



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:12 PM EDT

PDB ID : 2YVJ / pdb_00002yvj
Title : Crystal structure of the ferredoxin-ferredoxin reductase (BPHA3-BPHA4)complex
Authors : Senda, T.; Senda, M.
Deposited on : 2007-04-12
Resolution : 1.90 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

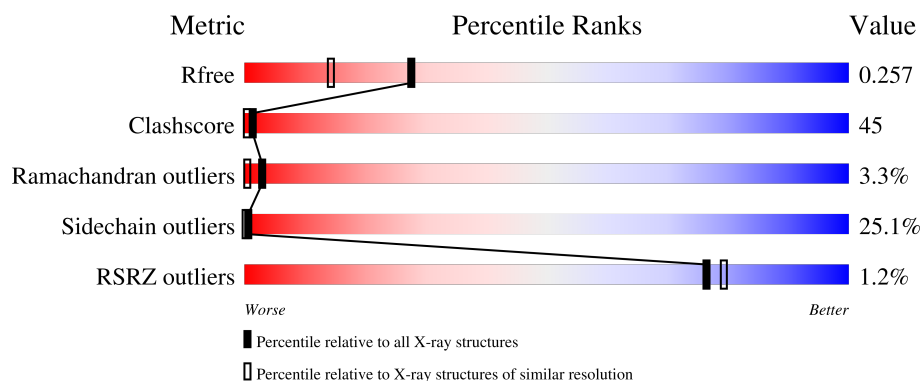
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

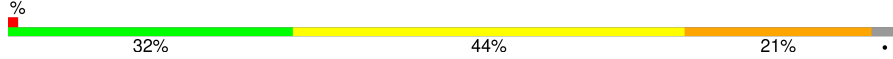
The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	408	
1	P	408	
2	B	109	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FES	B	500	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7045 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.

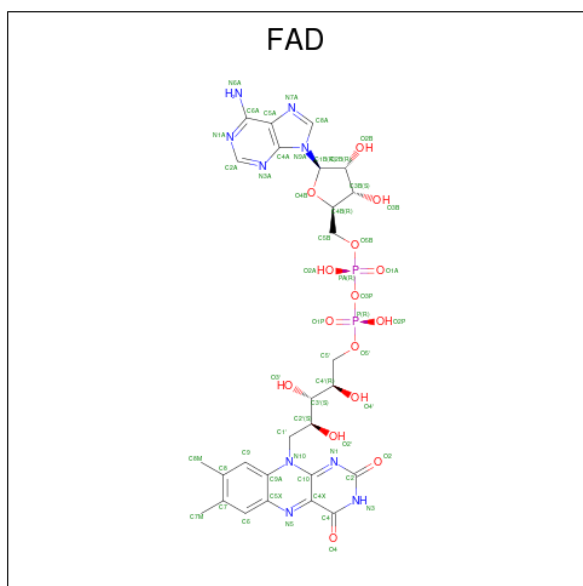
- Molecule 1 is a protein called Ferredoxin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			2992	1876	548	560	8			
1	P	401	Total	C	N	O	S	0	0	0
			2991	1876	548	559	8			

- Molecule 2 is a protein called Biphenyl dioxygenase ferredoxin subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	106	Total	C	N	O	S	0	0	0
			804	506	136	156	6			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



