



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:49 AM UTC

PDB ID : 1PJ2 / pdb_00001pj2
Title : Crystal structure of human mitochondrial NAD(P)+-dependent malic enzyme in a pentary complex with natural substrate malate, cofactor NADH, Mn⁺⁺, and allosteric activator fumarate
Authors : Tao, X.; Yang, Z.; Tong, L.
Deposited on : 2003-05-30
Resolution : 2.30 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

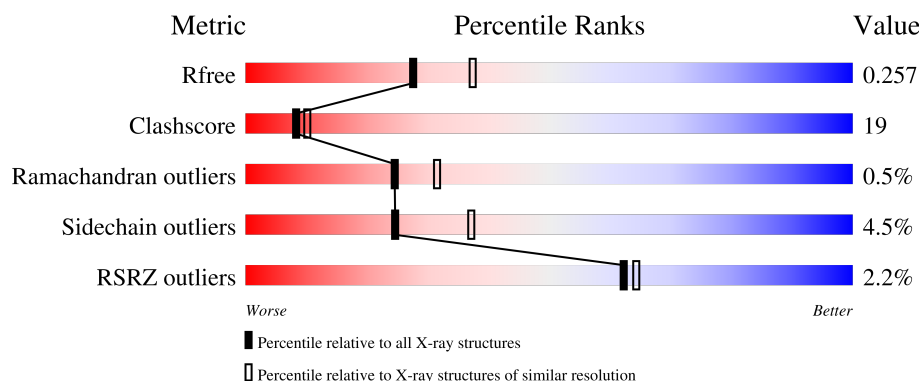
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	564	0% 64% 31% ..
1	B	564	3% 56% 38% ..
1	C	564	2% 68% 26% ..
1	D	564	2% 61% 33% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18640 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 NAD-dependent malic enzyme, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	B	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	C	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	D	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			

There are 56 discrepancies between the modelled and reference sequences:

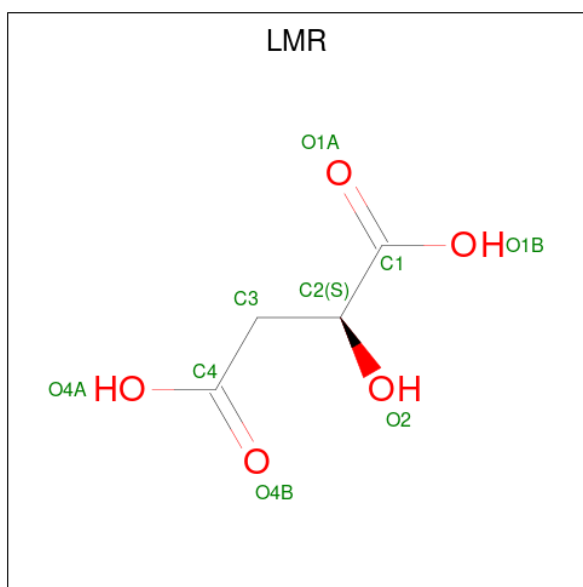
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MSE	MET	modified residue	UNP P23368
A	38	MSE	MET	modified residue	UNP P23368
A	47	MSE	MET	modified residue	UNP P23368
A	75	MSE	MET	modified residue	UNP P23368
A	86	MSE	MET	modified residue	UNP P23368
A	108	MSE	MET	modified residue	UNP P23368
A	177	MSE	MET	modified residue	UNP P23368
A	219	MSE	MET	modified residue	UNP P23368
A	239	MSE	MET	modified residue	UNP P23368
A	325	MSE	MET	modified residue	UNP P23368
A	327	MSE	MET	modified residue	UNP P23368
A	343	MSE	MET	modified residue	UNP P23368
A	407	MSE	MET	modified residue	UNP P23368
A	539	MSE	MET	modified residue	UNP P23368
B	1029	MSE	MET	modified residue	UNP P23368
B	1038	MSE	MET	modified residue	UNP P23368
B	1047	MSE	MET	modified residue	UNP P23368
B	1075	MSE	MET	modified residue	UNP P23368
B	1086	MSE	MET	modified residue	UNP P23368
B	1108	MSE	MET	modified residue	UNP P23368
B	1177	MSE	MET	modified residue	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1219	MSE	MET	modified residue	UNP P23368
B	1239	MSE	MET	modified residue	UNP P23368
B	1325	MSE	MET	modified residue	UNP P23368
B	1327	MSE	MET	modified residue	UNP P23368
B	1343	MSE	MET	modified residue	UNP P23368
B	1407	MSE	MET	modified residue	UNP P23368
B	1539	MSE	MET	modified residue	UNP P23368
C	2029	MSE	MET	modified residue	UNP P23368
C	2038	MSE	MET	modified residue	UNP P23368
C	2047	MSE	MET	modified residue	UNP P23368
C	2075	MSE	MET	modified residue	UNP P23368
C	2086	MSE	MET	modified residue	UNP P23368
C	2108	MSE	MET	modified residue	UNP P23368
C	2177	MSE	MET	modified residue	UNP P23368
C	2219	MSE	MET	modified residue	UNP P23368
C	2239	MSE	MET	modified residue	UNP P23368
C	2325	MSE	MET	modified residue	UNP P23368
C	2327	MSE	MET	modified residue	UNP P23368
C	2343	MSE	MET	modified residue	UNP P23368
C	2407	MSE	MET	modified residue	UNP P23368
C	2539	MSE	MET	modified residue	UNP P23368
D	3029	MSE	MET	modified residue	UNP P23368
D	3038	MSE	MET	modified residue	UNP P23368
D	3047	MSE	MET	modified residue	UNP P23368
D	3075	MSE	MET	modified residue	UNP P23368
D	3086	MSE	MET	modified residue	UNP P23368
D	3108	MSE	MET	modified residue	UNP P23368
D	3177	MSE	MET	modified residue	UNP P23368
D	3219	MSE	MET	modified residue	UNP P23368
D	3239	MSE	MET	modified residue	UNP P23368
D	3325	MSE	MET	modified residue	UNP P23368
D	3327	MSE	MET	modified residue	UNP P23368
D	3343	MSE	MET	modified residue	UNP P23368
D	3407	MSE	MET	modified residue	UNP P23368
D	3539	MSE	MET	modified residue	UNP P23368

- Molecule 2 is (2S)-2-hydroxybutanedioic acid (CCD ID: LMR) (formula: C₄H₆O₅).

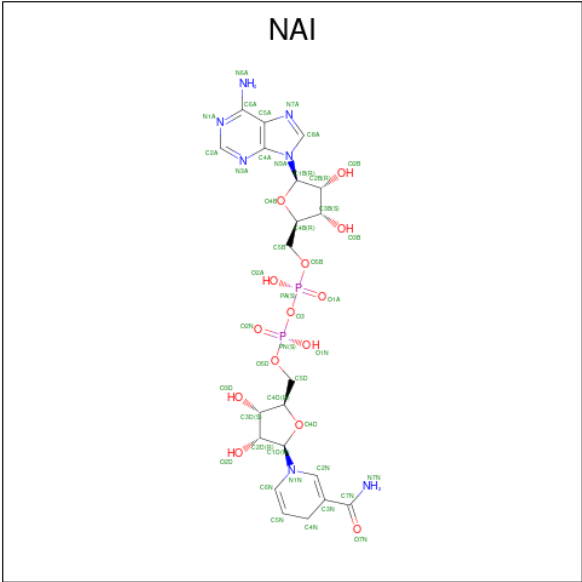


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		
2	B	1	Total	C	O	0	0
			9	4	5		
2	C	1	Total	C	O	0	0
			9	4	5		
2	D	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

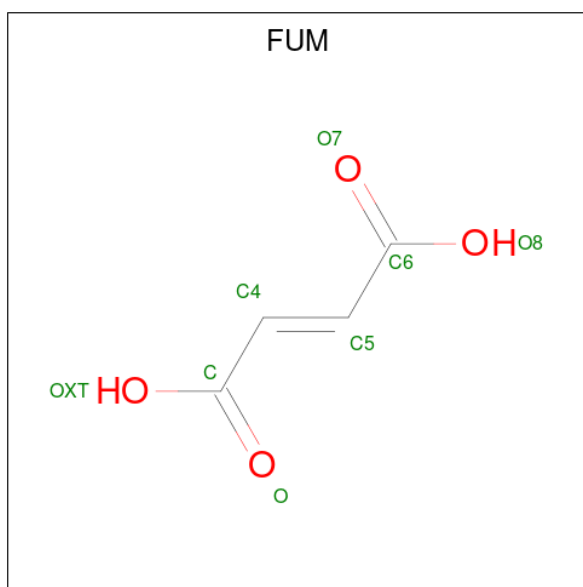
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	A	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	9	0
			44	21	7	14	2		

- Molecule 5 is FUMARIC ACID (CCD ID: FUM) (formula: C₄H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	4	4		
5	B	1	Total	C	O	0	0
			8	4	4		
5	C	1	Total	C	O	0	0
			8	4	4		
5	D	1	Total	C	O	0	0
			8	4	4		

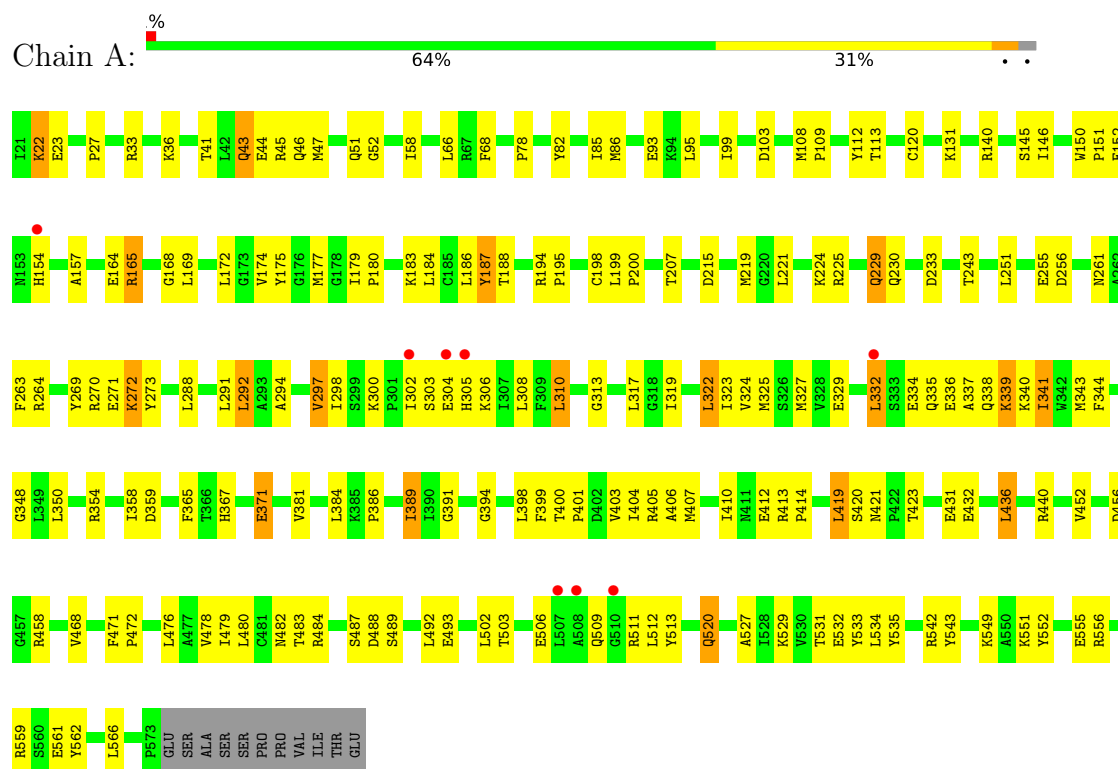
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	193	Total	O	0	0
			193	193		
6	B	164	Total	O	0	0
			164	164		
6	C	212	Total	O	0	0
			212	212		
6	D	179	Total	O	0	0
			179	179		

3 Residue-property plots

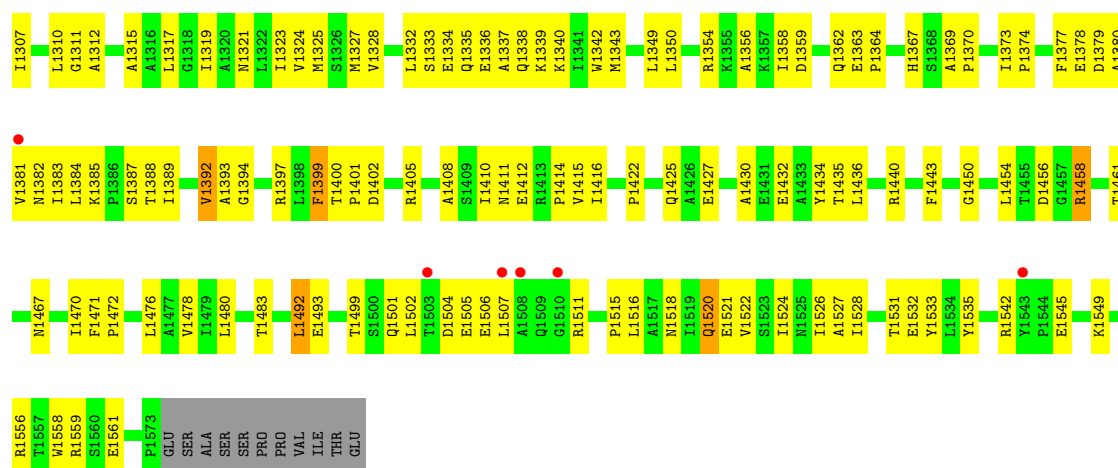
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NAD-dependent malic enzyme, mitochondrial

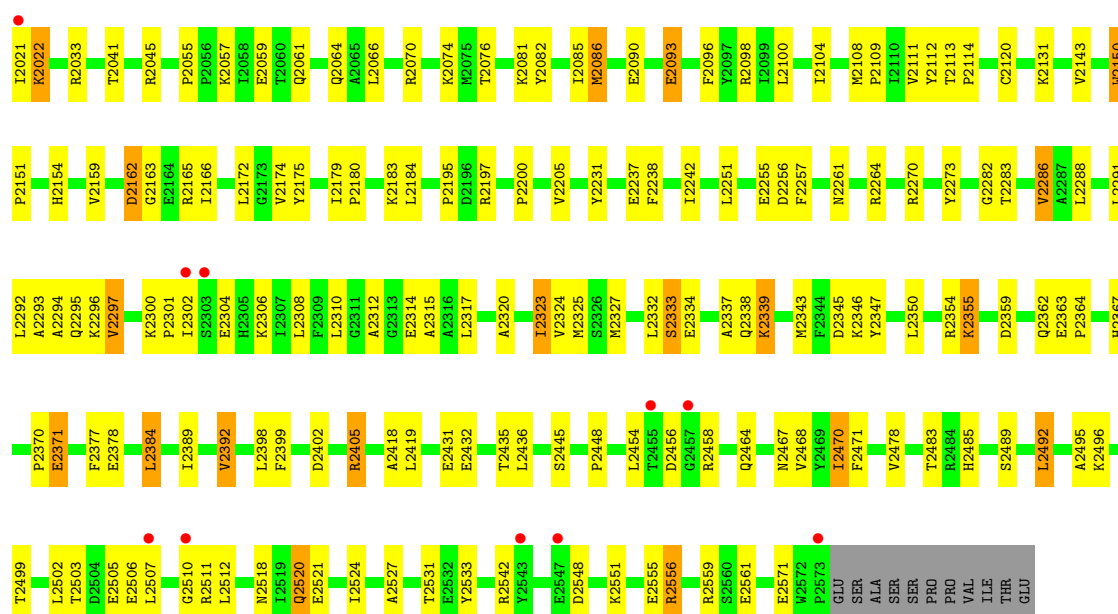


- Molecule 1: NAD-dependent malic enzyme, mitochondrial

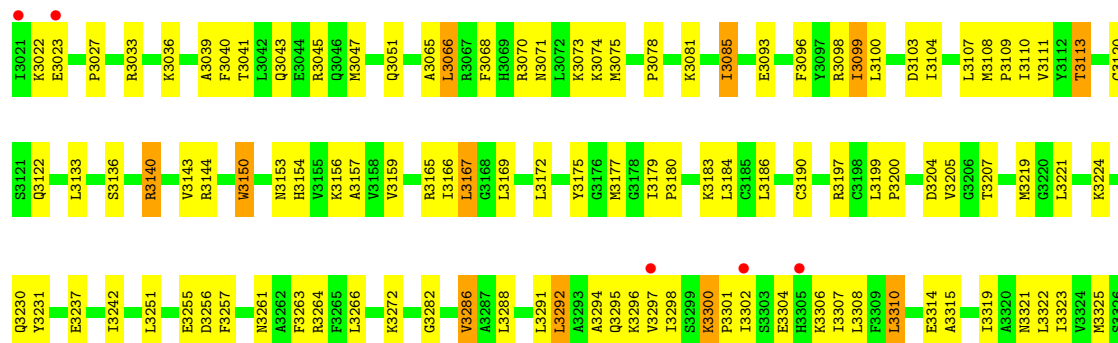


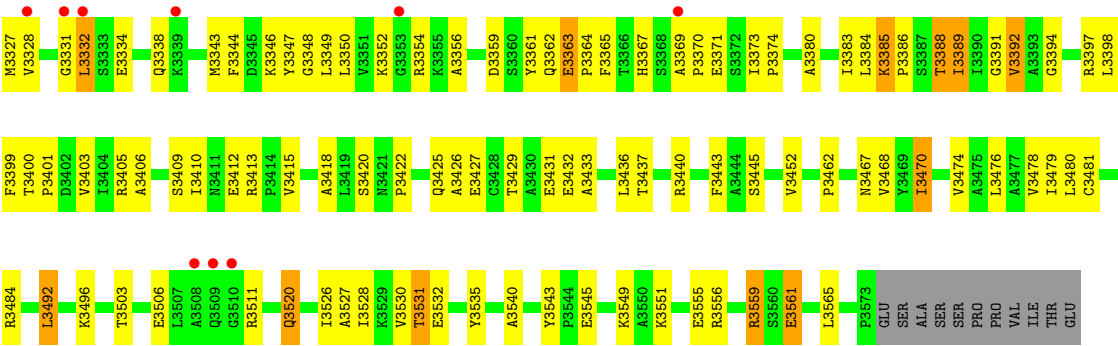


- Molecule 1: NAD-dependent malic enzyme, mitochondrial



- Molecule 1: NAD-dependent malic enzyme, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	227.28Å 117.34Å 113.02Å 90.00° 109.79° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.9 (20.00-2.30) 94.8 (20.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.256 0.206 , 0.257	Depositor DCC
R_{free} test set	8855 reflections (7.52%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18640	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% 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: LMR, MN, FUM, NAI

