



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:38 PM UTC

PDB ID : 5GTL / pdb_00005gtl
Title : NADPH complex structure of Aldehyde Dehydrogenase from Bacillus cereus
Authors : Ngo, H.P.T.; Hong, S.H.; Ho, T.H.; Oh, D.K.; Kang, L.W.
Deposited on : 2016-08-21
Resolution : 2.00 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

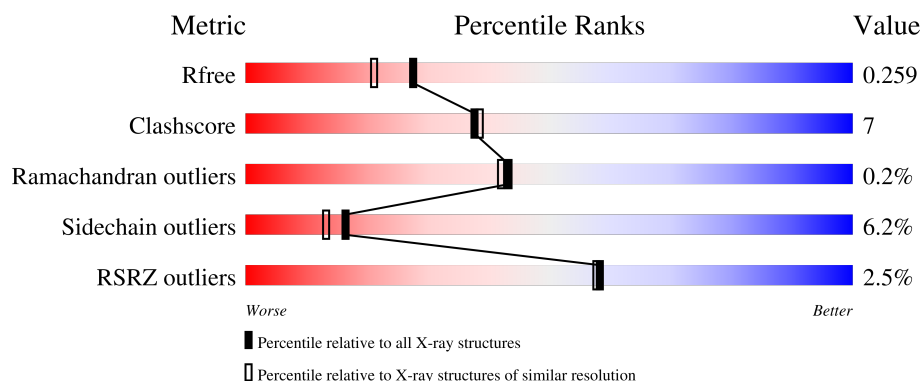
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	494	0% 72% 23% 0%
1	B	494	0% 74% 22% 0%
1	C	494	6% 71% 23% 0%
1	D	494	2% 73% 21% 0%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16824 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.

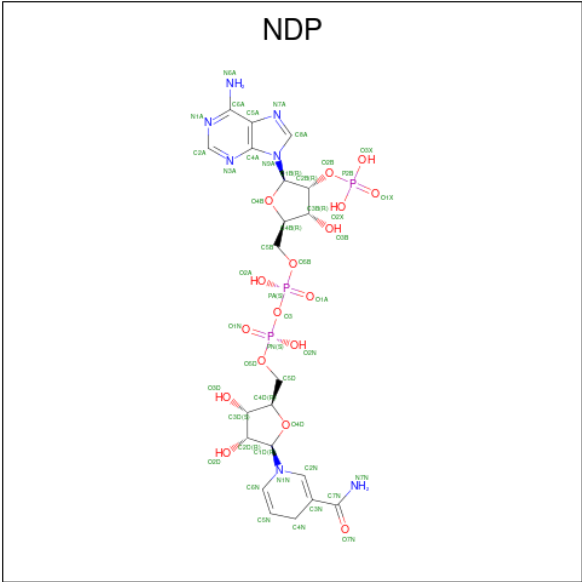
- Molecule 1 is a protein called Betaine-aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3791	2414	630	733	14			
1	B	491	Total	C	N	O	S	0	0	0
			3791	2414	630	733	14			
1	C	488	Total	C	N	O	S	0	0	0
			3768	2400	626	728	14			
1	D	489	Total	C	N	O	S	0	0	0
			3776	2406	627	729	14			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Na	0	0
			2	2		
2	B	2	Total	Na	0	0
			2	2		
2	C	2	Total	Na	0	0
			2	2		
2	D	1	Total	Na	0	0
			1	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

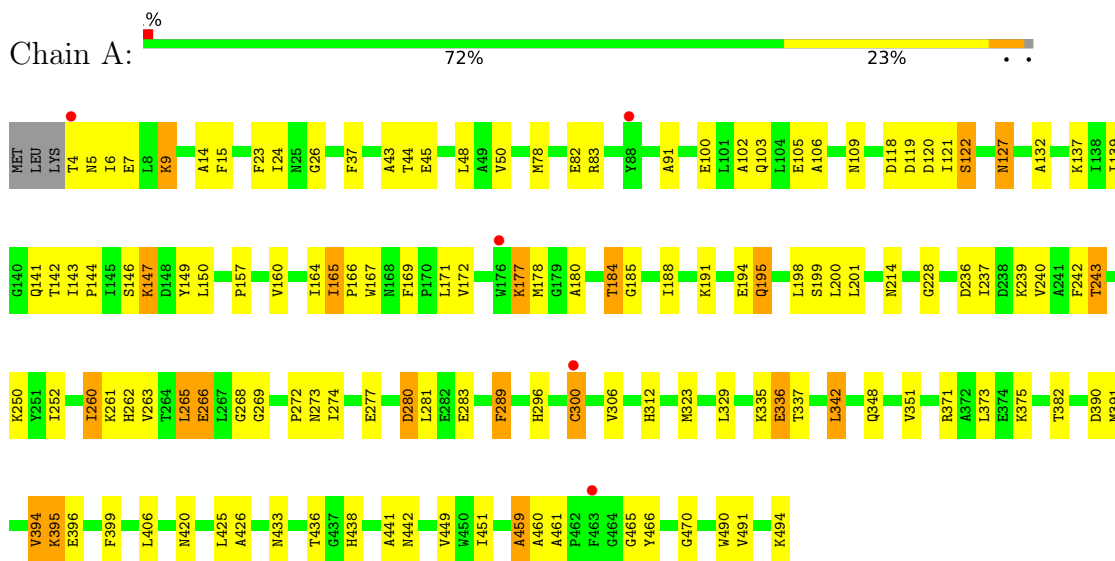
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	454	Total	O	0	0
			454	454		
4	B	421	Total	O	0	0
			421	421		
4	C	291	Total	O	0	0
			291	291		
4	D	333	Total	O	0	0
			333	333		

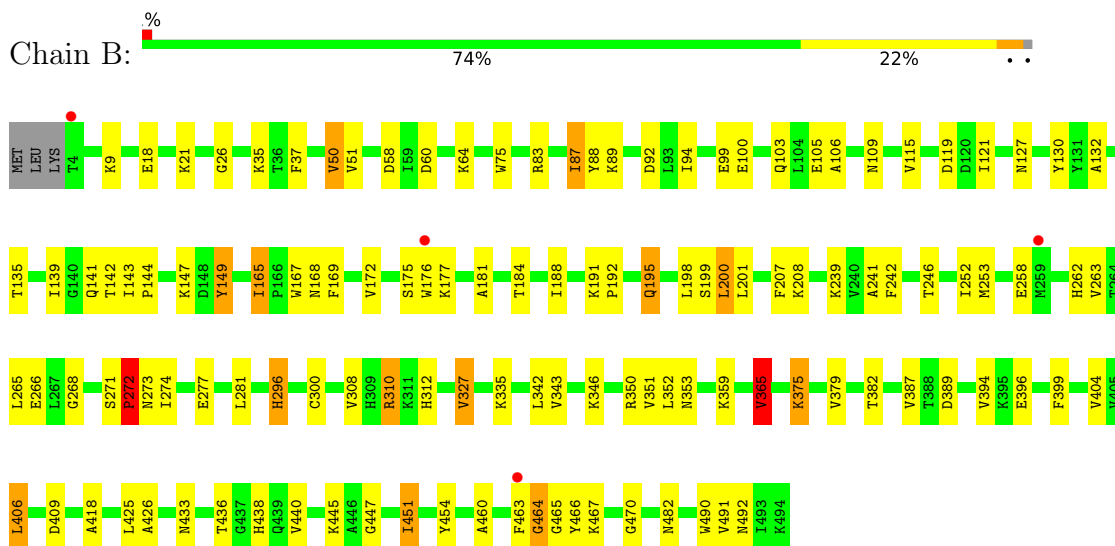
3 Residue-property plots

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: Betaine-aldehyde dehydrogenase

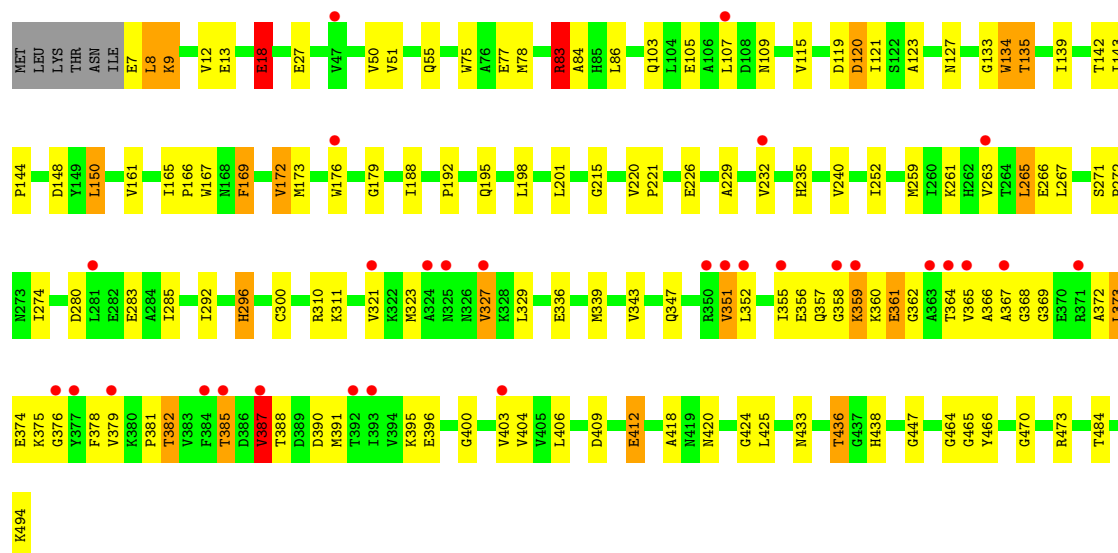


• Molecule 1: Betaine-aldehyde dehydrogenase

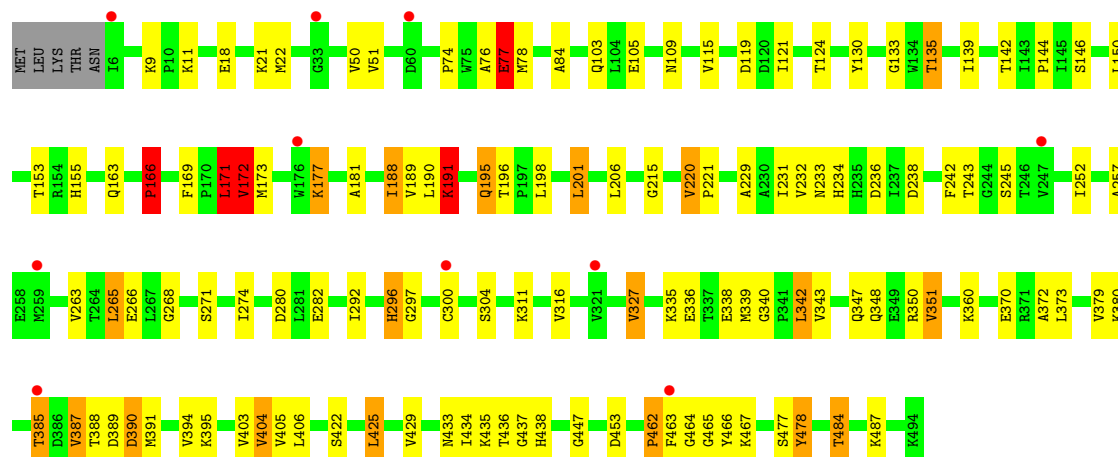


• Molecule 1: Betaine-aldehyde dehydrogenase





• Molecule 1: Betaine-aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.89Å 93.94Å 144.93Å 90.00° 97.67° 90.00°	Depositor
Resolution (Å)	47.88 – 2.00 47.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.88-2.00) 99.8 (47.88-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.91 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.189 , 0.252 0.203 , 0.259	Depositor DCC
R_{free} test set	7525 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16824	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: NDP, NA