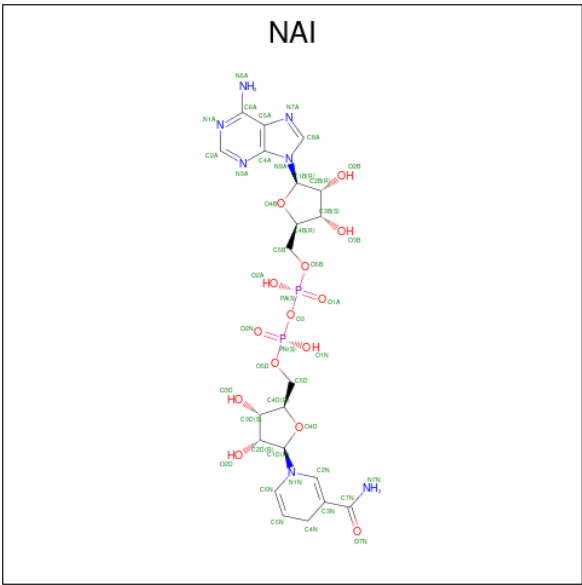
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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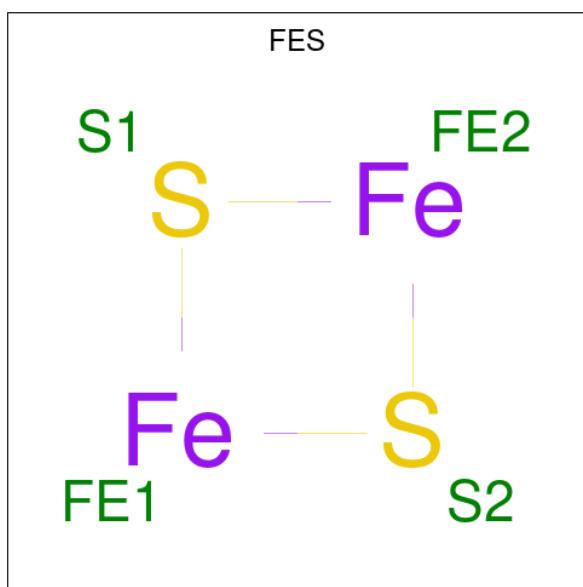
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	P	1	53	27	9	15	2	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	35	15	5	13	2	0	0
4	P	1	35	15	5	13	2	0	0

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	Fe	S	0	0
			4	2	2		

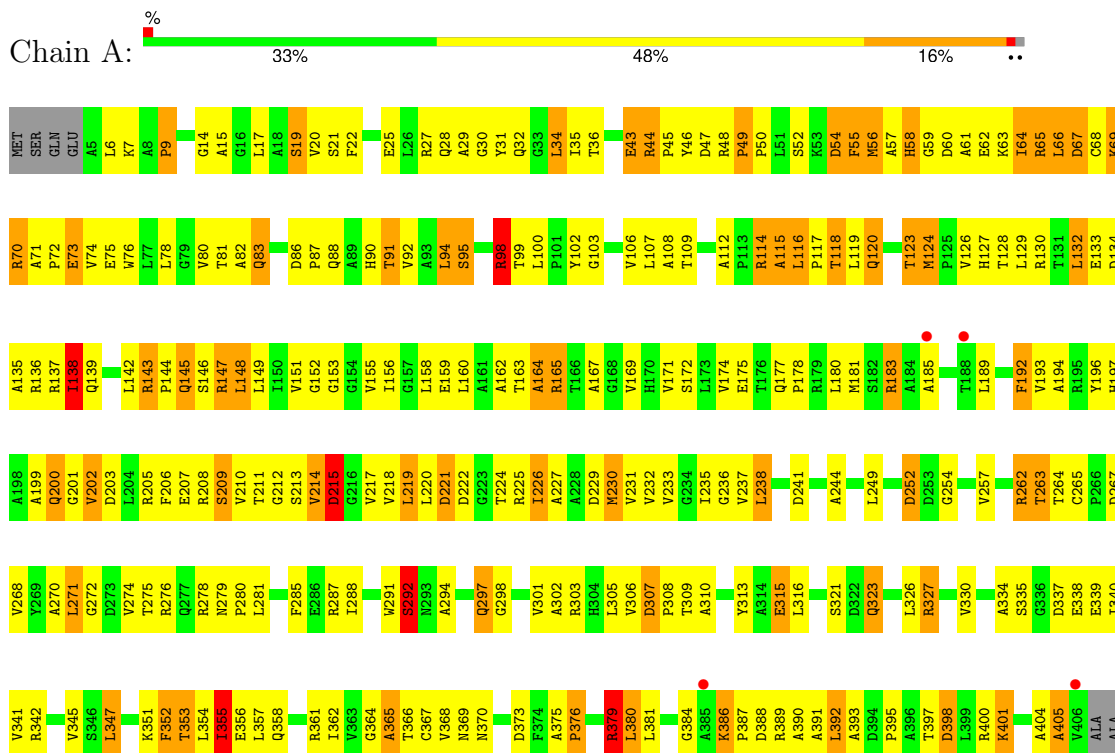
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total	O	0	0
			32	32		
6	B	4	Total	O	0	0
			4	4		
6	P	42	Total	O	0	0
			42	42		

