



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:44 PM UTC

PDB ID : 7PPI / pdb_00007ppi
Title : Crystal STRUCTURE OF NAMPT IN COMPLEX WITH Compound 11
Authors : Hillig, R.C.
Deposited on : 2021-09-13
Resolution : 2.33 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

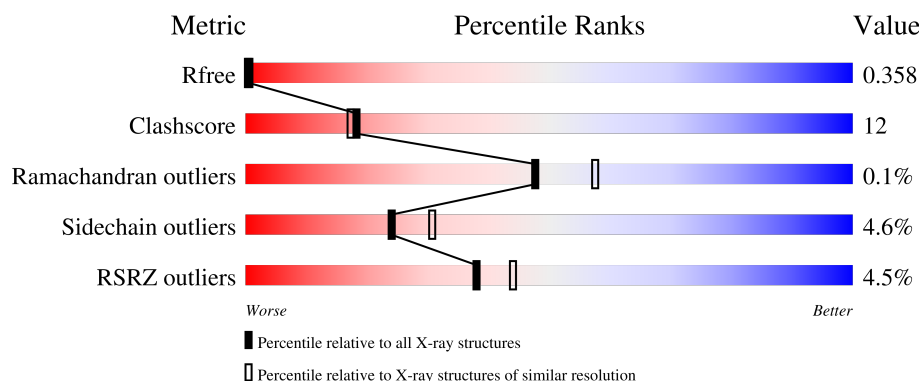
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

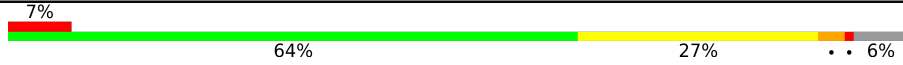
The reported resolution of this entry is 2.33 Å.

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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	492	
1	B	492	
1	C	492	
1	D	492	

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	502	-	-	X	-
3	PO4	D	502	-	-	X	-
4	CL	A	505	-	-	X	-
4	CL	B	503	-	-	X	-
4	CL	C	505	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16184 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.

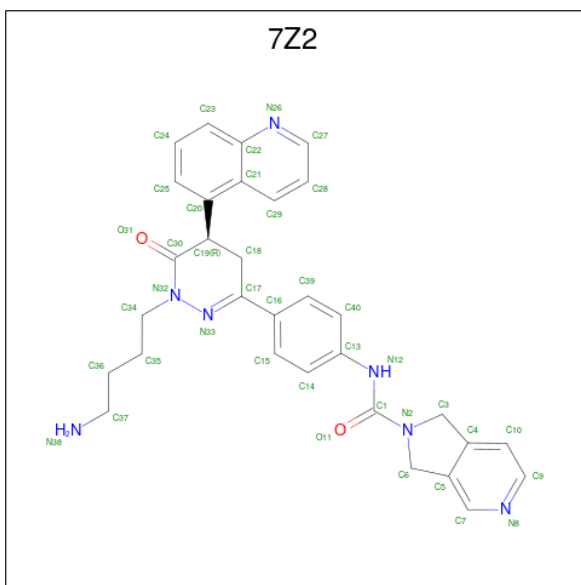
- Molecule 1 is a protein called Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3703	2382	612	702	7			
1	B	463	Total	C	N	O	S	0	1	0
			3707	2386	612	702	7			
1	C	464	Total	C	N	O	S	0	0	0
			3711	2388	613	703	7			
1	D	463	Total	C	N	O	S	0	2	0
			3712	2391	612	702	7			

There are 4 discrepancies between the modelled and reference sequences:

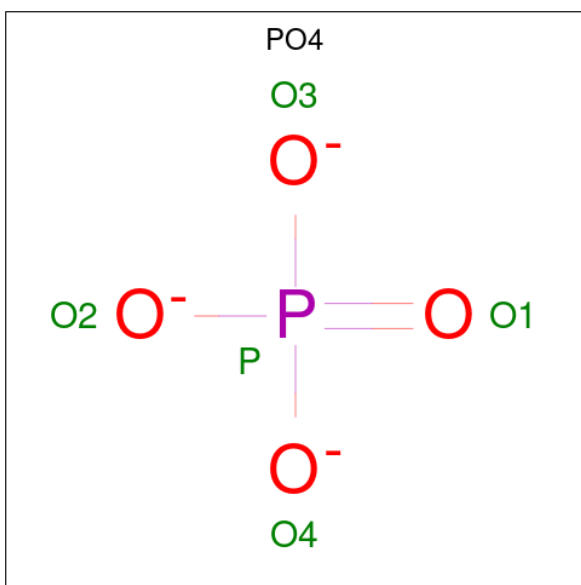
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P43490
B	0	GLY	-	expression tag	UNP P43490
C	0	GLY	-	expression tag	UNP P43490
D	0	GLY	-	expression tag	UNP P43490

- Molecule 2 is N-[4-[(5R)-1-(4-azanylbutyl)-6-oxidanylidene-5-quinolin-5-yl]-4,5-dihydropyridazin-3-yl]phenyl]-1,3-dihydropyrrolo[3,4-c]pyridine-2-carboxamide (CCD ID: 7Z2) (formula: C₃₁H₃₁N₇O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			40	31	7	2		
2	B	1	Total	C	N	O	0	0
			40	31	7	2		
2	C	1	Total	C	N	O	0	0
			40	31	7	2		
2	D	1	Total	C	N	O	0	0
			40	31	7	2		

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

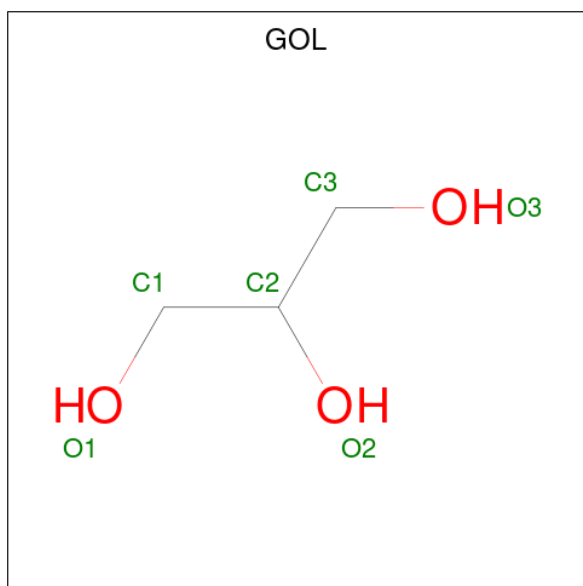


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Cl 3 3	0	0
4	B	1	Total Cl 1 1	0	0
4	C	3	Total Cl 3 3	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



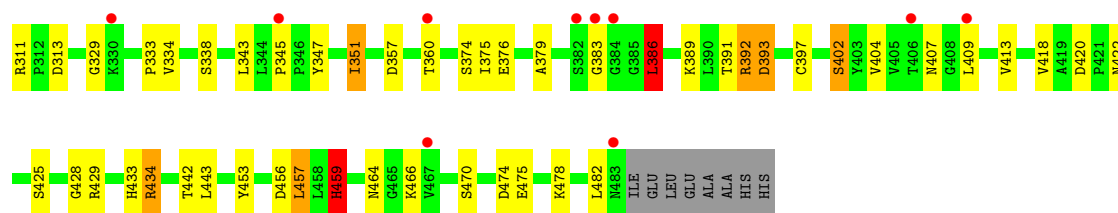
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

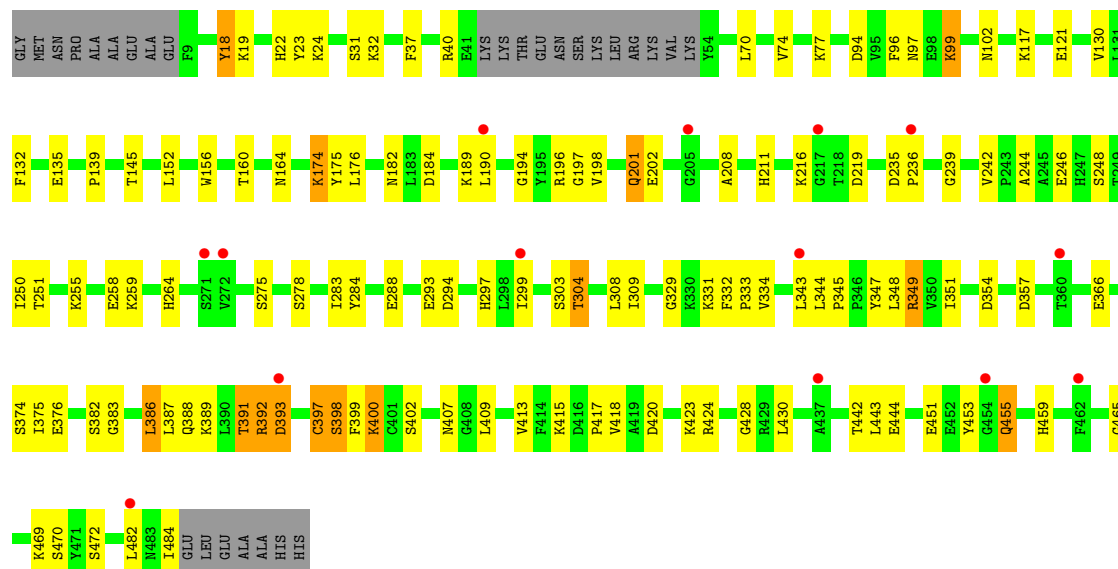
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	283	Total 283	O 283	0	0
6	B	280	Total 280	O 280	0	0
6	C	280	Total 280	O 280	0	0
6	D	303	Total 303	O 303	0	0

