



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:18 pm BST

PDB ID : 4I7F  
Title : HIV-1 Reverse Transcriptase in complex with a phosphonate analog of nevirapine  
Authors : Lansdon, E.B.; Parrish, J.  
Deposited on : 2012-11-30  
Resolution : 2.50 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 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

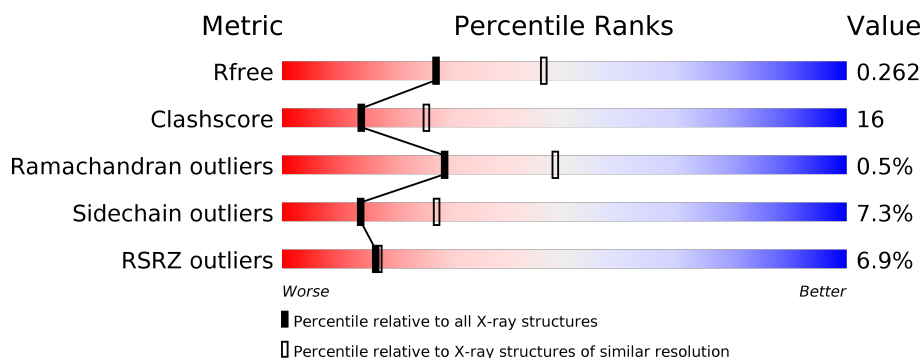
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	560	
2	B	440	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7999 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.

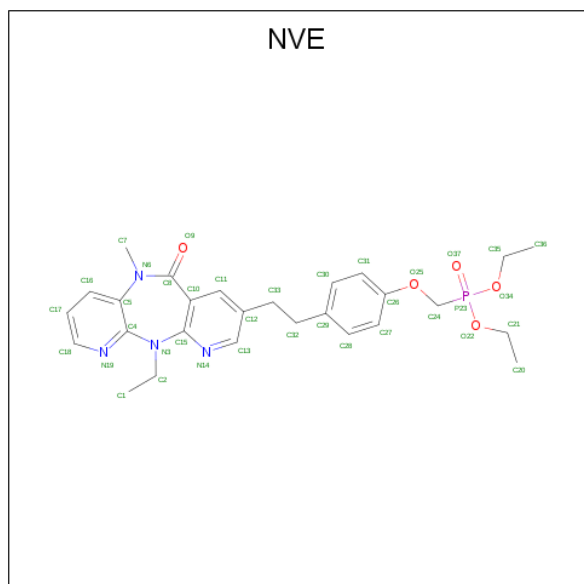
- Molecule 1 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4502	2911	751	832	8			

- Molecule 2 is a protein called Reverse transcriptase.

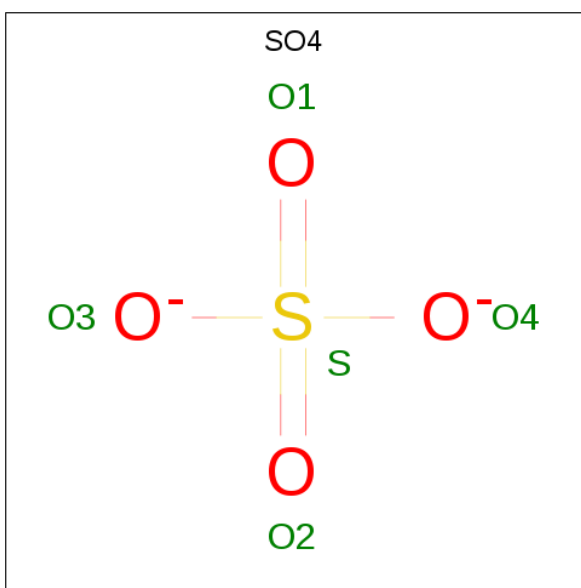
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	0	0
			3353	2184	553	610	6			

- Molecule 3 is diethyl ({4-[2-(11-ethyl-5-methyl-6-oxo-6,11-dihydro-5H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-8-yl)ethyl]phenoxy}methyl)phosphonate (three-letter code: NVE) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>4</sub>O<sub>5</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			37	27	4	5	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	A	1	Total	Cl	0	0
			1	1		

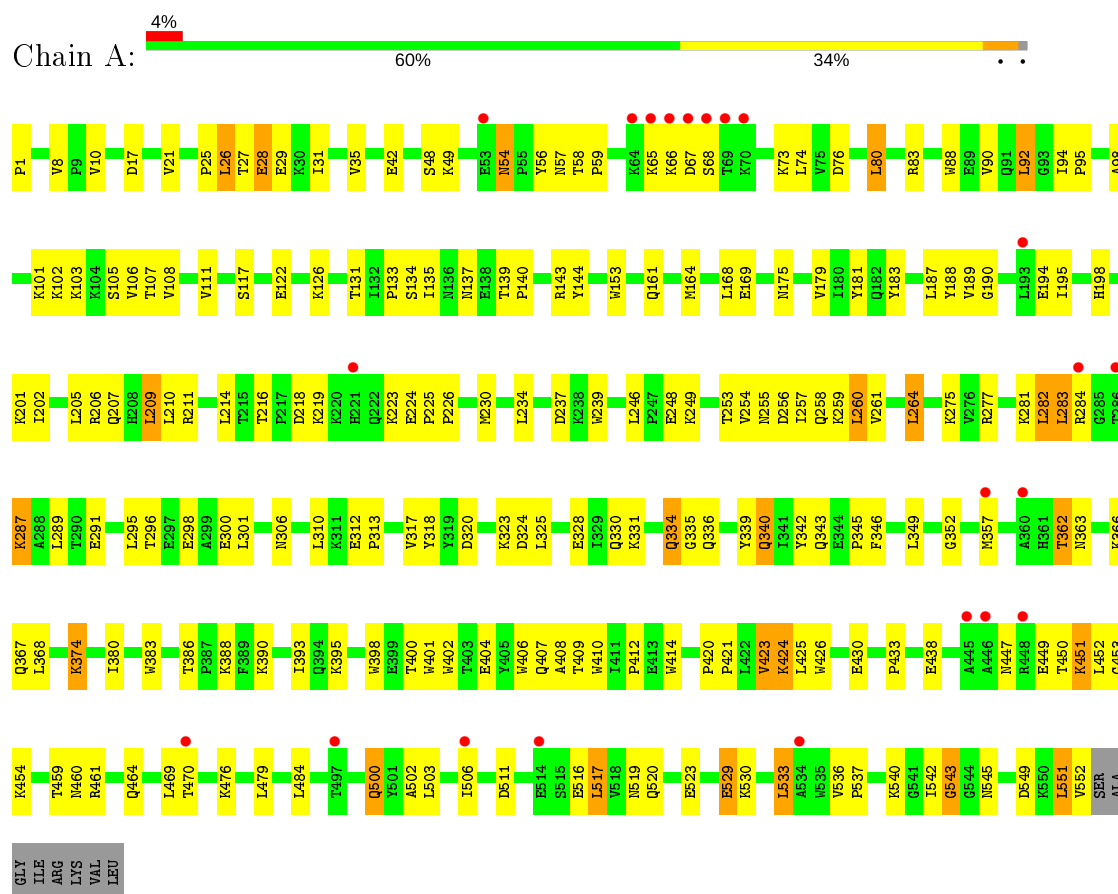
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	49	Total 49	O 49	0	0
7	B	35	Total 35	O 35	0	0

