



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:03 AM UTC

PDB ID : 8VF7 / pdb_00008vf7
EMDB ID : EMD-43187
Title : Modifying portion of human FASN with NADPH and the ACP at the ER domain
Authors : Schultz, K.; Marmorstein, R.
Deposited on : 2023-12-21
Resolution : 3.20 Å (reported)
Based on initial models : ., 2CG5

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

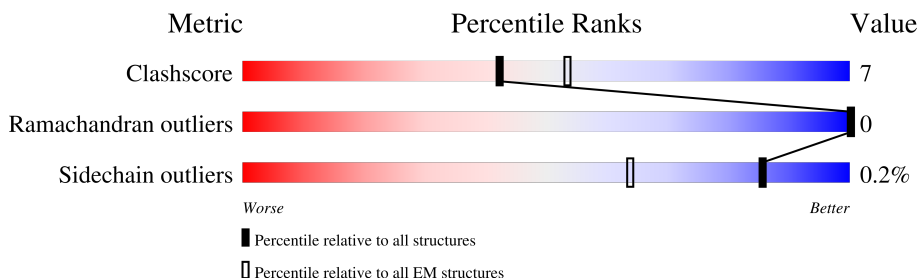
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	2553	
2	B	2553	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 38890 atoms, of which 19416 are hydrogens and 0 are deuteriums.

In the tables below, 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 Fatty acid synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1216	Total	C	H	N	O	S	0	0
			18703	5928	9357	1644	1735	39		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	MET	-	initiating methionine	UNP P49327
A	-30	SER	-	expression tag	UNP P49327
A	-29	TYR	-	expression tag	UNP P49327
A	-28	TYR	-	expression tag	UNP P49327
A	-27	ASP	-	expression tag	UNP P49327
A	-26	TYR	-	expression tag	UNP P49327
A	-25	LYS	-	expression tag	UNP P49327
A	-24	ASP	-	expression tag	UNP P49327
A	-23	ASP	-	expression tag	UNP P49327
A	-22	ASP	-	expression tag	UNP P49327
A	-21	ASP	-	expression tag	UNP P49327
A	-20	LYS	-	expression tag	UNP P49327
A	-19	ASP	-	expression tag	UNP P49327
A	-18	TYR	-	expression tag	UNP P49327
A	-17	ASP	-	expression tag	UNP P49327
A	-16	ILE	-	expression tag	UNP P49327
A	-15	PRO	-	expression tag	UNP P49327
A	-14	THR	-	expression tag	UNP P49327
A	-13	THR	-	expression tag	UNP P49327
A	-12	GLU	-	expression tag	UNP P49327
A	-11	ASN	-	expression tag	UNP P49327
A	-10	LEU	-	expression tag	UNP P49327
A	-9	TYR	-	expression tag	UNP P49327
A	-8	PHE	-	expression tag	UNP P49327
A	-7	GLN	-	expression tag	UNP P49327
A	-6	GLY	-	expression tag	UNP P49327
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327
A	1151	THR	LYS	conflict	UNP P49327
A	2512	LEU	-	expression tag	UNP P49327
A	2513	GLU	-	expression tag	UNP P49327
A	2514	HIS	-	expression tag	UNP P49327
A	2515	HIS	-	expression tag	UNP P49327
A	2516	HIS	-	expression tag	UNP P49327
A	2517	HIS	-	expression tag	UNP P49327
A	2518	HIS	-	expression tag	UNP P49327
A	2519	HIS	-	expression tag	UNP P49327
A	2520	HIS	-	expression tag	UNP P49327
A	2521	HIS	-	expression tag	UNP P49327

- Molecule 2 is a protein called Fatty acid synthase.

Mol	Chain	Residues	Atoms							AltConf	Trace
2	B	1289	Total	C	H	N	O	P	S	0	0
			19891	6290	9955	1750	1854	1	41		

There are 44 discrepancies between the modelled and reference sequences:

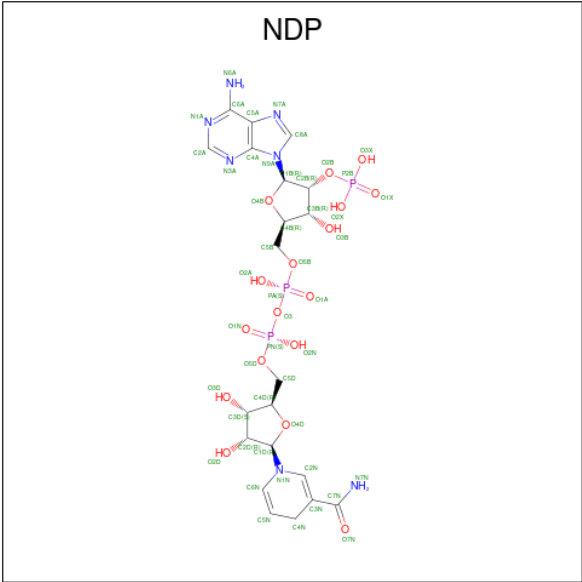
Chain	Residue	Modelled	Actual	Comment	Reference
B	-31	MET	-	initiating methionine	UNP P49327
B	-30	SER	-	expression tag	UNP P49327
B	-29	TYR	-	expression tag	UNP P49327
B	-28	TYR	-	expression tag	UNP P49327
B	-27	ASP	-	expression tag	UNP P49327
B	-26	TYR	-	expression tag	UNP P49327
B	-25	LYS	-	expression tag	UNP P49327
B	-24	ASP	-	expression tag	UNP P49327
B	-23	ASP	-	expression tag	UNP P49327
B	-22	ASP	-	expression tag	UNP P49327
B	-21	ASP	-	expression tag	UNP P49327
B	-20	LYS	-	expression tag	UNP P49327
B	-19	ASP	-	expression tag	UNP P49327
B	-18	TYR	-	expression tag	UNP P49327
B	-17	ASP	-	expression tag	UNP P49327
B	-16	ILE	-	expression tag	UNP P49327

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	PRO	-	expression tag	UNP P49327
B	-14	THR	-	expression tag	UNP P49327
B	-13	THR	-	expression tag	UNP P49327
B	-12	GLU	-	expression tag	UNP P49327
B	-11	ASN	-	expression tag	UNP P49327
B	-10	LEU	-	expression tag	UNP P49327
B	-9	TYR	-	expression tag	UNP P49327
B	-8	PHE	-	expression tag	UNP P49327
B	-7	GLN	-	expression tag	UNP P49327
B	-6	GLY	-	expression tag	UNP P49327
B	-5	ALA	-	expression tag	UNP P49327
B	-4	MET	-	expression tag	UNP P49327
B	-3	GLY	-	expression tag	UNP P49327
B	-2	SER	-	expression tag	UNP P49327
B	-1	GLY	-	expression tag	UNP P49327
B	0	ILE	-	expression tag	UNP P49327
B	1	PRO	-	expression tag	UNP P49327
B	1151	THR	LYS	conflict	UNP P49327
B	2512	LEU	-	expression tag	UNP P49327
B	2513	GLU	-	expression tag	UNP P49327
B	2514	HIS	-	expression tag	UNP P49327
B	2515	HIS	-	expression tag	UNP P49327
B	2516	HIS	-	expression tag	UNP P49327
B	2517	HIS	-	expression tag	UNP P49327
B	2518	HIS	-	expression tag	UNP P49327
B	2519	HIS	-	expression tag	UNP P49327
B	2520	HIS	-	expression tag	UNP P49327
B	2521	HIS	-	expression tag	UNP P49327

