



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:52 PM UTC

PDB ID : 2P9E / pdb_00002p9e
Title : Crystal Structure of G336V mutant of E.coli phosphoglycerate dehydrogenase
Authors : Dey, S.; Sacchettini, J.C.
Deposited on : 2007-03-25
Resolution : 2.60 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

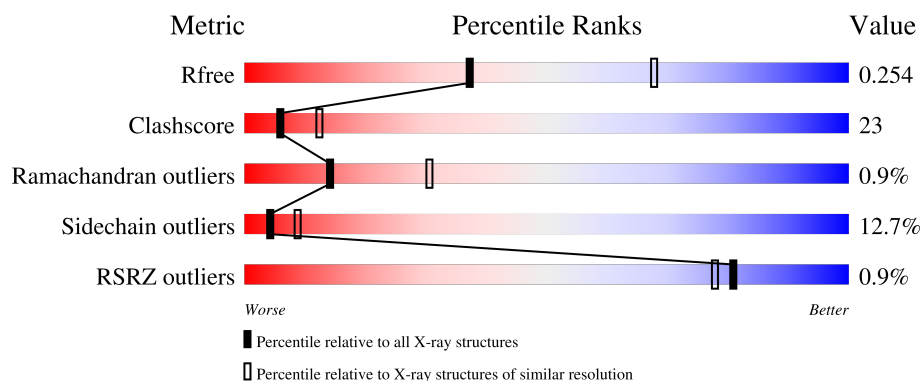
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	410	
1	B	410	
1	C	410	
1	D	410	

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
2	PO4	B	499	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12648 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.

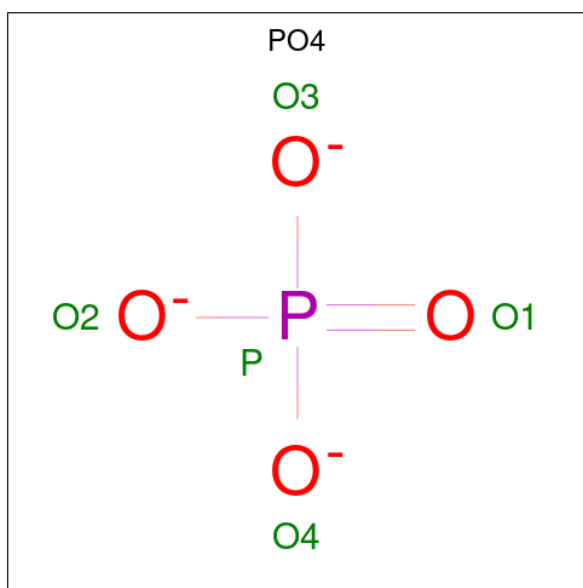
- Molecule 1 is a protein called D-3-phosphoglycerate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3076	1950	534	584	8			
1	B	404	Total	C	N	O	S	0	0	0
			3062	1941	532	581	8			
1	C	406	Total	C	N	O	S	0	0	0
			3076	1950	534	584	8			
1	D	403	Total	C	N	O	S	0	0	0
			3053	1936	531	578	8			

There are 20 discrepancies between the modelled and reference sequences:

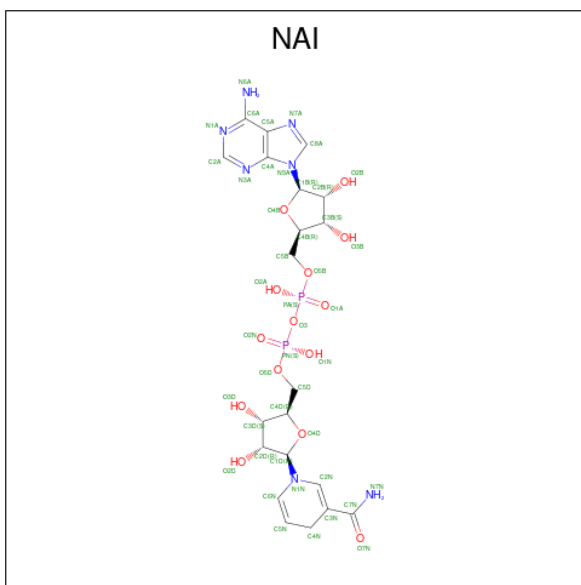
Chain	Residue	Modelled	Actual	Comment	Reference
A	81	ALA	CYS	engineered mutation	UNP P0A9T0
A	83	ALA	CYS	engineered mutation	UNP P0A9T0
A	250	ALA	CYS	engineered mutation	UNP P0A9T0
A	282	ALA	CYS	engineered mutation	UNP P0A9T0
A	336	VAL	GLY	engineered mutation	UNP P0A9T0
B	81	ALA	CYS	engineered mutation	UNP P0A9T0
B	83	ALA	CYS	engineered mutation	UNP P0A9T0
B	250	ALA	CYS	engineered mutation	UNP P0A9T0
B	282	ALA	CYS	engineered mutation	UNP P0A9T0
B	336	VAL	GLY	engineered mutation	UNP P0A9T0
C	81	ALA	CYS	engineered mutation	UNP P0A9T0
C	83	ALA	CYS	engineered mutation	UNP P0A9T0
C	250	ALA	CYS	engineered mutation	UNP P0A9T0
C	282	ALA	CYS	engineered mutation	UNP P0A9T0
C	336	VAL	GLY	engineered mutation	UNP P0A9T0
D	81	ALA	CYS	engineered mutation	UNP P0A9T0
D	83	ALA	CYS	engineered mutation	UNP P0A9T0
D	250	ALA	CYS	engineered mutation	UNP P0A9T0
D	282	ALA	CYS	engineered mutation	UNP P0A9T0
D	336	VAL	GLY	engineered mutation	UNP P0A9T0

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



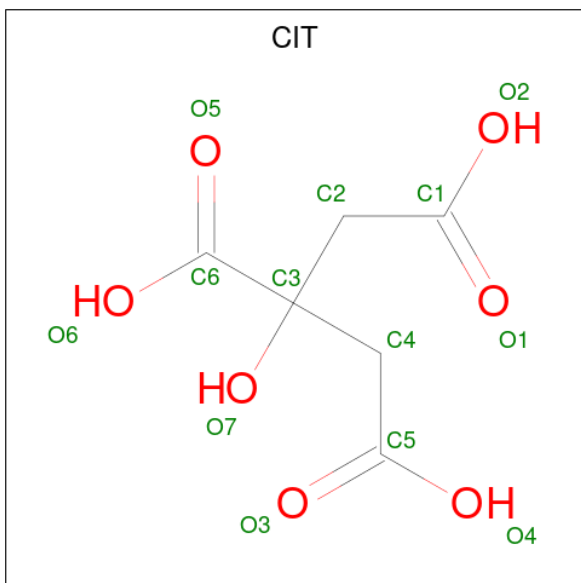
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



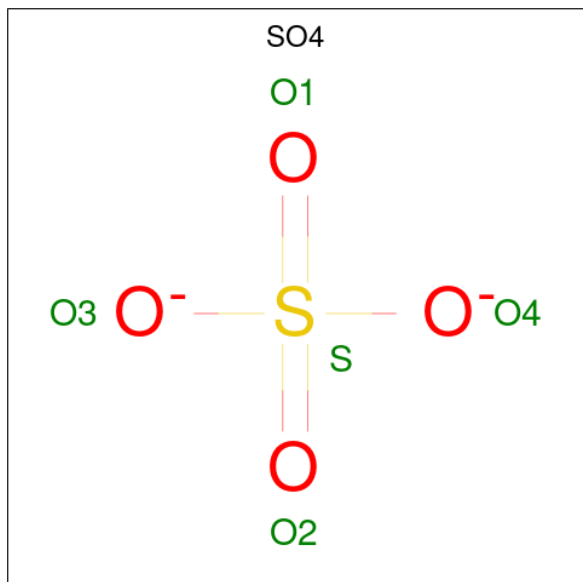
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	D	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $\text{C}_6\text{H}_8\text{O}_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0
4	A	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0
4	C	1	Total C O 13 6 7	0	0
4	C	1	Total C O 13 6 7	0	0
4	D	1	Total C O 13 6 7	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	24	Total O 24 24	0	0
6	B	16	Total O 16 16	0	0
6	C	15	Total O 15 15	0	0

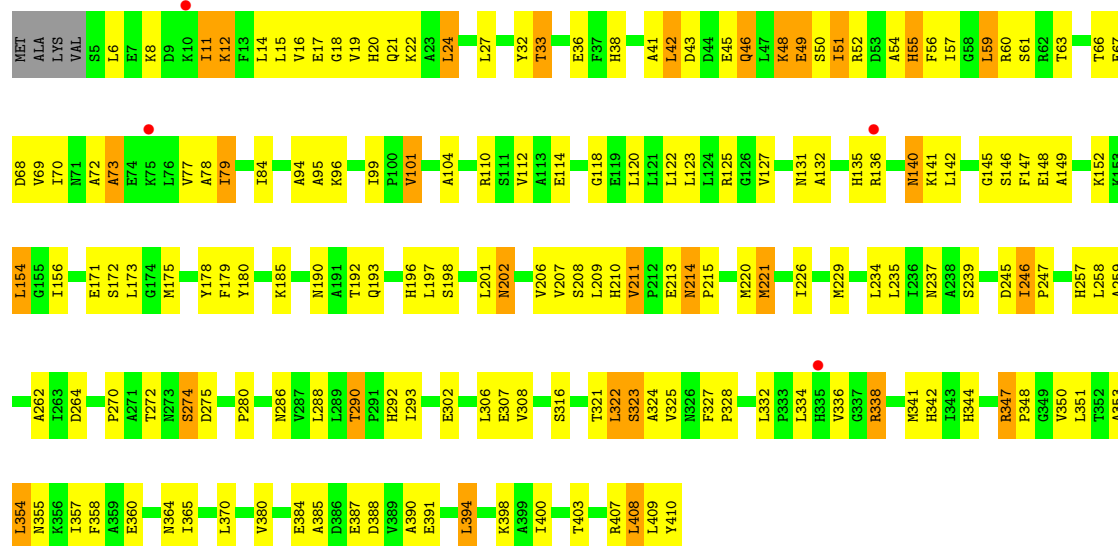
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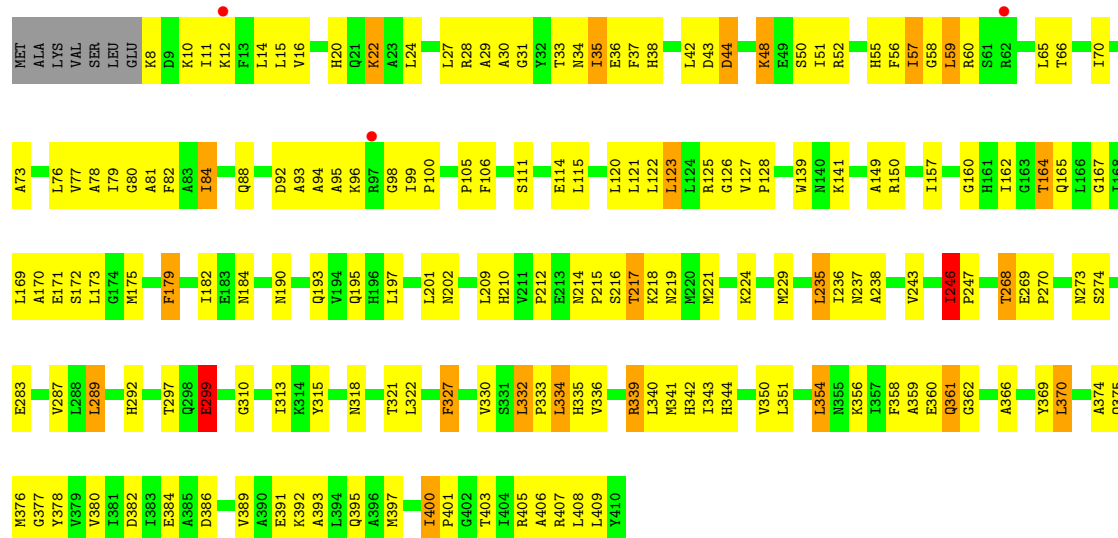
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	27	Total	O	0	0
			27	27		



• Molecule 1: D-3-phosphoglycerate dehydrogenase



• Molecule 1: D-3-phosphoglycerate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	76.24Å 76.24Å 353.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.60 35.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.00-2.60) 99.5 (35.00-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.279 (Not available) , 0.254	Depositor DCC
R_{free} test set	3107 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.215 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12648	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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: CIT, NAI, PO4, 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	1.02	1/3129 (0.0%)	1.24	20/4241 (0.5%)
1	B	1.03	3/3115 (0.1%)	1.23	18/4222 (0.4%)
1	C	1.01	2/3129 (0.1%)	1.28	19/4241 (0.4%)
1	D	1.04	3/3106 (0.1%)	1.25	21/4210 (0.5%)
All	All	1.03	9/12479 (0.1%)	1.25	78/16914 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	101	VAL	CA-CB	-7.73	1.45	1.54
1	D	81	ALA	CA-CB	-7.41	1.43	1.53
1	C	79	ILE	CA-CB	-7.04	1.45	1.54
1	B	308	VAL	CA-CB	-6.57	1.45	1.54
1	D	246	ILE	CA-CB	6.42	1.57	1.54
1	B	309	ALA	CA-CB	-5.49	1.44	1.53
1	A	19	VAL	CA-CB	5.42	1.60	1.54
1	D	182	ILE	CA-CB	-5.05	1.48	1.54
1	B	185	LYS	CE-NZ	5.01	1.64	1.49

