



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:21 AM UTC

PDB ID : 3S61 / pdb_00003s61
Title : Reduced Form of Ornithine Hydroxylase (PvdA) from *Pseudomonas aeruginosa*
Authors : Olucha, J.; Lamb, A.L.
Deposited on : 2011-05-23
Resolution : 3.03 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

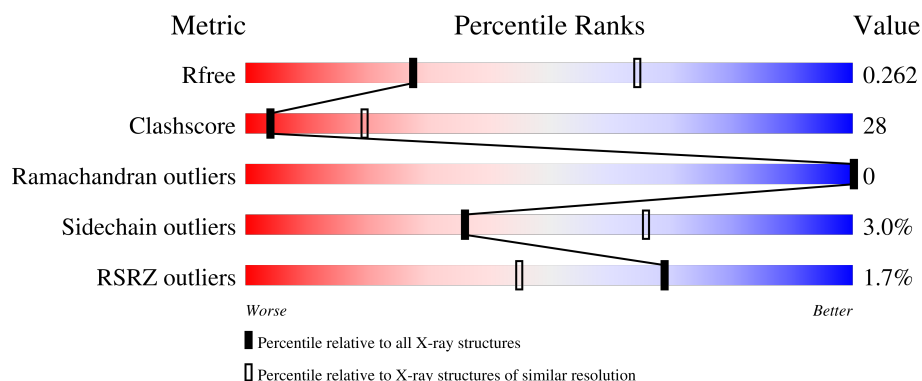
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	463	48% 36% • 11%
1	B	463	2% 43% 40% 6% 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6760 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 L-ornithine 5-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3284	2075	584	616	9			
1	B	410	Total	C	N	O	S	0	0	0
			3256	2057	577	613	9			

There are 40 discrepancies between the modelled and reference sequences:

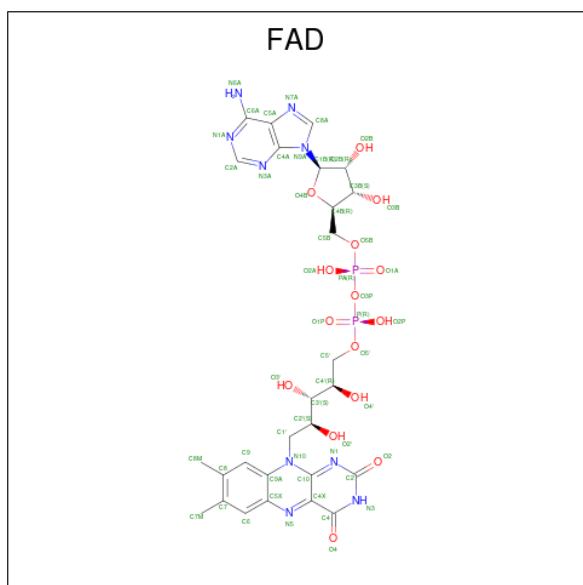
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q51548
A	-18	GLY	-	expression tag	UNP Q51548
A	-17	SER	-	expression tag	UNP Q51548
A	-16	SER	-	expression tag	UNP Q51548
A	-15	HIS	-	expression tag	UNP Q51548
A	-14	HIS	-	expression tag	UNP Q51548
A	-13	HIS	-	expression tag	UNP Q51548
A	-12	HIS	-	expression tag	UNP Q51548
A	-11	HIS	-	expression tag	UNP Q51548
A	-10	HIS	-	expression tag	UNP Q51548
A	-9	SER	-	expression tag	UNP Q51548
A	-8	SER	-	expression tag	UNP Q51548
A	-7	GLY	-	expression tag	UNP Q51548
A	-6	LEU	-	expression tag	UNP Q51548
A	-5	VAL	-	expression tag	UNP Q51548
A	-4	PRO	-	expression tag	UNP Q51548
A	-3	ARG	-	expression tag	UNP Q51548
A	-2	GLY	-	expression tag	UNP Q51548
A	-1	SER	-	expression tag	UNP Q51548
A	0	HIS	-	expression tag	UNP Q51548
B	-19	MET	-	expression tag	UNP Q51548
B	-18	GLY	-	expression tag	UNP Q51548
B	-17	SER	-	expression tag	UNP Q51548
B	-16	SER	-	expression tag	UNP Q51548
B	-15	HIS	-	expression tag	UNP Q51548

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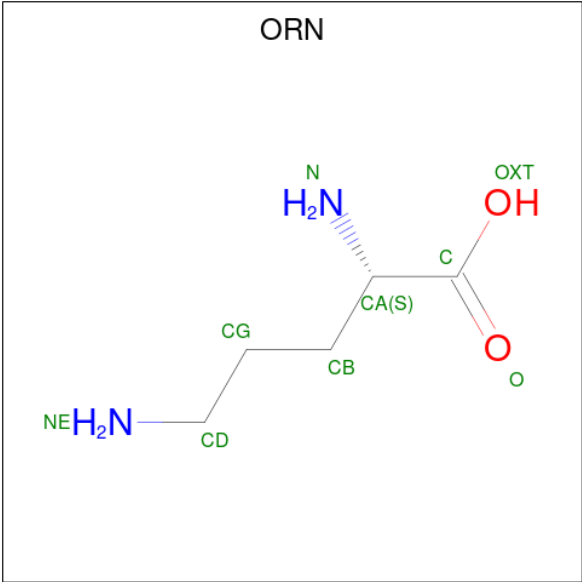
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q51548
B	-13	HIS	-	expression tag	UNP Q51548
B	-12	HIS	-	expression tag	UNP Q51548
B	-11	HIS	-	expression tag	UNP Q51548
B	-10	HIS	-	expression tag	UNP Q51548
B	-9	SER	-	expression tag	UNP Q51548
B	-8	SER	-	expression tag	UNP Q51548
B	-7	GLY	-	expression tag	UNP Q51548
B	-6	LEU	-	expression tag	UNP Q51548
B	-5	VAL	-	expression tag	UNP Q51548
B	-4	PRO	-	expression tag	UNP Q51548
B	-3	ARG	-	expression tag	UNP Q51548
B	-2	GLY	-	expression tag	UNP Q51548
B	-1	SER	-	expression tag	UNP Q51548
B	0	HIS	-	expression tag	UNP Q51548

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



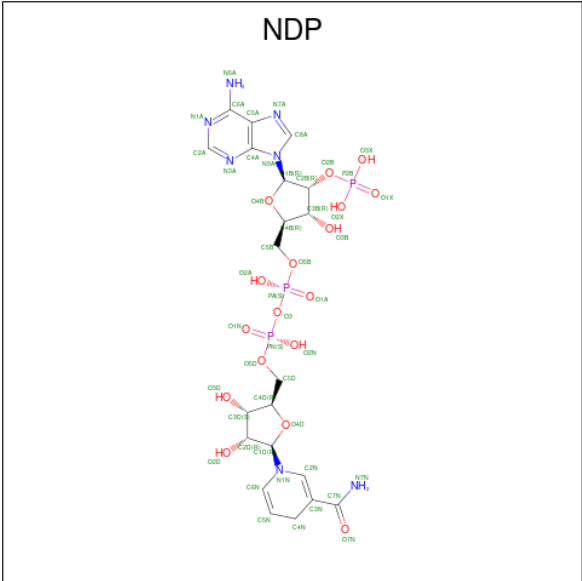
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is L-ornithine (CCD ID: ORN) (formula: $C_5H_{12}N_2O_2$).



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

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

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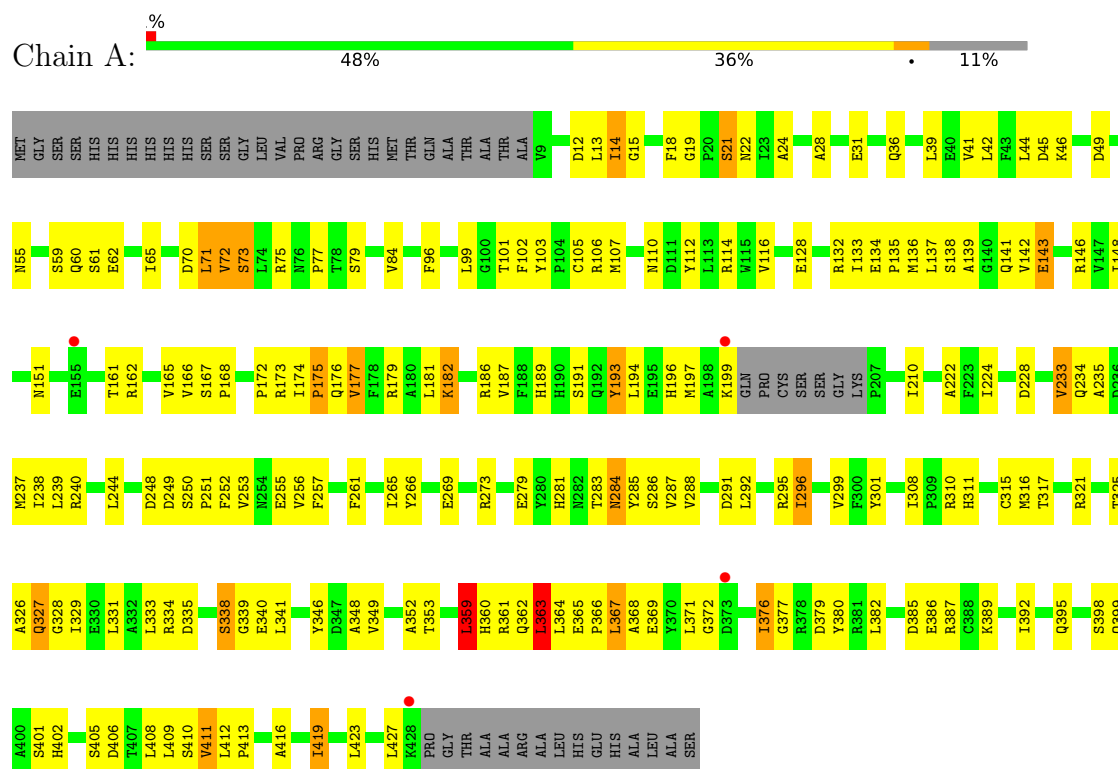
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