- Molecule 1: Nicotinamide phosphoribosyltransferase

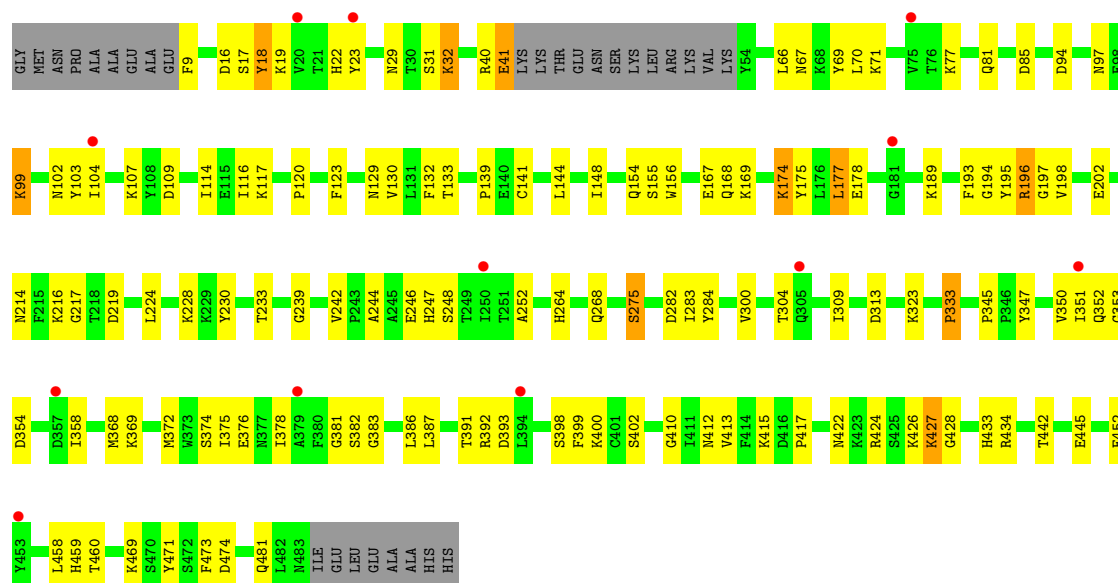




• Molecule 1: Nicotinamide phosphoribosyltransferase



• Molecule 1: Nicotinamide phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.21Å 106.26Å 120.95Å 90.00° 96.42° 90.00°	Depositor
Resolution (Å)	46.14 – 2.33 46.14 – 2.33	Depositor EDS
% Data completeness (in resolution range)	95.3 (46.14-2.33) 95.8 (46.14-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.292 , 0.359 0.294 , 0.358	Depositor DCC
R_{free} test set	2100 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.775	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	16184	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3190e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 7Z2, CL, GOL, 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	1.26	10/3791 (0.3%)	1.57	20/5138 (0.4%)
1	B	1.25	10/3798 (0.3%)	1.57	18/5148 (0.3%)
1	C	1.28	13/3799 (0.3%)	1.58	17/5149 (0.3%)
1	D	1.27	8/3806 (0.2%)	1.55	18/5159 (0.3%)
All	All	1.27	41/15194 (0.3%)	1.56	73/20594 (0.4%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	398	SER	C-O	8.72	1.34	1.23
1	A	277	VAL	C-O	7.80	1.32	1.24
1	C	201	GLN	C-O	7.48	1.32	1.24
1	A	206	ILE	C-O	7.34	1.32	1.24
1	A	250	ILE	C-O	7.34	1.31	1.24
1	C	397	CYS	C-O	6.75	1.32	1.23
1	A	244	ALA	C-O	6.71	1.32	1.23
1	D	417	PRO	C-O	-6.53	1.15	1.23
1	C	250	ILE	C-O	6.28	1.30	1.24
1	C	182	ASN	C-O	6.25	1.31	1.23
1	C	392	ARG	C-O	-6.16	1.16	1.24
1	D	353	GLY	C-O	-6.09	1.20	1.24
1	B	201	GLN	C-O	6.07	1.31	1.24
1	A	469	LYS	C-O	5.89	1.30	1.23
1	A	391	THR	C-O	5.88	1.31	1.23
1	D	196	ARG	C-O	5.78	1.31	1.24
1	B	404	VAL	C-O	5.76	1.29	1.23
1	B	393	ASP	C-O	5.68	1.30	1.24
1	C	482	LEU	C-O	5.67	1.30	1.23
1	B	262	PHE	C-O	5.67	1.30	1.24
1	C	308	LEU	C-O	5.58	1.30	1.24
1	D	433	HIS	CE1-NE2	5.49	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	314	SER	C-O	-5.46	1.17	1.23
1	D	129	ASN	C-O	5.43	1.30	1.23
1	D	350	VAL	C-O	5.41	1.29	1.24
1	C	297	HIS	CE1-NE2	5.34	1.37	1.32
1	C	264	HIS	CE1-NE2	5.31	1.37	1.32
1	B	402	SER	C-O	5.29	1.30	1.24
1	A	193	PHE	C-O	5.26	1.31	1.24
1	A	350	VAL	C-O	5.23	1.29	1.24
1	C	164	ASN	C-O	-5.22	1.17	1.24
1	C	354	ASP	CG-OD1	5.19	1.35	1.25
1	D	247	HIS	CG-ND1	-5.18	1.32	1.38
1	A	134	VAL	C-O	5.15	1.29	1.24
1	C	417	PRO	C-O	-5.10	1.17	1.23
1	B	470	SER	C-O	5.09	1.30	1.23
1	B	386	LEU	C-O	-5.08	1.17	1.24
1	B	282	ASP	CG-OD1	5.07	1.34	1.25
1	B	313	ASP	CG-OD2	-5.05	1.15	1.25
1	B	34	TYR	C-O	5.04	1.29	1.24
1	D	352	GLN	C-O	5.02	1.30	1.24

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	393	ASP	CA-CB-CG	10.16	122.76	112.60
1	C	393	ASP	CB-CA-C	-9.99	93.86	110.85
1	C	393	ASP	CA-CB-CG	8.39	120.99	112.60
1	A	167	GLU	CB-CG-CD	7.71	125.70	112.60
1	B	393	ASP	CB-CA-C	-7.19	99.31	110.81
1	A	132	PHE	CA-CB-CG	7.09	120.89	113.80
1	A	483	ASN	CA-C-O	-6.91	109.06	120.80
1	B	407	ASN	CB-CA-C	-6.63	101.04	111.51
1	B	392	ARG	CA-C-N	6.56	129.40	120.54
1	B	392	ARG	C-N-CA	6.56	129.40	120.54
1	D	391	THR	CA-CB-OG1	-6.27	100.20	109.60
1	C	184	ASP	CB-CA-C	-6.26	101.15	110.16
1	D	333	PRO	CB-CA-C	6.20	117.04	111.40
1	A	205	GLY	CA-C-N	6.15	128.31	120.56
1	A	205	GLY	C-N-CA	6.15	128.31	120.56
1	D	167	GLU	CB-CG-CD	6.15	123.06	112.60
1	A	422	ASN	CA-CB-CG	-6.05	106.55	112.60
1	B	132	PHE	CA-CB-CG	6.04	119.84	113.80
1	C	132	PHE	CA-CB-CG	5.97	119.77	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	GLU	CB-CG-CD	5.93	122.69	112.60
1	D	132	PHE	CA-CB-CG	5.89	119.69	113.80
1	B	305	GLN	CB-CA-C	-5.74	99.68	110.01
1	D	94	ASP	CA-C-O	-5.68	115.71	122.13
1	B	161	VAL	N-CA-C	-5.67	105.20	110.53
1	D	474	ASP	CA-CB-CG	-5.61	106.99	112.60
1	C	121	GLU	CB-CA-C	5.58	119.19	109.65
1	D	174	LYS	CA-C-O	-5.57	114.97	120.82
1	A	396	ASN	CB-CA-C	5.55	120.77	112.06
1	C	94	ASP	CA-C-N	5.45	129.25	121.02
1	C	94	ASP	C-N-CA	5.45	129.25	121.02
1	D	195	TYR	CA-C-O	-5.45	115.10	120.82
1	B	99	LYS	CA-C-N	5.43	126.01	119.98
1	B	99	LYS	C-N-CA	5.43	126.01	119.98
1	D	29	ASN	CA-CB-CG	-5.41	107.19	112.60
1	C	407	ASN	CB-CA-C	-5.39	102.99	111.51
1	B	459	HIS	CA-CB-CG	5.39	119.19	113.80
1	A	99	LYS	CA-C-N	5.38	125.91	119.94
1	A	99	LYS	C-N-CA	5.38	125.91	119.94
1	A	345	PRO	N-CA-CB	5.37	106.20	103.19
1	D	40	ARG	CA-C-N	5.34	131.32	121.70
1	D	40	ARG	C-N-CA	5.34	131.32	121.70
1	A	386	LEU	CA-C-O	-5.32	114.33	120.24
1	B	208	ALA	CA-C-O	-5.31	114.79	120.42
1	A	396	ASN	N-CA-CB	-5.28	103.68	111.71
1	A	395	LEU	CB-CA-C	-5.25	102.56	111.02
1	B	302	ARG	CA-C-N	5.23	128.65	120.75
1	B	302	ARG	C-N-CA	5.23	128.65	120.75
1	A	383	GLY	CA-C-N	5.21	125.73	119.94
1	A	383	GLY	C-N-CA	5.21	125.73	119.94
1	B	121	GLU	CB-CA-C	5.21	118.37	109.72
1	C	99	LYS	CA-C-N	5.21	125.76	119.98
1	C	99	LYS	C-N-CA	5.21	125.76	119.98
1	D	246	GLU	CA-C-O	-5.20	115.54	121.68
1	A	92	GLN	CB-CG-CD	-5.19	103.77	112.60
1	C	40	ARG	NE-CZ-NH1	-5.18	116.31	121.50
1	C	184	ASP	CA-CB-CG	5.17	117.77	112.60
1	C	349	ARG	CA-C-N	5.16	130.18	123.06
1	C	349	ARG	C-N-CA	5.16	130.18	123.06
1	A	155	SER	N-CA-C	-5.13	106.28	112.54
1	D	224	LEU	CA-C-O	-5.13	115.41	120.70
1	D	9	PHE	CB-CA-C	-5.12	100.37	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	VAL	CA-C-O	-5.12	115.73	121.05
1	C	145	THR	CA-CB-OG1	-5.10	101.96	109.60
1	B	40	ARG	O-C-N	5.09	129.13	122.87
1	D	40	ARG	CA-C-O	-5.07	116.18	121.55
1	D	99	LYS	CA-C-N	5.07	125.60	119.98
1	D	99	LYS	C-N-CA	5.07	125.60	119.98
1	A	461	VAL	N-CA-C	-5.05	107.91	112.96
1	D	452	GLU	N-CA-C	-5.05	106.97	113.23
1	B	360	THR	CB-CA-C	5.04	119.91	110.70
1	B	183	LEU	N-CA-CB	-5.01	102.95	111.17
1	C	420	ASP	N-CA-CB	-5.01	105.04	110.71
1	C	208	ALA	CA-C-O	-5.01	115.11	120.42

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	3703	0	3675	105	0
1	B	3707	0	3684	91	0
1	C	3711	0	3686	86	0
1	D	3712	0	3695	84	0
2	A	40	0	0	4	0
2	B	40	0	0	5	0
2	C	40	0	0	5	0
2	D	40	0	0	4	0
3	A	5	0	0	0	0
3	B	5	0	0	2	0
3	C	5	0	0	1	0
3	D	5	0	0	5	0
4	A	3	0	0	3	0
4	B	1	0	0	2	0
4	C	3	0	0	3	0
5	A	6	0	8	0	0
5	C	12	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	283	0	0	23	0
6	B	280	0	0	28	0
6	C	280	0	0	22	0
6	D	303	0	0	22	0
All	All	16184	0	14764	361	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 12.