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/4447	0.91	11/5998 (0.2%)
1	B	0.42	0/4447	0.94	14/5998 (0.2%)
1	C	0.44	0/4447	0.94	16/5998 (0.3%)
1	D	0.41	0/4447	0.91	10/5998 (0.2%)
All	All	0.42	0/17788	0.93	51/23992 (0.2%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1303	SER	N-CA-C	-9.55	101.83	113.19
1	C	2150	TRP	CA-C-N	8.70	128.71	119.05
1	C	2150	TRP	C-N-CA	8.70	128.71	119.05
1	D	3470	ILE	N-CA-C	8.68	119.63	111.48
1	C	2470	ILE	N-CA-C	6.80	117.87	111.48
1	C	2162	ASP	N-CA-C	-6.50	103.77	112.94
1	B	1399	PHE	N-CA-C	-6.40	101.79	110.68
1	D	3256	ASP	N-CA-C	6.38	120.19	111.39
1	D	3150	TRP	CA-C-N	6.35	125.84	119.24
1	D	3150	TRP	C-N-CA	6.35	125.84	119.24
1	A	256	ASP	N-CA-C	6.12	119.62	111.30
1	C	2333	SER	N-CA-C	-5.85	102.98	110.53
1	A	187	TYR	N-CA-C	-5.68	104.99	111.07
1	B	1269	TYR	N-CA-C	5.67	120.47	113.50
1	A	423	THR	N-CA-C	5.61	118.12	111.33
1	C	2323	ILE	N-CA-C	-5.61	105.06	110.72
1	C	2098	ARG	N-CA-C	-5.59	105.27	111.36
1	D	3470	ILE	CB-CA-C	-5.54	107.00	111.71
1	B	1307	ILE	N-CA-C	5.53	116.55	108.58
1	B	1461	THR	CA-C-N	5.53	125.29	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1461	THR	C-N-CA	5.53	125.29	119.76
1	A	419	LEU	N-CA-C	5.52	120.02	113.28
1	A	310	LEU	N-CA-C	-5.49	97.54	107.75
1	D	3310	LEU	N-CA-C	-5.48	97.56	107.75
1	C	2470	ILE	CB-CA-C	-5.46	107.07	111.71
1	B	1076	THR	N-CA-C	5.44	119.92	112.68
1	C	2310	LEU	N-CA-C	-5.44	98.90	108.20
1	D	3257	PHE	N-CA-C	-5.37	102.51	110.46
1	B	1443	PHE	N-CA-C	5.37	118.81	110.17
1	C	2076	THR	N-CA-C	5.34	119.79	113.12
1	D	3098	ARG	N-CA-C	-5.28	105.60	111.36
1	C	2256	ASP	N-CA-C	5.27	118.71	111.54
1	A	512	LEU	N-CA-C	-5.26	106.10	112.88
1	D	3443	PHE	N-CA-C	5.24	118.28	109.95
1	C	2093	GLU	N-CA-C	5.22	116.65	111.07
1	B	1310	LEU	N-CA-C	-5.17	99.35	108.20
1	A	269	TYR	N-CA-C	5.17	120.58	113.97
1	A	513	TYR	CA-C-N	5.16	123.43	119.66
1	A	513	TYR	C-N-CA	5.16	123.43	119.66
1	B	1194	ARG	CA-C-N	5.16	124.77	119.05
1	B	1194	ARG	C-N-CA	5.16	124.77	119.05
1	B	1450	GLY	CA-C-N	5.16	125.15	119.89
1	B	1450	GLY	C-N-CA	5.16	125.15	119.89
1	C	2257	PHE	N-CA-C	-5.14	102.91	110.52
1	A	297	VAL	N-CA-C	-5.13	108.28	113.20
1	A	341	ILE	N-CA-C	5.11	115.21	107.80
1	C	2556	ARG	N-CA-C	5.09	118.52	112.72
1	D	3167	LEU	CB-CA-C	-5.07	110.71	116.54
1	C	2510	GLY	N-CA-C	-5.07	108.07	115.63
1	C	2419	LEU	N-CA-C	5.06	119.45	113.28
1	B	1311	GLY	N-CA-C	-5.00	105.48	112.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4367	0	4407	158	0
1	B	4367	0	4407	213	0
1	C	4367	0	4407	136	0
1	D	4367	0	4407	180	0
2	A	9	0	3	1	0
2	B	9	0	3	2	0
2	C	9	0	3	2	0
2	D	9	0	3	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	88	0	54	4	0
4	B	88	0	54	1	0
4	C	88	0	54	7	0
4	D	88	0	54	4	0
5	A	8	0	1	0	0
5	B	8	0	1	0	0
5	C	8	0	1	0	0
5	D	8	0	1	0	0
6	A	193	0	0	12	0
6	B	164	0	0	3	0
6	C	212	0	0	5	0
6	D	179	0	0	6	0
All	All	18640	0	17860	684	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 19.