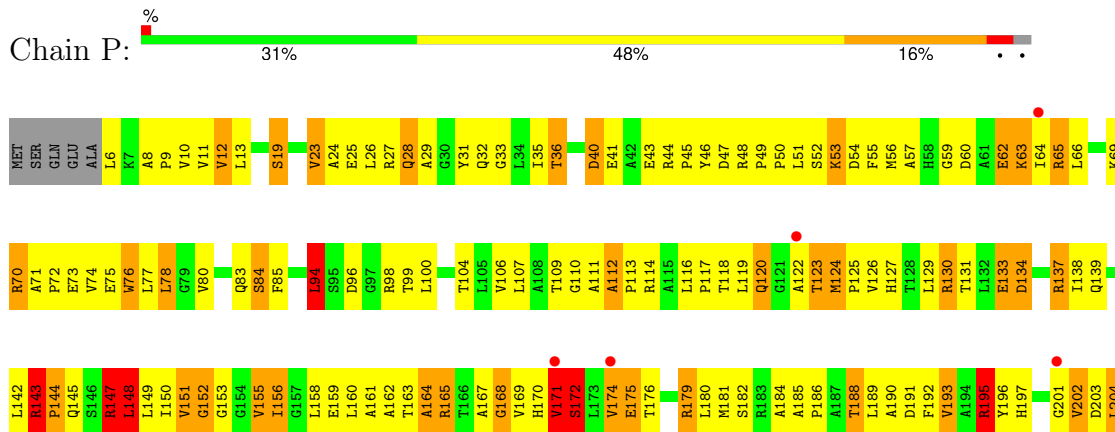
3 Residue-property plots

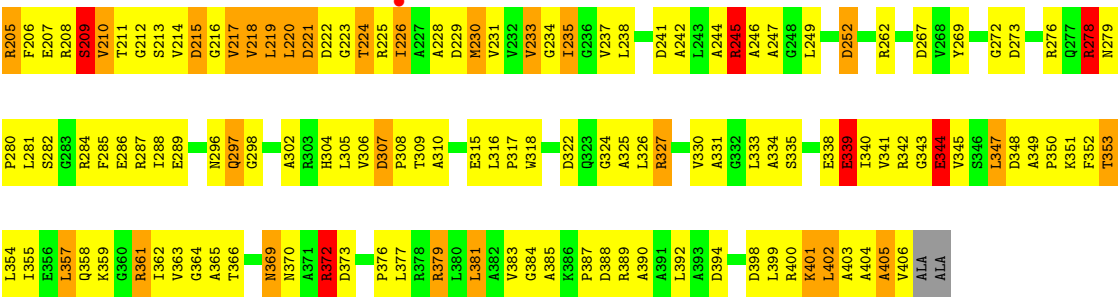
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

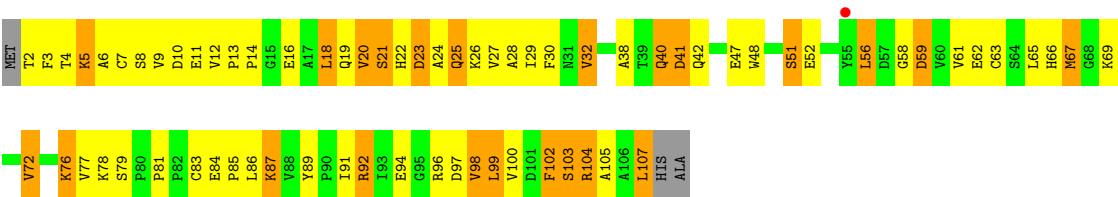


• Molecule 1: Ferredoxin reductase





● Molecule 2: Biphenyl dioxygenase ferredoxin subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.60Å 173.72Å 60.98Å 90.00° 115.81° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 10.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.5 (10.00-1.90) 95.1 (10.00-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 1.90Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.183 , 0.262 0.177 , 0.257	Depositor DCC
R_{free} test set	4123 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.427 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7045	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: FES, NAI, FAD

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	0.51	0/3044	1.69	61/4150 (1.5%)
1	P	0.51	0/3043	1.74	69/4147 (1.7%)
2	B	0.42	0/822	1.58	10/1115 (0.9%)
All	All	0.50	0/6909	1.70	140/9412 (1.5%)

There are no bond length outliers.