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
3	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
3	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
3	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

- Molecule 2: Fatty acid synthase



VAL	HIS	GLN	GLY	LEU	LYS	ARG	GLN	ASN	LEU	E2012
VAL	HIS	LEU	THR	LEU	THR	VAL	GLN	THR	VAL	V2018
ILE	ILE	SER	PRO	PRO	GLY	VAL	GLN	VAL	GLN	F2019
GLY	GLY	PHE	GLY	CYS	GLY	PRO	GLY	GLY	GLY	S2020
ASP	ASP	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	S2021
HIS	HIS	ARG	ALA	ALA	GLY	PRO	PRO	GLY	GLY	V2022
THR	THR	ARG	GLY	ALA	GLY	GLY	GLY	GLY	GLY	R2026
THR	THR	PHE	GLY	ALA	GLY	ARG	ARG	ARG	ARG	G2027
LEU	LEU	TYR	TYR	THR	THR	VAL	VAL	VAL	VAL	V2028
GLY	GLY	LYS	LYS	GLY	GLY	ALA	ALA	PHE	PHE	A2029
GLY	GLY	LEU	LEU	ALA	ALA	TYR	TYR	VAL	VAL	N2033
SER	SER	ARG	ILE	ILE	ILE	SER	HIS	HIS	HIS	V2034
GLY	GLY	ALA	CYS	CYS	PHE	TYR	TYR	PRO	PRO	E2167
LEU	LEU	ALA	PHE	PHE	ALA	GLY	GLY	ILE	ILE	R2168
SER	SER	GLN	VAL	VAL	VAL	ALA	ALA	GLY	GLY	E2169
ILE	ILE	TYR	GLN	GLN	VAL	CYS	CYS	GLY	GLY	L2170
ILE	ILE	THR	THR	GLN	ALA	VAL	VAL	SER	SER	Q2059
SER	SER	PRO	PHE	PHE	GLU	ALA	ALA	THR	THR	A2194
LYS	LYS	LYS	THR	THR	THR	GLY	GLY	VAL	VAL	ASP
GLY	GLY	ILE	ILE	ILE	ILE	MET	MET	ALA	ALA	GLU
LEU	LEU	GLY	GLY	GLY	GLY	CYS	CYS	SER	SER	V2066
ARG	ARG	LEU	LEU	LEU	LEU	SER	SER	GLY	GLY	ILE
VAL	VAL	SER	ARG	ARG	ALA	LEU	LEU	LEU	LEU	VAL
VAL	VAL	ALA	ALA	ALA	ALA	GLN	GLN	CYS	CYS	GLY
ARG	ARG	VAL	VAL	VAL	VAL	ALA	ALA	ARG	ARG	THR
PRO	PRO	MET	MET	LEU	LEU	ALA	ALA	PRO	PRO	THR
ARG	ARG	LEU	LEU	GLY	GLY	GLN	GLN	SER	SER	THR
VAL	VAL	LEU	LEU	ALA	ALA	SER	SER	ILE	ILE	THR
VAL	VAL	ARG	ARG	LEU	LEU	PRO	PRO	GLY	GLY	ASN
VAL	VAL	ALA	ALA	LEU	LEU	ALA	ALA	THR	THR	ASP
ARG	ARG	LYS	LYS	PRO	PRO	PRO	PRO	TYR	TYR	THR
GLY	GLY	THR	THR	LEU	LEU	THR	THR	GLY	GLY	ILE
GLY	GLY	GLY	GLY	LYS	LYS	HIS	HIS	LEU	LEU	VAL
LEU	LEU	GLY	GLY	GLY	GLY	ASN	ASN	GLN	GLN	S2081
LEU	LEU	ALA	ALA	LEU	LEU	SER	SER	GLN	GLN	V2096
HIS	HIS	TYR	TYR	GLY	GLY	LEU	LEU	GLN	GLN	L2097
HIS	HIS	GLY	GLY	GLY	GLY	PHE	PHE	THR	THR	D2096
HIS	HIS	GLU	GLU	ARG	ARG	LEU	LEU	GLN	GLN	L2097
HIS	HIS	ASP	ASP	VAL	VAL	PHE	PHE	LEU	LEU	N2100
HIS	HIS	LEU	LEU	ALA	ALA	ASP	ASP	ASN	ASN	E2113
HIS	HIS	GLY	GLY	ALA	ALA	GLY	GLY	LEU	LEU	LYS
HIS	HIS	ASP	ASP	VAL	VAL	SER	SER	SER	SER	ALA
HIS	HIS	TYR	TYR	ASP	ASP	PRO	PRO	LEU	LEU	ALA
ASN	ASN	ASN	ASN	LEU	LEU	THR	THR	ILE	ILE	ALA
LEU	LEU	SER	SER	ILE	ILE	TYR	TYR	HIS	HIS	ALA
GLN	GLN	GLN	GLN	LYS	LYS	VAL	VAL	SER	SER	ALA
VAL	VAL	VAL	VAL	VAL	VAL	ALA	ALA	ASN	ASN	ALA
CYS	CYS	VAL	VAL	THR	THR	ALA	ALA	PRO	PRO	ALA
ASP	ASP	GLN	GLN	HIS	HIS	THR	THR	GLY	GLY	ALA
GLY	GLY	ASP	ASP	GLY	GLY	SER	SER	TYR	TYR	ALA
LYS	LYS	VAL	VAL	LEU	LEU	TYR	TYR	PRO	PRO	ALA
VAL	VAL	ASP	ASP	ASP	ASP	ARG	ARG	THR	THR	ALA
SER	SER	SER	SER	ARG	ARG	ALA	ALA	ILE	ILE	ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103038	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4HH, NDP

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	0.11	0/9552	0.24	0/12985
2	B	0.11	0/10114	0.25	0/13741
All	All	0.11	0/19666	0.24	0/26726