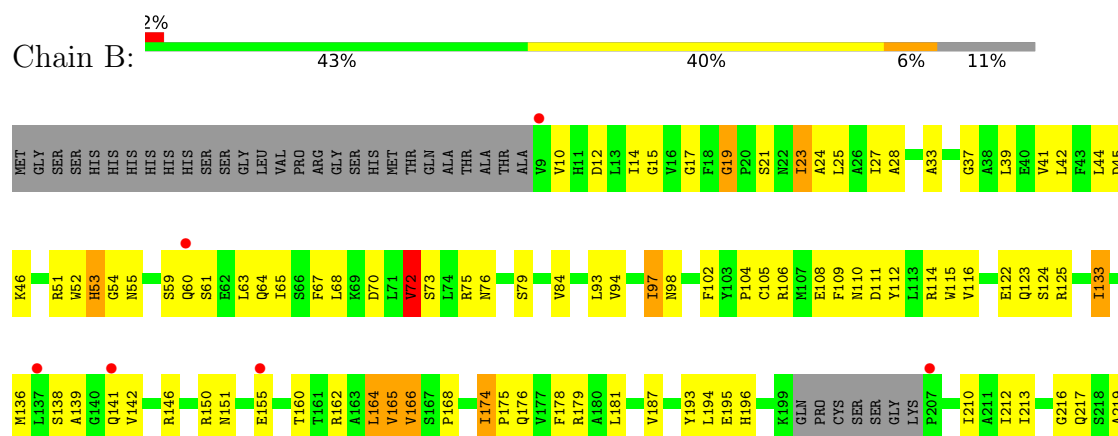
3 Residue-property plots

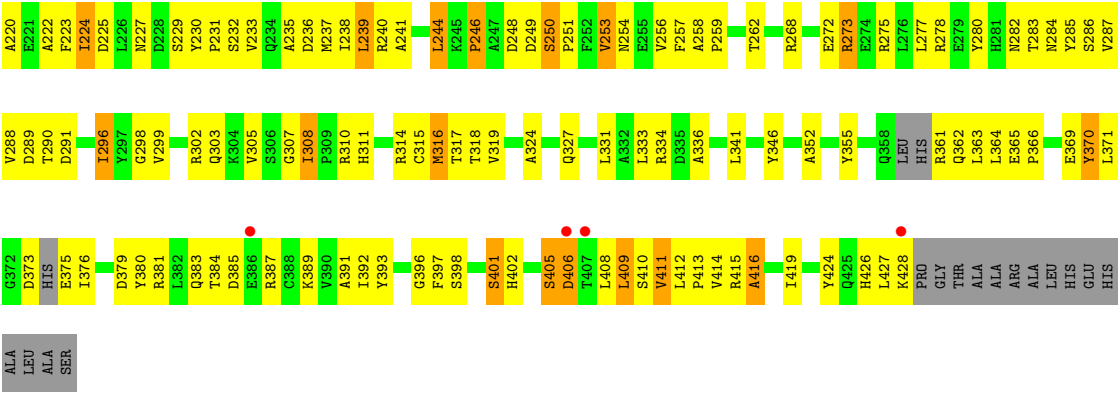
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: L-ornithine 5-monooxygenase



• Molecule 1: L-ornithine 5-monooxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	128.16Å 128.16Å 316.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.26 – 3.03 39.26 – 3.03	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.26-3.03) 99.4 (39.26-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.216 , 0.272 0.226 , 0.262	Depositor DCC
R_{free} test set	2616 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6760	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.41% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.91	15/3353 (0.4%)	1.25	34/4540 (0.7%)
1	B	1.92	23/3321 (0.7%)	1.34	48/4493 (1.1%)
All	All	1.92	38/6674 (0.6%)	1.30	82/9033 (0.9%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	ILE	CA-CB	-6.74	1.49	1.54
1	A	376	ILE	CA-CB	-6.49	1.48	1.54
1	B	165	VAL	CA-CB	-6.46	1.46	1.54
1	B	230	TYR	C-O	-6.37	1.19	1.24
1	B	84	VAL	CA-CB	-6.34	1.46	1.54
1	B	27	ILE	CA-CB	-6.32	1.46	1.54
1	B	76	ASN	C-O	-6.20	1.20	1.25
1	B	220	ALA	CA-CB	-6.16	1.43	1.53
1	B	246	PRO	N-CD	-6.12	1.39	1.47
1	A	416	ALA	CA-CB	-6.09	1.43	1.53
1	B	216	GLY	C-O	-6.05	1.17	1.23
1	B	219	ALA	CA-CB	-5.93	1.44	1.53
1	B	416	ALA	CA-CB	-5.83	1.44	1.53
1	B	187	VAL	CA-CB	-5.77	1.47	1.54
1	B	28	ALA	CA-CB	-5.64	1.44	1.53
1	B	53	HIS	CA-C	-5.61	1.46	1.53
1	B	241	ALA	CA-CB	-5.58	1.44	1.53
1	B	308	ILE	CA-C	-5.34	1.47	1.52
1	B	24	ALA	C-O	-5.29	1.18	1.24
1	A	28	ALA	CA-CB	-5.29	1.45	1.53
1	A	392	ILE	CA-CB	-5.28	1.47	1.54
1	A	296	ILE	CA-CB	-5.28	1.47	1.54
1	A	253	VAL	CA-CB	-5.25	1.48	1.54
1	B	212	ILE	CA-CB	-5.23	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	ALA	CA-CB	-5.15	1.45	1.53
1	B	237	MET	C-O	-5.14	1.18	1.24
1	A	84	VAL	CA-CB	-5.12	1.48	1.54
1	B	308	ILE	CA-CB	-5.09	1.47	1.54
1	B	251	PRO	N-CD	-5.09	1.40	1.47
1	A	24	ALA	CA-CB	-5.08	1.45	1.53
1	A	103	TYR	C-O	-5.07	1.20	1.25
1	B	210	ILE	C-O	-5.06	1.19	1.24
1	A	308	ILE	CA-C	-5.05	1.49	1.53
1	A	14	ILE	C-O	-5.04	1.19	1.24
1	A	174	ILE	CA-C	-5.03	1.48	1.52
1	A	392	ILE	C-O	-5.01	1.19	1.24
1	A	128	GLU	C-O	-5.01	1.18	1.24
1	B	213	ILE	CA-CB	-5.00	1.48	1.54

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	ARG	N-CA-C	10.11	123.57	111.33
1	B	239	LEU	N-CA-C	9.66	125.15	109.40
1	A	338	SER	N-CA-C	-9.59	101.47	113.55
1	B	419	ILE	N-CA-C	9.18	119.98	110.62
1	B	229	SER	N-CA-C	9.05	121.22	111.36
1	A	240	ARG	N-CA-CB	8.89	123.31	110.16
1	B	250	SER	N-CA-C	-8.79	97.63	109.84
1	A	359	LEU	N-CA-C	8.63	121.83	111.82
1	B	244	LEU	N-CA-C	-8.51	98.50	110.50
1	B	105	CYS	N-CA-C	-8.22	99.17	110.35
1	A	59	SER	N-CA-C	8.11	120.12	111.28
1	B	371	LEU	N-CA-C	7.92	119.91	111.28
1	B	73	SER	N-CA-C	7.62	119.59	111.28
1	A	240	ARG	N-CA-C	-7.47	103.22	111.36
1	B	233	VAL	N-CA-C	7.22	119.04	109.21
1	B	409	LEU	N-CA-C	-7.18	104.95	113.21
1	A	410	SER	N-CA-C	7.04	118.60	111.07
1	B	59	SER	N-CA-C	7.03	119.02	111.36
1	B	385	ASP	N-CA-C	6.88	118.88	110.41
1	A	182	LYS	N-CA-C	-6.84	100.31	110.23
1	B	196	HIS	N-CA-C	6.67	119.56	111.82
1	A	339	GLY	N-CA-C	-6.58	106.71	115.40
1	A	386	GLU	N-CA-C	-6.54	105.17	113.01
1	B	72	VAL	N-CA-C	6.51	119.90	113.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	CYS	N-CA-C	-6.43	100.52	110.10
1	B	401	SER	N-CA-C	6.41	118.35	111.36
1	A	363	LEU	N-CA-C	6.39	118.32	111.36
1	B	240	ARG	N-CA-CB	6.38	120.17	110.28
1	B	53	HIS	N-CA-C	-6.35	102.48	111.24
1	B	72	VAL	CB-CA-C	-6.31	104.70	110.63
1	B	150	ARG	N-CA-C	-6.28	99.59	109.50
1	A	193	TYR	N-CA-C	6.21	117.71	111.07
1	B	23	ILE	N-CA-C	-6.17	104.48	110.72
1	A	22	ASN	N-CA-C	6.17	118.97	111.82
1	B	352	ALA	N-CA-C	-6.16	101.10	109.54
1	A	352	ALA	N-CA-C	-6.13	101.15	109.54
1	B	193	TYR	N-CA-C	6.08	117.71	111.14
1	A	411	VAL	N-CA-C	6.07	118.31	111.88
1	B	327	GLN	N-CA-C	5.99	117.89	111.36
1	B	305	VAL	CB-CA-C	-5.97	104.32	111.97
1	B	336	ALA	CA-C-N	-5.96	113.45	119.94
1	B	336	ALA	C-N-CA	-5.96	113.45	119.94
1	A	18	PHE	N-CA-C	-5.93	103.32	110.44
1	A	253	VAL	CB-CA-C	-5.90	104.17	112.14
1	B	239	LEU	N-CA-CB	-5.85	100.65	110.83
1	B	262	THR	CB-CA-C	5.83	120.47	110.79
1	B	33	ALA	N-CA-C	5.82	117.30	111.07
1	B	19	GLY	N-CA-C	-5.81	100.49	112.34
1	B	142	VAL	N-CA-CB	-5.80	104.18	111.31
1	B	405	SER	N-CA-C	5.79	118.37	111.71
1	A	269	GLU	N-CA-C	-5.66	103.44	110.41
1	A	419	ILE	N-CA-C	5.66	116.39	110.62
1	B	232	SER	N-CA-C	-5.63	105.29	111.82
1	A	406	ASP	N-CA-C	5.60	117.06	111.07
1	B	291	ASP	N-CA-C	-5.56	105.22	111.28
1	A	233	VAL	N-CA-C	5.53	116.73	109.21
1	A	71	LEU	N-CA-C	5.49	118.02	111.71
1	B	27	ILE	N-CA-C	5.47	115.68	110.53
1	A	281	HIS	N-CA-C	-5.46	105.43	111.71
1	A	175	PRO	N-CA-C	-5.46	103.22	111.41
1	A	196	HIS	N-CA-C	5.40	118.09	111.82
1	B	166	VAL	N-CA-C	5.39	115.61	107.80
1	A	143	GLU	N-CA-C	5.37	117.22	111.36
1	B	54	GLY	N-CA-C	5.33	119.13	112.73
1	A	376	ILE	CB-CA-C	-5.31	103.28	111.08
1	A	291	ASP	N-CA-C	5.27	117.77	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	406	ASP	CA-C-O	5.27	126.14	120.55
1	A	73	SER	N-CA-C	5.27	117.02	111.28
1	B	111	ASP	N-CA-C	-5.24	105.57	111.28
1	B	411	VAL	CB-CA-C	-5.23	105.50	112.46
1	A	19	GLY	N-CA-C	-5.22	101.68	112.34
1	B	414	VAL	N-CA-C	5.18	115.95	110.72
1	B	289	ASP	N-CA-C	-5.15	102.43	110.10
1	A	308	ILE	CB-CA-C	-5.14	104.97	111.04
1	B	238	ILE	N-CA-C	5.14	114.97	107.37
1	B	222	ALA	N-CA-C	-5.10	105.72	111.28
1	A	284	ASN	N-CA-C	5.08	119.93	113.18
1	B	370	TYR	N-CA-C	5.07	119.61	113.38
1	A	72	VAL	N-CA-C	5.06	118.49	113.53
1	B	115	TRP	N-CA-C	-5.03	105.80	111.28
1	B	273	ARG	N-CA-C	5.02	116.75	111.28
1	A	36	GLN	N-CA-C	5.01	120.01	113.30

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	3284	0	3229	190	2
1	B	3256	0	3202	179	2
2	A	53	0	31	1	0
2	B	53	0	31	4	0
3	A	9	0	11	0	0
3	B	9	0	11	0	0
4	A	48	0	26	1	0
4	B	48	0	26	2	0
All	All	6760	0	6567	368	2

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 28.