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	209	SER	CA-C-N	15.96	150.43	121.70
1	P	209	SER	C-N-CA	15.96	150.43	121.70
1	A	28	GLN	CA-C-N	12.80	139.88	120.17
1	A	28	GLN	C-N-CA	12.80	139.88	120.17
2	B	98	VAL	CA-C-N	9.91	134.82	120.95
2	B	98	VAL	C-N-CA	9.91	134.82	120.95
1	A	298	GLY	CA-C-N	9.68	132.76	120.56
1	A	298	GLY	C-N-CA	9.68	132.76	120.56
1	P	302	ALA	CA-C-N	9.63	133.19	120.28
1	P	302	ALA	C-N-CA	9.63	133.19	120.28
1	P	195	ARG	CD-NE-CZ	9.23	137.32	124.40
1	A	352	PHE	O-C-N	8.58	132.17	122.99
1	P	134	ASP	CA-CB-CG	8.46	121.06	112.60
1	A	390	ALA	CA-C-O	7.80	128.97	119.38
1	P	12	VAL	CA-C-N	-7.76	112.45	122.77
1	P	12	VAL	C-N-CA	-7.76	112.45	122.77
1	P	278	ARG	CD-NE-CZ	7.76	135.26	124.40
1	P	85	PHE	CA-CB-CG	7.63	121.43	113.80
1	P	267	ASP	CA-CB-CG	-7.56	105.04	112.60
1	P	372	ARG	CD-NE-CZ	7.55	134.98	124.40
1	P	344	GLU	CA-C-O	7.37	128.42	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	11	VAL	CA-C-N	-7.28	114.16	123.19
1	P	11	VAL	C-N-CA	-7.28	114.16	123.19
1	P	94	LEU	CA-C-N	7.26	132.22	120.60
1	P	94	LEU	C-N-CA	7.26	132.22	120.60
1	A	55	PHE	CA-CB-CG	-7.13	106.67	113.80
1	P	327	ARG	CA-C-N	7.13	131.28	122.37
1	P	327	ARG	C-N-CA	7.13	131.28	122.37
1	P	40	ASP	CA-C-N	-7.04	110.03	122.07
1	P	40	ASP	C-N-CA	-7.04	110.03	122.07
1	P	262	ARG	NE-CZ-NH2	6.97	125.47	119.20
1	P	330	VAL	CA-C-N	6.95	132.78	123.05
1	P	330	VAL	C-N-CA	6.95	132.78	123.05
1	A	379	ARG	CD-NE-CZ	6.84	133.98	124.40
1	P	364	GLY	CA-C-N	6.71	132.87	121.87
1	P	364	GLY	C-N-CA	6.71	132.87	121.87
1	P	364	GLY	O-C-N	6.69	131.40	122.70
1	A	352	PHE	CA-C-N	6.67	133.84	122.37
1	A	352	PHE	C-N-CA	6.67	133.84	122.37
1	P	76	TRP	CA-C-N	-6.63	113.60	122.42
1	P	76	TRP	C-N-CA	-6.63	113.60	122.42
1	A	307	ASP	O-C-N	6.61	125.24	121.27
1	A	334	ALA	CA-C-N	6.54	132.22	122.99
1	A	334	ALA	C-N-CA	6.54	132.22	122.99
1	P	195	ARG	NE-CZ-NH2	6.54	125.09	119.20
1	A	98	ARG	CA-C-N	6.37	131.24	122.77
1	A	98	ARG	C-N-CA	6.37	131.24	122.77
1	A	354	LEU	CA-C-O	-6.36	113.97	120.71
1	P	383	VAL	CA-C-N	-6.21	112.07	121.51
1	P	383	VAL	C-N-CA	-6.21	112.07	121.51
1	P	133	GLU	CA-C-N	6.19	133.36	121.54
1	P	133	GLU	C-N-CA	6.19	133.36	121.54
1	A	183	ARG	CA-C-N	-6.17	112.70	121.83
1	A	183	ARG	C-N-CA	-6.17	112.70	121.83
2	B	51	SER	CA-C-N	-6.16	114.84	122.84
2	B	51	SER	C-N-CA	-6.16	114.84	122.84
1	A	9	PRO	CA-C-N	-6.14	115.19	122.93
1	A	9	PRO	C-N-CA	-6.14	115.19	122.93
1	A	297	GLN	O-C-N	6.13	130.54	122.33
1	P	343	GLY	CA-C-N	-6.09	114.60	123.00
1	P	343	GLY	C-N-CA	-6.09	114.60	123.00
1	P	133	GLU	O-C-N	6.07	129.74	122.27
1	P	76	TRP	CA-C-O	6.06	127.45	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	ALA	CA-C-O	6.05	126.95	120.24
1	A	353	THR	CA-C-N	6.04	131.69	122.93
1	A	353	THR	C-N-CA	6.04	131.69	122.93
1	A	285	PHE	CA-CB-CG	-6.02	107.78	113.80
1	A	309	THR	CA-C-N	6.01	130.65	121.03
1	A	309	THR	C-N-CA	6.01	130.65	121.03