All (361) 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)
4:A:505:CL:CL	6:B:773:HOH:O	1.91	1.19
1:C:391:THR:CG2	1:C:393:ASP:HB2	1.89	1.03
1:D:398:SER:OG	3:D:502:PO4:O4	1.78	1.00
1:A:391:THR:HG23	1:A:393:ASP:H	1.26	0.98
1:C:32:LYS:NZ	1:C:135:GLU:OE2	2.01	0.94
1:C:391:THR:HG22	1:C:393:ASP:HB2	1.48	0.94
1:A:272:VAL:HG22	1:A:273:PRO:HD2	1.50	0.92
1:B:216:LYS:HE3	6:B:744:HOH:O	1.71	0.91
1:D:114:ILE:HD11	1:D:144:LEU:HG	1.51	0.91
1:D:104:ILE:HD11	1:D:141:CYS:SG	2.11	0.89
4:C:505:CL:CL	6:D:774:HOH:O	2.27	0.89
4:A:505:CL:CL	6:A:668:HOH:O	2.35	0.81
1:D:264:HIS:O	1:D:268:GLN:HG2	1.80	0.80
4:A:505:CL:CL	1:B:311:ARG:NH2	2.51	0.79
1:B:459:HIS:HB3	6:B:809:HOH:O	1.81	0.79
4:B:503:CL:CL	6:B:802:HOH:O	2.36	0.79
1:A:441:VAL:HG11	1:A:453:TYR:CE2	2.19	0.78
4:C:506:CL:CL	6:C:813:HOH:O	2.39	0.77
1:A:56:GLU:OE1	1:A:166:ARG:NH1	2.17	0.77
1:A:391:THR:CG2	1:A:393:ASP:H	1.96	0.77
1:B:357:ASP:OD2	6:B:601:HOH:O	2.01	0.77
3:B:502:PO4:O2	6:B:602:HOH:O	2.01	0.76
1:D:374:SER:OG	1:D:376:GLU:HG2	1.85	0.76
1:C:174:LYS:HE2	1:C:175:TYR:CE2	2.20	0.75
4:C:505:CL:CL	6:D:863:HOH:O	2.41	0.75
1:A:149:GLU:OE2	6:A:601:HOH:O	2.05	0.75
1:A:38:GLU:OE2	1:A:40:ARG:HA	1.88	0.73
1:B:391:THR:OG1	1:B:393:ASP:HB2	1.89	0.72
1:B:434:ARG:HD2	1:B:457:LEU:HD21	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:THR:HG23	1:C:393:ASP:H	1.54	0.71
1:D:104:ILE:CD1	1:D:141:CYS:SG	2.78	0.71
1:B:334[A]:VAL:HG22	6:B:665:HOH:O	1.88	0.71
1:B:211:HIS:HB2	1:B:386:LEU:HD21	1.72	0.70
1:A:175:TYR:HB3	1:A:375:ILE:HG13	1.72	0.70
1:A:430:LEU:O	6:A:602:HOH:O	2.08	0.70
1:B:217:GLY:HA3	6:B:722:HOH:O	1.93	0.69
1:C:357:ASP:OD2	1:C:389:LYS:NZ	2.27	0.68
1:B:216:LYS:CE	6:B:744:HOH:O	2.36	0.67
1:D:175:TYR:HB3	1:D:375:ILE:HG13	1.78	0.67
1:B:41:GLU:OE2	1:B:422:ASN:ND2	2.28	0.66
1:C:392:ARG:HD3	1:D:197:GLY:HA2	1.77	0.66
1:B:175:TYR:HB3	1:B:375:ILE:HG13	1.78	0.66
1:C:391:THR:CG2	1:C:393:ASP:H	2.08	0.66
1:C:391:THR:HG21	1:C:393:ASP:HB2	1.76	0.66
1:A:466:LYS:HE2	6:A:855:HOH:O	1.96	0.66
1:A:469:LYS:HE3	1:A:471:TYR:CZ	2.31	0.66
2:B:501:7Z2:C35	2:B:501:7Z2:O31	2.45	0.64
1:C:175:TYR:HB3	1:C:375:ILE:HG13	1.80	0.64
1:C:37:PHE:CZ	1:C:397:CYS:HB3	2.33	0.63
1:A:444:GLU:OE2	6:A:603:HOH:O	2.15	0.63
1:C:96:PHE:O	5:C:507:GOL:H32	1.98	0.63
1:A:66:LEU:HD23	1:A:70:LEU:HD12	1.80	0.62
1:D:333:PRO:HA	6:D:718:HOH:O	1.98	0.62
1:D:400:LYS:NZ	3:D:502:PO4:O4	2.32	0.62
1:A:40:ARG:NE	1:A:422:ASN:O	2.29	0.62
1:A:374:SER:OG	1:A:376:GLU:HG2	1.99	0.62
1:C:304:THR:HB	6:C:847:HOH:O	2.00	0.61
1:B:211:HIS:CG	1:B:386:LEU:HD21	2.35	0.61
1:B:434:ARG:HG3	1:B:434:ARG:HH21	1.65	0.61
1:C:202:GLU:HA	6:C:720:HOH:O	2.00	0.61
1:D:458:LEU:HD12	6:D:707:HOH:O	1.99	0.61
1:C:398:SER:OG	3:C:502:PO4:O2	2.10	0.61
1:D:242:VAL:HG22	2:D:501:7Z2:C40	2.31	0.61
1:A:412:ASN:HB2	6:A:743:HOH:O	2.01	0.61
1:A:92:GLN:HA	1:A:92:GLN:NE2	2.16	0.60
1:A:173:ALA:HA	1:A:183:LEU:CD2	2.31	0.60
1:A:31:SER:O	1:A:139:PRO:HA	2.01	0.59
1:C:455:GLN:NE2	6:C:613:HOH:O	2.34	0.59
1:A:258:GLU:OE2	6:A:604:HOH:O	2.16	0.59
1:A:441:VAL:CG1	1:A:453:TYR:CE2	2.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:GLU:HA	6:C:697:HOH:O	2.01	0.59
1:A:24:LYS:HB3	1:B:268:GLN:HG2	1.85	0.59
1:D:41:GLU:OE2	1:D:422:ASN:ND2	2.35	0.59
1:A:174:LYS:O	1:A:178:GLU:HG3	2.03	0.58
3:B:502:PO4:O1	6:B:603:HOH:O	2.15	0.58
1:B:343:LEU:CD1	1:B:376:GLU:HG3	2.33	0.58
1:C:391:THR:CG2	1:C:393:ASP:CB	2.74	0.58
1:D:398:SER:HG	1:D:400:LYS:HZ3	1.47	0.58
1:B:17:SER:OG	1:B:90:HIS:NE2	2.34	0.58
1:B:31:SER:O	1:B:139:PRO:HA	2.03	0.58
1:C:31:SER:O	1:C:139:PRO:HA	2.03	0.58
1:B:184:ASP:HB2	6:B:764:HOH:O	2.04	0.57
1:A:130:VAL:HG12	1:A:442:THR:HG23	1.87	0.57
1:C:258:GLU:OE2	6:C:601:HOH:O	2.17	0.57
1:C:189:LYS:HE3	1:C:375:ILE:HG22	1.86	0.57
1:C:374:SER:OG	1:C:376:GLU:HG2	2.05	0.57
1:A:398:SER:OG	1:A:400:LYS:NZ	2.33	0.57
1:A:258:GLU:HB3	6:A:604:HOH:O	2.06	0.56
1:D:31:SER:O	1:D:139:PRO:HA	2.04	0.56
1:D:412:ASN:OD1	6:D:601:HOH:O	2.17	0.56
1:D:189:LYS:NZ	2:D:501:7Z2:N26	2.53	0.56
1:A:57:THR:HG21	1:A:395:LEU:HD13	1.86	0.56
1:B:433:HIS:HB3	1:B:453:TYR:HB3	1.87	0.56
1:B:418:VAL:N	6:B:613:HOH:O	2.40	0.55
1:B:62:LEU:HD12	1:B:62:LEU:O	2.07	0.55
1:D:372:MET:HE1	6:D:795:HOH:O	2.06	0.55
1:B:70:LEU:HD11	1:B:152:LEU:HD21	1.87	0.55
4:B:503:CL:CL	6:B:706:HOH:O	2.56	0.55
1:A:256:ASP:C	6:A:654:HOH:O	2.50	0.54
1:B:374:SER:OG	1:B:376:GLU:HG2	2.06	0.54
1:A:391:THR:CG2	1:A:393:ASP:N	2.68	0.54
1:D:69:TYR:OH	1:D:202:GLU:OE2	2.25	0.54
1:B:279:ASP:OD2	6:B:604:HOH:O	2.18	0.54
1:A:11:ILE:HG22	6:A:609:HOH:O	2.07	0.54
1:D:189:LYS:HE3	1:D:375:ILE:HG22	1.89	0.54
1:A:16:ASP:OD2	1:B:196:ARG:NH2	2.39	0.54
1:D:469:LYS:NZ	1:D:471:TYR:OH	2.23	0.54
1:A:349:ARG:CZ	6:A:661:HOH:O	2.56	0.53
1:B:211:HIS:CB	1:B:386:LEU:HD21	2.37	0.53
1:B:379:ALA:HB2	2:B:501:7Z2:C25	2.37	0.53
1:C:219:ASP:HA	1:D:17:SER:OG	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:LEU:CD1	1:C:376:GLU:HG3	2.39	0.53
1:B:130:VAL:HG12	1:B:442:THR:HG23	1.91	0.52
1:A:272:VAL:HG22	1:A:273:PRO:CD	2.31	0.52
1:A:453:TYR:C	1:A:454:GLY:O	2.52	0.52
2:D:501:7Z2:C29	2:D:501:7Z2:C30	2.87	0.52
1:C:174:LYS:HE2	1:C:175:TYR:CZ	2.44	0.52
1:A:24:LYS:HD3	1:B:268:GLN:OE1	2.10	0.52
1:C:211:HIS:CG	1:C:386:LEU:HD11	2.45	0.52
1:A:447:LYS:HE3	6:A:869:HOH:O	2.10	0.52
1:B:189:LYS:HE3	1:B:375:ILE:HG22	1.91	0.52
1:D:415:LYS:NZ	6:D:615:HOH:O	2.41	0.51
1:B:211:HIS:ND1	1:B:386:LEU:HD21	2.25	0.51
1:B:244:ALA:CB	1:B:275:SER:HB3	2.40	0.51
1:A:54:TYR:OH	1:A:164:ASN:OD1	2.27	0.51
1:A:338:SER:HB3	6:A:676:HOH:O	2.11	0.51
1:B:211:HIS:HB2	1:B:386:LEU:CD2	2.41	0.51
1:D:382:SER:HB3	1:D:386:LEU:HB2	1.92	0.51
2:C:501:7Z2:C29	2:C:501:7Z2:C30	2.89	0.51
1:C:251:THR:O	6:C:603:HOH:O	2.19	0.51
1:C:366:GLU:OE1	6:C:602:HOH:O	2.19	0.51
1:B:311:ARG:NH1	6:B:632:HOH:O	2.40	0.51
1:C:391:THR:HG22	1:C:393:ASP:CB	2.31	0.51
1:A:244:ALA:HA	1:A:275:SER:O	2.10	0.50
2:A:501:7Z2:C29	2:A:501:7Z2:C30	2.89	0.50
1:A:323:LYS:HD3	6:A:711:HOH:O	2.11	0.50
1:A:290:ILE:HD11	6:A:604:HOH:O	2.12	0.50
1:C:236:PRO:HD2	6:C:773:HOH:O	2.11	0.50
1:C:288:GLU:O	1:C:293:GLU:HG3	2.12	0.50
1:B:402:SER:O	1:B:428:GLY:N	2.42	0.50
1:B:429:ARG:HD3	6:B:817:HOH:O	2.12	0.50
1:A:402:SER:O	1:A:428:GLY:N	2.44	0.50
1:A:10:ASN:HB3	1:A:13:LEU:HD12	1.93	0.50
1:D:460:THR:HG21	6:D:879:HOH:O	2.11	0.50
1:B:351:ILE:HD12	1:B:379:ALA:HB3	1.94	0.49
1:B:420:ASP:OD1	1:B:422:ASN:HB2	2.12	0.49
1:D:427:LYS:HG3	6:D:639:HOH:O	2.12	0.49
1:C:130:VAL:HG12	1:C:442:THR:HG23	1.94	0.49
1:B:379:ALA:HB2	2:B:501:7Z2:C24	2.42	0.49
2:B:501:7Z2:C30	2:B:501:7Z2:C29	2.90	0.49
1:B:351:ILE:HD12	1:B:379:ALA:CB	2.42	0.49
1:C:196:ARG:NH2	1:D:16:ASP:OD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:PHE:O	6:D:602:HOH:O	2.19	0.49
1:A:92:GLN:HA	1:A:92:GLN:HE21	1.74	0.49
1:C:423:LYS:NZ	1:D:354:ASP:OD1	2.44	0.49
1:A:183:LEU:HD22	1:A:186:LEU:HD22	1.95	0.49
1:B:389:LYS:HE2	6:B:831:HOH:O	2.12	0.49
1:C:399:PHE:O	1:C:400:LYS:HD3	2.13	0.49
1:A:424:ARG:HH11	1:A:424:ARG:HG2	1.77	0.49
1:C:176:LEU:HD11	6:C:697:HOH:O	2.12	0.49
1:C:70:LEU:HD11	1:C:152:LEU:HD21	1.94	0.48
1:A:189:LYS:HE3	1:A:375:ILE:HG22	1.94	0.48
1:D:178:GLU:HG2	1:D:369:LYS:HE3	1.96	0.48
1:A:379:ALA:HB2	2:A:501:7Z2:C25	2.44	0.48
1:D:233:THR:HG22	1:D:473:PHE:HB3	1.96	0.48
1:A:194:GLY:CA	1:A:383:GLY:HA2	2.43	0.48
1:C:197:GLY:HA2	1:D:392:ARG:HD3	1.95	0.48
1:D:81:GLN:NE2	1:D:85:ASP:OD1	2.47	0.48
1:A:27:PRO:HA	1:B:253:TRP:CZ2	2.49	0.48
1:A:244:ALA:CB	1:A:275:SER:HB3	2.44	0.48
1:A:392:ARG:NE	1:B:196:ARG:HG3	2.29	0.48
1:B:68:LYS:HA	6:B:778:HOH:O	2.14	0.48
1:C:309:ILE:HG22	1:C:351:ILE:HG22	1.95	0.48
1:C:244:ALA:CB	1:C:275:SER:HB3	2.44	0.47
1:D:217:GLY:HA3	6:D:691:HOH:O	2.13	0.47
1:D:242:VAL:HG22	2:D:501:7Z2:C39	2.44	0.47
1:D:368:MET:SD	1:D:378:ILE:HG21	2.54	0.47
1:A:382:SER:HB3	1:A:386:LEU:HB2	1.95	0.47
1:D:114:ILE:HD12	1:D:148:ILE:HD11	1.95	0.47
1:A:132:PHE:HE2	1:A:152:LEU:HD13	1.80	0.47
1:A:481:GLN:NE2	6:A:643:HOH:O	2.47	0.47
1:B:134:VAL:HG21	1:B:152:LEU:CD1	2.45	0.47
1:B:343:LEU:HD11	1:B:376:GLU:HG3	1.95	0.47
1:A:309:ILE:HG22	1:A:351:ILE:HG22	1.96	0.47