All (684) 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:B:1029:MSE:HE2	1:B:1050:LEU:HD22	1.23	1.13
1:A:381:VAL:HG13	1:A:407:MSE:HE3	1.42	1.01
1:D:3315:ALA:HB3	1:D:3392:VAL:HG21	1.43	0.99
1:B:1210:ILE:HD12	1:B:1210:ILE:H	1.26	0.99
1:D:3343:MSE:HE2	1:D:3365:PHE:HB2	1.46	0.97
1:A:532:GLU:HG2	1:A:549:LYS:HG3	1.44	0.97
1:C:2286:VAL:HG21	1:C:2467:ASN:HA	1.45	0.95
1:A:323:ILE:HG22	1:A:327:MSE:HE2	1.47	0.94
1:C:2323:ILE:HG22	1:C:2327:MSE:HE2	1.46	0.93
1:B:1315:ALA:HB3	1:B:1392:VAL:HG21	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3286:VAL:HG21	1:D:3467:ASN:HA	1.52	0.90
1:B:1026:LYS:HA	1:B:1029:MSE:HE3	1.54	0.89
1:A:108:MSE:HE1	1:A:186:LEU:HD21	1.53	0.88
1:D:3113:THR:HB	6:D:4542:HOH:O	1.76	0.86
1:D:3334:GLU:O	1:D:3338:GLN:HG3	1.76	0.85
1:A:407:MSE:HA	1:A:407:MSE:HE2	1.58	0.84
1:D:3520:GLN:H	1:D:3520:GLN:HE21	1.25	0.83
1:C:2184:LEU:HD12	1:C:2200:PRO:HG3	1.60	0.83
1:B:1286:VAL:HG21	1:B:1467:ASN:HA	1.61	0.82
1:B:1323:ILE:HG22	1:B:1327:MSE:HE2	1.60	0.82
1:C:2355:LYS:HE3	1:C:2355:LYS:HA	1.61	0.80
1:B:1085:ILE:HD11	1:B:1111:VAL:HG12	1.64	0.80
1:B:1504:ASP:HA	1:B:1507:LEU:HD12	1.64	0.80
1:B:1301:PRO:HD2	1:B:1304:GLU:HG3	1.62	0.79
1:B:1339:LYS:HA	1:B:1367:HIS:CE1	2.18	0.79
1:B:1377:PHE:CZ	1:B:1389:ILE:HD11	2.18	0.79
1:D:3332:LEU:HD12	1:D:3332:LEU:H	1.48	0.79
1:B:1239:MSE:O	1:B:1243:THR:HG22	1.83	0.78
1:C:2520:GLN:H	1:C:2520:GLN:HE21	1.29	0.78
1:B:1300:LYS:HE2	1:B:1304:GLU:HB3	1.66	0.77
1:C:2086:MSE:HE1	1:C:2111:VAL:HG23	1.66	0.76
1:D:3371:GLU:CD	1:D:3371:GLU:H	1.93	0.76
1:D:3140:ARG:HH21	1:D:3230:GLN:HG2	1.50	0.75
1:A:108:MSE:HB3	1:A:109:PRO:HD3	1.67	0.75
1:B:1047:MSE:HE2	1:D:3047:MSE:SE	2.37	0.75
1:C:2332:LEU:HD12	1:C:2332:LEU:H	1.52	0.75
1:D:3068:PHE:CD2	1:D:3099:ILE:HG13	2.22	0.75
1:A:493:GLU:HG3	1:A:533:TYR:CD1	2.22	0.75
1:B:1377:PHE:O	1:B:1381:VAL:HG23	1.86	0.75
1:A:381:VAL:CG1	1:A:407:MSE:HE3	2.17	0.75
1:A:261:ASN:HD22	1:A:264:ARG:HE	1.33	0.75
1:A:43:GLN:HG2	1:A:47:MSE:HE3	1.68	0.74
1:B:1515:PRO:HG2	1:B:1518:ASN:HD22	1.52	0.74
1:C:2527:ALA:O	1:C:2531:THR:HG23	1.86	0.74
1:D:3315:ALA:HB3	1:D:3392:VAL:CG2	2.15	0.73
2:A:701:LMR:H2	4:A:601:NAI:H42N	1.70	0.73
1:D:3022:LYS:O	1:D:3022:LYS:HD3	1.88	0.73
1:D:3302:ILE:HG23	1:D:3327:MSE:HE2	1.70	0.72
1:B:1515:PRO:HG2	1:B:1518:ASN:ND2	2.04	0.71
1:C:2325:MSE:HE2	1:C:2492:LEU:HD12	1.72	0.71
1:A:261:ASN:ND2	1:A:264:ARG:HE	1.87	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2033:ARG:HD3	1:C:2093:GLU:OE2	1.89	0.71
1:D:3527:ALA:O	1:D:3531:THR:HG22	1.90	0.71
1:B:1456:ASP:OD2	1:B:1458:ARG:HB2	1.90	0.70
1:D:3184:LEU:HD12	1:D:3200:PRO:HG3	1.73	0.70
1:C:2315:ALA:HB3	1:C:2392:VAL:HG21	1.74	0.70
1:C:2154:HIS:O	1:C:2197:ARG:HD2	1.91	0.70
1:C:2506:GLU:O	1:C:2511:ARG:HB2	1.91	0.70
1:D:3374:PRO:HG3	1:D:3383:ILE:HD12	1.74	0.70
1:D:3476:LEU:O	1:D:3480:LEU:HG	1.91	0.69
1:D:3179:ILE:HB	1:D:3180:PRO:HD3	1.74	0.69
1:D:3520:GLN:H	1:D:3520:GLN:NE2	1.90	0.69
1:A:272:LYS:HB2	1:A:272:LYS:NZ	2.08	0.69
1:D:3294:ALA:O	1:D:3297:VAL:HG22	1.93	0.68
2:B:1701:LMR:H2	4:B:1601:NAI:H42N	1.76	0.68
1:A:302:ILE:HD12	1:A:305:HIS:ND1	2.09	0.68
1:C:2478:VAL:HG13	1:C:2483:THR:HB	1.75	0.68
1:A:334:GLU:O	1:A:338:GLN:HG3	1.94	0.67
1:B:1324:VAL:HA	1:B:1327:MSE:HE3	1.76	0.67
1:D:3400:THR:OG1	1:D:3403:VAL:HG23	1.95	0.67
1:A:108:MSE:HE1	1:A:186:LEU:CD2	2.22	0.67
1:B:1179:ILE:HB	1:B:1180:PRO:HD3	1.76	0.67
1:B:1377:PHE:HZ	1:B:1389:ILE:HD11	1.56	0.67
1:B:1520:GLN:H	1:B:1520:GLN:HE21	1.42	0.67
1:C:2327:MSE:HE3	1:C:2337:ALA:HB1	1.75	0.67
1:D:3108:MSE:HB3	1:D:3109:PRO:HD3	1.77	0.67
1:A:288:LEU:HD22	1:A:322:LEU:HD12	1.76	0.67
1:D:3288:LEU:HD22	1:D:3322:LEU:HG	1.75	0.67
1:B:1177:MSE:O	1:B:1180:PRO:HD2	1.95	0.67
1:D:3503:THR:OG1	1:D:3506:GLU:HG3	1.95	0.67
1:B:1132:GLY:HA3	1:B:1200:PRO:HG2	1.75	0.67
1:A:413:ARG:HA	1:A:440:ARG:O	1.95	0.66
1:B:1085:ILE:C	1:B:1085:ILE:HD12	2.21	0.66
1:B:1154:HIS:O	1:B:1197:ARG:HD3	1.95	0.66
1:B:1260:HIS:O	1:B:1264:ARG:HG2	1.96	0.66
1:B:1527:ALA:O	1:B:1531:THR:HG23	1.96	0.66
1:C:2286:VAL:CG2	1:C:2467:ASN:HA	2.25	0.66
1:B:1315:ALA:O	1:B:1319:ILE:HG13	1.96	0.66
1:C:2061:GLN:HA	1:C:2064:GLN:HE21	1.61	0.65
1:C:2183:LYS:HE3	1:C:2255:GLU:CD	2.20	0.65
2:D:3701:LMR:H2	4:D:3601:NAI:H42N	1.77	0.65
1:A:343:MSE:HE3	1:A:350:LEU:HD12	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1210:ILE:H	1:B:1210:ILE:CD1	2.03	0.65
1:D:3298:ILE:HD12	1:D:3300:LYS:HE3	1.78	0.65
1:B:1384:LEU:N	1:B:1384:LEU:HD12	2.12	0.65
1:B:1090:GLU:OE1	1:B:1131:LYS:HE2	1.97	0.65
1:D:3308:LEU:HD23	1:D:3389:ILE:HD11	1.79	0.64
1:B:1354:ARG:CZ	1:B:1356:ALA:HB3	2.28	0.64
1:A:343:MSE:HE2	1:A:365:PHE:HB2	1.80	0.64
1:C:2492:LEU:CD2	1:C:2496:LYS:HE3	2.26	0.64
1:B:1505:GLU:CD	1:B:1505:GLU:H	2.06	0.64
1:D:3308:LEU:HB3	1:D:3389:ILE:CD1	2.27	0.64
1:A:319:ILE:O	1:A:323:ILE:HG13	1.97	0.64
1:B:1029:MSE:HE1	1:B:1053:LEU:CD1	2.29	0.63
1:D:3492:LEU:HD22	1:D:3496:LYS:HE2	1.80	0.63
1:B:1108:MSE:HB3	1:B:1109:PRO:HD3	1.81	0.63
1:D:3085:ILE:HD11	1:D:3111:VAL:HG12	1.80	0.63
1:C:2108:MSE:HB3	1:C:2109:PRO:HD3	1.80	0.63
1:B:1075:MSE:HG2	1:B:1080:GLU:CD	2.23	0.63
1:B:1108:MSE:HE3	1:B:1516:LEU:HD11	1.81	0.63
1:B:1300:LYS:HG2	1:B:1304:GLU:CB	2.29	0.63
1:D:3301:PRO:HB2	1:D:3304:GLU:HG2	1.79	0.63
1:A:108:MSE:HE2	1:A:112:TYR:HB2	1.79	0.62
1:B:1305:HIS:HA	1:B:1387:SER:OG	1.99	0.62
1:A:272:LYS:HB2	1:A:272:LYS:HZ3	1.63	0.62
1:A:298:ILE:HG22	1:A:300:LYS:HB2	1.80	0.62
1:D:3266:LEU:HD13	1:D:3266:LEU:C	2.25	0.62
1:A:36:LYS:HE2	1:A:562:TYR:HB3	1.81	0.62
1:B:1238:PHE:O	1:B:1242:ILE:HD13	1.99	0.62
1:B:1286:VAL:CG2	1:B:1467:ASN:HA	2.30	0.62
1:D:3391:GLY:HA3	1:D:3427:GLU:HG2	1.80	0.62
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.81	0.62
1:A:184:LEU:HD12	1:A:200:PRO:HG3	1.82	0.62
1:C:2282:GLY:O	1:C:2286:VAL:HG23	1.99	0.62
1:D:3143:VAL:HB	1:D:3237:GLU:HG2	1.82	0.62
1:D:3363:GLU:HB3	1:D:3364:PRO:HD3	1.81	0.62
1:A:41:THR:OG1	1:A:44:GLU:HG3	2.00	0.61
1:B:1334:GLU:O	1:B:1338:GLN:HG3	2.00	0.61
1:D:3308:LEU:HB3	1:D:3389:ILE:HD12	1.82	0.61
1:D:3394:GLY:HA2	1:D:3420:SER:HB3	1.81	0.61
1:C:2402:ASP:HA	1:C:2405:ARG:NH1	2.15	0.61
1:C:2492:LEU:HD22	1:C:2496:LYS:HE3	1.82	0.61
1:A:288:LEU:CD2	1:A:322:LEU:HD12	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1379:ASP:O	1:B:1383:ILE:HD13	1.99	0.61
1:C:2306:LYS:HE3	1:C:2384:LEU:O	2.01	0.61
1:D:3051:GLN:HE21	1:D:3051:GLN:HA	1.66	0.61
1:D:3183:LYS:HE3	1:D:3255:GLU:OE2	2.00	0.61
1:A:108:MSE:HE2	1:A:112:TYR:CB	2.31	0.61
1:B:1085:ILE:CD1	1:B:1111:VAL:HG12	2.30	0.61
1:B:1298:ILE:HD12	1:B:1300:LYS:HB3	1.82	0.61
1:B:1524:ILE:O	1:B:1528:ILE:HG13	2.00	0.61
1:A:288:LEU:HG	1:A:292:LEU:CD2	2.31	0.61
1:B:1298:ILE:C	1:B:1300:LYS:H	2.08	0.61
1:D:3319:ILE:O	1:D:3323:ILE:HG13	1.99	0.61
1:B:1369:ALA:HB1	1:B:1373:ILE:HD11	1.83	0.60
1:B:1518:ASN:HB3	1:B:1521:GLU:OE2	2.01	0.60
1:A:371:GLU:H	1:A:371:GLU:CD	2.07	0.60
1:B:1350:LEU:HD23	1:B:1354:ARG:CZ	2.31	0.60
1:B:1085:ILE:HD12	1:B:1086:MSE:N	2.17	0.60
1:A:207:THR:O	1:A:224:LYS:HA	2.02	0.60
1:B:1068:PHE:CD2	1:B:1099:ILE:HG13	2.37	0.60
1:C:2286:VAL:HG22	1:C:2470:ILE:HG12	1.82	0.60
1:A:294:ALA:O	1:A:297:VAL:HG22	2.02	0.59
1:C:2179:ILE:HB	1:C:2180:PRO:HD3	1.84	0.59
1:D:3385:LYS:HA	1:D:3410:ILE:HD13	1.84	0.59
1:C:2195:PRO:HG2	6:C:4349:HOH:O	2.03	0.59
1:C:2346:LYS:HE2	1:C:2347:TYR:CE1	2.36	0.59
1:D:3392:VAL:HG22	1:D:3392:VAL:O	2.02	0.59
1:B:1342:TRP:HE3	1:B:1349:LEU:HD11	1.68	0.59
1:C:2431:GLU:O	1:C:2435:THR:HG23	2.01	0.59
1:B:1343:MSE:HE3	1:B:1350:LEU:HD13	1.83	0.59
1:D:3140:ARG:NH2	1:D:3230:GLN:HG2	2.17	0.59
1:D:3401:PRO:HA	1:D:3436:LEU:HD13	1.83	0.59
1:C:2448:PRO:HD3	1:C:2464:GLN:HE22	1.68	0.59
1:D:3120:CYS:O	1:D:3175:TYR:HB3	2.02	0.59
1:B:1389:ILE:HG22	1:B:1416:ILE:HA	1.83	0.59
1:B:1506:GLU:O	1:B:1511:ARG:HB2	2.02	0.59
1:D:3354:ARG:NE	1:D:3356:ALA:HB3	2.18	0.59
1:D:3085:ILE:HD12	1:D:3096:PHE:HE1	1.68	0.58
1:A:140:ARG:NH2	1:A:230:GLN:HA	2.18	0.58
1:B:1382:ASN:O	1:B:1385:LYS:HG3	2.03	0.58
1:D:3261:ASN:HD22	1:D:3264:ARG:HE	1.49	0.58
1:C:2363:GLU:HG2	6:C:4628:HOH:O	2.02	0.58
1:B:1325:MSE:HE2	1:B:1492:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1335:GLN:O	1:B:1339:LYS:HG3	2.03	0.58
1:D:3314:GLU:HB2	4:D:3601:NAI:O1N	2.03	0.58
1:C:2021:ILE:HG13	1:C:2022:LYS:N	2.18	0.58
1:B:1029:MSE:HE1	1:B:1053:LEU:HD13	1.86	0.58
1:C:2301:PRO:HD2	1:C:2304:GLU:OE2	2.03	0.58
1:D:3041:THR:O	1:D:3045:ARG:HG3	2.03	0.58
1:B:1506:GLU:OE1	1:B:1515:PRO:HD3	2.04	0.58
1:A:332:LEU:HG	1:A:336:GLU:OE2	2.04	0.58
1:B:1319:ILE:O	1:B:1323:ILE:HG13	2.03	0.58
1:D:3323:ILE:O	1:D:3327:MSE:HG3	2.03	0.58
1:D:3388:THR:OG1	1:D:3415:VAL:HB	2.04	0.58
1:C:2503:THR:OG1	1:C:2506:GLU:HG3	2.04	0.57
1:A:325:MSE:HE1	1:A:488:ASP:HB3	1.87	0.57
1:D:3066:LEU:O	1:D:3070:ARG:HG2	2.04	0.57
2:C:2701:LMR:H2	4:C:2601:NAI:H42N	1.87	0.57
1:B:1339:LYS:HA	1:B:1367:HIS:NE2	2.20	0.57
1:B:1476:LEU:O	1:B:1480:LEU:HG	2.03	0.57
1:C:2061:GLN:HA	1:C:2064:GLN:NE2	2.19	0.57
1:A:556:ARG:HG3	1:A:556:ARG:HH11	1.69	0.57
1:D:3385:LYS:HZ3	1:D:3410:ILE:HG23	1.70	0.57
1:D:3207:THR:O	1:D:3224:LYS:HA	2.05	0.56
1:A:140:ARG:NH2	1:A:233:ASP:HB2	2.20	0.56
1:A:288:LEU:HG	1:A:292:LEU:HD22	1.88	0.56
1:B:1036:LYS:HB3	1:B:1039:ALA:HB3	1.88	0.56
1:B:1401:PRO:O	1:B:1405:ARG:HG3	2.05	0.56
1:C:2402:ASP:HA	1:C:2405:ARG:HH12	1.69	0.56
1:A:484:ARG:NH1	1:D:3543:TYR:HB3	2.20	0.56
1:B:1042:LEU:O	1:B:1046:GLN:HG3	2.05	0.56
1:A:400:THR:OG1	1:A:403:VAL:HG23	2.05	0.56
1:A:506:GLU:HB3	1:A:511:ARG:HD2	1.87	0.56
1:B:1261:ASN:HA	1:B:1264:ARG:HD3	1.87	0.56
1:B:1402:ASP:HA	1:B:1405:ARG:NH1	2.21	0.56
1:B:1542:ARG:HD3	1:B:1542:ARG:C	2.31	0.56
1:C:2041:THR:O	1:C:2045:ARG:HG3	2.05	0.56
1:B:1401:PRO:HA	1:B:1436:LEU:HD23	1.87	0.56
1:B:1113:THR:HG21	2:B:1701:LMR:O4A	2.05	0.55
1:C:2324:VAL:HA	1:C:2327:MSE:HE3	1.87	0.55
1:D:3043:GLN:HG2	1:D:3047:MSE:HE3	1.87	0.55
1:B:1021:ILE:HG12	1:B:1028:LEU:HD21	1.87	0.55
1:B:1343:MSE:HB2	1:B:1350:LEU:CD1	2.36	0.55
1:D:3023:GLU:CG	1:D:3027:PRO:HB2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3085:ILE:HD12	1:D:3085:ILE:C	2.31	0.55
1:D:3023:GLU:HG3	1:D:3027:PRO:HB2	1.87	0.55
1:A:140:ARG:HH22	1:A:233:ASP:HB2	1.71	0.55
1:A:432:GLU:O	1:A:436:LEU:HB2	2.07	0.55
1:B:1363:GLU:HB3	1:B:1364:PRO:HD3	1.87	0.55
1:B:1456:ASP:OD2	1:B:1458:ARG:NH1	2.35	0.55
1:D:3099:ILE:HG22	1:D:3100:LEU:HD12	1.89	0.55
1:A:113:THR:HB	6:A:4543:HOH:O	2.07	0.55
1:D:3043:GLN:HG2	1:D:3047:MSE:CE	2.37	0.55
1:D:3073:LYS:HE3	6:D:4513:HOH:O	2.07	0.55
1:A:41:THR:O	1:A:45:ARG:HG3	2.06	0.55
1:D:3343:MSE:HE2	1:D:3365:PHE:CB	2.30	0.55
1:C:2520:GLN:H	1:C:2520:GLN:NE2	2.03	0.55
1:D:3385:LYS:HZ3	1:D:3385:LYS:HB3	1.72	0.55
1:D:3169:LEU:HD21	1:D:3422:PRO:HD3	1.89	0.54
1:D:3380:ALA:O	1:D:3384:LEU:HB2	2.06	0.54
1:A:46:GLN:HG2	1:A:51:GLN:HG3	1.89	0.54
1:B:1081:LYS:O	1:B:1085:ILE:HG23	2.08	0.54
1:D:3078:PRO:HD2	6:D:4257:HOH:O	2.07	0.54
1:C:2495:ALA:O	1:C:2499:THR:HG22	2.07	0.54
1:D:3397:ARG:HA	1:D:3427:GLU:O	2.08	0.54
1:B:1183:LYS:HE3	1:B:1255:GLU:CD	2.33	0.54
1:D:3040:PHE:HE2	1:D:3565:LEU:HD12	1.71	0.54
1:A:288:LEU:HD22	1:A:322:LEU:CD1	2.37	0.54
1:B:1132:GLY:CA	1:B:1200:PRO:HG2	2.37	0.54
1:C:2273:TYR:HB3	6:C:4008:HOH:O	2.08	0.54
1:D:3177:MSE:O	1:D:3180:PRO:HD2	2.08	0.54
1:D:3315:ALA:O	1:D:3319:ILE:HG13	2.07	0.54
1:D:3385:LYS:HB3	1:D:3385:LYS:NZ	2.23	0.54
1:D:3506:GLU:O	1:D:3511:ARG:HB2	2.08	0.54
1:D:3397:ARG:HD3	1:D:3426:ALA:O	2.08	0.54
1:C:2559:ARG:HH11	1:C:2559:ARG:HG2	1.72	0.54
1:C:2022:LYS:NZ	1:C:2022:LYS:HB3	2.23	0.54
1:D:3420:SER:HA	4:D:3601:NAI:H1D	1.90	0.54
1:C:2520:GLN:HG2	6:C:4597:HOH:O	2.08	0.53
1:A:529:LYS:HE2	1:A:529:LYS:HA	1.89	0.53
1:C:2302:ILE:HG21	1:C:2332:LEU:HD11	1.90	0.53
1:A:389:ILE:HG23	1:A:399:PHE:CE1	2.44	0.53
1:B:1343:MSE:HE1	1:B:1362:GLN:HG2	1.90	0.53
1:B:1383:ILE:HG22	1:B:1384:LEU:HD12	1.91	0.53
1:C:2456:ASP:OD2	1:C:2458:ARG:HD3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1504:ASP:HA	1:B:1507:LEU:CD1	2.36	0.53
1:A:483:THR:OG1	1:A:534:LEU:HD13	2.08	0.53
1:C:2082:TYR:O	1:C:2086:MSE:HB2	2.09	0.53
1:B:1248:ARG:HG2	1:B:1248:ARG:HH11	1.73	0.53
1:B:1261:ASN:HD22	1:B:1264:ARG:HD3	1.74	0.53
1:B:1324:VAL:O	1:B:1328:VAL:HG23	2.09	0.53
1:C:2021:ILE:HG13	1:C:2022:LYS:H	1.74	0.53
1:D:3315:ALA:CB	1:D:3392:VAL:HG21	2.27	0.53
1:A:108:MSE:HE3	1:A:108:MSE:HA	1.90	0.53
1:B:1559:ARG:HB3	1:B:1561:GLU:OE1	2.09	0.53
1:D:3065:ALA:HA	1:D:3099:ILE:HD11	1.89	0.53
1:B:1432:GLU:O	1:B:1436:LEU:HB2	2.09	0.52
1:C:2286:VAL:HG22	1:C:2470:ILE:CG1	2.39	0.52
1:B:1493:GLU:HG3	1:B:1533:TYR:CD1	2.44	0.52
1:D:3068:PHE:HE1	1:D:3085:ILE:HG22	1.74	0.52
1:A:68:PHE:CD2	1:A:99:ILE:HG13	2.44	0.52
1:A:341:ILE:O	1:A:367:HIS:HE1	1.92	0.52
1:B:1401:PRO:HA	1:B:1436:LEU:CD2	2.39	0.52
1:C:2312:ALA:HB1	1:C:2362:GLN:HE21	1.73	0.52
1:C:2432:GLU:O	1:C:2436:LEU:HD23	2.09	0.52
1:B:1343:MSE:HB2	1:B:1350:LEU:HD12	1.91	0.52
1:D:3559:ARG:HG3	1:D:3561:GLU:OE1	2.09	0.52
1:A:184:LEU:HD22	1:A:198:CYS:HB3	1.92	0.52
1:A:407:MSE:HA	1:A:407:MSE:CE	2.35	0.52
1:B:1099:ILE:HG22	1:B:1100:LEU:HD12	1.90	0.52
1:B:1302:ILE:C	1:B:1304:GLU:H	2.15	0.52
1:B:1282:GLY:O	1:B:1286:VAL:HG23	2.09	0.52
1:D:3022:LYS:HD3	1:D:3022:LYS:C	2.34	0.52
1:A:22:LYS:HD2	1:A:23:GLU:N	2.25	0.52
1:C:2327:MSE:CE	1:C:2337:ALA:HB1	2.40	0.52
1:A:551:LYS:O	1:A:555:GLU:HG3	2.09	0.52
1:D:3344:PHE:CZ	1:D:3348:GLY:HA2	2.45	0.52
1:A:165:ARG:O	1:A:165:ARG:NE	2.42	0.51
1:C:2165:ARG:NH2	2:C:2701:LMR:O1B	2.43	0.51
1:A:543:TYR:HB3	1:D:3484:ARG:NH1	2.25	0.51
1:C:2551:LYS:O	1:C:2555:GLU:HB2	2.09	0.51
1:D:3286:VAL:HG22	1:D:3470:ILE:CG1	2.41	0.51
1:B:1343:MSE:C	1:B:1350:LEU:HD12	2.35	0.51
1:D:3033:ARG:NH1	1:D:3093:GLU:OE2	2.43	0.51
1:A:371:GLU:CD	1:A:371:GLU:N	2.68	0.51
1:B:1335:GLN:HE21	1:B:1339:LYS:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2205:VAL:HG11	1:C:2231:TYR:HD1	1.74	0.51
1:D:3096:PHE:O	1:D:3100:LEU:HD13	2.10	0.51
1:B:1295:GLN:OE1	1:B:1302:ILE:HD11	2.10	0.51
1:B:1499:THR:C	1:B:1501:GLN:H	2.18	0.51
1:B:1298:ILE:HG13	1:B:1300:LYS:H	1.74	0.51
1:D:3343:MSE:O	1:D:3349:LEU:HD12	2.11	0.51
1:A:354:ARG:HD2	6:A:4396:HOH:O	2.11	0.51
1:A:503:THR:OG1	1:A:506:GLU:HG3	2.10	0.51
1:D:3418:ALA:O	1:D:3445:SER:HA	2.10	0.51
1:A:78:PRO:HD2	6:A:4088:HOH:O	2.10	0.51
1:A:298:ILE:CG2	1:A:300:LYS:HB2	2.41	0.51
1:A:468:VAL:HA	1:A:471:PHE:CE2	2.46	0.50
1:B:1380:ALA:O	1:B:1384:LEU:HD13	2.11	0.50
1:C:2333:SER:HB2	6:C:4596:HOH:O	2.10	0.50
1:B:1385:LYS:HG2	1:B:1410:ILE:HD13	1.93	0.50
1:C:2085:ILE:HD12	1:C:2096:PHE:HE1	1.76	0.50
1:B:1302:ILE:HA	6:B:4055:HOH:O	2.11	0.50
1:B:1515:PRO:CG	1:B:1518:ASN:ND2	2.74	0.50
1:C:2261:ASN:ND2	1:C:2264:ARG:HH21	2.09	0.50
1:B:1312:ALA:HB1	1:B:1343:MSE:CE	2.41	0.50
1:B:1384:LEU:N	1:B:1384:LEU:CD1	2.74	0.50
1:B:1478:VAL:HG13	1:B:1483:THR:HB	1.92	0.50
1:C:2378:GLU:OE1	1:C:2402:ASP:HB3	2.12	0.50
1:A:120:CYS:O	1:A:175:TYR:HB3	2.12	0.50
1:B:1120:CYS:O	1:B:1175:TYR:HB3	2.11	0.50
1:B:1315:ALA:CB	1:B:1392:VAL:HG21	2.32	0.50
1:C:2300:LYS:HG3	1:C:2301:PRO:HD2	1.93	0.50
1:C:2363:GLU:HB3	1:C:2364:PRO:HD3	1.92	0.50
1:A:68:PHE:CE1	1:A:85:ILE:HG22	2.47	0.50
1:A:308:LEU:HB3	1:A:389:ILE:HD12	1.94	0.50
1:A:394:GLY:HA2	1:A:420:SER:HB3	1.93	0.50
1:C:2317:LEU:HD23	1:C:2343:MSE:HE1	1.94	0.50
1:D:3282:GLY:O	1:D:3286:VAL:HG23	2.12	0.50
1:D:3346:LYS:HG2	4:D:3601:NAI:O2B	2.12	0.50
1:D:3431:GLU:OE1	1:D:3452:VAL:HG13	2.10	0.50
1:D:3535:TYR:CD2	1:D:3545:GLU:HG3	2.47	0.50
1:A:489:SER:HB3	1:A:533:TYR:OH	2.12	0.50
1:B:1096:PHE:O	1:B:1100:LEU:HD13	2.12	0.50
1:D:3051:GLN:HA	1:D:3051:GLN:NE2	2.27	0.50
1:A:157:ALA:HB2	1:A:479:ILE:HD11	1.93	0.49
1:A:43:GLN:HG2	1:A:47:MSE:CE	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:O	1:A:99:ILE:HD13	2.12	0.49
1:A:324:VAL:HA	1:A:327:MSE:HE3	1.95	0.49
1:B:1556:ARG:HH11	1:B:1556:ARG:HG3	1.76	0.49
1:C:2104:ILE:HG13	1:C:2108:MSE:HE2	1.94	0.49
1:D:3150:TRP:CE2	1:D:3199:LEU:HD13	2.47	0.49
1:D:3302:ILE:HD12	1:D:3327:MSE:HE2	1.94	0.49
1:A:535:TYR:OH	1:A:542:ARG:HB3	2.11	0.49