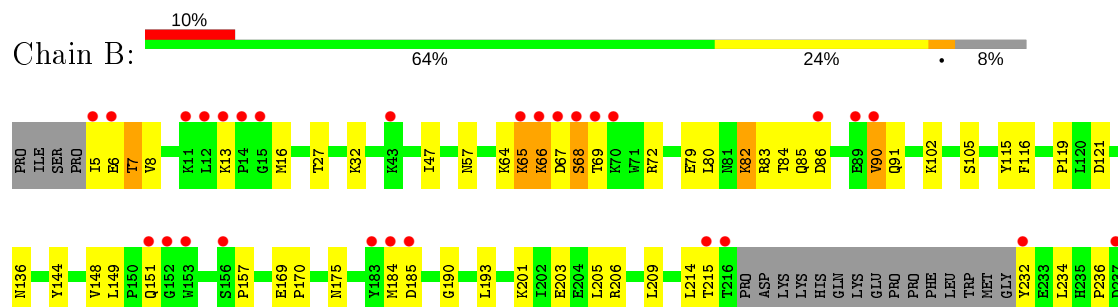
### 3 Residue-property plots

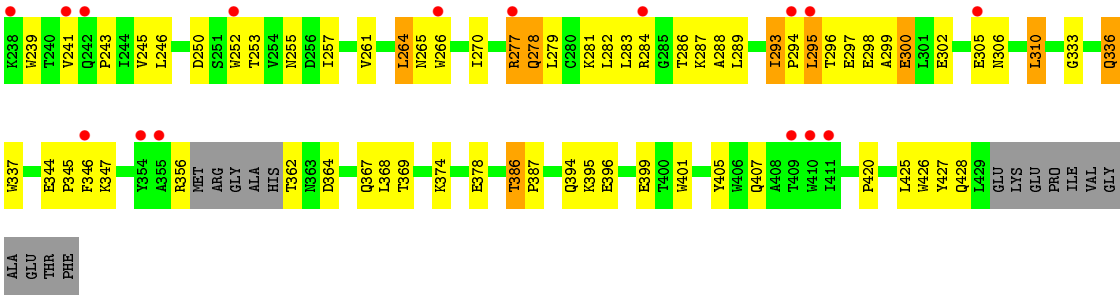
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Reverse transcriptase



#### • Molecule 2: Reverse transcriptase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.32Å 154.70Å 154.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.50) 91.3 (29.93-2.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.28 (at 2.51Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.221 , 0.267 0.215 , 0.262	Depositor DCC
$R_{free}$ test set	2411 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7999	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: NVE, CL, MG, SO4

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	0.37	0/4619	0.52	0/6276
2	B	0.36	0/3446	0.51	0/4683
All	All	0.36	0/8065	0.52	0/10959

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	362	THR	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4502	0	4553	166	0
2	B	3353	0	3388	97	0
3	A	37	0	33	2	0
4	A	20	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	49	0	0	3	0
7	B	35	0	0	0	0
All	All	7999	0	7974	250	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 16.