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9346	9357	9351	122	0
2	B	9936	9955	9971	143	0
3	A	96	52	52	7	0
3	B	96	52	52	11	0
All	All	19474	19416	19426	262	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 (262) 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)
2:B:2156:4HH:HT3	3:B:2601:NDP:H2D	1.56	0.88
2:B:1577:MET:HE1	2:B:2156:4HH:HO2	1.57	0.84
2:B:1552:ARG:O	2:B:1555:GLN:NE2	2.14	0.81
1:A:1994:PRO:HB3	3:A:2602:NDP:N6A	1.99	0.77
2:B:1241:LYS:NZ	2:B:1307:LEU:O	2.19	0.76
1:A:1994:PRO:HB3	3:A:2602:NDP:H61A	1.50	0.76
1:A:1404:ARG:NH1	1:A:1500:ASP:O	2.20	0.74
1:A:1617:VAL:HG12	1:A:1628:LEU:HD13	1.69	0.72
1:A:1940:GLN:NE2	1:A:1958:GLU:OE2	2.23	0.72
1:A:1244:GLU:OE1	1:A:1270:TYR:OH	2.07	0.72
2:B:973:GLU:N	2:B:973:GLU:OE1	2.23	0.72
2:B:1950:GLU:N	2:B:1950:GLU:OE1	2.23	0.72
1:A:1714:GLN:N	1:A:1714:GLN:OE1	2.23	0.71
2:B:2134:ILE:HD11	2:B:2165:THR:HG21	1.72	0.71
2:B:1230:THR:O	2:B:1234:ASN:ND2	2.23	0.71
2:B:1606:ARG:NH1	2:B:1860:GLU:OE1	2.24	0.70
1:A:1457:VAL:HG21	1:A:1471:CYS:HB2	1.74	0.70
1:A:1933:ARG:NH1	1:A:1939:VAL:O	2.24	0.70
2:B:1986:GLU:OE1	2:B:1986:GLU:N	2.25	0.69
1:A:1176:GLN:N	1:A:1176:GLN:OE1	2.25	0.69
2:B:1478:SER:O	2:B:1481:SER:OG	2.10	0.69
2:B:1680:VAL:HG23	3:B:2601:NDP:O1N	1.93	0.69
2:B:1177:GLU:N	2:B:1177:GLU:OE1	2.26	0.68
2:B:1540:ASP:OD2	2:B:1543:SER:N	2.27	0.68
2:B:1835:GLN:N	2:B:1835:GLN:OE1	2.26	0.68
2:B:1837:GLU:N	2:B:1837:GLU:OE1	2.27	0.68
2:B:2096:ASP:O	2:B:2100:ASN:ND2	2.27	0.68
1:A:995:ARG:NH1	1:A:2065:ASP:O	2.29	0.66
1:A:1521:GLU:N	1:A:1521:GLU:OE1	2.28	0.66
1:A:1294:GLN:OE1	1:A:1294:GLN:N	2.28	0.66
1:A:1333:VAL:HG21	1:A:1384:VAL:HG21	1.76	0.65
2:B:1940:GLN:NE2	2:B:1958:GLU:OE2	2.28	0.65
1:A:1107:GLN:N	1:A:1107:GLN:OE1	2.30	0.64
1:A:1917:ARG:CZ	3:A:2602:NDP:O3X	2.46	0.64
2:B:1274:ASP:OD1	2:B:1275:ARG:N	2.29	0.64
1:A:981:GLU:OE1	1:A:981:GLU:N	2.29	0.64
1:A:1202:LEU:HD12	1:A:1202:LEU:O	1.98	0.63
1:A:1343:LEU:HD21	1:A:1400:LEU:HD11	1.78	0.63
2:B:2042:GLU:OE2	2:B:2059:GLN:NE2	2.31	0.63
1:A:1071:ASP:OD1	1:A:1072:LYS:N	2.32	0.62
2:B:1801:ASN:ND2	2:B:1802:GLU:OE1	2.30	0.62
1:A:934:GLU:N	1:A:934:GLU:OE1	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1628:LEU:HD12	2:B:1629:SER:O	2.00	0.61
1:A:1286:GLU:OE1	1:A:1286:GLU:N	2.34	0.61
2:B:1794:VAL:O	2:B:1795:LEU:HD12	2.01	0.61
2:B:1525:GLU:OE2	2:B:1545:ARG:NH2	2.34	0.60
2:B:2156:4HH:HP3	3:B:2601:NDP:O2D	2.01	0.60
1:A:939:GLU:N	1:A:939:GLU:OE1	2.34	0.60
1:A:1175:GLN:OE1	1:A:1175:GLN:N	2.35	0.60
2:B:2148:SER:N	2:B:2151:ASP:OD2	2.35	0.60
1:A:1297:TRP:NE1	1:A:1301:ASP:O	2.34	0.59
1:A:1730:GLN:OE1	1:A:1730:GLN:N	2.34	0.59
2:B:1141:CYS:O	2:B:1145:VAL:HG23	2.02	0.59
1:A:1174:SER:OG	1:A:1176:GLN:OE1	2.20	0.59
1:A:1145:VAL:HG12	1:A:1145:VAL:O	2.02	0.59
2:B:1663:GLY:O	2:B:1765:ARG:NH1	2.36	0.59
1:A:1928:GLN:OE1	1:A:1931:ARG:NH2	2.36	0.58
2:B:2028:ASN:OD1	2:B:2029:ALA:N	2.37	0.58
1:A:1329:LEU:HD12	1:A:1330:SER:N	2.19	0.57
2:B:1460:LEU:HD22	2:B:1980:LEU:HD22	1.87	0.57
2:B:2156:4HH:CT	3:B:2601:NDP:H2D	2.31	0.57
1:A:869:GLU:N	1:A:869:GLU:OE1	2.36	0.57
1:A:1413:ILE:HG21	1:A:1431:ILE:HD12	1.85	0.57
1:A:1210:PRO:HB3	1:A:1319:VAL:HG11	1.87	0.56
1:A:1238:LEU:HD13	1:A:1265:LEU:O	2.05	0.56
1:A:1483:VAL:HG23	1:A:1483:VAL:O	2.05	0.56
2:B:1597:SER:C	2:B:1598:LEU:HD12	2.30	0.56
2:B:2161:GLU:O	2:B:2165:THR:HG23	2.05	0.56
1:A:1726:THR:O	1:A:1726:THR:HG22	2.05	0.56
2:B:1628:LEU:CD1	2:B:1629:SER:O	2.53	0.56
1:A:1723:SER:CB	3:A:2601:NDP:O3X	2.54	0.56
1:A:2042:GLU:OE2	1:A:2059:GLN:NE2	2.39	0.56
1:A:1177:GLU:OE1	1:A:1180:ARG:NH2	2.37	0.56
2:B:1457:VAL:HG21	2:B:1471:CYS:HB2	1.88	0.56
1:A:1662:ARG:NH1	2:B:1788:ASN:OD1	2.40	0.55
1:A:1628:LEU:HD23	1:A:1633:LEU:HD21	1.89	0.55
1:A:1669:GLU:OE1	1:A:1765:ARG:NH2	2.39	0.55
2:B:879:THR:HG22	2:B:884:VAL:HG22	1.88	0.55
2:B:1596:ASP:OD1	2:B:1597:SER:N	2.40	0.54
2:B:1726:THR:HG22	2:B:1726:THR:O	2.06	0.54
2:B:2018:VAL:HB	2:B:2041:MET:HE3	1.90	0.54
2:B:1565:THR:HG23	2:B:1870:PRO:HB3	1.89	0.54
1:A:1198:LEU:O	1:A:1204:GLN:NE2	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1763:HIS:N	2:B:1788:ASN:O	2.40	0.54
1:A:945:GLU:OE1	2:B:941:SER:OG	2.18	0.54
2:B:1411:SER:O	2:B:1439:ARG:NE	2.39	0.54
2:B:1431:ILE:O	2:B:1468:ARG:NH2	2.41	0.54
2:B:1576:ILE:HD12	2:B:1577:MET:N	2.23	0.54
2:B:2165:THR:HG22	2:B:2168:ARG:NH2	2.23	0.54
2:B:1128:LEU:HD11	2:B:1218:LEU:HD23	1.90	0.53
2:B:1443:LEU:HD12	2:B:1457:VAL:HG22	1.90	0.53
1:A:1019:ARG:HD3	1:A:1075:VAL:HG21	1.90	0.53
1:A:1596:ASP:OD1	1:A:1597:SER:N	2.42	0.53
2:B:1391:LEU:HD23	2:B:1392:LYS:N	2.23	0.53
1:A:877:ASP:OD2	1:A:1004:HIS:ND1	2.42	0.53
1:A:1833:GLY:O	1:A:1836:VAL:HG23	2.09	0.53
2:B:1280:LEU:HD21	2:B:1294:GLN:HB3	1.91	0.53
2:B:1274:ASP:O	2:B:1296:GLN:NE2	2.42	0.52
1:A:1662:ARG:NH2	2:B:1790:THR:OG1	2.41	0.52
2:B:1925:GLN:O	2:B:1929:VAL:HG23	2.09	0.52
2:B:1413:ILE:HD11	2:B:1439:ARG:NE	2.24	0.52
1:A:1413:ILE:HG21	1:A:1431:ILE:CD1	2.39	0.52
1:A:1570:SER:OG	1:A:1646:ALA:O	2.19	0.52
1:A:1831:PHE:O	1:A:1855:GLN:N	2.44	0.51
1:A:1860:GLU:N	1:A:1860:GLU:OE1	2.43	0.51
2:B:1366:GLN:O	2:B:1370:GLY:N	2.42	0.51
1:A:1602:GLU:OE1	1:A:1851:LYS:NZ	2.42	0.51
2:B:1297:TRP:NE1	2:B:1301:ASP:O	2.39	0.51
2:B:1366:GLN:N	2:B:1366:GLN:OE1	2.43	0.51
2:B:2157:LEU:O	2:B:2160:VAL:HG12	2.11	0.51
2:B:1771:LYS:HG3	2:B:2156:4HH:HS2	1.93	0.51
1:A:2006:THR:OG1	1:A:2013:LEU:HD22	2.11	0.51
1:A:1058:ASP:OD2	1:A:1061:THR:OG1	2.25	0.51
2:B:1125:GLU:N	2:B:1125:GLU:OE1	2.43	0.51
2:B:2033:ASN:OD1	2:B:2034:TYR:N	2.43	0.51
1:A:1602:GLU:HG3	1:A:1650:VAL:HG23	1.92	0.51
1:A:1322:LEU:HD12	1:A:1322:LEU:O	2.10	0.51
2:B:1286:GLU:N	2:B:1286:GLU:OE1	2.44	0.51
1:A:1670:THR:C	1:A:1671:LEU:HD12	2.37	0.50
1:A:1244:GLU:O	1:A:1273:THR:OG1	2.16	0.50
1:A:1493:LEU:O	1:A:1497:LEU:HD23	2.11	0.50
2:B:879:THR:C	2:B:880:LEU:HD12	2.36	0.50
1:A:1622:LEU:HD11	1:A:1854:VAL:HG11	1.94	0.49
1:A:1422:PHE:O	1:A:1425:VAL:HG12	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1020:LEU:HD22	2:B:1032:THR:HG22	1.94	0.49
2:B:1372:LEU:HG	2:B:1376:ALA:HB3	1.95	0.49
2:B:1128:LEU:HD13	2:B:1394:SER:OG	2.12	0.49
1:A:1238:LEU:HD12	1:A:1238:LEU:C	2.38	0.49
1:A:1545:ARG:HD2	1:A:1876:ILE:HD11	1.94	0.49
2:B:866:THR:HG22	2:B:866:THR:O	2.13	0.49
1:A:1723:SER:OG	3:A:2601:NDP:O3X	2.26	0.48