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	347	ARG	CA-C-N	-10.29	108.92	119.93
1	C	347	ARG	C-N-CA	-10.29	108.92	119.93
1	C	48	LYS	N-CA-C	-9.50	100.90	111.07
1	A	186	LEU	CA-C-N	8.37	128.43	119.89
1	A	186	LEU	C-N-CA	8.37	128.43	119.89
1	D	332	LEU	CA-C-N	-7.68	111.51	120.11
1	D	332	LEU	C-N-CA	-7.68	111.51	120.11
1	D	123	LEU	N-CA-C	-7.43	103.26	111.36
1	D	374	ALA	N-CA-C	-7.42	102.56	111.69
1	D	216	SER	N-CA-C	-7.39	103.52	112.54
1	B	211	VAL	CA-C-N	7.26	127.42	120.31
1	B	211	VAL	C-N-CA	7.26	127.42	120.31
1	B	347	ARG	CA-C-N	-7.22	113.23	120.31
1	B	347	ARG	C-N-CA	-7.22	113.23	120.31
1	C	112	VAL	N-CA-C	7.16	117.26	110.53
1	A	177	VAL	N-CA-C	7.08	118.08	108.17
1	A	269	GLU	CA-C-N	7.01	126.98	119.76
1	A	269	GLU	C-N-CA	7.01	126.98	119.76
1	B	177	VAL	N-CA-C	7.00	117.73	107.37
1	C	350	VAL	N-CA-C	6.62	117.32	110.36
1	A	309	ALA	N-CA-C	-6.61	104.00	111.14
1	C	207	VAL	CB-CA-C	-6.59	101.42	110.77
1	D	321	THR	N-CA-C	-6.55	103.89	112.41
1	C	308	VAL	N-CA-C	6.53	117.31	110.72
1	C	69	VAL	CB-CA-C	-6.43	103.62	112.04
1	D	35	ILE	N-CA-C	6.31	117.32	107.28
1	A	17	GLU	N-CA-C	6.28	120.72	113.38
1	B	312	LEU	N-CA-C	-6.25	104.40	111.14
1	C	408	LEU	N-CA-C	-6.22	99.02	108.67
1	B	179	PHE	N-CA-C	6.20	118.72	108.99
1	C	246	ILE	CB-CA-C	-6.08	107.90	114.35
1	B	16	VAL	N-CA-C	5.93	117.71	109.29
1	B	162	ILE	N-CA-C	5.91	116.94	111.45
1	C	280	PRO	N-CA-C	-5.79	106.90	114.03
1	D	299	GLU	N-CA-CB	5.79	118.73	110.16
1	B	99	ILE	CA-C-N	-5.77	114.66	120.31
1	B	99	ILE	C-N-CA	-5.77	114.66	120.31
1	D	179	PHE	N-CA-C	5.74	118.00	108.99
1	A	99	ILE	CA-C-N	-5.73	114.07	120.14
1	A	99	ILE	C-N-CA	-5.73	114.07	120.14
1	C	6	LEU	N-CA-C	-5.70	105.05	112.23
1	C	11	ILE	N-CA-C	5.68	115.51	106.88
1	D	361	GLN	N-CA-C	-5.63	106.45	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	ASN	N-CA-C	5.60	117.82	108.02
1	A	302	GLU	N-CA-C	-5.58	105.27	111.36
1	A	385	ALA	N-CA-C	5.56	116.68	107.73
1	D	400	ILE	CA-C-N	-5.53	114.01	119.93
1	D	400	ILE	C-N-CA	-5.53	114.01	119.93
1	A	179	PHE	N-CA-C	5.48	117.40	109.07
1	B	393	ALA	N-CA-C	-5.46	105.23	111.07
1	C	118	GLY	N-CA-C	-5.43	106.20	112.50
1	D	238	ALA	N-CA-C	-5.42	105.37	112.41
1	D	214	ASN	CA-C-N	-5.41	114.05	119.56
1	D	214	ASN	C-N-CA	-5.41	114.05	119.56
1	D	33	THR	N-CA-C	5.40	120.14	113.50
1	D	162	ILE	N-CA-C	5.39	116.17	110.72
1	A	315	TYR	N-CA-C	-5.38	105.49	111.36
1	B	293	ILE	N-CA-C	-5.36	106.20	111.88
1	A	296	SER	N-CA-C	5.29	117.81	109.39
1	C	201	LEU	N-CA-C	-5.28	106.10	112.54
1	A	226	ILE	N-CA-C	-5.28	104.45	111.05
1	D	35	ILE	CB-CA-C	-5.24	104.18	110.99
1	B	230	LYS	CA-C-N	-5.23	114.37	119.76
1	B	230	LYS	C-N-CA	-5.23	114.37	119.76
1	C	211	VAL	CA-C-N	-5.18	115.44	120.98
1	C	211	VAL	C-N-CA	-5.18	115.44	120.98
1	D	79	ILE	N-CA-C	5.18	115.42	108.17
1	A	238	ALA	N-CA-C	-5.15	104.45	111.56
1	A	378	TYR	CA-C-N	-5.14	115.30	122.71
1	A	378	TYR	C-N-CA	-5.14	115.30	122.71
1	B	84	ILE	CB-CA-C	-5.12	105.22	111.92
1	D	44	ASP	N-CA-C	5.11	121.68	110.80
1	B	204	SER	N-CA-C	5.11	117.94	109.46
1	C	140	ASN	N-CA-C	5.09	116.89	108.49
1	A	160	GLY	N-CA-C	-5.06	105.35	112.13
1	A	37	PHE	N-CA-C	5.05	116.99	108.96
1	C	385	ALA	N-CA-C	5.02	115.82	107.73
1	D	126	GLY	N-CA-C	-5.01	107.19	114.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	334	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3076	0	3122	147	0
1	B	3062	0	3106	151	0
1	C	3076	0	3122	149	0
1	D	3053	0	3100	138	0
2	A	10	0	0	0	0
2	B	10	0	0	3	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	44	0	27	2	0
3	B	44	0	27	4	0
3	C	44	0	27	0	0
3	D	44	0	27	1	0
4	A	26	0	10	7	0
4	B	13	0	5	4	0
4	C	26	0	10	6	0
4	D	13	0	5	4	0
5	C	5	0	0	1	0
6	A	24	0	0	4	0
6	B	16	0	0	0	0
6	C	15	0	0	1	0
6	D	27	0	0	2	0
All	All	12648	0	12588	575	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 23.

