HB	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ASN:C	1:A:464:SER:OG[2_464]	2.00	0.20
1:A:301:ASN:O	1:A:464:SER:N[2_464]	2.09	0.11

## 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	328/353 (93%)	317 (97%)	11 (3%)	0	<a href="#">100</a> <a href="#">100</a>

There are no Ramachandran outliers to report.

### 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	302/311 (97%)	301 (100%)	1 (0%)	86 91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	ASN
1	A	425	ASN
1	A	432	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

11 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	XKR	A	509	-	30,31,31	2.29	7 (23%)	38,44,44	2.42	14 (36%)
2	NAG	A	506	1	14,14,15	0.34	0	17,19,21	0.43	0
3	XKR	A	510	-	30,31,31	2.35	10 (33%)	38,44,44	2.32	13 (34%)
2	NAG	A	505	1	14,14,15	0.39	0	17,19,21	0.62	0
2	NAG	A	501	1	14,14,15	0.27	0	17,19,21	0.35	0
2	NAG	A	504	1	14,14,15	0.36	0	17,19,21	0.56	0
4	EPE	A	511	-	15,15,15	0.87	1 (6%)	19,20,20	1.58	4 (21%)
2	NAG	A	502	1	14,14,15	0.39	0	17,19,21	0.51	0
2	NAG	A	507	1	14,14,15	0.40	0	17,19,21	0.70	1 (5%)
2	NAG	A	508	1	14,14,15	0.22	0	17,19,21	0.49	0
2	NAG	A	503	1	14,14,15	0.36	0	17,19,21	0.64	0

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	XKR	A	509	-	-	7/21/22/22	0/3/3/3
2	NAG	A	506	1	-	0/6/23/26	0/1/1/1
3	XKR	A	510	-	-	3/21/22/22	0/3/3/3
2	NAG	A	505	1	-	0/6/23/26	0/1/1/1
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	504	1	-	2/6/23/26	0/1/1/1
4	EPE	A	511	-	-	6/9/19/19	0/1/1/1
2	NAG	A	502	1	-	0/6/23/26	0/1/1/1
2	NAG	A	507	1	-	0/6/23/26	0/1/1/1
2	NAG	A	508	1	-	0/6/23/26	0/1/1/1
2	NAG	A	503	1	-	0/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	509	XKR	C02-N01	-6.44	1.17	1.48
3	A	510	XKR	C02-N01	-6.17	1.18	1.48
3	A	509	XKR	C05-N04	5.20	1.45	1.34
3	A	510	XKR	C03-C21	4.82	1.63	1.50
3	A	510	XKR	C23-N22	4.42	1.46	1.38
3	A	509	XKR	C23-N22	4.35	1.46	1.38
3	A	509	XKR	C24-C23	4.33	1.56	1.50
