



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:39 PM UTC

PDB ID : 6PEB / pdb_00006peb
Title : Crystal Structure of human NAMPT in complex with NVP-LTM976
Authors : Weihofen, W.A.
Deposited on : 2019-06-20
Resolution : 2.46 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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)
Xtriage (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

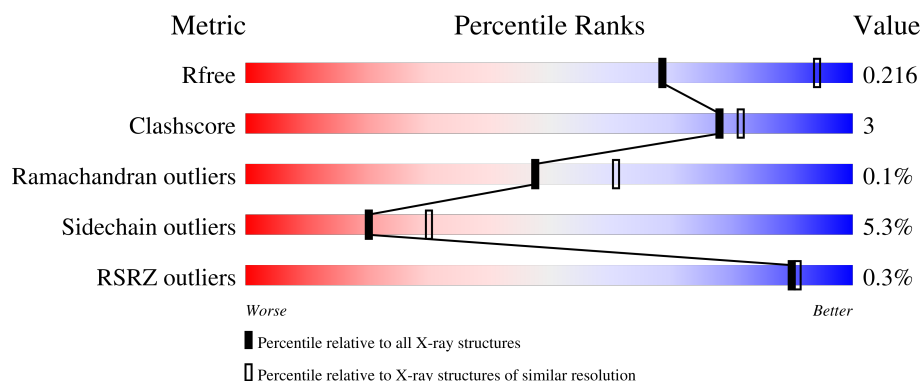
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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 ≥ 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	500	 82% 12% • 6%
1	B	500	 82% 10% • 6%
1	C	500	 81% 12% • 6%
1	D	500	 80% 13% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	B	604	-	X	-	-
3	PO4	D	602	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15757 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 Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	0	0
			3754	2416	621	710	7			
1	B	468	Total	C	N	O	S	0	0	0
			3743	2408	619	709	7			
1	C	469	Total	C	N	O	S	0	0	0
			3754	2415	620	712	7			
1	D	471	Total	C	N	O	S	0	0	0
			3768	2423	623	715	7			

There are 40 discrepancies between the modelled and reference sequences:

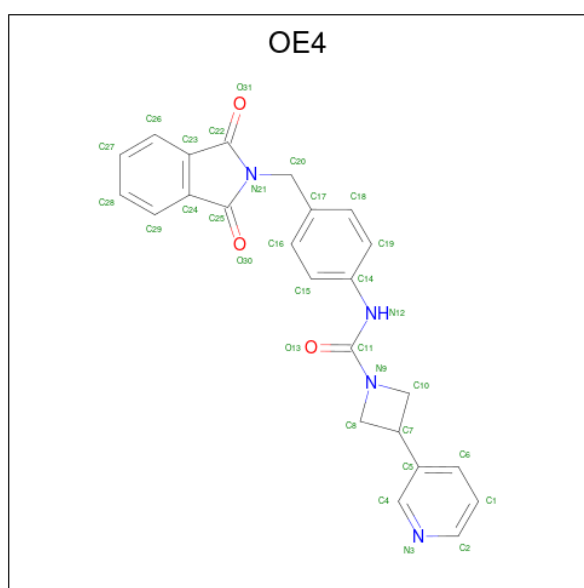
Chain	Residue	Modelled	Actual	Comment	Reference
A	492	LEU	-	expression tag	UNP P43490
A	493	GLU	-	expression tag	UNP P43490
A	494	HIS	-	expression tag	UNP P43490
A	495	HIS	-	expression tag	UNP P43490
A	496	HIS	-	expression tag	UNP P43490
A	497	HIS	-	expression tag	UNP P43490
A	498	HIS	-	expression tag	UNP P43490
A	499	HIS	-	expression tag	UNP P43490
A	500	HIS	-	expression tag	UNP P43490
A	501	HIS	-	expression tag	UNP P43490
B	492	LEU	-	expression tag	UNP P43490
B	493	GLU	-	expression tag	UNP P43490
B	494	HIS	-	expression tag	UNP P43490
B	495	HIS	-	expression tag	UNP P43490
B	496	HIS	-	expression tag	UNP P43490
B	497	HIS	-	expression tag	UNP P43490
B	498	HIS	-	expression tag	UNP P43490
B	499	HIS	-	expression tag	UNP P43490
B	500	HIS	-	expression tag	UNP P43490
B	501	HIS	-	expression tag	UNP P43490
C	492	LEU	-	expression tag	UNP P43490

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Chain	Residue	Modelled	Actual	Comment	Reference
C	493	GLU	-	expression tag	UNP P43490
C	494	HIS	-	expression tag	UNP P43490
C	495	HIS	-	expression tag	UNP P43490
C	496	HIS	-	expression tag	UNP P43490
C	497	HIS	-	expression tag	UNP P43490
C	498	HIS	-	expression tag	UNP P43490
C	499	HIS	-	expression tag	UNP P43490
C	500	HIS	-	expression tag	UNP P43490
C	501	HIS	-	expression tag	UNP P43490
D	492	LEU	-	expression tag	UNP P43490
D	493	GLU	-	expression tag	UNP P43490
D	494	HIS	-	expression tag	UNP P43490
D	495	HIS	-	expression tag	UNP P43490
D	496	HIS	-	expression tag	UNP P43490
D	497	HIS	-	expression tag	UNP P43490
D	498	HIS	-	expression tag	UNP P43490
D	499	HIS	-	expression tag	UNP P43490
D	500	HIS	-	expression tag	UNP P43490
D	501	HIS	-	expression tag	UNP P43490

- Molecule 2 is N-{4-[(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)methyl]phenyl}-3-(pyridin-3-yl)azetidine-1-carboxamide (CCD ID: OE4) (formula: C₂₄H₂₀N₄O₃) (labeled as "Ligand of Interest" by depositor).



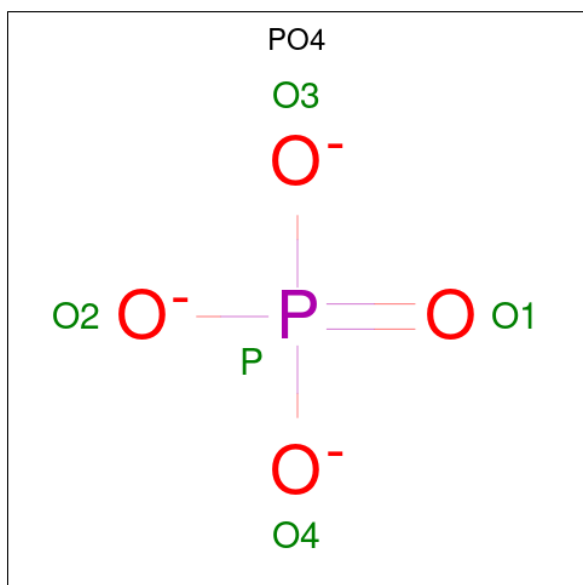
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	24	4	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			31	24	4	3		
2	C	1	Total	C	N	O	0	0
			31	24	4	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