All (575) 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:D:268:THR:HB	6:D:590:HOH:O	1.39	1.17
1:C:342:HIS:CD2	1:C:344:HIS:HD2	1.63	1.16
1:B:196:HIS:HB3	2:B:499:PO4:O4	1.52	1.09
1:C:229:MET:HE1	1:C:235:LEU:HD13	1.08	1.07
1:B:214:ASN:HB2	1:B:215:PRO:HD3	1.42	1.01
1:A:62:ARG:HH21	1:A:272:THR:HB	1.25	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:HH11	1:B:62:ARG:CG	1.76	0.99
1:B:62:ARG:HH11	1:B:62:ARG:HG3	0.84	0.98
1:B:62:ARG:HG3	1:B:62:ARG:NH1	1.64	0.98
1:B:342:HIS:ND1	1:B:344:HIS:HD2	1.62	0.97
1:C:20:HIS:HD2	1:C:22:LYS:H	1.10	0.96
1:B:88:GLN:N	1:B:88:GLN:HE21	1.64	0.95
1:C:342:HIS:CD2	1:C:344:HIS:CD2	2.55	0.94
1:C:342:HIS:HD2	1:C:344:HIS:HD2	1.09	0.93
1:D:229:MET:HE1	1:D:235:LEU:HG	1.50	0.93
1:A:59:LEU:HD23	1:A:59:LEU:H	1.31	0.92
1:B:161:HIS:HD2	3:B:509:NAI:O2A	1.52	0.92
1:B:214:ASN:HB2	1:B:215:PRO:CD	1.99	0.92
1:A:342:HIS:HD2	1:A:344:HIS:HD2	1.06	0.91
1:C:229:MET:HE1	1:C:235:LEU:CD1	1.99	0.91
1:A:94:ALA:HB1	1:A:99:ILE:HB	1.53	0.90
1:B:88:GLN:HE21	1:B:88:GLN:H	0.98	0.90
1:C:322:LEU:O	1:C:323:SER:HB3	1.72	0.89
1:B:340:LEU:HD13	1:B:397:MET:HE1	1.54	0.88
1:B:88:GLN:H	1:B:88:GLN:NE2	1.71	0.88
1:A:335:HIS:HB3	6:A:571:HOH:O	1.74	0.87
1:B:180:TYR:CD1	1:B:197:LEU:HD13	2.09	0.87
1:B:409:LEU:O	1:B:410:TYR:HB3	1.74	0.86
1:A:11:ILE:HG23	1:A:55:HIS:CG	2.10	0.86
1:B:42:LEU:HB3	1:B:46:GLN:HG3	1.57	0.86
1:D:12:LYS:H	1:D:55:HIS:HD2	1.20	0.85
1:A:141:LYS:O	1:A:141:LYS:HG3	1.79	0.82
1:A:342:HIS:HD2	1:A:344:HIS:CD2	1.94	0.82
1:A:125:ARG:HB2	1:A:127:VAL:HG23	1.62	0.82
1:A:150:ARG:CG	1:A:150:ARG:HH11	1.93	0.82
1:C:342:HIS:HD2	1:C:344:HIS:CD2	1.94	0.82
1:B:342:HIS:ND1	1:B:344:HIS:CD2	2.46	0.82
1:A:62:ARG:NH2	1:A:272:THR:HB	1.93	0.81
1:C:221:MET:HE1	1:C:229:MET:HE3	1.61	0.81
1:C:20:HIS:CD2	1:C:22:LYS:H	1.97	0.81
1:B:332:LEU:HB3	1:B:339:ARG:NH2	1.95	0.80
1:C:78:ALA:HA	1:C:99:ILE:HG23	1.64	0.80
1:B:83:ALA:HB1	4:B:516:CIT:H41	1.64	0.79
4:C:517:CIT:C6	4:C:517:CIT:O3	2.25	0.79
1:D:212:PRO:O	1:D:217:THR:HG21	1.82	0.79
1:D:339:ARG:HD2	1:D:380:VAL:CG1	2.13	0.79
1:A:332:LEU:CD1	1:A:369:TYR:HB2	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ILE:HD13	1:C:73:ALA:HB2	1.64	0.78
1:A:150:ARG:HG3	1:A:150:ARG:NH1	1.99	0.78
1:A:11:ILE:HG22	1:A:55:HIS:HB2	1.67	0.77
1:B:291:PRO:HD2	1:B:293:ILE:HD13	1.66	0.77
1:D:339:ARG:HD3	1:D:382:ASP:OD1	1.83	0.77
1:A:150:ARG:HH11	1:A:150:ARG:HG3	1.48	0.77
1:A:342:HIS:CD2	1:A:344:HIS:HD2	1.97	0.77
1:D:160:GLY:O	1:D:164:THR:HB	1.84	0.76
1:B:201:LEU:HD23	1:B:225:GLU:O	1.86	0.76
1:A:291:PRO:HD2	1:A:293:ILE:HG12	1.66	0.76
1:C:45:GLU:O	1:C:49:GLU:HB2	1.86	0.76
1:C:11:ILE:HG23	1:C:55:HIS:CD2	2.20	0.75
1:C:229:MET:CE	1:C:235:LEU:HD13	2.03	0.75
1:A:332:LEU:HD13	1:A:369:TYR:HB2	1.67	0.75
1:B:196:HIS:CB	2:B:499:PO4:O4	2.31	0.75
1:A:38:HIS:CD2	1:A:42:LEU:HD21	2.21	0.74
1:B:212:PRO:O	1:B:217:THR:HG21	1.87	0.74
1:C:38:HIS:HD2	1:C:42:LEU:HD21	1.52	0.74
1:C:322:LEU:O	1:C:323:SER:CB	2.33	0.74
1:B:248:ALA:O	1:B:251:ASP:HB2	1.88	0.74
1:B:85:GLY:N	4:B:516:CIT:O4	2.21	0.74
1:C:123:LEU:HB3	1:C:234:LEU:HD13	1.70	0.74
1:A:213:GLU:HB2	1:A:240:ARG:HD2	1.70	0.73
1:C:8:LYS:HA	1:C:11:ILE:HD12	1.69	0.73
1:B:156:ILE:HG12	1:B:166:LEU:HD23	1.71	0.73
1:C:226:ILE:O	1:C:229:MET:HB2	1.88	0.73
1:D:57:ILE:HG21	1:D:65:LEU:HD11	1.71	0.73
1:B:201:LEU:CD2	1:B:225:GLU:O	2.37	0.72
1:A:209:LEU:C	1:A:210:HIS:CD2	2.68	0.72
1:A:36:GLU:OE2	1:A:50:SER:HB2	1.90	0.72
4:A:514:CIT:C6	4:A:514:CIT:O3	2.37	0.72
1:D:179:PHE:CZ	1:D:193:GLN:HB2	2.25	0.71
1:C:21:GLN:O	1:C:24:LEU:N	2.23	0.71
1:D:125:ARG:HB2	1:D:127:VAL:HG23	1.71	0.71
1:B:340:LEU:HD13	1:B:397:MET:CE	2.21	0.70
1:A:388:ASP:OD1	1:A:389:VAL:N	2.25	0.70
1:B:355:ASN:ND2	1:C:351:LEU:HB3	2.06	0.70
1:D:12:LYS:HD2	1:D:34:ASN:HD21	1.56	0.70
1:A:11:ILE:CG2	1:A:55:HIS:CB	2.68	0.70
1:C:20:HIS:HD2	1:C:22:LYS:N	1.87	0.70
4:D:513:CIT:C6	4:D:513:CIT:O1	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:TYR:HD1	1:B:197:LEU:HD13	1.56	0.69
1:D:59:LEU:HD23	1:D:59:LEU:H	1.57	0.68
1:B:161:HIS:CD2	3:B:509:NAI:O2A	2.42	0.68
1:A:131:ASN:O	1:A:135:HIS:HD2	1.76	0.67
1:B:201:LEU:HD23	1:B:228:LEU:HB2	1.75	0.67
1:C:211:VAL:HG21	1:C:220:MET:HE2	1.76	0.67
1:D:38:HIS:CD2	1:D:42:LEU:HD11	2.29	0.67
1:D:342:HIS:CE1	1:D:403:THR:HG23	2.29	0.67
1:A:272:THR:N	1:A:275:ASP:OD1	2.27	0.67
1:A:290:THR:HB	1:A:293:ILE:HD11	1.76	0.67
1:A:197:LEU:O	1:A:201:LEU:HG	1.94	0.67
1:D:24:LEU:HD23	1:D:28:ARG:NH2	2.09	0.67
1:A:409:LEU:O	1:A:410:TYR:HB3	1.95	0.66
1:B:201:LEU:HD11	1:B:221:MET:HE1	1.76	0.66
1:A:150:ARG:CG	1:A:150:ARG:NH1	2.57	0.66
1:A:33:THR:O	1:A:33:THR:HG22	1.94	0.66
1:C:104:ALA:HA	1:C:307:GLU:OE1	1.96	0.66
1:A:214:ASN:HB2	1:A:215:PRO:HD2	1.78	0.66
1:A:59:LEU:HD23	1:A:59:LEU:N	2.05	0.66
1:D:221:MET:CE	1:D:229:MET:HE3	2.26	0.65
1:A:120:LEU:C	1:A:120:LEU:HD12	2.21	0.65
1:C:59:LEU:HD12	1:C:60:ARG:O	1.96	0.65
1:C:213:GLU:O	1:C:214:ASN:HB3	1.95	0.65
1:A:245:ASP:OD1	1:A:247:PRO:HD2	1.97	0.65
1:A:14:LEU:HD23	1:A:57:ILE:HG13	1.78	0.65
1:B:120:LEU:O	1:B:121:LEU:C	2.40	0.65
1:B:249:LEU:CD1	1:B:253:LEU:HD22	2.26	0.65
1:A:11:ILE:HG23	1:A:55:HIS:CB	2.25	0.65
1:B:157:ILE:HB	1:B:209:LEU:HD23	1.78	0.65
1:B:339:ARG:HG2	1:B:409:LEU:HD12	1.79	0.65
1:B:108:ASN:ND2	1:B:295:GLY:HA3	2.11	0.64
1:C:221:MET:CE	1:C:229:MET:HE3	2.26	0.64
4:C:515:CIT:O1	4:C:515:CIT:C6	2.41	0.64
1:B:27:LEU:HD23	1:B:313:ILE:HD11	1.79	0.64
1:A:11:ILE:CG2	1:A:55:HIS:HB2	2.27	0.64
1:B:123:LEU:HD23	1:B:128:PRO:HG2	1.80	0.64
1:C:125:ARG:HH12	1:D:115:LEU:HB2	1.62	0.64
1:D:287:VAL:HG12	1:D:289:LEU:HD13	1.78	0.64
1:A:328:PRO:HB3	1:A:371:GLN:HG3	1.80	0.64
1:B:108:ASN:HD22	1:B:295:GLY:HA3	1.62	0.64
1:A:12:LYS:HZ3	1:A:12:LYS:HB2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:LEU:HD12	1:C:237:ASN:HB2	1.79	0.64
1:A:342:HIS:CD2	1:A:344:HIS:CD2	2.80	0.63
4:C:517:CIT:C6	4:C:517:CIT:O1	2.47	0.63
1:B:42:LEU:HB3	1:B:46:GLN:CG	2.27	0.63
1:C:61:SER:HB3	4:C:517:CIT:O3	1.98	0.63
1:B:81:ALA:O	1:B:103:ASN:HA	1.98	0.63
1:A:367:ALA:HB3	1:A:382:ASP:HB2	1.79	0.63
1:B:279:SER:OG	1:B:280:PRO:HD2	1.99	0.62
1:A:5:SER:HA	1:A:8:LYS:HG3	1.81	0.62
1:C:147:PHE:HB3	1:C:152:LYS:HE2	1.81	0.62
1:A:185:LYS:O	1:A:187:PRO:HD3	1.98	0.62
1:C:154:LEU:HD23	1:C:206:VAL:HB	1.81	0.62
1:D:92:ASP:O	1:D:93:ALA:C	2.41	0.62
1:B:116:VAL:CG1	1:B:166:LEU:HD11	2.29	0.62
1:D:376:MET:HG2	1:D:377:GLY:N	2.13	0.62
1:B:386:ASP:OD1	1:B:389:VAL:HG23	1.99	0.62
1:C:229:MET:O	1:C:257:HIS:CE1	2.53	0.62
1:D:318:ASN:HB2	1:D:339:ARG:HH11	1.65	0.62
1:A:164:THR:CG2	1:A:188:LEU:HD11	2.30	0.61
1:D:15:LEU:CD1	1:D:35:ILE:HG23	2.30	0.61
1:C:391:GLU:HG2	1:C:408:LEU:HD22	1.82	0.61
1:B:181:ASP:C	1:B:183:GLU:H	2.08	0.60
1:B:181:ASP:OD1	3:B:509:NAI:H1B	2.01	0.60
1:D:70:ILE:O	1:D:73:ALA:HB3	2.00	0.60
1:A:196:HIS:ND1	4:A:514:CIT:O5	2.34	0.60
1:A:38:HIS:HD2	1:A:42:LEU:HD21	1.66	0.60
1:D:66:THR:O	1:D:70:ILE:HG13	2.01	0.60
1:D:48:LYS:O	1:D:52:ARG:HB3	2.01	0.60
1:A:186:LEU:HD12	1:A:187:PRO:HD2	1.84	0.59
1:A:373:SER:O	1:A:374:ALA:C	2.45	0.59
1:C:179:PHE:CZ	1:C:193:GLN:HB2	2.37	0.59
1:A:332:LEU:HB3	1:A:339:ARG:NH1	2.17	0.59
1:C:123:LEU:HB3	1:C:234:LEU:CD1	2.31	0.59
1:C:125:ARG:NH2	1:D:111:SER:O	2.35	0.59
1:D:105:PRO:HB2	1:D:106:PHE:CD2	2.37	0.59
1:B:217:THR:OG1	1:B:243:VAL:HG22	2.02	0.59
1:B:308:VAL:O	1:B:312:LEU:HG	2.02	0.59
1:D:59:LEU:H	1:D:59:LEU:CD2	2.16	0.59
1:D:12:LYS:HD2	1:D:34:ASN:ND2	2.18	0.59
1:C:211:VAL:HG11	1:C:220:MET:HE1	1.86	0.58
1:B:214:ASN:CB	1:B:215:PRO:CD	2.76	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:SER:OG	1:A:210:HIS:NE2	2.30	0.58
1:D:20:HIS:HD2	1:D:22:LYS:HB2	1.67	0.58
1:A:73:ALA:O	1:A:97:ARG:NH1	2.31	0.58
1:C:171:GLU:OE1	1:C:190:ASN:HB2	2.04	0.58
1:B:157:ILE:HD13	1:B:221:MET:HE3	1.86	0.58
1:C:11:ILE:HG23	1:C:55:HIS:HD2	1.67	0.58
1:C:245:ASP:OD1	1:C:247:PRO:HD2	2.04	0.58
1:C:347:ARG:O	1:C:348:PRO:C	2.39	0.58
1:B:249:LEU:HD11	1:B:253:LEU:HD22	1.86	0.58
1:C:38:HIS:CD2	1:C:42:LEU:HD21	2.37	0.58
1:C:43:ASP:H	1:C:46:GLN:HE21	1.51	0.58
1:C:122:LEU:HD22	1:C:127:VAL:HG11	1.85	0.58
1:B:342:HIS:CE1	1:B:344:HIS:HB3	2.38	0.57
1:B:253:LEU:HD13	1:B:258:LEU:HB2	1.87	0.57
1:C:264:ASP:OD1	1:C:290:THR:HB	2.03	0.57
1:A:334:LEU:O	1:A:335:HIS:CD2	2.57	0.57
1:D:43:ASP:C	1:D:43:ASP:OD1	2.47	0.57
1:C:148:GLU:HG3	1:D:299:GLU:HG2	1.85	0.57
1:A:12:LYS:HB3	1:A:54:ALA:HA	1.86	0.57
1:C:12:LYS:HD2	1:C:54:ALA:HA	1.87	0.57
1:C:132:ALA:O	1:C:136:ARG:HG2	2.05	0.57
1:A:407:ARG:HD2	6:A:588:HOH:O	2.04	0.56
1:D:197:LEU:HB3	4:D:513:CIT:O7	2.05	0.56
1:D:287:VAL:HG12	1:D:289:LEU:CD1	2.36	0.56
1:B:211:VAL:HB	1:B:212:PRO:HD2	1.87	0.56
1:D:171:GLU:OE2	1:D:190:ASN:HB2	2.04	0.56
1:B:332:LEU:HB3	1:B:339:ARG:HH22	1.71	0.56
1:A:8:LYS:O	1:A:10:LYS:N	2.38	0.56
1:A:12:LYS:HB2	1:A:12:LYS:NZ	2.21	0.56
1:C:146:SER:C	1:C:147:PHE:CD2	2.85	0.55
1:B:254:ALA:C	1:B:256:LYS:H	2.14	0.55
1:A:51:ILE:O	1:A:52:ARG:C	2.49	0.55
1:A:24:LEU:HD23	1:A:24:LEU:H	1.71	0.55
1:B:17:GLU:OE1	1:B:60:ARG:N	2.38	0.55
1:B:369:TYR:O	1:B:379:VAL:HA	2.07	0.55
1:C:154:LEU:HD13	1:C:156:ILE:HG13	1.89	0.55
1:B:59:LEU:HD22	1:B:65:LEU:HD11	1.88	0.55
1:D:221:MET:HE2	1:D:229:MET:HE3	1.88	0.55
1:C:41:ALA:O	1:C:42:LEU:HD12	2.06	0.55
1:B:314:LYS:O	1:B:318:ASN:N	2.33	0.55
1:C:122:LEU:HD12	1:D:122:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:GLU:CG	1:D:299:GLU:HG2	2.37	0.55
1:A:384:GLU:O	1:A:385:ALA:HB2	2.07	0.55
1:B:207:VAL:CG2	1:B:229:MET:HE3	2.37	0.55
1:B:103:ASN:N	1:B:103:ASN:HD22	2.05	0.55
1:C:125:ARG:HE	1:D:297:THR:HG21	1.72	0.55
1:D:221:MET:HE1	1:D:229:MET:HE3	1.87	0.55
1:A:76:LEU:O	1:A:99:ILE:HD13	2.07	0.54
1:A:332:LEU:HD13	1:A:369:TYR:CB	2.35	0.54
1:A:341:MET:HE1	1:A:343:ILE:HD11	1.88	0.54
1:B:287:VAL:HG12	1:B:289:LEU:HD13	1.89	0.54
1:D:330:VAL:HG13	1:D:369:TYR:CG	2.42	0.54
1:D:24:LEU:HD23	1:D:28:ARG:HH21	1.72	0.54
1:B:179:PHE:CE1	1:B:193:GLN:HB2	2.42	0.54
1:C:16:VAL:HG23	1:C:17:GLU:HG3	1.88	0.54
1:B:78:ALA:HA	1:B:99:ILE:HG23	1.88	0.54
1:C:123:LEU:CB	1:C:234:LEU:HD13	2.38	0.54
1:D:105:PRO:HB2	1:D:106:PHE:CE2	2.43	0.54
1:B:115:LEU:O	1:B:119:GLU:HG3	2.08	0.54
1:C:36:GLU:OE2	1:C:50:SER:HB2	2.07	0.54
1:B:188:LEU:O	1:B:189:GLY:C	2.50	0.53
1:C:41:ALA:C	1:C:42:LEU:HD12	2.33	0.53
1:A:33:THR:O	1:A:33:THR:CG2	2.56	0.53
1:C:246:ILE:N	1:C:247:PRO:CD	2.71	0.53
1:A:164:THR:HG21	1:A:188:LEU:HD11	1.90	0.53
1:B:201:LEU:HG	1:B:229:MET:HG3	1.89	0.53
1:B:342:HIS:CE1	1:B:344:HIS:CD2	2.95	0.53
1:C:56:PHE:CZ	1:C:316:SER:HB2	2.44	0.53
1:C:211:VAL:HG21	1:C:220:MET:CE	2.38	0.53
1:A:65:LEU:HD23	1:A:69:VAL:HG11	1.91	0.53
1:B:409:LEU:O	1:B:410:TYR:CB	2.49	0.53
1:C:178:TYR:CD2	1:C:192:THR:HB	2.44	0.53
4:C:517:CIT:O6	4:C:517:CIT:C5	2.54	0.53
1:D:342:HIS:HD2	1:D:344:HIS:CD2	2.25	0.53
1:C:131:ASN:OD1	1:C:135:HIS:HE1	1.91	0.52
1:C:208:SER:OG	1:C:210:HIS:NE2	2.42	0.52
1:A:212:PRO:HD2	1:A:217:THR:HG21	1.91	0.52
1:A:405:ARG:HD3	6:A:588:HOH:O	2.09	0.52
1:B:160:GLY:HA3	3:B:509:NAI:O5B	2.09	0.52
1:C:11:ILE:HG23	1:C:55:HIS:CB	2.38	0.52
1:B:124:LEU:HD13	1:B:234:LEU:HD12	1.90	0.52
1:C:33:THR:HG23	1:C:33:THR:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:LEU:HD12	1:D:121:LEU:N	2.24	0.52
1:A:28:ARG:HD2	6:A:544:HOH:O	2.09	0.52
1:D:77:VAL:O	1:D:100:PRO:HD2	2.10	0.52
1:A:225:GLU:OE1	1:A:225:GLU:N	2.39	0.52
1:B:201:LEU:HD21	1:B:225:GLU:O	2.10	0.52
1:D:350:VAL:HG12	1:D:354:LEU:CD2	2.40	0.52
1:B:17:GLU:HB2	1:B:60:ARG:HG2	1.92	0.52
1:C:110:ARG:HE	1:C:114:GLU:HG3	1.75	0.52
1:A:87:ASN:HD22	1:A:87:ASN:H	1.58	0.51
1:B:20:HIS:HD2	1:B:22:LYS:H	1.56	0.51
1:B:116:VAL:HG11	1:B:166:LEU:HD11	1.92	0.51
1:B:124:LEU:HD13	1:B:234:LEU:CD1	2.41	0.51
1:B:222:GLY:O	1:B:223:ALA:C	2.52	0.51
1:C:20:HIS:CE1	1:C:302:GLU:HB2	2.45	0.51
1:C:120:LEU:C	1:C:120:LEU:HD12	2.35	0.51
1:A:43:ASP:O	1:A:44:ASP:C	2.53	0.51
1:A:196:HIS:HB3	4:A:514:CIT:O3	2.11	0.51
1:A:210:HIS:CD2	1:A:210:HIS:N	2.78	0.51
1:C:259:ALA:O	1:C:286:ASN:ND2	2.39	0.51
1:C:338:ARG:HG3	1:C:410:TYR:O	2.10	0.51
1:C:196:HIS:HB3	4:C:515:CIT:O5	2.11	0.51
1:A:131:ASN:O	1:A:135:HIS:CD2	2.62	0.51
1:C:22:LYS:HB3	1:C:306:LEU:HD21	1.92	0.51
1:B:264:ASP:O	1:B:292:HIS:HA	2.10	0.51
1:B:214:ASN:CB	1:B:215:PRO:HD3	2.27	0.50
1:A:164:THR:CG2	1:A:188:LEU:CD1	2.89	0.50
1:A:179:PHE:C	1:A:179:PHE:CD1	2.88	0.50
1:C:270:PRO:HB3	1:C:275:ASP:HB2	1.94	0.50
1:B:8:LYS:HA	1:B:11:ILE:HD12	1.93	0.50
1:B:156:ILE:CG1	1:B:166:LEU:HD23	2.41	0.50
1:B:259:ALA:O	1:B:286:ASN:ND2	2.35	0.50
1:C:14:LEU:C	1:C:15:LEU:HD23	2.37	0.50
1:B:246:ILE:HB	1:B:247:PRO:HD3	1.93	0.50
1:C:148:GLU:HA	1:D:114:GLU:OE2	2.12	0.50
1:D:37:PHE:CD1	1:D:37:PHE:C	2.89	0.50
1:D:56:PHE:CE2	1:D:78:ALA:HB3	2.46	0.50