3	A	510	XKR	C05-N04	4.31	1.43	1.34
3	A	509	XKR	C03-C21	3.80	1.60	1.50
3	A	510	XKR	C24-C23	3.39	1.54	1.50
3	A	510	XKR	C03-N04	3.01	1.52	1.45
4	A	511	EPE	C10-S	2.94	1.81	1.77
3	A	510	XKR	C20-C18	2.49	1.41	1.37
3	A	509	XKR	C13-C14	2.42	1.41	1.37
3	A	510	XKR	C21-S29	2.31	1.81	1.75
3	A	509	XKR	C20-C18	2.17	1.41	1.37
3	A	510	XKR	C07-N11	2.09	1.41	1.37
3	A	510	XKR	C02-C03	-2.06	1.49	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	509	XKR	C03-C21-N22	6.13	133.59	123.61
3	A	509	XKR	C27-C26-C23	5.17	133.17	126.84
3	A	510	XKR	C03-C21-N22	5.10	131.90	123.61
3	A	510	XKR	C27-C26-C23	5.03	133.01	126.84
3	A	510	XKR	C07-C05-N04	4.90	123.41	116.86
3	A	509	XKR	C20-C12-C13	-4.57	114.30	119.65
3	A	509	XKR	C03-C21-S29	-4.52	115.36	121.80
3	A	510	XKR	C20-C12-C13	-4.50	114.39	119.65
3	A	509	XKR	C07-C05-N04	4.36	122.67	116.86
3	A	510	XKR	S29-C21-N22	-4.29	110.13	116.00
3	A	509	XKR	C02-C03-C21	-3.90	100.62	108.65
4	A	511	EPE	C5-N4-C3	3.82	117.08	108.84
3	A	509	XKR	S29-C21-N22	-3.64	111.02	116.00
3	A	510	XKR	C24-C23-N22	3.15	123.87	118.42
3	A	509	XKR	C12-C13-C14	3.04	123.22	119.07
3	A	510	XKR	C20-C12-C10	3.00	125.07	120.43
3	A	510	XKR	C12-C13-C14	2.95	123.09	119.07
3	A	510	XKR	O06-C05-N04	-2.95	117.89	123.09
3	A	509	XKR	C12-C20-C18	2.73	122.79	119.07
3	A	510	XKR	C03-C21-S29	-2.70	117.96	121.80
3	A	509	XKR	O06-C05-N04	-2.65	118.42	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	509	XKR	C20-C12-C10	2.62	124.49	120.43
3	A	510	XKR	C12-C20-C18	2.60	122.61	119.07
3	A	509	XKR	C24-C23-N22	2.56	122.85	118.42
4	A	511	EPE	O1S-S-C10	2.50	110.51	106.73
4	A	511	EPE	C7-N4-C5	2.49	117.88	111.24
3	A	509	XKR	C10-N11-C07	2.42	112.86	109.65
2	A	507	NAG	C1-O5-C5	2.32	115.30	112.19
3	A	510	XKR	C03-N04-C05	2.22	125.73	122.00
4	A	511	EPE	C7-N4-C3	2.18	117.05	111.24
3	A	509	XKR	C18-C16-C14	-2.13	115.21	117.87
3	A	510	XKR	C09-C10-N11	-2.03	104.69	107.10