1	P	339	GLU	CA-C-N	-6.00	115.75	123.19
1	P	339	GLU	C-N-CA	-6.00	115.75	123.19
1	A	95	SER	CA-C-N	-5.97	113.10	122.65
1	A	95	SER	C-N-CA	-5.97	113.10	122.65
1	P	307	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	397	THR	CA-C-N	-5.92	114.55	122.72
1	A	397	THR	C-N-CA	-5.92	114.55	122.72
2	B	102	PHE	CA-CB-CG	-5.90	107.90	113.80
1	P	298	GLY	CA-C-N	5.87	128.50	120.46
1	P	298	GLY	C-N-CA	5.87	128.50	120.46
1	P	245	ARG	CD-NE-CZ	5.84	132.57	124.40
1	A	91	THR	CA-C-N	5.83	131.25	122.98
1	A	91	THR	C-N-CA	5.83	131.25	122.98
1	A	138	ILE	CB-CA-C	-5.81	104.55	111.81
1	P	201	GLY	CA-C-N	5.78	132.37	121.97
1	P	201	GLY	C-N-CA	5.78	132.37	121.97
1	P	267	ASP	CA-C-N	-5.72	115.65	123.14
1	P	267	ASP	C-N-CA	-5.72	115.65	123.14
1	P	297	GLN	O-C-N	5.67	128.13	122.12
2	B	59	ASP	CA-C-N	5.58	130.37	123.12
2	B	59	ASP	C-N-CA	5.58	130.37	123.12
1	P	13	LEU	O-C-N	5.57	129.57	123.22
1	P	252	ASP	CA-C-N	5.53	130.21	122.36
1	P	252	ASP	C-N-CA	5.53	130.21	122.36
1	A	252	ASP	CA-CB-CG	5.51	118.11	112.60
1	P	168	GLY	CA-C-N	5.50	130.41	123.10
1	P	168	GLY	C-N-CA	5.50	130.41	123.10
1	P	285	PHE	CA-CB-CG	-5.50	108.31	113.80
1	A	355	ILE	CA-C-O	5.49	126.10	120.39
1	A	390	ALA	CA-C-N	-5.46	111.24	120.58
1	A	390	ALA	C-N-CA	-5.46	111.24	120.58
1	A	298	GLY	O-C-N	5.45	129.79	122.70
1	P	379	ARG	O-C-N	-5.45	116.35	122.12
1	A	268	VAL	O-C-N	5.44	129.08	123.20
1	P	155	VAL	CA-C-N	-5.38	112.48	120.82
1	P	155	VAL	C-N-CA	-5.38	112.48	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	VAL	N-CA-C	5.34	116.17	108.48
1	P	112	ALA	CA-C-N	5.34	126.51	119.84
1	P	112	ALA	C-N-CA	5.34	126.51	119.84
2	B	67	MET	CA-C-N	5.31	129.23	121.05
2	B	67	MET	C-N-CA	5.31	129.23	121.05
1	A	367	CYS	CA-C-N	-5.30	115.89	123.10
1	A	367	CYS	C-N-CA	-5.30	115.89	123.10
1	A	80	VAL	CA-C-N	5.28	129.90	122.09
1	A	80	VAL	C-N-CA	5.28	129.90	122.09
1	P	209	SER	CA-C-O	-5.26	115.89	121.94
1	A	388	ASP	CA-C-N	5.23	128.66	120.82
1	A	388	ASP	C-N-CA	5.23	128.66	120.82
2	B	10	ASP	CA-CB-CG	5.22	117.82	112.60
1	P	143	ARG	CA-C-N	5.21	126.36	119.84
1	P	143	ARG	C-N-CA	5.21	126.36	119.84
1	A	355	ILE	CA-C-N	-5.20	115.83	123.00
1	A	355	ILE	C-N-CA	-5.20	115.83	123.00
1	P	99	THR	CA-C-N	-5.20	116.14	122.64
1	P	99	THR	C-N-CA	-5.20	116.14	122.64
1	P	109	THR	CA-C-N	5.17	127.79	119.98
1	P	109	THR	C-N-CA	5.17	127.79	119.98
1	P	143	ARG	O-C-N	5.15	125.79	121.31
1	A	292	SER	CA-C-N	5.13	127.57	120.29
1	A	292	SER	C-N-CA	5.13	127.57	120.29
1	A	268	VAL	CA-C-N	5.10	132.17	123.05
1	A	268	VAL	C-N-CA	5.10	132.17	123.05
1	A	376	PRO	CA-C-N	-5.06	113.10	120.29
1	A	376	PRO	C-N-CA	-5.06	113.10	120.29
1	A	297	GLN	N-CA-C	-5.06	105.86	112.23
1	A	133	GLU	N-CA-C	-5.04	107.21	113.55
1	A	164	ALA	CA-C-N	5.02	127.46	120.63
1	A	164	ALA	C-N-CA	5.02	127.46	120.63
1	P	384	GLY	O-C-N	-5.02	116.41	122.38
1	A	192	PHE	CA-C-N	5.00	127.58	120.53
1	A	192	PHE	C-N-CA	5.00	127.58	120.53