1:A:8:LYS:C	1:A:10:LYS:H	2.19	0.50
1:B:13:PHE:CZ	1:B:56:PHE:CD1	3.00	0.50
1:C:154:LEU:HB2	1:C:175:MET:HE2	1.92	0.50
1:A:239:SER:OG	1:A:240:ARG:N	2.45	0.50
1:B:59:LEU:HD22	1:B:65:LEU:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:CG	1:B:62:ARG:NH1	2.48	0.50
1:B:181:ASP:O	1:B:183:GLU:N	2.45	0.50
1:D:167:GLY:O	1:D:171:GLU:HG3	2.12	0.50
1:A:59:LEU:N	1:A:59:LEU:CD2	2.74	0.49
1:D:351:LEU:HA	1:D:354:LEU:HD23	1.94	0.49
1:B:218:LYS:O	1:B:219:ASN:HB2	2.11	0.49
1:C:43:ASP:H	1:C:46:GLN:NE2	2.10	0.49
1:B:133:LYS:HB3	1:B:138:VAL:HB	1.92	0.49
1:C:11:ILE:HG23	1:C:55:HIS:CG	2.46	0.49
1:C:125:ARG:HE	1:D:297:THR:CG2	2.24	0.49
1:C:131:ASN:OD1	1:C:135:HIS:CE1	2.64	0.49
1:C:214:ASN:C	1:C:214:ASN:OD1	2.54	0.49
1:C:323:SER:O	1:C:324:ALA:C	2.56	0.49
1:D:121:LEU:HD23	1:D:149:ALA:HB2	1.93	0.49
1:D:393:ALA:O	1:D:397:MET:HG3	2.11	0.49
1:B:16:VAL:HG23	1:B:59:LEU:HA	1.93	0.49
1:B:254:ALA:C	1:B:256:LYS:N	2.68	0.49
1:D:229:MET:HE1	1:D:235:LEU:CG	2.31	0.49
1:D:342:HIS:CE1	1:D:403:THR:CG2	2.95	0.49
1:D:400:ILE:O	1:D:401:PRO:C	2.54	0.49
1:A:188:LEU:O	1:A:189:GLY:C	2.56	0.49
1:C:321:THR:O	1:C:322:LEU:C	2.55	0.49
1:D:340:LEU:HD23	1:D:408:LEU:HB2	1.93	0.49
1:A:291:PRO:HD3	1:B:130:ALA:HB1	1.95	0.49
1:D:120:LEU:HD12	1:D:120:LEU:C	2.38	0.49
1:A:360:GLU:O	1:A:360:GLU:HG2	2.12	0.48
1:A:368:GLN:NE2	1:A:381:ILE:HG12	2.27	0.48
1:C:141:LYS:HE3	1:D:292:HIS:O	2.13	0.48
1:D:14:LEU:HD13	1:D:50:SER:HB3	1.95	0.48
1:D:95:ALA:O	1:D:98:GLY:N	2.33	0.48
1:B:214:ASN:N	1:B:217:THR:HG22	2.28	0.48
1:D:29:ALA:C	1:D:31:GLY:H	2.21	0.48
1:D:342:HIS:HD2	1:D:344:HIS:HD2	1.61	0.48
1:A:55:HIS:HA	1:A:75:LYS:O	2.14	0.48
1:C:110:ARG:HE	1:C:114:GLU:CG	2.26	0.48
1:D:243:VAL:O	1:D:243:VAL:HG12	2.13	0.48
1:A:36:GLU:CD	1:A:50:SER:HB2	2.38	0.48
1:A:51:ILE:O	1:A:54:ALA:N	2.47	0.48
1:A:318:ASN:HD21	1:A:320:SER:HB2	1.79	0.48
1:B:95:ALA:HB1	1:B:376:MET:HE1	1.95	0.48
1:A:341:MET:HE2	1:A:378:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LEU:O	1:A:410:TYR:CB	2.58	0.48
1:B:338:ARG:HA	1:B:410:TYR:O	2.13	0.48
1:D:43:ASP:OD1	1:D:43:ASP:O	2.31	0.48
1:B:358:PHE:CE1	1:B:383:ILE:HG21	2.48	0.48
1:C:16:VAL:HG21	1:C:63:THR:OG1	2.14	0.48
1:D:376:MET:CG	1:D:377:GLY:N	2.75	0.48
1:D:407:ARG:NH1	1:D:409:LEU:HD22	2.29	0.48
1:A:318:ASN:O	1:A:339:ARG:NH2	2.40	0.48
1:B:83:ALA:HA	4:B:516:CIT:O6	2.14	0.48
1:D:28:ARG:NH1	1:D:35:ILE:HD12	2.29	0.48
1:C:70:ILE:C	1:C:72:ALA:H	2.21	0.47
1:C:246:ILE:HB	1:C:247:PRO:HD3	1.95	0.47
1:A:235:LEU:O	1:A:261:ALA:HA	2.14	0.47
1:C:264:ASP:OD1	1:C:290:THR:CB	2.61	0.47
1:A:340:LEU:HD22	1:A:397:MET:SD	2.54	0.47
1:B:201:LEU:HD23	1:B:228:LEU:CB	2.44	0.47
1:C:59:LEU:HD13	1:C:63:THR:HB	1.96	0.47
1:C:292:HIS:HB3	1:D:141:LYS:HE2	1.96	0.47
1:A:243:VAL:HG12	1:A:243:VAL:O	2.13	0.47
1:C:214:ASN:HB2	1:C:215:PRO:HD2	1.96	0.47
1:A:168:ILE:HD11	1:A:188:LEU:HD12	1.95	0.47
1:B:197:LEU:HB3	2:B:499:PO4:O2	2.15	0.47
1:C:41:ALA:C	1:C:42:LEU:CD1	2.88	0.47
1:C:327:PHE:CG	1:C:328:PRO:HD2	2.49	0.47
1:D:327:PHE:HZ	1:D:343:ILE:HD13	1.79	0.47
1:A:230:LYS:O	1:A:233:SER:HB3	2.14	0.47
1:B:321:THR:O	1:B:322:LEU:C	2.55	0.47
1:D:82:PHE:N	1:D:82:PHE:CD1	2.82	0.47
1:B:291:PRO:HD2	1:B:293:ILE:CD1	2.39	0.47
1:C:293:ILE:HD12	1:C:293:ILE:C	2.40	0.47
1:D:11:ILE:HA	1:D:55:HIS:CD2	2.50	0.47
1:D:157:ILE:HB	1:D:209:LEU:HD23	1.97	0.47
1:D:209:LEU:HB2	1:D:237:ASN:HD22	1.80	0.47
1:B:393:ALA:O	1:B:394:LEU:C	2.56	0.47
1:D:34:ASN:ND2	1:D:34:ASN:C	2.72	0.47
1:A:122:LEU:HD12	1:B:122:LEU:HD12	1.97	0.46
1:D:339:ARG:HD2	1:D:380:VAL:HG12	1.94	0.46
1:A:240:ARG:HB2	1:A:243:VAL:HG23	1.97	0.46
1:B:394:LEU:HA	1:B:397:MET:HE3	1.97	0.46
1:C:12:LYS:NZ	1:C:50:SER:O	2.43	0.46
1:A:169:LEU:HD22	1:B:173:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:VAL:HB	1:A:212:PRO:CD	2.45	0.46
1:B:48:LYS:HG3	1:B:49:GLU:N	2.29	0.46
1:D:44:ASP:OD1	1:D:44:ASP:N	2.45	0.46
1:D:332:LEU:HB3	1:D:339:ARG:NH2	2.30	0.46
1:B:42:LEU:HD22	1:B:46:GLN:HE21	1.81	0.46
1:B:109:THR:O	1:B:110:ARG:C	2.57	0.46
1:B:241:GLY:O	1:B:267:PRO:HD3	2.15	0.46
1:A:38:HIS:CG	4:A:518:CIT:O5	2.68	0.46
1:B:207:VAL:HG21	1:B:229:MET:HE3	1.96	0.46
4:B:516:CIT:O3	4:B:516:CIT:O7	2.32	0.46
1:D:15:LEU:CD1	1:D:35:ILE:CG2	2.93	0.46
1:D:215:PRO:C	1:D:217:THR:H	2.22	0.46
1:C:24:LEU:N	1:C:24:LEU:HD23	2.30	0.46
1:C:38:HIS:HB3	5:C:506:SO4:O4	2.15	0.46
1:A:209:LEU:C	1:A:210:HIS:CG	2.94	0.46
1:B:264:ASP:OD1	1:B:293:ILE:N	2.46	0.46
1:C:94:ALA:HB1	1:C:99:ILE:HB	1.98	0.46
1:D:95:ALA:O	1:D:96:LYS:C	2.59	0.46
1:A:38:HIS:ND1	4:A:518:CIT:O5	2.49	0.46
1:B:115:LEU:HD22	1:B:294:GLY:HA2	1.98	0.46
1:C:292:HIS:O	1:C:292:HIS:CD2	2.69	0.46
1:A:24:LEU:H	1:A:24:LEU:CD2	2.28	0.46
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.81	0.46
1:B:220:MET:HG2	1:B:243:VAL:HG13	1.97	0.46
1:C:20:HIS:CD2	1:C:21:GLN:N	2.84	0.46
1:C:354:LEU:O	1:C:358:PHE:CD2	2.69	0.46
1:D:77:VAL:CG1	1:D:315:TYR:HE2	2.28	0.46
1:A:156:ILE:HG12	1:A:166:LEU:HD23	1.97	0.46
1:A:196:HIS:O	1:A:199:ASP:HB2	2.15	0.46
1:B:133:LYS:O	1:B:134:ALA:C	2.54	0.46
1:D:92:ASP:C	1:D:94:ALA:N	2.71	0.46
1:A:13:PHE:CD2	1:A:56:PHE:HB2	2.51	0.45
1:C:407:ARG:NH2	6:C:539:HOH:O	2.45	0.45
1:A:24:LEU:CD2	1:A:24:LEU:N	2.79	0.45
1:B:43:ASP:CG	1:B:46:GLN:OE1	2.60	0.45
1:D:287:VAL:CG1	1:D:289:LEU:CD1	2.94	0.45
1:A:229:MET:HE2	1:A:233:SER:OG	2.16	0.45
1:C:154:LEU:HD13	1:C:156:ILE:CG1	2.45	0.45
1:C:258:LEU:N	1:C:258:LEU:HD12	2.31	0.45
1:D:370:LEU:HA	1:D:378:TYR:O	2.16	0.45
1:A:88:GLN:HG2	1:A:89:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ALA:HB1	1:B:376:MET:CE	2.45	0.45
1:A:214:ASN:HB2	1:A:215:PRO:CD	2.46	0.45
1:D:197:LEU:O	1:D:201:LEU:HG	2.17	0.45
1:B:181:ASP:C	1:B:183:GLU:N	2.75	0.45
1:C:214:ASN:HB2	1:C:215:PRO:CD	2.46	0.45
1:B:344:HIS:CD2	1:B:350:VAL:HG11	2.52	0.45
1:B:163:GLY:O	1:B:164:THR:C	2.60	0.45
1:C:257:HIS:C	1:C:258:LEU:HD12	2.42	0.45
1:D:14:LEU:HD23	1:D:57:ILE:HG12	1.98	0.45
1:D:169:LEU:O	1:D:170:ALA:C	2.58	0.45
1:B:340:LEU:CD1	1:B:397:MET:HE1	2.38	0.44
1:D:14:LEU:HB3	1:D:57:ILE:HG12	1.98	0.44
1:D:335:HIS:O	1:D:336:VAL:C	2.59	0.44
1:D:405:ARG:HG2	1:D:406:ALA:N	2.32	0.44
1:A:104:ALA:HA	1:A:307:GLU:OE2	2.17	0.44
1:C:79:ILE:O	1:C:101:VAL:HA	2.17	0.44
1:D:209:LEU:HD11	1:D:221:MET:HG3	1.99	0.44
1:D:360:GLU:C	1:D:362:GLY:H	2.25	0.44
1:D:12:LYS:H	1:D:55:HIS:CD2	2.12	0.44
1:A:120:LEU:HD12	1:A:121:LEU:N	2.31	0.44
1:D:59:LEU:CD2	1:D:59:LEU:N	2.79	0.44
1:D:334:LEU:HD13	1:D:334:LEU:O	2.17	0.44
1:A:383:ILE:O	1:A:383:ILE:HG13	2.16	0.44
1:D:269:GLU:O	1:D:270:PRO:C	2.58	0.44
1:D:310:GLY:HA3	6:D:565:HOH:O	2.17	0.44
1:D:358:PHE:O	1:D:359:ALA:C	2.59	0.44
1:A:103:ASN:OD1	1:A:105:PRO:HD3	2.18	0.44
1:B:46:GLN:O	1:B:47:LEU:C	2.60	0.44
1:D:15:LEU:HD12	1:D:35:ILE:HG23	1.99	0.44
1:B:186:LEU:HD12	1:B:187:PRO:N	2.32	0.44
1:C:394:LEU:HG	1:C:398:LYS:HE2	1.99	0.44
3:D:511:NAI:H2D	3:D:511:NAI:H6N	1.69	0.44
1:A:57:ILE:HD12	1:A:65:LEU:HD11	1.98	0.44
1:B:16:VAL:HG12	1:B:38:HIS:HB2	1.98	0.44
1:C:141:LYS:H	1:D:273:ASN:ND2	2.16	0.44
1:A:322:LEU:HA	1:A:329:GLU:HG2	2.00	0.43
1:C:27:LEU:O	1:C:32:TYR:HB2	2.18	0.43
1:D:57:ILE:HG21	1:D:65:LEU:CD1	2.46	0.43
1:D:100:PRO:HG3	1:D:315:TYR:CE1	2.52	0.43
1:A:34:ASN:C	1:A:35:ILE:HG13	2.43	0.43
1:C:409:LEU:HD23	1:C:409:LEU:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:LEU:HD23	1:D:128:PRO:HG2	2.00	0.43
1:A:162:ILE:O	1:A:163:GLY:C	2.60	0.43
1:C:270:PRO:HG2	1:D:139:TRP:CG	2.53	0.43
1:A:341:MET:HE2	1:A:378:TYR:HE1	1.82	0.43
4:A:514:CIT:O1	4:A:514:CIT:O7	2.36	0.43
1:B:314:LYS:HG2	1:B:318:ASN:HD21	1.84	0.43
1:D:246:ILE:N	1:D:247:PRO:CD	2.82	0.43
1:B:355:ASN:HD21	1:C:351:LEU:HB3	1.83	0.43
1:D:58:GLY:HA2	1:D:80:GLY:O	2.18	0.43
1:D:350:VAL:HG12	1:D:354:LEU:HD22	2.00	0.43
1:C:125:ARG:NH1	1:D:115:LEU:HB2	2.30	0.43
1:C:327:PHE:O	1:C:328:PRO:C	2.62	0.43
1:D:209:LEU:C	1:D:210:HIS:CG	2.96	0.43
1:D:16:VAL:HA	1:D:38:HIS:HB2	1.99	0.43
1:D:334:LEU:O	1:D:335:HIS:ND1	2.51	0.43
1:D:386:ASP:OD1	1:D:389:VAL:HG23	2.18	0.43
1:C:353:ALA:HB3	1:C:400:ILE:HD13	1.99	0.43
1:D:20:HIS:HD2	1:D:22:LYS:H	1.67	0.43
1:D:27:LEU:HD23	1:D:313:ILE:HD11	2.01	0.43
1:A:12:LYS:NZ	1:A:12:LYS:CB	2.82	0.43
1:A:43:ASP:OD2	1:A:44:ASP:N	2.52	0.43
4:A:514:CIT:O6	4:A:514:CIT:C5	2.62	0.43
1:D:120:LEU:HD11	1:D:175:MET:HE1	2.01	0.43
1:D:209:LEU:O	1:D:210:HIS:CG	2.71	0.43
1:A:74:GLU:OE2	1:A:74:GLU:HA	2.18	0.43
1:A:108:ASN:N	1:A:108:ASN:HD22	2.17	0.43
1:D:340:LEU:CD2	1:D:408:LEU:HB2	2.49	0.43
1:A:209:LEU:HD11	1:A:221:MET:HG3	2.01	0.42
1:B:228:LEU:HD23	1:B:228:LEU:HA	1.84	0.42
1:C:42:LEU:CD1	1:C:42:LEU:N	2.82	0.42
1:B:27:LEU:HD23	1:B:27:LEU:HA	1.78	0.42
1:B:201:LEU:HG	1:B:229:MET:CG	2.49	0.42
1:B:214:ASN:H	1:B:217:THR:CG2	2.32	0.42
1:C:262:ALA:HA	1:C:288:LEU:O	2.19	0.42
1:B:214:ASN:H	1:B:217:THR:HG22	1.84	0.42
1:D:76:LEU:O	1:D:99:ILE:HD11	2.18	0.42
1:D:235:LEU:HD22	1:D:236:ILE:N	2.35	0.42
1:B:330:VAL:HG12	1:B:331:SER:N	2.35	0.42
1:C:66:THR:O	1:C:70:ILE:HG13	2.18	0.42
1:C:229:MET:O	1:C:257:HIS:HE1	2.02	0.42
4:D:513:CIT:O1	4:D:513:CIT:O6	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LYS:HE2	1:A:323:SER:OG	2.20	0.42
1:C:22:LYS:HE3	1:C:306:LEU:HD11	2.02	0.42
1:C:172:SER:HB3	1:D:172:SER:HB3	2.01	0.42
1:C:198:SER:O	1:C:202:ASN:HB2	2.20	0.42
1:A:160:GLY:HA3	3:A:508:NAI:O5B	2.19	0.42
1:B:131:ASN:O	1:B:135:HIS:HD2	2.03	0.42
1:B:186:LEU:HD12	1:B:186:LEU:C	2.45	0.42
1:B:214:ASN:N	1:B:217:THR:CG2	2.83	0.42
1:B:249:LEU:HD12	1:B:253:LEU:HD22	2.01	0.42
1:B:394:LEU:HA	1:B:394:LEU:HD12	1.86	0.42
1:C:221:MET:HE2	1:C:221:MET:HB3	1.86	0.42
1:A:65:LEU:CD2	1:A:69:VAL:HG11	2.50	0.42
1:A:258:LEU:HD12	1:A:258:LEU:HA	1.73	0.42
1:B:262:ALA:HA	1:B:288:LEU:O	2.20	0.42
1:C:148:GLU:CD	1:D:299:GLU:HG2	2.44	0.42
1:D:29:ALA:C	1:D:31:GLY:N	2.78	0.42
1:D:55:HIS:HA	1:D:76:LEU:HA	2.02	0.42
1:A:41:ALA:O	1:A:42:LEU:HD12	2.20	0.42
1:A:169:LEU:HA	1:A:169:LEU:HD23	1.76	0.42
1:B:340:LEU:HD22	1:B:397:MET:HE1	2.01	0.42
1:C:272:THR:C	1:C:274:SER:H	2.27	0.42
1:C:95:ALA:O	1:C:96:LYS:C	2.59	0.42
1:C:173:LEU:HD11	1:D:173:LEU:HD11	2.00	0.42
1:C:357:ILE:O	1:C:358:PHE:C	2.62	0.42
1:A:81:ALA:O	1:A:103:ASN:HA	2.19	0.42
1:B:166:LEU:O	1:B:167:GLY:C	2.62	0.42
1:D:38:HIS:HD2	1:D:42:LEU:HD11	1.80	0.42
1:A:152:LYS:HD3	1:A:152:LYS:HA	1.77	0.41
1:A:357:ILE:HD12	1:A:400:ILE:HD11	2.02	0.41
1:C:149:ALA:O	1:C:175:MET:HG2	2.20	0.41
1:A:59:LEU:HB2	1:A:63:THR:HB	2.02	0.41
1:C:332:LEU:HD12	1:C:380:VAL:HG12	2.01	0.41
1:D:92:ASP:O	1:D:94:ALA:N	2.53	0.41
1:B:291:PRO:O	1:B:292:HIS:C	2.63	0.41
1:C:145:GLY:O	1:C:147:PHE:CE2	2.72	0.41
1:C:398:LYS:HA	1:C:403:THR:HG21	2.02	0.41
1:A:127:VAL:HB	1:A:128:PRO:HD3	2.03	0.41
1:A:149:ALA:O	1:A:152:LYS:HB2	2.21	0.41
1:C:180:TYR:CE1	1:C:197:LEU:HB2	2.55	0.41
1:C:237:ASN:OD1	1:C:239:SER:OG	2.33	0.41
1:C:390:ALA:HB1	1:C:408:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:GLU:CB	1:B:60:ARG:HG2	2.51	0.41
1:C:78:ALA:HA	1:C:99:ILE:CG2	2.43	0.41
1:B:214:ASN:O	1:B:217:THR:HG22	2.21	0.41
4:D:513:CIT:O7	4:D:513:CIT:O3	2.33	0.41
1:B:318:ASN:OD1	1:B:320:SER:HB2	2.21	0.41
1:B:355:ASN:HD21	1:C:351:LEU:HD13	1.84	0.41
1:D:20:HIS:CD2	1:D:22:LYS:H	2.39	0.41
1:D:20:HIS:CD2	1:D:22:LYS:HB2	2.52	0.41
1:D:60:ARG:O	1:D:88:GLN:NE2	2.54	0.41
1:D:215:PRO:C	1:D:217:THR:N	2.75	0.41
1:D:217:THR:HG23	1:D:243:VAL:HG22	2.03	0.41
1:D:287:VAL:CG1	1:D:289:LEU:HD13	2.49	0.41
1:D:332:LEU:O	1:D:333:PRO:C	2.59	0.41
1:A:38:HIS:HD2	1:A:42:LEU:CD2	2.33	0.41
1:B:219:ASN:C	1:B:221:MET:N	2.77	0.41
1:B:387:GLU:O	1:B:391:GLU:HG3	2.21	0.41
1:C:43:ASP:OD1	1:C:46:GLN:HB2	2.21	0.41
1:C:394:LEU:HG	1:C:394:LEU:O	2.21	0.41
1:A:121:LEU:HD23	1:A:121:LEU:HA	1.94	0.40
1:A:331:SER:O	1:A:369:TYR:CD2	2.74	0.40
1:A:368:GLN:HE21	1:A:381:ILE:HG12	1.85	0.40
1:A:291:PRO:HD2	1:A:293:ILE:CG1	2.41	0.40
1:D:84:ILE:O	1:D:84:ILE:HG12	2.22	0.40
1:A:142:LEU:C	1:A:142:LEU:HD23	2.46	0.40
1:A:184:ASN:N	1:A:184:ASN:HD22	2.18	0.40
1:A:211:VAL:O	3:A:508:NAI:H4D	2.22	0.40
1:B:173:LEU:HD12	1:B:173:LEU:HA	1.83	0.40
1:C:147:PHE:CD2	1:C:147:PHE:N	2.89	0.40
1:C:407:ARG:HD3	1:C:407:ARG:HA	1.96	0.40
1:B:78:ALA:HA	1:B:99:ILE:CG2	2.51	0.40
1:C:290:THR:O	1:C:292:HIS:N	2.48	0.40
1:A:79:ILE:HB	1:A:101:VAL:HG22	2.04	0.40
1:B:346:ASN:HD21	1:B:372:THR:CG2	2.34	0.40
1:C:70:ILE:C	1:C:72:ALA:N	2.79	0.40
1:C:351:LEU:HA	1:C:351:LEU:HD23	1.88	0.40
1:D:366:ALA:N	1:D:382:ASP:O	2.51	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	404/410 (98%)	365 (90%)	33 (8%)	6 (2%)	8	18
1	B	402/410 (98%)	363 (90%)	37 (9%)	2 (0%)	24	46
1	C	404/410 (98%)	373 (92%)	26 (6%)	5 (1%)	10	23
1	D	401/410 (98%)	374 (93%)	25 (6%)	2 (0%)	24	46
All	All	1611/1640 (98%)	1475 (92%)	121 (8%)	15 (1%)	14	30