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	509	XKR	C26-C23-C24-O25
3	A	509	XKR	N04-C05-C07-C08
3	A	509	XKR	N04-C05-C07-N11
3	A	509	XKR	O06-C05-C07-N11
3	A	510	XKR	C21-C03-N04-C05
4	A	511	EPE	C9-C10-S-O1S
4	A	511	EPE	C9-C10-S-O2S
4	A	511	EPE	C9-C10-S-O3S
3	A	509	XKR	O06-C05-C07-C08
4	A	511	EPE	S-C10-C9-N1
2	A	504	NAG	C4-C5-C6-O6
4	A	511	EPE	C10-C9-N1-C2
4	A	511	EPE	C10-C9-N1-C6
2	A	504	NAG	O5-C5-C6-O6
3	A	509	XKR	N22-C23-C24-O25
3	A	510	XKR	N04-C03-C21-N22
3	A	510	XKR	N22-C23-C24-O25
3	A	509	XKR	N04-C03-C21-N22

There are no ring outliers.

3 monomers are involved in 4 short contacts:

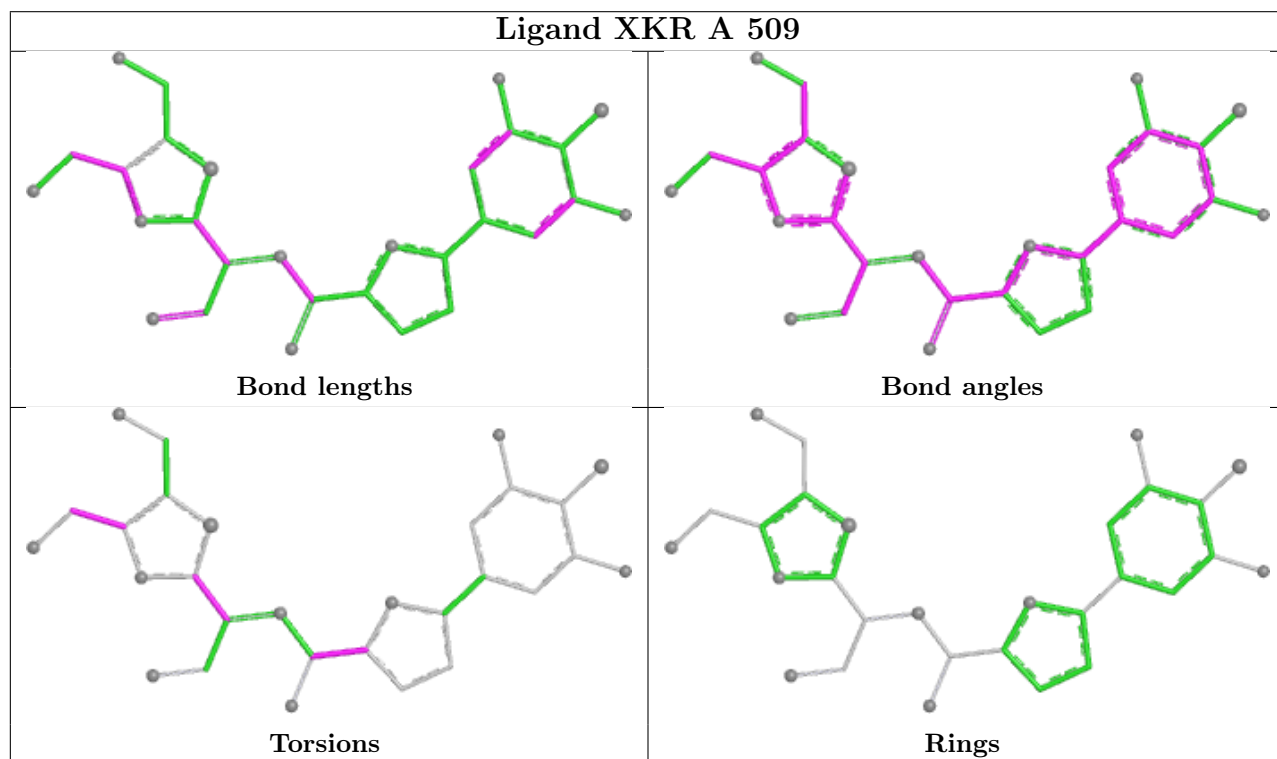
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	510	XKR	1	0
4	A	511	EPE	2	0