All (368) 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:A:359:LEU:O	1:A:359:LEU:HD12	1.36	1.25
1:A:363:LEU:C	1:A:363:LEU:HD23	1.59	1.24
1:B:231:PRO:HA	1:B:310:ARG:NH2	1.52	1.22
1:A:363:LEU:HD23	1:A:363:LEU:O	1.35	1.20
1:B:112:TYR:O	1:B:116:VAL:HG23	1.41	1.20
1:A:334:ARG:NH1	1:A:341:LEU:HB2	1.53	1.20
1:A:39:LEU:HD13	1:A:427:LEU:CD1	1.77	1.12
1:A:61:SER:OG	1:A:106:ARG:HD3	1.53	1.09
1:A:361:ARG:HG2	1:A:362:GLN:H	1.17	1.09
1:B:361:ARG:HD3	1:B:362:GLN:H	1.22	1.03
1:B:381:ARG:NE	1:B:391:ALA:HB1	1.75	1.01
1:B:60:GLN:O	1:B:60:GLN:HG3	1.58	1.00
1:B:231:PRO:HA	1:B:310:ARG:HH22	1.27	0.97
1:B:280:TYR:O	1:B:283:THR:HG23	1.62	0.97
1:A:224:ILE:HD11	1:A:296:ILE:HG12	1.45	0.97
1:A:363:LEU:C	1:A:363:LEU:CD2	2.36	0.96
1:B:138:SER:O	1:B:139:ALA:HB3	1.61	0.96
1:A:235:ALA:H	1:A:311:HIS:HD2	1.05	0.95
1:B:381:ARG:NH2	1:B:391:ALA:HB2	1.81	0.95
1:B:165:VAL:HG13	1:B:165:VAL:O	1.66	0.94
1:B:268:ARG:HD2	1:B:272:GLU:HG2	1.52	0.92
1:A:60:GLN:O	1:A:60:GLN:HG3	1.69	0.91
1:A:239:LEU:O	1:A:316:MET:N	2.07	0.87
1:A:315:CYS:O	1:A:316:MET:HB2	1.73	0.87
1:B:246:PRO:HA	1:B:288:VAL:O	1.75	0.86
1:A:96:PHE:O	1:A:99:LEU:HB2	1.76	0.86
1:A:39:LEU:CD1	1:A:427:LEU:HD12	2.06	0.85
1:A:39:LEU:HD13	1:A:427:LEU:HD12	1.59	0.85
1:B:361:ARG:NE	1:B:361:ARG:HA	1.91	0.85
1:B:381:ARG:NE	1:B:391:ALA:CB	2.39	0.84
1:B:381:ARG:CZ	1:B:391:ALA:HB2	2.07	0.84
1:A:284:ASN:ND2	1:A:408:LEU:HD21	1.93	0.84
1:B:246:PRO:HB3	1:B:290:THR:HG22	1.58	0.84
1:A:361:ARG:HG2	1:A:362:GLN:N	1.92	0.83
1:B:45:ASP:OD1	2:B:444:FAD:H1B	1.78	0.83
1:B:381:ARG:HE	1:B:391:ALA:HB1	1.43	0.82
1:A:359:LEU:HD12	1:A:359:LEU:C	1.98	0.82
1:B:427:LEU:O	1:B:428:LYS:CG	2.27	0.82
1:A:325:THR:HG22	1:A:326:ALA:N	1.93	0.81
1:A:39:LEU:CD1	1:A:427:LEU:CD1	2.58	0.81
1:B:235:ALA:H	1:B:311:HIS:HD2	1.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:TYR:O	1:A:116:VAL:HG23	1.81	0.80
1:A:235:ALA:H	1:A:311:HIS:CD2	1.96	0.80
1:A:363:LEU:HD22	1:A:364:LEU:HG	1.63	0.79
1:B:55:ASN:ND2	1:B:195:GLU:HB2	1.98	0.79
1:B:246:PRO:CB	1:B:290:THR:HG22	2.11	0.79
1:B:256:VAL:O	1:B:256:VAL:HG22	1.83	0.79
1:B:427:LEU:C	1:B:428:LYS:HG3	2.05	0.79
1:B:361:ARG:HA	1:B:361:ARG:HE	1.47	0.79
1:B:165:VAL:O	1:B:165:VAL:CG1	2.30	0.78
1:A:166:VAL:HG12	1:A:168:PRO:HD3	1.65	0.77
1:B:138:SER:O	1:B:139:ALA:CB	2.31	0.76
1:A:39:LEU:HD13	1:A:427:LEU:HD11	1.64	0.76
1:B:61:SER:HB2	1:B:106:ARG:HH11	1.51	0.75
1:B:60:GLN:O	1:B:60:GLN:CG	2.33	0.75
1:B:12:ASP:OD1	1:B:162:ARG:NH1	2.19	0.75
1:A:248:ASP:OD1	1:A:248:ASP:C	2.29	0.75
1:B:315:CYS:O	1:B:316:MET:HB2	1.86	0.75
1:A:73:SER:O	1:A:77:PRO:HD3	1.88	0.74
1:B:381:ARG:CZ	1:B:391:ALA:CB	2.66	0.74
1:A:284:ASN:HD21	1:A:408:LEU:HD21	1.52	0.74
1:B:334:ARG:NH1	1:B:341:LEU:HB2	2.02	0.73
1:A:70:ASP:C	1:A:70:ASP:OD2	2.30	0.73
1:A:49:ASP:OD1	1:A:114:ARG:NH2	2.22	0.72
1:A:361:ARG:CG	1:A:362:GLN:H	1.96	0.72
1:A:365:GLU:HB3	1:A:366:PRO:HD3	1.71	0.72
1:B:141:GLN:OE1	1:B:389:LYS:NZ	2.22	0.72
1:A:257:PHE:HZ	1:A:283:THR:HB	1.55	0.72
1:A:369:GLU:CG	1:A:387:ARG:HH22	2.02	0.72
1:B:176:GLN:OE1	1:B:179:ARG:NH1	2.22	0.72
1:B:55:ASN:HD21	1:B:195:GLU:HB2	1.52	0.71
1:A:367:LEU:N	1:A:367:LEU:HD23	2.04	0.71
1:A:31:GLU:OE2	1:A:75:ARG:NH1	2.15	0.71
1:B:427:LEU:O	1:B:428:LYS:HG2	1.88	0.71
1:A:176:GLN:HE21	1:A:176:GLN:HA	1.55	0.70
1:B:427:LEU:C	1:B:428:LYS:CG	2.64	0.70
1:A:256:VAL:HG22	1:A:256:VAL:O	1.90	0.70
1:A:325:THR:HG22	1:A:327:GLN:H	1.54	0.70
1:A:412:LEU:N	1:A:413:PRO:CD	2.54	0.69
1:B:401:SER:OG	1:B:402:HIS:HD2	1.75	0.69
1:A:334:ARG:HH12	1:A:341:LEU:HB2	1.53	0.69
1:B:406:ASP:OD1	1:B:415:ARG:NH1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:HG23	1:A:317:THR:HB	1.75	0.68
1:B:166:VAL:HG12	1:B:168:PRO:CD	2.24	0.68
1:B:370:TYR:N	1:B:370:TYR:CD2	2.61	0.68
1:A:325:THR:CG2	1:A:326:ALA:N	2.57	0.68
1:B:41:VAL:HB	1:B:123:GLN:HE21	1.58	0.67
1:A:235:ALA:N	1:A:311:HIS:HD2	1.87	0.67
1:A:237:MET:HB3	1:A:239:LEU:HD11	1.76	0.67
1:B:361:ARG:CD	1:B:362:GLN:H	2.02	0.67
1:A:13:LEU:HD13	1:A:423:LEU:HD21	1.76	0.67
1:B:72:VAL:O	1:B:72:VAL:CG2	2.42	0.67
1:A:224:ILE:HD11	1:A:296:ILE:CG1	2.23	0.66
1:A:187:VAL:HG23	1:A:329:ILE:CD1	2.25	0.66
1:A:359:LEU:O	1:A:359:LEU:CD1	2.30	0.66
1:B:236:ASP:OD2	1:B:314:ARG:NH1	2.28	0.66
1:B:122:GLU:O	1:B:125:ARG:NH1	2.26	0.66
1:A:176:GLN:NE2	1:A:179:ARG:HD2	2.10	0.65
1:B:284:ASN:ND2	1:B:408:LEU:HD11	2.11	0.65
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.60	0.65
1:A:239:LEU:N	1:A:239:LEU:HD12	2.11	0.65
1:B:52:TRP:O	1:B:53:HIS:C	2.39	0.65
1:B:376:ILE:HD13	1:B:398:SER:OG	1.98	0.64
1:A:239:LEU:HD21	1:A:244:LEU:HD21	1.78	0.64
1:B:93:LEU:O	1:B:97:ILE:HG13	1.98	0.64
1:B:376:ILE:HG23	1:B:376:ILE:O	1.99	0.63
1:B:298:GLY:O	1:B:302:ARG:HG3	1.98	0.63
1:A:60:GLN:NE2	1:A:62:GLU:HG3	2.14	0.63
1:B:373:ASP:C	1:B:375:GLU:N	2.57	0.63
1:A:239:LEU:HB2	1:A:315:CYS:HA	1.81	0.63
1:A:137:LEU:CD2	1:A:142:VAL:HG22	2.29	0.63
1:A:317:THR:CG2	1:A:333:LEU:HB3	2.28	0.63
1:A:132:ARG:HG3	1:A:148:ILE:HD12	1.81	0.62
1:A:72:VAL:HG21	1:A:79:SER:HB3	1.81	0.62
1:A:176:GLN:NE2	1:A:179:ARG:HH11	1.98	0.62
1:B:427:LEU:O	1:B:428:LYS:HG3	1.94	0.62
1:B:136:MET:HG3	1:B:146:ARG:HG2	1.81	0.62
1:A:238:ILE:C	1:A:239:LEU:HD12	2.25	0.61
1:A:176:GLN:HA	1:A:176:GLN:NE2	2.14	0.61
1:B:373:ASP:O	1:B:375:GLU:N	2.32	0.61
1:A:39:LEU:HD11	1:A:427:LEU:HD12	1.81	0.61
1:A:335:ASP:C	1:A:335:ASP:OD1	2.42	0.61
1:B:398:SER:HB3	1:B:402:HIS:CD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:SER:OG	1:A:106:ARG:CD	2.42	0.60
1:B:380:TYR:CE2	1:B:415:ARG:HG3	2.36	0.60
1:B:401:SER:OG	1:B:402:HIS:CD2	2.54	0.60
1:A:137:LEU:HD21	1:A:142:VAL:HG22	1.82	0.60
1:A:224:ILE:CD1	1:A:296:ILE:HG12	2.28	0.60
1:A:186:ARG:NH2	1:A:325:THR:O	2.34	0.60
1:A:315:CYS:O	1:A:316:MET:CB	2.45	0.60
1:A:187:VAL:CG2	1:A:329:ILE:HD13	2.31	0.60
1:A:287:VAL:HG23	1:A:287:VAL:O	2.02	0.59
1:A:360:HIS:NE2	1:A:371:LEU:HD13	2.18	0.59
1:A:372:GLY:HA2	1:B:176:GLN:HG2	1.84	0.59
1:A:369:GLU:OE2	1:A:387:ARG:NH1	2.30	0.59
1:B:365:GLU:N	1:B:366:PRO:CD	2.66	0.58
1:B:272:GLU:OE2	1:B:275:ARG:NH2	2.35	0.58
1:A:256:VAL:HG23	1:A:261:PHE:CE2	2.37	0.58
1:B:361:ARG:HD3	1:B:362:GLN:N	2.06	0.57
1:B:166:VAL:HG12	1:B:168:PRO:HD2	1.85	0.57
1:A:177:VAL:O	1:A:177:VAL:CG2	2.50	0.57
1:A:266:TYR:O	1:A:273:ARG:NH2	2.33	0.57
1:A:376:ILE:CD1	1:A:398:SER:OG	2.53	0.57
1:A:365:GLU:HB3	1:A:366:PRO:CD	2.34	0.57
1:B:15:GLY:HA2	1:B:165:VAL:HG12	1.87	0.57
1:B:282:ASN:O	1:B:287:VAL:HG11	2.04	0.57
1:B:379:ASP:O	1:B:380:TYR:HB2	2.04	0.57
1:A:21:SER:HB2	2:A:444:FAD:O2P	2.05	0.56
1:A:365:GLU:N	1:A:366:PRO:HD2	2.20	0.56
1:A:369:GLU:HG2	1:A:387:ARG:NH2	2.20	0.56
1:B:246:PRO:HB2	1:B:290:THR:HG22	1.88	0.56
1:B:112:TYR:O	1:B:116:VAL:CG2	2.35	0.56
1:B:412:LEU:N	1:B:413:PRO:CD	2.69	0.56
1:A:369:GLU:HG2	1:A:387:ARG:HH22	1.70	0.56
1:A:189:HIS:HD2	1:A:191:SER:OG	1.89	0.56
1:B:70:ASP:OD2	1:B:70:ASP:C	2.46	0.56
1:A:395:GLN:HE21	1:A:419:ILE:HD12	1.71	0.55
1:B:331:LEU:HD12	1:B:346:TYR:CE2	2.41	0.55
1:A:341:LEU:HD23	1:A:341:LEU:C	2.31	0.55
1:B:166:VAL:CG1	1:B:168:PRO:HD3	2.37	0.55
1:A:55:ASN:O	1:A:194:LEU:HG	2.06	0.55
1:B:381:ARG:HH21	1:B:391:ALA:HB2	1.68	0.55
1:B:19:GLY:O	1:B:23:ILE:HG13	2.07	0.55
1:B:223:PHE:CD2	1:B:296:ILE:HD13	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:PHE:HA	1:A:405:SER:OG	2.08	0.55
1:A:181:LEU:O	1:A:182:LYS:C	2.49	0.54
1:B:164:LEU:HD23	1:B:392:ILE:HG23	1.89	0.54
1:A:376:ILE:HG22	1:A:376:ILE:O	2.07	0.54
1:A:366:PRO:C	1:A:367:LEU:HD23	2.31	0.54
1:B:268:ARG:HB3	1:B:272:GLU:HB3	1.88	0.54
1:A:173:ARG:O	1:A:353:THR:OG1	2.22	0.54
1:A:325:THR:HB	1:A:328:GLY:O	2.07	0.54
1:B:133:ILE:O	1:B:366:PRO:HB2	2.06	0.54
1:B:141:GLN:CD	1:B:389:LYS:NZ	2.66	0.54
1:B:278:ARG:HH11	1:B:278:ARG:HG3	1.73	0.54
1:B:166:VAL:HG12	1:B:168:PRO:HD3	1.88	0.54
1:B:365:GLU:N	1:B:366:PRO:HD2	2.23	0.54
1:A:224:ILE:HG13	1:A:292:LEU:HD11	1.90	0.53
1:A:175:PRO:HB3	4:A:446:NDP:N6A	2.23	0.53
1:A:187:VAL:HG23	1:A:329:ILE:HD13	1.90	0.53
1:B:45:ASP:OD1	1:B:46:LYS:N	2.41	0.53
1:B:256:VAL:O	1:B:256:VAL:CG2	2.55	0.53
1:B:318:THR:HG22	1:B:319:VAL:N	2.24	0.53
1:B:273:ARG:O	1:B:277:LEU:HG	2.08	0.53