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	374	ALA
1	B	224	LYS
1	A	44	ASP
1	A	336	VAL
1	B	182	ILE
1	C	323	SER
1	C	73	ALA
1	D	30	ALA
1	A	47	LEU
1	A	48	LYS
1	C	18	GLY
1	C	336	VAL
1	D	219	ASN
1	C	214	ASN

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	325/328 (99%)	276 (85%)	49 (15%)	3	5
1	B	323/328 (98%)	285 (88%)	38 (12%)	5	10
1	C	325/328 (99%)	286 (88%)	39 (12%)	5	10
1	D	322/328 (98%)	283 (88%)	39 (12%)	5	10
All	All	1295/1312 (99%)	1130 (87%)	165 (13%)	4	9

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	7	GLU
1	A	8	LYS
1	A	10	LYS
1	A	11	ILE
1	A	12	LYS
1	A	15	LEU
1	A	24	LEU
1	A	34	ASN
1	A	44	ASP
1	A	51	ILE
1	A	52	ARG
1	A	57	ILE
1	A	64	HIS
1	A	75	LYS
1	A	87	ASN
1	A	99	ILE
1	A	108	ASN
1	A	120	LEU
1	A	141	LYS
1	A	142	LEU
1	A	150	ARG
1	A	183	GLU
1	A	188	LEU
1	A	200	LEU
1	A	220	MET
1	A	224	LYS
1	A	256	LYS
1	A	258	LEU
1	A	268	THR
1	A	274	SER

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Mol	Chain	Res	Type
1	A	283	GLU
1	A	293	ILE
1	A	307	GLU
1	A	312	LEU
1	A	318	ASN
1	A	332	LEU
1	A	338	ARG
1	A	352	THR
1	A	354	LEU
1	A	356	LYS
1	A	360	GLU
1	A	361	GLN
1	A	368	GLN
1	A	370	LEU
1	A	384	GLU
1	A	404	ILE
1	A	405	ARG
1	A	407	ARG
1	B	16	VAL
1	B	39	LYS
1	B	48	LYS
1	B	51	ILE
1	B	52	ARG
1	B	59	LEU
1	B	61	SER
1	B	62	ARG
1	B	67	GLU
1	B	88	GLN
1	B	103	ASN
1	B	124	LEU
1	B	141	LYS
1	B	142	LEU
1	B	150	ARG
1	B	173	LEU
1	B	186	LEU
1	B	188	LEU
1	B	192	THR
1	B	194	VAL
1	B	220	MET
1	B	224	LYS
1	B	245	ASP
1	B	246	ILE

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Mol	Chain	Res	Type
1	B	253	LEU
1	B	268	THR
1	B	274	SER
1	B	278	THR
1	B	289	LEU
1	B	293	ILE
1	B	331	SER
1	B	334	LEU
1	B	338	ARG
1	B	341	MET
1	B	345	GLU
1	B	347	ARG
1	B	351	LEU
1	B	407	ARG
1	C	12	LYS
1	C	19	VAL
1	C	24	LEU
1	C	33	THR
1	C	42	LEU
1	C	46	GLN
1	C	48	LYS
1	C	49	GLU
1	C	51	ILE
1	C	52	ARG
1	C	55	HIS
1	C	57	ILE
1	C	59	LEU
1	C	67	GLU
1	C	68	ASP
1	C	77	VAL
1	C	84	ILE
1	C	140	ASN
1	C	142	LEU
1	C	154	LEU
1	C	185	LYS
1	C	202	ASN
1	C	221	MET
1	C	274	SER
1	C	290	THR
1	C	322	LEU
1	C	325	VAL
1	C	338	ARG