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	1.68	62/3870 (1.6%)	1.33	32/5250 (0.6%)
1	B	1.68	51/3870 (1.3%)	1.33	25/5250 (0.5%)
1	C	1.49	18/3847 (0.5%)	1.31	37/5218 (0.7%)
1	D	1.55	29/3855 (0.8%)	1.31	38/5229 (0.7%)
All	All	1.60	160/15442 (1.0%)	1.32	132/20947 (0.6%)

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	477	SER	C-O	-8.21	1.14	1.24
1	A	171	LEU	C-O	-7.60	1.15	1.24
1	A	406	LEU	CA-C	-7.38	1.46	1.52
1	A	100	GLU	N-CA	-7.14	1.37	1.46
1	B	308	VAL	C-O	-7.13	1.17	1.24
1	B	191	LYS	C-O	-7.07	1.17	1.24
1	A	149	TYR	C-O	-7.05	1.15	1.23
1	B	50	VAL	C-O	-7.05	1.16	1.24
1	C	143	ILE	C-N	6.78	1.39	1.33
1	A	269	GLY	C-O	-6.73	1.17	1.23
1	D	181	ALA	C-O	6.68	1.31	1.24
1	C	144	PRO	C-O	-6.63	1.17	1.23
1	B	451	ILE	C-O	-6.57	1.16	1.24
1	C	240	VAL	C-O	-6.50	1.17	1.24
1	A	441	ALA	N-CA	6.45	1.54	1.46
1	A	106	ALA	C-O	-6.37	1.16	1.24
1	A	178	MET	C-O	-6.35	1.16	1.24
1	D	379	VAL	C-O	-6.32	1.17	1.24
1	B	346	LYS	C-O	-6.28	1.16	1.24
1	B	89	LYS	C-O	-6.25	1.16	1.24
1	B	144	PRO	C-O	6.23	1.28	1.24
1	A	48	LEU	C-O	-6.22	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	ALA	N-CA	6.18	1.54	1.46
1	D	130	TYR	C-O	-6.17	1.17	1.24
1	B	272	PRO	C-O	-6.11	1.17	1.23
1	A	188	ILE	C-O	-6.09	1.18	1.24
1	A	289	PHE	C-O	-6.08	1.17	1.24
1	A	420	ASN	C-O	-6.08	1.17	1.23
1	B	208	LYS	N-CA	6.02	1.53	1.46
1	B	149	TYR	C-O	-6.01	1.16	1.23
1	B	106	ALA	C-O	-6.00	1.17	1.24
1	D	435	LYS	C-O	-5.99	1.17	1.24
1	A	451	ILE	C-O	-5.95	1.17	1.24
1	A	119	ASP	C-O	-5.94	1.16	1.24
1	B	491	VAL	C-O	-5.94	1.17	1.24
1	B	241	ALA	C-O	-5.94	1.17	1.24
1	B	181	ALA	N-CA	-5.92	1.39	1.46
1	B	51	VAL	C-O	-5.92	1.18	1.24
1	A	273	ASN	C-O	-5.91	1.17	1.24
1	C	226	GLU	CA-C	5.87	1.57	1.52
1	A	127	ASN	N-CA	-5.84	1.39	1.46
1	A	200	LEU	C-O	-5.81	1.17	1.24
1	C	134	TRP	C-O	-5.81	1.16	1.24
1	A	43	ALA	C-O	-5.80	1.16	1.24
1	C	436	THR	C-O	-5.79	1.17	1.24
1	B	200	LEU	C-O	-5.76	1.17	1.24
1	A	122	SER	C-O	-5.74	1.16	1.24
1	A	15	PHE	C-O	-5.73	1.17	1.24
1	A	7	GLU	C-O	-5.73	1.17	1.24
1	B	490	TRP	C-O	-5.72	1.17	1.24
1	A	177	LYS	C-O	-5.69	1.17	1.24
1	B	482	ASN	C-O	-5.68	1.16	1.24
1	B	87	ILE	C-O	-5.65	1.17	1.24
1	C	135	THR	C-O	-5.65	1.17	1.24
1	D	425	LEU	C-O	-5.64	1.17	1.24
1	D	257	ALA	C-O	-5.62	1.17	1.24
1	B	141	GLN	C-O	-5.61	1.16	1.23
1	B	394	VAL	C-O	-5.61	1.17	1.24
1	D	215	GLY	C-O	-5.60	1.16	1.24
1	A	337	THR	C-O	-5.60	1.17	1.23
1	B	115	VAL	C-O	-5.59	1.18	1.24
1	A	426	ALA	C-O	-5.59	1.17	1.23
1	B	21	LYS	C-O	-5.58	1.16	1.23
1	B	26	GLY	C-O	-5.57	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	37	PHE	C-O	-5.57	1.16	1.23
1	A	118	ASP	C-O	-5.55	1.17	1.24
1	B	127	ASN	N-CA	-5.54	1.39	1.46
1	A	260	ILE	C-O	-5.54	1.17	1.24
1	B	88	TYR	C-O	-5.54	1.17	1.24
1	B	119	ASP	C-O	-5.52	1.17	1.24
1	A	132	ALA	C-O	-5.52	1.17	1.24
1	A	449	VAL	C-O	-5.52	1.18	1.24
1	C	127	ASN	N-CA	-5.49	1.39	1.46
1	D	462	PRO	C-O	-5.47	1.17	1.23
1	A	144	PRO	C-O	-5.47	1.19	1.24
1	A	191	LYS	C-O	-5.46	1.18	1.24
1	A	460	ALA	C-O	-5.46	1.16	1.24
1	D	144	PRO	C-O	-5.44	1.19	1.24
1	A	214	ASN	C-O	-5.44	1.17	1.23
1	D	206	LEU	C-O	-5.43	1.17	1.24
1	A	184	THR	C-O	-5.42	1.16	1.24
1	A	105	GLU	C-O	-5.42	1.17	1.24
1	B	18	GLU	C-O	-5.42	1.17	1.23
1	B	94	ILE	C-O	-5.41	1.18	1.24
1	A	306	VAL	C-O	-5.37	1.18	1.24
1	B	139	ILE	C-O	-5.37	1.16	1.24
1	A	261	LYS	C-O	-5.36	1.17	1.24
1	A	442	ASN	C-O	-5.36	1.17	1.24
1	C	83	ARG	C-O	-5.36	1.17	1.24
1	D	434	ILE	C-O	-5.33	1.18	1.24
1	B	199	SER	C-O	-5.31	1.18	1.24
1	C	119	ASP	C-O	-5.31	1.17	1.24
1	A	185	GLY	C-O	-5.30	1.16	1.24
1	A	490	TRP	C-O	-5.30	1.17	1.24
1	B	92	ASP	C-O	-5.30	1.18	1.24
1	B	406	LEU	CA-C	-5.29	1.47	1.53
1	B	310	ARG	C-O	-5.29	1.17	1.24
1	D	76	ALA	C-O	-5.28	1.17	1.24
1	D	146	SER	C-O	-5.28	1.17	1.23
1	D	119	ASP	C-O	-5.27	1.17	1.24
1	A	146	SER	N-CA	-5.27	1.39	1.46
1	A	395	LYS	C-O	-5.27	1.17	1.24
1	D	171	LEU	C-O	-5.27	1.18	1.24
1	C	169	PHE	C-O	-5.27	1.18	1.24
1	D	297	GLY	C-O	-5.25	1.17	1.24
1	B	175	SER	C-O	-5.23	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	LEU	C-O	-5.22	1.17	1.24
1	B	100	GLU	N-CA	-5.22	1.40	1.46
1	C	123	ALA	C-O	-5.22	1.17	1.24
1	D	268	GLY	C-O	-5.22	1.18	1.23
1	B	135	THR	C-O	-5.22	1.18	1.24
1	D	169	PHE	C-O	-5.22	1.18	1.24
1	C	133	GLY	C-O	-5.21	1.17	1.23
1	A	237	ILE	C-O	-5.21	1.18	1.24
1	D	11	LYS	C-O	-5.21	1.17	1.24
1	D	463	PHE	C-O	-5.21	1.17	1.23
1	A	160	VAL	C-O	-5.21	1.18	1.24
1	D	133	GLY	C-O	-5.20	1.17	1.24
1	D	236	ASP	C-O	-5.20	1.17	1.24
1	C	215	GLY	C-O	-5.20	1.16	1.24
1	D	265	LEU	C-O	-5.19	1.17	1.23
1	B	460	ALA	C-O	-5.19	1.17	1.24
1	D	201	LEU	C-O	-5.18	1.17	1.24
1	C	484	THR	C-O	-5.16	1.17	1.23
1	A	165	ILE	C-O	-5.16	1.18	1.24
1	A	199	SER	C-O	-5.16	1.18	1.24
1	A	102	ALA	N-CA	5.15	1.52	1.46
1	B	281	LEU	C-O	-5.15	1.17	1.24
1	A	120	ASP	C-O	-5.15	1.18	1.24
1	B	184	THR	C-O	-5.15	1.17	1.24
1	B	273	ASN	C-O	-5.13	1.18	1.24
1	A	141	GLN	C-O	-5.13	1.17	1.23
1	B	454	TYR	C-O	-5.13	1.17	1.23
1	A	459	ALA	C-O	-5.13	1.18	1.24
1	A	268	GLY	C-O	-5.13	1.18	1.23
1	A	14	ALA	C-O	-5.12	1.18	1.24
1	A	461	ALA	C-O	-5.11	1.18	1.24
1	D	135	THR	C-O	-5.10	1.18	1.24
1	D	77	GLU	C-O	-5.10	1.17	1.24
1	B	268	GLY	C-O	-5.09	1.19	1.23
1	A	26	GLY	C-O	-5.08	1.17	1.24
1	A	265	LEU	C-O	-5.08	1.17	1.23
1	A	166	PRO	C-O	-5.08	1.17	1.24
1	B	99	GLU	C-O	-5.08	1.18	1.24
1	C	188	ILE	C-O	-5.07	1.18	1.24
1	B	58	ASP	C-O	-5.06	1.18	1.24
1	D	327	VAL	CA-CB	5.06	1.59	1.54
1	B	440	VAL	CA-C	5.05	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	LYS	C-O	-5.04	1.17	1.24
1	A	300	CYS	C-O	-5.04	1.18	1.24
1	B	352	LEU	C-O	-5.04	1.18	1.24
1	A	37	PHE	C-O	-5.04	1.17	1.23
1	C	179	GLY	N-CA	5.04	1.52	1.45
1	B	143	ILE	C-O	-5.03	1.18	1.24
1	B	130	TYR	C-O	-5.02	1.18	1.24
1	D	453	ASP	C-O	-5.02	1.18	1.24
1	C	387	VAL	C-O	-5.02	1.17	1.23
1	A	272	PRO	C-O	-5.01	1.18	1.23
1	A	180	ALA	C-O	-5.01	1.18	1.24
1	B	201	LEU	C-O	-5.00	1.17	1.24