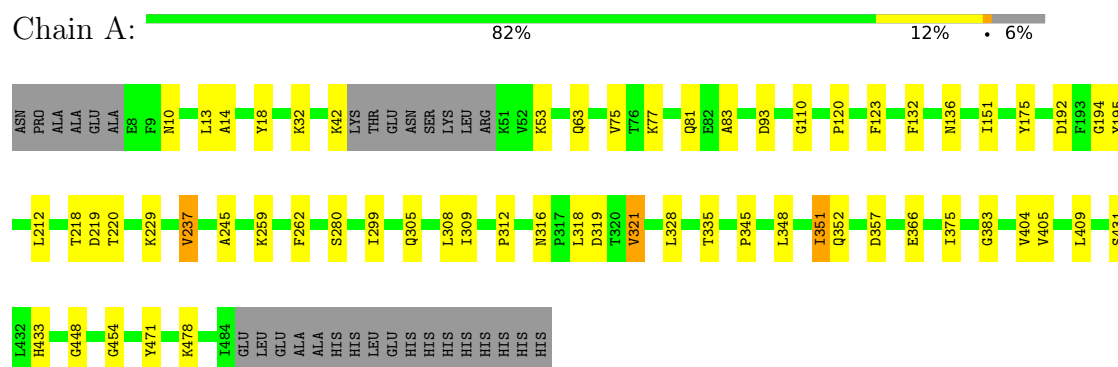
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	230	Total	O	0	0
			230	230		
4	B	127	Total	O	0	0
			127	127		
4	C	134	Total	O	0	0
			134	134		
4	D	94	Total	O	0	0
			94	94		

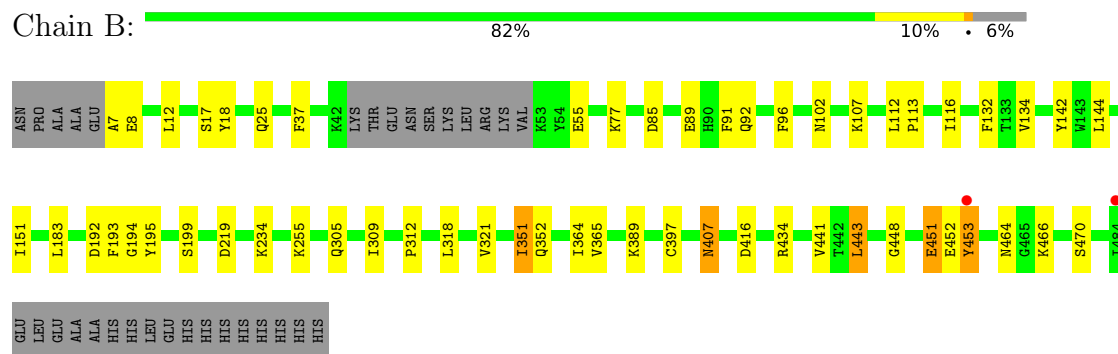
3 Residue-property plots

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.

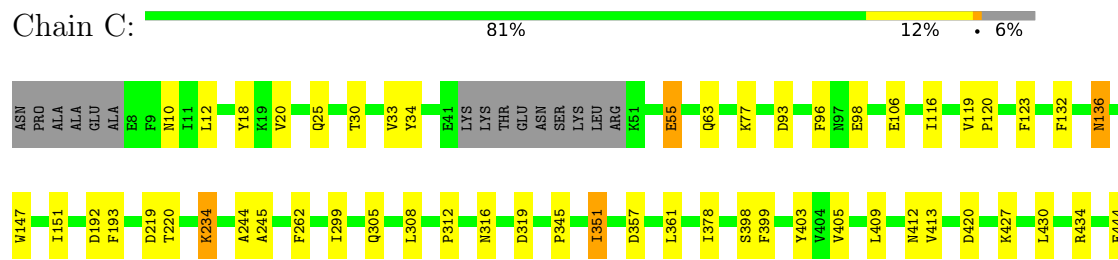
- Molecule 1: Nicotinamide phosphoribosyltransferase

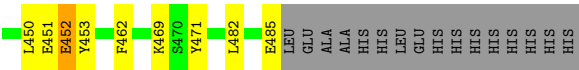


- Molecule 1: Nicotinamide phosphoribosyltransferase

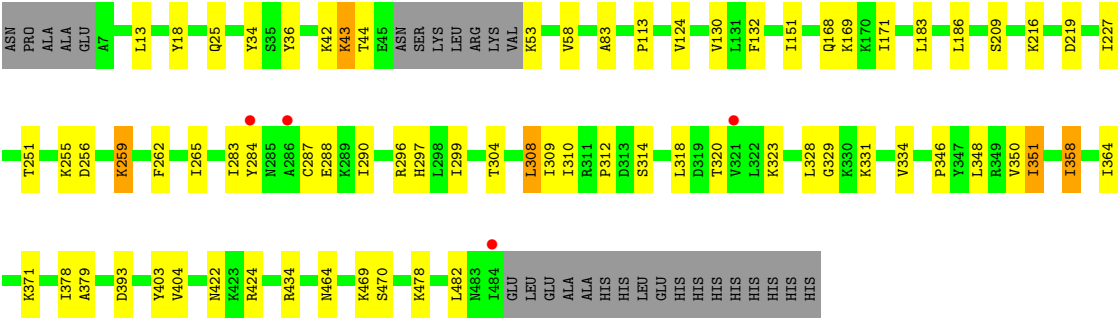
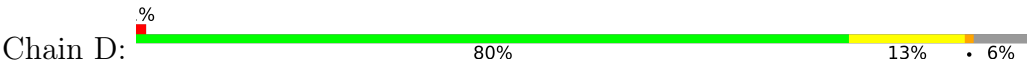


- Molecule 1: Nicotinamide phosphoribosyltransferase





● Molecule 1: Nicotinamide phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.74Å 96.16Å 246.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.94 – 2.46 34.94 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.94-2.46) 99.8 (34.94-2.46)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.159 , 0.209 0.167 , 0.216	Depositor DCC
R_{free} test set	3962 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15757	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OE4, PO4