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Mol	Chain	Res	Type
1	C	341	MET
1	C	354	LEU
1	C	355	ASN
1	C	360	GLU
1	C	364	ASN
1	C	365	ILE
1	C	370	LEU
1	C	384	GLU
1	C	387	GLU
1	C	388	ASP
1	C	394	LEU
1	D	8	LYS
1	D	10	LYS
1	D	22	LYS
1	D	36	GLU
1	D	48	LYS
1	D	51	ILE
1	D	57	ILE
1	D	59	LEU
1	D	84	ILE
1	D	150	ARG
1	D	164	THR
1	D	165	GLN
1	D	184	ASN
1	D	195	GLN
1	D	202	ASN
1	D	217	THR
1	D	218	LYS
1	D	224	LYS
1	D	235	LEU
1	D	246	ILE
1	D	268	THR
1	D	274	SER
1	D	283	GLU
1	D	289	LEU
1	D	299	GLU
1	D	322	LEU
1	D	327	PHE
1	D	334	LEU
1	D	339	ARG
1	D	341	MET
1	D	354	LEU

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Mol	Chain	Res	Type
1	D	356	LYS
1	D	361	GLN
1	D	370	LEU
1	D	375	GLN
1	D	384	GLU
1	D	391	GLU
1	D	392	LYS
1	D	395	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	87	ASN
1	A	135	HIS
1	A	165	GLN
1	A	184	ASN
1	A	219	ASN
1	A	273	ASN
1	A	292	HIS
1	A	303	ASN
1	A	318	ASN
1	A	335	HIS
1	A	342	HIS
1	A	344	HIS
1	A	364	ASN
1	A	368	GLN
1	B	20	HIS
1	B	88	GLN
1	B	103	ASN
1	B	108	ASN
1	B	161	HIS
1	B	190	ASN
1	B	219	ASN
1	B	344	HIS
1	B	346	ASN
1	B	355	ASN
1	B	368	GLN
1	C	20	HIS
1	C	34	ASN
1	C	46	GLN
1	C	55	HIS

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Mol	Chain	Res	Type
1	C	71	ASN
1	C	135	HIS
1	C	140	ASN
1	C	190	ASN
1	C	301	GLN
1	C	303	ASN
1	C	342	HIS
1	C	344	HIS
1	C	355	ASN
1	D	20	HIS
1	D	38	HIS
1	D	55	HIS
1	D	87	ASN
1	D	135	HIS
1	D	140	ASN
1	D	184	ASN
1	D	190	ASN
1	D	195	GLN
1	D	237	ASN
1	D	318	ASN
1	D	342	HIS
1	D	344	HIS
1	D	346	ASN
1	D	355	ASN
1	D	368	GLN
1	D	395	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

19 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
4	CIT	C	517	-	12,12,12	1.35	1 (8%)	17,17,17	1.52	3 (17%)
3	NAI	A	508	-	47,48,48	1.81	7 (14%)	64,73,73	1.72	16 (25%)
2	PO4	A	504	-	4,4,4	0.92	0	6,6,6	1.07	0
3	NAI	B	509	-	47,48,48	1.91	11 (23%)	64,73,73	1.91	16 (25%)
2	PO4	D	507	-	4,4,4	0.71	0	6,6,6	1.24	1 (16%)
2	PO4	C	501	-	4,4,4	1.28	0	6,6,6	0.87	0
2	PO4	B	503	-	4,4,4	1.38	1 (25%)	6,6,6	0.54	0
2	PO4	B	499	-	4,4,4	0.83	0	6,6,6	1.20	0
2	PO4	C	502	-	4,4,4	0.88	0	6,6,6	1.36	1 (16%)
2	PO4	A	500	-	4,4,4	1.54	1 (25%)	6,6,6	1.06	1 (16%)
2	PO4	D	505	-	4,4,4	1.12	0	6,6,6	0.85	0
4	CIT	C	515	-	12,12,12	1.28	1 (8%)	17,17,17	1.86	6 (35%)
3	NAI	D	511	-	47,48,48	1.83	8 (17%)	64,73,73	1.92	17 (26%)
3	NAI	C	510	-	47,48,48	1.78	9 (19%)	64,73,73	1.77	13 (20%)
4	CIT	B	516	-	12,12,12	1.33	0	17,17,17	2.03	5 (29%)
4	CIT	D	513	-	12,12,12	1.36	1 (8%)	17,17,17	2.13	7 (41%)
4	CIT	A	514	-	12,12,12	1.08	0	17,17,17	1.84	5 (29%)
4	CIT	A	518	-	12,12,12	0.97	0	17,17,17	2.47	10 (58%)
5	SO4	C	506	-	4,4,4	0.46	0	6,6,6	0.51	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
4	CIT	C	517	-	-	1/16/16/16	-
3	NAI	A	508	-	-	6/29/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	A	518	-	-	1/16/16/16	-
3	NAI	D	511	-	-	7/29/72/72	0/5/5/5
3	NAI	C	510	-	-	11/29/72/72	0/5/5/5
4	CIT	C	515	-	-	0/16/16/16	-
4	CIT	B	516	-	-	3/16/16/16	-
4	CIT	D	513	-	-	8/16/16/16	-
3	NAI	B	509	-	-	7/29/72/72	0/5/5/5
4	CIT	A	514	-	-	3/16/16/16	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	511	NAI	O7N-C7N	7.32	1.41	1.24
3	B	509	NAI	O7N-C7N	6.92	1.40	1.24
3	A	508	NAI	O7N-C7N	6.77	1.40	1.24
3	C	510	NAI	O7N-C7N	6.50	1.39	1.24
3	A	508	NAI	C4N-C3N	-6.00	1.38	1.50
3	C	510	NAI	C4N-C3N	-5.74	1.39	1.50
3	B	509	NAI	C4N-C3N	-5.69	1.39	1.50
3	D	511	NAI	C4N-C3N	-5.63	1.39	1.50
3	D	511	NAI	C4N-C5N	-3.81	1.39	1.49
3	C	510	NAI	C4N-C5N	-3.76	1.39	1.49
3	A	508	NAI	C4N-C5N	-3.73	1.39	1.49
3	B	509	NAI	PA-O3	3.49	1.63	1.59
3	B	509	NAI	C4N-C5N	-3.41	1.40	1.49
3	B	509	NAI	PN-O3	3.34	1.63	1.59
3	A	508	NAI	C2A-N3A	3.02	1.39	1.33
3	D	511	NAI	PN-O3	3.02	1.62	1.59
4	D	513	CIT	C3-C6	-2.92	1.50	1.53
3	A	508	NAI	C2A-N1A	2.81	1.38	1.33
3	C	510	NAI	C8A-N7A	2.81	1.37	1.31
3	D	511	NAI	C8A-N7A	2.74	1.36	1.31
3	C	510	NAI	C2A-N1A	2.70	1.38	1.33
3	B	509	NAI	C2A-N1A	2.60	1.38	1.33
2	A	500	PO4	P-O4	-2.59	1.47	1.54
3	C	510	NAI	C2A-N3A	2.51	1.38	1.33
3	A	508	NAI	PN-O3	2.47	1.62	1.59
4	C	515	CIT	C3-C6	-2.43	1.50	1.53
3	B	509	NAI	C8A-N7A	2.41	1.36	1.31
3	B	509	NAI	C2A-N3A	2.35	1.38	1.33
3	D	511	NAI	C2A-N3A	2.32	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	511	NAI	C2A-N1A	2.31	1.38	1.33
3	C	510	NAI	C6N-C5N	2.30	1.40	1.33
3	B	509	NAI	C2N-C3N	2.30	1.41	1.35
3	B	509	NAI	C5A-N7A	-2.24	1.35	1.39
3	A	508	NAI	C8A-N7A	2.19	1.35	1.31
4	C	517	CIT	C3-C6	-2.19	1.51	1.53
3	B	509	NAI	C6N-C5N	2.12	1.39	1.33
3	D	511	NAI	C6N-C5N	2.12	1.39	1.33
3	C	510	NAI	C5A-N7A	-2.08	1.35	1.39
2	B	503	PO4	P-O2	-2.07	1.48	1.54
3	C	510	NAI	PN-O1N	-2.05	1.45	1.55

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	511	NAI	N3A-C2A-N1A	-5.51	120.25	128.58
3	B	509	NAI	N3A-C2A-N1A	-5.39	120.42	128.58
3	C	510	NAI	N3A-C2A-N1A	-5.39	120.42	128.58
3	B	509	NAI	O4D-C1D-N1N	4.89	117.42	108.08
3	D	511	NAI	N9A-C8A-N7A	-4.77	107.17	113.94
3	C	510	NAI	C5A-C4A-N3A	-4.67	120.29	126.72
3	C	510	NAI	O7N-C7N-C3N	-4.60	112.24	120.90
3	A	508	NAI	C5A-C4A-N3A	-4.34	120.73	126.72
3	B	509	NAI	C5A-C4A-N3A	-4.32	120.77	126.72
4	A	518	CIT	O6-C6-C3	4.14	121.09	113.14
3	B	509	NAI	C5A-C6A-N6A	-4.04	113.29	123.29
4	D	513	CIT	O7-C3-C6	-4.01	103.27	108.96
4	A	514	CIT	O6-C6-C3	3.95	120.72	113.14
4	B	516	CIT	O6-C6-C3	3.94	120.71	113.14
3	C	510	NAI	N9A-C8A-N7A	-3.91	108.39	113.94
3	A	508	NAI	O7N-C7N-C3N	-3.87	113.61	120.90
3	B	509	NAI	N9A-C8A-N7A	-3.83	108.51	113.94
3	A	508	NAI	N3A-C2A-N1A	-3.82	122.81	128.58
4	C	515	CIT	O6-C6-C3	3.75	120.33	113.14
4	D	513	CIT	C3-C4-C5	-3.73	103.71	113.92
3	D	511	NAI	C5A-N7A-C8A	3.67	109.22	103.45
3	C	510	NAI	C3N-C7N-N7N	3.63	124.12	117.67
3	A	508	NAI	C3N-C2N-N1N	-3.62	117.88	123.20
4	A	518	CIT	C3-C4-C5	-3.62	104.03	113.92
3	D	511	NAI	C4A-N9A-C1B	-3.58	118.26	126.63
4	A	518	CIT	C4-C3-C2	3.53	118.37	109.31
4	B	516	CIT	C2-C3-C6	3.51	117.80	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	511	NAI	C2D-C1D-N1N	-3.47	104.76	113.31
4	A	514	CIT	O4-C5-O3	-3.47	114.42	123.33
3	C	510	NAI	C2A-N3A-C4A	3.44	120.24	111.83
4	C	517	CIT	C3-C4-C5	-3.34	104.78	113.92
3	B	509	NAI	C5A-N7A-C8A	3.34	108.69	103.45
4	D	513	CIT	O6-C6-C3	3.33	119.53	113.14
3	D	511	NAI	O3D-C3D-C2D	-3.23	101.45	111.82
3	C	510	NAI	C5A-N7A-C8A	3.22	108.51	103.45
4	B	516	CIT	O2-C1-O1	-3.20	115.11	123.33
3	D	511	NAI	C4A-C5A-N7A	-3.16	106.96	110.58
4	C	515	CIT	O7-C3-C6	-3.14	104.50	108.96
3	D	511	NAI	C2A-N3A-C4A	3.13	119.48	111.83
3	A	508	NAI	C4A-C5A-N7A	-3.07	107.07	110.58
3	B	509	NAI	O2A-PA-O3	3.05	115.52	107.27
3	B	509	NAI	C6A-C5A-C4A	3.04	121.33	117.18
4	C	517	CIT	O6-C6-C3	3.03	118.96	113.14
3	D	511	NAI	C5A-C4A-N3A	-3.03	122.54	126.72
4	A	518	CIT	O2-C1-C2	3.03	123.95	114.35
3	A	508	NAI	C5A-N7A-C8A	3.03	108.21	103.45
4	A	518	CIT	O7-C3-C6	3.00	113.22	108.96
3	A	508	NAI	N9A-C8A-N7A	-2.98	109.71	113.94
3	B	509	NAI	C2A-N3A-C4A	2.96	119.07	111.83
3	D	511	NAI	C4A-N9A-C8A	2.96	108.84	105.74
3	C	510	NAI	O3D-C3D-C2D	-2.95	102.36	111.82
4	D	513	CIT	C3-C2-C1	-2.94	105.89	113.92
4	D	513	CIT	O4-C5-C4	2.90	123.55	114.35
3	B	509	NAI	N3A-C4A-N9A	2.90	132.09	127.17
3	A	508	NAI	O4D-C1D-N1N	2.89	113.60	108.08
3	A	508	NAI	C6N-N1N-C2N	2.88	122.41	119.32
4	B	516	CIT	O7-C3-C6	-2.86	104.90	108.96
2	C	502	PO4	O4-P-O3	2.81	116.67	107.91
3	A	508	NAI	C5A-C4A-N9A	2.80	108.86	105.81
3	A	508	NAI	O1N-PN-O3	2.78	114.79	107.27
4	A	518	CIT	O2-C1-O1	-2.71	116.38	123.33
4	A	518	CIT	O7-C3-C4	-2.69	103.23	109.38
3	C	510	NAI	N3A-C4A-N9A	2.69	131.74	127.17
3	B	509	NAI	C3N-C2N-N1N	-2.67	119.29	123.20
3	C	510	NAI	C4A-C5A-N7A	-2.64	107.56	110.58
4	C	517	CIT	O4-C5-C4	2.63	122.67	114.35
4	A	518	CIT	O4-C5-C4	2.63	122.67	114.35
3	D	511	NAI	C1B-N9A-C8A	2.61	132.90	127.09
4	A	514	CIT	O4-C5-C4	2.60	122.58	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	NAI	C2A-N3A-C4A	2.59	118.16	111.83
4	A	514	CIT	O2-C1-O1	-2.57	116.72	123.33
3	A	508	NAI	C6A-C5A-C4A	2.57	120.69	117.18
3	D	511	NAI	C2B-C3B-C4B	2.53	107.51	102.61
3	D	511	NAI	O4B-C1B-N9A	2.53	112.95	108.09
2	D	507	PO4	O4-P-O2	2.52	115.74	107.91
4	C	515	CIT	C3-C2-C1	-2.49	107.11	113.92
3	D	511	NAI	O4D-C1D-C2D	-2.49	101.29	106.62
4	C	515	CIT	O2-C1-C2	2.48	122.22	114.35
3	D	511	NAI	C3N-C2N-N1N	-2.46	119.59	123.20
3	C	510	NAI	C3N-C2N-N1N	-2.45	119.61	123.20
3	B	509	NAI	C6N-N1N-C2N	2.43	121.92	119.32
4	B	516	CIT	C3-C4-C5	-2.42	107.30	113.92
4	D	513	CIT	C4-C3-C6	2.37	115.28	110.03
3	B	509	NAI	C4A-C5A-N7A	-2.36	107.89	110.58
3	D	511	NAI	O3-PA-O1A	-2.36	103.61	110.70
4	C	515	CIT	O2-C1-O1	-2.35	117.29	123.33
4	A	518	CIT	O4-C5-O3	-2.27	117.50	123.33
4	A	514	CIT	O2-C1-C2	2.26	121.52	114.35
4	A	518	CIT	C3-C2-C1	-2.25	107.76	113.92
4	C	515	CIT	C3-C4-C5	-2.23	107.83	113.92
3	C	510	NAI	O3D-C3D-C4D	-2.21	104.72	111.08
3	A	508	NAI	C2D-C1D-N1N	-2.21	107.86	113.31
3	B	509	NAI	C2B-C3B-C4B	2.20	106.86	102.61
3	B	509	NAI	C3D-C2D-C1D	-2.19	97.33	101.46
3	C	510	NAI	O4D-C1D-N1N	2.16	112.21	108.08
3	A	508	NAI	C3N-C7N-N7N	2.13	121.46	117.67
3	B	509	NAI	O4B-C4B-C5B	2.12	116.12	109.33
3	A	508	NAI	O3B-C3B-C4B	-2.10	105.06	111.08
3	D	511	NAI	O4D-C1D-N1N	2.08	112.05	108.08
2	A	500	PO4	O4-P-O1	-2.07	103.64	110.95
4	D	513	CIT	O3-C5-C4	-2.06	117.13	122.95