1:B:341:LEU:C	1:B:341:LEU:HD23	2.33	0.52
1:B:15:GLY:CA	1:B:165:VAL:HG12	2.39	0.52
1:A:250:SER:HB2	1:A:251:PRO:HD2	1.90	0.52
1:B:249:ASP:OD1	1:B:249:ASP:N	2.37	0.52
1:A:233:VAL:O	1:A:310:ARG:NH2	2.40	0.52
1:A:239:LEU:HD21	1:A:244:LEU:CD2	2.40	0.52
1:B:287:VAL:HG23	1:B:287:VAL:O	2.08	0.52
1:A:331:LEU:HD12	1:A:346:TYR:CE2	2.45	0.52
1:B:278:ARG:HG3	1:B:278:ARG:NH1	2.24	0.52
1:B:355:TYR:CE2	2:B:444:FAD:HM83	2.45	0.52
1:B:63:LEU:HD22	1:B:104:PRO:HD2	1.92	0.51
1:B:412:LEU:HD21	1:B:415:ARG:NH2	2.26	0.51
1:A:284:ASN:OD1	1:A:284:ASN:C	2.54	0.51
1:A:334:ARG:CZ	1:A:341:LEU:HD12	2.41	0.51
1:A:321:ARG:HG2	1:A:321:ARG:NH1	2.26	0.51
1:A:193:TYR:CD1	1:A:193:TYR:C	2.89	0.51
1:A:325:THR:HG22	1:A:326:ALA:H	1.73	0.50
1:A:165:VAL:HG13	1:A:165:VAL:O	2.09	0.50
1:A:325:THR:CG2	1:A:326:ALA:H	2.21	0.50
1:A:363:LEU:O	1:A:363:LEU:CD2	2.30	0.50
1:B:355:TYR:CE2	2:B:444:FAD:C8M	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:VAL:O	1:A:177:VAL:HG23	2.12	0.50
1:B:109:PHE:O	1:B:112:TYR:HB3	2.12	0.49
1:B:376:ILE:O	1:B:376:ILE:CG2	2.59	0.49
1:A:161:THR:HG23	1:A:161:THR:O	2.12	0.49
1:A:256:VAL:O	1:A:256:VAL:CG2	2.59	0.49
1:A:334:ARG:HH11	1:A:341:LEU:HB2	1.67	0.49
1:A:132:ARG:CG	1:A:148:ILE:HD12	2.42	0.49
1:A:284:ASN:OD1	1:A:284:ASN:O	2.30	0.49
1:A:285:TYR:O	1:A:286:SER:HB2	2.13	0.49
1:A:186:ARG:NH1	1:A:325:THR:O	2.45	0.49
1:A:233:VAL:O	1:A:310:ARG:NE	2.44	0.49
1:B:61:SER:CB	1:B:106:ARG:HH11	2.23	0.49
1:B:21:SER:HA	1:B:412:LEU:HD22	1.95	0.49
1:A:239:LEU:N	1:A:239:LEU:CD1	2.75	0.48
1:B:64:GLN:NE2	1:B:217:GLN:OE1	2.46	0.48
1:B:380:TYR:CZ	1:B:415:ARG:HG3	2.48	0.48
1:A:15:GLY:HA2	1:A:165:VAL:O	2.14	0.48
1:A:176:GLN:HE22	1:A:179:ARG:HH11	1.60	0.48
1:B:383:GLN:C	1:B:384:THR:HG23	2.38	0.48
1:A:197:MET:C	1:A:199:LYS:H	2.20	0.48
1:B:227:ASN:OD1	1:B:311:HIS:HE1	1.95	0.48
1:A:138:SER:HB3	1:A:143:GLU:HG3	1.95	0.48
1:B:257:PHE:HA	1:B:405:SER:OG	2.13	0.48
1:B:72:VAL:O	1:B:72:VAL:HG22	2.05	0.48
1:B:396:GLY:HA2	1:B:406:ASP:OD1	2.14	0.48
1:B:406:ASP:OD1	1:B:406:ASP:O	2.31	0.48
1:B:94:VAL:O	1:B:98:ASN:ND2	2.46	0.48
1:A:70:ASP:OD2	1:A:72:VAL:N	2.45	0.47
1:B:231:PRO:CA	1:B:310:ARG:HH22	2.13	0.47
1:B:334:ARG:CZ	1:B:341:LEU:HD12	2.44	0.47
1:B:369:GLU:HB3	1:B:370:TYR:CE2	2.49	0.47
1:A:41:VAL:HG12	1:A:42:LEU:N	2.29	0.47
1:B:12:ASP:OD2	1:B:39:LEU:HA	2.13	0.47
1:A:101:THR:O	1:A:101:THR:HG23	2.15	0.47
1:A:365:GLU:N	1:A:366:PRO:CD	2.77	0.47
1:B:398:SER:HB3	1:B:402:HIS:HD2	1.75	0.47
1:A:107:MET:O	1:A:110:ASN:HB3	2.14	0.47
1:A:228:ASP:OD2	1:A:295:ARG:NH2	2.47	0.47
1:A:411:VAL:C	1:A:413:PRO:HD2	2.39	0.47
1:B:25:LEU:HA	1:B:416:ALA:HB1	1.97	0.47
1:A:61:SER:CB	1:A:106:ARG:HD3	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ILE:HD13	1:A:398:SER:OG	2.13	0.47
1:B:63:LEU:HG	1:B:65:ILE:HG22	1.95	0.47
1:B:72:VAL:HG21	1:B:79:SER:CB	2.43	0.47
1:A:172:PRO:HB3	1:A:189:HIS:CD2	2.50	0.47
1:A:376:ILE:HD12	1:A:398:SER:OG	2.14	0.47
1:A:412:LEU:N	1:A:413:PRO:HD3	2.30	0.47
1:B:363:LEU:C	1:B:363:LEU:HD23	2.40	0.47
1:B:408:LEU:HD23	2:B:444:FAD:H1'2	1.96	0.47
1:A:176:GLN:O	1:A:177:VAL:C	2.56	0.47
1:A:239:LEU:O	1:A:317:THR:N	2.48	0.47
1:B:284:ASN:O	1:B:284:ASN:OD1	2.32	0.47
1:B:381:ARG:HE	1:B:391:ALA:CB	2.13	0.47
1:A:70:ASP:OD2	1:A:71:LEU:N	2.48	0.46
1:A:176:GLN:HE21	1:A:176:GLN:CA	2.21	0.46
1:B:37:GLY:O	1:B:424:TYR:OH	2.17	0.46
1:B:181:LEU:HD21	1:B:324:ALA:HB2	1.96	0.46
1:B:280:TYR:O	1:B:283:THR:CG2	2.49	0.46
1:A:365:GLU:CB	1:A:366:PRO:CD	2.92	0.46
1:A:14:ILE:HG13	1:A:161:THR:HB	1.97	0.46
1:A:101:THR:OG1	1:A:102:PHE:N	2.49	0.46
1:A:55:ASN:HB2	1:A:191:SER:O	2.15	0.46
1:A:325:THR:HG22	1:A:327:GLN:N	2.28	0.46
1:B:14:ILE:HG12	1:B:42:LEU:HB2	1.97	0.46
1:A:317:THR:HG23	1:A:333:LEU:HB3	1.97	0.46
1:A:398:SER:HB3	1:A:402:HIS:HD2	1.80	0.46
1:B:303:GLN:O	1:B:307:GLY:N	2.36	0.46
1:B:318:THR:CG2	1:B:319:VAL:N	2.79	0.46
1:B:308:ILE:O	1:B:308:ILE:HG22	2.15	0.46
1:A:369:GLU:CD	1:A:387:ARG:HH22	2.24	0.46
1:B:317:THR:CG2	1:B:333:LEU:HB3	2.46	0.46
1:A:61:SER:OG	1:A:106:ARG:NH1	2.32	0.46
1:A:287:VAL:O	1:A:287:VAL:CG2	2.63	0.46
1:A:13:LEU:HD13	1:A:423:LEU:CD2	2.46	0.45
1:B:52:TRP:O	1:B:53:HIS:HB2	2.15	0.45
1:B:175:PRO:HB2	1:B:178:PHE:HD2	1.81	0.45
1:A:12:ASP:OD2	1:A:162:ARG:NH1	2.50	0.45
1:B:363:LEU:HD23	1:B:364:LEU:HG	1.98	0.45
1:A:279:GLU:O	1:A:279:GLU:HG2	2.17	0.45
1:B:254:ASN:C	1:B:256:VAL:H	2.25	0.45
1:A:295:ARG:O	1:A:299:VAL:HG23	2.17	0.45
1:B:68:LEU:HD23	1:B:68:LEU:HA	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ASP:OD1	1:B:406:ASP:C	2.55	0.45
1:B:249:ASP:O	1:B:250:SER:C	2.54	0.45
1:A:167:SER:N	1:A:168:PRO:HD3	2.32	0.45
1:A:187:VAL:HG22	1:A:349:VAL:HB	1.99	0.45
1:B:380:TYR:CE1	1:B:415:ARG:HD2	2.52	0.45
1:A:65:ILE:HG21	1:A:409:LEU:HD12	1.99	0.44
1:B:61:SER:HB2	1:B:106:ARG:NH1	2.27	0.44
1:A:151:ASN:C	1:A:151:ASN:OD1	2.58	0.44
1:A:252:PHE:O	1:A:255:GLU:HB2	2.17	0.44
1:A:233:VAL:CG1	1:A:234:GLN:N	2.78	0.44
1:B:72:VAL:O	1:B:72:VAL:HG23	2.17	0.44
1:A:317:THR:HG21	1:A:333:LEU:HB3	1.98	0.44
1:A:135:PRO:HD3	1:A:367:LEU:CD2	2.48	0.44
1:B:51:ARG:HE	1:B:51:ARG:HB2	1.56	0.44
1:B:64:GLN:NE2	1:B:217:GLN:CD	2.75	0.44
1:B:72:VAL:HG21	1:B:79:SER:HB2	1.99	0.44
1:A:60:GLN:HE22	1:A:62:GLU:HG3	1.83	0.44
1:B:223:PHE:CE2	1:B:296:ILE:HG23	2.53	0.44
1:B:224:ILE:O	1:B:225:ASP:C	2.57	0.44
1:B:396:GLY:HA2	1:B:406:ASP:CG	2.42	0.44
1:A:361:ARG:C	1:A:363:LEU:N	2.72	0.44
1:B:165:VAL:HA	1:B:393:TYR:O	2.17	0.44
1:A:55:ASN:HD22	1:A:194:LEU:HB2	1.81	0.44
1:A:187:VAL:HG23	1:A:329:ILE:HD11	1.99	0.44
1:A:338:SER:C	1:A:340:GLU:H	2.26	0.43
1:B:408:LEU:C	1:B:410:SER:H	2.27	0.43
1:B:412:LEU:HD23	1:B:412:LEU:HA	1.81	0.43
1:A:361:ARG:CG	1:A:362:GLN:N	2.61	0.43
1:A:210:ILE:HA	1:A:348:ALA:O	2.18	0.43
1:B:409:LEU:HA	1:B:412:LEU:HG	2.00	0.43
1:A:186:ARG:HH22	1:A:325:THR:H	1.66	0.43
1:A:134:GLU:HB2	1:A:146:ARG:HB2	2.01	0.43
1:B:67:PHE:CD2	1:B:102:PHE:HA	2.54	0.43
1:B:412:LEU:CD2	1:B:415:ARG:NH2	2.82	0.43
1:B:110:ASN:O	1:B:114:ARG:HG3	2.18	0.43
1:B:397:PHE:CD2	1:B:397:PHE:N	2.86	0.43
1:A:166:VAL:HG12	1:A:168:PRO:CD	2.44	0.43
1:B:124:SER:O	1:B:124:SER:OG	2.30	0.43
1:B:411:VAL:O	1:B:412:LEU:C	2.60	0.43
1:B:248:ASP:OD2	1:B:253:VAL:HG21	2.18	0.42
1:B:286:SER:N	4:B:446:NDP:O1A	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASP:OD2	1:A:46:LYS:N	2.53	0.42
1:B:375:GLU:HG3	1:B:376:ILE:N	2.34	0.42
1:A:233:VAL:HG12	1:A:234:GLN:N	2.32	0.42
1:A:249:ASP:OD1	1:A:249:ASP:N	2.53	0.42
1:A:141:GLN:NE2	1:A:389:LYS:HE3	2.35	0.42
1:A:367:LEU:O	1:A:368:ALA:C	2.59	0.42
1:A:382:LEU:HD12	1:A:382:LEU:N	2.35	0.42
1:B:286:SER:OG	4:B:446:NDP:H3B	2.19	0.42
1:A:379:ASP:O	1:A:380:TYR:HB2	2.18	0.42
1:A:405:SER:HB3	1:A:411:VAL:HG22	2.02	0.42
1:B:151:ASN:OD1	1:B:155:GLU:HB2	2.20	0.42
1:A:371:LEU:HD22	1:A:382:LEU:HD23	2.01	0.41
1:B:299:VAL:O	1:B:303:GLN:HG3	2.20	0.41
1:A:369:GLU:OE2	1:A:387:ARG:NH2	2.53	0.41
1:B:285:TYR:O	1:B:287:VAL:HG13	2.20	0.41
1:B:426:HIS:O	1:B:426:HIS:CG	2.73	0.41
1:B:42:LEU:HD23	1:B:123:GLN:O	2.20	0.41
1:B:239:LEU:HD21	1:B:244:LEU:HD23	2.02	0.41
1:B:168:PRO:HG2	1:B:397:PHE:HZ	1.84	0.41
1:A:136:MET:HE2	1:A:136:MET:HB3	1.75	0.41
1:A:189:HIS:CD2	1:A:191:SER:H	2.38	0.41
1:B:75:ARG:HH21	1:B:75:ARG:HD3	1.75	0.41
1:B:284:ASN:OD1	1:B:284:ASN:C	2.62	0.41
1:B:406:ASP:C	1:B:408:LEU:H	2.29	0.41
1:A:376:ILE:HG23	1:A:377:GLY:O	2.20	0.41
1:A:133:ILE:HG12	1:A:363:LEU:HD21	2.02	0.41
1:A:361:ARG:C	1:A:363:LEU:H	2.29	0.41
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.65	0.41
1:B:258:ALA:HA	1:B:259:PRO:HD3	1.85	0.41
1:B:283:THR:HG23	1:B:283:THR:H	1.59	0.41
1:A:321:ARG:NH1	1:A:321:ARG:CG	2.83	0.41
1:B:141:GLN:CD	1:B:389:LYS:HZ1	2.29	0.40
1:B:363:LEU:CD2	1:B:364:LEU:HG	2.51	0.40
1:A:261:PHE:O	1:A:265:ILE:HG22	2.21	0.40
1:A:134:GLU:OE1	1:A:146:ARG:NE	2.42	0.40
1:B:12:ASP:OD2	1:B:39:LEU:CD2	2.70	0.40
1:B:17:GLY:N	1:B:44:LEU:O	2.47	0.40
1:B:275:ARG:O	1:B:275:ARG:HG2	2.21	0.40
1:A:385:ASP:C	1:A:387:ARG:N	2.79	0.40
1:B:102:PHE:O	1:B:104:PRO:HD3	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ALA:O	1:B:146:ARG:NH1[10_545]	2.00	0.20
1:A:301:TYR:OH	1:B:108:GLU:OE2[4_554]	2.18	0.02