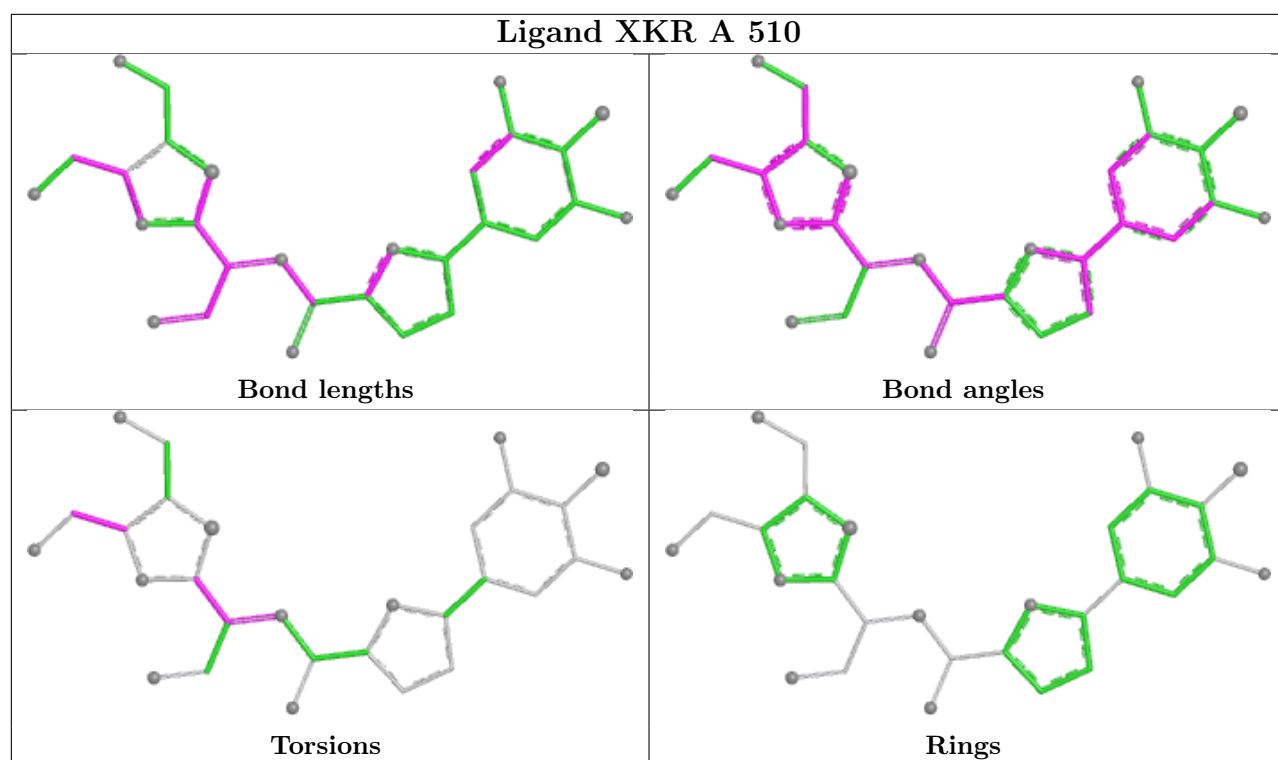
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	507	NAG	1	0

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





## 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, 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	336/353 (95%)	0.81	36 (10%) <b>11</b> <b>11</b>	37, 58, 83, 107	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	LEU	4.3
1	A	394	THR	4.2
1	A	339	ASN	3.2
1	A	122	LEU	3.2
1	A	71	THR	3.1
1	A	86	LEU	3.1
1	A	83	GLU	3.0
1	A	48	ALA	3.0
1	A	61	HIS	3.0
1	A	383	PHE	3.0
1	A	330	TYR	2.9
1	A	92	ASN	2.9
1	A	342	LEU	2.8
1	A	392	ASN	2.8
1	A	492	GLU	2.8
1	A	199	SER	2.7
1	A	251	ILE	2.6
1	A	376	PHE	2.5
1	A	395	CYS	2.4
1	A	225	ILE	2.4
1	A	418	CYS	2.3
1	A	411	ASN	2.3
1	A	299	PRO	2.3
1	A	419	LYS	2.3
1	A	326	ILE	2.2
1	A	453	LEU	2.1
1	A	264	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	68	VAL	2.1
1	A	433	ALA	2.1
1	A	252	LYS	2.1
1	A	230	ASP	2.1
1	A	491	ILE	2.1
1	A	106	GLU	2.1
1	A	414	ILE	2.1
1	A	360	ILE	2.0
1	A	239	CYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