1:C:2389:ILE:HG23	1:C:2399:PHE:CE1	2.46	0.49
1:D:3081:LYS:O	1:D:3085:ILE:HG23	2.11	0.49
1:D:3167:LEU:HB2	1:D:3169:LEU:CD2	2.43	0.49
1:D:3286:VAL:HG22	1:D:3470:ILE:HG12	1.93	0.49
1:B:1041:THR:O	1:B:1045:ARG:HG3	2.12	0.49
1:C:2081:LYS:O	1:C:2085:ILE:HG23	2.13	0.49
1:C:2154:HIS:O	1:C:2197:ARG:CD	2.60	0.49
1:D:3429:THR:OG1	1:D:3432:GLU:HG3	2.12	0.49
1:B:1302:ILE:C	1:B:1304:GLU:N	2.69	0.49
1:D:3528:ILE:O	1:D:3531:THR:HG23	2.12	0.49
1:A:532:GLU:HG2	1:A:549:LYS:CG	2.31	0.49
1:B:1312:ALA:HB1	1:B:1343:MSE:HE3	1.95	0.49
1:B:1196:ASP:OD1	1:B:1197:ARG:HG2	2.12	0.49
1:C:2163:GLY:HA2	1:C:2166:ILE:HD11	1.94	0.49
1:C:2300:LYS:HG3	1:C:2304:GLU:OE2	2.13	0.49
1:C:2392:VAL:O	1:C:2392:VAL:HG13	2.13	0.49
1:D:3302:ILE:HG23	1:D:3327:MSE:CE	2.42	0.49
1:D:3389:ILE:HG23	1:D:3399:PHE:CZ	2.47	0.49
1:C:2315:ALA:CB	1:C:2392:VAL:HG21	2.42	0.49
1:B:1359:ASP:OD2	1:B:1362:GLN:HG3	2.13	0.49
1:B:1422:PRO:HD2	1:B:1425:GLN:NE2	2.28	0.49
1:D:3169:LEU:CD2	1:D:3422:PRO:HD3	2.43	0.49
1:A:302:ILE:HD12	1:A:305:HIS:HD1	1.75	0.48
1:A:420:SER:HA	4:A:601:NAI:H1D	1.95	0.48
1:D:3308:LEU:HB3	1:D:3389:ILE:HD11	1.95	0.48
1:A:310:LEU:HD21	1:A:398:LEU:HB2	1.95	0.48
1:B:1515:PRO:CG	1:B:1518:ASN:HD22	2.23	0.48
1:D:3292:LEU:O	1:D:3296:LYS:HE2	2.13	0.48
1:B:1163:GLY:HA2	1:B:1166:ILE:HD11	1.95	0.48
1:B:1343:MSE:O	1:B:1350:LEU:HD12	2.13	0.48
1:B:1532:GLU:HG2	1:B:1549:LYS:HG2	1.95	0.48
1:D:3401:PRO:O	1:D:3405:ARG:HG3	2.13	0.48
1:D:3535:TYR:CE2	1:D:3545:GLU:HG3	2.49	0.48
1:A:177:MSE:O	1:A:180:PRO:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:THR:HG21	1:A:273:TYR:CD2	2.49	0.48
1:A:520:GLN:HE21	1:A:520:GLN:H	1.61	0.48
1:B:1333:SER:OG	1:B:1336:GLU:HG2	2.12	0.48
1:A:339:LYS:HB2	1:A:339:LYS:NZ	2.28	0.48
1:A:412:GLU:O	1:A:440:ARG:NH1	2.46	0.48
1:B:1248:ARG:CZ	4:C:2602:NAI:O2N	2.61	0.48
1:B:1298:ILE:C	1:B:1300:LYS:N	2.71	0.48
1:D:3359:ASP:OD2	1:D:3362:GLN:HG3	2.12	0.48
1:A:168:GLY:N	1:A:421:ASN:O	2.47	0.48
1:B:1029:MSE:HE1	1:B:1053:LEU:HD12	1.96	0.48
1:D:3307:ILE:HD13	1:D:3323:ILE:HD13	1.95	0.48
1:B:1210:ILE:HD12	1:B:1210:ILE:N	2.10	0.48
1:B:1400:THR:HB	1:B:1401:PRO:HD2	1.95	0.48
1:A:151:PRO:HG2	1:A:152:GLU:OE1	2.13	0.48
1:B:1273:TYR:HB3	6:B:4691:HOH:O	2.12	0.48
1:C:2090:GLU:OE1	1:C:2131:LYS:HE2	2.14	0.48
1:D:3172:LEU:O	1:D:3175:TYR:HB2	2.13	0.48
1:A:332:LEU:HD12	1:A:332:LEU:H	1.79	0.47
1:B:1287:ALA:O	1:B:1291:LEU:HD23	2.14	0.47
1:B:1383:ILE:HD12	1:B:1383:ILE:N	2.29	0.47
1:D:3369:ALA:HB1	1:D:3373:ILE:CD1	2.44	0.47
1:D:3036:LYS:HB3	1:D:3039:ALA:HB3	1.96	0.47
1:A:329:GLU:HA	6:A:4296:HOH:O	2.13	0.47
1:A:476:LEU:O	1:A:480:LEU:HG	2.15	0.47
1:C:2542:ARG:HD3	1:C:2542:ARG:C	2.40	0.47
1:D:3556:ARG:HH11	1:D:3556:ARG:HG3	1.79	0.47
1:C:2288:LEU:O	1:C:2292:LEU:HD13	2.14	0.47
1:A:51:GLN:NE2	6:A:4239:HOH:O	2.48	0.47
1:C:2312:ALA:CB	1:C:2362:GLN:HE21	2.28	0.47
1:D:3154:HIS:HD2	1:D:3197:ARG:CZ	2.27	0.47
1:A:68:PHE:HE1	1:A:85:ILE:HG22	1.80	0.47
1:A:471:PHE:CG	1:A:472:PRO:HD3	2.50	0.47
1:A:527:ALA:O	1:A:531:THR:HG23	2.15	0.47
1:B:1060:THR:OG1	1:B:1063:ILE:HG13	2.15	0.47
1:B:1286:VAL:HG22	1:B:1470:ILE:HG12	1.96	0.47
1:B:1556:ARG:HG3	1:B:1556:ARG:NH1	2.30	0.47
1:C:2339:LYS:HA	1:C:2367:HIS:CE1	2.50	0.47
1:D:3186:LEU:HD13	1:D:3468:VAL:HG23	1.96	0.47
1:B:1188:THR:HG21	1:B:1195:PRO:HG3	1.97	0.47
1:C:2143:VAL:HB	1:C:2237:GLU:HG2	1.96	0.47
1:A:45:ARG:NH2	1:A:58:ILE:HD13	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2085:ILE:HD12	1:C:2085:ILE:C	2.39	0.47
1:B:1161:THR:HG22	1:B:1180:PRO:HG2	1.97	0.46
1:D:3165:ARG:O	1:D:3165:ARG:NE	2.47	0.46
1:D:3331:GLY:O	1:D:3332:LEU:O	2.33	0.46
1:D:3526:ILE:O	1:D:3530:VAL:HG23	2.14	0.46
1:A:401:PRO:O	1:A:405:ARG:HG3	2.14	0.46
1:C:2503:THR:HG1	1:C:2506:GLU:HG3	1.79	0.46
1:D:3328:VAL:HA	1:D:3332:LEU:O	2.14	0.46
1:B:1232:ASP:CG	1:B:1264:ARG:HH22	2.21	0.46
1:C:2293:ALA:O	1:C:2296:LYS:HB2	2.15	0.46
1:B:1232:ASP:OD1	1:B:1264:ARG:NH2	2.49	0.46
1:C:2197:ARG:HG3	1:C:2197:ARG:HH11	1.79	0.46
1:D:3532:GLU:HG2	1:D:3549:LYS:HG2	1.96	0.46
1:A:145:SER:HB2	6:A:4288:HOH:O	2.15	0.46
1:A:229:GLN:O	1:A:229:GLN:HG2	2.15	0.46
1:C:2489:SER:HB3	1:C:2533:TYR:OH	2.16	0.46
1:D:3261:ASN:ND2	1:D:3264:ARG:HE	2.13	0.46
1:D:3350:LEU:HD13	1:D:3354:ARG:CZ	2.45	0.46
1:A:406:ALA:O	1:A:410:ILE:HG13	2.15	0.46
1:B:1150:TRP:CE2	1:B:1199:LEU:HD13	2.50	0.46
1:B:1328:VAL:HA	1:B:1332:LEU:O	2.15	0.46
1:C:2086:MSE:CE	1:C:2111:VAL:HG23	2.41	0.46
1:D:3346:LYS:HG3	1:D:3347:TYR:CD1	2.51	0.46
1:C:2295:GLN:NE2	1:C:2300:LYS:O	2.47	0.46
1:D:3321:ASN:O	1:D:3325:MSE:HG3	2.16	0.46
1:A:354:ARG:NE	1:A:358:ILE:HD11	2.31	0.46
1:B:1294:ALA:O	1:B:1297:VAL:HB	2.16	0.45
1:C:2120:CYS:O	1:C:2175:TYR:HB3	2.15	0.45
1:D:3136:SER:HA	1:D:3204:ASP:O	2.16	0.45
1:A:401:PRO:HA	1:A:436:LEU:HD23	1.98	0.45
1:B:1288:LEU:HG	1:B:1292:LEU:HD13	1.99	0.45
1:C:2302:ILE:CG2	1:C:2332:LEU:HD11	2.46	0.45
1:C:2315:ALA:HB3	1:C:2392:VAL:CG2	2.45	0.45
1:D:3263:PHE:CZ	1:D:3314:GLU:HA	2.52	0.45
1:A:327:MSE:HE3	1:A:337:ALA:HB1	1.99	0.45
1:C:2270:ARG:O	1:C:2485:HIS:HD2	1.99	0.45
1:A:219:MSE:HG2	1:B:1038:MSE:HE1	1.99	0.45
1:A:306:LYS:HB3	1:A:386:PRO:HA	1.98	0.45
1:C:2057:LYS:HE2	1:C:2059:GLU:HG2	1.97	0.45
1:C:2468:VAL:HA	1:C:2471:PHE:CE2	2.51	0.45
1:D:3051:GLN:HE21	1:D:3051:GLN:CA	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLY:HA3	1:B:1146:ILE:HG23	1.98	0.45
1:B:1079:LEU:O	1:B:1082:TYR:HB3	2.17	0.45
1:B:1392:VAL:O	1:B:1392:VAL:HG13	2.16	0.45
1:A:43:GLN:NE2	1:A:566:LEU:HD11	2.32	0.45
1:A:271:GLU:HB2	6:A:4614:HOH:O	2.16	0.45
1:A:520:GLN:H	1:A:520:GLN:NE2	2.15	0.45
1:C:2085:ILE:HD11	1:C:2086:MSE:SE	2.66	0.45
1:D:3068:PHE:CE1	1:D:3085:ILE:HG22	2.50	0.45
1:A:343:MSE:HE3	1:A:350:LEU:CD1	2.45	0.45
1:D:3297:VAL:HG23	1:D:3298:ILE:HG23	1.99	0.45
1:D:3306:LYS:HE3	1:D:3384:LEU:O	2.16	0.45
1:A:172:LEU:O	1:A:175:TYR:HB2	2.17	0.45
1:B:1154:HIS:O	1:B:1197:ARG:CD	2.63	0.45
1:B:1229:GLN:HG3	1:B:1233:ASP:OD2	2.16	0.45
1:B:1422:PRO:HD2	1:B:1425:GLN:HE21	1.82	0.45
1:A:146:ILE:HG23	1:B:1052:GLY:HA3	1.99	0.45
1:A:194:ARG:HA	1:A:195:PRO:HD3	1.87	0.45
1:C:2370:PRO:O	1:C:2371:GLU:C	2.59	0.45
1:D:3412:GLU:HG3	1:D:3413:ARG:HG2	1.99	0.45
1:A:33:ARG:HD2	1:A:93:GLU:OE2	2.17	0.45
1:A:509:GLN:NE2	1:A:511:ARG:HE	2.15	0.45
1:B:1300:LYS:HG2	1:B:1304:GLU:HB3	1.97	0.45
1:B:1321:ASN:O	1:B:1325:MSE:HG3	2.17	0.45
1:C:2205:VAL:HG11	1:C:2231:TYR:CD1	2.52	0.44
1:A:86:MSE:HE3	1:A:131:LYS:NZ	2.31	0.44
1:B:1392:VAL:O	1:B:1392:VAL:HG22	2.16	0.44
1:C:2070:ARG:O	1:C:2074:LYS:HD3	2.17	0.44
1:B:1518:ASN:O	1:B:1521:GLU:HG2	2.18	0.44
1:B:1520:GLN:O	1:B:1524:ILE:HG12	2.18	0.44
1:C:2172:LEU:O	1:C:2175:TYR:HB2	2.17	0.44
1:D:3369:ALA:HA	1:D:3370:PRO:HD3	1.80	0.44
1:D:3474:VAL:O	1:D:3478:VAL:HG23	2.17	0.44
1:D:3528:ILE:O	1:D:3531:THR:CG2	2.65	0.44
1:A:154:HIS:CD2	6:A:4548:HOH:O	2.70	0.44
1:B:1069:HIS:HE1	1:B:1102:ASP:OD2	2.00	0.44
1:B:1342:TRP:CZ3	1:B:1349:LEU:HD21	2.53	0.44
1:C:2150:TRP:HA	1:C:2151:PRO:HD3	1.80	0.44
1:B:1458:ARG:HB2	1:B:1458:ARG:HH11	1.82	0.44
1:D:3036:LYS:HE3	1:D:3565:LEU:HG	2.00	0.44
1:D:3186:LEU:HD13	1:D:3468:VAL:CG2	2.47	0.44
1:B:1122:GLN:HG2	1:B:1125:HIS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2162:ASP:C	1:C:2162:ASP:OD1	2.60	0.44
1:C:2308:LEU:HD23	1:C:2389:ILE:HD11	1.99	0.44
1:C:2518:ASN:O	1:C:2521:GLU:HG2	2.17	0.44
1:C:2520:GLN:O	1:C:2524:ILE:HG12	2.18	0.44
1:A:263:PHE:HZ	1:A:317:LEU:HB2	1.81	0.44
1:A:350:LEU:HD22	1:A:354:ARG:CZ	2.48	0.44
1:C:2350:LEU:HD13	1:C:2354:ARG:CZ	2.48	0.44
1:D:3159:VAL:HG23	1:D:3184:LEU:HD21	1.99	0.44
1:D:3385:LYS:N	1:D:3386:PRO:CD	2.80	0.44
1:A:306:LYS:CG	1:A:386:PRO:HA	2.48	0.44
1:B:1471:PHE:CG	1:B:1472:PRO:HD3	2.53	0.44
1:D:3413:ARG:HA	1:D:3440:ARG:O	2.18	0.44
1:A:552:TYR:O	1:A:556:ARG:HG3	2.17	0.43
1:D:3199:LEU:HA	1:D:3200:PRO:HD3	1.89	0.43
1:D:3406:ALA:O	1:D:3409:SER:HB3	2.17	0.43
1:B:1239:MSE:SE	1:B:1252:ILE:HD13	2.69	0.43
1:D:3272:LYS:HE3	1:D:3272:LYS:HB3	1.92	0.43
1:A:183:LYS:HE3	1:A:255:GLU:CD	2.43	0.43
1:A:478:VAL:HG13	1:A:483:THR:HB	1.99	0.43
1:A:482:ASN:HD21	4:A:602:NAI:H4B	1.84	0.43
1:B:1184:LEU:O	1:B:1187:TYR:HB2	2.18	0.43
1:B:1378:GLU:OE1	1:B:1402:ASP:HB3	2.18	0.43
1:B:1399:PHE:CG	1:B:1427:GLU:HB3	2.53	0.43
1:B:1522:VAL:O	1:B:1526:ILE:HG13	2.18	0.43
1:C:2334:GLU:O	1:C:2338:GLN:HG3	2.17	0.43
1:C:2454:LEU:C	1:C:2456:ASP:H	2.26	0.43
1:D:3071:ASN:O	1:D:3075:MSE:HG3	2.18	0.43
1:A:23:GLU:CG	1:A:27:PRO:HB2	2.48	0.43
1:A:188:THR:HG21	1:A:195:PRO:HG3	1.99	0.43
1:A:306:LYS:HE3	6:A:4713:HOH:O	2.18	0.43
1:C:2066:LEU:O	1:C:2070:ARG:HB2	2.18	0.43
1:D:3157:ALA:HB2	1:D:3479:ILE:HD11	2.00	0.43
1:A:332:LEU:H	1:A:332:LEU:CD1	2.32	0.43
1:A:344:PHE:CZ	1:A:348:GLY:HA2	2.53	0.43
1:B:1298:ILE:O	1:B:1299:SER:HB2	2.18	0.43
1:C:2556:ARG:HH11	1:C:2556:ARG:HG3	1.84	0.43
1:D:3156:LYS:HA	1:D:3156:LYS:HE2	2.00	0.43
1:A:184:LEU:O	1:A:187:TYR:HB2	2.19	0.43
1:A:506:GLU:O	1:A:511:ARG:HB2	2.19	0.43
1:B:1327:MSE:HE3	1:B:1337:ALA:HB1	2.01	0.43
1:B:1068:PHE:CE1	1:B:1085:ILE:HG22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1094:LYS:HD2	1:B:1558:TRP:CZ2	2.53	0.43
1:B:1300:LYS:HA	1:B:1301:PRO:HD3	1.91	0.43
1:A:288:LEU:CD2	1:A:322:LEU:CD1	2.95	0.43
1:B:1184:LEU:HD12	1:B:1200:PRO:HB3	2.01	0.43
1:C:2448:PRO:HD3	1:C:2464:GLN:NE2	2.33	0.43
1:D:3140:ARG:O	1:D:3140:ARG:HG3	2.18	0.43
1:B:1261:ASN:HA	1:B:1264:ARG:CG	2.48	0.43
1:B:1411:ASN:HB2	1:B:1414:PRO:HB3	2.00	0.43
1:C:2082:TYR:CE1	1:C:2086:MSE:HE2	2.54	0.43
1:D:3310:LEU:HB3	1:D:3391:GLY:HA2	2.00	0.43
1:D:3352:LYS:HG3	1:D:3367:HIS:C	2.44	0.43
1:A:414:PRO:HD2	1:A:440:ARG:O	2.19	0.42
1:B:1405:ARG:O	1:B:1408:ALA:HB3	2.18	0.42
1:D:3310:LEU:HD21	1:D:3398:LEU:HB2	2.01	0.42
1:D:3481:CYS:HB3	1:D:3540:ALA:CB	2.49	0.42
1:A:251:LEU:C	1:A:251:LEU:HD13	2.43	0.42
1:B:1229:GLN:HE21	1:B:1229:GLN:HA	1.84	0.42
1:D:3104:ILE:O	1:D:3108:MSE:HB2	2.19	0.42
1:D:3143:VAL:CB	1:D:3237:GLU:HG2	2.49	0.42
1:D:3295:GLN:O	1:D:3295:GLN:HG3	2.19	0.42
1:B:1260:HIS:NE2	1:B:1264:ARG:HD2	2.34	0.42
1:D:3085:ILE:HD11	1:D:3111:VAL:CG1	2.48	0.42
1:D:3144:ARG:HA	1:D:3144:ARG:HD2	1.86	0.42
1:D:3186:LEU:O	1:D:3190:CYS:HB2	2.19	0.42
1:B:1138:SER:OG	1:B:1221:LEU:HD21	2.20	0.42
1:C:2418:ALA:O	1:C:2445:SER:HA	2.20	0.42
1:D:3462:PRO:HB2	6:D:4170:HOH:O	2.20	0.42
1:B:1097:TYR:CE2	1:B:1188:THR:HB	2.55	0.42
1:D:3085:ILE:CD1	1:D:3096:PHE:HE1	2.29	0.42
1:D:3107:LEU:HA	1:D:3110:ILE:HD12	2.01	0.42
1:A:174:VAL:O	1:A:174:VAL:HG12	2.19	0.42
1:A:302:ILE:HG13	1:A:340:LYS:HE2	2.02	0.42
1:B:1085:ILE:HD11	1:B:1086:MSE:SE	2.69	0.42
1:B:1393:ALA:O	1:B:1394:GLY:C	2.62	0.42
1:C:2165:ARG:NH1	4:C:2601:NAI:O1N	2.49	0.42
1:A:108:MSE:N	1:A:109:PRO:CD	2.83	0.42
1:A:313:GLY:HA2	6:A:4407:HOH:O	2.19	0.42
1:A:407:MSE:CE	1:A:410:ILE:HD12	2.50	0.42
1:B:1243:THR:OG1	1:B:1248:ARG:HA	2.19	0.42
1:B:1298:ILE:HG13	1:B:1299:SER:N	2.35	0.42
1:B:1412:GLU:O	1:B:1440:ARG:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1535:TYR:CE2	1:B:1545:GLU:HG3	2.55	0.42
1:D:3551:LYS:O	1:D:3555:GLU:HG3	2.19	0.42
1:C:2184:LEU:HD12	1:C:2200:PRO:CG	2.40	0.42
1:C:2238:PHE:CE1	1:C:2242:ILE:HG13	2.54	0.42
1:A:270:ARG:HH21	1:A:487:SER:HA	1.85	0.42
1:B:1243:THR:HG23	1:B:1244:ASP:N	2.34	0.42
1:D:3166:ILE:O	1:D:3167:LEU:C	2.63	0.42
1:B:1499:THR:C	1:B:1501:GLN:N	2.77	0.42
1:C:2096:PHE:O	1:C:2100:LEU:HD13	2.20	0.42
1:D:3307:ILE:HG23	1:D:3388:THR:HG22	2.01	0.42
1:D:3362:GLN:O	1:D:3363:GLU:C	2.62	0.42
1:B:1094:LYS:HD2	1:B:1558:TRP:HZ2	1.85	0.41
1:B:1104:ILE:HG23	1:B:1105:GLU:N	2.35	0.41
1:B:1194:ARG:HA	1:B:1195:PRO:HD3	1.85	0.41
1:B:1229:GLN:HA	1:B:1229:GLN:NE2	2.34	0.41
1:C:2502:LEU:HD11	1:C:2512:LEU:C	2.45	0.41
1:A:215:ASP:C	1:A:215:ASP:OD1	2.63	0.41
1:A:556:ARG:HH11	1:A:556:ARG:CG	2.31	0.41
1:B:1150:TRP:HA	1:B:1151:PRO:HD3	1.91	0.41
1:B:1400:THR:HB	1:B:1401:PRO:CD	2.51	0.41
1:C:2086:MSE:HE1	1:C:2111:VAL:CG2	2.44	0.41
1:C:2288:LEU:HG	1:C:2292:LEU:HD13	2.02	0.41
1:B:1177:MSE:C	1:B:1180:PRO:HD2	2.44	0.41
1:C:2112:TYR:CG	1:C:2113:THR:N	2.89	0.41
1:C:2314:GLU:HB2	4:C:2601:NAI:O1N	2.20	0.41
1:D:3556:ARG:HG3	1:D:3556:ARG:NH1	2.35	0.41
1:A:154:HIS:HD2	6:A:4548:HOH:O	2.02	0.41
1:B:1159:VAL:HG23	1:B:1184:LEU:HD21	2.01	0.41
1:B:1215:ASP:HA	1:B:1216:PRO:HD3	1.86	0.41
1:B:1349:LEU:HD22	1:B:1374:PRO:HG2	2.02	0.41
1:D:3167:LEU:HB2	1:D:3169:LEU:HD23	2.01	0.41
1:B:1286:VAL:HG21	1:B:1467:ASN:CA	2.39	0.41
1:B:1295:GLN:C	1:B:1297:VAL:H	2.29	0.41
1:C:2022:LYS:HB3	1:C:2022:LYS:HZ2	1.85	0.41
1:D:3122:GLN:HE21	1:D:3122:GLN:HB3	1.64	0.41
1:D:3177:MSE:C	1:D:3180:PRO:HD2	2.46	0.41
1:A:556:ARG:CG	1:A:556:ARG:NH1	2.84	0.41
1:B:1077:SER:HB2	6:B:4206:HOH:O	2.21	0.41
1:C:2283:THR:CG2	4:C:2601:NAI:H4N	2.51	0.41
1:C:2505:GLU:CD	1:C:2505:GLU:H	2.29	0.41
1:D:3361:TYR:H	1:D:3361:TYR:HD1	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1354:ARG:NE	1:B:1358:ILE:HD11	2.35	0.41
1:B:1388:THR:HG23	1:B:1415:VAL:CG1	2.50	0.41
1:C:2294:ALA:O	1:C:2297:VAL:HG13	2.20	0.41
1:D:3294:ALA:C	1:D:3296:LYS:H	2.29	0.41
1:D:3549:LYS:HB2	6:D:4386:HOH:O	2.20	0.41
1:A:431:GLU:OE2	1:A:452:VAL:HG13	2.21	0.41
1:B:1383:ILE:CG2	1:B:1384:LEU:HD12	2.51	0.41
1:B:1430:ALA:O	1:B:1434:TYR:HD1	2.03	0.41
1:C:2055:PRO:HG2	1:D:3219:MSE:HE3	2.02	0.41
1:C:2295:GLN:OE1	1:C:2295:GLN:HA	2.21	0.41
1:A:164:GLU:HB2	1:A:225:ARG:CZ	2.51	0.41
1:A:302:ILE:HD11	1:A:327:MSE:SE	2.70	0.41
1:A:310:LEU:HB3	1:A:391:GLY:HA2	2.03	0.41
1:B:1061:GLN:HA	1:B:1064:GLN:HE21	1.85	0.41
1:B:1304:GLU:O	1:B:1305:HIS:HB2	2.20	0.41
1:B:1381:VAL:O	1:B:1385:LYS:HA	2.20	0.41
1:C:2108:MSE:N	1:C:2109:PRO:CD	2.84	0.41
1:C:2197:ARG:HG3	1:C:2197:ARG:NH1	2.36	0.41
1:C:2332:LEU:H	1:C:2332:LEU:CD1	2.26	0.41
1:C:2355:LYS:HA	1:C:2355:LYS:CE	2.40	0.41
1:C:2359:ASP:OD2	1:C:2359:ASP:C	2.64	0.41
1:D:3068:PHE:CD2	1:D:3099:ILE:CG1	3.00	0.41
1:D:3093:GLU:O	1:D:3096:PHE:HB3	2.21	0.41
1:D:3350:LEU:HD13	1:D:3354:ARG:NH1	2.36	0.41
1:D:3433:ALA:O	1:D:3437:THR:HG23	2.21	0.41
1:A:82:TYR:CZ	1:A:86:MSE:HG3	2.55	0.41
1:A:359:ASP:OD2	1:A:359:ASP:C	2.64	0.41
1:A:419:LEU:O	4:A:601:NAI:H2N	2.21	0.41
1:B:1298:ILE:HD12	1:B:1300:LYS:CB	2.50	0.41
1:B:1312:ALA:CB	1:B:1343:MSE:HE3	2.51	0.41
1:B:1435:THR:HG22	1:B:1454:LEU:CD2	2.50	0.41
1:C:2345:ASP:HB2	4:C:2601:NAI:O2B	2.21	0.41
1:C:2548:ASP:OD2	1:C:2551:LYS:HB2	2.21	0.41
1:A:302:ILE:HG23	1:A:303:SER:N	2.36	0.40
1:A:456:ASP:OD1	1:A:458:ARG:HD3	2.21	0.40
1:B:1286:VAL:HG22	1:B:1470:ILE:CG1	2.52	0.40
1:B:1430:ALA:O	1:B:1434:TYR:CD1	2.74	0.40
1:C:2159:VAL:HG23	1:C:2184:LEU:HD21	2.03	0.40
1:C:2346:LYS:HG2	4:C:2601:NAI:O2B	2.21	0.40
1:D:3205:VAL:HG11	1:D:3231:TYR:HD1	1.86	0.40
1:A:150:TRP:CE2	1:A:199:LEU:HD13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:HB3	1:A:389:ILE:CD1	2.51	0.40
1:B:1317:LEU:HD21	1:B:1362:GLN:HG2	2.02	0.40
1:D:3099:ILE:HD12	1:D:3099:ILE:HA	1.82	0.40
1:A:233:ASP:HB3	6:A:4438:HOH:O	2.22	0.40
1:B:1055:PRO:HA	1:B:1056:PRO:HD3	1.99	0.40
1:B:1108:MSE:O	1:B:1112:TYR:HB3	2.21	0.40
1:B:1342:TRP:CH2	1:B:1370:PRO:HG3	2.56	0.40
1:C:2377:PHE:CZ	1:C:2389:ILE:HD11	2.56	0.40
1:D:3113:THR:CB	6:D:4542:HOH:O	2.48	0.40
1:A:68:PHE:CE2	1:A:99:ILE:HG23	2.56	0.40
1:A:412:GLU:O	1:A:440:ARG:HB3	2.22	0.40
1:C:2174:VAL:O	1:C:2174:VAL:HG12	2.21	0.40
1:C:2183:LYS:HE3	1:C:2255:GLU:OE1	2.21	0.40
1:C:2294:ALA:O	1:C:2297:VAL:CG1	2.69	0.40
1:D:3023:GLU:HA	1:D:3023:GLU:OE1	2.22	0.40
1:D:3108:MSE:N	1:D:3109:PRO:CD	2.85	0.40
1:A:400:THR:O	1:A:404:ILE:HG13	2.21	0.40
1:C:2320:ALA:O	1:C:2324:VAL:HG23	2.22	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	551/564 (98%)	522 (95%)	27 (5%)	2 (0%)	30	38
1	B	551/564 (98%)	518 (94%)	29 (5%)	4 (1%)	18	23
1	C	551/564 (98%)	530 (96%)	19 (3%)	2 (0%)	30	38
1	D	551/564 (98%)	518 (94%)	30 (5%)	3 (0%)	24	31
All	All	2204/2256 (98%)	2088 (95%)	105 (5%)	11 (0%)	24	31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	3332	LEU
1	B	1392	VAL
1	B	1301	PRO
1	C	2392	VAL
1	B	1305	HIS
1	B	1397	ARG
1	C	2371	GLU
1	D	3103	ASP
1	D	3392	VAL
1	A	103	ASP
1	A	332	LEU