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	409/463 (88%)	401 (98%)	8 (2%)	0	100	100
1	B	402/463 (87%)	392 (98%)	10 (2%)	0	100	100
All	All	811/926 (88%)	793 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/386 (90%)	339 (97%)	10 (3%)	37	67
1	B	346/386 (90%)	335 (97%)	11 (3%)	34	64
All	All	695/772 (90%)	674 (97%)	21 (3%)	36	66

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	44	LEU
1	A	177	VAL
1	A	288	VAL
1	A	327	GLN
1	A	359	LEU
1	A	363	LEU
1	A	367	LEU
1	A	399	GLN
1	A	401	SER
1	B	10	VAL
1	B	72	VAL
1	B	97	ILE
1	B	133	ILE
1	B	160	THR
1	B	164	LEU
1	B	174	ILE
1	B	224	ILE
1	B	253	VAL
1	B	296	ILE
1	B	316	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	36	GLN
1	A	47	GLN
1	A	55	ASN
1	A	60	GLN
1	A	141	GLN
1	A	176	GLN
1	A	189	HIS
1	A	190	HIS
1	A	311	HIS
1	A	399	GLN
1	A	402	HIS
1	A	426	HIS
1	B	30	GLN
1	B	55	ASN
1	B	64	GLN
1	B	76	ASN
1	B	98	ASN

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Mol	Chain	Res	Type
1	B	119	HIS
1	B	123	GLN
1	B	311	HIS
1	B	395	GLN
1	B	399	GLN
1	B	402	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NDP	A	446	-	51,52,52	1.56	5 (9%)	71,80,80	1.58	11 (15%)
4	NDP	B	446	-	51,52,52	1.74	8 (15%)	71,80,80	1.80	16 (22%)
2	FAD	B	444	-	58,58,58	1.17	5 (8%)	85,89,89	1.68	19 (22%)
2	FAD	A	444	-	58,58,58	1.08	5 (8%)	85,89,89	1.62	16 (18%)
3	ORN	A	445	-	7,8,8	0.60	0	6,9,9	0.71	0
3	ORN	B	445	-	7,8,8	0.61	0	6,9,9	0.71	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	NDP	A	446	-	-	7/34/77/77	0/5/5/5
4	NDP	B	446	-	-	10/34/77/77	0/5/5/5
2	FAD	B	444	-	-	11/34/50/50	0/6/6/6
2	FAD	A	444	-	-	10/34/50/50	0/6/6/6
3	ORN	A	445	-	-	0/8/8/8	-
3	ORN	B	445	-	-	0/8/8/8	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	446	NDP	O7N-C7N	7.54	1.42	1.24
4	A	446	NDP	O7N-C7N	7.05	1.41	1.24
4	B	446	NDP	PN-O3	3.97	1.63	1.59
4	B	446	NDP	C2A-N3A	3.53	1.40	1.33
2	B	444	FAD	C4X-N5	3.35	1.38	1.30
4	A	446	NDP	C2A-N1A	3.24	1.39	1.33
4	A	446	NDP	C2A-N3A	3.24	1.39	1.33
2	A	444	FAD	C4X-N5	3.02	1.37	1.30
4	B	446	NDP	C2A-N1A	2.98	1.39	1.33
2	B	444	FAD	C2A-N3A	2.94	1.39	1.33
2	B	444	FAD	C2A-N1A	2.70	1.38	1.33
2	B	444	FAD	C10-N1	2.65	1.38	1.33
2	A	444	FAD	C2A-N1A	2.65	1.38	1.33
4	B	446	NDP	PA-O3	2.52	1.62	1.59
4	B	446	NDP	C8A-N7A	2.45	1.36	1.31
2	A	444	FAD	C10-N1	2.30	1.37	1.33
4	B	446	NDP	C6N-C5N	2.27	1.40	1.33
4	A	446	NDP	PN-O3	2.20	1.61	1.59
2	A	444	FAD	C2A-N3A	2.20	1.37	1.33
4	A	446	NDP	C6N-C5N	2.17	1.39	1.33
2	A	444	FAD	C8A-N7A	2.13	1.35	1.31
2	B	444	FAD	C8A-N7A	2.04	1.35	1.31
4	B	446	NDP	C4A-N3A	2.02	1.38	1.34