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	0.87	1/3842 (0.0%)	1.33	10/5204 (0.2%)
1	B	0.84	0/3831	1.34	14/5190 (0.3%)
1	C	0.88	2/3842 (0.1%)	1.32	14/5205 (0.3%)
1	D	0.88	0/3856	1.34	6/5223 (0.1%)
All	All	0.87	3/15371 (0.0%)	1.33	44/20822 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	PRO	CA-C	5.61	1.54	1.51
1	C	345	PRO	CA-C	5.34	1.54	1.51
1	C	119	VAL	CA-C	5.05	1.57	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	193	PHE	CA-CB-CG	8.15	121.95	113.80
1	A	194	GLY	N-CA-C	7.56	125.23	115.32
1	C	262	PHE	CA-CB-CG	7.46	121.26	113.80
1	B	142	TYR	CA-C-N	6.82	130.68	120.31
1	B	142	TYR	C-N-CA	6.82	130.68	120.31
1	A	132	PHE	CA-CB-CG	6.70	120.50	113.80
1	C	361	LEU	CA-C-N	6.36	128.80	120.28
1	C	361	LEU	C-N-CA	6.36	128.80	120.28
1	C	399	PHE	CA-CB-CG	6.29	120.09	113.80
1	B	416	ASP	CA-CB-CG	6.18	118.78	112.60
1	D	132	PHE	CA-CB-CG	6.18	119.98	113.80
1	B	234	LYS	N-CA-C	-6.17	104.63	111.36
1	C	234	LYS	N-CA-C	-6.12	104.61	111.28
1	A	262	PHE	CA-CB-CG	5.93	119.73	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	VAL	N-CA-CB	5.91	119.32	111.64
1	B	193	PHE	CA-CB-CG	5.84	119.64	113.80
1	B	451	GLU	CA-C-N	5.83	128.10	120.28
1	B	451	GLU	C-N-CA	5.83	128.10	120.28
1	A	93	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	132	PHE	CA-CB-CG	5.61	119.41	113.80
1	B	192	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	357	ASP	CA-CB-CG	5.55	118.15	112.60
1	B	407	ASN	CA-CB-CG	5.50	118.10	112.60
1	B	194	GLY	N-CA-C	5.46	122.47	115.32
1	C	220	THR	CA-C-N	5.44	128.20	120.53
1	C	220	THR	C-N-CA	5.44	128.20	120.53
1	B	85	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	365	VAL	CA-C-N	5.39	127.45	120.44
1	B	365	VAL	C-N-CA	5.39	127.45	120.44
1	D	283	ILE	CA-C-N	5.32	127.67	120.65
1	D	283	ILE	C-N-CA	5.32	127.67	120.65
1	C	192	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	192	ASP	CA-CB-CG	5.26	117.86	112.60
1	D	262	PHE	CA-CB-CG	5.24	119.03	113.80
1	C	10	ASN	CA-CB-CG	5.21	117.81	112.60
1	A	10	ASN	CA-CB-CG	5.21	117.81	112.60
1	C	132	PHE	CA-CB-CG	5.20	119.00	113.80
1	C	55	GLU	CB-CG-CD	5.12	121.31	112.60
1	D	320	THR	CA-C-N	5.12	127.21	120.60
1	D	320	THR	C-N-CA	5.12	127.21	120.60
1	A	383	GLY	CA-C-N	5.09	125.73	120.03
1	A	383	GLY	C-N-CA	5.09	125.73	120.03
1	C	357	ASP	CA-CB-CG	5.05	117.65	112.60
1	C	420	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3754	0	3740	22	0
1	B	3743	0	3723	17	0
1	C	3754	0	3733	25	0
1	D	3768	0	3749	27	0
2	A	31	0	0	0	0
2	B	31	0	0	0	0
2	C	31	0	0	0	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0
4	A	230	0	0	0	0
4	B	127	0	0	0	0
4	C	134	0	0	0	0
4	D	94	0	0	0	0
All	All	15757	0	14945	83	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 3.