2:B:1573:PHE:CE1	3:B:2601:NDP:H52A	2.48	0.48
2:B:1122:HIS:ND1	2:B:1511:TRP:O	2.46	0.48
2:B:1111:VAL:O	2:B:1111:VAL:HG13	2.13	0.48
1:A:1145:VAL:HG11	1:A:1356:ILE:HD12	1.95	0.48
2:B:1476:ASN:ND2	2:B:1481:SER:OG	2.42	0.48
2:B:1602:GLU:HB3	2:B:1650:VAL:HG23	1.95	0.48
2:B:1141:CYS:HB3	2:B:1356:ILE:HD13	1.95	0.48
2:B:1215:LEU:C	2:B:1215:LEU:HD23	2.39	0.48
2:B:1996:TYR:CE1	2:B:2000:LEU:HD11	2.49	0.48
2:B:1127:CYS:C	2:B:1128:LEU:HD12	2.39	0.48
2:B:2134:ILE:CD1	2:B:2165:THR:HG21	2.41	0.48
1:A:872:ASP:OD1	1:A:875:LEU:HD12	2.14	0.47
2:B:1970:ASN:C	2:B:1971:LEU:HD12	2.39	0.47
1:A:1628:LEU:HD11	1:A:1632:PHE:HB2	1.94	0.47
1:A:2033:ASN:OD1	1:A:2034:TYR:N	2.48	0.47
1:A:1555:GLN:N	1:A:1556:PRO:CD	2.78	0.47
2:B:2148:SER:OG	2:B:2151:ASP:OD2	2.26	0.47
1:A:1732:VAL:O	1:A:1736:THR:HG22	2.15	0.47
1:A:1726:THR:HG23	1:A:1755:ALA:CB	2.44	0.47
1:A:1917:ARG:NH1	3:A:2602:NDP:O3X	2.47	0.47
2:B:1144:LEU:HD13	2:B:1182:LEU:CB	2.45	0.47
2:B:1344:LEU:O	2:B:1401:PHE:N	2.46	0.47
1:A:1418:ASP:OD2	1:A:1447:ASN:N	2.47	0.47
2:B:1267:GLN:N	2:B:1267:GLN:OE1	2.47	0.47
1:A:1185:ALA:O	1:A:1193:ASN:ND2	2.46	0.46
1:A:1607:ASP:OD1	1:A:1611:LYS:N	2.46	0.46
2:B:863:ASN:ND2	2:B:930:THR:OG1	2.48	0.46
1:A:1425:VAL:HG21	1:A:1988:PHE:CE1	2.50	0.46
2:B:1128:LEU:HD13	2:B:1394:SER:CB	2.46	0.46
2:B:1384:VAL:O	2:B:1385:SER:OG	2.25	0.46
1:A:1246:LEU:HD12	1:A:1246:LEU:N	2.30	0.46
1:A:1410:ASP:OD1	1:A:1410:ASP:N	2.49	0.46
1:A:1019:ARG:NH1	1:A:1067:TYR:OH	2.48	0.46
1:A:1971:LEU:N	1:A:1971:LEU:HD12	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2156:4HH:HS3	3:B:2601:NDP:O2D	2.15	0.45
2:B:1375:ASP:OD1	2:B:1376:ALA:N	2.49	0.45
1:A:1384:VAL:HG22	1:A:1385:SER:N	2.32	0.45
1:A:1420:THR:HG22	1:A:1421:SER:N	2.31	0.45
2:B:1453:VAL:O	2:B:1457:VAL:HG23	2.16	0.45
2:B:1454:VAL:O	2:B:1458:ASN:ND2	2.43	0.45
1:A:1343:LEU:HD23	1:A:1343:LEU:C	2.41	0.45
1:A:1733:LEU:O	1:A:1738:GLY:N	2.48	0.45
2:B:1287:LEU:HD22	2:B:1292:VAL:HG21	1.98	0.45
2:B:1313:LEU:O	2:B:1342:LEU:HD12	2.17	0.45
2:B:1337:ARG:NE	2:B:1338:GLU:O	2.50	0.45
1:A:1893:LEU:HD12	1:A:1916:SER:OG	2.16	0.45
1:A:1453:VAL:O	1:A:1457:VAL:HG23	2.17	0.45
1:A:1329:LEU:HD12	1:A:1329:LEU:C	2.42	0.45
1:A:1477:LEU:HD11	1:A:2047:LYS:HA	1.97	0.45
2:B:1347:LEU:N	2:B:1347:LEU:HD12	2.32	0.45
1:A:1750:GLU:O	1:A:1753:LEU:N	2.50	0.44
2:B:2063:ILE:HD13	3:B:2602:NDP:C7N	2.47	0.44
1:A:1707:TYR:CD2	1:A:1849:ILE:HD11	2.52	0.44
2:B:1114:LEU:N	2:B:1114:LEU:HD12	2.33	0.44
2:B:2020:SER:OG	2:B:2021:SER:N	2.50	0.44
1:A:1322:LEU:HD12	1:A:1322:LEU:C	2.43	0.44
2:B:1033:MET:SD	2:B:1089:ALA:HB3	2.58	0.44
2:B:1933:ARG:NH1	2:B:1939:VAL:O	2.51	0.44
2:B:2097:LEU:C	2:B:2097:LEU:HD23	2.42	0.44
2:B:2097:LEU:HD23	2:B:2097:LEU:O	2.18	0.44
1:A:2020:SER:OG	1:A:2021:SER:N	2.49	0.44
2:B:1209:LEU:N	2:B:1210:PRO:HD2	2.33	0.43
1:A:1014:GLU:OE1	1:A:1014:GLU:N	2.48	0.43
2:B:991:TYR:CZ	2:B:1006:GLN:HA	2.54	0.43
2:B:1364:GLU:N	2:B:1365:PRO:HD2	2.33	0.43
2:B:1894:GLY:HA3	3:B:2602:NDP:H4B	1.99	0.43
2:B:1196:LEU:C	2:B:1196:LEU:HD23	2.43	0.43
2:B:1202:LEU:C	2:B:1202:LEU:HD12	2.43	0.43
1:A:1009:LEU:HD11	1:A:1021:LEU:HG	2.00	0.43
1:A:1033:MET:SD	1:A:1089:ALA:HB3	2.59	0.43
1:A:1081:SER:O	1:A:1085:ARG:N	2.51	0.43
1:A:1617:VAL:HG11	1:A:1626:VAL:HG21	2.00	0.43
2:B:1348:LEU:HD22	2:B:1374:GLN:HB3	2.00	0.43
2:B:1413:ILE:HD12	2:B:1440:PRO:O	2.19	0.43
2:B:1628:LEU:HD12	2:B:1628:LEU:C	2.43	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1411:SER:OG	1:A:1439:ARG:NE	2.52	0.43
1:A:1914:LEU:HD12	1:A:1914:LEU:N	2.34	0.43
1:A:1651:VAL:HG23	1:A:1652:TYR:N	2.34	0.42
2:B:1237:SER:OG	2:B:1239:LYS:O	2.37	0.42
2:B:1497:LEU:HD12	2:B:1497:LEU:C	2.44	0.42
2:B:1535:THR:HG22	2:B:1544:ILE:CD1	2.49	0.42
2:B:2022:VAL:O	2:B:2026:ARG:N	2.49	0.42
2:B:2156:4HH:HL12	2:B:2156:4HH:O2P	2.19	0.42
1:A:1338:GLU:OE1	1:A:1405:ARG:NH2	2.53	0.42
1:A:1198:LEU:HD12	1:A:1198:LEU:C	2.43	0.42
2:B:1977:ASP:OD1	2:B:1977:ASP:N	2.53	0.42
1:A:905:LEU:N	1:A:905:LEU:HD12	2.35	0.42
2:B:1128:LEU:HD21	2:B:1217:GLY:C	2.44	0.42
2:B:1651:VAL:HG23	2:B:1652:TYR:N	2.35	0.42
2:B:2134:ILE:HG21	2:B:2162:VAL:HG13	2.00	0.42
1:A:1235:MET:HE3	1:A:1240:MET:SD	2.60	0.42
2:B:1602:GLU:OE2	2:B:1851:LYS:NZ	2.53	0.42
2:B:1894:GLY:HA3	3:B:2602:NDP:O2A	2.20	0.42
2:B:880:LEU:HD23	2:B:1048:LEU:HD21	2.02	0.42
2:B:1215:LEU:HD11	2:B:1319:VAL:HG22	2.02	0.42
2:B:1105:ARG:NH2	2:B:2167:GLU:OE2	2.48	0.42
2:B:1127:CYS:HB3	2:B:1128:LEU:HD12	2.00	0.42
2:B:1144:LEU:HD13	2:B:1182:LEU:HB3	2.01	0.42
2:B:1573:PHE:CD1	3:B:2601:NDP:H52A	2.54	0.42
2:B:2169:GLU:HG3	2:B:2170:LEU:HD13	2.02	0.42
2:B:1573:PHE:CE2	2:B:1577:MET:HE3	2.55	0.41
2:B:1535:THR:HG23	2:B:1599:LEU:HD11	2.01	0.41
2:B:1435:GLU:O	2:B:1468:ARG:NH2	2.53	0.41
2:B:2012:GLU:OE1	2:B:2012:GLU:N	2.53	0.41
2:B:2165:THR:HG22	2:B:2168:ARG:HH22	1.82	0.41
1:A:1769:ILE:HG22	1:A:1794:VAL:CG2	2.50	0.41
2:B:1178:LEU:C	2:B:1178:LEU:HD23	2.46	0.41
2:B:1984:THR:HG23	2:B:1987:PHE:H	1.85	0.41
1:A:1556:PRO:HG2	1:A:1627:LEU:HD22	2.02	0.41
2:B:1726:THR:HG23	2:B:1755:ALA:CB	2.50	0.41
1:A:899:LEU:HD22	1:A:958:VAL:HG22	2.02	0.41
2:B:1391:LEU:HD23	2:B:1391:LEU:C	2.45	0.41
1:A:991:TYR:CZ	1:A:1006:GLN:HA	2.56	0.41
1:A:1020:LEU:HD22	1:A:1032:THR:HG22	2.02	0.41
1:A:1973:VAL:CG1	3:A:2602:NDP:H3D	2.50	0.41
2:B:1404:ARG:NH1	2:B:1500:ASP:O	2.47	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1680:VAL:HG21	3:B:2601:NDP:C6N	2.51	0.41
2:B:2151:ASP:OD1	2:B:2152:LEU:N	2.54	0.41
1:A:1245:VAL:HG11	1:A:1332:MET:SD	2.61	0.41
1:A:1428:LEU:HA	1:A:1431:ILE:HG22	2.03	0.41
1:A:1502:VAL:HG23	1:A:1503:MET:N	2.36	0.41
2:B:905:LEU:N	2:B:905:LEU:HD12	2.36	0.41
2:B:1081:SER:O	2:B:1085:ARG:N	2.54	0.41
1:A:864:ILE:HD12	1:A:864:ILE:N	2.36	0.40
2:B:1657:TYR:CE2	2:B:1794:VAL:HG13	2.56	0.40
1:A:1121:PRO:O	1:A:1392:LYS:NZ	2.54	0.40
1:A:1300:ALA:O	1:A:1331:ASN:ND2	2.55	0.40
1:A:1384:VAL:HG22	1:A:1385:SER:H	1.87	0.40
1:A:1419:ASP:OD1	1:A:1420:THR:N	2.55	0.40
1:A:1261:SER:N	1:A:1262:PRO:CD	2.85	0.40
1:A:1794:VAL:O	1:A:1794:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1210/2553 (47%)	1182 (98%)	28 (2%)	0	100	100
2	B	1280/2553 (50%)	1250 (98%)	30 (2%)	0	100	100
All	All	2490/5106 (49%)	2432 (98%)	58 (2%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM