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	444	FAD	N3A-C2A-N1A	-6.62	118.55	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	444	FAD	N3A-C2A-N1A	-5.57	120.15	128.58
4	B	446	NDP	C5A-C4A-N3A	-5.36	119.34	126.72
4	B	446	NDP	N3A-C2A-N1A	-5.24	120.65	128.58
4	A	446	NDP	N3A-C2A-N1A	-5.17	120.75	128.58
2	B	444	FAD	C5A-C4A-N3A	-4.93	119.92	126.72
2	A	444	FAD	N9A-C8A-N7A	-4.26	107.89	113.94
4	A	446	NDP	O4D-C1D-N1N	4.26	116.21	108.08
4	A	446	NDP	C5A-C4A-N3A	-4.08	121.11	126.72
4	B	446	NDP	N9A-C8A-N7A	-4.04	108.20	113.94
4	B	446	NDP	N3A-C4A-N9A	4.03	134.02	127.17
2	B	444	FAD	C4-N3-C2	-3.79	118.91	125.64
4	B	446	NDP	C5A-N7A-C8A	3.74	109.33	103.45
4	B	446	NDP	C2A-N3A-C4A	3.68	120.81	111.83
2	A	444	FAD	C5A-C4A-N3A	-3.64	121.70	126.72
2	A	444	FAD	C2A-N3A-C4A	3.50	120.37	111.83
2	B	444	FAD	C2A-N3A-C4A	3.45	120.25	111.83
4	A	446	NDP	N9A-C8A-N7A	-3.39	109.13	113.94
2	B	444	FAD	N9A-C8A-N7A	-3.38	109.14	113.94
2	B	444	FAD	C5A-N7A-C8A	3.37	108.74	103.45
2	A	444	FAD	C5A-N7A-C8A	3.33	108.68	103.45
2	B	444	FAD	N3A-C4A-N9A	3.27	132.73	127.17
4	A	446	NDP	C5A-N7A-C8A	3.27	108.59	103.45
4	A	446	NDP	C2A-N3A-C4A	3.08	119.36	111.83
2	B	444	FAD	C4X-C10-N10	2.99	120.77	116.48
2	A	444	FAD	C4X-C10-N10	2.95	120.71	116.48
2	A	444	FAD	C5A-C6A-N6A	-2.95	115.99	123.29
2	B	444	FAD	O2A-PA-O3P	2.94	115.22	107.27
4	A	446	NDP	C1D-N1N-C2N	-2.93	116.31	121.14
4	B	446	NDP	O2A-PA-O3	2.91	115.15	107.27
4	A	446	NDP	O4B-C1B-N9A	2.87	113.60	108.09
2	A	444	FAD	C4-N3-C2	-2.76	120.74	125.64
2	B	444	FAD	C4X-C4-N3	2.73	120.19	113.25
4	A	446	NDP	N3A-C4A-N9A	2.72	131.80	127.17
4	B	446	NDP	O4B-C1B-C2B	-2.72	101.90	106.59
2	B	444	FAD	C4A-C5A-N7A	-2.69	107.51	110.58
2	B	444	FAD	C4X-C10-N1	-2.63	118.14	124.59
2	B	444	FAD	C10-C4X-N5	-2.59	119.52	124.81
4	B	446	NDP	O4D-C1D-C2D	-2.56	101.14	106.62
4	B	446	NDP	C5A-C6A-N6A	-2.50	117.09	123.29
2	A	444	FAD	N3A-C4A-N9A	2.49	131.40	127.17
4	B	446	NDP	O2A-PA-O5B	2.45	118.68	107.57
2	A	444	FAD	C4A-N9A-C8A	2.40	108.25	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	446	NDP	C5B-C4B-C3B	-2.33	106.82	115.21
4	A	446	NDP	C4A-C5A-N7A	-2.32	107.93	110.58
4	B	446	NDP	O5B-C5B-C4B	-2.28	101.22	108.99
2	A	444	FAD	C10-C4X-N5	-2.24	120.23	124.81
2	B	444	FAD	C4-C4X-C10	2.24	120.78	116.93
4	B	446	NDP	O3D-C3D-C4D	-2.23	104.67	111.08
2	A	444	FAD	C5X-C9A-N10	2.22	119.97	117.97
2	B	444	FAD	C5X-C9A-N10	2.18	119.94	117.97
2	B	444	FAD	C5B-C4B-C3B	-2.17	107.41	115.21
4	B	446	NDP	C1D-N1N-C2N	-2.16	117.58	121.14
4	A	446	NDP	C2D-C1D-N1N	-2.15	108.02	113.31
2	A	444	FAD	O4-C4-C4X	-2.11	120.97	126.53
4	B	446	NDP	C4A-C5A-N7A	-2.10	108.19	110.58
2	B	444	FAD	O4-C4-C4X	-2.10	121.00	126.53
2	B	444	FAD	C6A-C5A-C4A	2.06	119.99	117.18
2	A	444	FAD	C4-C4X-C10	2.05	120.45	116.93
2	A	444	FAD	C4A-N9A-C1B	-2.02	121.90	126.63
2	A	444	FAD	C4A-C5A-N7A	-2.02	108.28	110.58
2	B	444	FAD	C9A-C5X-N5	-2.01	120.33	122.45

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	444	FAD	N10-C1'-C2'-C3'
2	B	444	FAD	C5B-O5B-PA-O1A
2	B	444	FAD	C5B-O5B-PA-O2A
2	B	444	FAD	C5B-O5B-PA-O3P
2	B	444	FAD	N10-C1'-C2'-C3'
4	A	446	NDP	C5B-O5B-PA-O2A
4	A	446	NDP	C5B-O5B-PA-O3
4	B	446	NDP	C5B-O5B-PA-O1A
4	B	446	NDP	O4D-C1D-N1N-C2N
2	B	444	FAD	O4B-C4B-C5B-O5B
4	B	446	NDP	O4D-C4D-C5D-O5D
4	A	446	NDP	O4D-C1D-N1N-C2N
2	B	444	FAD	C3B-C4B-C5B-O5B
4	B	446	NDP	C3B-C4B-C5B-O5B
4	B	446	NDP	O4B-C4B-C5B-O5B
2	A	444	FAD	C2'-C3'-C4'-O4'
2	A	444	FAD	O3'-C3'-C4'-C5'
2	A	444	FAD	C2'-C3'-C4'-C5'

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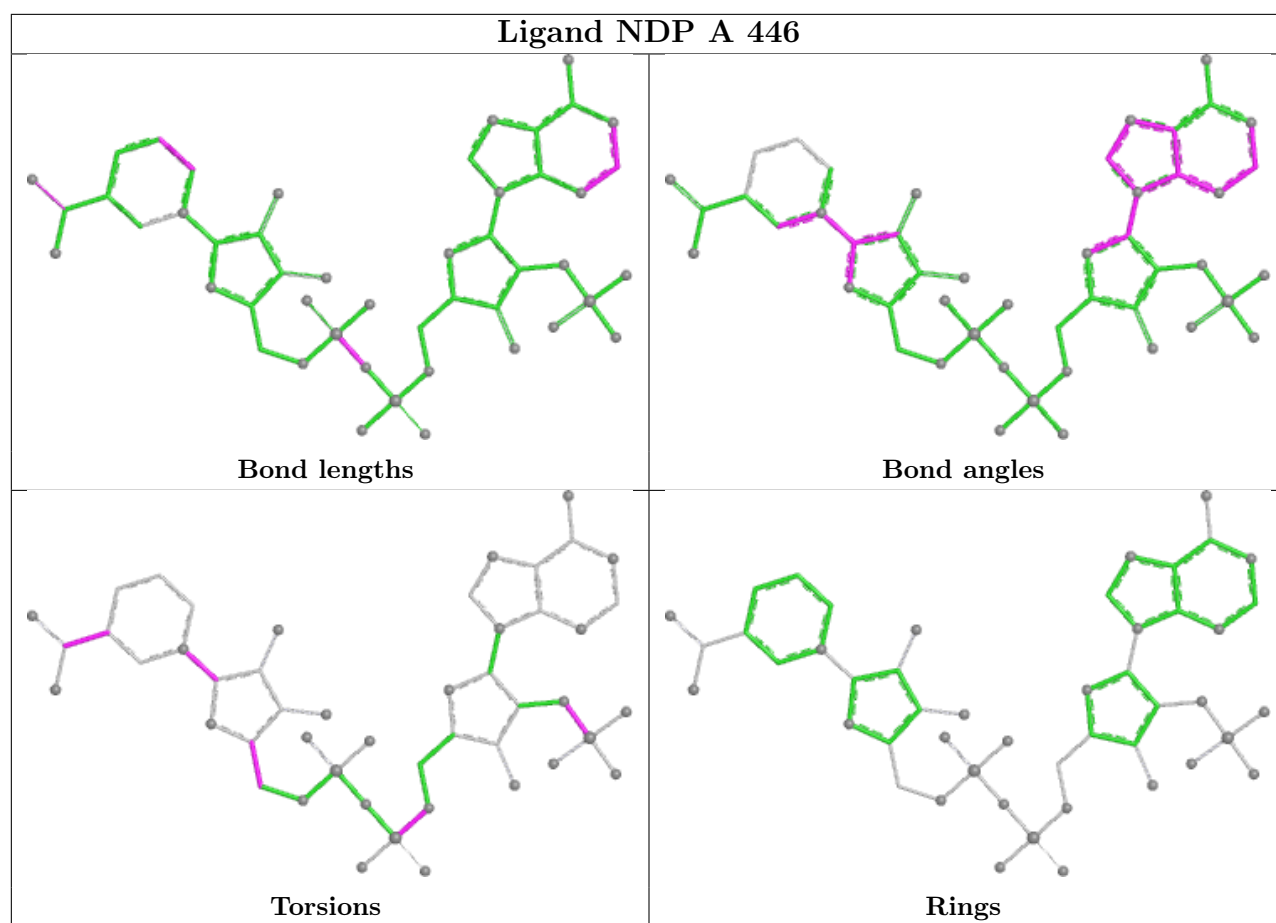
Mol	Chain	Res	Type	Atoms
2	A	444	FAD	O3'-C3'-C4'-O4'
2	A	444	FAD	O4B-C4B-C5B-O5B
2	B	444	FAD	C2'-C3'-C4'-C5'
2	A	444	FAD	C3B-C4B-C5B-O5B
2	B	444	FAD	O3'-C3'-C4'-C5'
4	B	446	NDP	C3D-C4D-C5D-O5D
2	A	444	FAD	C2B-C1B-N9A-C8A
2	A	444	FAD	N10-C1'-C2'-O2'
4	A	446	NDP	O4D-C4D-C5D-O5D
4	A	446	NDP	C5B-O5B-PA-O1A
4	B	446	NDP	C5D-O5D-PN-O1N
4	B	446	NDP	C2B-O2B-P2B-O3X
4	A	446	NDP	C2N-C3N-C7N-N7N
2	B	444	FAD	O3'-C3'-C4'-O4'
2	A	444	FAD	O4B-C1B-N9A-C8A
2	B	444	FAD	C2'-C3'-C4'-O4'
4	B	446	NDP	PA-O3-PN-O1N
4	A	446	NDP	C2B-O2B-P2B-O3X
2	B	444	FAD	N10-C1'-C2'-O2'
4	B	446	NDP	PA-O3-PN-O2N