All (83) 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:33:VAL:H	1:C:136:ASN:HD21	1.23	0.85
1:C:63:GLN:HE22	1:C:471:TYR:H	1.25	0.84
1:A:316:ASN:HD22	1:A:319:ASP:H	1.33	0.74
1:D:43:LYS:HG2	1:D:44:THR:H	1.54	0.72
1:C:450:LEU:HB3	1:C:452:GLU:HG3	1.75	0.68
1:C:245:ALA:HA	1:D:25:GLN:HE22	1.60	0.66
1:C:316:ASN:HD22	1:C:319:ASP:H	1.41	0.65
1:D:328:LEU:HD22	1:D:348:LEU:HD21	1.78	0.64
1:A:321:VAL:HG23	1:A:352:GLN:HE21	1.63	0.64
1:A:63:GLN:HE22	1:A:471:TYR:H	1.47	0.62
1:C:120:PRO:O	1:C:123:PHE:HB2	1.99	0.61
1:A:245:ALA:HA	1:B:25:GLN:HE22	1.64	0.61
1:D:304:THR:HG23	1:D:346:PRO:HB2	1.83	0.61
1:C:299:ILE:HD12	1:C:308:LEU:HD22	1.84	0.59
1:D:183:LEU:HD23	1:D:186:LEU:HD22	1.84	0.59
1:D:299:ILE:HD12	1:D:308:LEU:HD22	1.85	0.57
1:B:453:TYR:CD1	1:B:453:TYR:N	2.72	0.57
1:B:321:VAL:HG23	1:B:352:GLN:HE21	1.70	0.56
1:B:17:SER:O	1:B:91:PHE:HZ	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LYS:NZ	1:B:7:ALA:HB2	2.22	0.55
1:C:33:VAL:H	1:C:136:ASN:ND2	1.99	0.55
1:D:113:PRO:HA	1:D:464:ASN:HD22	1.72	0.54
1:B:453:TYR:N	1:B:453:TYR:HD1	2.06	0.54
1:C:25:GLN:HG2	1:D:265:ILE:HG12	1.89	0.54
1:A:328:LEU:HD22	1:A:348:LEU:HD21	1.90	0.53
1:D:296:ARG:HH12	1:D:331:LYS:C	2.17	0.52
1:D:169:LYS:HG2	1:D:482:LEU:HD11	1.91	0.52
1:C:30:THR:HA	1:C:405:VAL:O	2.09	0.52
1:A:32:LYS:HA	1:A:136:ASN:HD21	1.75	0.51
1:A:299:ILE:HD12	1:A:308:LEU:HD22	1.91	0.51
1:B:112:LEU:O	1:B:464:ASN:HA	2.11	0.51
1:B:318:LEU:HD13	1:B:364:ILE:HA	1.93	0.50
1:C:116:ILE:HB	1:C:462:PHE:HB3	1.93	0.50
1:C:312:PRO:HD2	1:C:351:ILE:O	2.12	0.50
1:A:75:VAL:HB	1:A:110:GLY:HA2	1.94	0.50
1:A:309:ILE:HG22	1:A:351:ILE:HG22	1.92	0.49
1:D:36:TYR:HB2	1:D:130:VAL:HG23	1.94	0.49
1:B:312:PRO:HD2	1:B:351:ILE:O	2.12	0.48
1:B:443:LEU:HD23	1:B:448:GLY:HA2	1.96	0.48
1:A:312:PRO:HD2	1:A:351:ILE:O	2.14	0.47
1:D:297:HIS:H	1:D:297:HIS:CD2	2.33	0.46
1:D:318:LEU:HD13	1:D:364:ILE:HA	1.97	0.46
1:D:378:ILE:HG13	1:D:379:ALA:N	2.30	0.46
1:D:34:TYR:HB3	1:D:403:TYR:HB3	1.97	0.46
1:D:168:GLN:HG3	1:D:358:ILE:HD12	1.98	0.46
1:B:12:LEU:HD23	1:B:96:PHE:HZ	1.81	0.46
1:C:63:GLN:NE2	1:C:471:TYR:H	2.04	0.45
1:A:316:ASN:HB3	1:A:319:ASP:HB2	1.97	0.45
1:C:20:VAL:HG22	1:C:147:TRP:CH2	2.52	0.45
1:D:310:ILE:HB	1:D:350:VAL:HG12	1.98	0.45
1:A:212:LEU:HD11	1:A:218:THR:HG21	1.98	0.45
1:A:431:SER:OG	1:A:433:HIS:HE1	2.00	0.45
1:D:13:LEU:HD21	1:D:83:ALA:HA	1.98	0.44
1:D:58:VAL:HG22	1:D:124:VAL:HG22	1.98	0.44
1:A:195:TYR:CG	1:A:220:THR:HG23	2.52	0.44
1:C:12:LEU:HD23	1:C:96:PHE:CZ	2.53	0.44
1:D:259:LYS:HG3	1:D:290:ILE:HG23	1.99	0.44
1:A:13:LEU:HD21	1:A:83:ALA:HA	2.00	0.44
1:B:116:ILE:HG12	1:B:134:VAL:HG22	2.00	0.44
1:C:55:GLU:H	1:C:55:GLU:CD	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ASN:ND2	1:C:136:ASN:H	2.15	0.44
1:C:412:ASN:HB3	1:C:427:LYS:HB3	2.00	0.44
1:B:37:PHE:CZ	1:B:397:CYS:HB3	2.53	0.44
1:A:237:VAL:HG22	1:B:89:GLU:HB3	1.99	0.43
1:C:136:ASN:H	1:C:136:ASN:HD22	1.66	0.43
1:D:329:GLY:HA2	1:D:334:VAL:HG13	1.99	0.43
1:D:168:GLN:HA	1:D:171:ILE:HD12	1.99	0.43
1:B:309:ILE:HG22	1:B:351:ILE:HG22	2.01	0.42
1:C:413:VAL:HB	1:D:251:THR:HB	2.01	0.42
1:C:34:TYR:HB3	1:C:403:TYR:HB3	2.02	0.42
1:C:244:ALA:HB3	1:D:18:TYR:HB2	2.02	0.42
1:D:312:PRO:HD2	1:D:351:ILE:O	2.19	0.42
1:A:431:SER:OG	1:A:448:GLY:HA3	2.20	0.42
1:A:14:ALA:HA	1:B:195:TYR:OH	2.19	0.41
1:B:113:PRO:HD2	1:B:144:LEU:CD2	2.50	0.41
1:C:482:LEU:HB2	1:C:485:GLU:HG3	2.02	0.41
1:A:120:PRO:O	1:A:123:PHE:HB2	2.20	0.41
1:A:433:HIS:HD2	1:A:454:GLY:O	2.03	0.41
1:D:43:LYS:CG	1:D:44:THR:H	2.28	0.41
1:A:175:TYR:HB3	1:A:375:ILE:HG13	2.02	0.41
1:C:12:LEU:HD23	1:C:96:PHE:HZ	1.84	0.41
1:C:430:LEU:HD23	1:C:444:GLU:HA	2.03	0.40
1:D:209:SER:HA	1:D:227:ILE:HD11	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	465/500 (93%)	452 (97%)	13 (3%)	0	100	100
1	B	464/500 (93%)	449 (97%)	14 (3%)	1 (0%)	43	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	465/500 (93%)	451 (97%)	14 (3%)	0	100	100
1	D	467/500 (93%)	447 (96%)	19 (4%)	1 (0%)	43	54
All	All	1861/2000 (93%)	1799 (97%)	60 (3%)	2 (0%)	48	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	43	LYS
1	B	8	GLU

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	413/439 (94%)	394 (95%)	19 (5%)	24	36
1	B	411/439 (94%)	388 (94%)	23 (6%)	19	27
1	C	413/439 (94%)	394 (95%)	19 (5%)	24	36
1	D	414/439 (94%)	388 (94%)	26 (6%)	16	23
All	All	1651/1756 (94%)	1564 (95%)	87 (5%)	20	30

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	TYR
1	A	42	LYS
1	A	53	LYS
1	A	77	LYS
1	A	81	GLN
1	A	151	ILE
1	A	219	ASP
1	A	237	VAL
1	A	259	LYS
1	A	280	SER

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Mol	Chain	Res	Type
1	A	305	GLN
1	A	318	LEU
1	A	321	VAL
1	A	335	THR
1	A	351	ILE
1	A	366	GLU
1	A	404	VAL
1	A	409	LEU
1	A	478	LYS
1	B	18	TYR
1	B	55	GLU
1	B	77	LYS
1	B	92	GLN
1	B	102	ASN
1	B	107	LYS
1	B	151	ILE
1	B	183	LEU
1	B	199	SER
1	B	219	ASP
1	B	255	LYS
1	B	305	GLN
1	B	351	ILE
1	B	389	LYS
1	B	407	ASN
1	B	434	ARG
1	B	441	VAL
1	B	443	LEU
1	B	451	GLU
1	B	452	GLU
1	B	453	TYR
1	B	466	LYS
1	B	470	SER
1	C	18	TYR
1	C	77	LYS
1	C	93	ASP
1	C	98	GLU
1	C	106	GLU
1	C	136	ASN
1	C	151	ILE
1	C	219	ASP
1	C	234	LYS
1	C	305	GLN

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Mol	Chain	Res	Type
1	C	351	ILE
1	C	378	ILE
1	C	398	SER
1	C	409	LEU
1	C	434	ARG
1	C	451	GLU
1	C	452	GLU
1	C	453	TYR
1	C	469	LYS
1	D	42	LYS
1	D	53	LYS
1	D	151	ILE
1	D	216	LYS
1	D	219	ASP
1	D	255	LYS
1	D	256	ASP
1	D	259	LYS
1	D	284	TYR
1	D	287	CYS
1	D	288	GLU
1	D	308	LEU
1	D	309	ILE
1	D	314	SER
1	D	323	LYS
1	D	351	ILE
1	D	358	ILE
1	D	371	LYS
1	D	393	ASP
1	D	404	VAL
1	D	422	ASN
1	D	424	ARG
1	D	434	ARG
1	D	469	LYS
1	D	470	SER
1	D	478	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	81	GLN
1	A	102	ASN