entries.

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	1009/2117 (48%)	1006 (100%)	3 (0%)	86	88
2	B	1073/2116 (51%)	1072 (100%)	1 (0%)	88	91
All	All	2082/4233 (49%)	2078 (100%)	4 (0%)	85	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	985	LEU
1	A	1602	GLU
1	A	1854	VAL
2	B	1463	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1035	GLN
1	A	1139	GLN
1	A	1276	HIS
1	A	1290	HIS
1	A	1731	HIS
1	A	1735	HIS
1	A	1845	GLN
1	A	1906	GLN
1	A	1961	GLN
2	B	863	ASN
2	B	971	HIS
2	B	1004	HIS
2	B	1006	GLN
2	B	1044	HIS
2	B	1107	GLN
2	B	1200	GLN
2	B	1251	HIS
2	B	1351	HIS
2	B	1482	HIS
2	B	1709	GLN
2	B	1845	GLN
2	B	1855	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	4HH	B	2156	2	22,26,27	0.43	0	27,35,37	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4HH	B	2156	2	-	20/33/35/37	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2156	4HH	C-CA-CB-OG
2	B	2156	4HH	CB-OG-P-O2P
2	B	2156	4HH	CB-OG-P-O3P
2	B	2156	4HH	O3P-CJ-CK-CL1
2	B	2156	4HH	O3P-CJ-CK-CL2
2	B	2156	4HH	O3P-CJ-CK-CM
2	B	2156	4HH	CK-CJ-O3P-P
2	B	2156	4HH	CM-CL3-NN-CO
2	B	2156	4HH	ON-CL3-NN-CO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	2156	4HH	CJ-O3P-P-OG
2	B	2156	4HH	CP-CQ-NR-CS
2	B	2156	4HH	OR-CQ-NR-CS
2	B	2156	4HH	NN-CL3-CM-CK
2	B	2156	4HH	NN-CL3-CM-OM
2	B	2156	4HH	NR-CS-CT-SU
2	B	2156	4HH	CB-OG-P-O1P
2	B	2156	4HH	CJ-O3P-P-O2P
2	B	2156	4HH	N-CA-CB-OG
2	B	2156	4HH	NN-CO-CP-CQ
2	B	2156	4HH	ON-CL3-CM-CK