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	198	LEU	N-CA-C	11.29	123.15	111.07
1	A	188	ILE	N-CA-C	9.96	123.29	108.46
1	C	198	LEU	N-CA-C	9.90	121.66	111.07
1	B	188	ILE	N-CA-C	9.59	122.29	108.48
1	D	343	VAL	N-CA-C	9.47	124.13	111.44
1	A	198	LEU	N-CA-C	9.31	121.12	110.97
1	B	342	LEU	N-CA-C	-8.63	99.40	110.53
1	D	274	ILE	N-CA-C	8.33	120.16	107.99
1	D	188	ILE	N-CA-C	8.32	120.45	108.48
1	C	188	ILE	N-CA-C	8.04	120.06	108.48
1	B	198	LEU	N-CA-C	8.04	119.73	110.97
1	A	165	ILE	N-CA-C	7.97	117.45	108.05
1	A	165	ILE	CB-CA-C	-7.63	102.45	110.53
1	A	470	GLY	N-CA-C	7.58	120.87	110.56
1	A	274	ILE	N-CA-C	7.57	119.04	107.99
1	C	267	LEU	CA-C-N	-7.56	114.24	122.55
1	C	267	LEU	C-N-CA	-7.56	114.24	122.55
1	C	343	VAL	N-CA-C	7.53	122.96	112.50
1	B	343	VAL	N-CA-C	7.47	120.43	111.09
1	C	274	ILE	N-CA-C	7.34	118.71	107.99
1	D	342	LEU	N-CA-C	-7.29	101.13	110.53
1	A	335	LYS	N-CA-C	7.27	120.07	111.71
1	B	149	TYR	N-CA-C	7.07	120.19	109.23
1	A	466	TYR	N-CA-C	-7.02	100.41	110.59
1	D	51	VAL	N-CA-C	6.98	118.53	108.48
1	C	466	TYR	N-CA-C	-6.88	100.62	110.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	ILE	N-CA-C	6.87	118.02	107.99
1	C	465	GLY	N-CA-C	6.79	125.40	112.51
1	D	172	VAL	N-CA-CB	6.78	119.77	110.54
1	B	139	ILE	N-CA-C	6.75	119.44	108.97
1	C	271	SER	N-CA-C	6.72	118.18	109.64
1	D	389	ASP	N-CA-C	6.68	120.30	111.75
1	D	142	THR	N-CA-C	-6.61	98.44	109.07
1	C	167	TRP	N-CA-C	6.55	121.42	113.17
1	C	359	LYS	N-CA-C	-6.54	104.23	111.36
1	C	165	ILE	N-CA-C	6.52	114.99	107.89
1	C	352	LEU	N-CA-C	-6.51	103.69	111.69
1	A	167	TRP	N-CA-C	6.46	121.31	113.17
1	B	177	LYS	N-CA-C	6.45	118.11	111.14
1	A	7	GLU	N-CA-C	6.44	119.06	109.59
1	A	132	ALA	N-CA-C	-6.43	104.27	111.28
1	C	470	GLY	N-CA-C	6.40	119.27	110.56
1	D	465	GLY	N-CA-C	6.39	124.66	112.51
1	B	365	VAL	N-CA-CB	6.39	118.94	111.66
1	A	5	ASN	N-CA-C	6.38	119.72	110.28
1	C	8	LEU	N-CA-C	6.37	119.22	110.24
1	C	51	VAL	N-CA-C	6.34	117.61	108.48
1	A	396	GLU	N-CA-C	6.28	120.28	110.17
1	C	142	THR	N-CA-C	-6.25	99.00	109.07
1	A	281	LEU	N-CA-C	6.25	118.89	111.33
1	B	382	THR	N-CA-C	6.22	119.54	109.40
1	D	335	LYS	N-CA-C	6.20	120.45	113.01
1	B	389	ASP	N-CA-C	6.17	119.64	111.75
1	A	139	ILE	N-CA-C	6.16	117.89	108.71
1	C	120	ASP	N-CA-C	6.16	118.54	111.02
1	D	466	TYR	N-CA-C	-6.15	101.36	110.46
1	A	6	ILE	N-CA-C	-6.13	99.75	108.58
1	A	465	GLY	N-CA-C	6.06	124.28	112.04
1	D	234	HIS	N-CA-C	5.99	118.39	109.59
1	D	220	VAL	CA-C-N	-5.95	114.48	120.31
1	D	220	VAL	C-N-CA	-5.95	114.48	120.31
1	B	281	LEU	N-CA-C	5.92	119.32	111.75
1	C	400	GLY	N-CA-C	-5.89	100.33	112.34
1	A	191	LYS	CA-C-N	-5.87	114.70	120.52
1	A	191	LYS	C-N-CA	-5.87	114.70	120.52
1	B	141	GLN	N-CA-C	5.87	119.11	109.72
1	A	280	ASP	N-CA-C	-5.86	97.68	107.99
1	D	327	VAL	N-CA-CB	5.83	117.48	110.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	437	GLY	N-CA-C	-5.83	105.44	112.49
1	A	382	THR	N-CA-C	5.82	118.89	109.40
1	C	9	LYS	N-CA-C	-5.80	102.77	110.07
1	A	236	ASP	N-CA-C	5.78	119.64	112.59
1	B	142	THR	N-CA-C	-5.78	99.77	109.07
1	C	169	PHE	N-CA-C	-5.76	100.47	108.76
1	D	177	LYS	N-CA-C	5.74	117.21	111.07
1	A	142	THR	N-CA-C	-5.67	99.94	109.07
1	C	139	ILE	N-CA-C	5.66	118.06	109.12
1	D	150	LEU	N-CA-C	-5.66	99.51	108.73
1	D	271	SER	N-CA-C	5.62	117.58	109.48
1	D	478	TYR	N-CA-C	5.62	117.86	111.11
1	D	406	LEU	CA-C-N	-5.62	114.54	120.66
1	D	406	LEU	C-N-CA	-5.62	114.54	120.66
1	C	280	ASP	N-CA-C	-5.61	98.12	107.99
1	C	327	VAL	N-CA-C	5.60	116.49	108.93
1	A	406	LEU	CA-C-N	-5.59	114.56	120.66
1	A	406	LEU	C-N-CA	-5.59	114.56	120.66
1	B	207	PHE	N-CA-C	-5.59	105.11	111.14
1	A	141	GLN	N-CA-C	5.54	118.60	109.85
1	B	470	GLY	N-CA-C	5.51	118.06	110.56
1	C	382	THR	N-CA-C	5.46	117.79	108.90
1	A	237	ILE	N-CA-C	-5.45	100.57	108.36
1	A	143	ILE	N-CA-C	5.43	113.92	107.73
1	A	342	LEU	N-CA-C	-5.43	103.22	110.55
1	C	150	LEU	N-CA-C	-5.41	99.91	108.73
1	D	434	ILE	N-CA-C	5.40	116.13	110.62
1	D	21	LYS	N-CA-C	5.40	117.84	110.55
1	B	167	TRP	N-CA-C	5.40	119.97	113.17
1	A	228	GLY	N-CA-C	5.40	118.76	112.50
1	D	189	VAL	N-CA-C	-5.39	98.71	107.28
1	B	327	VAL	N-CA-CB	5.39	118.54	110.13
1	D	139	ILE	N-CA-C	5.39	117.64	109.12
1	D	405	VAL	N-CA-C	5.36	115.81	107.99
1	D	280	ASP	N-CA-C	-5.36	99.02	108.23
1	B	35	LYS	N-CA-C	5.34	118.03	110.50
1	C	368	GLY	N-CA-C	5.32	120.65	110.86
1	D	196	THR	CA-C-N	-5.32	114.78	120.47
1	D	196	THR	C-N-CA	-5.32	114.78	120.47
1	D	191	LYS	CA-C-N	-5.31	115.10	120.31
1	D	191	LYS	C-N-CA	-5.31	115.10	120.31
1	B	466	TYR	N-CA-C	-5.30	102.90	110.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	362	GLY	N-CA-C	5.29	122.61	115.00
1	C	235	HIS	N-CA-C	5.28	118.82	112.38
1	B	465	GLY	N-CA-C	5.26	122.67	112.04
1	B	467	LYS	CB-CA-C	-5.25	110.50	116.54
1	D	338	GLU	N-CA-C	-5.22	107.46	113.88
1	D	340	GLY	CA-C-N	-5.22	115.39	120.98
1	D	340	GLY	C-N-CA	-5.22	115.39	120.98
1	A	9	LYS	N-CA-C	-5.21	103.50	110.07
1	C	55	GLN	N-CA-C	-5.18	102.53	110.14
1	D	387	VAL	N-CA-C	5.15	116.61	109.29
1	C	373	LEU	N-CA-C	5.15	121.77	110.80
1	B	396	GLU	N-CA-C	5.15	118.50	110.32
1	A	150	LEU	N-CA-C	-5.12	100.39	108.73
1	C	396	GLU	N-CA-C	5.12	118.08	109.95
1	B	168	ASN	N-CA-C	5.07	118.61	112.23
1	C	220	VAL	CA-C-N	-5.06	115.35	120.21
1	C	220	VAL	C-N-CA	-5.06	115.35	120.21
1	C	376	GLY	N-CA-C	-5.06	101.20	113.18
1	C	18	GLU	N-CA-CB	-5.03	103.72	111.46
1	B	464	GLY	N-CA-C	5.02	118.08	110.75
1	C	107	LEU	N-CA-C	5.02	117.86	111.69
1	D	238	ASP	N-CA-C	5.01	119.10	112.89

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	3791	0	3740	54	0
1	B	3791	0	3740	43	0
1	C	3768	0	3716	60	0
1	D	3776	0	3727	67	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	1	0
3	A	48	0	26	1	0
3	B	48	0	26	0	0
3	C	48	0	26	0	0
3	D	48	0	26	4	0
4	A	454	0	0	6	0
4	B	421	0	0	6	0
4	C	291	0	0	10	0
4	D	333	0	0	8	0
All	All	16824	0	15027	211	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 7.