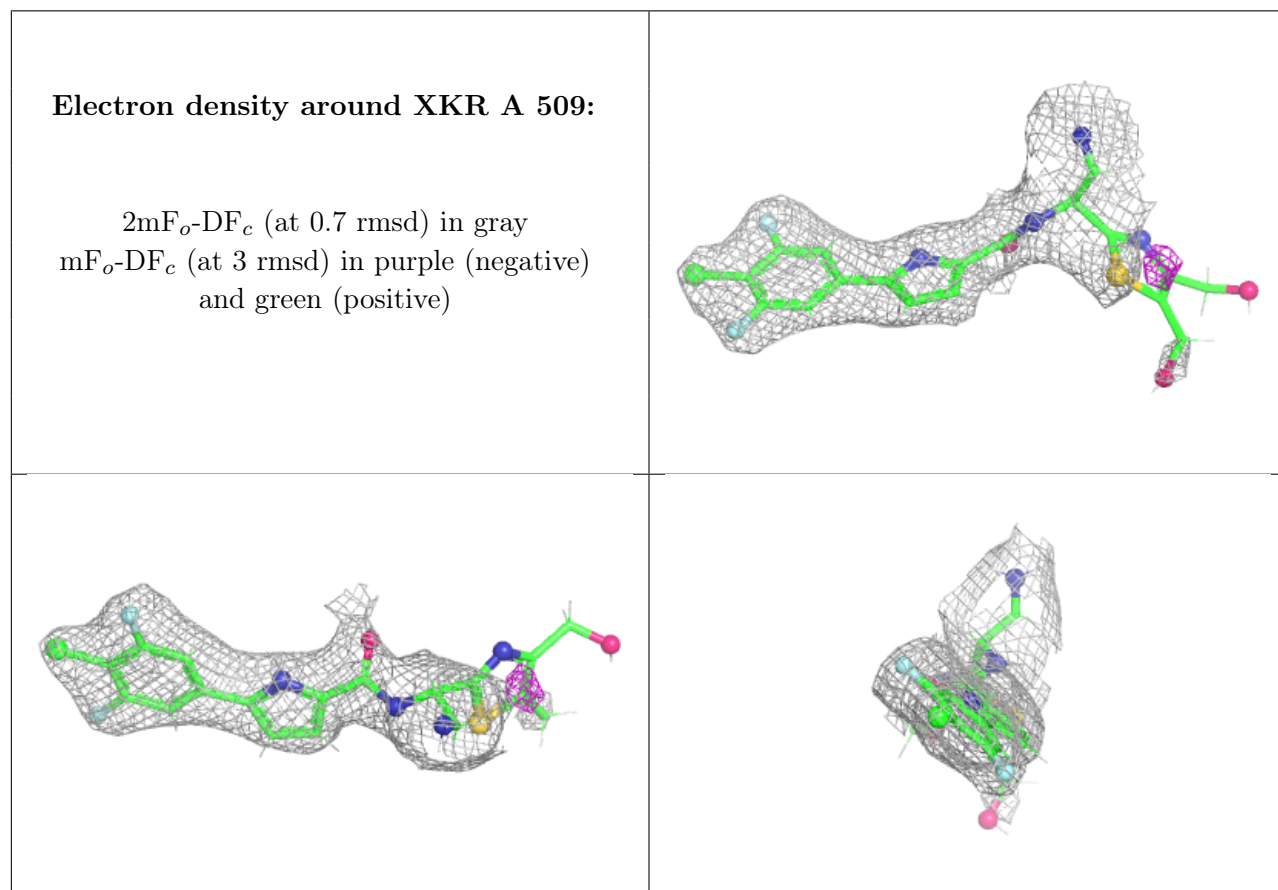
## 6.4 Ligands [i](#)