All (250) 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:459:THR:HG22	1:A:461:ARG:H	0.97	1.09
1:A:131:THR:HG22	1:A:143:ARG:HD2	1.36	1.08
1:A:459:THR:HG22	1:A:461:ARG:N	1.79	0.97
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.49	0.92
1:A:393:ILE:HB	1:A:423:VAL:HG13	1.51	0.91
1:A:275:LYS:H	1:A:306:ASN:HD21	1.20	0.89
1:A:459:THR:CG2	1:A:461:ARG:H	1.87	0.83
1:A:131:THR:CG2	1:A:143:ARG:HD2	2.13	0.79
1:A:320:ASP:H	1:A:343:GLN:HE22	1.32	0.78
2:B:333:GLY:O	2:B:336:GLN:HG3	1.83	0.78
1:A:102:LYS:HE3	1:A:237:ASP:HB3	1.67	0.75
2:B:86:ASP:O	2:B:90:VAL:HG22	1.86	0.75
1:A:194:GLU:H	1:A:194:GLU:CD	1.89	0.74
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.32	0.74
1:A:287:LYS:HD3	1:A:291:GLU:HG2	1.67	0.73
2:B:281:LYS:O	2:B:284:ARG:HG2	1.89	0.72
1:A:25:PRO:HG3	1:A:137:ASN:ND2	2.03	0.72
1:A:503:LEU:HD12	1:A:533:LEU:HD13	1.72	0.72
2:B:425:LEU:HD12	2:B:428:GLN:NE2	2.06	0.70
1:A:460:ASN:HD22	2:B:288:ALA:HB2	1.57	0.70
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.91	0.69
2:B:5:ILE:HG22	2:B:6:GLU:H	1.57	0.69
1:A:438:GLU:OE2	1:A:459:THR:HG21	1.91	0.69
2:B:278:GLN:HB3	2:B:298:GLU:HG3	1.73	0.69
2:B:395:LYS:O	2:B:399:GLU:HG2	1.91	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:GLN:HG2	2:B:396:GLU:OE2	1.93	0.69
1:A:503:LEU:HD12	1:A:533:LEU:CD1	2.23	0.68
2:B:278:GLN:HE21	2:B:278:GLN:HA	1.56	0.68
1:A:54:ASN:ND2	1:A:56:TYR:H	1.92	0.67
1:A:460:ASN:ND2	2:B:288:ALA:HB2	2.09	0.67
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.10	0.67
1:A:57:ASN:OD1	1:A:131:THR:HG23	1.95	0.66
2:B:13:LYS:HB2	2:B:16:MET:SD	2.35	0.66
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.30	0.66
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.25	0.66
1:A:255:ASN:HB2	1:A:289:LEU:HG	1.77	0.66
1:A:25:PRO:HG3	1:A:137:ASN:HD21	1.59	0.66
2:B:306:ASN:O	2:B:310:LEU:HD22	1.96	0.65
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.31	0.65
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.46	0.64
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.79	0.63
1:A:536:VAL:HG11	1:A:542:ILE:HG21	1.81	0.63
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.80	0.63
1:A:380:ILE:HD12	2:B:27:THR:HG22	1.80	0.63
1:A:406:TRP:HD1	1:A:407:GLN:HE21	1.47	0.63
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.14	0.62
1:A:424:LYS:HD2	1:A:426:TRP:CE2	2.34	0.62
1:A:54:ASN:HB3	1:A:143:ARG:HH21	1.64	0.62
2:B:175:ASN:HD21	2:B:201:LYS:HZ3	1.47	0.62
1:A:536:VAL:HG13	1:A:537:PRO:HD2	1.82	0.61
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.36	0.61
2:B:5:ILE:HG22	2:B:6:GLU:N	2.15	0.61
1:A:94:ILE:HD13	1:A:230:MET:CE	2.31	0.61
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.83	0.61
1:A:103:LYS:HE3	1:A:179:VAL:HG21	1.82	0.60
2:B:241:VAL:O	2:B:243:PRO:HD3	2.02	0.60
1:A:223:LYS:HD3	1:A:224:GLU:H	1.65	0.60
1:A:260:LEU:HD22	1:A:264:LEU:HD22	1.84	0.60
2:B:253:THR:O	2:B:257:ILE:HG12	2.02	0.60
1:A:27:THR:HG22	1:A:29:GLU:H	1.66	0.60
1:A:139:THR:OG1	1:A:140:PRO:HD2	2.01	0.59
2:B:344:GLU:HG2	2:B:347:LYS:HE3	1.83	0.59
1:A:94:ILE:HD13	1:A:230:MET:HE2	1.84	0.59
1:A:334:GLN:NE2	7:A:735:HOH:O	2.34	0.59
2:B:295:LEU:HD23	2:B:295:LEU:N	2.18	0.59
1:A:320:ASP:H	1:A:343:GLN:NE2	1.99	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LYS:CD	1:A:291:GLU:HG2	2.32	0.59
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.38	0.59
2:B:66:LYS:HA	2:B:407:GLN:NE2	2.17	0.58
1:A:542:ILE:O	1:A:543:GLY:O	2.22	0.58
1:A:27:THR:HG22	1:A:28:GLU:N	2.17	0.58
1:A:545:ASN:O	1:A:549:ASP:HB2	2.04	0.58
2:B:296:THR:O	2:B:300:GLU:HB2	2.04	0.57
2:B:297:GLU:HG2	2:B:298:GLU:N	2.19	0.57
1:A:42:GLU:OE1	1:A:49:LYS:HE2	2.05	0.56
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.41	0.56
1:A:296:THR:HB	1:A:298:GLU:OE2	2.04	0.56
1:A:401:TRP:HD1	1:A:402:TRP:CD1	2.24	0.56
1:A:102:LYS:HE3	1:A:237:ASP:CB	2.34	0.56
1:A:343:GLN:CG	1:A:349:LEU:HD11	2.31	0.56
1:A:209:LEU:HD23	1:A:216:THR:HG21	1.87	0.56