All (211) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:VAL:O	1:C:355:ILE:HD12	1.32	1.28
1:C:391:MET:SD	4:C:806:HOH:O	2.00	1.17
1:D:347:GLN:O	1:D:351:VAL:HG12	1.66	0.95
1:A:195:GLN:H	1:A:195:GLN:HE21	1.22	0.86
1:D:385:THR:HG21	4:D:883:HOH:O	1.76	0.85
1:D:342:LEU:CD1	1:D:351:VAL:HG11	2.06	0.85
1:B:375:LYS:HE3	4:B:671:HOH:O	1.76	0.84
1:C:351:VAL:O	1:C:355:ILE:CD1	2.24	0.83
1:A:277:GLU:HG2	4:A:968:HOH:O	1.78	0.82
1:C:18:GLU:HG3	4:C:764:HOH:O	1.79	0.80
1:C:387:VAL:HA	4:C:806:HOH:O	1.84	0.76
1:B:83:ARG:HD3	4:B:614:HOH:O	1.85	0.76
1:D:9:LYS:H	1:D:103:GLN:HE22	1.34	0.75
1:B:195:GLN:HE21	1:B:195:GLN:H	1.36	0.74
1:C:148:ASP:HB3	1:C:494:LYS:HG3	1.71	0.72
1:D:84:ALA:HB2	1:D:135:THR:OG1	1.91	0.70
1:C:84:ALA:HB2	1:C:135:THR:OG1	1.91	0.70
1:B:165:ILE:HD11	4:B:859:HOH:O	1.91	0.70
1:B:438:HIS:HE1	1:C:438:HIS:HE1	1.41	0.69
1:A:243:THR:HG21	4:A:636:HOH:O	1.93	0.68
1:C:300:CYS:SG	1:C:425:LEU:HD21	2.34	0.68
1:C:192:PRO:HA	4:C:605:HOH:O	1.94	0.67
1:D:347:GLN:O	1:D:351:VAL:CG1	2.41	0.67
1:C:169:PHE:HB3	1:C:172:VAL:HG22	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:LYS:H	1:C:103:GLN:HE22	1.44	0.66
1:D:370:GLU:O	1:D:380:LYS:HG3	1.96	0.66
1:D:467:LYS:O	4:D:603:HOH:O	2.15	0.65
1:D:388:THR:OG1	4:D:602:HOH:O	2.14	0.65
1:A:169:PHE:HB3	1:A:172:VAL:CG1	2.27	0.64
1:B:9:LYS:H	1:B:103:GLN:HE22	1.43	0.64
1:B:239:LYS:HZ1	1:B:262:HIS:CD2	2.16	0.63
1:B:350:ARG:NH1	4:B:601:HOH:O	2.31	0.63
1:C:83:ARG:HH11	1:C:83:ARG:HG3	1.65	0.62
1:A:177:LYS:HZ1	1:A:243:THR:CG2	2.13	0.62
1:C:259:MET:HE3	1:C:261:LYS:HE3	1.82	0.61
1:C:387:VAL:HG12	4:C:806:HOH:O	2.00	0.61
1:D:342:LEU:HD11	1:D:351:VAL:HG11	1.81	0.60
1:A:9:LYS:H	1:A:103:GLN:HE22	1.49	0.60
1:D:229:ALA:HA	1:D:232:VAL:HG12	1.82	0.60
1:D:387:VAL:HG23	1:D:391:MET:SD	2.41	0.60
2:D:501:NA:NA	4:D:601:HOH:O	1.74	0.60
1:A:494:LYS:HE3	4:A:767:HOH:O	2.02	0.60
1:C:356:GLU:O	1:C:359:LYS:N	2.35	0.59
1:A:300:CYS:SG	1:A:425:LEU:HD21	2.43	0.59
1:C:8:LEU:HB3	1:C:13:GLU:HG3	1.83	0.59
1:A:391:MET:HB2	1:A:394:VAL:HG13	1.85	0.58
1:B:239:LYS:NZ	1:B:262:HIS:HD2	2.02	0.58
1:B:75:TRP:CH2	1:B:83:ARG:HD2	2.39	0.57
1:C:355:ILE:HG21	1:C:369:GLY:HA2	1.86	0.57
1:D:433:ASN:HD22	1:D:436:THR:H	1.51	0.57
1:C:310:ARG:HD2	1:C:409:ASP:OD1	2.04	0.57
1:A:263:VAL:HG12	1:A:265:LEU:HG	1.86	0.56
1:D:387:VAL:CG2	1:D:391:MET:SD	2.93	0.56
1:A:240:VAL:CG1	1:A:263:VAL:HG22	2.35	0.56
1:B:438:HIS:HE1	1:C:438:HIS:CE1	2.24	0.56
1:C:347:GLN:O	1:C:351:VAL:HG13	2.04	0.56
1:D:350:ARG:HG2	1:D:350:ARG:HH11	1.68	0.56
1:C:173:MET:HG2	1:C:176:TRP:CZ3	2.42	0.55
1:B:359:LYS:HE2	1:B:365:VAL:HG11	1.89	0.54
1:D:229:ALA:O	1:D:232:VAL:HG12	2.07	0.54
1:B:263:VAL:HG12	1:B:265:LEU:HG	1.89	0.54
1:A:438:HIS:CE1	1:D:438:HIS:HE1	2.25	0.54
1:D:22:MET:CG	1:D:221:PRO:HD2	2.37	0.54
1:C:388:THR:OG1	1:C:390:ASP:OD1	2.21	0.54
1:B:195:GLN:HG3	4:B:967:HOH:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:HIS:CE1	1:C:438:HIS:HE1	2.22	0.53
1:C:433:ASN:HD22	1:C:436:THR:H	1.57	0.53
1:A:195:GLN:H	1:A:195:GLN:NE2	2.01	0.53
1:C:359:LYS:HE2	1:C:365:VAL:HG11	1.92	0.52
1:A:433:ASN:HD22	1:A:436:THR:H	1.58	0.52
1:D:242:PHE:CD1	1:D:252:ILE:HD13	2.45	0.52
1:D:342:LEU:HD13	1:D:351:VAL:HG11	1.91	0.52
1:C:272:PRO:HG3	1:C:418:ALA:HB1	1.91	0.52
1:D:245:SER:HB3	3:D:502:NDP:O4D	2.11	0.52
1:C:78:MET:HE1	1:C:86:LEU:HD11	1.90	0.51
1:D:447:GLY:HA3	1:D:464:GLY:O	2.11	0.51
1:A:260:ILE:HA	1:B:253:MET:HE1	1.93	0.50
1:D:195:GLN:NE2	3:D:502:NDP:O1X	2.44	0.50
1:D:201:LEU:HD11	1:D:221:PRO:HG3	1.94	0.50
1:C:192:PRO:CA	4:C:605:HOH:O	2.56	0.50
1:A:300:CYS:HB2	1:A:425:LEU:CD2	2.41	0.50
1:D:191:LYS:HG2	1:D:220:VAL:O	2.11	0.50
1:A:78:MET:HG2	1:A:82:GLU:HB2	1.93	0.49
1:A:147:LYS:HE2	1:D:77:GLU:HG3	1.93	0.49
1:D:163:GLN:NE2	1:D:177:LYS:HB3	2.27	0.49
1:A:289:PHE:CD2	1:A:323:MET:HE2	2.47	0.49
1:C:412:GLU:H	1:C:412:GLU:CD	2.19	0.49
1:A:277:GLU:O	1:A:312:HIS:HE1	1.95	0.49
1:B:239:LYS:NZ	1:B:262:HIS:CD2	2.80	0.49
1:C:229:ALA:HA	1:C:232:VAL:HG12	1.93	0.49
1:A:438:HIS:HE1	1:D:438:HIS:HE1	1.58	0.49
1:C:263:VAL:HG12	1:C:265:LEU:HG	1.94	0.49
1:A:4:THR:N	4:A:608:HOH:O	2.46	0.49
1:D:263:VAL:HG12	1:D:265:LEU:HG	1.95	0.49
1:D:390:ASP:CB	4:D:865:HOH:O	2.61	0.48
1:C:172:VAL:HG13	4:C:653:HOH:O	2.12	0.48
1:A:390:ASP:O	1:A:395:LYS:HE2	2.13	0.48
1:B:272:PRO:HG3	1:B:418:ALA:HB1	1.94	0.48
1:C:367:ALA:O	1:C:382:THR:HG23	2.13	0.48
1:A:242:PHE:CD1	1:A:252:ILE:CD1	2.97	0.48
1:C:75:TRP:CZ2	1:C:83:ARG:HD3	2.48	0.48
1:D:390:ASP:HB3	4:D:865:HOH:O	2.13	0.48
1:B:447:GLY:HA3	1:B:464:GLY:O	2.13	0.48
1:A:243:THR:HA	1:A:266:GLU:O	2.13	0.48
1:C:201:LEU:HD11	1:C:221:PRO:HG3	1.96	0.48
1:D:191:LYS:HD2	1:D:191:LYS:C	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:THR:HG21	1:D:171:LEU:HD13	1.95	0.47
1:A:147:LYS:HE2	1:D:77:GLU:CG	2.44	0.47
1:D:232:VAL:HG13	1:D:233:ASN:N	2.29	0.47
1:A:44:THR:O	1:A:45:GLU:HB2	2.14	0.47
1:D:296:HIS:CD2	1:D:296:HIS:N	2.80	0.47
1:A:240:VAL:HG12	1:A:263:VAL:HG22	1.97	0.47
1:B:195:GLN:CG	4:B:967:HOH:O	2.62	0.47
1:C:356:GLU:C	1:C:358:GLY:N	2.72	0.47
1:D:191:LYS:NZ	3:D:502:NDP:O2X	2.48	0.47
1:B:310:ARG:HD2	1:B:409:ASP:OD1	2.15	0.47
1:D:394:VAL:HG22	1:D:404:VAL:HG11	1.97	0.47
1:A:177:LYS:NZ	1:A:243:THR:CG2	2.78	0.47
1:D:166:PRO:HD2	1:D:173:MET:SD	2.55	0.47
1:C:420:ASN:HB3	4:C:701:HOH:O	2.15	0.46
1:C:447:GLY:HA3	1:C:464:GLY:O	2.16	0.46
1:B:169:PHE:HB3	1:B:172:VAL:HG12	1.98	0.46
1:D:163:GLN:HB2	1:D:190:LEU:HD23	1.98	0.46
1:D:242:PHE:CG	1:D:252:ILE:HD13	2.51	0.46
1:D:300:CYS:HB3	3:D:502:NDP:H72N	1.80	0.46
1:A:239:LYS:NZ	1:A:262:HIS:HD2	2.13	0.46
1:A:312:HIS:HD2	4:A:928:HOH:O	1.97	0.46
1:C:391:MET:CE	4:C:806:HOH:O	2.54	0.46
1:D:74:PRO:O	1:D:78:MET:HB2	2.14	0.46
1:A:194:GLU:HG2	1:A:195:GLN:NE2	2.31	0.46
1:B:296:HIS:N	1:B:296:HIS:CD2	2.82	0.46
1:C:12:VAL:HG21	1:C:103:GLN:HE21	1.80	0.46
1:D:292:ILE:HG21	1:D:403:VAL:HB	1.98	0.46
1:C:365:VAL:O	1:C:365:VAL:HG23	2.16	0.45
1:C:263:VAL:CG1	1:C:265:LEU:HD21	2.47	0.45
1:B:75:TRP:CH2	1:B:83:ARG:CD	3.00	0.45
1:A:78:MET:HG2	1:A:82:GLU:CB	2.46	0.45
1:A:169:PHE:HB3	1:A:172:VAL:HG12	1.99	0.45
1:B:404:VAL:HG23	1:B:406:LEU:HD11	1.98	0.45
1:C:321:VAL:HG21	1:C:366:ALA:HB1	1.99	0.45
1:D:300:CYS:SG	1:D:425:LEU:HD21	2.57	0.45
1:A:491:VAL:HG22	1:B:451:ILE:HD12	1.99	0.45
1:B:242:PHE:CD1	1:B:252:ILE:CD1	3.00	0.45
1:D:296:HIS:CD2	1:D:339:MET:HG3	2.52	0.45
1:A:263:VAL:CG1	1:A:265:LEU:HG	2.46	0.45
1:C:404:VAL:HG23	1:C:404:VAL:O	2.15	0.45
1:C:473:ARG:CZ	4:C:691:HOH:O	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:LEU:HD12	1:D:348:GLN:HA	1.98	0.45
1:A:137:LYS:HE3	1:C:134:TRP:CD1	2.52	0.44
1:C:120:ASP:O	1:C:172:VAL:HG12	2.17	0.44
1:D:372:ALA:HB2	1:D:380:LYS:HG2	1.98	0.44
1:A:177:LYS:HZ1	1:A:243:THR:HG22	1.83	0.44
1:A:164:ILE:HD13	3:A:503:NDP:H2A	1.98	0.44
1:A:280:ASP:OD1	1:A:283:GLU:HG2	2.17	0.44
1:C:372:ALA:HB3	1:C:378:PHE:HB3	1.98	0.44
1:D:22:MET:HG2	1:D:221:PRO:HD2	1.97	0.44
1:D:292:ILE:HD13	1:D:304:SER:HA	1.99	0.44
1:C:285:ILE:HG22	1:C:323:MET:HE1	1.99	0.44
1:B:300:CYS:SG	1:B:425:LEU:HD21	2.57	0.44
1:D:263:VAL:CG1	1:D:265:LEU:HD21	2.48	0.44
1:D:229:ALA:HA	1:D:232:VAL:CG1	2.47	0.43
1:B:149:TYR:CD1	1:B:492:ASN:HA	2.53	0.43
1:C:296:HIS:CD2	1:C:339:MET:HG3	2.53	0.43
1:D:166:PRO:HD3	1:D:243:THR:HB	2.01	0.43
1:B:192:PRO:HG3	1:B:200:LEU:HD23	2.00	0.43
1:C:364:THR:OG1	1:C:385:THR:HG22	2.19	0.43
1:D:388:THR:CB	4:D:602:HOH:O	2.66	0.43
1:B:75:TRP:CZ2	1:B:83:ARG:HD2	2.54	0.43
1:D:9:LYS:N	1:D:103:GLN:HE22	2.09	0.43
1:D:391:MET:O	1:D:395:LYS:HG3	2.19	0.43
1:A:342:LEU:HD12	1:A:348:GLN:HA	2.01	0.42
1:A:425:LEU:HA	1:A:425:LEU:HD12	1.78	0.42
1:B:277:GLU:O	1:B:312:HIS:HE1	2.01	0.42
1:A:9:LYS:N	1:A:103:GLN:HE22	2.15	0.42
1:B:176:TRP:CZ3	1:B:463:PHE:CD2	3.07	0.42
1:D:387:VAL:HG22	1:D:391:MET:SD	2.60	0.42
1:A:147:LYS:HE3	1:D:77:GLU:O	2.19	0.42
1:B:169:PHE:HB3	1:B:172:VAL:CG1	2.49	0.42
1:B:438:HIS:CE1	1:C:438:HIS:CE1	3.04	0.42
1:C:327:VAL:HG11	1:C:339:MET:HE3	2.01	0.42
1:A:78:MET:SD	1:A:83:ARG:HG2	2.58	0.42
4:A:815:HOH:O	1:B:445:LYS:CE	2.67	0.42
1:D:229:ALA:CA	1:D:232:VAL:HG12	2.50	0.42
1:D:191:LYS:HB2	1:D:231:ILE:CD1	2.50	0.42
1:D:155:HIS:HB3	1:D:484:THR:HG21	2.01	0.42
1:B:9:LYS:N	1:B:103:GLN:HE22	2.15	0.41
1:D:22:MET:HG3	1:D:221:PRO:HD2	2.02	0.41
1:D:172:VAL:HG13	4:D:607:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:PRO:HG3	1:D:478:TYR:CD2	2.55	0.41
1:A:157:PRO:HB3	1:A:184:THR:O	2.19	0.41
1:A:336:GLU:H	1:A:336:GLU:CD	2.27	0.41
1:A:243:THR:HB	1:A:266:GLU:HB3	2.03	0.41
1:A:137:LYS:HE3	1:C:134:TRP:NE1	2.35	0.41
1:A:260:ILE:O	1:A:260:ILE:HG22	2.21	0.41
1:C:292:ILE:HG21	1:C:403:VAL:HB	2.02	0.41
1:C:357:GLN:NE2	1:C:361:GLU:OE2	2.54	0.41
1:C:412:GLU:CD	1:C:412:GLU:N	2.79	0.41
1:A:165:ILE:CD1	1:A:177:LYS:HG3	2.49	0.41
1:B:60:ASP:OD2	1:B:64:LYS:NZ	2.53	0.41
1:B:263:VAL:CG1	1:B:265:LEU:HG	2.50	0.41
1:B:271:SER:HB3	1:B:426:ALA:O	2.20	0.41
1:B:433:ASN:HD22	1:B:436:THR:H	1.68	0.41
1:A:250:LYS:HE2	1:B:258:GLU:O	2.20	0.41
1:B:87:ILE:HG22	1:B:132:ALA:HB2	2.03	0.41
1:D:229:ALA:C	1:D:232:VAL:HG12	2.46	0.41
1:C:359:LYS:HE2	1:C:365:VAL:CG1	2.50	0.41
1:D:153:THR:HA	1:D:487:LYS:O	2.21	0.41
1:A:23:PHE:C	1:A:24:ILE:HG13	2.46	0.40
1:D:403:VAL:HG22	1:D:404:VAL:N	2.37	0.40
1:A:127:ASN:OD1	1:A:459:ALA:HB2	2.21	0.40
1:C:395:LYS:HE2	1:C:395:LYS:HB2	1.89	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	489/494 (99%)	474 (97%)	15 (3%)	0	100	100
1	B	489/494 (99%)	470 (96%)	19 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	486/494 (98%)	463 (95%)	21 (4%)	2 (0%)	30	27
1	D	487/494 (99%)	466 (96%)	20 (4%)	1 (0%)	43	42
All	All	1951/1976 (99%)	1873 (96%)	75 (4%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	373	LEU
1	C	424	GLY
1	D	166	PRO