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2156	4HH	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NDP	A	2601	-	51,52,52	0.48	0	71,80,80	0.75	1 (1%)
3	NDP	B	2601	-	51,52,52	0.49	0	71,80,80	0.70	1 (1%)
3	NDP	B	2602	-	51,52,52	0.49	0	71,80,80	0.71	2 (2%)
3	NDP	A	2602	-	51,52,52	0.51	0	71,80,80	0.68	1 (1%)

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	A	2601	-	-	9/34/77/77	0/5/5/5
3	NDP	B	2601	-	-	14/34/77/77	0/5/5/5
3	NDP	B	2602	-	-	9/34/77/77	0/5/5/5
3	NDP	A	2602	-	-	8/34/77/77	0/5/5/5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2601	NDP	P2B-O2B-C2B	-4.50	111.42	123.43
3	A	2602	NDP	P2B-O2B-C2B	-4.28	111.99	123.43
3	B	2601	NDP	P2B-O2B-C2B	-4.01	112.72	123.43
3	B	2602	NDP	P2B-O2B-C2B	-3.43	114.27	123.43
3	B	2602	NDP	C3N-C2N-N1N	-2.23	119.93	123.20

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2601	NDP	C5B-O5B-PA-O3
3	A	2601	NDP	C2N-C3N-C7N-N7N
3	A	2602	NDP	O4B-C4B-C5B-O5B
3	A	2602	NDP	C3B-C4B-C5B-O5B
3	A	2602	NDP	C5D-O5D-PN-O3
3	A	2602	NDP	C5D-O5D-PN-O2N
3	B	2601	NDP	C5B-O5B-PA-O1A
3	B	2601	NDP	O4D-C4D-C5D-O5D
3	B	2601	NDP	C2N-C3N-C7N-O7N
3	B	2601	NDP	C2N-C3N-C7N-N7N
3	B	2602	NDP	O4D-C1D-N1N-C6N
3	B	2601	NDP	O4D-C1D-N1N-C2N
3	B	2601	NDP	O4B-C4B-C5B-O5B
3	B	2601	NDP	C3B-C4B-C5B-O5B
3	B	2602	NDP	C1B-C2B-O2B-P2B
3	A	2602	NDP	O4D-C1D-N1N-C6N
3	B	2602	NDP	O4D-C4D-C5D-O5D
3	B	2602	NDP	C3D-C4D-C5D-O5D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	2601	NDP	C1B-C2B-O2B-P2B
3	B	2601	NDP	C3B-C2B-O2B-P2B
3	B	2601	NDP	C3D-C4D-C5D-O5D
3	A	2601	NDP	C2D-C1D-N1N-C2N
3	A	2601	NDP	C2D-C1D-N1N-C6N
3	B	2602	NDP	C3B-C2B-O2B-P2B
3	B	2602	NDP	C4B-C5B-O5B-PA
3	B	2601	NDP	PA-O3-PN-O1N
3	A	2601	NDP	O4D-C1D-N1N-C2N
3	A	2602	NDP	C4B-C5B-O5B-PA
3	A	2601	NDP	C5B-O5B-PA-O1A
3	B	2602	NDP	C5D-O5D-PN-O1N
3	A	2601	NDP	O4D-C1D-N1N-C6N
3	B	2601	NDP	PA-O3-PN-O2N
3	B	2601	NDP	C4B-C5B-O5B-PA
3	B	2602	NDP	O4B-C4B-C5B-O5B
3	A	2601	NDP	C3B-C4B-C5B-O5B
3	A	2602	NDP	PA-O3-PN-O1N
3	A	2602	NDP	PA-O3-PN-O2N
3	B	2601	NDP	C2B-O2B-P2B-O3X
3	B	2602	NDP	C2B-O2B-P2B-O1X
3	A	2601	NDP	C2N-C3N-C7N-O7N