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.88	0.56
1:A:210:LEU:O	1:A:210:LEU:HD12	2.05	0.56
1:A:27:THR:CG2	1:A:28:GLU:N	2.68	0.56
1:A:281:LYS:HD2	1:A:284:ARG:NH2	2.21	0.55
1:A:194:GLU:N	1:A:194:GLU:CD	2.59	0.55
1:A:54:ASN:HD22	1:A:56:TYR:H	1.54	0.55
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.71	0.55
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.42	0.55
1:A:529:GLU:O	1:A:530:LYS:HG3	2.06	0.55
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.90	0.54
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.07	0.54
1:A:401:TRP:HB2	1:A:425:LEU:HD11	1.90	0.54
2:B:175:ASN:ND2	2:B:201:LYS:NZ	2.55	0.54
1:A:254:VAL:O	1:A:258:GLN:HG3	2.07	0.54
2:B:302:GLU:HA	2:B:305:GLU:OE2	2.08	0.53
1:A:253:THR:HA	1:A:291:GLU:O	2.08	0.53
1:A:368:LEU:HD22	1:A:423:VAL:HG11	1.89	0.53
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.74	0.53
1:A:542:ILE:HD11	2:B:261:VAL:HG11	1.89	0.53
1:A:28:GLU:OE1	1:A:135:ILE:HD13	2.08	0.53
1:A:17:ASP:O	1:A:83:ARG:NE	2.39	0.53
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.09	0.53
2:B:396:GLU:N	2:B:396:GLU:OE2	2.33	0.53
2:B:84:THR:O	2:B:84:THR:HG22	2.08	0.53
2:B:296:THR:HG22	2:B:297:GLU:N	2.24	0.53
1:A:459:THR:CG2	1:A:460:ASN:N	2.72	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASP:OD2	1:A:323:LYS:NZ	2.40	0.52
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.33	0.52
2:B:214:LEU:HG	2:B:215:THR:N	2.25	0.52
2:B:65:LYS:HD2	2:B:72:ARG:HD2	1.92	0.52
2:B:13:LYS:HD2	2:B:16:MET:SD	2.50	0.52
1:A:95:PRO:HG2	3:A:601:NVE:H12	1.91	0.51
2:B:345:PRO:O	2:B:346:PHE:HB2	2.09	0.51
1:A:452:LEU:HD12	1:A:470:THR:HA	1.93	0.51
1:A:108:VAL:HG22	1:A:188:TYR:CE2	2.46	0.51
1:A:516:GLU:HG3	1:A:520:GLN:NE2	2.25	0.51
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.92	0.51
1:A:105:SER:O	1:A:190:GLY:HA2	2.11	0.50
1:A:454:LYS:HE3	1:A:552:VAL:O	2.12	0.50
1:A:106:VAL:HA	1:A:189:VAL:O	2.11	0.50
1:A:459:THR:HG22	1:A:460:ASN:N	2.26	0.50
1:A:66:LYS:O	1:A:67:ASP:HB3	2.12	0.50
1:A:107:THR:CG2	3:A:601:NVE:H33	2.41	0.50
1:A:255:ASN:O	1:A:259:LYS:HG3	2.12	0.50
1:A:400:THR:O	1:A:404:GLU:HG3	2.12	0.50
1:A:402:TRP:CD2	1:A:409:THR:HG21	2.47	0.50
2:B:66:LYS:HA	2:B:407:GLN:HE21	1.75	0.50
1:A:295:LEU:HD12	1:A:300:GLU:OE1	2.12	0.50
1:A:287:LYS:NZ	1:A:287:LYS:HB3	2.25	0.50
1:A:134:SER:CB	1:A:139:THR:HG23	2.42	0.49
1:A:345:PRO:HA	1:A:346:PHE:HA	1.61	0.49
1:A:420:PRO:HA	1:A:421:PRO:C	2.33	0.49
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.94	0.49
1:A:223:LYS:CD	1:A:224:GLU:H	2.25	0.49
2:B:279:LEU:HD13	2:B:282:LEU:HD12	1.94	0.49
1:A:54:ASN:HD21	1:A:56:TYR:HB2	1.78	0.48
1:A:175:ASN:OD1	1:A:201:LYS:HD2	2.13	0.48
1:A:54:ASN:O	1:A:143:ARG:NH2	2.46	0.48
1:A:27:THR:O	1:A:31:ILE:HG13	2.13	0.48
1:A:1:PRO:O	1:A:117:SER:HA	2.14	0.48
1:A:363:ASN:HA	1:A:511:ASP:CG	2.33	0.48
1:A:430:GLU:OE2	1:A:530:LYS:HG2	2.13	0.48
1:A:282:LEU:HD11	1:A:296:THR:HG23	1.96	0.48
1:A:65:LYS:HG2	1:A:66:LYS:HG2	1.95	0.48
1:A:131:THR:CG2	1:A:143:ARG:HH11	2.27	0.47
2:B:175:ASN:ND2	2:B:201:LYS:HD2	2.29	0.47
2:B:286:THR:O	2:B:286:THR:HG23	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LYS:HE2	2:B:69:THR:HA	1.96	0.47
2:B:374:LYS:O	2:B:378:GLU:HG3	2.13	0.47
1:A:48:SER:O	1:A:144:TYR:HA	2.14	0.47
1:A:500:GLN:HE22	2:B:420:PRO:HB3	1.80	0.47
1:A:8:VAL:O	1:A:10:VAL:HG23	2.15	0.47
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.97	0.47
1:A:249:LYS:HE3	1:A:256:ASP:OD2	2.15	0.47
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.50	0.47
1:A:54:ASN:HD22	1:A:54:ASN:C	2.18	0.47
1:A:80:LEU:HD13	1:A:153:TRP:CD1	2.50	0.47
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.97	0.47
2:B:296:THR:CG2	2:B:298:GLU:HG2	2.45	0.46
2:B:7:THR:HG22	2:B:7:THR:O	2.15	0.46
2:B:90:VAL:CG2	2:B:91:GLN:N	2.78	0.46
2:B:278:GLN:NE2	2:B:278:GLN:HA	2.27	0.46
1:A:73:LYS:HG2	1:A:74:LEU:N	2.30	0.46
1:A:95:PRO:HB3	2:B:136:ASN:O	2.16	0.46
1:A:323:LYS:HG3	1:A:323:LYS:HZ2	1.55	0.46