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	398/401 (99%)	382 (96%)	16 (4%)	28	27
1	B	398/401 (99%)	378 (95%)	20 (5%)	22	20
1	C	395/401 (98%)	361 (91%)	34 (9%)	10	6
1	D	396/401 (99%)	367 (93%)	29 (7%)	13	9
All	All	1587/1604 (99%)	1488 (94%)	99 (6%)	16	13

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	VAL
1	A	109	ASN
1	A	121	ILE
1	A	122	SER
1	A	195	GLN
1	A	243	THR
1	A	266	GLU
1	A	296	HIS
1	A	329	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	336	GLU
1	A	351	VAL
1	A	371	ARG
1	A	373	LEU
1	A	375	LYS
1	A	394	VAL
1	A	399	PHE
1	B	50	VAL
1	B	105	GLU
1	B	109	ASN
1	B	121	ILE
1	B	147	LYS
1	B	165	ILE
1	B	195	GLN
1	B	246	THR
1	B	266	GLU
1	B	272	PRO
1	B	296	HIS
1	B	327	VAL
1	B	335	LYS
1	B	351	VAL
1	B	353	ASN
1	B	365	VAL
1	B	375	LYS
1	B	379	VAL
1	B	387	VAL
1	B	399	PHE
1	C	7	GLU
1	C	18	GLU
1	C	27	GLU
1	C	50	VAL
1	C	77	GLU
1	C	83	ARG
1	C	105	GLU
1	C	109	ASN
1	C	115	VAL
1	C	121	ILE
1	C	150	LEU
1	C	161	VAL
1	C	166	PRO
1	C	172	VAL
1	C	195	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	252	ILE
1	C	265	LEU
1	C	266	GLU
1	C	283	GLU
1	C	296	HIS
1	C	311	LYS
1	C	329	LEU
1	C	336	GLU
1	C	351	VAL
1	C	360	LYS
1	C	361	GLU
1	C	374	GLU
1	C	375	LYS
1	C	379	VAL
1	C	381	PRO
1	C	385	THR
1	C	387	VAL
1	C	406	LEU
1	C	412	GLU
1	D	18	GLU
1	D	50	VAL
1	D	77	GLU
1	D	105	GLU
1	D	109	ASN
1	D	115	VAL
1	D	121	ILE
1	D	166	PRO
1	D	171	LEU
1	D	172	VAL
1	D	188	ILE
1	D	191	LYS
1	D	195	GLN
1	D	266	GLU
1	D	282	GLU
1	D	296	HIS
1	D	311	LYS
1	D	316	VAL
1	D	327	VAL
1	D	336	GLU
1	D	351	VAL
1	D	360	LYS
1	D	373	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	385	THR
1	D	390	ASP
1	D	404	VAL
1	D	422	SER
1	D	429	VAL
1	D	484	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	114	GLN
1	A	141	GLN
1	A	195	GLN
1	A	214	ASN
1	A	233	ASN
1	A	255	GLN
1	A	262	HIS
1	A	312	HIS
1	A	326	ASN
1	A	432	GLN
1	A	433	ASN
1	A	438	HIS
1	A	482	ASN
1	B	55	GLN
1	B	85	HIS
1	B	103	GLN
1	B	114	GLN
1	B	141	GLN
1	B	195	GLN
1	B	214	ASN
1	B	233	ASN
1	B	255	GLN
1	B	262	HIS
1	B	312	HIS
1	B	347	GLN
1	B	432	GLN
1	B	433	ASN
1	B	438	HIS
1	B	482	ASN
1	C	103	GLN
1	C	114	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	233	ASN
1	C	235	HIS
1	C	255	GLN
1	C	262	HIS
1	C	325	ASN
1	C	326	ASN
1	C	347	GLN
1	C	353	ASN
1	C	432	GLN
1	C	433	ASN
1	C	438	HIS
1	C	482	ASN
1	D	85	HIS
1	D	103	GLN
1	D	114	GLN
1	D	141	GLN
1	D	163	GLN
1	D	214	ASN
1	D	262	HIS
1	D	299	ASN
1	D	309	HIS
1	D	312	HIS
1	D	325	ASN
1	D	326	ASN
1	D	353	ASN
1	D	432	GLN
1	D	433	ASN
1	D	438	HIS
1	D	455	ASN
1	D	482	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NDP	B	503	-	51,52,52	1.51	8 (15%)	71,80,80	1.65	15 (21%)
3	NDP	C	503	-	51,52,52	1.47	8 (15%)	71,80,80	1.57	11 (15%)
3	NDP	A	503	-	51,52,52	1.48	7 (13%)	71,80,80	1.83	16 (22%)
3	NDP	D	502	-	51,52,52	1.51	10 (19%)	71,80,80	1.74	11 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	B	503	-	-	6/34/77/77	0/5/5/5
3	NDP	C	503	-	-	5/34/77/77	0/5/5/5
3	NDP	A	503	-	-	6/34/77/77	0/5/5/5
3	NDP	D	502	-	-	5/34/77/77	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	NDP	C5A-C4A	5.63	1.49	1.39
3	C	503	NDP	C5A-C4A	5.44	1.48	1.39
3	D	502	NDP	C5A-C4A	5.34	1.48	1.39
3	A	503	NDP	C5A-C4A	4.49	1.47	1.39
3	B	503	NDP	PA-O3	4.34	1.64	1.59
3	A	503	NDP	PN-O3	4.27	1.64	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	NDP	PA-O3	3.73	1.63	1.59
3	D	502	NDP	PA-O3	3.72	1.63	1.59
3	D	502	NDP	PN-O3	3.41	1.63	1.59
3	B	503	NDP	C5A-N7A	-3.19	1.33	1.39
3	C	503	NDP	PA-O3	3.04	1.62	1.59
3	C	503	NDP	C5A-N7A	-2.99	1.33	1.39
3	C	503	NDP	PN-O3	2.77	1.62	1.59
3	D	502	NDP	C2N-C3N	2.73	1.42	1.35
3	C	503	NDP	C8A-N7A	2.67	1.36	1.31
3	A	503	NDP	C5A-N7A	-2.67	1.34	1.39
3	A	503	NDP	P2B-O2B	2.65	1.64	1.59
3	D	502	NDP	C5A-N7A	-2.56	1.34	1.39
3	C	503	NDP	C4A-N9A	-2.53	1.32	1.37
3	B	503	NDP	C4A-N9A	-2.52	1.32	1.37
3	D	502	NDP	C5A-C6A	2.51	1.48	1.41
3	A	503	NDP	C5A-C6A	2.49	1.47	1.41
3	B	503	NDP	C5A-C6A	2.48	1.47	1.41
3	D	502	NDP	C8A-N7A	2.48	1.36	1.31
3	C	503	NDP	C2N-C3N	2.48	1.42	1.35
3	B	503	NDP	C7N-C3N	2.46	1.54	1.48
3	D	502	NDP	C7N-C3N	2.46	1.54	1.48
3	C	503	NDP	C6N-C5N	2.41	1.40	1.33
3	B	503	NDP	P2B-O2B	2.35	1.63	1.59
3	D	502	NDP	P2B-O2B	2.34	1.63	1.59
3	B	503	NDP	C8A-N7A	2.31	1.36	1.31
3	A	503	NDP	C2N-C3N	2.20	1.41	1.35
3	D	502	NDP	C6N-C5N	2.03	1.39	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	NDP	C5A-C4A-N3A	-6.62	117.60	126.72
3	A	503	NDP	C5A-C4A-N3A	-5.93	118.55	126.72
3	D	502	NDP	N3A-C4A-N9A	5.06	135.77	127.17
3	B	503	NDP	C5A-C4A-N3A	-5.01	119.82	126.72
3	C	503	NDP	C5A-C4A-N3A	-4.76	120.16	126.72
3	C	503	NDP	O4D-C1D-N1N	4.52	116.70	108.08
3	A	503	NDP	N3A-C4A-N9A	4.51	134.84	127.17
3	A	503	NDP	O4B-C1B-N9A	4.19	116.13	108.09
3	D	502	NDP	C2A-N3A-C4A	4.16	122.00	111.83
3	A	503	NDP	O4D-C1D-N1N	4.15	116.00	108.08
3	D	502	NDP	O4D-C1D-N1N	4.10	115.90	108.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	NDP	C4A-C5A-N7A	-4.06	105.94	110.58
3	B	503	NDP	N3A-C4A-N9A	4.00	133.97	127.17
3	B	503	NDP	O4B-C1B-N9A	3.74	115.26	108.09
3	C	503	NDP	N3A-C2A-N1A	-3.68	123.01	128.58
3	C	503	NDP	C2D-C1D-N1N	-3.56	104.56	113.31
3	A	503	NDP	C5A-N7A-C8A	3.47	108.90	103.45
3	A	503	NDP	C2A-N3A-C4A	3.35	120.02	111.83
3	B	503	NDP	N3A-C2A-N1A	-3.32	123.56	128.58
3	A	503	NDP	O3X-P2B-O2X	3.31	120.22	107.80
3	D	502	NDP	N3A-C2A-N1A	-3.24	123.67	128.58
3	C	503	NDP	C2A-N3A-C4A	3.23	119.71	111.83
3	D	502	NDP	C2D-C1D-N1N	-3.20	105.42	113.31
3	D	502	NDP	C4A-C5A-N7A	-3.15	106.98	110.58
3	C	503	NDP	N3A-C4A-N9A	3.14	132.51	127.17
3	B	503	NDP	C2A-N3A-C4A	3.05	119.29	111.83
3	A	503	NDP	C6N-N1N-C2N	3.00	122.53	119.32
3	B	503	NDP	C4A-C5A-N7A	-3.00	107.15	110.58
3	A	503	NDP	C2D-C1D-N1N	-2.90	106.17	113.31
3	B	503	NDP	C2A-N1A-C6A	2.82	123.37	118.73
3	C	503	NDP	O4B-C1B-N9A	2.80	113.47	108.09
3	A	503	NDP	N9A-C8A-N7A	-2.77	110.01	113.94
3	B	503	NDP	O4D-C1D-N1N	2.75	113.33	108.08
3	A	503	NDP	N3A-C2A-N1A	-2.69	124.50	128.58
3	B	503	NDP	C2D-C1D-N1N	-2.68	106.70	113.31
3	B	503	NDP	C1D-N1N-C2N	-2.68	116.72	121.14
3	A	503	NDP	C4A-N9A-C8A	2.64	108.51	105.74
3	B	503	NDP	O3D-C3D-C2D	2.64	120.29	111.82
3	C	503	NDP	C4A-C5A-N7A	-2.64	107.57	110.58
3	D	502	NDP	C5A-N7A-C8A	2.56	107.48	103.45
3	B	503	NDP	C6N-N1N-C2N	2.50	122.00	119.32
3	A	503	NDP	O2N-PN-O1N	2.39	123.56	112.44
3	D	502	NDP	O4D-C4D-C5D	2.31	116.72	109.33
3	B	503	NDP	C5A-N7A-C8A	2.29	107.05	103.45
3	C	503	NDP	C2A-N1A-C6A	2.28	122.48	118.73
3	B	503	NDP	O2N-PN-O3	2.25	113.37	107.27
3	C	503	NDP	C3D-C2D-C1D	2.20	105.62	101.46
3	D	502	NDP	C6N-N1N-C2N	2.11	121.58	119.32
3	B	503	NDP	C4A-N9A-C8A	2.11	107.95	105.74
3	A	503	NDP	C1D-N1N-C2N	-2.10	117.68	121.14
3	D	502	NDP	C5A-C6A-N6A	-2.10	118.09	123.29
3	A	503	NDP	C6A-C5A-N7A	2.04	136.03	132.09
3	C	503	NDP	O2X-P2B-O1X	2.03	118.76	110.83