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	469/465 (101%)	446 (95%)	23 (5%)	22	34
1	B	469/465 (101%)	450 (96%)	19 (4%)	27	41
1	C	469/465 (101%)	452 (96%)	17 (4%)	31	47
1	D	469/465 (101%)	444 (95%)	25 (5%)	20	30
All	All	1876/1860 (101%)	1792 (96%)	84 (4%)	24	37

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	43	GLN
1	A	66	LEU
1	A	165	ARG
1	A	169	LEU
1	A	221	LEU
1	A	229	GLN
1	A	272	LYS
1	A	291	LEU
1	A	292	LEU
1	A	304	GLU

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Mol	Chain	Res	Type
1	A	322	LEU
1	A	335	GLN
1	A	339	LYS
1	A	371	GLU
1	A	384	LEU
1	A	389	ILE
1	A	436	LEU
1	A	492	LEU
1	A	502	LEU
1	A	520	GLN
1	A	559	ARG
1	A	561	GLU
1	B	1070	ARG
1	B	1075	MSE
1	B	1085	ILE
1	B	1099	ILE
1	B	1105	GLU
1	B	1113	THR
1	B	1123	TYR
1	B	1169	LEU
1	B	1210	ILE
1	B	1221	LEU
1	B	1232	ASP
1	B	1248	ARG
1	B	1271	GLU
1	B	1286	VAL
1	B	1340	LYS
1	B	1458	ARG
1	B	1492	LEU
1	B	1502	LEU
1	B	1520	GLN
1	C	2022	LYS
1	C	2086	MSE
1	C	2114	PRO
1	C	2251	LEU
1	C	2286	VAL
1	C	2291	LEU
1	C	2297	VAL
1	C	2339	LYS
1	C	2355	LYS
1	C	2384	LEU
1	C	2398	LEU

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Mol	Chain	Res	Type
1	C	2405	ARG
1	C	2492	LEU
1	C	2507	LEU
1	C	2520	GLN
1	C	2561	GLU
1	C	2571	GLU
1	D	3066	LEU
1	D	3074	LYS
1	D	3085	ILE
1	D	3099	ILE
1	D	3113	THR
1	D	3133	LEU
1	D	3140	ARG
1	D	3153	ASN
1	D	3221	LEU
1	D	3242	ILE
1	D	3251	LEU
1	D	3286	VAL
1	D	3291	LEU
1	D	3292	LEU
1	D	3300	LYS
1	D	3363	GLU
1	D	3385	LYS
1	D	3388	THR
1	D	3389	ILE
1	D	3425	GLN
1	D	3492	LEU
1	D	3520	GLN
1	D	3531	THR
1	D	3559	ARG
1	D	3561	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	51	GLN
1	A	64	GLN
1	A	125	HIS
1	A	153	ASN
1	A	253	GLN
1	A	260	HIS

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Mol	Chain	Res	Type
1	A	261	ASN
1	A	295	GLN
1	A	330	ASN
1	A	335	GLN
1	A	367	HIS
1	A	411	ASN
1	A	482	ASN
1	A	485	HIS
1	A	509	GLN
1	A	518	ASN
1	A	520	GLN
1	B	1043	GLN
1	B	1064	GLN
1	B	1069	HIS
1	B	1089	GLN
1	B	1229	GLN
1	B	1230	GLN
1	B	1261	ASN
1	B	1335	GLN
1	B	1338	GLN
1	B	1362	GLN
1	B	1382	ASN
1	B	1425	GLN
1	B	1482	ASN
1	B	1509	GLN
1	B	1518	ASN
1	B	1520	GLN
1	C	2064	GLN
1	C	2229	GLN
1	C	2230	GLN
1	C	2261	ASN
1	C	2362	GLN
1	C	2425	GLN
1	C	2464	GLN
1	C	2482	ASN
1	C	2485	HIS
1	C	2518	ASN
1	C	2520	GLN
1	D	3043	GLN
1	D	3051	GLN
1	D	3064	GLN
1	D	3122	GLN

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Mol	Chain	Res	Type
1	D	3142	HIS
1	D	3153	ASN
1	D	3229	GLN
1	D	3230	GLN
1	D	3261	ASN
1	D	3305	HIS
1	D	3330	ASN
1	D	3338	GLN
1	D	3425	GLN
1	D	3509	GLN
1	D	3520	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	$\# Z > 2$
4	NAI	C	2602	-	47,48,48	1.66	12 (25%)	64,73,73	1.83	12 (18%)
4	NAI	D	3602	-	47,48,48	1.68	11 (23%)	64,73,73	1.82	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LMR	A	701	3	8,8,8	1.36	2 (25%)	10,10,10	1.56	2 (20%)
4	NAI	C	2601	-	47,48,48	1.70	12 (25%)	64,73,73	1.83	10 (15%)
4	NAI	A	602	-	47,48,48	1.71	12 (25%)	64,73,73	1.84	13 (20%)
2	LMR	B	1701	3	8,8,8	1.34	2 (25%)	10,10,10	1.58	2 (20%)
5	FUM	D	3700	-	7,7,7	1.73	2 (28%)	8,8,8	1.01	0
5	FUM	B	1700	-	7,7,7	1.93	3 (42%)	8,8,8	0.86	0
4	NAI	A	601	-	47,48,48	1.62	10 (21%)	64,73,73	1.84	10 (15%)
4	NAI	B	1601	-	47,48,48	1.75	12 (25%)	64,73,73	1.84	10 (15%)
4	NAI	B	1602	-	47,48,48	1.70	12 (25%)	64,73,73	1.80	10 (15%)
5	FUM	A	700	-	7,7,7	1.93	3 (42%)	8,8,8	0.83	0
4	NAI	D	3601	-	47,48,48	1.68	13 (27%)	64,73,73	1.87	9 (14%)
2	LMR	C	2701	3	8,8,8	1.20	1 (12%)	10,10,10	1.70	3 (30%)
2	LMR	D	3701	3	8,8,8	1.23	2 (25%)	10,10,10	1.73	2 (20%)
5	FUM	C	2700	-	7,7,7	1.93	3 (42%)	8,8,8	1.02	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	NAI	C	2602	-	-	6/29/72/72	0/5/5/5
4	NAI	D	3602	-	-	3/29/72/72	0/5/5/5
2	LMR	A	701	3	-	0/8/8/8	-
4	NAI	C	2601	-	-	3/29/72/72	0/5/5/5
4	NAI	A	602	-	-	10/29/72/72	0/5/5/5
2	LMR	B	1701	3	-	0/8/8/8	-
5	FUM	D	3700	-	-	2/5/5/5	-
5	FUM	B	1700	-	-	0/5/5/5	-
4	NAI	A	601	-	-	3/29/72/72	0/5/5/5
4	NAI	B	1601	-	-	5/29/72/72	0/5/5/5
4	NAI	B	1602	-	-	5/29/72/72	0/5/5/5
5	FUM	A	700	-	-	0/5/5/5	-
4	NAI	D	3601	-	-	4/29/72/72	0/5/5/5
2	LMR	C	2701	3	-	3/8/8/8	-
2	LMR	D	3701	3	-	4/8/8/8	-
5	FUM	C	2700	-	-	2/5/5/5	-

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3601	NAI	C5A-N7A	-4.55	1.30	1.39
4	C	2601	NAI	C4N-C3N	-4.48	1.41	1.50
4	B	1601	NAI	C5A-N7A	-4.35	1.31	1.39
4	C	2601	NAI	C5A-N7A	-4.32	1.31	1.39
4	B	1601	NAI	C4N-C3N	-4.26	1.42	1.50
4	A	602	NAI	C5A-N7A	-4.22	1.31	1.39
4	D	3601	NAI	C4N-C3N	-4.17	1.42	1.50
4	B	1602	NAI	C5A-N7A	-4.15	1.31	1.39
4	A	601	NAI	C5A-N7A	-4.07	1.31	1.39
4	C	2602	NAI	C5A-N7A	-4.07	1.31	1.39
4	D	3602	NAI	C5A-N7A	-3.99	1.31	1.39
4	A	601	NAI	C4N-C3N	-3.91	1.42	1.50
4	C	2602	NAI	C4N-C3N	-3.84	1.42	1.50
4	B	1602	NAI	C4N-C3N	-3.83	1.42	1.50
4	D	3602	NAI	C4N-C3N	-3.81	1.42	1.50
4	A	602	NAI	C4N-C3N	-3.73	1.43	1.50
4	A	601	NAI	C6N-N1N	3.42	1.45	1.37
4	A	601	NAI	C5A-C4A	-3.34	1.33	1.39
4	C	2601	NAI	C5A-C4A	-3.33	1.33	1.39
4	C	2601	NAI	C7N-C3N	3.24	1.55	1.48
4	C	2602	NAI	C7N-C3N	3.16	1.55	1.48
4	D	3601	NAI	C6N-N1N	3.16	1.44	1.37
4	A	602	NAI	C7N-C3N	3.16	1.55	1.48
4	D	3602	NAI	C7N-C3N	3.14	1.55	1.48
4	C	2602	NAI	C5A-C4A	-3.06	1.33	1.39
4	A	601	NAI	C7N-C3N	3.05	1.55	1.48
4	B	1602	NAI	C4N-C5N	-3.04	1.41	1.49
4	D	3602	NAI	C5A-C4A	-3.04	1.33	1.39
4	D	3601	NAI	C5A-C4A	-3.02	1.33	1.39
4	D	3601	NAI	C7N-C3N	3.02	1.55	1.48
4	A	602	NAI	C6N-N1N	2.99	1.44	1.37
4	B	1601	NAI	C6N-N1N	2.99	1.44	1.37
4	D	3602	NAI	C6N-N1N	2.98	1.44	1.37
5	B	1700	FUM	OXT-C	-2.95	1.22	1.30
4	B	1602	NAI	C5A-C4A	-2.92	1.33	1.39
4	B	1601	NAI	C7N-C3N	2.89	1.54	1.48
5	C	2700	FUM	C5-C6	2.80	1.55	1.48
4	B	1602	NAI	C7N-C3N	2.79	1.54	1.48
4	C	2601	NAI	C6N-N1N	2.77	1.44	1.37
4	D	3602	NAI	C8A-N7A	2.73	1.36	1.31
4	B	1601	NAI	C5A-C4A	-2.73	1.34	1.39
4	A	602	NAI	C5A-C4A	-2.71	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	700	FUM	OXT-C	-2.71	1.23	1.30
4	A	602	NAI	C8A-N7A	2.69	1.36	1.31
4	D	3602	NAI	C6N-C5N	2.67	1.41	1.33
4	A	602	NAI	C6N-C5N	2.66	1.41	1.33
4	B	1601	NAI	C4N-C5N	-2.65	1.42	1.49
4	D	3601	NAI	C4N-C5N	-2.63	1.42	1.49
5	D	3700	FUM	C5-C6	2.63	1.54	1.48
4	C	2602	NAI	C6N-C5N	2.59	1.41	1.33
4	B	1602	NAI	C8A-N7A	2.58	1.36	1.31
4	D	3602	NAI	C4N-C5N	-2.58	1.42	1.49
4	A	602	NAI	C4N-C5N	-2.57	1.42	1.49
4	B	1602	NAI	C6N-C5N	2.57	1.40	1.33
4	B	1601	NAI	C8A-N7A	2.57	1.36	1.31
4	B	1602	NAI	C2N-C3N	2.55	1.42	1.35
5	C	2700	FUM	C5-C4	2.50	1.40	1.33
4	A	601	NAI	C6N-C5N	2.49	1.40	1.33
4	C	2602	NAI	PA-O3	-2.48	1.56	1.59
4	D	3602	NAI	C2N-C3N	2.46	1.41	1.35
4	C	2601	NAI	C4N-C5N	-2.46	1.42	1.49
4	B	1602	NAI	C6N-N1N	2.46	1.43	1.37
2	B	1701	LMR	O1B-C1	-2.44	1.22	1.30
4	A	602	NAI	O4D-C1D	2.44	1.47	1.42
4	D	3602	NAI	O4D-C1D	2.41	1.47	1.42
4	D	3601	NAI	C6N-C5N	2.39	1.40	1.33
4	A	602	NAI	C2N-C3N	2.39	1.41	1.35
5	A	700	FUM	C5-C4	2.39	1.40	1.33
4	B	1601	NAI	C2A-N1A	2.36	1.38	1.33
4	B	1601	NAI	C2A-N3A	2.36	1.38	1.33
4	B	1601	NAI	C6N-C5N	2.34	1.40	1.33
4	C	2602	NAI	C2N-C3N	2.34	1.41	1.35
4	D	3601	NAI	C2A-N3A	2.33	1.38	1.33
4	B	1601	NAI	O4D-C1D	2.32	1.47	1.42
4	C	2601	NAI	C4A-N9A	-2.31	1.32	1.37
4	A	601	NAI	C4A-N9A	-2.31	1.32	1.37
4	A	601	NAI	C8A-N7A	2.30	1.36	1.31
5	B	1700	FUM	C5-C4	2.30	1.40	1.33
2	D	3701	LMR	O1B-C1	-2.29	1.23	1.30
5	A	700	FUM	C5-C6	2.29	1.54	1.48
4	C	2601	NAI	O4B-C4B	2.29	1.50	1.45
4	D	3601	NAI	O4D-C1D	2.28	1.47	1.42
4	D	3601	NAI	C8A-N7A	2.27	1.36	1.31
2	B	1701	LMR	O4A-C4	-2.26	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2601	NAI	C6N-C5N	2.26	1.40	1.33
4	C	2602	NAI	C8A-N7A	2.25	1.36	1.31
4	D	3601	NAI	C2A-N1A	2.22	1.37	1.33
5	B	1700	FUM	C5-C6	2.21	1.53	1.48
4	C	2602	NAI	C4A-N9A	-2.21	1.33	1.37
4	C	2601	NAI	C8A-N7A	2.19	1.35	1.31
4	A	602	NAI	C2A-N1A	2.18	1.37	1.33
4	B	1602	NAI	O4B-C1B	2.18	1.47	1.42
2	C	2701	LMR	O1B-C1	-2.18	1.23	1.30
4	D	3601	NAI	O4B-C1B	2.18	1.47	1.42
4	A	601	NAI	C4N-C5N	-2.18	1.43	1.49
2	A	701	LMR	O1B-C1	-2.17	1.23	1.30
4	C	2602	NAI	C6N-N1N	2.17	1.42	1.37
4	C	2602	NAI	C4N-C5N	-2.16	1.43	1.49
4	A	602	NAI	C2A-N3A	2.16	1.37	1.33
4	A	601	NAI	C2A-N1A	2.15	1.37	1.33
5	D	3700	FUM	C5-C4	2.15	1.39	1.33
4	D	3602	NAI	C4A-N9A	-2.13	1.33	1.37
4	B	1602	NAI	C4A-N9A	-2.12	1.33	1.37
4	C	2601	NAI	C2A-N1A	2.11	1.37	1.33
4	C	2601	NAI	C2N-C3N	2.10	1.41	1.35
5	C	2700	FUM	O8-C6	-2.09	1.25	1.30
4	D	3601	NAI	C2N-C3N	2.07	1.40	1.35
4	B	1601	NAI	PN-O3	2.07	1.61	1.59
4	C	2602	NAI	O4B-C1B	2.03	1.46	1.42
2	D	3701	LMR	O4A-C4	-2.02	1.24	1.30
2	A	701	LMR	O4A-C4	-2.02	1.24	1.30
4	B	1602	NAI	C1D-N1N	2.01	1.51	1.46