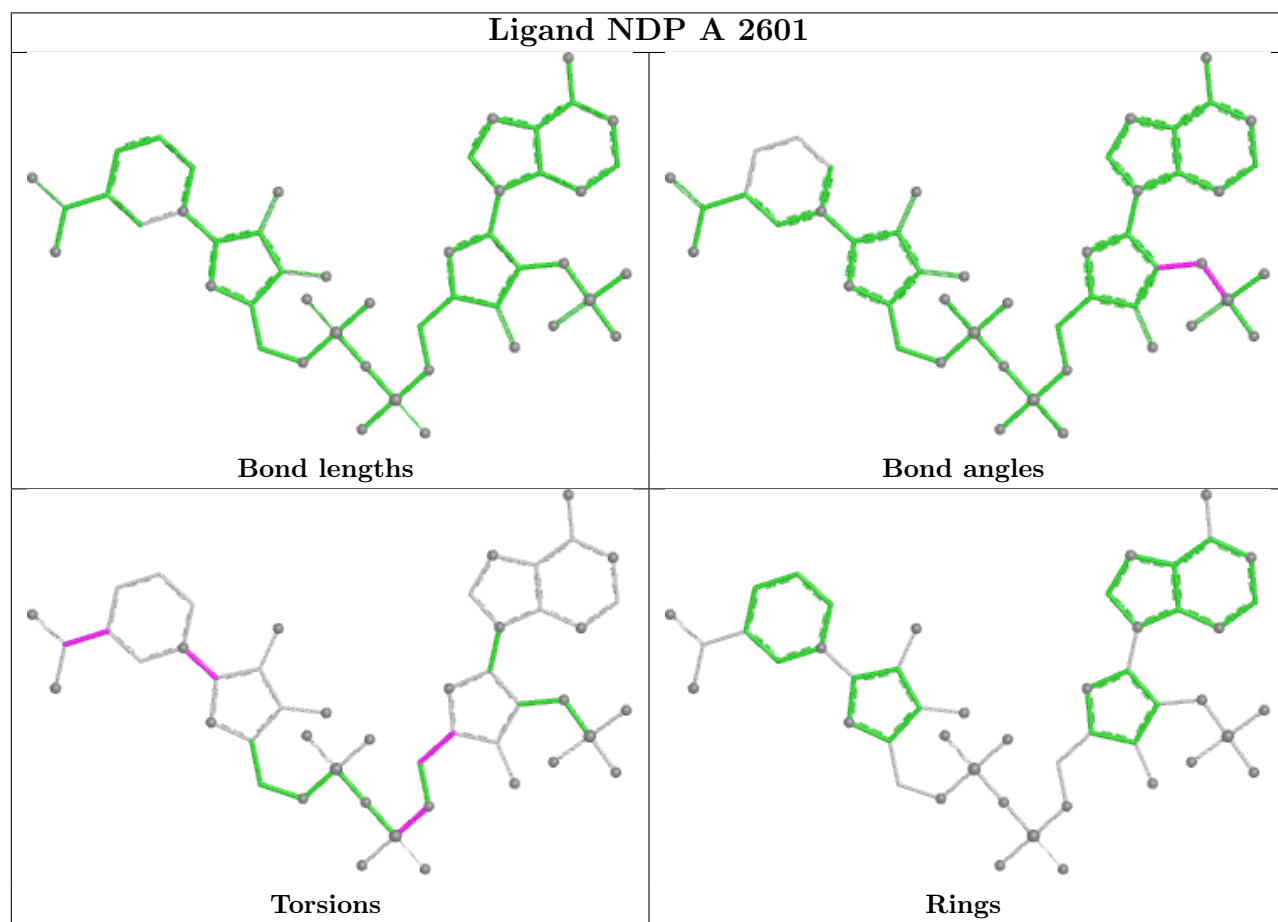
There are no ring outliers.

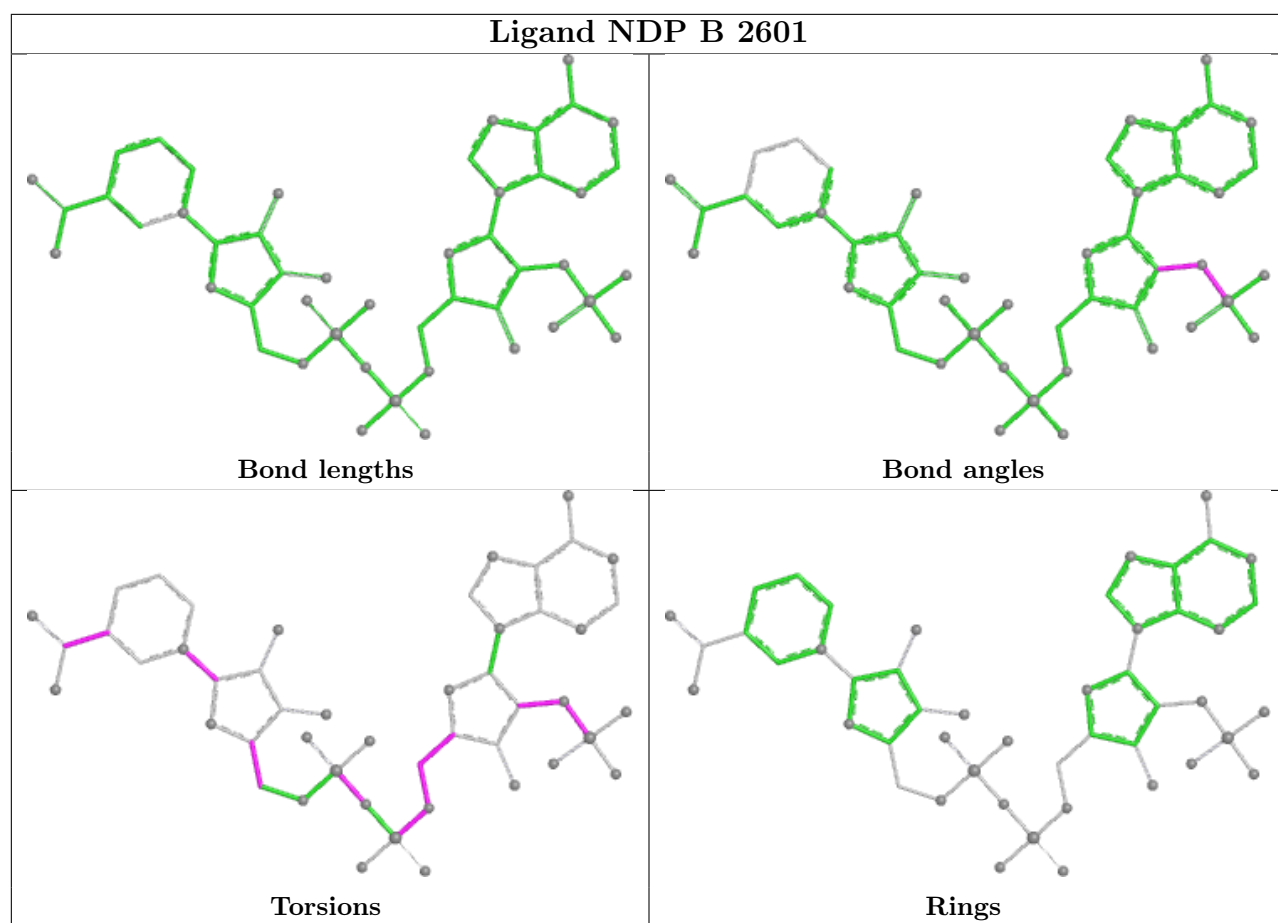
4 monomers are involved in 18 short contacts:

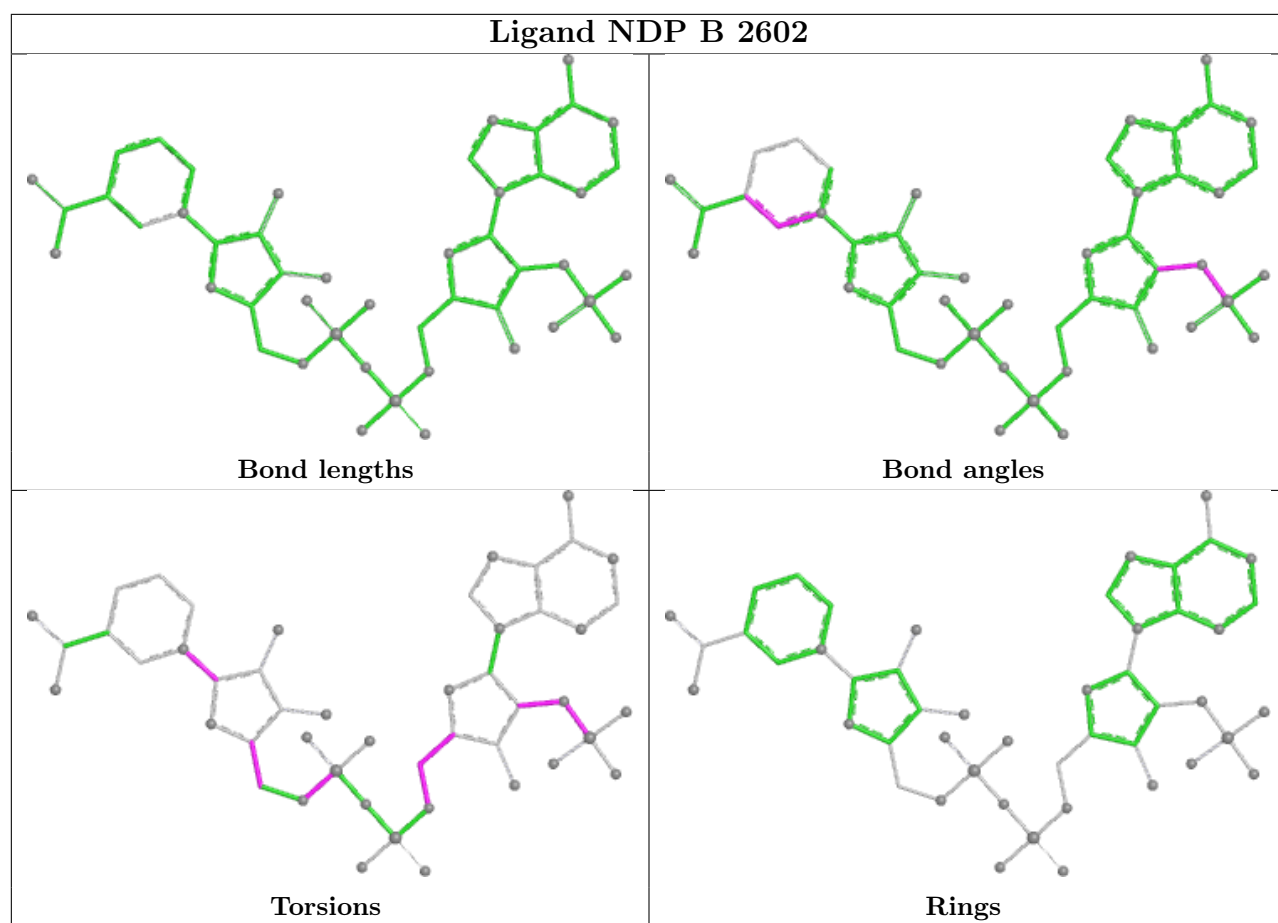
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2601	NDP	2	0
3	B	2601	NDP	8	0
3	B	2602	NDP	3	0
3	A	2602	NDP	5	0

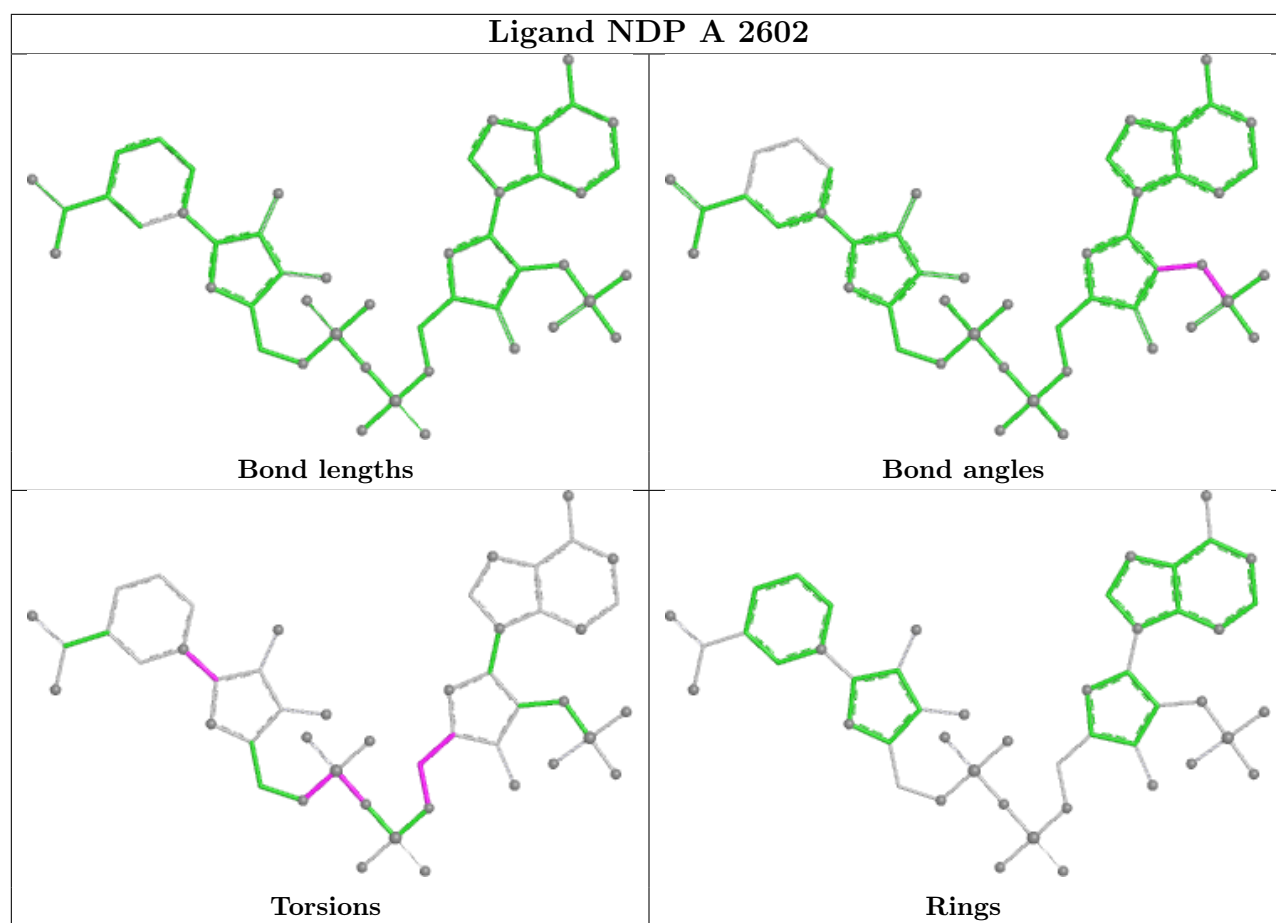
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 Map visualisation

This section contains visualisations of the EMDB entry EMD-43187. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.