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	NDP	O4D-C1D-N1N-C2N
3	A	503	NDP	C2N-C3N-C7N-N7N
3	B	503	NDP	O4D-C1D-N1N-C2N
3	B	503	NDP	C2N-C3N-C7N-N7N
3	C	503	NDP	O4D-C1D-N1N-C2N
3	C	503	NDP	C2N-C3N-C7N-N7N
3	D	502	NDP	O4D-C1D-N1N-C2N
3	A	503	NDP	C1B-C2B-O2B-P2B
3	A	503	NDP	C3B-C2B-O2B-P2B
3	B	503	NDP	C3B-C2B-O2B-P2B
3	B	503	NDP	C1B-C2B-O2B-P2B
3	D	502	NDP	PN-O3-PA-O5B
3	B	503	NDP	C2B-C1B-N9A-C8A
3	C	503	NDP	C2B-C1B-N9A-C8A
3	D	502	NDP	C2B-C1B-N9A-C8A
3	C	503	NDP	C3B-C2B-O2B-P2B
3	A	503	NDP	C2B-C1B-N9A-C8A
3	D	502	NDP	C4D-C5D-O5D-PN
3	A	503	NDP	O4B-C1B-N9A-C8A
3	C	503	NDP	O4B-C1B-N9A-C8A
3	D	502	NDP	O4B-C1B-N9A-C8A
3	B	503	NDP	O4B-C1B-N9A-C8A

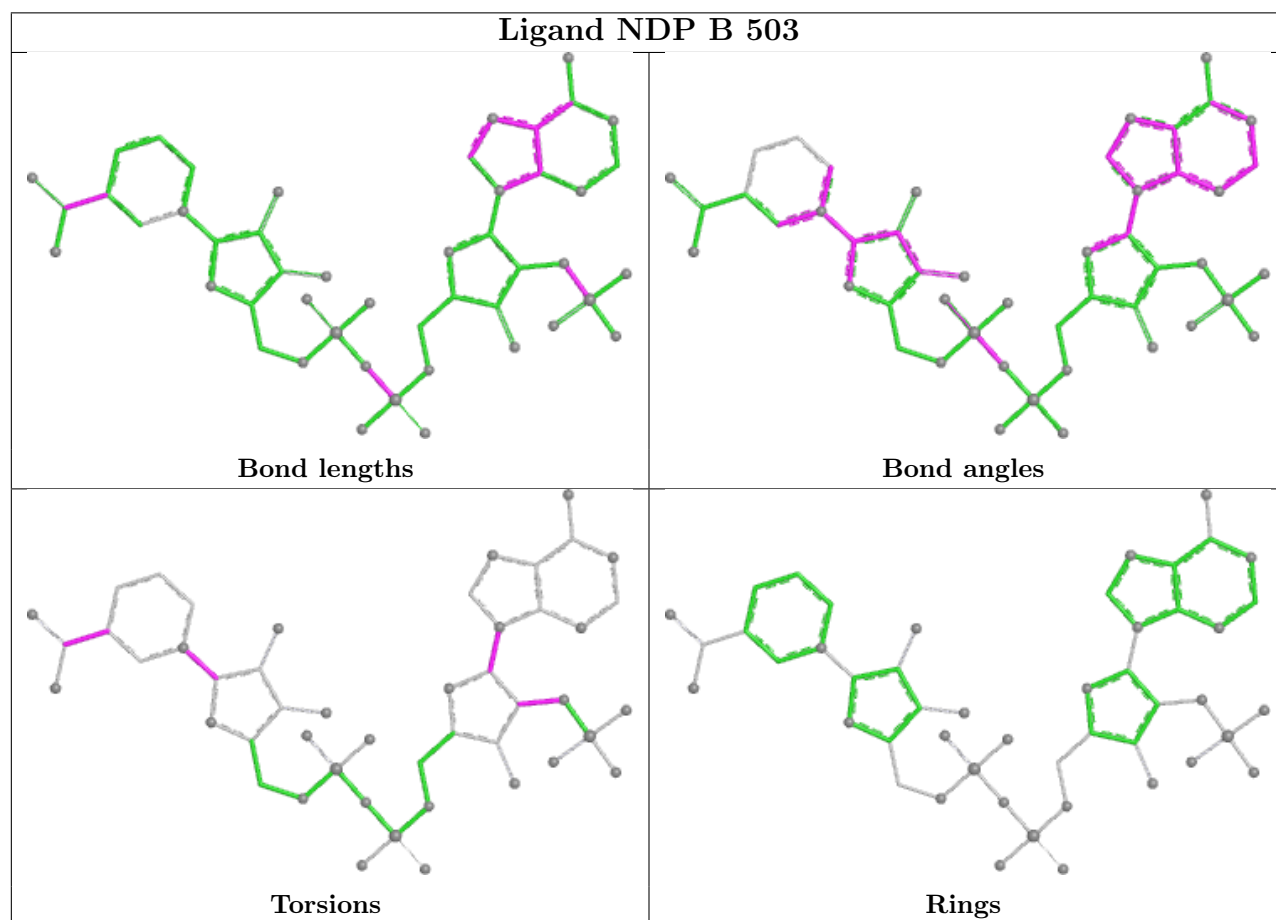
There are no ring outliers.