1:D:402:SER:O	1:D:428:GLY:N	2.43	0.47
1:A:193:PHE:CE2	1:A:381:GLY:HA3	2.50	0.47
1:D:99:LYS:HD2	6:D:743:HOH:O	2.14	0.47
1:A:198:VAL:CG1	1:A:387:LEU:HB3	2.45	0.47
1:D:130:VAL:HG12	1:D:442:THR:HG23	1.97	0.47
1:A:40:ARG:NE	1:A:423:LYS:HA	2.30	0.47
1:A:113:PRO:HD2	1:A:144:LEU:CD2	2.44	0.47
1:C:246:GLU:OE2	1:D:22:HIS:CE1	2.68	0.47
1:A:326:GLU:HG3	6:A:800:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:PHE:CZ	1:B:397:CYS:HB3	2.50	0.46
1:B:169:LYS:HG2	1:B:482:LEU:HD11	1.98	0.46
1:C:216:LYS:O	1:C:239:GLY:HA2	2.15	0.46
1:A:173:ALA:HA	1:A:183:LEU:HD21	1.96	0.46
1:C:156:TRP:O	1:C:160:THR:OG1	2.21	0.46
1:B:392:ARG:NH1	6:B:644:HOH:O	2.49	0.46
1:D:194:GLY:CA	1:D:383:GLY:HA2	2.46	0.46
1:D:244:ALA:HA	1:D:275:SER:O	2.15	0.46
1:D:189:LYS:HZ1	1:D:376:GLU:HA	1.81	0.46
1:D:333:PRO:O	1:D:345:PRO:HD3	2.16	0.46
1:D:400:LYS:HZ1	3:D:502:PO4:P	2.38	0.46
1:A:21:THR:HG21	1:B:243:PRO:HA	1.98	0.46
1:D:109:ASP:CG	6:D:690:HOH:O	2.58	0.46
1:C:99:LYS:HD2	5:C:507:GOL:O1	2.15	0.46
1:A:40:ARG:HD3	6:A:832:HOH:O	2.15	0.45
1:A:244:ALA:HB2	1:A:275:SER:HB3	1.98	0.45
1:A:441:VAL:HG11	1:A:453:TYR:CZ	2.49	0.45
1:A:63:GLN:NE2	1:A:230:TYR:O	2.50	0.45
1:A:219:ASP:HA	1:B:17:SER:HB2	1.98	0.45
1:B:123:PHE:HB3	1:B:125:ILE:HD11	1.97	0.45
1:B:474:ASP:OD1	6:B:605:HOH:O	2.21	0.45
1:C:391:THR:HG23	6:C:843:HOH:O	2.15	0.45
1:B:456:ASP:HB2	6:B:823:HOH:O	2.16	0.45
1:C:242:VAL:HG22	2:C:501:7Z2:C40	2.46	0.45
1:C:409:LEU:HD12	6:C:766:HOH:O	2.15	0.45
1:A:199:SER:O	1:A:200:SER:HB3	2.16	0.45
1:A:255:LYS:HA	1:A:281:TYR:CZ	2.52	0.45
1:A:391:THR:CG2	1:A:393:ASP:HB2	2.47	0.45
1:B:309:ILE:HG22	1:B:351:ILE:HG22	1.99	0.45
1:C:19:LYS:HA	1:C:22:HIS:ND1	2.31	0.45
1:D:216:LYS:O	1:D:239:GLY:HA2	2.16	0.45
1:C:293:GLU:OE2	1:C:331:LYS:NZ	2.29	0.45
1:C:484:ILE:O	1:C:484:ILE:HG13	2.16	0.45
1:A:259:LYS:HD2	1:A:294:ASP:HB3	1.99	0.45
1:B:194:GLY:CA	1:B:383:GLY:HA2	2.46	0.45
1:B:193:PHE:CZ	2:B:501:7Z2:C6	2.99	0.45
1:B:418:VAL:HG12	6:B:613:HOH:O	2.16	0.45
1:C:349:ARG:HB3	2:C:501:7Z2:C24	2.47	0.45
1:D:66:LEU:HD23	1:D:70:LEU:HD12	1.98	0.45
1:C:389:LYS:HE2	6:C:826:HOH:O	2.15	0.45
1:D:103:TYR:O	1:D:107:LYS:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LYS:HA	1:C:459:HIS:O	2.17	0.45
1:C:402:SER:O	1:C:428:GLY:N	2.44	0.45
1:A:117:LYS:HA	1:A:459:HIS:O	2.17	0.44
1:A:413:VAL:HG11	1:B:252:ALA:HA	1.99	0.44
2:A:501:7Z2:O11	2:A:501:7Z2:C14	2.64	0.44
1:B:464:ASN:HA	6:B:688:HOH:O	2.17	0.44
1:C:194:GLY:CA	1:C:383:GLY:HA2	2.47	0.44
1:C:415:LYS:NZ	6:C:606:HOH:O	2.26	0.44
1:A:92:GLN:NE2	1:A:92:GLN:CA	2.81	0.44
1:A:13:LEU:HD11	1:A:82:GLU:OE2	2.18	0.44
1:B:19:LYS:HA	1:B:22:HIS:ND1	2.33	0.44
1:D:193:PHE:CE2	1:D:381:GLY:HA3	2.52	0.44
1:B:81:GLN:HE22	1:B:84:LYS:HD3	1.82	0.44
1:B:278:SER:O	1:B:283:ILE:HA	2.18	0.44
1:B:466:LYS:HA	6:B:794:HOH:O	2.16	0.44
1:C:329:GLY:HA2	1:C:334:VAL:CG2	2.47	0.44
1:B:9:PHE:N	6:B:645:HOH:O	2.49	0.44
1:C:23:TYR:CE1	1:C:97:ASN:HB2	2.53	0.44
1:C:443:LEU:HA	6:C:629:HOH:O	2.16	0.44
1:A:155:SER:O	1:A:156:TRP:C	2.61	0.44
1:A:199:SER:HB2	1:B:157:TYR:CD2	2.53	0.44
1:C:388:GLN:NE2	1:D:156:TRP:HH2	2.16	0.44
1:D:398:SER:CB	3:D:502:PO4:O4	2.64	0.44
1:A:19:LYS:HA	1:A:22:HIS:ND1	2.32	0.44
1:A:66:LEU:HD13	1:A:462:PHE:HB2	2.00	0.44
1:C:333:PRO:O	1:C:345:PRO:HD3	2.17	0.44
1:D:103:TYR:CE1	1:D:107:LYS:HG3	2.53	0.44
1:D:469:LYS:HE2	6:D:714:HOH:O	2.16	0.44
1:A:116:ILE:HA	1:A:133:THR:O	2.17	0.43
1:A:277:VAL:HA	1:A:311:ARG:HB3	2.00	0.43
1:A:57:THR:CG2	1:A:395:LEU:HD13	2.48	0.43
1:C:74:VAL:HG12	6:C:621:HOH:O	2.18	0.43
1:C:198:VAL:CG1	1:C:387:LEU:HB3	2.48	0.43
1:C:278:SER:O	1:C:283:ILE:HA	2.18	0.43
1:C:344:LEU:HD22	1:C:348:LEU:HD23	2.00	0.43
1:D:120:PRO:HB2	1:D:123:PHE:CD1	2.53	0.43
1:D:198:VAL:CG1	1:D:387:LEU:HB3	2.48	0.43
1:C:18:TYR:HB3	6:D:723:HOH:O	2.17	0.43
1:C:418:VAL:HG12	6:C:723:HOH:O	2.18	0.43
1:D:155:SER:O	1:D:156:TRP:C	2.61	0.43
1:B:37:PHE:HZ	1:B:397:CYS:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LYS:HA	1:B:459:HIS:O	2.19	0.43
1:D:23:TYR:CE1	1:D:97:ASN:HB2	2.53	0.43
1:D:120:PRO:O	1:D:123:PHE:HB2	2.17	0.43
1:A:391:THR:HG23	1:A:393:ASP:N	2.10	0.43
1:B:114:ILE:HD13	1:B:136:ASN:HA	2.01	0.43
1:D:230:TYR:HE2	6:D:888:HOH:O	2.02	0.43
1:B:433:HIS:CD2	1:B:443:LEU:HD12	2.53	0.43
1:C:283:ILE:HG23	1:C:284:TYR:N	2.34	0.43
1:C:472:SER:HB2	6:C:686:HOH:O	2.18	0.43
1:D:177[A]:LEU:HD22	1:D:177[A]:LEU:HA	1.91	0.43
1:B:243:PRO:O	1:B:274:VAL:HA	2.19	0.43
1:B:277:VAL:HA	1:B:311:ARG:HB3	2.01	0.43
1:C:382:SER:HB3	1:C:386:LEU:HB2	2.01	0.43
1:B:209:SER:HA	1:B:227:ILE:HD11	2.00	0.43
1:B:345:PRO:HG2	1:B:347:TYR:CE1	2.54	0.43
1:B:434:ARG:NE	6:B:628:HOH:O	2.38	0.43
1:D:410:GLY:HA3	6:D:818:HOH:O	2.19	0.43
1:A:209:SER:HA	1:A:227:ILE:HD11	2.00	0.42
1:B:116:ILE:HA	1:B:133:THR:O	2.19	0.42
1:D:323:LYS:NZ	6:D:627:HOH:O	2.42	0.42
1:D:333:PRO:HD2	1:D:345:PRO:HG3	2.01	0.42
2:A:501:7Z2:C27	6:A:813:HOH:O	2.67	0.42
1:A:199:SER:HB3	1:B:157:TYR:CD1	2.54	0.42
1:C:174:LYS:HG3	6:C:879:HOH:O	2.18	0.42
1:C:345:PRO:HG2	1:C:347:TYR:CE1	2.54	0.42
1:A:17:SER:O	1:A:20:VAL:HB	2.19	0.42
1:B:333:PRO:HD2	1:B:345:PRO:HG3	2.02	0.42
1:B:140:GLU:OE1	1:B:140:GLU:HA	2.20	0.42
1:B:474:ASP:O	1:B:478:LYS:HD2	2.19	0.42
1:C:244:ALA:HA	1:C:275:SER:O	2.20	0.42
1:D:116:ILE:HA	1:D:133:THR:O	2.19	0.42
1:D:300:VAL:HG12	1:D:347:TYR:OH	2.20	0.42
1:A:192:ASP:OD2	1:A:220:THR:HB	2.19	0.42
1:A:338:SER:CB	6:A:676:HOH:O	2.68	0.42
1:D:19:LYS:HA	1:D:22:HIS:ND1	2.35	0.42
1:A:329:GLY:HA2	1:A:334:VAL:CG2	2.50	0.42
1:A:176:LEU:HD13	1:A:189:LYS:HE3	2.00	0.42
1:D:424:ARG:NH1	6:D:639:HOH:O	2.53	0.42
1:B:155:SER:O	1:B:156:TRP:C	2.63	0.42
1:C:242:VAL:HG22	2:C:501:7Z2:C39	2.50	0.42
1:A:120:PRO:O	1:A:123:PHE:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:LYS:HE2	1:D:32:LYS:HB2	1.82	0.41
1:C:201:GLN:NE2	1:D:154:GLN:OE1	2.48	0.41
1:C:423:LYS:NZ	6:C:610:HOH:O	2.30	0.41
1:A:224:LEU:HB2	6:A:657:HOH:O	2.19	0.41
1:A:321:VAL:HG23	1:A:352:GLN:HE21	1.85	0.41
1:A:333:PRO:O	1:A:345:PRO:HD3	2.21	0.41
1:B:172:LEU:HD13	1:B:189:LYS:HB3	2.01	0.41
1:C:443:LEU:HD11	1:C:453:TYR:CD2	2.55	0.41
1:D:426:LYS:HA	6:D:639:HOH:O	2.19	0.41
1:A:38:GLU:OE2	1:A:128:GLY:HA2	2.20	0.41
1:D:282:ASP:N	6:D:614:HOH:O	2.34	0.41
1:C:259:LYS:CE	1:C:294:ASP:HB3	2.50	0.41
1:D:283:ILE:HG23	1:D:284:TYR:N	2.36	0.41
1:A:253:TRP:CZ2	1:B:27:PRO:HA	2.56	0.41
1:A:386:LEU:HD13	1:A:387:LEU:HD23	2.03	0.41
1:B:329:GLY:HA2	1:B:334[A]:VAL:CG1	2.50	0.41
1:B:244:ALA:HA	1:B:275:SER:O	2.21	0.41
1:C:465:GLY:HA2	6:C:694:HOH:O	2.20	0.41
1:A:268:GLN:NE2	1:A:268:GLN:HA	2.35	0.41
1:A:277:VAL:N	6:A:611:HOH:O	2.32	0.41
1:A:438:GLY:HA3	6:A:845:HOH:O	2.21	0.41
1:B:422:ASN:HB3	6:B:757:HOH:O	2.20	0.41
1:D:117:LYS:HA	1:D:459:HIS:O	2.21	0.41
1:D:169:LYS:NZ	1:D:214:ASN:O	2.38	0.41
1:A:216:LYS:O	1:A:239:GLY:HA2	2.20	0.41
1:C:202:GLU:HB2	6:D:804:HOH:O	2.21	0.41
1:D:309:ILE:HG22	1:D:351:ILE:HG22	2.03	0.41
1:A:37:PHE:CG	1:A:132:PHE:CE1	3.09	0.40
1:B:425:SER:HB2	6:B:637:HOH:O	2.20	0.40
1:C:430:LEU:HD23	1:C:444:GLU:HA	2.03	0.40
2:C:501:7Z2:C10	1:D:18:TYR:CE1	3.04	0.40
1:D:168:GLN:HG3	1:D:358:ILE:HD12	2.03	0.40
1:D:400:LYS:NZ	3:D:502:PO4:P	2.94	0.40
1:C:391:THR:CG2	1:C:393:ASP:N	2.80	0.40
1:C:413:VAL:HG11	1:D:252:ALA:HA	2.03	0.40
1:A:92:GLN:HE21	1:A:92:GLN:CA	2.35	0.40
1:C:418:VAL:HG21	1:D:282:ASP:OD2	2.21	0.40
1:D:67:ASN:HA	1:D:71:LYS:HD3	2.03	0.40
1:D:313:ASP:O	1:D:313:ASP:CG	2.65	0.40
1:B:23:TYR:CE1	1:B:97:ASN:HB2	2.56	0.40
1:B:329:GLY:HA2	1:B:334[B]:VAL:CG2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:PHE:CD2	1:C:348:LEU:CD2	3.05	0.40
1:A:332:PHE:CD2	1:A:348:LEU:CD2	3.05	0.40
1:B:333:PRO:O	1:B:345:PRO:HD3	2.21	0.40
1:C:424:ARG:NH2	6:C:653:HOH:O	2.53	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	459/492 (93%)	435 (95%)	23 (5%)	1 (0%)	43	50
1	B	460/492 (94%)	443 (96%)	17 (4%)	0	100	100
1	C	460/492 (94%)	437 (95%)	23 (5%)	0	100	100
1	D	461/492 (94%)	442 (96%)	18 (4%)	1 (0%)	43	50
All	All	1840/1968 (94%)	1757 (96%)	81 (4%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	454	GLY
1	D	481	GLN