1:A:398:TRP:CE2	1:A:402:TRP:CD1	3.04	0.46
1:A:409:THR:O	2:B:364:ASP:HB2	2.16	0.46
2:B:116:PHE:HA	2:B:148:VAL:HG21	1.97	0.46
1:A:516:GLU:HG3	1:A:520:GLN:HE21	1.80	0.46
1:A:66:LYS:C	1:A:68:SER:H	2.20	0.45
1:A:194:GLU:O	1:A:195:ILE:C	2.55	0.45
1:A:205:LEU:HD13	1:A:209:LEU:HD22	1.98	0.45
1:A:380:ILE:HD11	1:A:386:THR:CG2	2.47	0.45
1:A:395:LYS:HD2	1:A:414:TRP:CZ3	2.52	0.45
2:B:65:LYS:HE2	2:B:66:LYS:H	1.82	0.45
1:A:169:GLU:O	1:A:169:GLU:OE1	2.35	0.45
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.53	0.44
2:B:175:ASN:ND2	2:B:201:LYS:HZ2	2.15	0.44
1:A:281:LYS:O	1:A:284:ARG:HG3	2.16	0.44
2:B:293:ILE:HD13	2:B:294:PRO:N	2.32	0.44
1:A:225:PRO:HA	1:A:226:PRO:C	2.38	0.44
1:A:312:GLU:HA	1:A:313:PRO:HD3	1.81	0.44
1:A:464:GLN:OE1	1:A:551:LEU:HD11	2.18	0.44
2:B:266:TRP:CH2	2:B:427:TYR:OH	2.71	0.44
1:A:224:GLU:HA	1:A:225:PRO:HD3	1.84	0.44
1:A:298:GLU:OE2	1:A:298:GLU:N	2.32	0.44
1:A:449:GLU:O	1:A:451:LYS:HE2	2.17	0.44
1:A:453:GLY:O	1:A:469:LEU:N	2.49	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:O	1:A:94:ILE:HG13	2.17	0.43
2:B:7:THR:CG2	2:B:121:ASP:HA	2.47	0.43
1:A:336:GLN:NE2	7:A:725:HOH:O	2.50	0.43
2:B:296:THR:CG2	2:B:297:GLU:N	2.82	0.43
2:B:293:ILE:HA	2:B:294:PRO:HD3	1.76	0.43
1:A:374:LYS:HE3	1:A:374:LYS:HB3	1.78	0.43
2:B:270:ILE:HG12	2:B:346:PHE:O	2.18	0.43
1:A:479:LEU:HB3	1:A:517:LEU:HD13	2.00	0.43
2:B:5:ILE:HB	2:B:119:PRO:HD2	2.00	0.43
2:B:82:LYS:HE2	2:B:82:LYS:HB2	1.66	0.43
1:A:542:ILE:HG22	1:A:543:GLY:N	2.34	0.43
2:B:206:ARG:NH2	2:B:215:THR:O	2.52	0.42
2:B:243:PRO:O	2:B:245:VAL:HG13	2.20	0.42
2:B:67:ASP:O	2:B:68:SER:HB2	2.19	0.42
1:A:198:HIS:O	1:A:202:ILE:HG12	2.19	0.42
1:A:502:ALA:O	1:A:506:ILE:HG12	2.18	0.42
2:B:289:LEU:HD12	2:B:289:LEU:HA	1.85	0.42
1:A:26:LEU:HD22	1:A:133:PRO:HG3	2.02	0.42
2:B:266:TRP:HZ3	2:B:427:TYR:HH	1.65	0.42
1:A:283:LEU:HD12	1:A:283:LEU:HA	1.81	0.42
1:A:65:LYS:HZ2	1:A:66:LYS:HG2	1.85	0.42
1:A:98:ALA:HB1	1:A:349:LEU:HB3	2.01	0.42
2:B:214:LEU:HG	2:B:215:THR:H	1.85	0.42
2:B:296:THR:HG22	2:B:298:GLU:H	1.84	0.42
2:B:386:THR:HA	2:B:387:PRO:HD3	1.82	0.42
1:A:331:LYS:HB3	1:A:421:PRO:HG2	2.01	0.42
2:B:116:PHE:CD1	2:B:116:PHE:N	2.87	0.42
2:B:293:ILE:HD13	2:B:294:PRO:O	2.20	0.42
1:A:317:VAL:CG1	1:A:318:TYR:N	2.82	0.42
1:A:424:LYS:HD2	1:A:426:TRP:CZ2	2.54	0.42
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.18	0.42
2:B:232:TYR:N	2:B:232:TYR:CD2	2.88	0.42
1:A:234:LEU:HD23	1:A:239:TRP:HB2	2.02	0.41
2:B:116:PHE:CE1	2:B:151:GLN:HG3	2.55	0.41
2:B:32:LYS:HD3	2:B:32:LYS:HA	1.72	0.41
1:A:540:LYS:HE2	2:B:265:ASN:OD1	2.20	0.41
1:A:88:TRP:CZ2	1:A:92:LEU:HD21	2.55	0.41
2:B:266:TRP:CD1	2:B:426:TRP:CZ3	3.08	0.41
2:B:105:SER:O	2:B:190:GLY:HA2	2.20	0.41
1:A:362:THR:HG22	1:A:366:LYS:HD2	2.02	0.41
2:B:157:PRO:HG3	2:B:184:MET:HA	2.01	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:GLU:CG	2:B:299:ALA:N	2.84	0.41
1:A:94:ILE:CD1	1:A:230:MET:HE2	2.50	0.41
2:B:293:ILE:C	2:B:293:ILE:HD13	2.41	0.41
1:A:209:LEU:HA	1:A:209:LEU:HD12	1.90	0.41
2:B:252:TRP:HB3	2:B:257:ILE:HD11	2.01	0.41
2:B:246:LEU:HD11	2:B:264:LEU:HD11	2.01	0.41
1:A:88:TRP:CZ3	2:B:57:ASN:HB2	2.54	0.41
1:A:260:LEU:HD22	1:A:264:LEU:CD2	2.50	0.41
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.93	0.41
2:B:13:LYS:CE	2:B:85:GLN:HB3	2.51	0.41
1:A:211:ARG:NH2	7:A:734:HOH:O	2.54	0.41
1:A:31:ILE:O	1:A:35:VAL:HG23	2.21	0.41
1:A:519:ASN:O	1:A:523:GLU:HG2	2.21	0.41
1:A:433:PRO:CG	2:B:255:ASN:ND2	2.84	0.41
2:B:277:ARG:O	2:B:281:LYS:HG3	2.21	0.41
1:A:257:ILE:O	1:A:261:VAL:HG23	2.21	0.40
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.21	0.40
2:B:283:LEU:O	2:B:284:ARG:C	2.60	0.40
1:A:246:LEU:HD11	1:A:310:LEU:HD12	2.04	0.40
2:B:203:GLU:HA	2:B:203:GLU:OE2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	550/560 (98%)	528 (96%)	19 (4%)	3 (0%)	29	48
2	B	399/440 (91%)	377 (94%)	20 (5%)	2 (0%)	29	48
All	All	949/1000 (95%)	905 (95%)	39 (4%)	5 (0%)	29	48