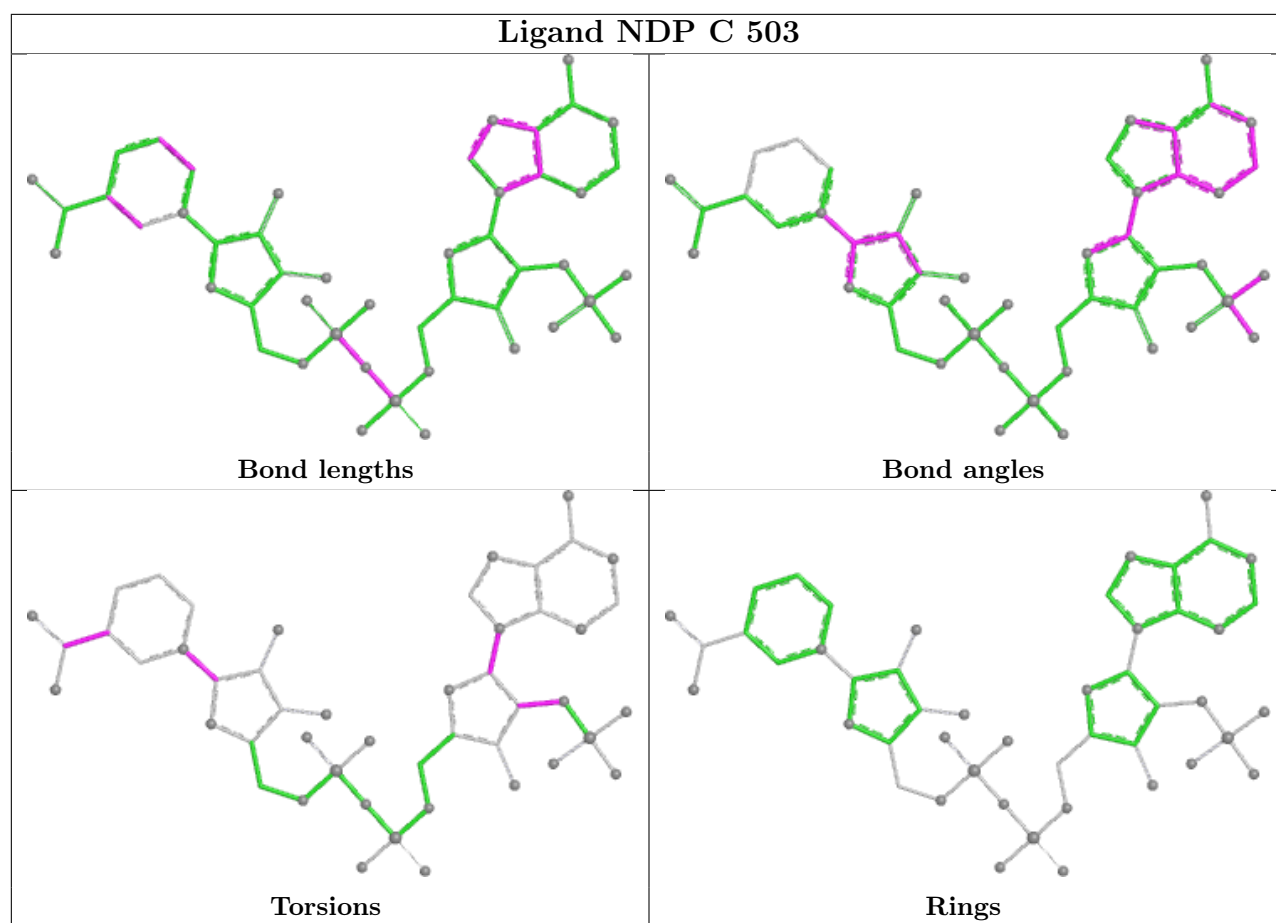
2 monomers are involved in 5 short contacts:

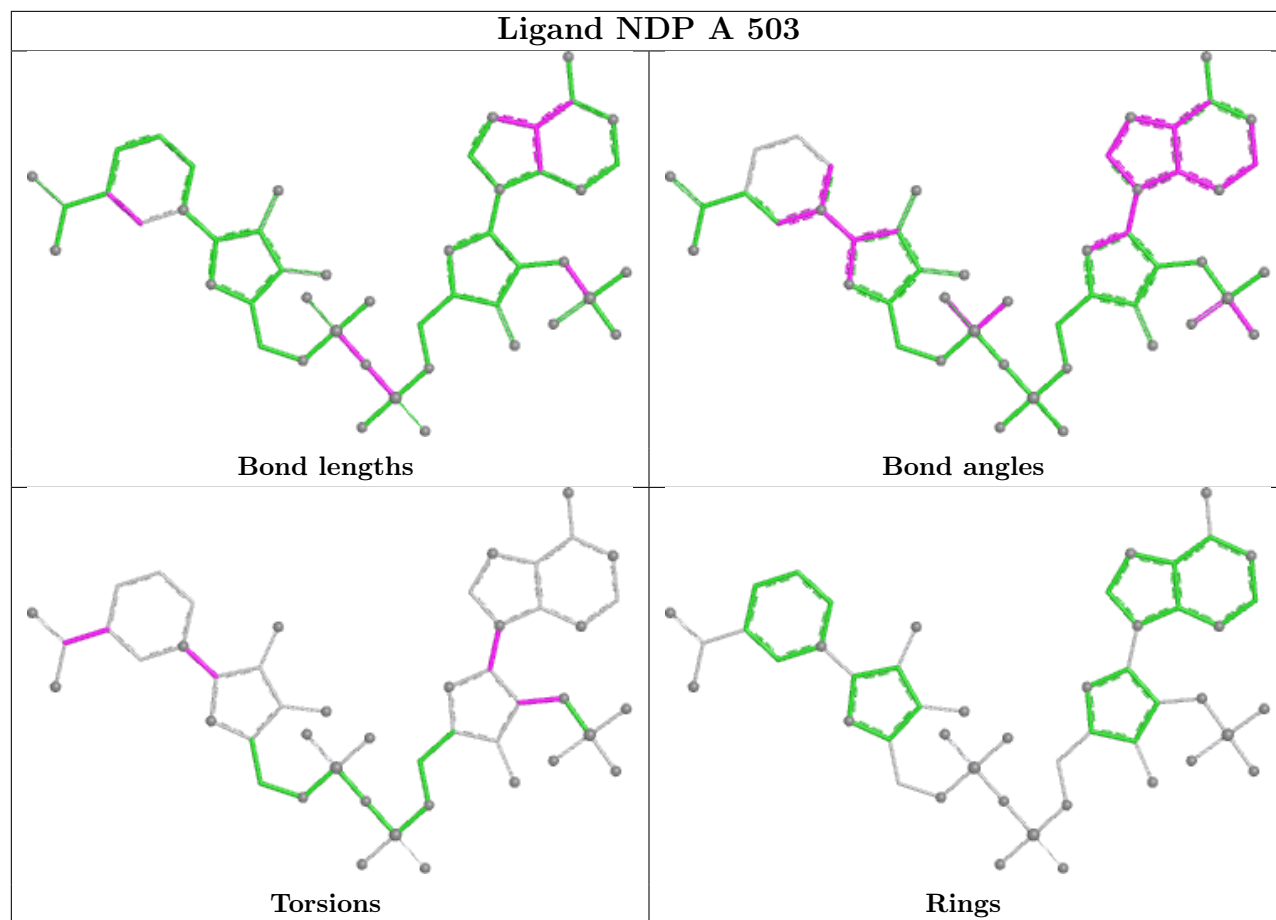
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	NDP	1	0
3	D	502	NDP	4	0

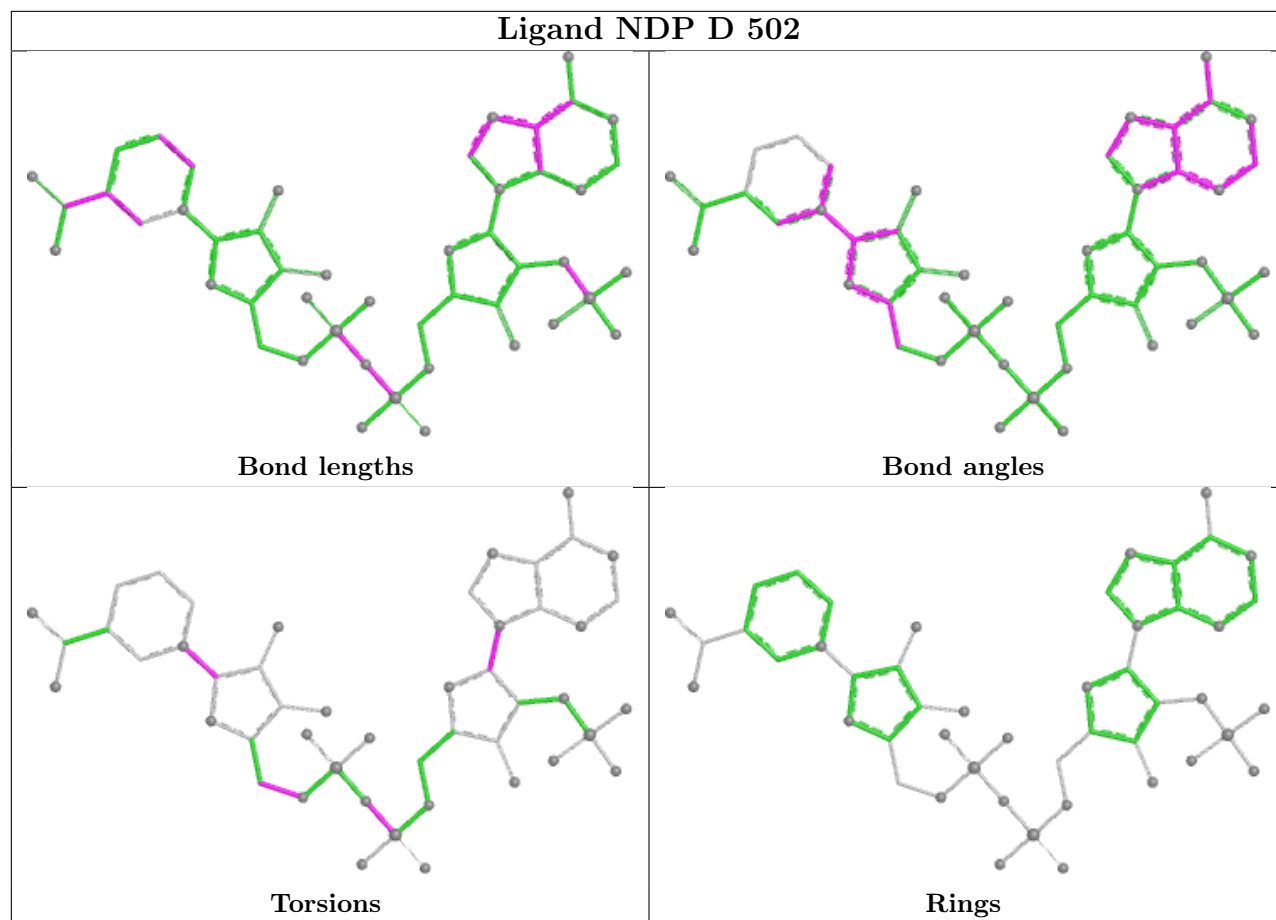
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	491/494 (99%)	0.05	5 (1%) 79 79	13, 27, 42, 60	0
1	B	491/494 (99%)	0.08	4 (0%) 82 82	15, 28, 43, 60	0
1	C	488/494 (98%)	0.58	30 (6%) 27 26	19, 35, 58, 76	0
1	D	489/494 (98%)	0.46	10 (2%) 65 64	18, 33, 50, 72	0
All	All	1959/1976 (99%)	0.29	49 (2%) 58 58	13, 30, 50, 76	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	176	TRP	4.0
1	A	176	TRP	3.8
1	C	321	VAL	3.8
1	D	6	ILE	3.6
1	C	358	GLY	3.6
1	B	176	TRP	3.5
1	C	363	ALA	3.4
1	B	463	PHE	3.1
1	C	385	THR	3.1
1	A	463	PHE	3.0
1	C	351	VAL	2.9
1	D	463	PHE	2.9
1	C	232	VAL	2.8
1	C	379	VAL	2.8
1	C	352	LEU	2.8
1	C	364	THR	2.8
1	C	384	PHE	2.7
1	C	367	ALA	2.6
1	C	47	VAL	2.6
1	C	371	ARG	2.5
1	B	4	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	359	LYS	2.5
1	C	355	ILE	2.5
1	C	107	LEU	2.4
1	C	327	VAL	2.4
1	C	376	GLY	2.4
1	B	259	MET	2.4
1	A	300	CYS	2.4
1	C	393	ILE	2.3
1	D	385	THR	2.3
1	C	263	VAL	2.3
1	C	387	VAL	2.3
1	D	247	VAL	2.3
1	D	259	MET	2.3
1	D	60	ASP	2.2
1	D	33	GLY	2.2
1	C	176	TRP	2.2
1	C	392	THR	2.2
1	C	403	VAL	2.1
1	C	324	ALA	2.1
1	C	281	LEU	2.1
1	A	4	THR	2.1
1	C	365	VAL	2.1
1	A	88	TYR	2.1
1	C	350	ARG	2.1
1	C	325	ASN	2.0
1	C	377	TYR	2.0
1	D	321	VAL	2.0
1	D	300	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