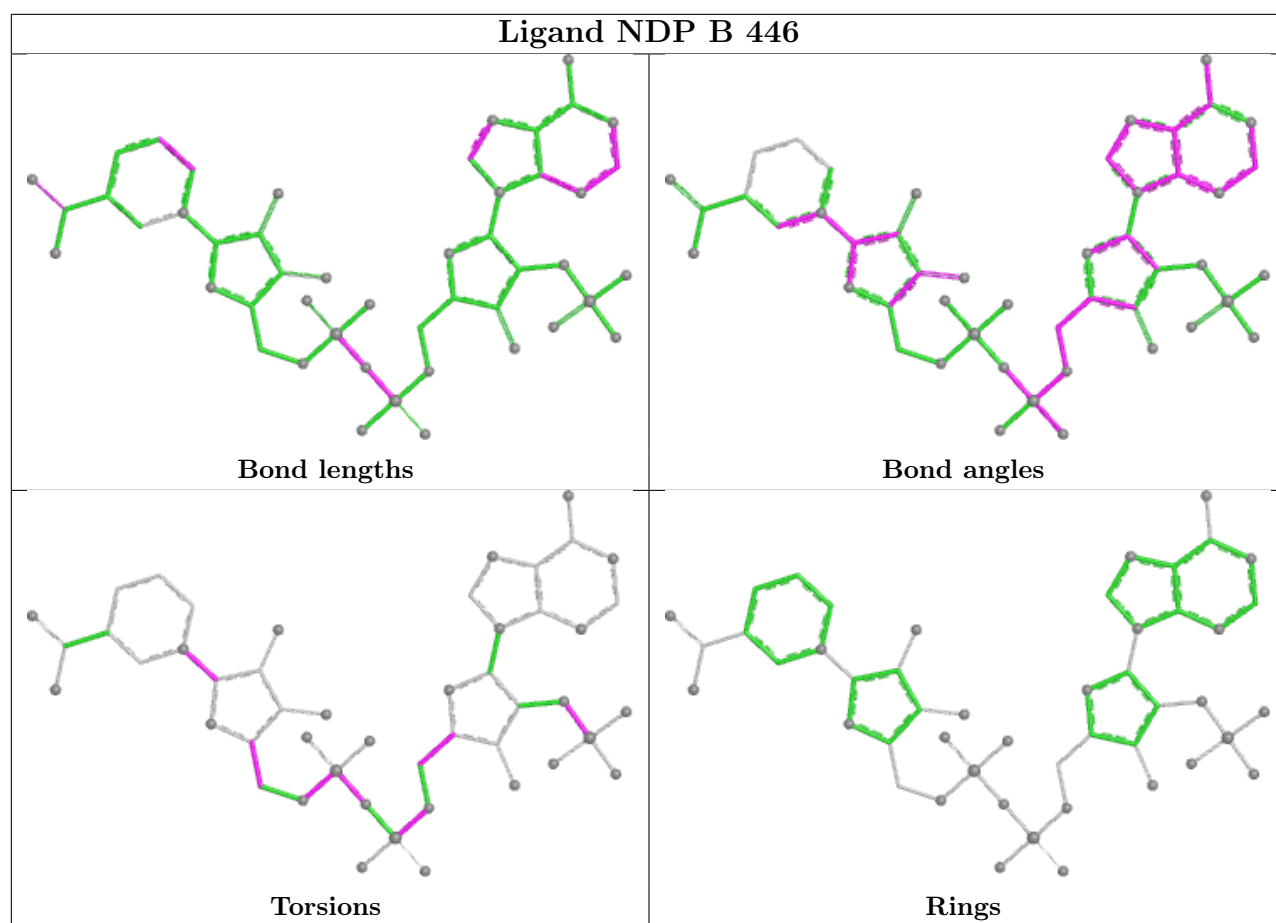
There are no ring outliers.

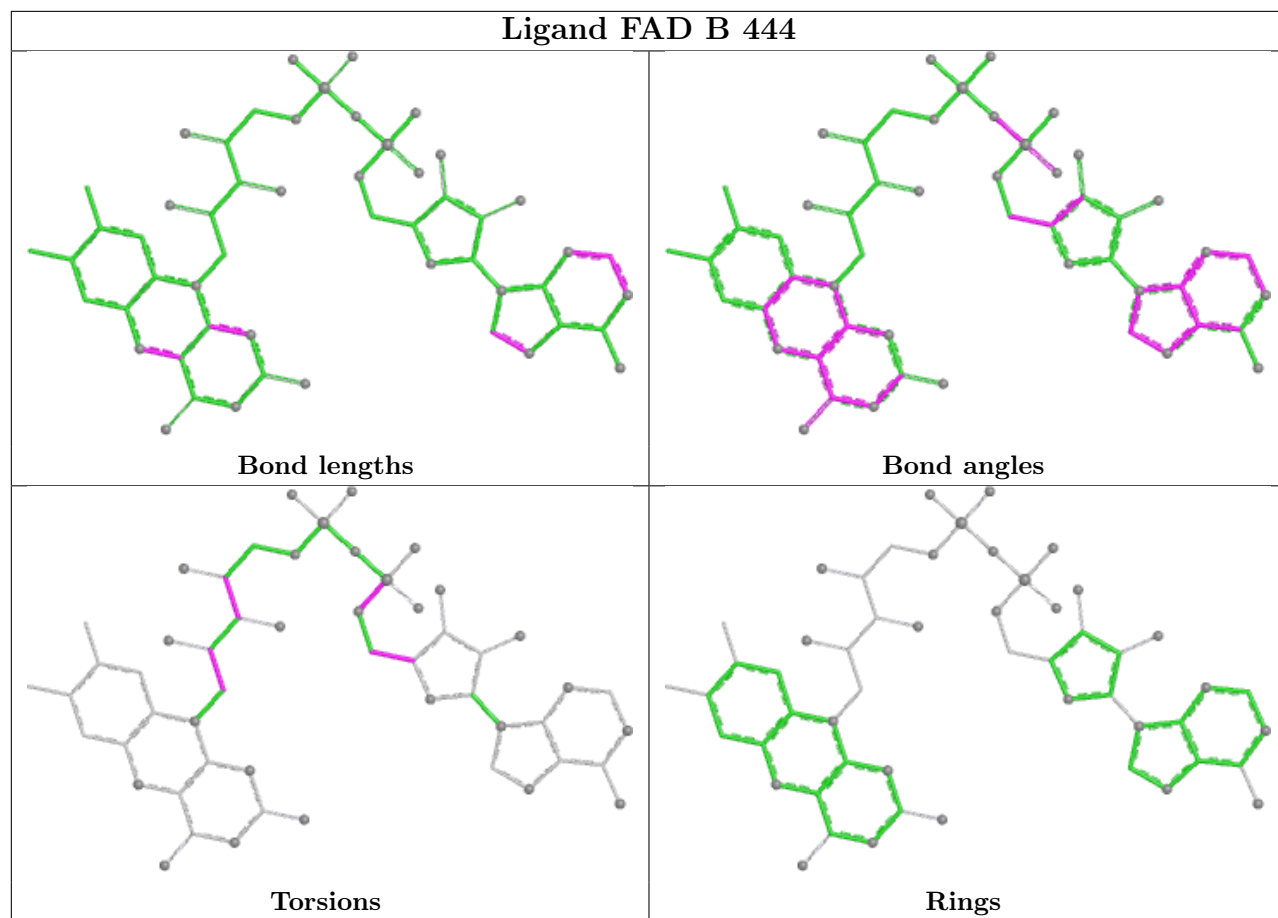
4 monomers are involved in 8 short contacts:

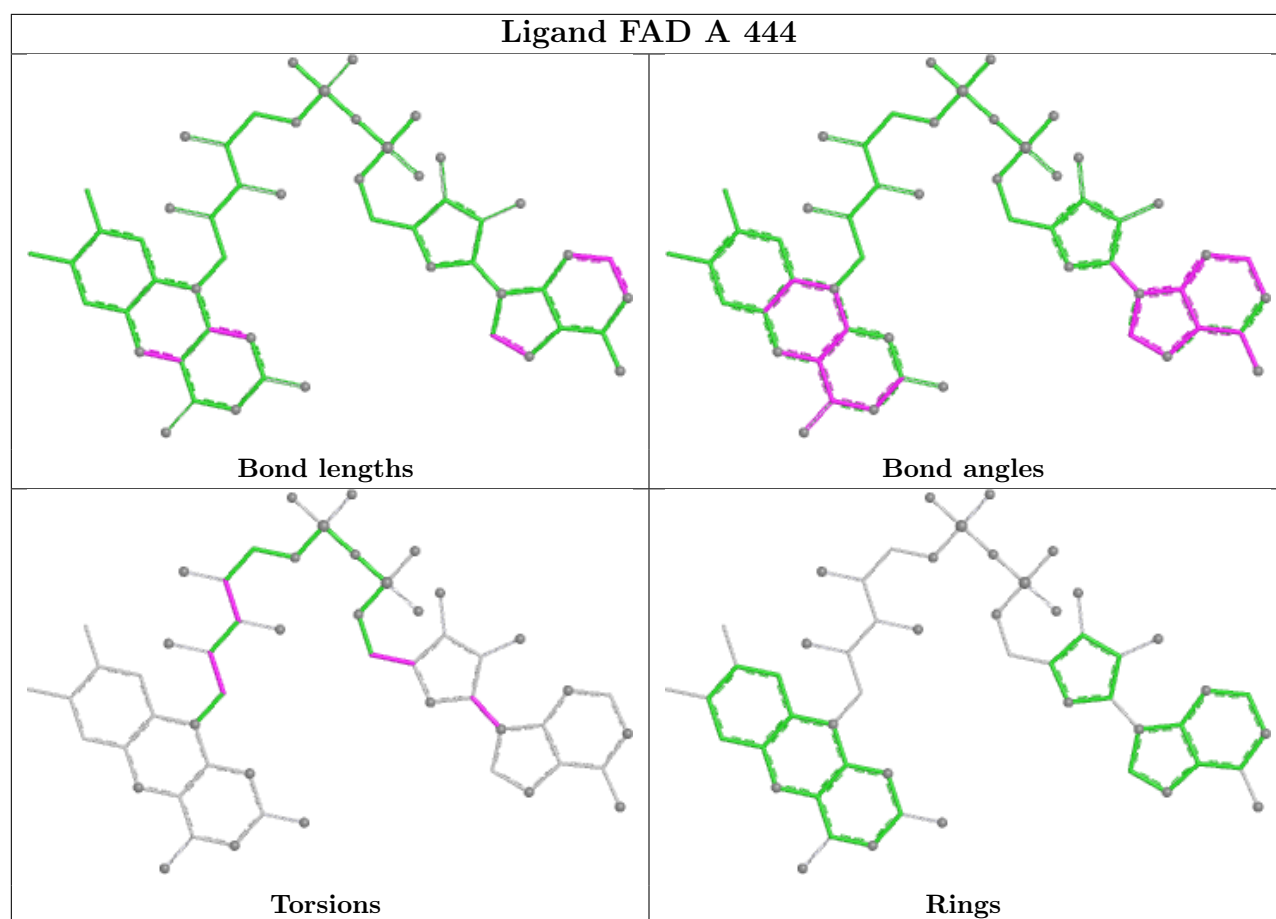
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	446	NDP	1	0
4	B	446	NDP	2	0
2	B	444	FAD	4	0
2	A	444	FAD	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	413/463 (89%)	0.09	4 (0%) 79 58	40, 58, 82, 102	0
1	B	410/463 (88%)	0.14	10 (2%) 59 36	43, 58, 83, 96	0
All	All	823/926 (88%)	0.12	14 (1%) 69 45	40, 58, 83, 102	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	406	ASP	4.0
1	B	9	VAL	3.8
1	B	137	LEU	3.3
1	B	60	GLN	2.5
1	A	373	ASP	2.4
1	B	407	THR	2.3
1	B	428	LYS	2.3
1	A	155	GLU	2.2
1	B	386	GLU	2.1
1	A	199	LYS	2.1
1	B	141	GLN	2.1
1	B	207	PRO	2.1
1	A	428	LYS	2.1
1	B	155	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](#)