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	509	NAI	C5D-O5D-PN-O3
3	B	509	NAI	C5D-O5D-PN-O2N
4	D	513	CIT	C2-C3-C4-C5
4	D	513	CIT	O7-C3-C4-C5
4	D	513	CIT	C6-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	D	513	CIT	C2-C3-C6-O5
4	D	513	CIT	C2-C3-C6-O6
4	D	513	CIT	O7-C3-C6-O5
4	D	513	CIT	O7-C3-C6-O6
4	A	514	CIT	C6-C3-C4-C5
4	A	514	CIT	O7-C3-C4-C5
4	A	514	CIT	C2-C3-C4-C5
3	D	511	NAI	O4B-C4B-C5B-O5B
3	A	508	NAI	O4B-C4B-C5B-O5B
4	B	516	CIT	O7-C3-C6-O6
3	C	510	NAI	O4B-C4B-C5B-O5B
3	C	510	NAI	C3B-C4B-C5B-O5B
3	D	511	NAI	C3B-C4B-C5B-O5B
3	C	510	NAI	C2B-C1B-N9A-C8A
3	A	508	NAI	C2B-C1B-N9A-C8A
3	C	510	NAI	C2D-C1D-N1N-C2N
3	C	510	NAI	C2D-C1D-N1N-C6N
3	C	510	NAI	C5D-O5D-PN-O2N
3	D	511	NAI	PN-O3-PA-O1A
3	C	510	NAI	C2B-C1B-N9A-C4A
4	D	513	CIT	C4-C3-C6-O5
3	A	508	NAI	O4D-C1D-N1N-C2N
3	B	509	NAI	O4D-C1D-N1N-C2N
3	C	510	NAI	O4D-C1D-N1N-C2N
3	D	511	NAI	O4D-C1D-N1N-C2N
3	A	508	NAI	C3B-C4B-C5B-O5B
3	B	509	NAI	O4D-C4D-C5D-O5D
3	C	510	NAI	O4D-C1D-N1N-C6N
3	B	509	NAI	PN-O3-PA-O1A
3	C	510	NAI	PN-O3-PA-O1A
3	D	511	NAI	PN-O3-PA-O2A
4	B	516	CIT	C2-C3-C6-O6
3	D	511	NAI	C2D-C1D-N1N-C2N
4	C	517	CIT	C6-C3-C4-C5
3	C	510	NAI	O4B-C1B-N9A-C8A
3	A	508	NAI	C2D-C1D-N1N-C2N
3	B	509	NAI	O4B-C4B-C5B-O5B
4	B	516	CIT	O7-C3-C6-O5
4	A	518	CIT	C1-C2-C3-C6
3	B	509	NAI	C2B-C1B-N9A-C8A
3	A	508	NAI	O4B-C1B-N9A-C8A
3	D	511	NAI	C2D-C1D-N1N-C6N

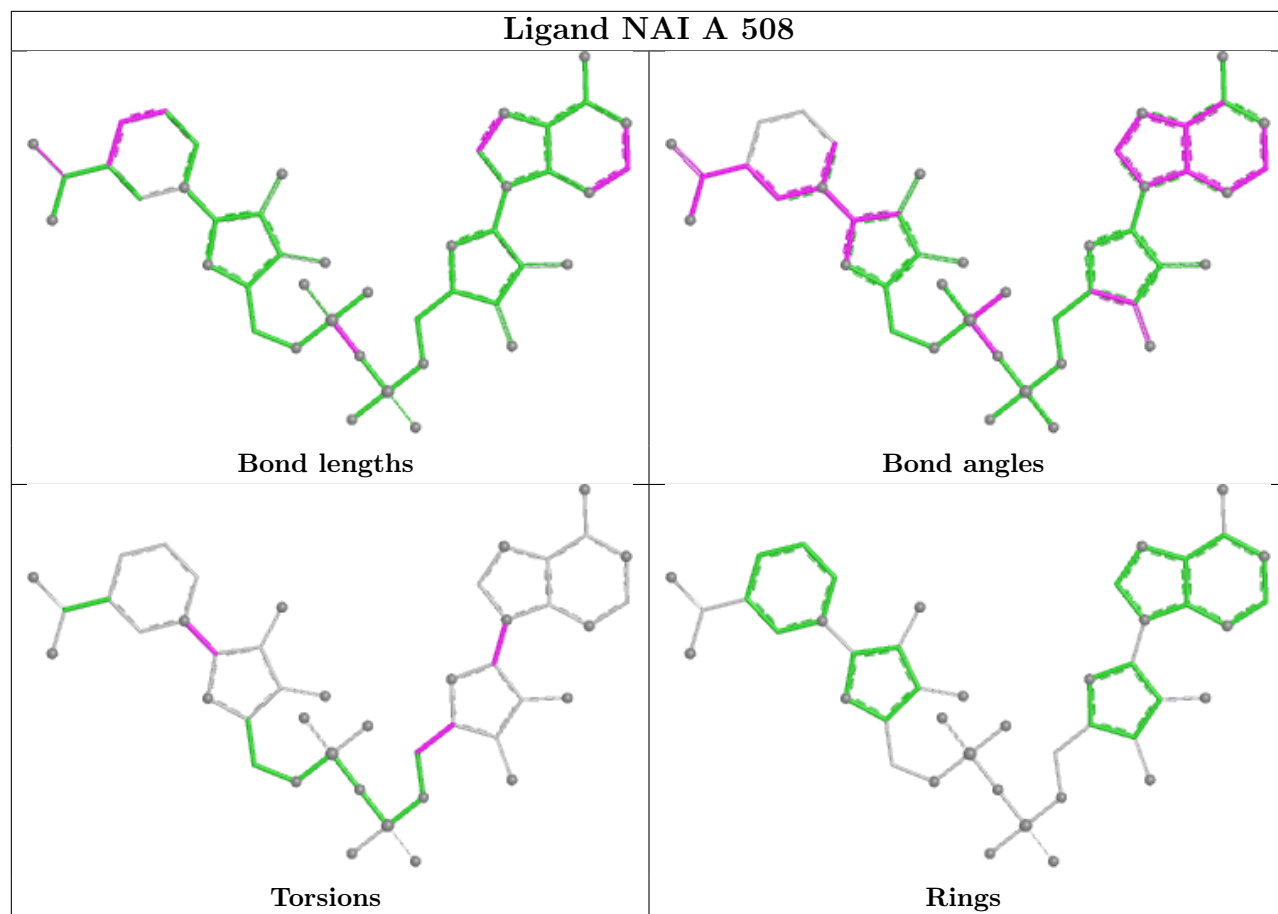
There are no ring outliers.

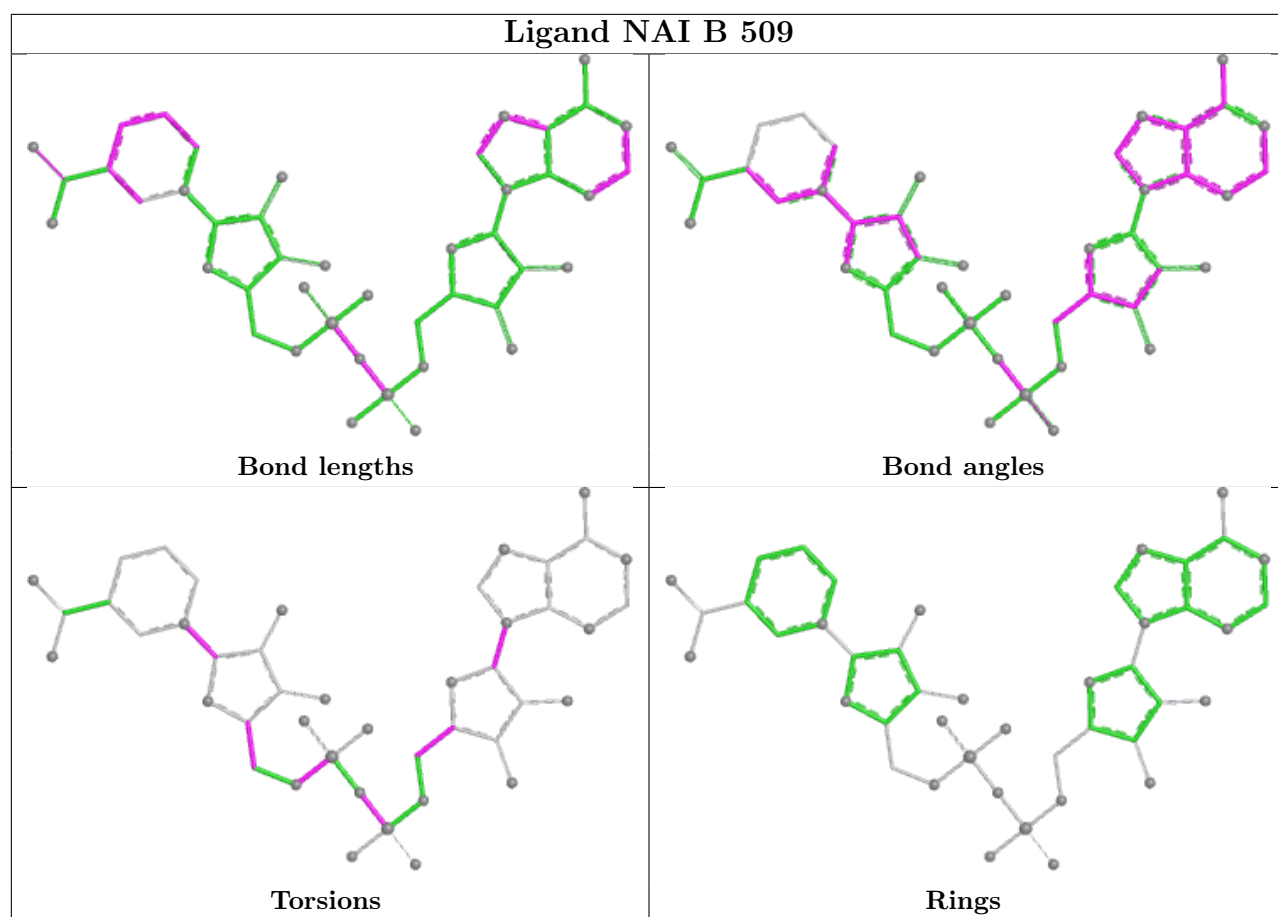
11 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	517	CIT	4	0
3	A	508	NAI	2	0
3	B	509	NAI	4	0
2	B	499	PO4	3	0
4	C	515	CIT	2	0
3	D	511	NAI	1	0
4	B	516	CIT	4	0
4	D	513	CIT	4	0
4	A	514	CIT	5	0
4	A	518	CIT	2	0
5	C	506	SO4	1	0

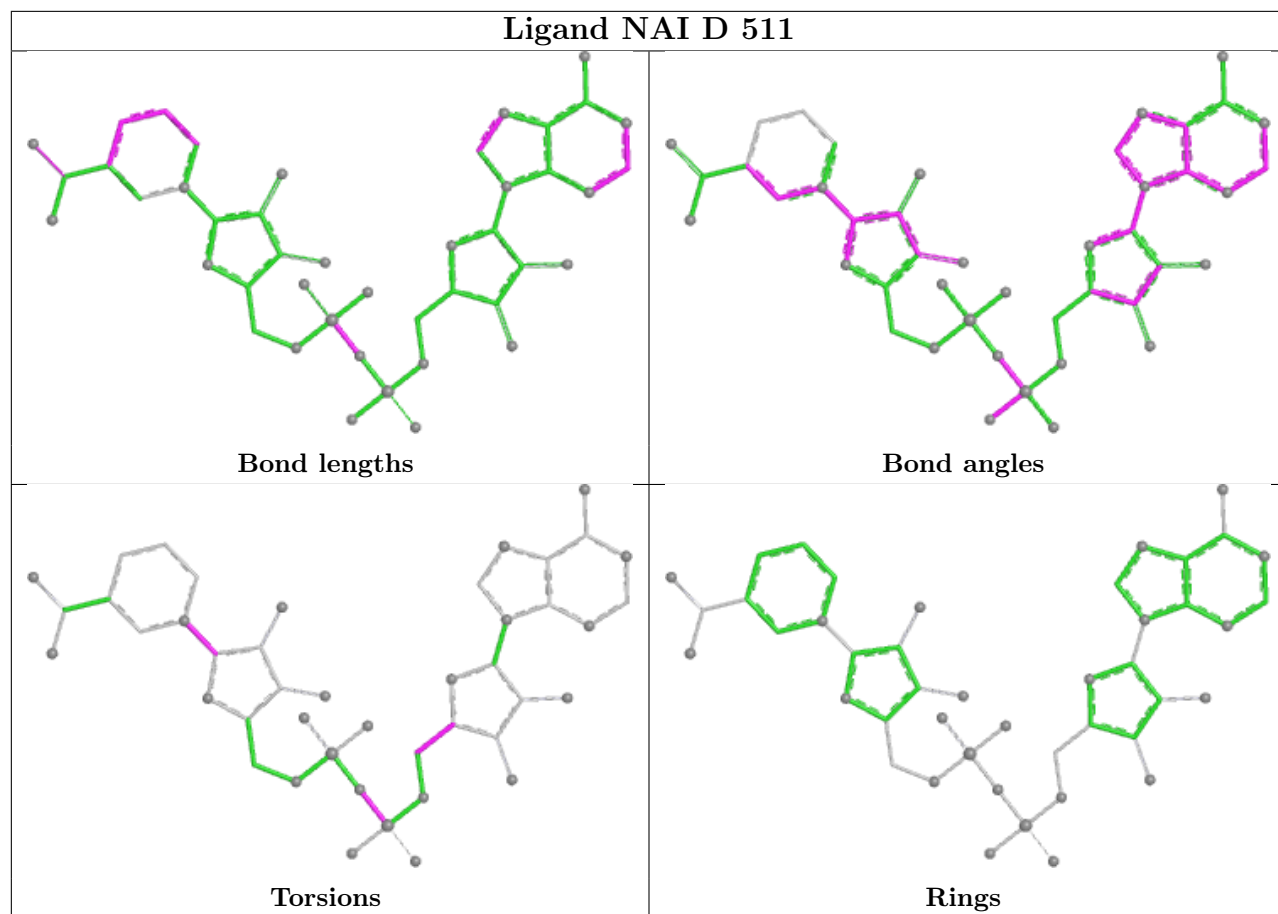
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