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	407/430 (95%)	391 (96%)	16 (4%)	28	37
1	B	408/430 (95%)	386 (95%)	22 (5%)	20	24
1	C	408/430 (95%)	389 (95%)	19 (5%)	23	30
1	D	409/430 (95%)	390 (95%)	19 (5%)	24	31
All	All	1632/1720 (95%)	1556 (95%)	76 (5%)	24	30

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	TYR
1	A	32	LYS
1	A	57	THR
1	A	77	LYS
1	A	102	ASN
1	A	190	LEU
1	A	196	ARG
1	A	234	LYS
1	A	235	ASP
1	A	248	SER
1	A	304	THR
1	A	386	LEU
1	A	391	THR
1	A	393	ASP
1	A	455	GLN
1	A	469	LYS
1	B	18	TYR
1	B	32	LYS
1	B	41	GLU
1	B	102	ASN
1	B	155	SER
1	B	183	LEU
1	B	187	GLU
1	B	190	LEU
1	B	228	LYS
1	B	248	SER
1	B	255	LYS
1	B	265	ILE
1	B	299	ILE
1	B	338	SER
1	B	351	ILE
1	B	386	LEU
1	B	409	LEU

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Mol	Chain	Res	Type
1	B	413	VAL
1	B	434	ARG
1	B	457	LEU
1	B	459	HIS
1	B	475	GLU
1	C	18	TYR
1	C	24	LYS
1	C	77	LYS
1	C	102	ASN
1	C	174	LYS
1	C	190	LEU
1	C	235	ASP
1	C	248	SER
1	C	255	LYS
1	C	299	ILE
1	C	303	SER
1	C	304	THR
1	C	386	LEU
1	C	391	THR
1	C	400	LYS
1	C	451	GLU
1	C	455	GLN
1	C	469	LYS
1	C	470	SER
1	D	18	TYR
1	D	32	LYS
1	D	41	GLU
1	D	77	LYS
1	D	102	ASN
1	D	174	LYS
1	D	177[A]	LEU
1	D	177[B]	LEU
1	D	196	ARG
1	D	219	ASP
1	D	228	LYS
1	D	248	SER
1	D	275	SER
1	D	304	THR
1	D	393	ASP
1	D	413	VAL
1	D	427	LYS
1	D	434	ARG

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Mol	Chain	Res	Type
1	D	445	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	92	GLN
1	A	201	GLN
1	A	268	GLN
1	A	352	GLN
1	A	362	GLN
1	A	433	HIS
1	A	481	GLN
1	B	81	GLN
1	B	129	ASN
1	B	201	GLN
1	B	285	ASN
1	B	352	GLN
1	B	412	ASN
1	B	481	GLN
1	C	154	GLN
1	C	264	HIS
1	C	268	GLN
1	C	285	ASN
1	C	305	GLN
1	C	407	ASN
1	D	129	ASN
1	D	214	ASN
1	D	285	ASN
1	D	422	ASN
1	D	481	GLN
1	D	483	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 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	PO4	D	502	-	4,4,4	0.78	0	6,6,6	0.65	0
3	PO4	B	502	-	4,4,4	1.05	0	6,6,6	0.61	0
2	7Z2	C	501	-	43,45,45	1.90	11 (25%)	51,63,63	2.57	15 (29%)
5	GOL	C	504	-	5,5,5	0.16	0	5,5,5	0.42	0
3	PO4	C	502	-	4,4,4	0.66	0	6,6,6	0.67	0
2	7Z2	D	501	-	43,45,45	1.88	11 (25%)	51,63,63	1.90	14 (27%)
3	PO4	A	502	-	4,4,4	0.88	0	6,6,6	0.67	0
2	7Z2	B	501	-	43,45,45	2.00	10 (23%)	51,63,63	2.83	18 (35%)
5	GOL	C	507	-	5,5,5	0.13	0	5,5,5	0.29	0
5	GOL	A	504	-	5,5,5	0.12	0	5,5,5	0.15	0
2	7Z2	A	501	-	43,45,45	1.90	8 (18%)	51,63,63	1.86	15 (29%)

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
5	GOL	C	504	-	-	4/4/4/4	-
2	7Z2	C	501	-	-	5/21/45/45	0/6/6/6
2	7Z2	D	501	-	-	6/21/45/45	0/6/6/6
2	7Z2	B	501	-	-	8/21/45/45	0/6/6/6
5	GOL	C	507	-	-	2/4/4/4	-
5	GOL	A	504	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	7Z2	A	501	-	-	4/21/45/45	0/6/6/6