All (5) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	543	GLY
2	B	66	LYS
2	B	68	SER
1	A	90	VAL
1	A	410	TRP

### 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	494/500 (99%)	455 (92%)	39 (8%)	12	24
2	B	370/400 (92%)	346 (94%)	24 (6%)	17	33
All	All	864/900 (96%)	801 (93%)	63 (7%)	14	27

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	28	GLU
1	A	54	ASN
1	A	58	THR
1	A	80	LEU
1	A	92	LEU
1	A	101	LYS
1	A	122	GLU
1	A	126	LYS
1	A	161	GLN
1	A	168	LEU
1	A	187	LEU
1	A	207	GLN
1	A	209	LEU
1	A	214	LEU
1	A	219	LYS
1	A	248	GLU
1	A	260	LEU
1	A	264	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	282	LEU
1	A	283	LEU
1	A	287	LYS
1	A	301	LEU
1	A	324	ASP
1	A	334	GLN
1	A	340	GLN
1	A	357	MET
1	A	362	THR
1	A	374	LYS
1	A	388	LYS
1	A	423	VAL
1	A	424	LYS
1	A	451	LYS
1	A	476	LYS
1	A	500	GLN
1	A	517	LEU
1	A	529	GLU
1	A	533	LEU
1	A	551	LEU
2	B	7	THR
2	B	8	VAL
2	B	65	LYS
2	B	80	LEU
2	B	82	LYS
2	B	90	VAL
2	B	102	LYS
2	B	193	LEU
2	B	205	LEU
2	B	209	LEU
2	B	234	LEU
2	B	250	ASP
2	B	264	LEU
2	B	277	ARG
2	B	278	GLN
2	B	287	LYS
2	B	293	ILE
2	B	295	LEU
2	B	300	GLU
2	B	310	LEU
2	B	336	GLN
2	B	356	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	368	LEU
2	B	386	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	137	ASN
1	A	207	GLN
1	A	258	GLN
1	A	306	ASN
1	A	336	GLN
1	A	340	GLN
1	A	343	GLN
1	A	373	GLN
1	A	407	GLN
1	A	475	GLN
1	A	500	GLN
1	A	520	GLN
2	B	147	ASN
2	B	161	GLN
2	B	175	ASN
2	B	182	GLN
2	B	242	GLN
2	B	258	GLN
2	B	278	GLN
2	B	334	GLN
2	B	336	GLN
2	B	348	ASN
2	B	367	GLN
2	B	407	GLN
2	B	428	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

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	NVE	A	601	-	35,40,40	2.75	19 (54%)	36,56,56	2.32	11 (30%)
4	SO4	A	603	-	4,4,4	0.26	0	6,6,6	0.21	0
4	SO4	A	604	-	4,4,4	0.27	0	6,6,6	0.10	0
4	SO4	A	602	-	4,4,4	0.27	0	6,6,6	0.14	0
4	SO4	A	605	-	4,4,4	0.26	0	6,6,6	0.06	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	NVE	A	601	-	-	11/19/21/21	0/3/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	NVE	C31-C26	5.34	1.49	1.38
3	A	601	NVE	C5-C4	5.09	1.46	1.40
3	A	601	NVE	C10-C15	4.79	1.45	1.41
3	A	601	NVE	C28-C29	4.28	1.48	1.38
3	A	601	NVE	C15-N14	4.13	1.41	1.35
3	A	601	NVE	C11-C12	4.02	1.46	1.37
3	A	601	NVE	P23-O22	3.86	1.66	1.57
3	A	601	NVE	C18-N19	3.64	1.39	1.32
3	A	601	NVE	C31-C30	3.48	1.45	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	NVE	C30-C29	3.47	1.46	1.38
3	A	601	NVE	C4-N19	3.25	1.40	1.35
3	A	601	NVE	C33-C12	3.14	1.60	1.51
3	A	601	NVE	C27-C26	3.09	1.44	1.38
3	A	601	NVE	P23-O34	2.82	1.64	1.57
3	A	601	NVE	C13-N14	2.78	1.36	1.31
3	A	601	NVE	C17-C16	2.48	1.42	1.36
3	A	601	NVE	C16-C5	2.41	1.45	1.41
3	A	601	NVE	C17-C18	2.18	1.44	1.37
3	A	601	NVE	C7-N6	2.13	1.51	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NVE	C13-N14-C15	6.36	124.85	116.73
3	A	601	NVE	C18-N19-C4	5.21	123.24	116.77
3	A	601	NVE	C33-C12-C13	-4.81	114.08	121.83
3	A	601	NVE	C1-C2-N3	4.15	118.67	111.37
3	A	601	NVE	C10-C15-N14	-3.79	118.78	124.62
3	A	601	NVE	C12-C13-N14	-3.30	118.78	123.98
3	A	601	NVE	C11-C12-C13	3.01	119.50	116.71
3	A	601	NVE	C17-C18-N19	-2.65	119.88	123.94
3	A	601	NVE	C33-C12-C11	2.60	126.42	121.04
3	A	601	NVE	O37-P23-C24	-2.49	105.30	113.50
3	A	601	NVE	P23-O34-C35	-2.46	113.18	122.30

There are no chirality outliers.