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Mol	Chain	Res	Type
1	A	129	ASN
1	A	136	ASN
1	A	154	GLN
1	A	316	ASN
1	A	352	GLN
1	A	412	ASN
1	A	433	HIS
1	A	439	ASN
1	A	464	ASN
1	B	25	GLN
1	B	92	GLN
1	B	102	ASN
1	B	146	ASN
1	B	164	ASN
1	B	201	GLN
1	B	362	GLN
1	B	439	ASN
1	B	455	GLN
1	C	63	GLN
1	C	92	GLN
1	C	136	ASN
1	C	201	GLN
1	C	214	ASN
1	C	268	GLN
1	C	305	GLN
1	C	316	ASN
1	C	352	GLN
1	C	359	ASN
1	C	388	GLN
1	C	407	ASN
1	C	433	HIS
1	C	459	HIS
1	C	464	ASN
1	D	25	GLN
1	D	29	ASN
1	D	102	ASN
1	D	154	GLN
1	D	164	ASN
1	D	182	ASN
1	D	247	HIS
1	D	285	ASN
1	D	297	HIS

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Mol	Chain	Res	Type
1	D	352	GLN
1	D	362	GLN
1	D	407	ASN
1	D	412	ASN
1	D	439	ASN
1	D	464	ASN

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](#)

15 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	PO4	C	603	-	4,4,4	2.59	3 (75%)	6,6,6	0.70	0
3	PO4	D	603	-	4,4,4	2.18	3 (75%)	6,6,6	0.37	0
2	OE4	B	601	-	33,35,35	1.47	6 (18%)	46,50,50	4.40	17 (36%)
3	PO4	B	603	-	4,4,4	2.55	1 (25%)	6,6,6	0.54	0
3	PO4	B	604	-	4,4,4	1.82	2 (50%)	6,6,6	1.73	2 (33%)
3	PO4	B	602	-	4,4,4	2.54	2 (50%)	6,6,6	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	A	603	-	4,4,4	2.56	3 (75%)	6,6,6	0.61	0
2	OE4	A	601	-	33,35,35	1.50	4 (12%)	46,50,50	4.00	16 (34%)
3	PO4	A	604	-	4,4,4	2.14	2 (50%)	6,6,6	0.86	0
3	PO4	A	602	-	4,4,4	1.77	1 (25%)	6,6,6	1.05	0
2	OE4	C	601	-	33,35,35	1.37	4 (12%)	46,50,50	4.24	17 (36%)
3	PO4	C	602	-	4,4,4	2.61	2 (50%)	6,6,6	0.78	0
3	PO4	C	604	-	4,4,4	2.65	2 (50%)	6,6,6	0.85	0
3	PO4	D	602	-	4,4,4	2.04	4 (100%)	6,6,6	0.69	0
3	PO4	D	601	-	4,4,4	2.52	2 (50%)	6,6,6	0.83	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
2	OE4	A	601	-	-	0/12/40/40	0/5/5/5
2	OE4	B	601	-	-	0/12/40/40	0/5/5/5
2	OE4	C	601	-	-	0/12/40/40	0/5/5/5

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	604	PO4	P-O1	4.47	1.61	1.50
3	B	603	PO4	P-O1	4.27	1.60	1.50
3	C	602	PO4	P-O1	4.27	1.60	1.50
3	B	602	PO4	P-O1	4.23	1.60	1.50
3	C	603	PO4	P-O1	4.23	1.60	1.50
3	A	603	PO4	P-O1	4.22	1.60	1.50
3	D	601	PO4	P-O1	4.11	1.60	1.50
2	C	601	OE4	C22-N21	-3.54	1.35	1.39
2	A	601	OE4	C10-N9	-3.30	1.44	1.47
2	B	601	OE4	C10-N9	-3.02	1.44	1.47
2	B	601	OE4	C25-N21	-2.90	1.36	1.39
2	C	601	OE4	C25-N21	-2.90	1.36	1.39
2	A	601	OE4	C22-N21	-2.70	1.36	1.39
3	D	603	PO4	P-O1	2.66	1.56	1.50
3	A	604	PO4	P-O1	2.53	1.56	1.50
2	A	601	OE4	C25-N21	-2.48	1.36	1.39
2	B	601	OE4	C4-C5	2.48	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	OE4	C22-N21	-2.39	1.36	1.39
2	C	601	OE4	C10-N9	-2.38	1.45	1.47
2	B	601	OE4	C6-C5	2.30	1.42	1.39
2	A	601	OE4	C8-N9	-2.30	1.45	1.47
2	B	601	OE4	C8-N9	-2.25	1.45	1.47
3	D	601	PO4	P-O4	2.13	1.60	1.54
3	A	602	PO4	P-O4	2.11	1.60	1.54
3	B	604	PO4	P-O3	2.10	1.60	1.54
3	D	602	PO4	P-O1	2.09	1.55	1.50
3	B	604	PO4	P-O2	2.08	1.60	1.54
3	A	604	PO4	P-O3	2.07	1.60	1.54
3	C	603	PO4	P-O3	2.06	1.60	1.54
2	C	601	OE4	C28-C27	2.05	1.42	1.38
3	A	603	PO4	P-O3	2.04	1.60	1.54
3	D	603	PO4	P-O3	2.04	1.60	1.54
3	D	602	PO4	P-O4	2.04	1.60	1.54
3	C	603	PO4	P-O4	2.03	1.60	1.54
3	C	604	PO4	P-O4	2.02	1.60	1.54
3	D	602	PO4	P-O3	2.01	1.60	1.54
3	D	602	PO4	P-O2	2.01	1.60	1.54
3	A	603	PO4	P-O4	2.01	1.60	1.54
3	B	602	PO4	P-O3	2.01	1.60	1.54
3	C	602	PO4	P-O4	2.00	1.60	1.54
3	D	603	PO4	P-O4	2.00	1.60	1.54