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	7Z2	C16-C17	-6.18	1.36	1.47
2	A	501	7Z2	C17-N33	5.63	1.38	1.29
2	D	501	7Z2	N32-N33	-5.00	1.25	1.37
2	B	501	7Z2	N32-N33	-4.92	1.25	1.37
2	A	501	7Z2	C6-C5	4.83	1.56	1.50
2	A	501	7Z2	N32-N33	-4.81	1.25	1.37
2	C	501	7Z2	C17-N33	4.72	1.36	1.29
2	D	501	7Z2	C17-N33	4.57	1.36	1.29
2	C	501	7Z2	N32-N33	-4.55	1.26	1.37
2	C	501	7Z2	C16-C17	-4.44	1.39	1.47
2	B	501	7Z2	C34-N32	4.03	1.52	1.46
2	A	501	7Z2	C13-N12	-3.79	1.34	1.41
2	D	501	7Z2	C16-C17	-3.76	1.40	1.47
2	D	501	7Z2	C6-C5	3.71	1.55	1.50
2	D	501	7Z2	C1-N2	-3.37	1.30	1.36
2	A	501	7Z2	C30-N32	3.25	1.43	1.36
2	B	501	7Z2	C17-N33	3.25	1.34	1.29
2	D	501	7Z2	C3-C4	3.16	1.54	1.50
2	D	501	7Z2	C13-N12	-3.12	1.35	1.41
2	B	501	7Z2	C13-N12	-3.06	1.35	1.41
2	B	501	7Z2	C23-C22	-3.05	1.36	1.41
2	D	501	7Z2	C30-N32	2.98	1.42	1.36
2	A	501	7Z2	C18-C17	2.96	1.58	1.50
2	A	501	7Z2	C16-C17	-2.91	1.42	1.47
2	C	501	7Z2	C6-C5	2.85	1.54	1.50
2	C	501	7Z2	C39-C40	2.83	1.43	1.38
2	D	501	7Z2	C20-C21	-2.79	1.38	1.43
2	B	501	7Z2	C40-C13	2.68	1.43	1.39
2	C	501	7Z2	C22-N26	-2.67	1.33	1.37
2	D	501	7Z2	C34-N32	2.58	1.50	1.46
2	C	501	7Z2	C40-C13	2.53	1.43	1.39
2	C	501	7Z2	C34-N32	2.52	1.50	1.46
2	A	501	7Z2	C3-C4	2.41	1.53	1.50
2	B	501	7Z2	C20-C21	-2.24	1.39	1.43
2	C	501	7Z2	C3-C4	2.24	1.53	1.50
2	C	501	7Z2	C18-C19	-2.22	1.51	1.54
2	C	501	7Z2	C21-C22	-2.18	1.39	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	7Z2	C39-C40	2.17	1.42	1.38
2	D	501	7Z2	C18-C17	2.14	1.55	1.50
2	B	501	7Z2	C24-C23	2.02	1.41	1.36

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	7Z2	C15-C16-C17	-7.81	111.59	120.84
2	B	501	7Z2	C15-C16-C17	-7.78	111.63	120.84
2	B	501	7Z2	C5-C6-N2	-7.46	98.92	102.42
2	C	501	7Z2	C39-C16-C17	7.41	129.61	120.84
2	B	501	7Z2	O11-C1-N2	-7.38	111.38	121.67
2	D	501	7Z2	O11-C1-N2	-6.97	111.95	121.67
2	C	501	7Z2	O11-C1-N2	-5.44	114.08	121.67
2	C	501	7Z2	C9-C10-C4	-5.24	114.67	119.58
2	B	501	7Z2	C39-C16-C17	5.20	127.00	120.84
2	B	501	7Z2	C5-C7-N8	-4.93	118.04	124.58
2	B	501	7Z2	C40-C39-C16	-4.85	115.61	120.80
2	A	501	7Z2	C39-C16-C17	4.81	126.53	120.84
2	C	501	7Z2	C5-C7-N8	-4.61	118.47	124.58
2	C	501	7Z2	C16-C17-N33	4.59	120.28	116.17
2	B	501	7Z2	C34-N32-N33	4.57	121.63	113.90
2	A	501	7Z2	C18-C19-C20	4.24	117.29	111.70
2	B	501	7Z2	C9-N8-C7	4.20	124.20	116.85
2	B	501	7Z2	O31-C30-N32	-4.18	114.54	121.93
2	C	501	7Z2	C34-N32-N33	4.00	120.65	113.90
2	A	501	7Z2	C5-C6-N2	-3.92	100.58	102.42
2	D	501	7Z2	N12-C1-N2	3.53	120.05	115.91
2	D	501	7Z2	C15-C16-C17	-3.52	116.67	120.84
2	C	501	7Z2	C40-C39-C16	-3.40	117.17	120.80
2	B	501	7Z2	C39-C40-C13	3.38	124.19	120.30
2	D	501	7Z2	C9-N8-C7	3.36	122.74	116.85
2	B	501	7Z2	C9-C10-C4	-3.32	116.47	119.58
2	B	501	7Z2	O11-C1-N12	3.25	130.60	123.46
2	C	501	7Z2	C39-C40-C13	3.21	124.00	120.30
2	B	501	7Z2	C18-C19-C20	3.17	115.88	111.70
2	C	501	7Z2	C14-C15-C16	3.09	124.10	120.80
2	D	501	7Z2	C16-C17-N33	3.05	118.90	116.17
2	D	501	7Z2	C39-C16-C17	3.05	124.45	120.84
2	C	501	7Z2	C27-N26-C22	3.04	121.53	116.93
2	A	501	7Z2	C15-C16-C17	-3.03	117.26	120.84
2	A	501	7Z2	C35-C34-N32	-3.02	106.35	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	7Z2	C4-C3-N2	-3.02	101.00	102.42
2	A	501	7Z2	C16-C17-N33	2.84	118.71	116.17
2	A	501	7Z2	O11-C1-N2	-2.83	117.73	121.67
2	A	501	7Z2	C10-C9-N8	-2.78	118.86	123.60
2	D	501	7Z2	C18-C17-N33	-2.73	117.84	122.86
2	C	501	7Z2	C21-C22-N26	-2.64	120.02	122.82
2	B	501	7Z2	C29-C21-C20	-2.61	120.20	123.37
2	D	501	7Z2	C27-N26-C22	2.60	120.87	116.93
2	A	501	7Z2	C34-N32-N33	2.56	118.22	113.90
2	D	501	7Z2	C20-C21-C22	2.52	120.63	117.47
2	A	501	7Z2	C18-C17-N33	-2.48	118.29	122.86
2	D	501	7Z2	C5-C7-N8	-2.47	121.30	124.58
2	A	501	7Z2	C27-N26-C22	2.43	120.61	116.93
2	D	501	7Z2	C10-C9-N8	-2.43	119.46	123.60
2	D	501	7Z2	C28-C27-N26	-2.42	120.42	123.97
2	A	501	7Z2	C6-C5-C7	2.35	134.24	128.43
2	A	501	7Z2	C9-N8-C7	2.32	120.92	116.85
2	B	501	7Z2	C20-C21-C22	2.31	120.37	117.47
2	C	501	7Z2	C18-C17-N33	-2.30	118.63	122.86
2	D	501	7Z2	C28-C29-C21	-2.29	117.82	120.91
2	B	501	7Z2	C35-C34-N32	2.14	116.37	112.21
2	A	501	7Z2	C40-C39-C16	2.12	123.07	120.80
2	C	501	7Z2	C13-N12-C1	2.12	130.32	126.04
2	B	501	7Z2	C27-N26-C22	2.10	120.10	116.93
2	C	501	7Z2	O11-C1-N12	2.07	128.00	123.46
2	D	501	7Z2	O11-C1-N12	2.03	127.92	123.46
2	A	501	7Z2	C39-C16-C15	-2.02	115.99	118.57

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	7Z2	C35-C34-N32-N33
2	B	501	7Z2	C35-C34-N32-C30
2	D	501	7Z2	C30-C19-C20-C21
5	C	504	GOL	C1-C2-C3-O3
5	C	507	GOL	C1-C2-C3-O3
2	B	501	7Z2	C34-C35-C36-C37
2	A	501	7Z2	N32-C34-C35-C36
2	D	501	7Z2	N32-C34-C35-C36
2	B	501	7Z2	N32-C34-C35-C36
5	C	504	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	D	501	7Z2	C34-C35-C36-C37
5	C	504	GOL	O2-C2-C3-O3
5	C	507	GOL	O2-C2-C3-O3
2	C	501	7Z2	N32-C34-C35-C36
2	A	501	7Z2	C30-C19-C20-C25
2	B	501	7Z2	C30-C19-C20-C25
2	C	501	7Z2	C30-C19-C20-C25
2	D	501	7Z2	C30-C19-C20-C25
2	A	501	7Z2	C30-C19-C20-C21
2	B	501	7Z2	C30-C19-C20-C21
2	C	501	7Z2	C30-C19-C20-C21
5	C	504	GOL	O1-C1-C2-O2
2	B	501	7Z2	C15-C16-C17-N33
2	D	501	7Z2	C35-C34-N32-N33
2	B	501	7Z2	C35-C36-C37-N38
2	A	501	7Z2	C35-C34-N32-C30
2	C	501	7Z2	C34-C35-C36-C37
2	C	501	7Z2	C15-C16-C17-N33
2	D	501	7Z2	C15-C16-C17-N33

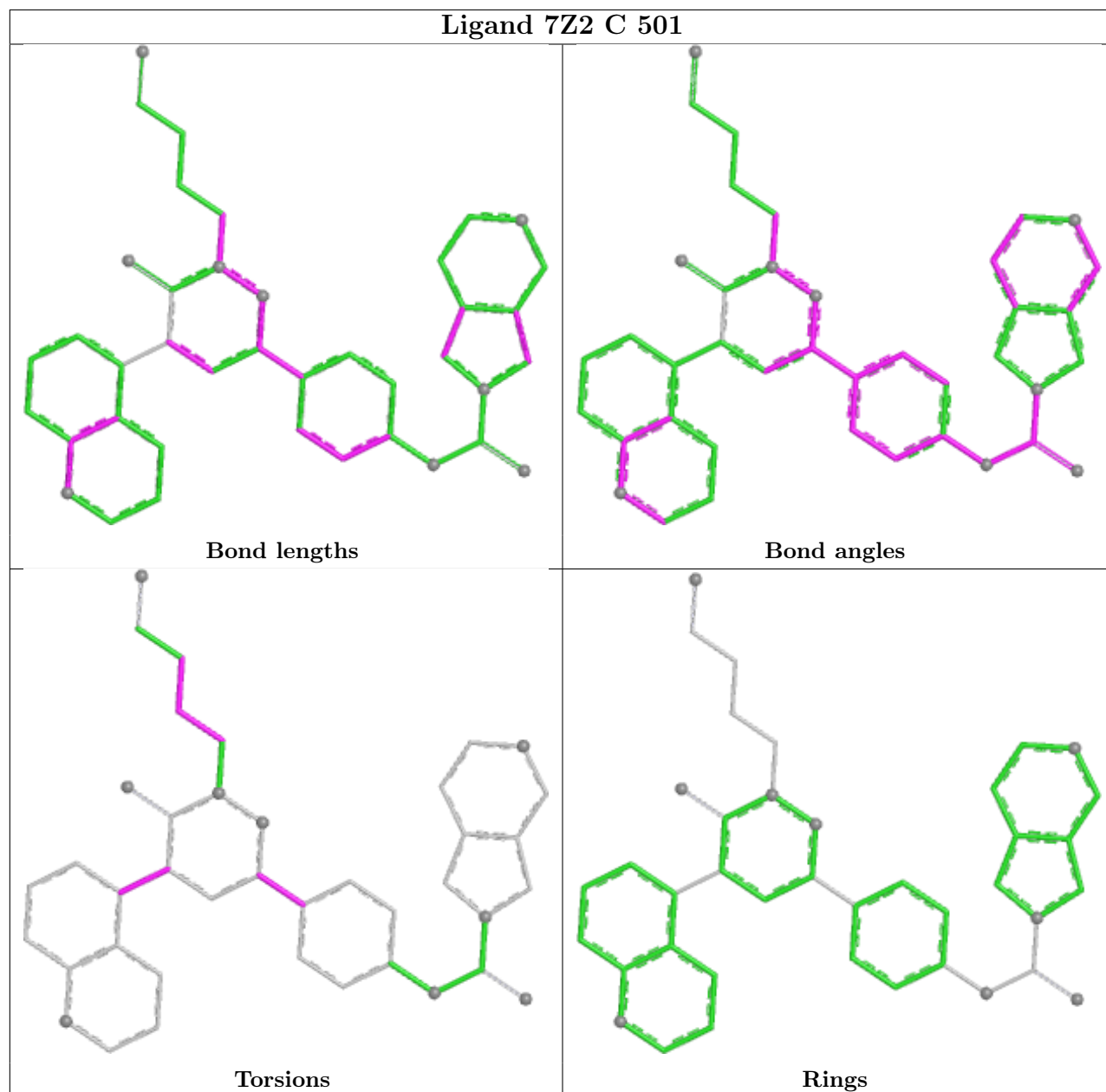
There are no ring outliers.