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	2992	0	3024	251	0
1	P	2991	0	3029	309	0
2	B	804	0	775	73	0
3	A	53	0	31	1	0
3	P	53	0	31	0	0
4	A	35	0	19	8	0
4	P	35	0	19	6	0
5	B	4	0	0	2	0
6	A	32	0	0	3	0
6	B	4	0	0	2	0
6	P	42	0	0	1	0
All	All	7045	0	6928	629	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 45.

All (629) 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:P:206:PHE:O	1:P:208:ARG:HG2	1.57	1.04
1:P:36:THR:HG23	1:P:75:GLU:HB2	1.38	1.00
1:A:126:VAL:HG22	1:A:231:VAL:HB	1.42	0.98
1:A:165:ARG:HH21	1:A:201:GLY:HA3	1.29	0.97
1:A:56:MET:HE2	1:A:56:MET:HA	1.47	0.95
2:B:63:CYS:HG	5:B:500:FES:FE1	0.64	0.94
1:A:249:LEU:HD23	1:A:263:THR:HG21	1.47	0.92
1:A:20:VAL:HG11	1:A:66:LEU:HD22	1.52	0.92
1:P:370:ASN:HD22	1:P:372:ARG:HE	1.18	0.90
1:A:218:VAL:HB	1:A:226:ILE:HB	1.55	0.87
1:P:189:LEU:HD13	1:P:366:THR:HG21	1.57	0.86
1:P:147:ARG:HA	1:P:170:HIS:HB3	1.58	0.85
1:P:220:LEU:HG	1:P:226:ILE:HD11	1.58	0.85
1:P:158:LEU:HD11	1:P:180:LEU:HD13	1.59	0.84
1:P:143:ARG:HD3	1:P:144:PRO:HD2	1.58	0.84
1:P:119:LEU:HG	1:P:219:LEU:HD21	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:138:ILE:HG23	1:P:230:MET:HE1	1.60	0.83
2:B:13:PRO:HG2	2:B:16:GLU:HG3	1.60	0.82
1:A:171:VAL:HB	1:A:202:VAL:HG23	1.61	0.82
1:A:56:MET:CE	1:A:139:GLN:HB2	2.09	0.81
1:A:276:ARG:HG2	1:A:287:ARG:HG3	1.61	0.81
1:A:129:LEU:HD22	1:A:160:LEU:HD22	1.61	0.81
1:P:151:VAL:HG12	1:P:234:GLY:H	1.45	0.81
1:A:56:MET:HE2	1:A:139:GLN:HB2	1.62	0.80
1:P:118:THR:HG22	1:P:219:LEU:HD22	1.61	0.79
1:P:370:ASN:HA	1:P:372:ARG:HH21	1.47	0.79
1:P:195:ARG:HG2	1:P:195:ARG:HH21	1.48	0.79
1:P:213:SER:HA	1:P:217:VAL:O	1.83	0.79
1:P:398:ASP:HB3	1:P:401:LYS:HB2	1.63	0.79
1:P:184:ALA:O	1:P:334:ALA:HB2	1.83	0.78
1:A:34:LEU:HD12	1:A:34:LEU:H	1.49	0.78
1:P:180:LEU:HD12	1:P:193:VAL:HG12	1.64	0.78
1:P:220:LEU:HD13	1:P:222:ASP:OD1	1.85	0.77
1:P:124:MET:HE1	1:P:218:VAL:HG23	1.67	0.77
1:A:116:LEU:HG	1:A:119:LEU:HD23	1.67	0.77
1:A:275:THR:O	1:A:287:ARG:HG2	1.84	0.76
1:A:355:ILE:HD13	1:A:392:LEU:HD22	1.64	0.76
1:P:125:PRO:HD2	1:P:229:ASP:O	1.86	0.76
1:A:337:ASP:OD1	1:A:358:GLN:HA	1.86	0.75