All (11) torsion outliers are listed below:

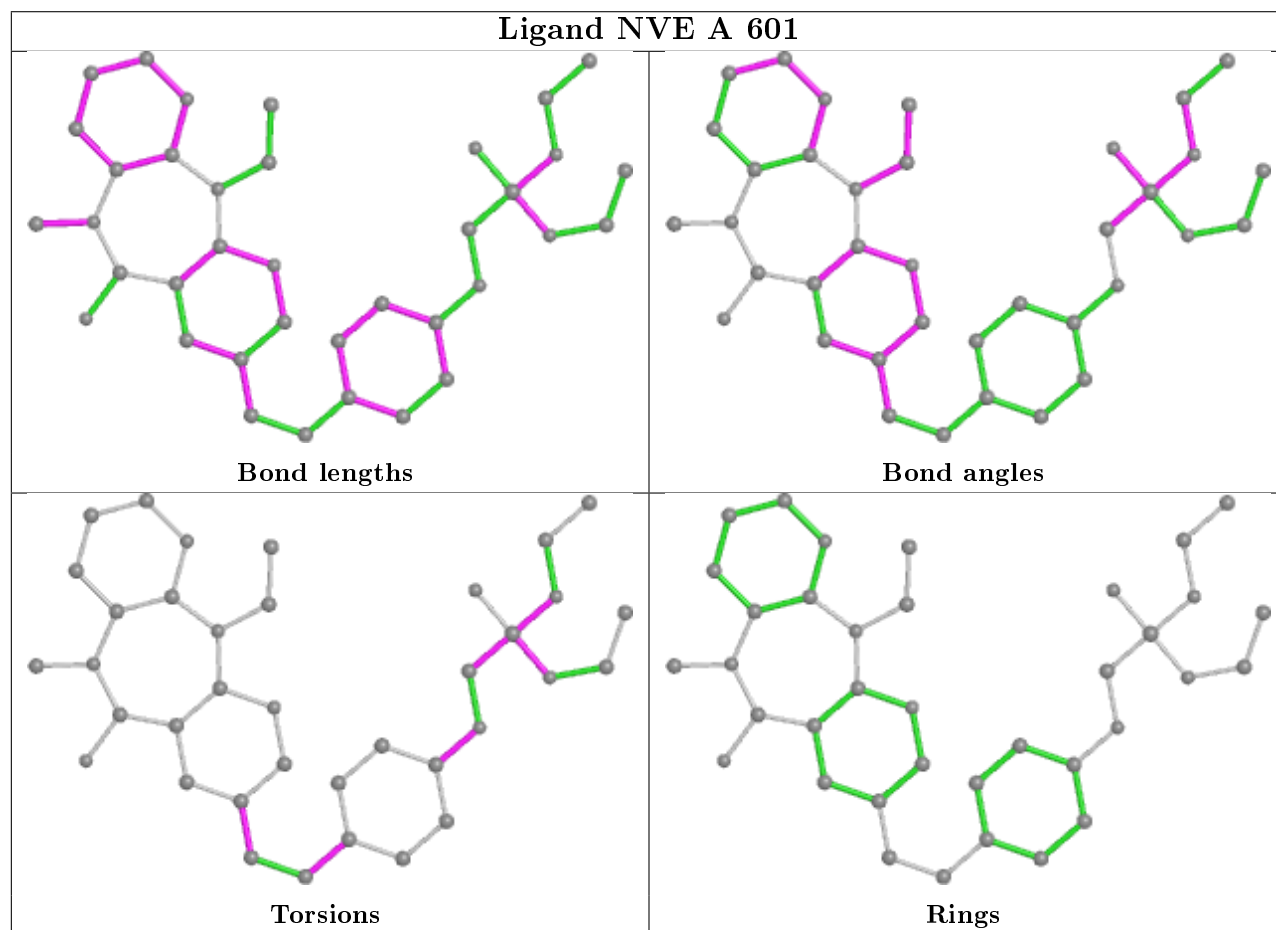
Mol	Chain	Res	Type	Atoms
3	A	601	NVE	C21-O22-P23-C24
3	A	601	NVE	O25-C24-P23-O37
3	A	601	NVE	O25-C24-P23-O22
3	A	601	NVE	O25-C24-P23-O34
3	A	601	NVE	C27-C26-O25-C24
3	A	601	NVE	C31-C26-O25-C24
3	A	601	NVE	C13-C12-C33-C32
3	A	601	NVE	C11-C12-C33-C32
3	A	601	NVE	C35-O34-P23-O37
3	A	601	NVE	C28-C29-C32-C33
3	A	601	NVE	C30-C29-C32-C33