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3601	NAI	C5A-C4A-N3A	-6.05	118.38	126.72
4	B	1601	NAI	C5A-C4A-N3A	-5.98	118.49	126.72
4	A	602	NAI	C5A-C4A-N3A	-5.95	118.52	126.72
4	B	1602	NAI	C5A-C4A-N3A	-5.94	118.53	126.72
4	D	3602	NAI	C5A-C4A-N3A	-5.89	118.61	126.72
4	C	2602	NAI	C5A-C4A-N3A	-5.89	118.61	126.72
4	A	601	NAI	C5A-C4A-N3A	-5.76	118.78	126.72
4	C	2601	NAI	C5A-C4A-N3A	-5.75	118.80	126.72
4	A	601	NAI	N3A-C2A-N1A	-5.37	120.46	128.58
4	D	3601	NAI	C6A-C5A-N7A	-5.33	121.82	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3601	NAI	C6A-C5A-C4A	5.31	124.43	117.18
4	C	2601	NAI	N3A-C2A-N1A	-5.31	120.55	128.58
4	A	602	NAI	N3A-C2A-N1A	-5.24	120.64	128.58
4	D	3602	NAI	N3A-C2A-N1A	-5.23	120.66	128.58
4	B	1601	NAI	N3A-C2A-N1A	-5.22	120.69	128.58
4	B	1602	NAI	N3A-C2A-N1A	-5.21	120.70	128.58
4	C	2602	NAI	N3A-C2A-N1A	-5.20	120.71	128.58
4	B	1601	NAI	C6A-C5A-N7A	-5.18	122.11	132.09
4	D	3601	NAI	N3A-C4A-N9A	5.11	135.86	127.17
4	B	1601	NAI	C6A-C5A-C4A	5.11	124.15	117.18
4	D	3601	NAI	N3A-C2A-N1A	-5.10	120.86	128.58
4	C	2601	NAI	C6A-C5A-N7A	-5.10	122.27	132.09
4	A	602	NAI	C6A-C5A-N7A	-5.04	122.36	132.09
4	A	601	NAI	C6A-C5A-N7A	-5.04	122.37	132.09
4	C	2601	NAI	C6A-C5A-C4A	4.98	123.98	117.18
4	C	2602	NAI	C6A-C5A-N7A	-4.98	122.49	132.09
4	B	1601	NAI	N3A-C4A-N9A	4.97	135.62	127.17
4	B	1602	NAI	C6A-C5A-N7A	-4.96	122.52	132.09
4	A	602	NAI	C6A-C5A-C4A	4.96	123.96	117.18
4	A	601	NAI	C6A-C5A-C4A	4.94	123.92	117.18
4	D	3602	NAI	C6A-C5A-N7A	-4.91	122.62	132.09
4	C	2601	NAI	N3A-C4A-N9A	4.85	135.41	127.17
4	C	2602	NAI	C6A-C5A-C4A	4.83	123.78	117.18
4	A	601	NAI	N3A-C4A-N9A	4.82	135.36	127.17
4	A	602	NAI	N3A-C4A-N9A	4.81	135.34	127.17
4	B	1602	NAI	C6A-C5A-C4A	4.80	123.73	117.18
4	C	2602	NAI	N3A-C4A-N9A	4.79	135.31	127.17
4	B	1602	NAI	N3A-C4A-N9A	4.74	135.23	127.17
4	D	3602	NAI	C6A-C5A-C4A	4.72	123.62	117.18
4	D	3602	NAI	N3A-C4A-N9A	4.64	135.05	127.17
4	A	601	NAI	N9A-C8A-N7A	-4.04	108.21	113.94
2	D	3701	LMR	O1B-C1-C2	3.86	120.91	112.74
2	C	2701	LMR	O1B-C1-C2	3.82	120.82	112.74
4	C	2601	NAI	N9A-C8A-N7A	-3.80	108.54	113.94
4	C	2602	NAI	N9A-C8A-N7A	-3.71	108.67	113.94
4	D	3602	NAI	N9A-C8A-N7A	-3.69	108.70	113.94
4	D	3601	NAI	N9A-C8A-N7A	-3.66	108.74	113.94
4	B	1602	NAI	N9A-C8A-N7A	-3.65	108.75	113.94
4	A	602	NAI	N9A-C8A-N7A	-3.59	108.84	113.94
4	B	1601	NAI	N9A-C8A-N7A	-3.59	108.84	113.94
2	B	1701	LMR	O1B-C1-C2	3.44	120.01	112.74
2	A	701	LMR	O1B-C1-C2	3.39	119.90	112.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1602	NAI	C2A-N3A-C4A	3.35	120.01	111.83
4	D	3602	NAI	C2A-N3A-C4A	3.28	119.84	111.83
4	A	602	NAI	C2A-N3A-C4A	3.25	119.77	111.83
4	C	2602	NAI	C2A-N3A-C4A	3.25	119.76	111.83
4	C	2601	NAI	C2A-N3A-C4A	3.22	119.70	111.83
4	B	1601	NAI	C2A-N3A-C4A	3.21	119.67	111.83
4	A	601	NAI	C2A-N3A-C4A	3.20	119.65	111.83
4	D	3601	NAI	C2A-N3A-C4A	3.18	119.59	111.83
4	D	3602	NAI	C4A-C5A-N7A	2.78	113.76	110.58
4	C	2601	NAI	C4A-C5A-N7A	2.78	113.76	110.58
4	B	1602	NAI	C4A-C5A-N7A	2.77	113.75	110.58
4	D	3601	NAI	C4A-C5A-N7A	2.77	113.75	110.58
4	B	1601	NAI	C4A-C5A-N7A	2.76	113.74	110.58
4	C	2602	NAI	C4A-C5A-N7A	2.75	113.72	110.58
4	A	601	NAI	C4A-C5A-N7A	2.74	113.71	110.58
4	C	2601	NAI	O4B-C1B-N9A	2.72	113.32	108.09
4	A	602	NAI	C4A-C5A-N7A	2.71	113.68	110.58
4	C	2602	NAI	C3D-C2D-C1D	2.62	106.42	101.46
4	B	1602	NAI	C3N-C2N-N1N	-2.44	119.62	123.20
4	B	1602	NAI	C3D-C2D-C1D	2.44	106.07	101.46
4	D	3602	NAI	C3D-C2D-C1D	2.43	106.06	101.46
4	A	602	NAI	C3D-C2D-C1D	2.36	105.93	101.46
2	B	1701	LMR	O1B-C1-O1A	-2.28	118.90	124.08
4	C	2602	NAI	C3B-C2B-C1B	2.24	105.70	101.46
2	D	3701	LMR	O1B-C1-O1A	-2.23	119.02	124.08
4	D	3601	NAI	C3N-C2N-N1N	-2.20	119.97	123.20
4	A	602	NAI	O4D-C1D-N1N	2.19	112.26	108.08
4	A	602	NAI	C3B-C2B-C1B	2.19	105.60	101.46
4	D	3602	NAI	C3N-C2N-N1N	-2.17	120.02	123.20
4	C	2601	NAI	C3N-C2N-N1N	-2.15	120.04	123.20
4	A	601	NAI	C1D-N1N-C2N	-2.15	117.60	121.14
4	D	3602	NAI	O4D-C1D-N1N	2.15	112.19	108.08
4	B	1601	NAI	O4B-C1B-N9A	2.15	112.21	108.09
2	C	2701	LMR	O1B-C1-O1A	-2.14	119.23	124.08
4	A	601	NAI	O4B-C1B-N9A	2.13	112.19	108.09
2	A	701	LMR	O1B-C1-O1A	-2.13	119.25	124.08
4	A	602	NAI	C2D-C3D-C4D	2.10	106.67	102.61
4	C	2602	NAI	C3N-C2N-N1N	-2.10	120.13	123.20
4	C	2602	NAI	O4D-C1D-N1N	2.08	112.06	108.08
4	A	602	NAI	C3N-C2N-N1N	-2.08	120.16	123.20
2	C	2701	LMR	O4A-C4-C3	2.06	120.40	114.00
4	B	1601	NAI	C3N-C2N-N1N	-2.03	120.22	123.20

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3701	LMR	O1A-C1-C2-C3
4	A	602	NAI	C5B-O5B-PA-O1A
4	A	602	NAI	C5B-O5B-PA-O2A
4	A	602	NAI	C5B-O5B-PA-O3
4	A	602	NAI	C5D-O5D-PN-O2N
4	A	602	NAI	O4D-C1D-N1N-C2N
4	C	2602	NAI	C5D-O5D-PN-O3
4	C	2602	NAI	C5D-O5D-PN-O1N
4	A	602	NAI	C3D-C4D-C5D-O5D
4	D	3602	NAI	O4D-C1D-N1N-C2N
5	C	2700	FUM	O-C-C4-C5
5	C	2700	FUM	OXT-C-C4-C5
2	C	2701	LMR	O1B-C1-C2-C3
2	D	3701	LMR	O1B-C1-C2-C3
4	A	602	NAI	O4D-C4D-C5D-O5D
4	A	602	NAI	PA-O3-PN-O5D
4	B	1601	NAI	O4B-C4B-C5B-O5B
5	D	3700	FUM	O-C-C4-C5
4	C	2602	NAI	O4D-C1D-N1N-C6N
4	D	3601	NAI	O4D-C1D-N1N-C2N
4	A	601	NAI	C5D-O5D-PN-O2N
4	B	1601	NAI	C5D-O5D-PN-O2N
4	B	1602	NAI	C5B-O5B-PA-O1A
4	C	2602	NAI	C5B-O5B-PA-O1A
4	C	2602	NAI	C5D-O5D-PN-O2N
4	D	3601	NAI	C5D-O5D-PN-O2N
4	A	602	NAI	C4D-C5D-O5D-PN
2	C	2701	LMR	O1A-C1-C2-C3
5	D	3700	FUM	OXT-C-C4-C5
4	B	1602	NAI	C4D-C5D-O5D-PN
4	C	2602	NAI	PA-O3-PN-O1N
4	A	601	NAI	O4D-C1D-N1N-C2N
4	B	1601	NAI	O4D-C1D-N1N-C2N
4	C	2601	NAI	O4D-C1D-N1N-C2N
4	B	1602	NAI	O4D-C1D-N1N-C6N
4	A	601	NAI	C2N-C3N-C7N-N7N
4	B	1601	NAI	C3B-C4B-C5B-O5B
4	B	1601	NAI	C2N-C3N-C7N-N7N
4	C	2601	NAI	C2N-C3N-C7N-N7N
4	D	3601	NAI	C2N-C3N-C7N-N7N

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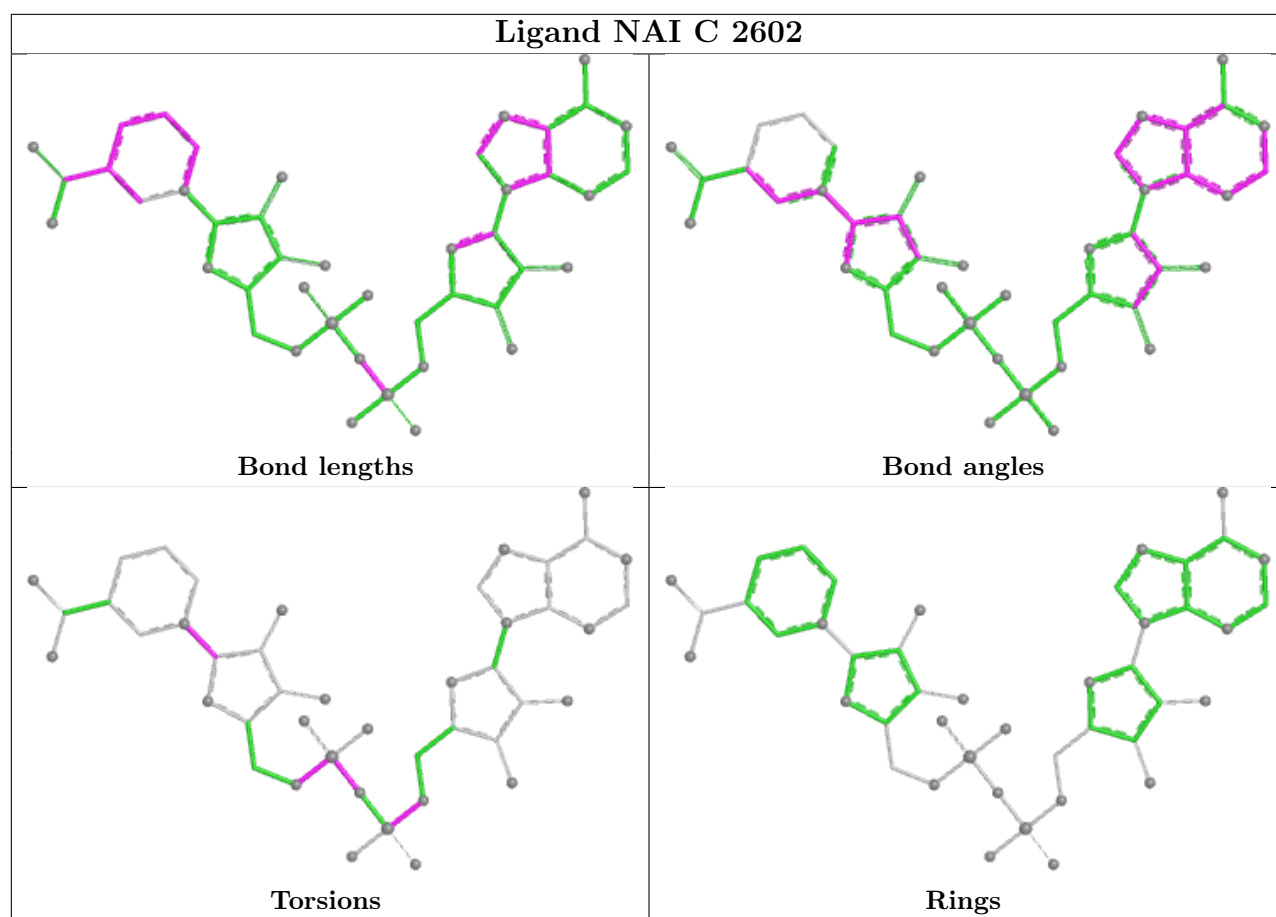
Mol	Chain	Res	Type	Atoms
4	D	3602	NAI	C2N-C3N-C7N-N7N
4	B	1602	NAI	C2D-C1D-N1N-C6N
2	D	3701	LMR	O1B-C1-C2-O2
4	D	3602	NAI	O4B-C4B-C5B-O5B
4	C	2601	NAI	O4B-C4B-C5B-O5B
4	D	3601	NAI	O4B-C4B-C5B-O5B
4	B	1602	NAI	O4D-C1D-N1N-C2N
2	C	2701	LMR	O1B-C1-C2-O2
2	D	3701	LMR	O1A-C1-C2-O2
4	A	602	NAI	PN-O3-PA-O2A

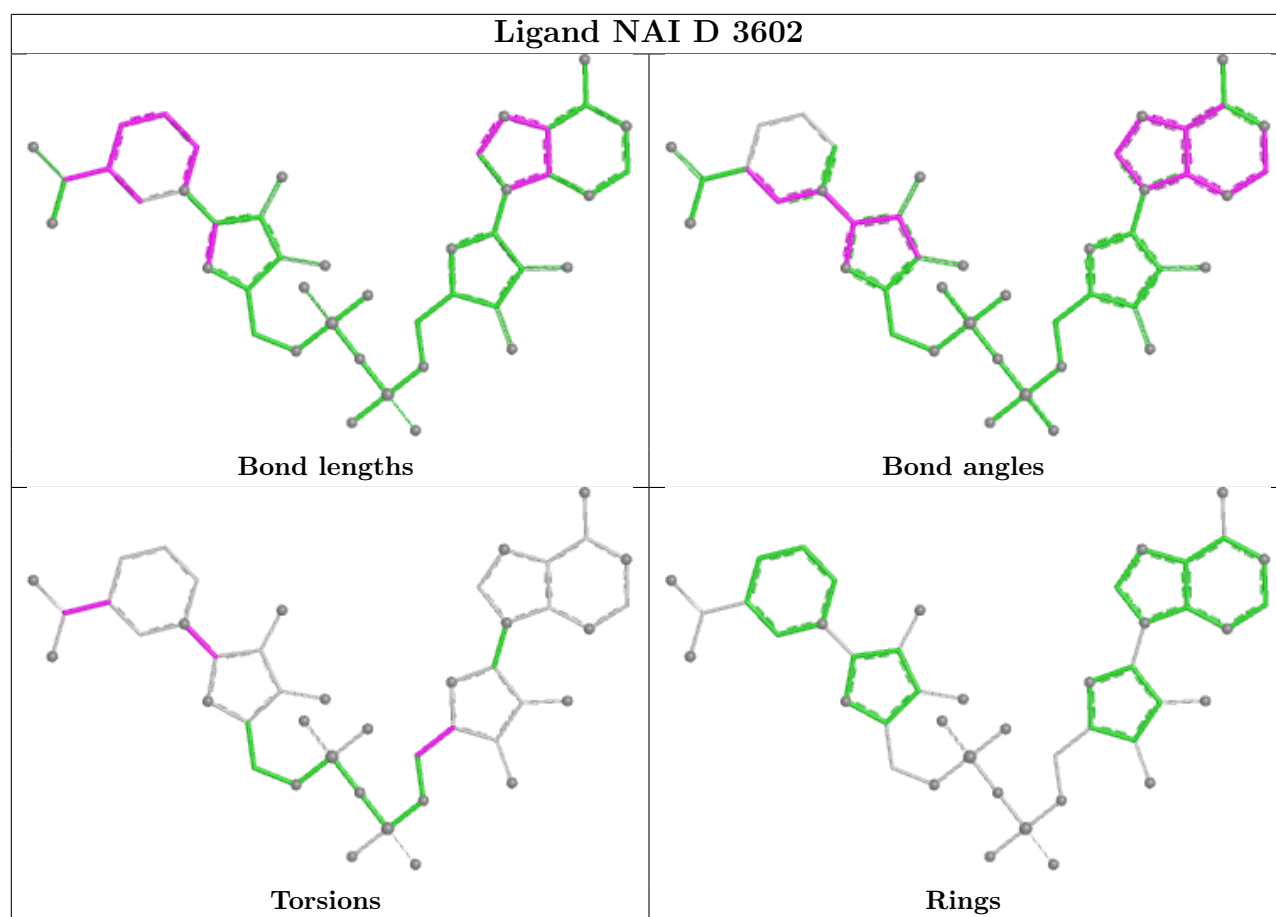
There are no ring outliers.