1:A:143:ARG:HG3	1:A:146:SER:HB3	1.67	0.75
1:P:211:THR:H	1:P:220:LEU:N	1.84	0.75
1:A:56:MET:HE2	1:A:56:MET:CA	2.17	0.75
1:A:119:LEU:HD21	1:A:210:VAL:HG11	1.68	0.74
2:B:38:ALA:HB2	2:B:91:ILE:HD12	1.66	0.74
1:P:279:ASN:HD21	1:P:317:PRO:HG2	1.52	0.74
2:B:18:LEU:HD23	2:B:29:ILE:HD12	1.70	0.74
1:A:165:ARG:NH2	1:A:201:GLY:HA3	2.03	0.73
1:A:44:ARG:HB2	1:A:65:ARG:HD3	1.68	0.73
1:P:165:ARG:HH21	1:P:324:GLY:HA3	1.52	0.73
1:P:242:ALA:HA	1:P:245:ARG:HD3	1.69	0.72
1:P:213:SER:HB3	1:P:219:LEU:HD23	1.71	0.72
1:P:217:VAL:HG22	1:P:225:ARG:HD2	1.70	0.72
2:B:13:PRO:HD2	2:B:16:GLU:HB2	1.72	0.72
1:A:218:VAL:HG23	1:A:226:ILE:O	1.90	0.72
1:P:210:VAL:HG13	1:P:219:LEU:HD13	1.72	0.72
2:B:20:VAL:HG23	2:B:27:VAL:HB	1.72	0.72
1:P:272:GLY:H	1:P:297:GLN:NE2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:209:SER:HA	1:P:210:VAL:HG23	1.72	0.71
1:A:180:LEU:HG	1:A:206:PHE:HE2	1.55	0.71
1:A:134:ASP:O	1:A:138:ILE:HG12	1.90	0.71
1:P:47:ASP:OD2	1:P:49:PRO:HD2	1.91	0.71
2:B:6:ALA:HB1	2:B:20:VAL:HG11	1.73	0.70
1:P:113:PRO:HA	1:P:237:VAL:HG12	1.73	0.70
1:P:220:LEU:HD12	1:P:224:THR:OG1	1.90	0.70
1:P:326:LEU:HA	1:P:369:ASN:HD21	1.56	0.70
1:A:164:ALA:O	1:A:167:ALA:HB3	1.91	0.70
1:P:149:LEU:HD11	1:P:231:VAL:HG22	1.73	0.70
1:P:327:ARG:H	1:P:369:ASN:ND2	1.90	0.70
1:P:24:ALA:HA	1:P:71:ALA:HB2	1.74	0.70
1:A:387:PRO:HG2	1:A:392:LEU:HD11	1.73	0.70
1:P:402:LEU:HD22	1:P:406:VAL:HG21	1.73	0.70
1:P:129:LEU:HD12	1:P:134:ASP:O	1.92	0.69
1:P:155:VAL:HG21	4:P:504:NAI:H2D	1.73	0.69
1:A:327:ARG:H	1:A:327:ARG:HE	1.39	0.69
1:P:244:ALA:HB1	1:P:249:LEU:HD22	1.75	0.69
1:P:342:ARG:HD2	1:P:392:LEU:O	1.93	0.69
1:A:47:ASP:O	1:A:64:ILE:HD12	1.93	0.68
1:P:209:SER:OG	1:P:210:VAL:HB	1.92	0.68
1:P:209:SER:O	1:P:221:ASP:HB3	1.94	0.68
1:P:35:ILE:HG22	1:P:74:VAL:HG13	1.76	0.67
1:P:23:VAL:HG23	1:P:35:ILE:HD13	1.77	0.67
2:B:22:HIS:O	2:B:25:GLN:HB2	1.95	0.67
1:A:212:GLY:O	1:A:219:LEU:HB2	1.95	0.67
1:A:330:VAL:HG22	1:A:366:THR:HG23	1.76	0.67
1:P:149:LEU:HD21	1:P:218:VAL:HG21	1.76	0.67
1:A:178:PRO:HB3	1:A:207:GLU:OE1	1.94	0.66
1:A:60:ASP:OD1	1:A:62:GLU:HB2	1.95	0.66
1:P:242:ALA:HB1	1:P:245:ARG:NH1	2.11	0.66