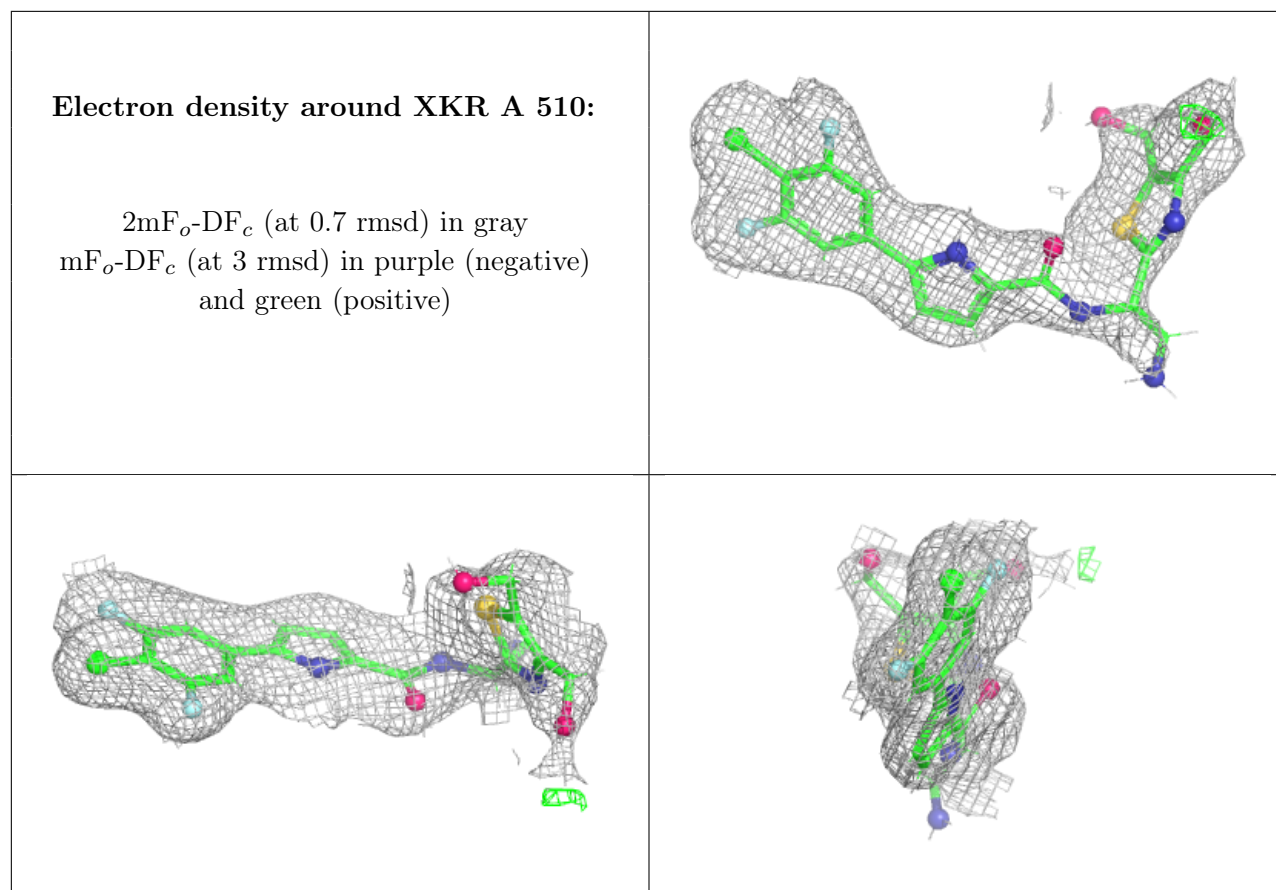
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	NAG	A	502	14/15	0.68	0.11	77,86,89,90	0
2	NAG	A	507	14/15	0.71	0.15	56,67,78,80	0
2	NAG	A	504	14/15	0.74	0.11	68,79,86,87	0
2	NAG	A	508	14/15	0.75	0.12	74,88,93,95	0
4	EPE	A	511	15/15	0.76	0.16	76,82,110,110	0
3	XKR	A	509	29/29	0.80	0.12	66,93,149,151	0
2	NAG	A	501	14/15	0.81	0.10	60,69,82,83	0
2	NAG	A	506	14/15	0.82	0.09	59,68,77,80	0
3	XKR	A	510	29/29	0.85	0.10	56,86,120,122	0
2	NAG	A	505	14/15	0.87	0.09	52,61,69,70	0
2	NAG	A	503	14/15	0.90	0.07	40,45,55,58	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.