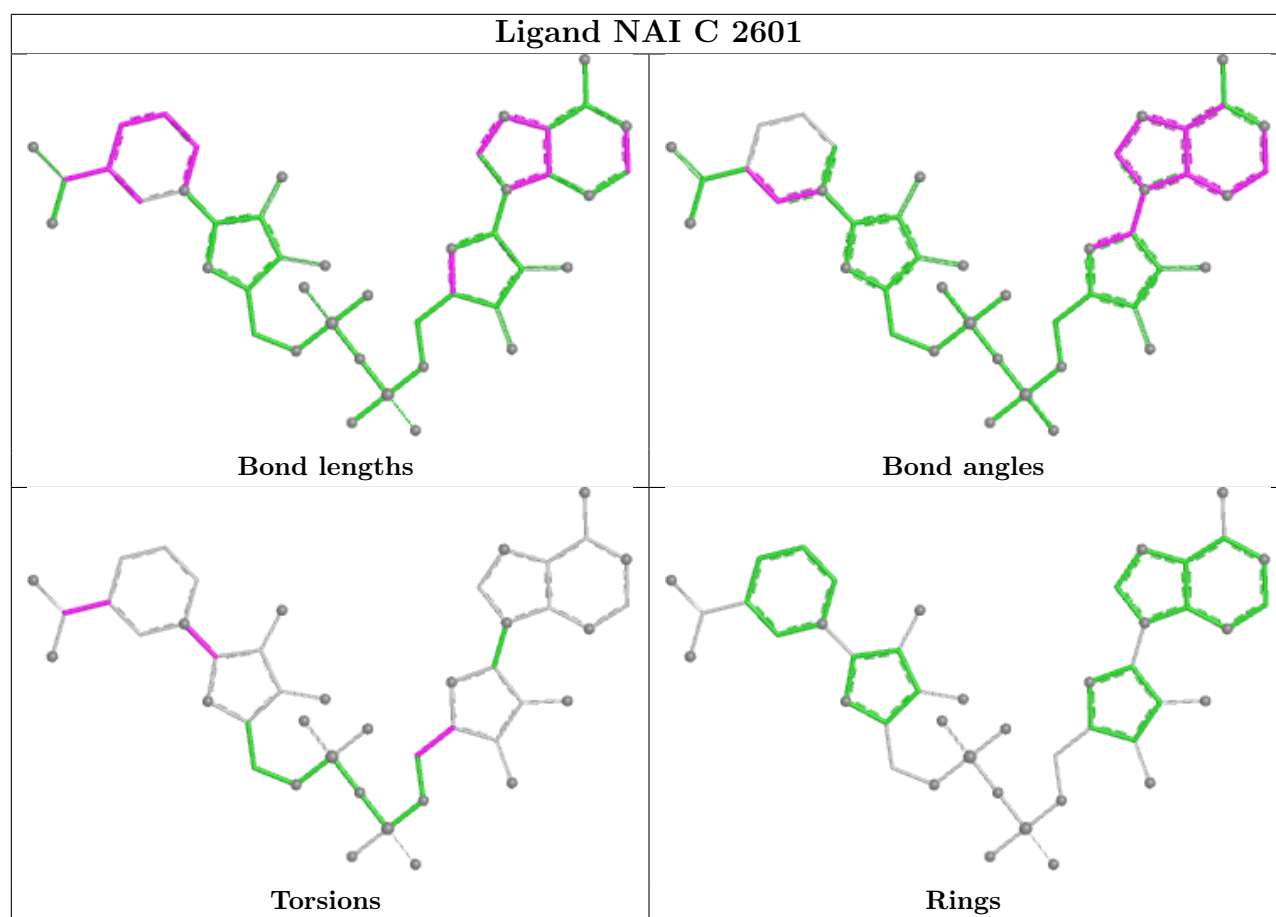
10 monomers are involved in 18 short contacts:

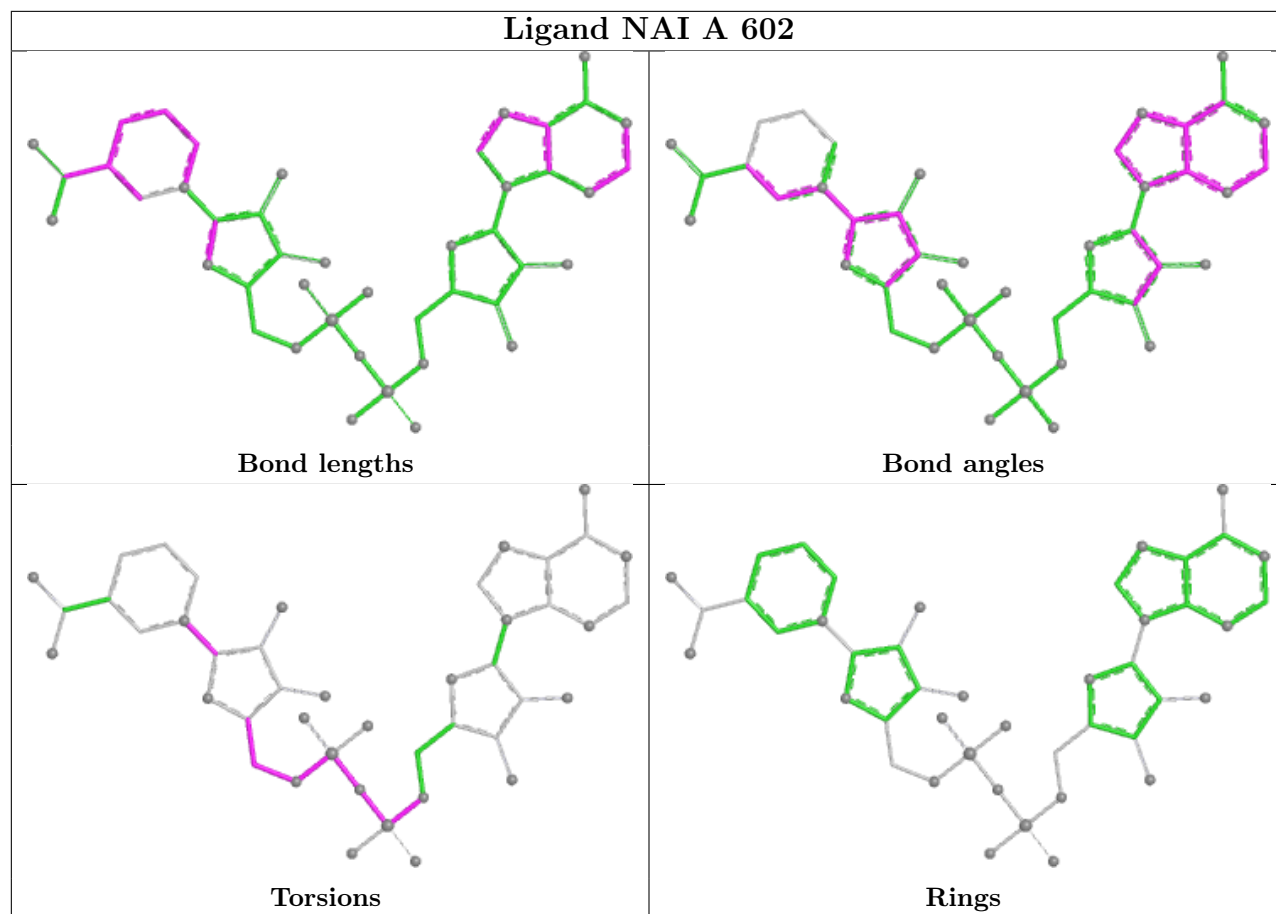
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2602	NAI	1	0
2	A	701	LMR	1	0
4	C	2601	NAI	6	0
4	A	602	NAI	1	0
2	B	1701	LMR	2	0
4	A	601	NAI	3	0
4	B	1601	NAI	1	0
4	D	3601	NAI	4	0
2	C	2701	LMR	2	0
2	D	3701	LMR	1	0

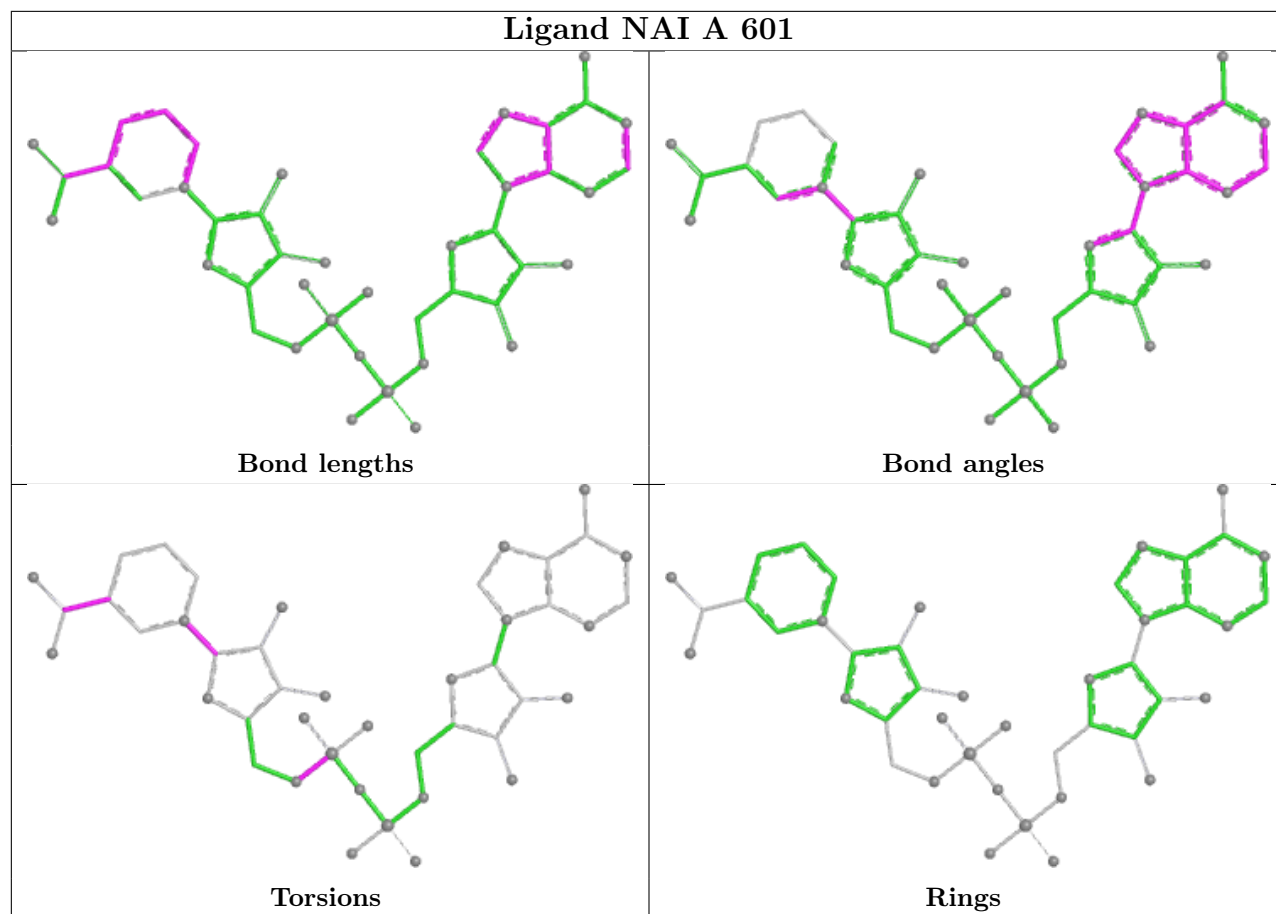
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