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	OE4	C10-N9-C8	18.53	107.67	94.69
2	C	601	OE4	C10-N9-C8	18.48	107.64	94.69
2	A	601	OE4	C10-N9-C8	16.61	106.33	94.69
2	B	601	OE4	C7-C8-N9	-13.63	76.97	88.22
2	C	601	OE4	C7-C8-N9	-13.57	77.01	88.22
2	B	601	OE4	C7-C10-N9	-13.44	77.12	88.22
2	C	601	OE4	C7-C10-N9	-13.18	77.34	88.22
2	A	601	OE4	C7-C8-N9	-12.19	78.15	88.22
2	A	601	OE4	C7-C10-N9	-11.39	78.81	88.22
2	A	601	OE4	C23-C22-N21	4.87	109.48	105.88
2	B	601	OE4	C23-C22-N21	4.48	109.19	105.88
2	A	601	OE4	C24-C25-N21	4.24	109.02	105.88
2	A	601	OE4	N12-C11-N9	4.15	120.78	115.91
2	B	601	OE4	C5-C4-N3	-4.07	117.69	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	OE4	O31-C22-N21	4.05	128.88	124.79
2	B	601	OE4	O31-C22-N21	3.91	128.75	124.79
2	B	601	OE4	C24-C25-N21	3.86	108.73	105.88
2	C	601	OE4	C24-C25-N21	3.84	108.72	105.88
2	A	601	OE4	O30-C25-N21	3.74	128.58	124.79
2	C	601	OE4	O30-C25-N21	3.69	128.52	124.79
2	A	601	OE4	O31-C22-C23	-3.68	121.52	128.66
2	C	601	OE4	C23-C22-N21	3.65	108.58	105.88
2	B	601	OE4	C2-N3-C4	3.53	123.04	116.85
2	B	601	OE4	O31-C22-C23	-3.42	122.03	128.66
2	B	601	OE4	O13-C11-N9	-3.31	117.05	121.67
2	B	601	OE4	N12-C11-N9	3.26	119.74	115.91
2	A	601	OE4	O30-C25-C24	-3.23	122.39	128.66
2	C	601	OE4	O30-C25-C24	-3.05	122.76	128.66
2	C	601	OE4	C2-N3-C4	2.94	121.99	116.85
2	A	601	OE4	O13-C11-N9	-2.92	117.59	121.67
3	B	604	PO4	O4-P-O1	-2.86	100.84	110.95
2	A	601	OE4	C25-N21-C22	-2.85	109.59	112.02
2	B	601	OE4	C6-C5-C4	2.84	119.82	116.89
3	B	604	PO4	O4-P-O2	2.81	116.64	107.91
2	C	601	OE4	C24-C23-C22	-2.75	105.85	108.26
2	A	601	OE4	C24-C23-C22	-2.75	105.85	108.26
2	B	601	OE4	C24-C23-C22	-2.72	105.87	108.26
2	C	601	OE4	C23-C24-C25	-2.72	105.88	108.26
2	A	601	OE4	C23-C24-C25	-2.66	105.92	108.26
2	B	601	OE4	O30-C25-N21	2.61	127.43	124.79
2	A	601	OE4	C2-N3-C4	2.57	121.35	116.85
2	B	601	OE4	O30-C25-C24	-2.50	123.83	128.66
2	B	601	OE4	C23-C24-C25	-2.42	106.14	108.26
2	C	601	OE4	O31-C22-N21	2.33	127.15	124.79
2	B	601	OE4	C25-N21-C22	-2.31	110.04	112.02
2	C	601	OE4	O31-C22-C23	-2.30	124.21	128.66
2	C	601	OE4	C28-C29-C24	-2.12	115.97	119.80
2	C	601	OE4	C5-C4-N3	-2.09	120.80	124.05
2	A	601	OE4	C14-N12-C11	2.08	130.24	126.04
2	C	601	OE4	O13-C11-N9	-2.08	118.77	121.67
2	C	601	OE4	N12-C11-N9	2.06	118.33	115.91
2	C	601	OE4	C27-C26-C23	-2.02	116.14	119.80

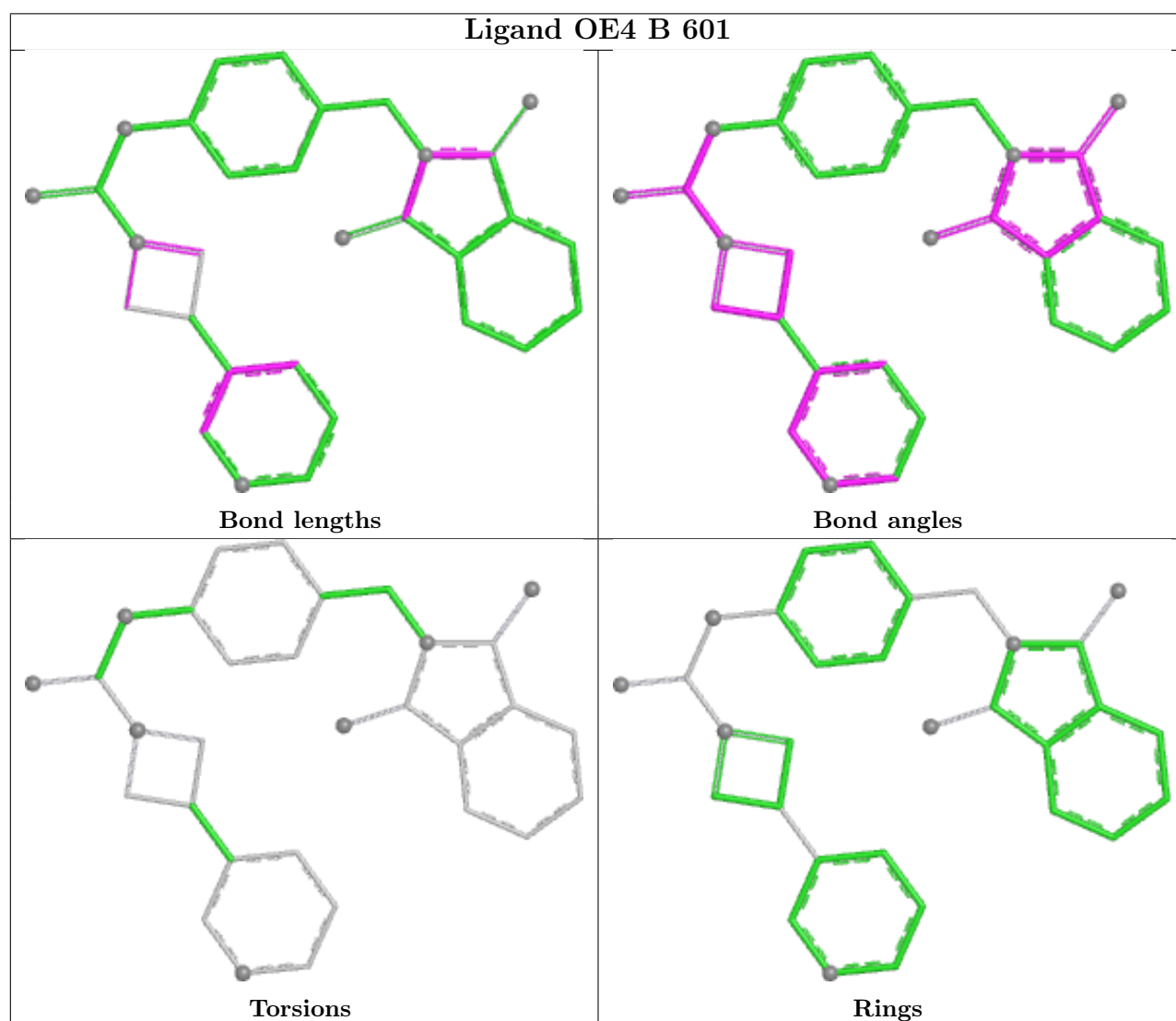
There are no chirality outliers.