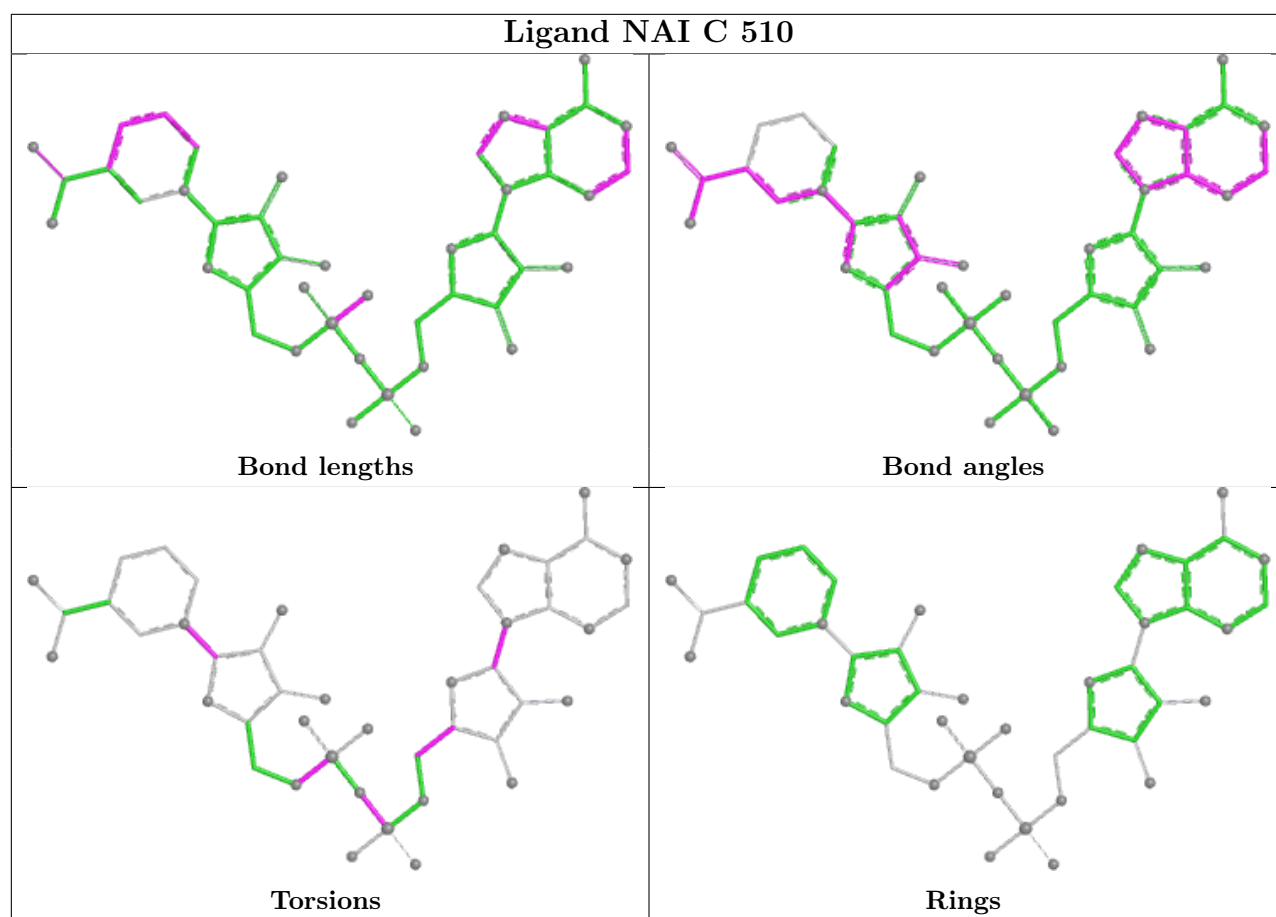
Ligand NAI A 508





Ligand NAI D 511





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	406/410 (99%)	-0.37	5 (1%) 76 73	20, 38, 66, 87	3 (0%)
1	B	404/410 (98%)	-0.43	3 (0%) 84 82	11, 37, 59, 73	3 (0%)
1	C	406/410 (99%)	-0.46	4 (0%) 79 76	11, 37, 63, 92	8 (1%)
1	D	403/410 (98%)	-0.43	3 (0%) 84 82	16, 36, 68, 87	6 (1%)
All	All	1619/1640 (98%)	-0.42	15 (0%) 81 78	11, 37, 65, 92	20 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	45	GLU	4.5
1	B	407	ARG	3.9
1	A	52	ARG	3.7
1	C	136	ARG	3.6
1	D	62	ARG	3.6
1	A	62	ARG	3.4
1	D	97	ARG	3.1
1	A	50	SER	2.7
1	A	45	GLU	2.4
1	C	10	LYS	2.4
1	D	12	LYS	2.3
1	B	186	LEU	2.3
1	C	335	HIS	2.3
1	C	75	LYS	2.0
1	A	334	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](#)

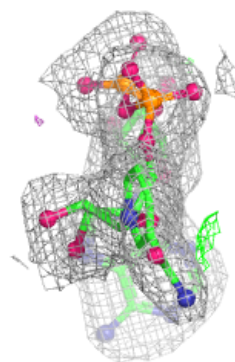
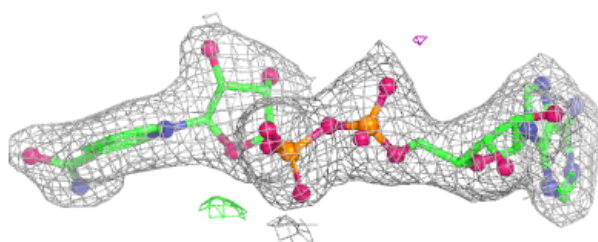
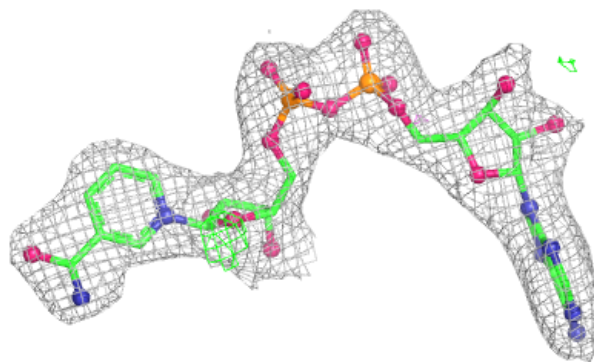
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CIT	A	514	13/13	0.76	0.13	58,72,97,102	0
2	PO4	B	499	5/5	0.82	0.10	62,62,75,76	0
2	PO4	A	504	5/5	0.82	0.13	61,67,69,79	0
4	CIT	A	518	13/13	0.82	0.11	59,68,81,96	0
4	CIT	B	516	13/13	0.83	0.10	29,53,60,66	0
4	CIT	C	515	13/13	0.87	0.10	44,62,73,81	0
4	CIT	D	513	13/13	0.88	0.12	49,69,77,85	0
4	CIT	C	517	13/13	0.89	0.12	61,71,82,89	0
2	PO4	D	507	5/5	0.92	0.10	54,56,59,64	0
2	PO4	D	505	5/5	0.93	0.11	51,61,71,71	0
5	SO4	C	506	5/5	0.93	0.10	56,57,70,72	0
3	NAI	C	510	44/44	0.96	0.06	21,41,49,53	0
3	NAI	B	509	44/44	0.96	0.06	26,45,51,59	0
3	NAI	A	508	44/44	0.97	0.06	18,37,48,51	0
3	NAI	D	511	44/44	0.97	0.06	27,39,49,53	0
2	PO4	B	503	5/5	0.97	0.05	35,39,45,48	0
2	PO4	C	501	5/5	0.98	0.05	28,32,36,41	0
2	PO4	C	502	5/5	0.99	0.04	25,28,35,37	0
2	PO4	A	500	5/5	0.99	0.04	16,25,29,30	0

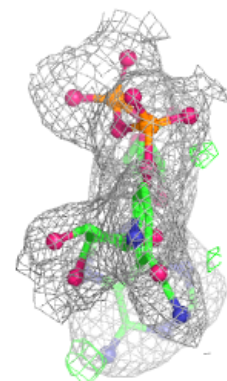
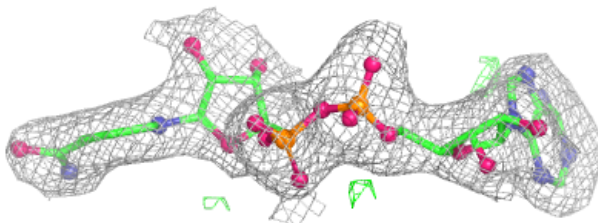
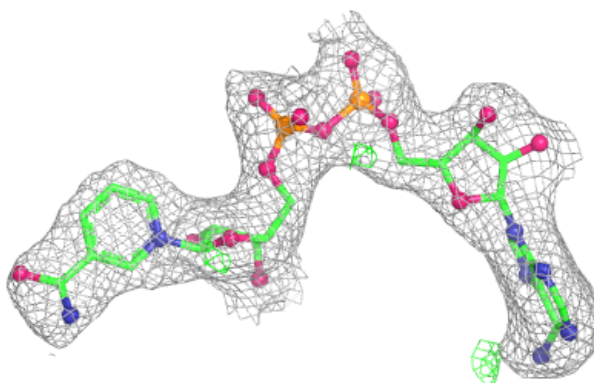
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAI C 510:

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

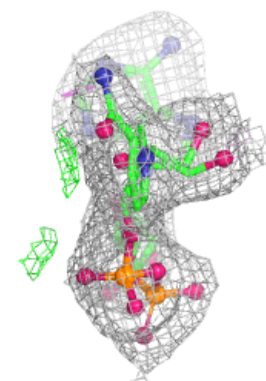
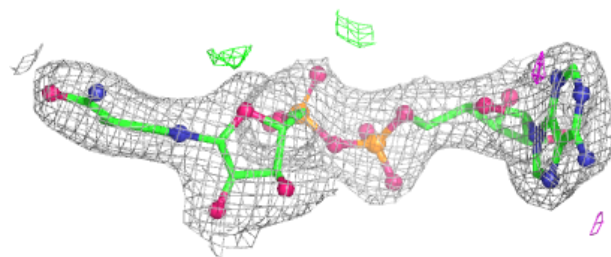
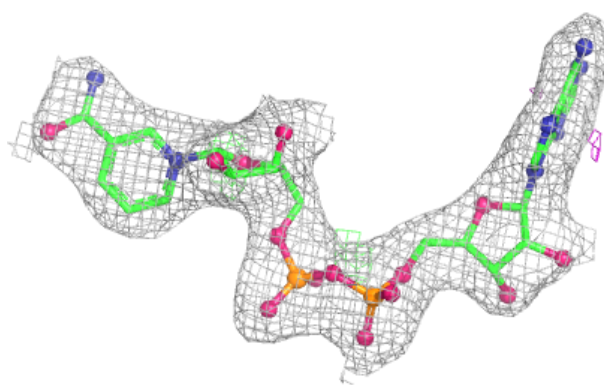
**Electron density around NAI B 509:**

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

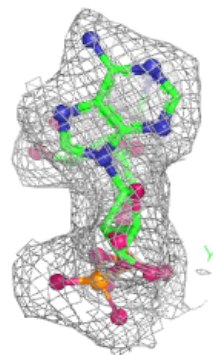
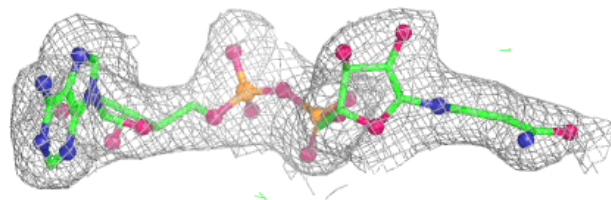
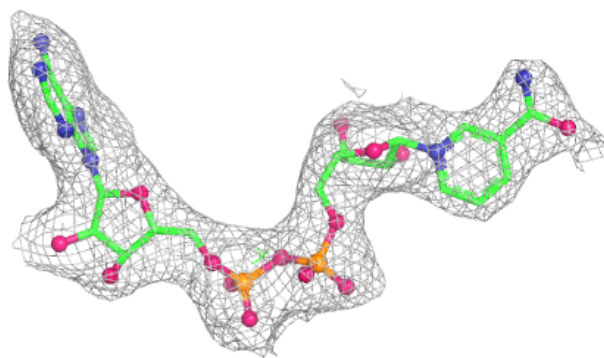


Electron density around NAI A 508:

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

**Electron density around NAI D 511:**

$2mF_o-DF_c$ (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.