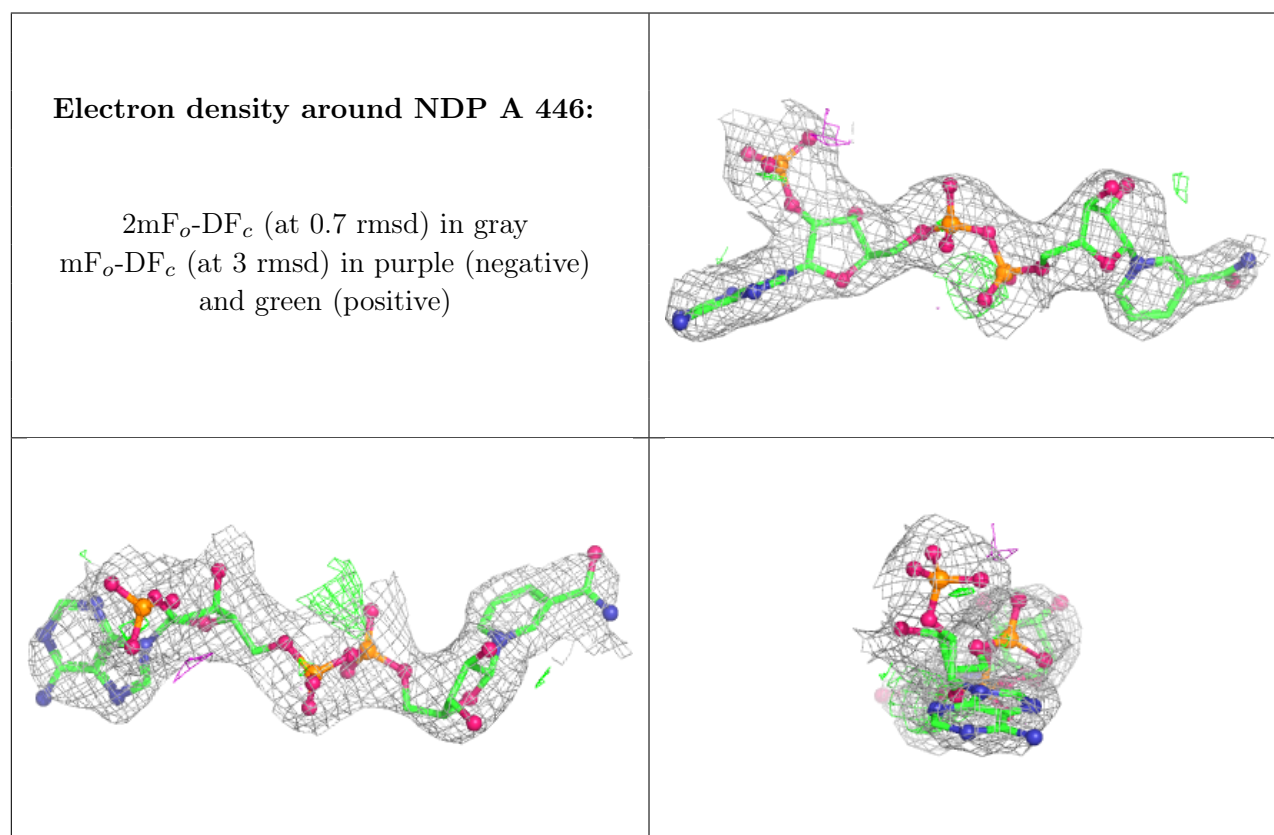
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

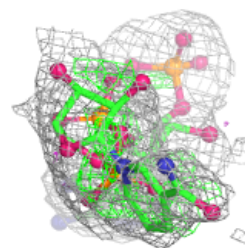
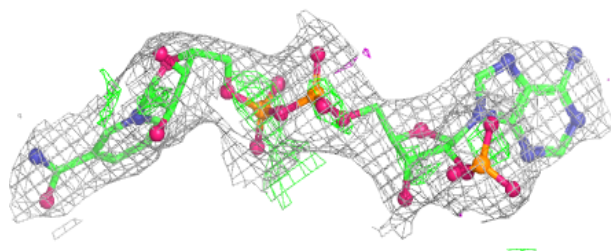
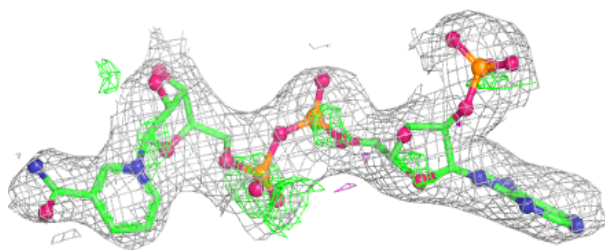
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ORN	B	445	9/9	0.83	0.23	22,23,27,28	0
3	ORN	A	445	9/9	0.84	0.24	22,23,27,28	0
4	NDP	A	446	48/48	0.92	0.14	79,84,90,91	0
4	NDP	B	446	48/48	0.92	0.16	73,78,80,80	0
2	FAD	A	444	53/53	0.95	0.16	68,77,81,82	0
2	FAD	B	444	53/53	0.95	0.16	71,77,80,83	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.

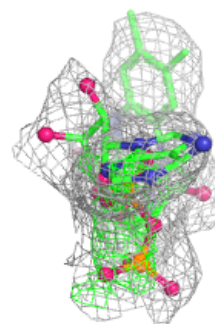
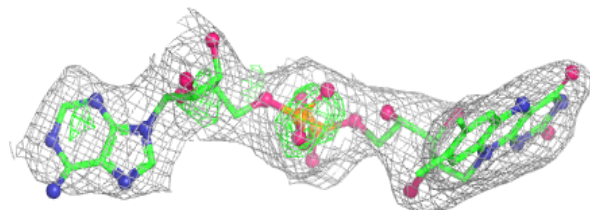
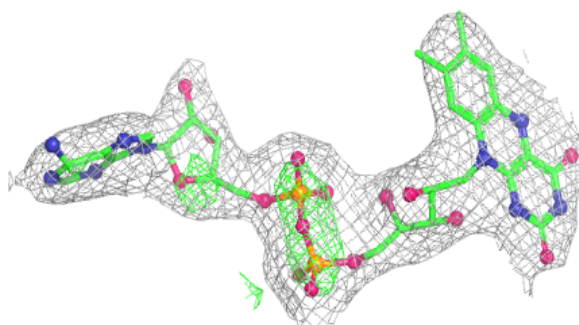


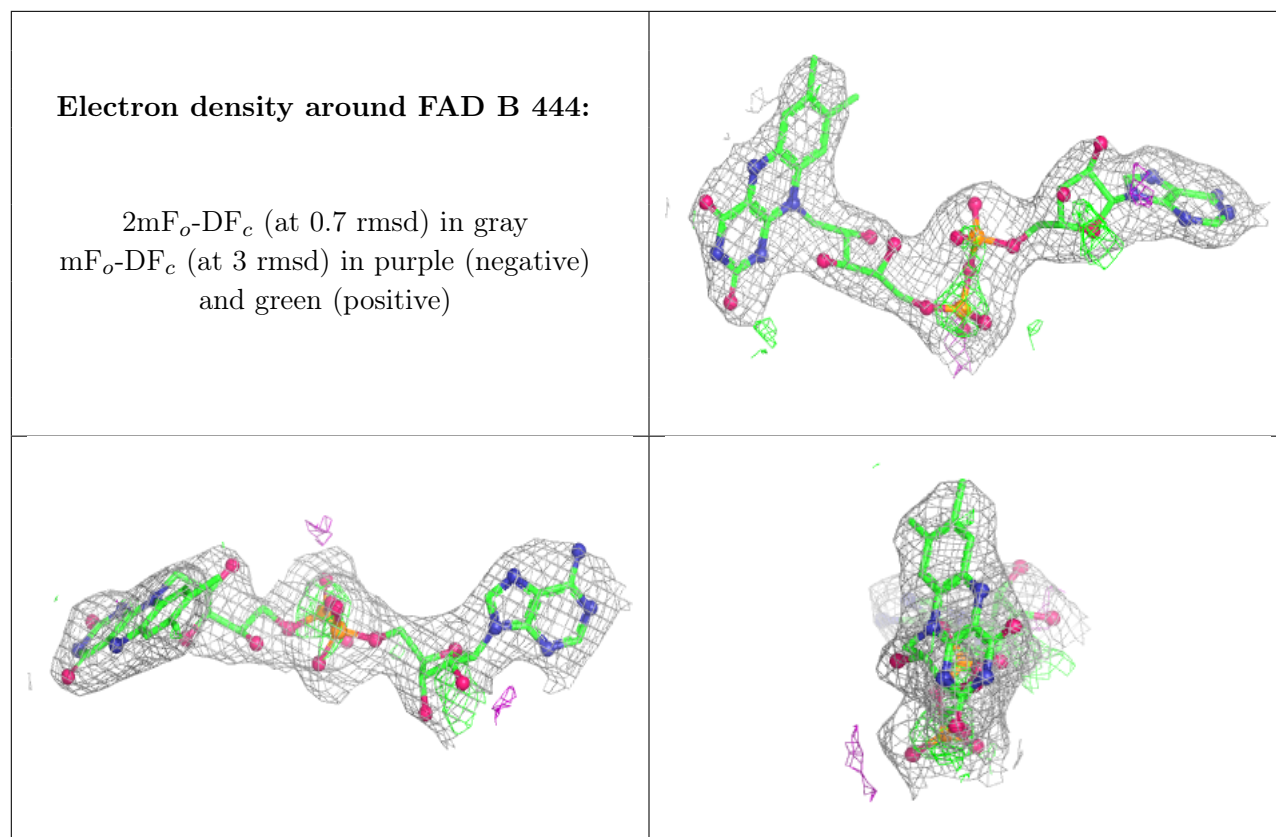
Electron density around NDP B 446:

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

**Electron density around FAD A 444:**

$2mF_o-DF_c$ (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.