8 monomers are involved in 28 short contacts:

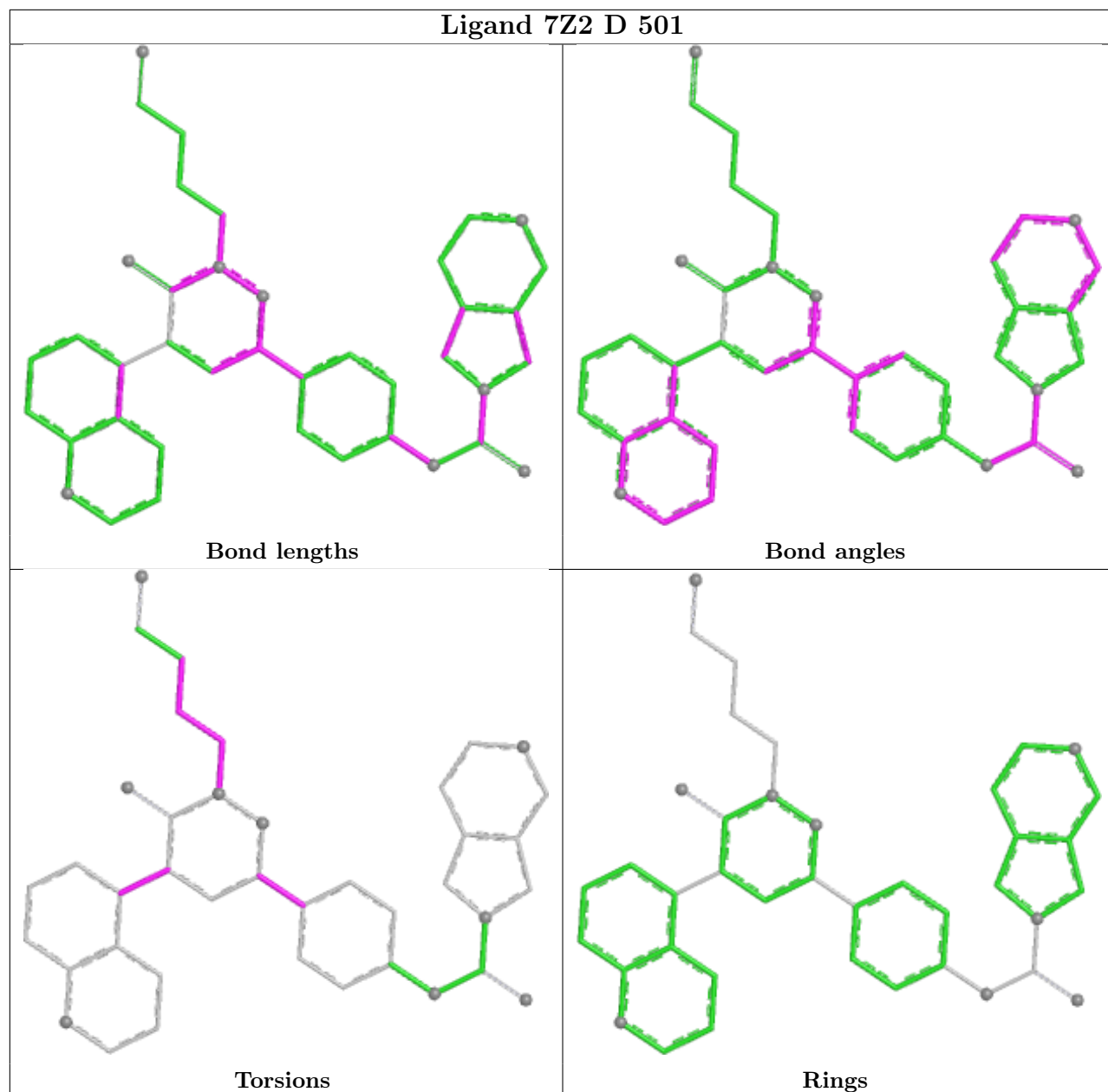
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	PO4	5	0
3	B	502	PO4	2	0
2	C	501	7Z2	5	0
3	C	502	PO4	1	0
2	D	501	7Z2	4	0
2	B	501	7Z2	5	0
5	C	507	GOL	2	0
2	A	501	7Z2	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

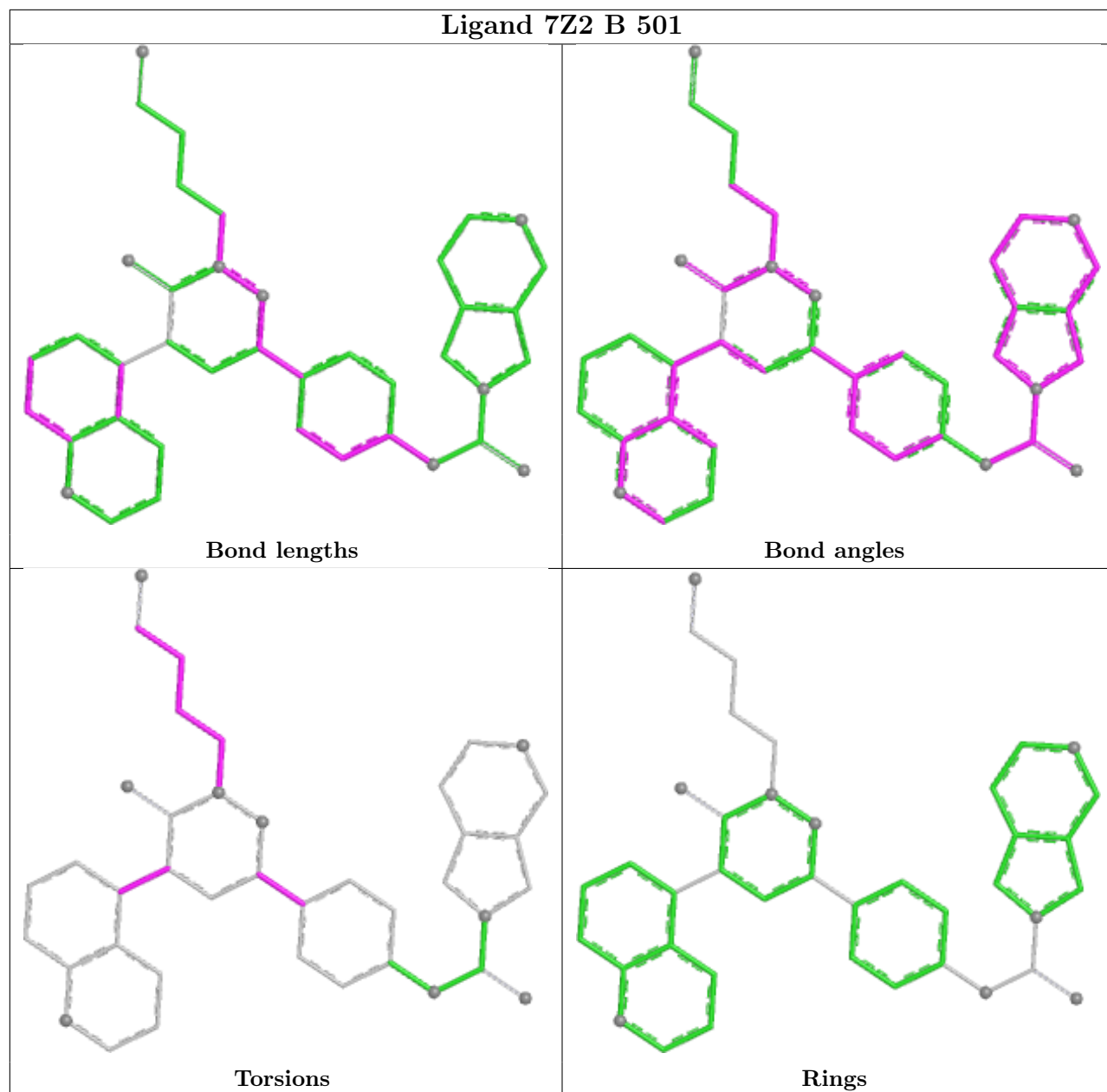
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