There are no torsion outliers.

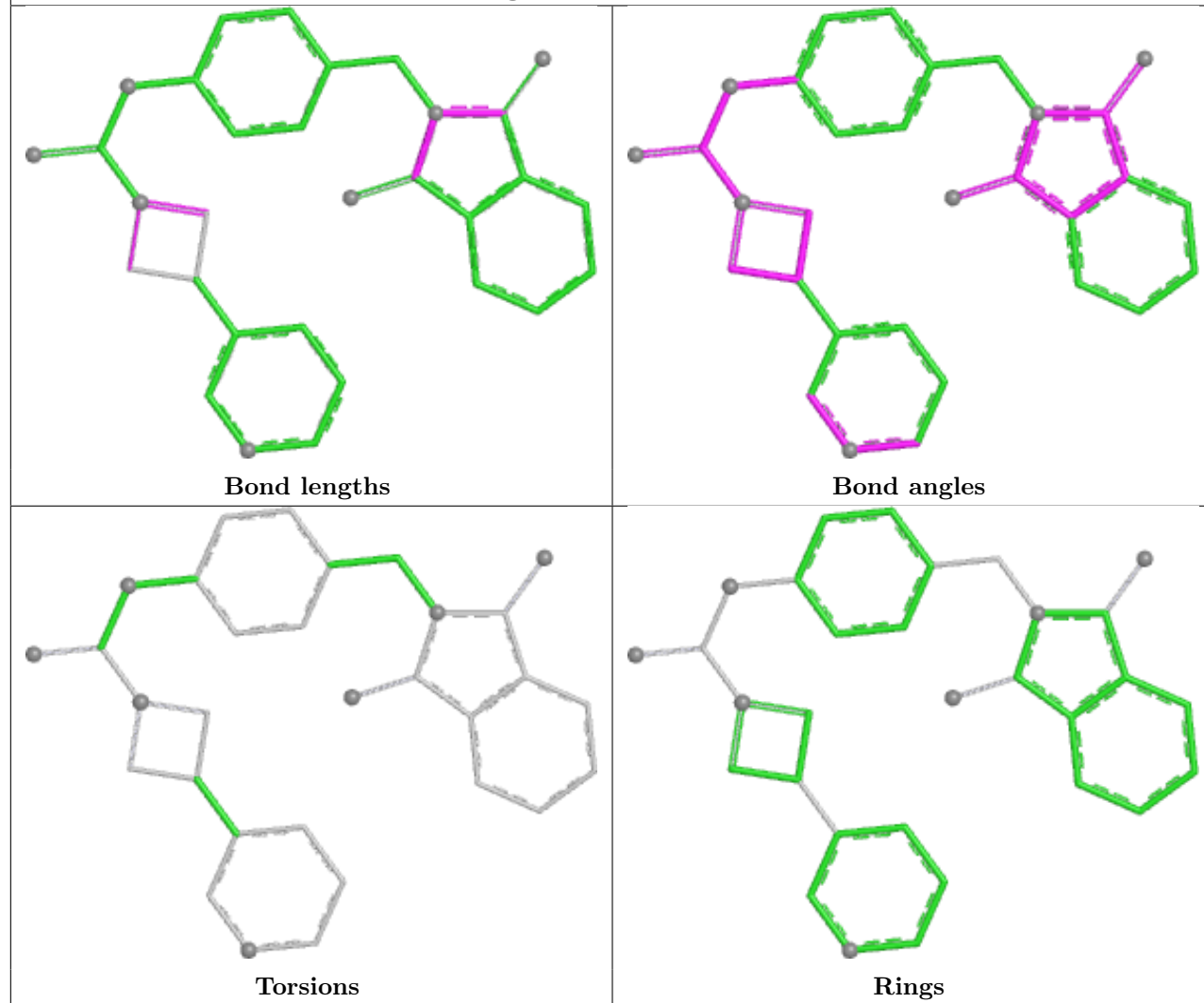
There are no ring outliers.

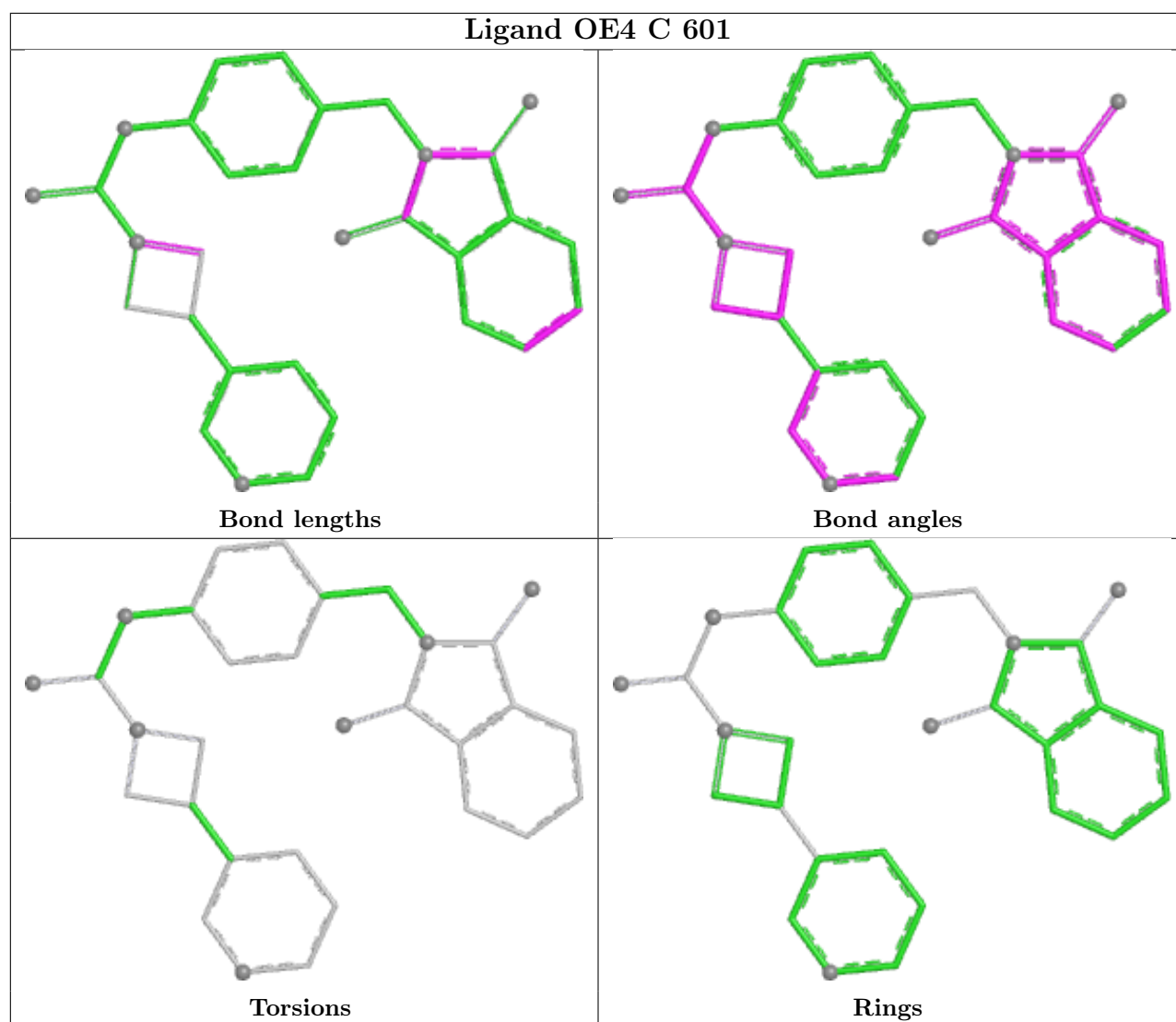
No monomer is involved in short contacts.