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NVE	2	0

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



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	552/560 (98%)	0.24	22 (3%) 38 41	34, 59, 89, 113	0
2	B	405/440 (92%)	0.38	44 (10%) 5 5	35, 58, 101, 117	0
All	All	957/1000 (95%)	0.29	66 (6%) 16 17	34, 59, 96, 117	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	67	ASP	6.5
2	B	66	LYS	6.3
2	B	70	LYS	5.5
2	B	14	PRO	5.5
2	B	68	SER	5.3
1	A	70	LYS	5.0
1	A	65	LYS	4.5
2	B	69	THR	4.3
1	A	67	ASP	4.2
2	B	409	THR	4.2
2	B	232	TYR	4.0
2	B	90	VAL	4.0
2	B	284	ARG	4.0
2	B	65	LYS	3.9
2	B	216	THR	3.6
1	A	66	LYS	3.5
1	A	357	MET	3.4
1	A	69	THR	3.3
1	A	445	ALA	3.2
1	A	286	THR	3.1
2	B	183	TYR	3.1
2	B	242	GLN	3.1
1	A	446	ALA	3.1
2	B	411	ILE	3.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	13	LYS	3.0
2	B	277	ARG	3.0
2	B	305	GLU	3.0
2	B	184	MET	2.9
2	B	252	TRP	2.8
1	A	284	ARG	2.8
2	B	410	TRP	2.8
1	A	68	SER	2.7
2	B	43	LYS	2.5
1	A	53	GLU	2.5
1	A	497	THR	2.5
1	A	448	ARG	2.4
2	B	215	THR	2.4
2	B	153	TRP	2.3
2	B	15	GLY	2.2
2	B	238	LYS	2.2
1	A	360	ALA	2.2
2	B	5	ILE	2.2
2	B	266	TRP	2.2
2	B	185	ASP	2.2
2	B	6	GLU	2.2
2	B	156	SER	2.2
2	B	346	PHE	2.2
2	B	295	LEU	2.2
1	A	534	ALA	2.1
1	A	221	HIS	2.1
1	A	193	LEU	2.1
2	B	12	LEU	2.1
2	B	152	GLY	2.1
2	B	355	ALA	2.1
2	B	354	TYR	2.1
2	B	294	PRO	2.0
1	A	506	ILE	2.0
1	A	514	GLU	2.0
2	B	89	GLU	2.0
2	B	241	VAL	2.0
1	A	64	LYS	2.0
2	B	86	ASP	2.0
1	A	470	THR	2.0
2	B	151	GLN	2.0
2	B	237	ASP	2.0
2	B	11	LYS	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 ⓘ

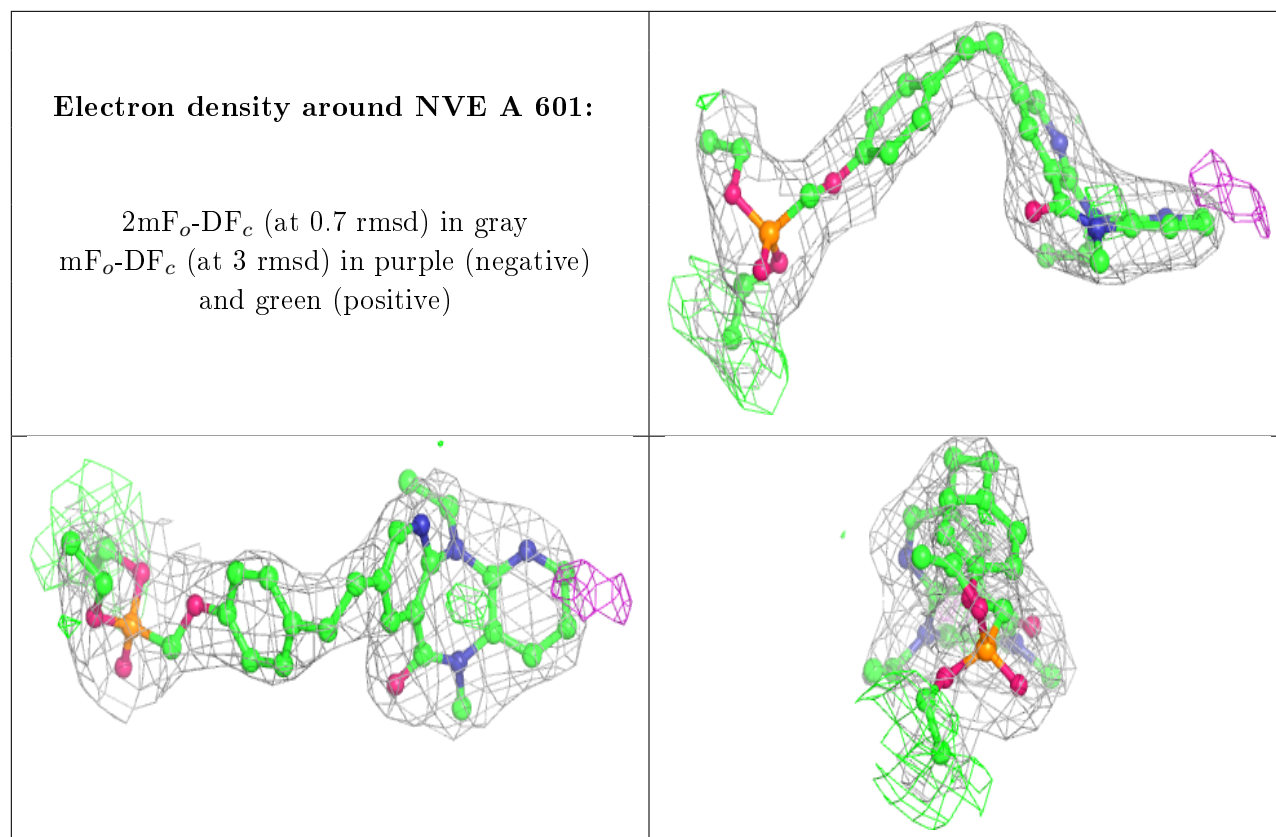
There are no carbohydrates in this entry.

## 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, 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
6	CL	B	501	1/1	0.82	0.14	68,68,68,68	0
6	CL	A	607	1/1	0.88	0.25	94,94,94,94	0
4	SO4	A	604	5/5	0.91	0.17	119,119,119,120	0
5	MG	A	606	1/1	0.92	0.24	77,77,77,77	0
4	SO4	A	602	5/5	0.92	0.15	94,96,96,96	0
4	SO4	A	605	5/5	0.92	0.12	119,119,119,120	0
3	NVE	A	601	37/37	0.94	0.19	37,45,67,68	0
4	SO4	A	603	5/5	0.95	0.12	75,78,79,79	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.