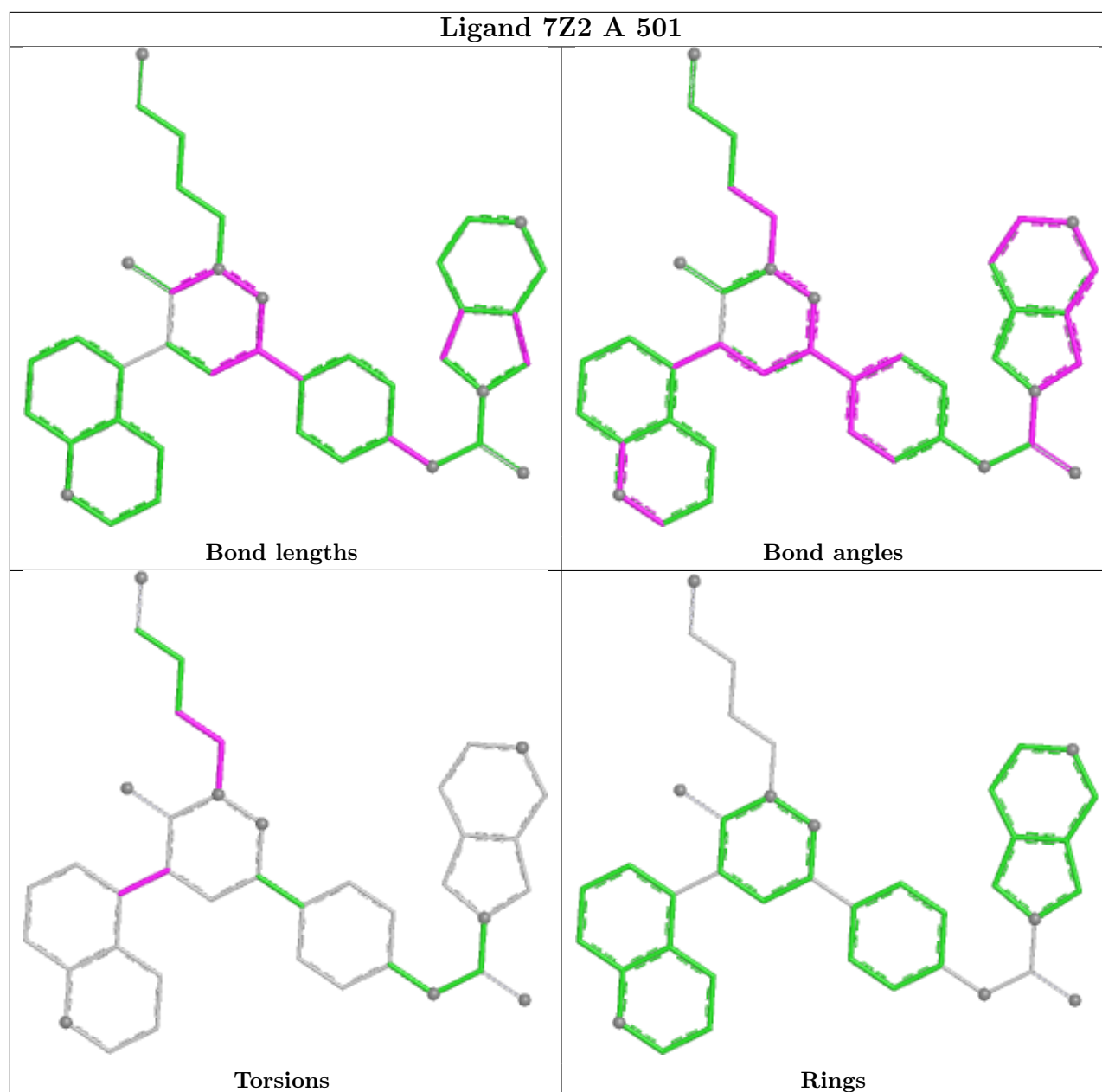


Ligand 7Z2 D 501



Ligand 7Z2 B 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	463/492 (94%)	0.84	32 (6%) 23 27	8, 19, 34, 56	0
1	B	463/492 (94%)	0.80	25 (5%) 31 37	8, 19, 35, 50	1 (0%)
1	C	464/492 (94%)	0.67	14 (3%) 52 59	8, 17, 33, 56	0
1	D	463/492 (94%)	0.61	12 (2%) 57 63	6, 16, 33, 47	2 (0%)
All	All	1853/1968 (94%)	0.73	83 (4%) 38 44	6, 18, 34, 56	3 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	GLY	4.9
1	D	75	VAL	4.9
1	C	454	GLY	4.6
1	B	185	GLY	4.2
1	B	29	ASN	4.1
1	A	480	ALA	3.8
1	B	384	GLY	3.6
1	B	230	TYR	3.6
1	B	409	LEU	3.6
1	C	393	ASP	3.2
1	C	236	PRO	3.2
1	C	205	GLY	3.2
1	A	95	VAL	3.1
1	A	379	ALA	3.1
1	A	102	ASN	3.1
1	A	462	PHE	3.0
1	B	360	THR	3.0
1	A	70	LEU	2.9
1	A	250	ILE	2.9
1	C	343	LEU	2.8
1	B	304	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	383	GLY	2.7
1	C	437	ALA	2.6
1	A	397	CYS	2.6
1	A	185	GLY	2.6
1	A	74	VAL	2.6
1	A	23	TYR	2.6
1	A	147	TRP	2.5
1	C	360	THR	2.5
1	B	406	THR	2.4
1	A	261	ALA	2.4
1	A	183	LEU	2.4
1	D	394	LEU	2.4
1	A	244	ALA	2.4
1	B	236	PRO	2.4
1	A	96	PHE	2.4
1	C	462	PHE	2.4
1	C	482	LEU	2.4
1	B	64	TYR	2.3
1	A	353	GLY	2.3
1	B	110	GLY	2.3
1	D	181	GLY	2.3
1	A	186	LEU	2.3
1	A	226	LEU	2.3
1	B	142	TYR	2.3
1	D	453	TYR	2.3
1	D	104	ILE	2.3
1	D	250	ILE	2.3
1	B	92	GLN	2.3
1	B	266	VAL	2.3
1	B	382	SER	2.3
1	B	104	ILE	2.3
1	A	236	PRO	2.3
1	A	453	TYR	2.3
1	D	23	TYR	2.3
1	A	101	TRP	2.3
1	A	350	VAL	2.2
1	D	379	ALA	2.2
1	C	299	ILE	2.2
1	B	107	LYS	2.2
1	A	343	LEU	2.2
1	D	20	VAL	2.2
1	B	161	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	467	VAL	2.1
1	B	483	ASN	2.1
1	A	438	GLY	2.1
1	C	271	SER	2.1
1	B	177	LEU	2.1
1	A	82	GLU	2.1
1	D	305	GLN	2.1
1	A	348	LEU	2.1
1	A	351	ILE	2.1
1	B	345	PRO	2.1
1	C	272	VAL	2.1
1	A	242	VAL	2.1
1	A	367	GLY	2.1
1	A	446	GLY	2.1
1	C	217	GLY	2.1
1	D	357	ASP	2.0
1	B	125	ILE	2.0
1	D	351	ILE	2.0
1	B	330	LYS	2.0
1	C	190	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
5	GOL	C	507	6/6	0.70	0.17	24,36,41,43	0
2	7Z2	D	501	40/40	0.84	0.15	12,22,38,45	0
2	7Z2	B	501	40/40	0.85	0.14	6,13,34,41	0

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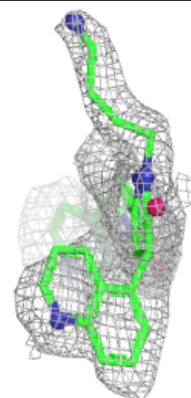
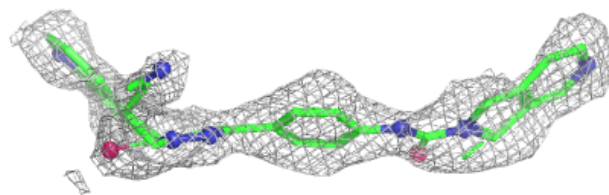
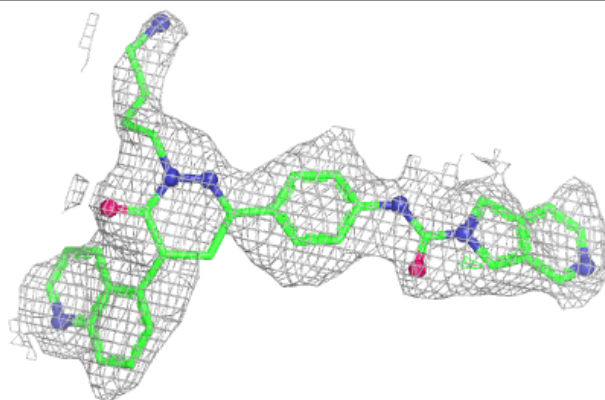
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	7Z2	A	501	40/40	0.86	0.14	8,26,40,50	0
5	GOL	A	504	6/6	0.88	0.11	21,23,24,24	0
2	7Z2	C	501	40/40	0.88	0.11	8,13,19,21	0
5	GOL	C	504	6/6	0.89	0.11	18,24,29,31	0
3	PO4	D	502	5/5	0.91	0.10	21,25,36,41	0
4	CL	A	506	1/1	0.93	0.08	31,31,31,31	0
3	PO4	C	502	5/5	0.93	0.10	17,18,21,27	0
4	CL	A	503	1/1	0.94	0.12	23,23,23,23	0
3	PO4	A	502	5/5	0.94	0.13	20,22,24,25	0
4	CL	C	503	1/1	0.94	0.13	31,31,31,31	0
4	CL	C	506	1/1	0.98	0.08	22,22,22,22	0
3	PO4	B	502	5/5	0.98	0.07	13,17,24,26	0
4	CL	B	503	1/1	0.98	0.09	29,29,29,29	0
4	CL	A	505	1/1	0.98	0.03	22,22,22,22	0
4	CL	C	505	1/1	0.99	0.04	18,18,18,18	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.

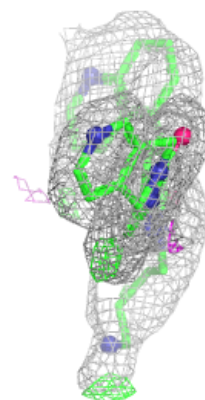
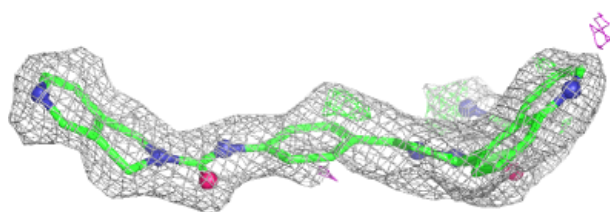
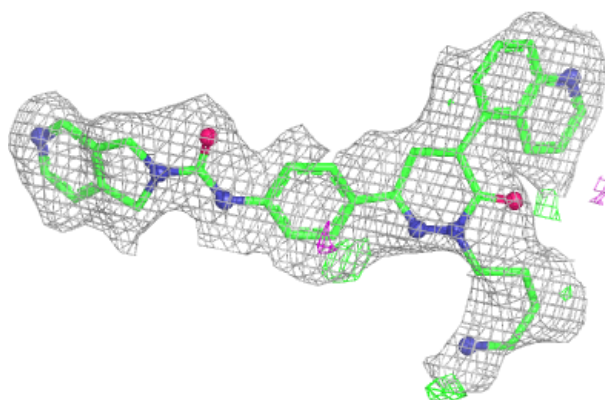
Electron density around 7Z2 D 501:

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

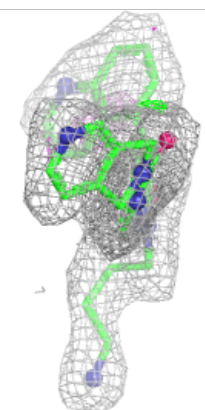
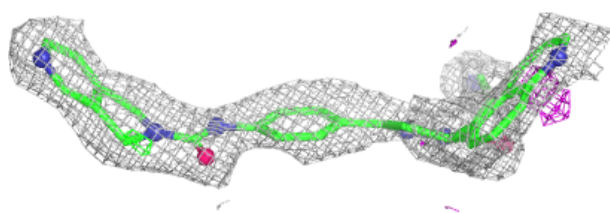
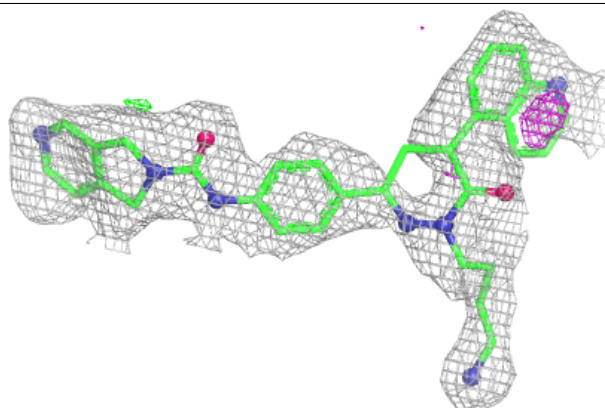


Electron density around 7Z2 B 501:

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

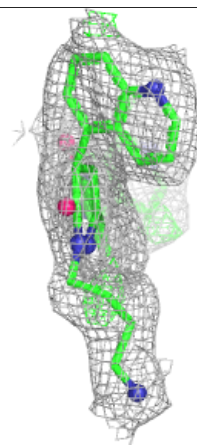
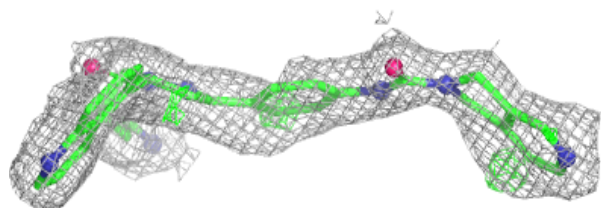
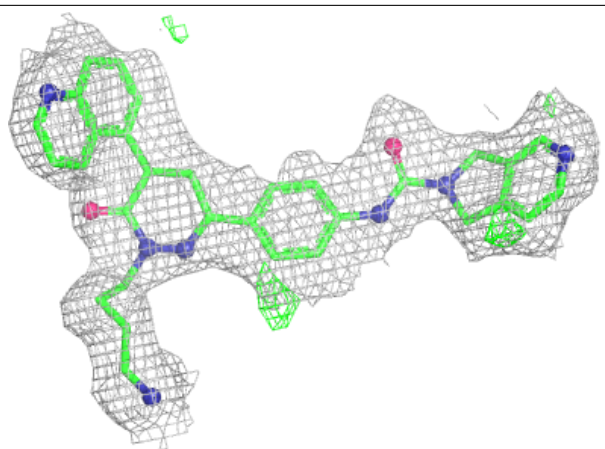
**Electron density around 7Z2 A 501:**

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



Electron density around 7Z2 C 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.