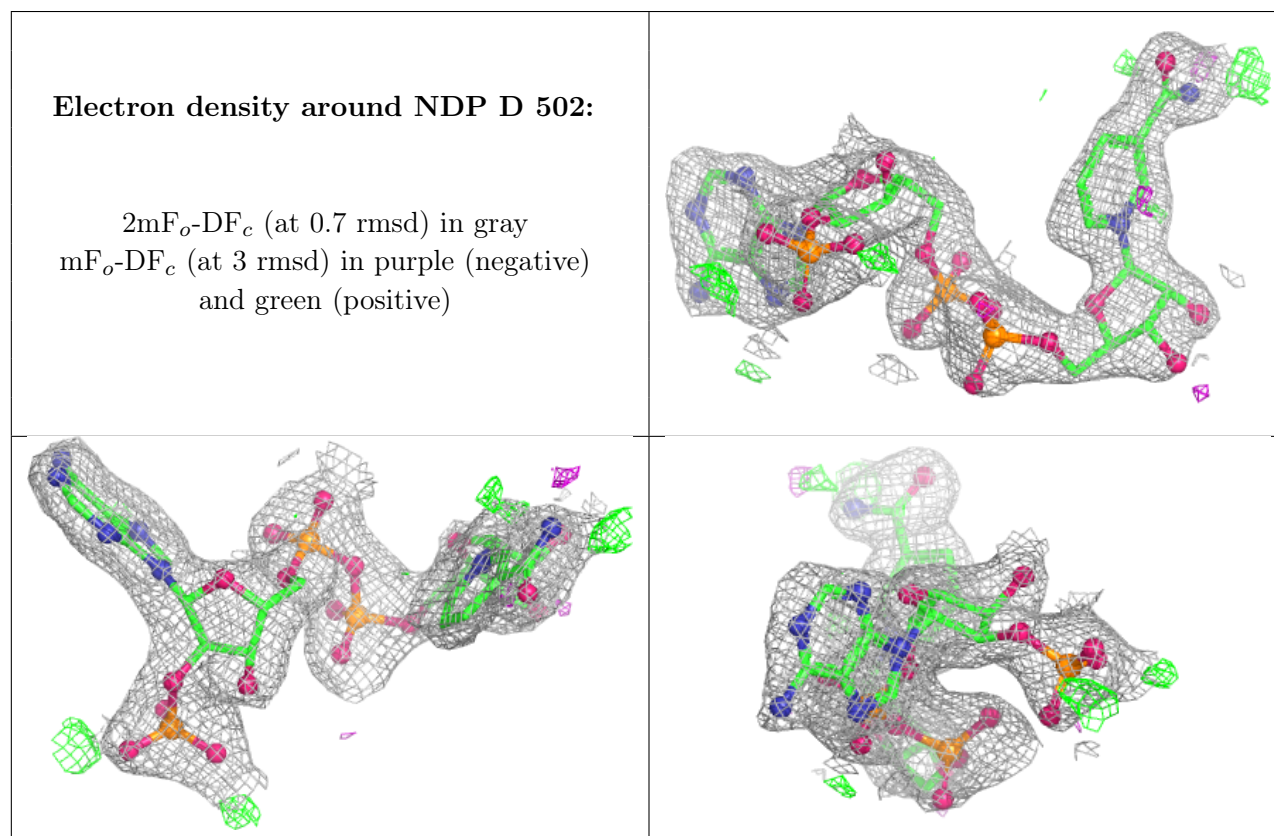
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

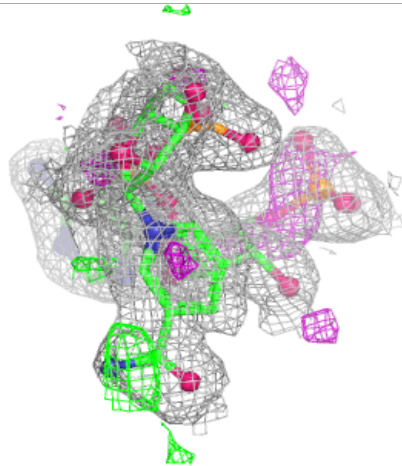
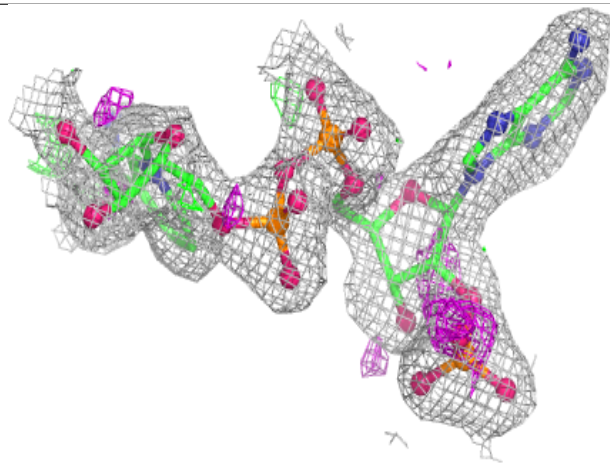
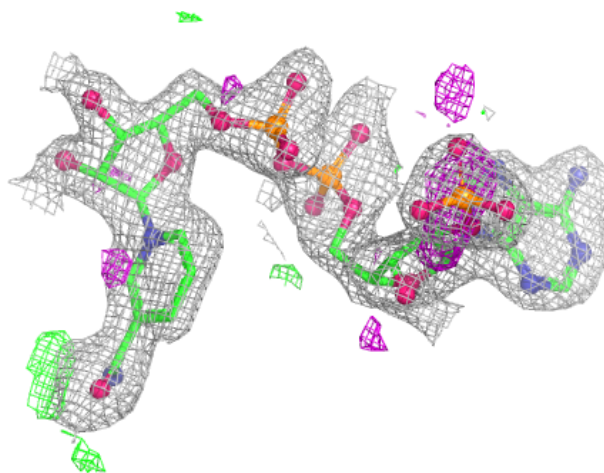
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NDP	D	502	48/48	0.87	0.11	43,54,69,73	0
3	NDP	A	503	48/48	0.90	0.11	36,45,51,52	0
3	NDP	C	503	48/48	0.90	0.11	41,49,56,60	0
2	NA	C	502	1/1	0.90	0.08	40,40,40,40	0
3	NDP	B	503	48/48	0.92	0.09	32,39,44,46	0
2	NA	D	501	1/1	0.94	0.10	35,35,35,35	0
2	NA	C	501	1/1	0.95	0.10	42,42,42,42	0
2	NA	B	501	1/1	0.96	0.07	27,27,27,27	0
2	NA	B	502	1/1	0.96	0.06	32,32,32,32	0
2	NA	A	501	1/1	0.96	0.06	23,23,23,23	0
2	NA	A	502	1/1	0.97	0.06	28,28,28,28	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.



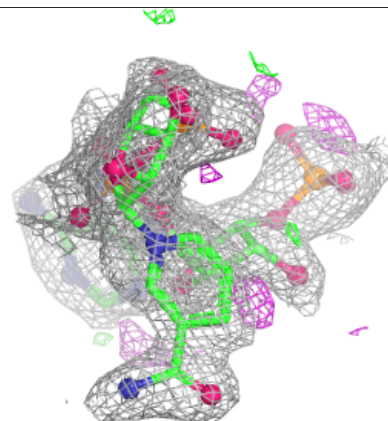
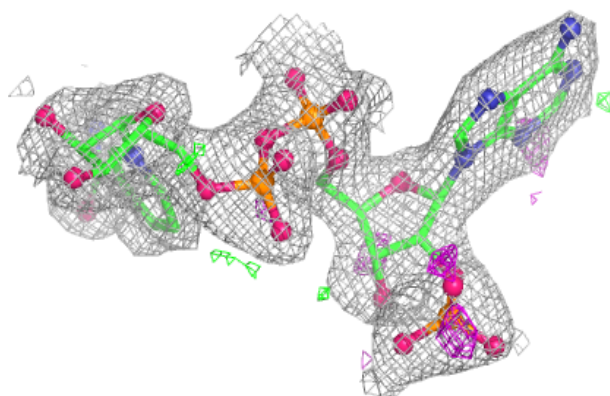
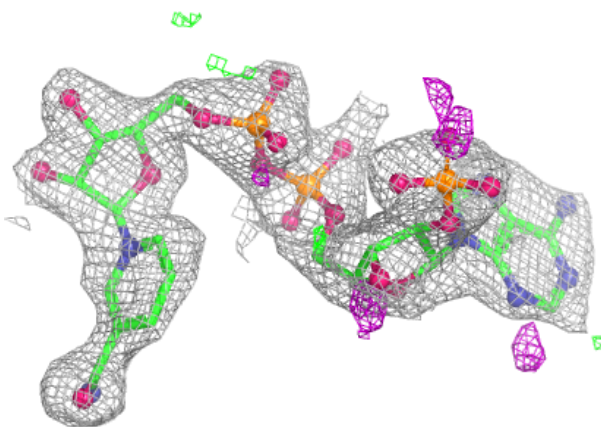
Electron density around NDP A 503:

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



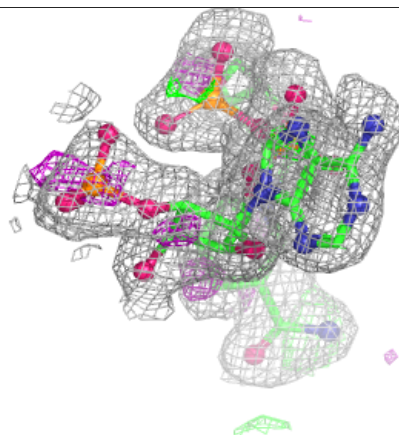
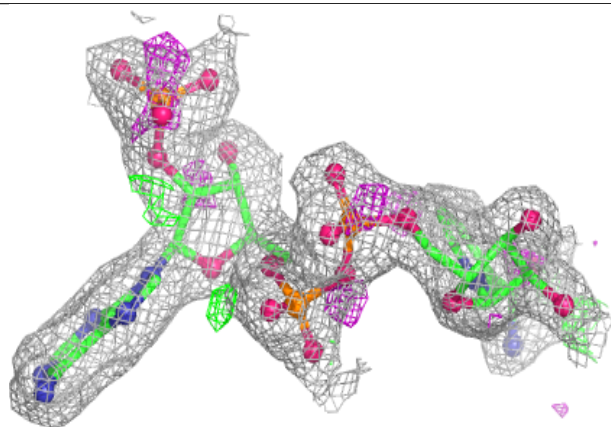
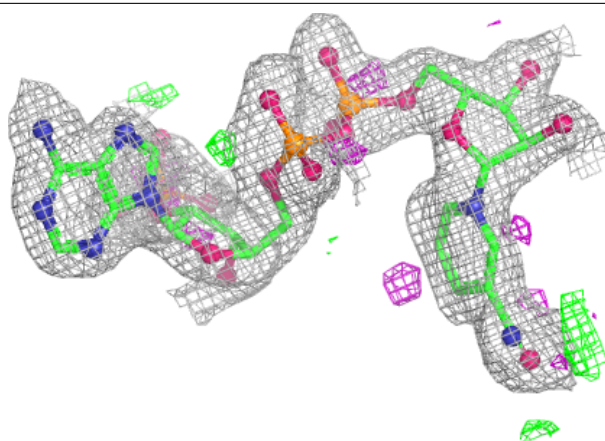
Electron density around NDP C 503:

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



Electron density around NDP B 503:

$2mF_o-DF_c$ (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.