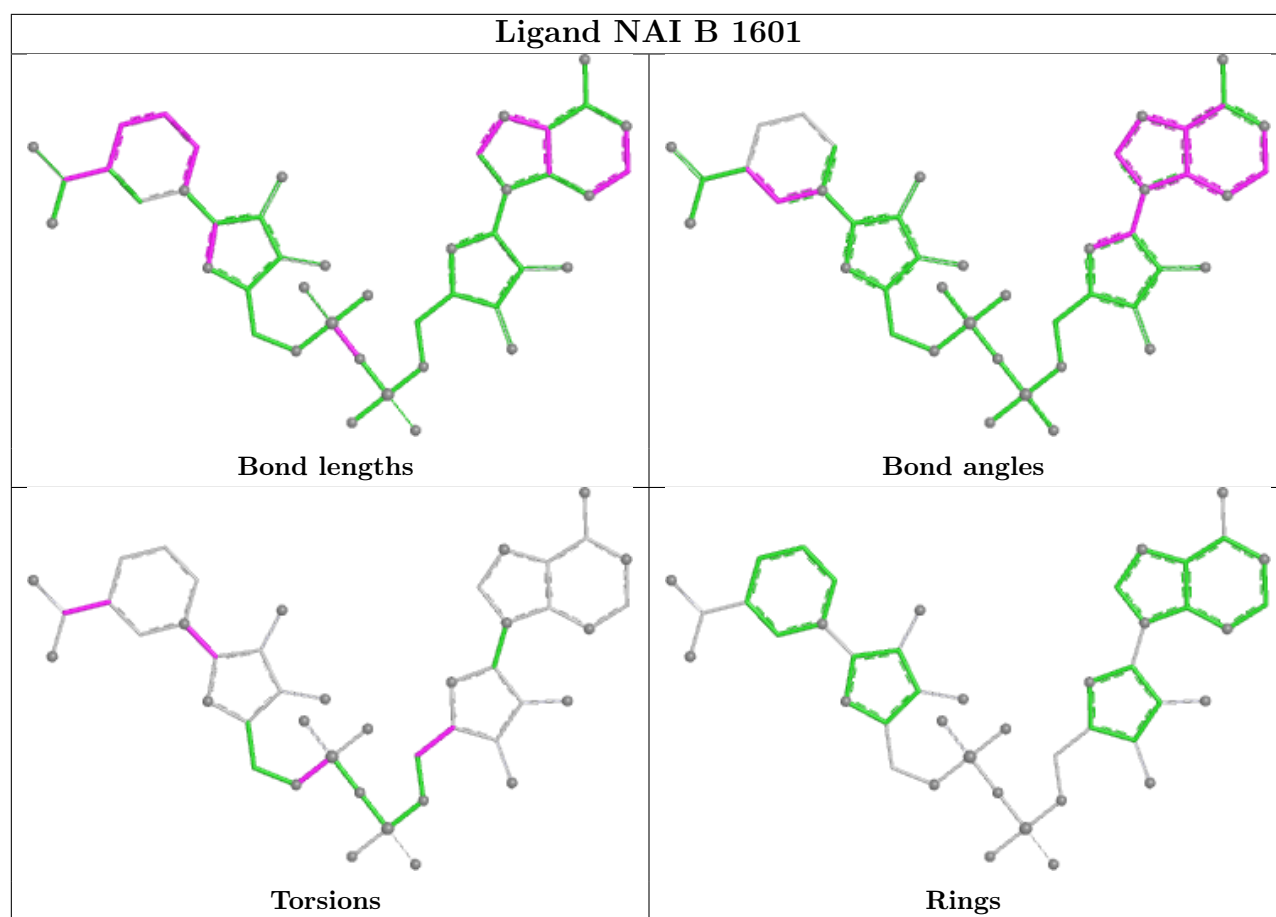


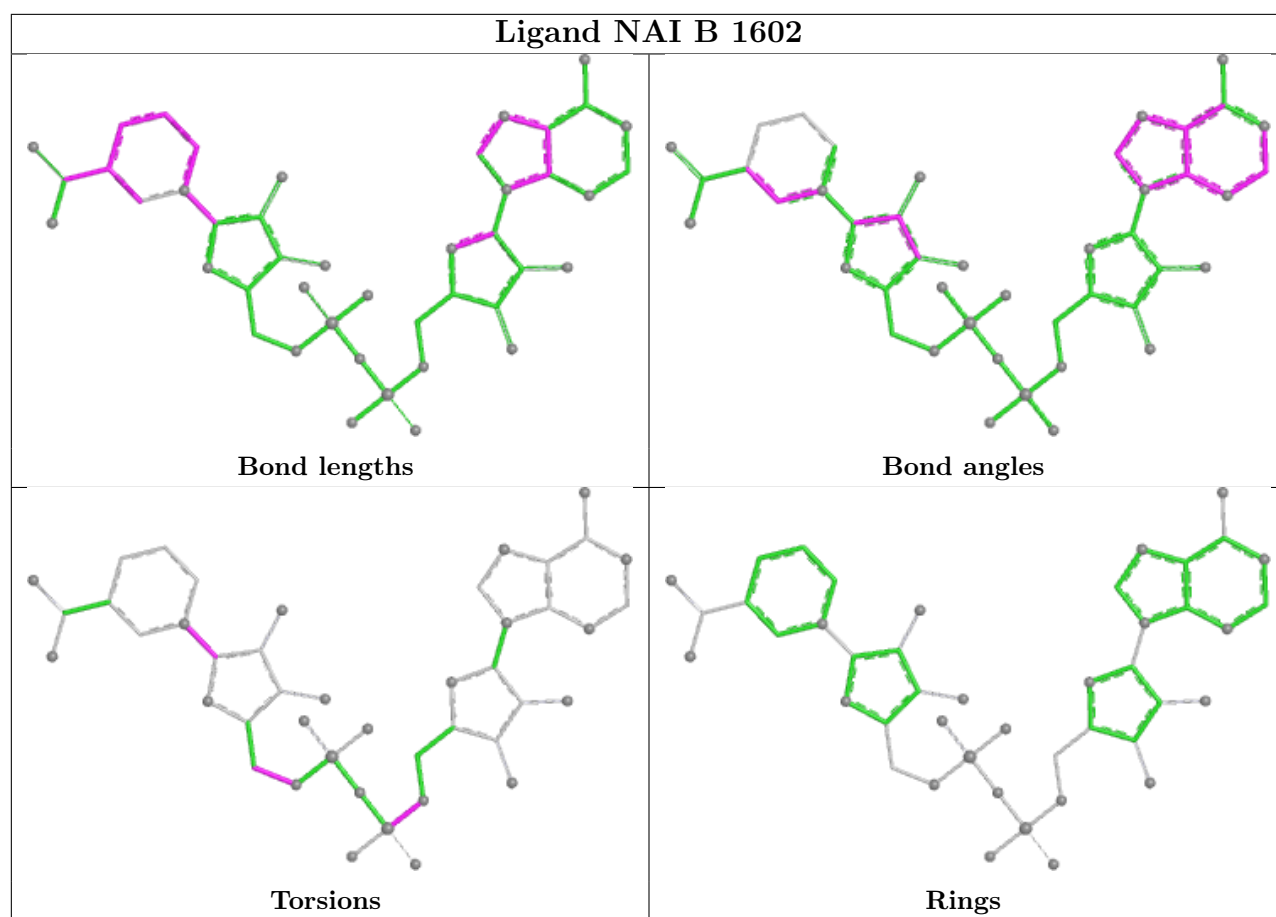


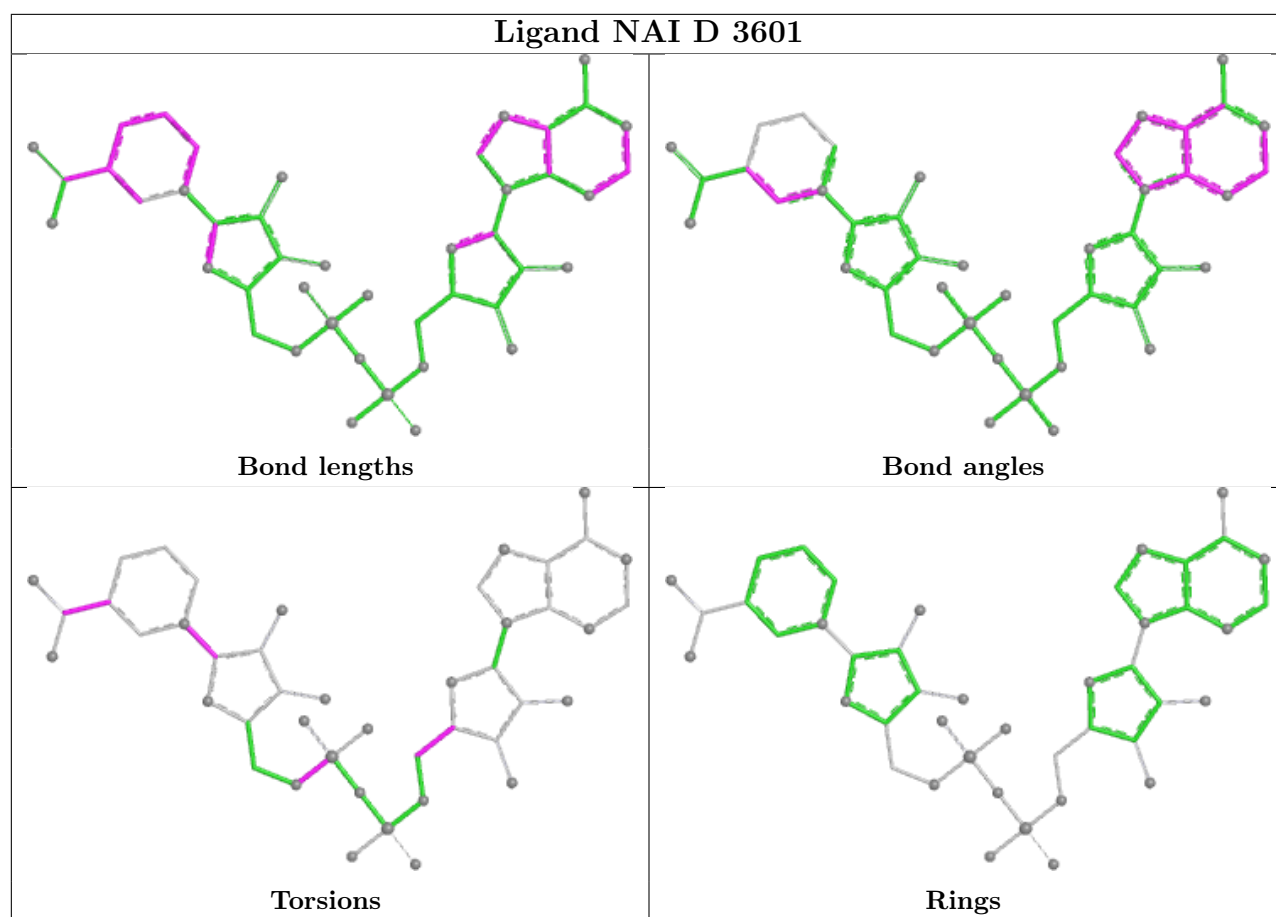












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	539/564 (95%)	-0.07	8 (1%) 72 73	16, 33, 61, 79	0
1	B	539/564 (95%)	0.15	16 (2%) 52 54	18, 36, 67, 97	0
1	C	539/564 (95%)	-0.16	10 (1%) 66 68	16, 31, 54, 68	0
1	D	539/564 (95%)	0.13	14 (2%) 57 59	20, 37, 69, 93	0
All	All	2156/2256 (95%)	0.01	48 (2%) 62 64	16, 34, 64, 97	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1301	PRO	5.9
1	D	3302	ILE	5.1
1	B	1302	ILE	5.1
1	C	2302	ILE	4.5
1	B	1303	SER	4.0
1	B	1543	TYR	3.5
1	B	1304	GLU	3.3
1	D	3328	VAL	3.2
1	B	1021	ILE	3.1
1	D	3508	ALA	3.1
1	A	510	GLY	3.0
1	C	2507	LEU	2.9
1	C	2510	GLY	2.8
1	C	2543	TYR	2.8
1	D	3509	GLN	2.8
1	A	154	HIS	2.7
1	B	1507	LEU	2.7
1	A	302	ILE	2.7
1	B	1508	ALA	2.6
1	C	2455	THR	2.6
1	C	2457	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	304	GLU	2.5
1	B	1260	HIS	2.5
1	C	2303	SER	2.4
1	C	2021	ILE	2.4
1	D	3021	ILE	2.4
1	A	507	LEU	2.4
1	A	508	ALA	2.4
1	A	305	HIS	2.4
1	D	3510	GLY	2.3
1	B	1510	GLY	2.3
1	B	1249	ASN	2.2
1	C	2573	PRO	2.2
1	B	1248	ARG	2.1
1	A	332	LEU	2.1
1	B	1298	ILE	2.1
1	D	3331	GLY	2.1
1	D	3369	ALA	2.1
1	D	3023	GLU	2.1
1	B	1297	VAL	2.1
1	B	1381	VAL	2.1
1	D	3339	LYS	2.0
1	D	3305	HIS	2.0
1	D	3332	LEU	2.0
1	D	3297	VAL	2.0
1	D	3353	GLY	2.0
1	B	1503	THR	2.0
1	C	2547	GLU	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,

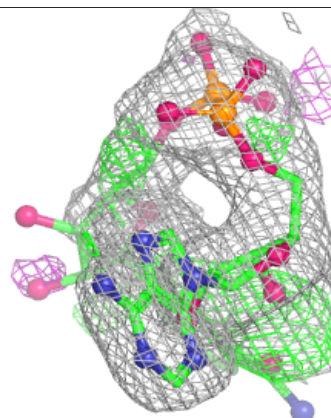
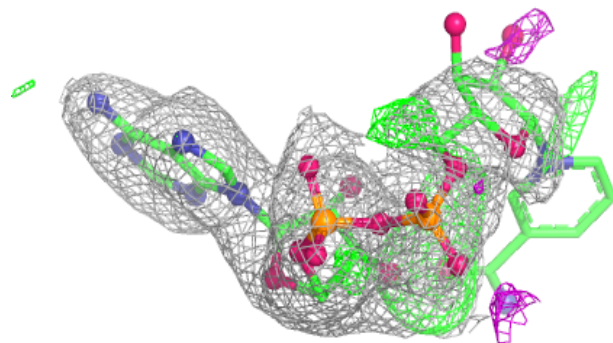
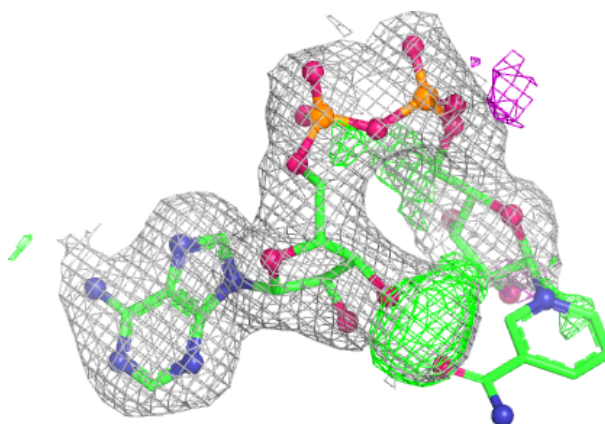
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAI	C	2602	44/44	0.87	0.14	36,58,91,92	9
4	NAI	A	602	44/44	0.88	0.13	37,54,82,82	9
4	NAI	B	1602	44/44	0.89	0.10	30,55,79,79	9
4	NAI	D	3602	44/44	0.89	0.12	30,51,79,79	9
5	FUM	A	700	8/8	0.91	0.07	32,35,37,39	0
5	FUM	B	1700	8/8	0.91	0.10	42,44,46,46	0
4	NAI	B	1601	44/44	0.92	0.10	28,35,41,42	0
5	FUM	C	2700	8/8	0.93	0.08	34,38,41,42	0
2	LMR	B	1701	9/9	0.94	0.07	25,28,32,33	0
2	LMR	C	2701	9/9	0.95	0.07	18,20,24,25	0
4	NAI	D	3601	44/44	0.95	0.07	22,39,45,47	0
5	FUM	D	3700	8/8	0.95	0.06	35,37,38,38	0
2	LMR	D	3701	9/9	0.96	0.07	24,30,32,35	0
4	NAI	A	601	44/44	0.96	0.07	24,30,32,36	0
4	NAI	C	2601	44/44	0.97	0.06	22,30,36,37	0
2	LMR	A	701	9/9	0.97	0.06	15,20,21,22	0
3	MN	B	1604	1/1	0.99	0.05	31,31,31,31	0
3	MN	C	2604	1/1	0.99	0.04	27,27,27,27	0
3	MN	D	3604	1/1	0.99	0.04	30,30,30,30	0
3	MN	A	604	1/1	1.00	0.03	25,25,25,25	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.

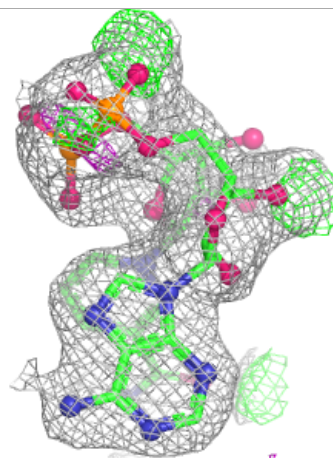
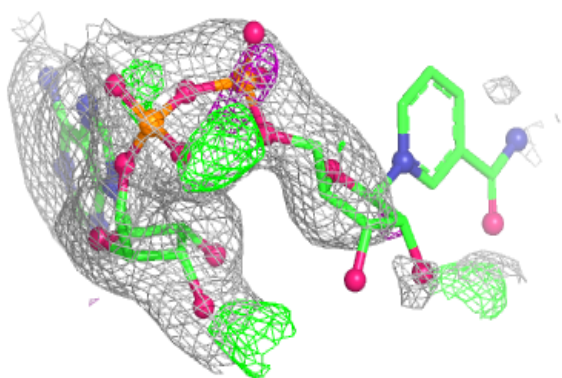
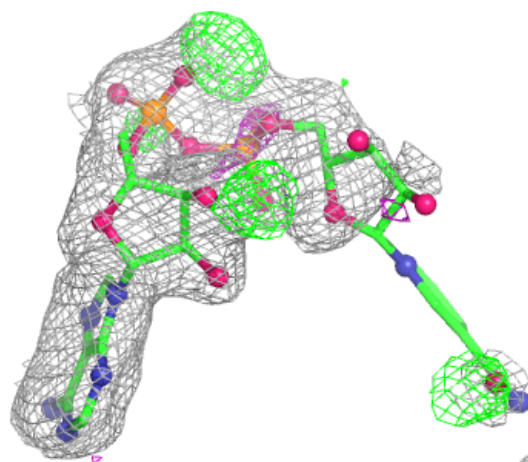
Electron density around NAI C 2602:

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



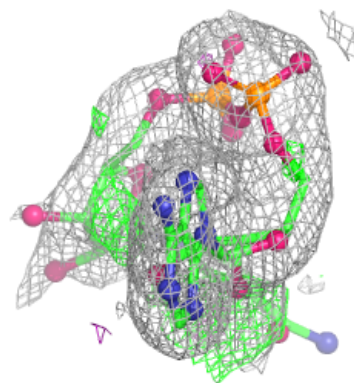
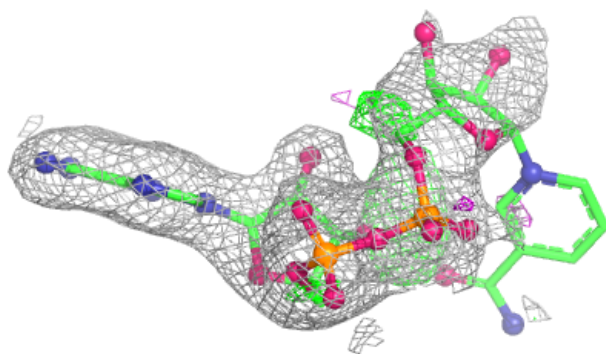
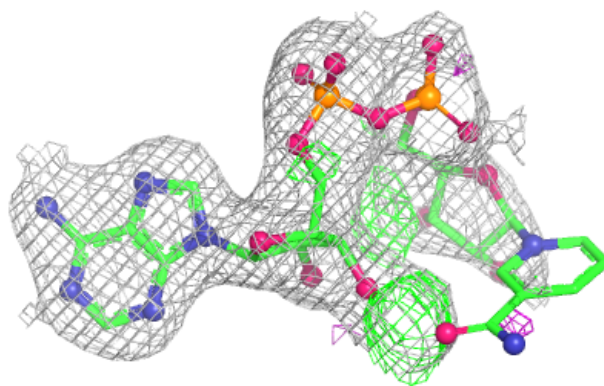
Electron density around NAI A 602:

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

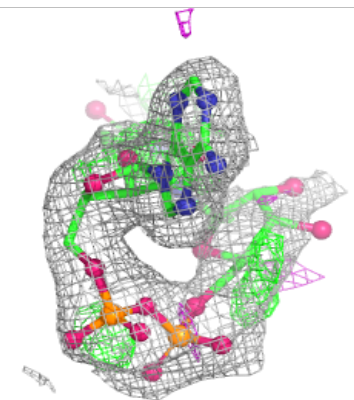
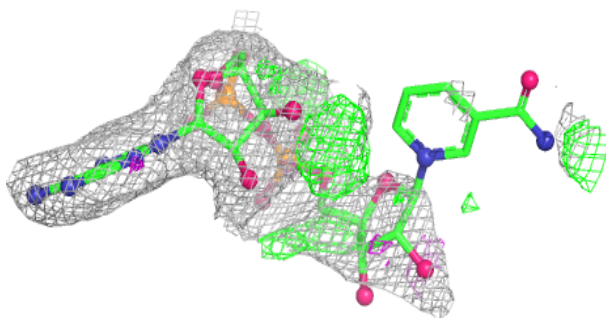
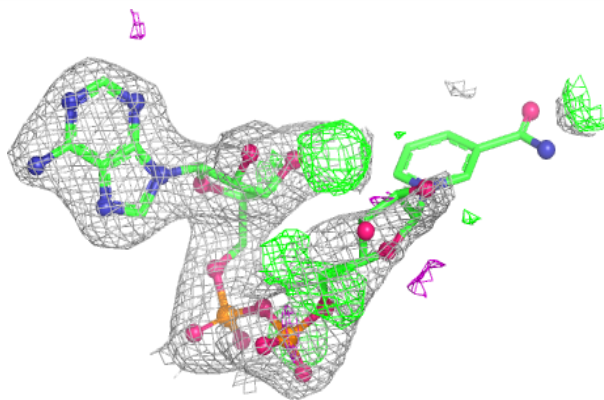


Electron density around NAI B 1602:

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

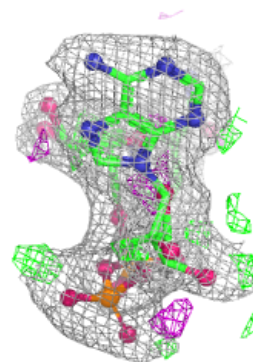
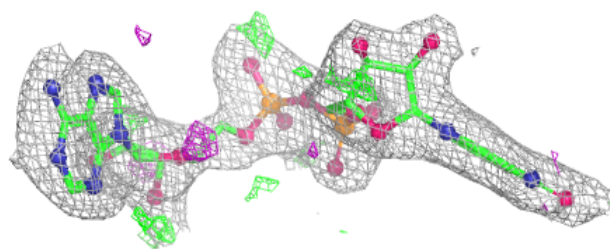
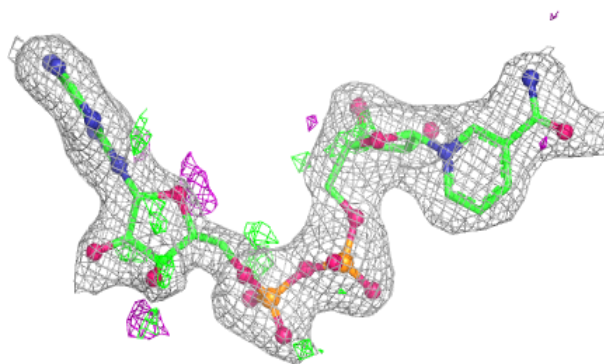
**Electron density around NAI D 3602:**

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

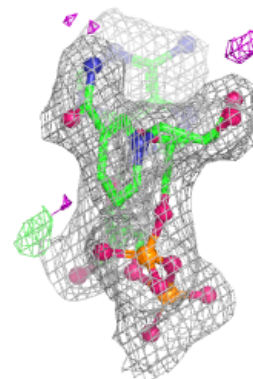
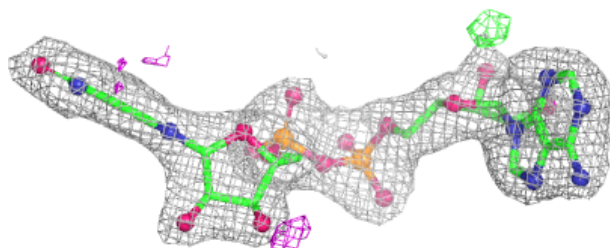
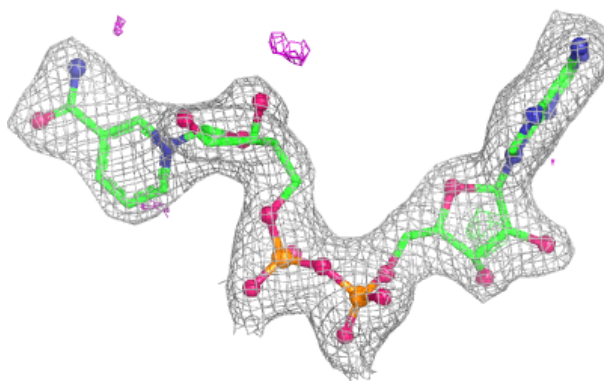


Electron density around NAI B 1601:

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

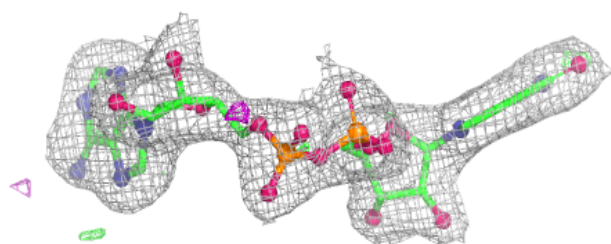
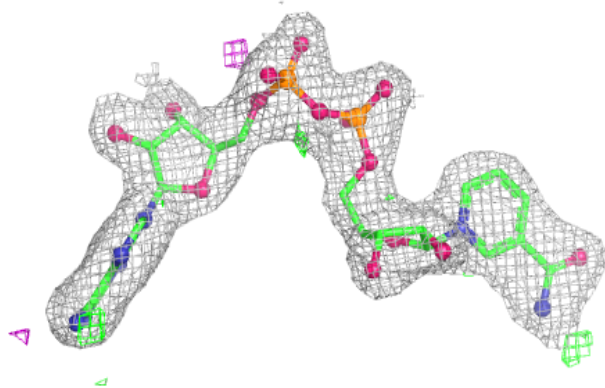
**Electron density around NAI D 3601:**

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

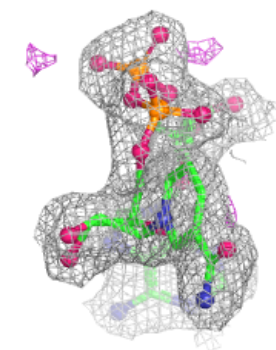
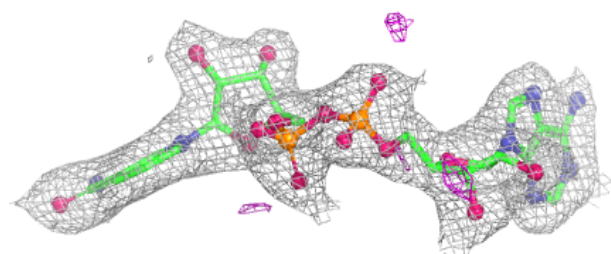
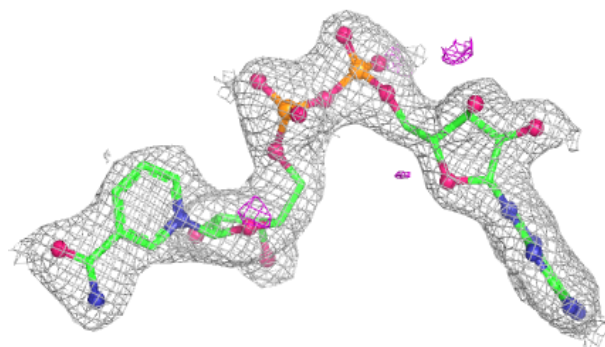


Electron density around NAI A 601:

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

**Electron density around NAI C 2601:**

$2mF_o-DF_c$ (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.