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



Ligand OE4 A 601





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	469/500 (93%)	-0.59	0 100 100	33, 53, 101, 122	0
1	B	468/500 (93%)	-0.49	2 (0%) 88 89	39, 64, 95, 132	0
1	C	469/500 (93%)	-0.33	0 100 100	40, 68, 121, 161	0
1	D	471/500 (94%)	-0.12	4 (0%) 82 83	47, 80, 144, 160	0
All	All	1877/2000 (93%)	-0.38	6 (0%) 90 91	33, 67, 126, 161	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	453	TYR	3.7
1	B	484	ILE	3.2
1	D	284	TYR	2.8
1	D	484	ILE	2.7
1	D	321	VAL	2.1
1	D	286	ALA	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,

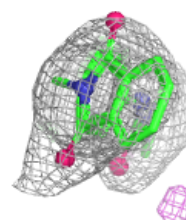
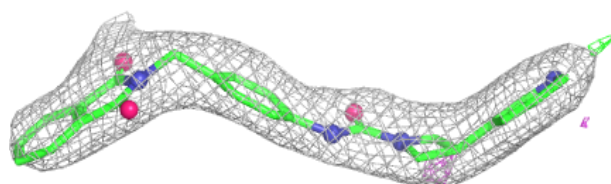
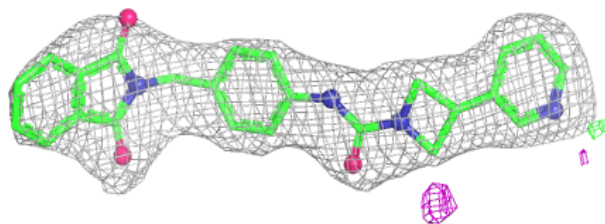
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	D	602	5/5	0.59	0.15	142,142,143,144	0
3	PO4	D	603	5/5	0.72	0.14	134,134,135,137	0
3	PO4	A	604	5/5	0.83	0.14	94,95,99,103	0
3	PO4	C	602	5/5	0.85	0.11	110,110,111,112	0
3	PO4	C	603	5/5	0.85	0.13	108,111,111,111	0
3	PO4	B	604	5/5	0.87	0.20	73,82,85,90	0
3	PO4	B	603	5/5	0.89	0.13	107,108,111,113	0
3	PO4	A	603	5/5	0.89	0.14	133,133,134,136	0
3	PO4	D	601	5/5	0.90	0.11	71,74,76,77	0
3	PO4	B	602	5/5	0.92	0.09	80,86,89,89	0
3	PO4	C	604	5/5	0.93	0.17	62,77,81,82	0
3	PO4	A	602	5/5	0.94	0.08	59,63,65,69	0
2	OE4	A	601	31/31	0.94	0.09	44,62,83,85	0
2	OE4	B	601	31/31	0.94	0.08	35,65,78,80	0
2	OE4	C	601	31/31	0.95	0.08	40,52,68,69	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.

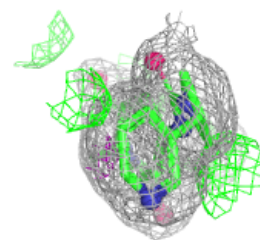
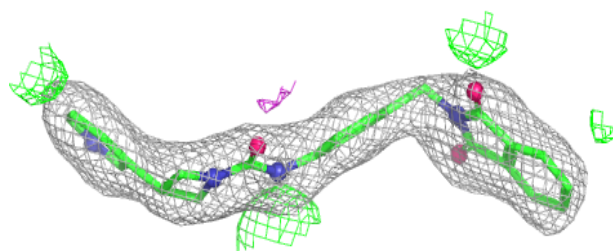
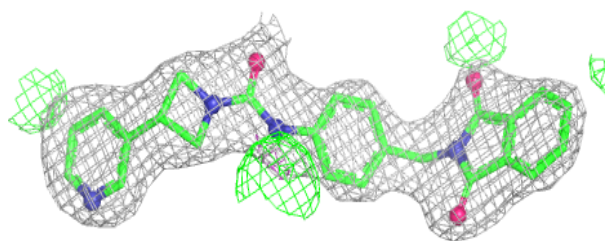
Electron density around OE4 A 601:

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

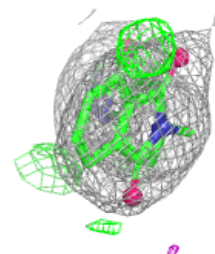
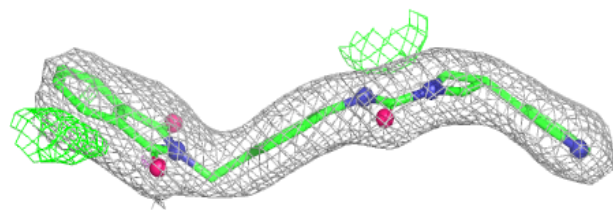
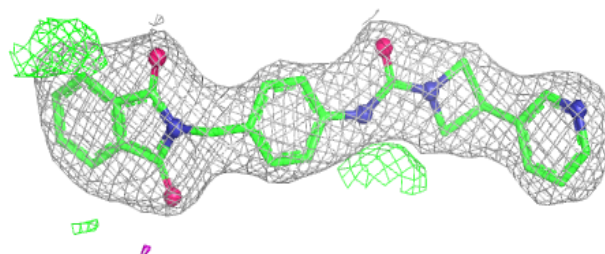


Electron density around OE4 B 601:

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

**Electron density around OE4 C 601:**

$2mF_o-DF_c$ (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.