1:P:370:ASN:ND2	1:P:372:ARG:HE	1.93	0.66
1:A:6:LEU:HB2	1:A:305:LEU:HD22	1.77	0.65
1:P:272:GLY:H	1:P:297:GLN:HE22	1.44	0.65
1:A:159:GLU:HG3	1:A:323:GLN:HG2	1.79	0.65
1:P:56:MET:HE3	1:P:160:LEU:HD21	1.78	0.65
1:P:119:LEU:HB3	1:P:126:VAL:HG21	1.79	0.65
1:A:252:ASP:O	1:A:276:ARG:HD2	1.95	0.65
1:P:242:ALA:HB1	1:P:245:ARG:HH11	1.61	0.65
1:A:91:THR:OG1	1:A:99:THR:HG23	1.96	0.64
1:A:373:ASP:O	1:A:376:PRO:HD2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:111:ALA:HB1	1:P:238:LEU:O	1.97	0.64
1:P:147:ARG:O	1:P:148:LEU:HB3	1.98	0.64
2:B:92:ARG:O	2:B:99:LEU:HB2	1.97	0.64
1:P:50:PRO:HA	1:P:53:LYS:HB2	1.79	0.64
1:P:60:ASP:O	1:P:63:LYS:HB2	1.97	0.64
1:A:272:GLY:H	1:A:297:GLN:NE2	1.95	0.64
1:P:29:ALA:HB3	1:P:306:VAL:HG21	1.79	0.64
1:A:17:LEU:HD23	1:A:294:ALA:HB3	1.80	0.64
1:A:400:ARG:HH21	1:A:404:ALA:N	1.96	0.64
2:B:24:ALA:HA	6:B:504:HOH:O	1.98	0.64
1:A:55:PHE:CZ	1:A:136:ARG:HG3	2.33	0.63
1:A:278:ARG:NH1	1:A:280:PRO:HA	2.13	0.63
1:P:370:ASN:HA	1:P:372:ARG:NH2	2.13	0.63
1:A:235:ILE:HG23	4:A:503:NAI:N7A	2.13	0.63
1:A:339:GLU:HG3	1:A:356:GLU:OE2	1.99	0.63
1:A:209:SER:O	1:A:220:LEU:HA	1.98	0.63
1:P:153:GLY:O	1:P:158:LEU:HD12	1.99	0.63
1:A:27:ARG:NH2	1:A:35:ILE:HG13	2.13	0.63
1:P:205:ARG:HH22	1:P:224:THR:HG21	1.65	0.62
1:P:44:ARG:HD2	1:P:78:LEU:HD12	1.81	0.62
1:P:377:LEU:O	1:P:381:LEU:HB2	1.99	0.62
1:P:151:VAL:HG11	1:P:235:ILE:HG23	1.81	0.62
1:A:19:SER:O	1:A:22:PHE:HB3	1.99	0.62
1:A:22:PHE:CD1	1:A:302:ALA:HB2	2.34	0.62
1:P:358:GLN:OE1	1:P:359:LYS:HG3	2.00	0.62
1:P:114:ARG:HB3	1:P:235:ILE:HD12	1.81	0.62
1:P:341:VAL:HG22	1:P:354:LEU:HD23	1.82	0.62
2:B:8:SER:OG	2:B:11:GLU:HG3	1.99	0.61
1:P:119:LEU:HD22	1:P:231:VAL:HG11	1.82	0.61
1:A:108:ALA:HB2	1:A:271:LEU:HD12	1.81	0.61
1:A:132:LEU:HD12	1:A:136:ARG:HD2	1.81	0.61
1:A:142:LEU:HD23	1:A:169:VAL:HG21	1.81	0.61
1:A:76:TRP:HB3	1:A:78:LEU:HD21	1.81	0.61
1:P:149:LEU:HD21	1:P:231:VAL:HG22	1.82	0.61
1:P:196:TYR:OH	1:P:325:ALA:HB3	2.00	0.61
1:A:152:GLY:HA2	4:A:503:NAI:N3A	2.16	0.60
1:P:358:GLN:HG3	1:P:359:LYS:HE3	1.81	0.60
1:A:257:VAL:HA	1:A:262:ARG:O	2.01	0.60
1:A:381:LEU:HD23	6:A:517:HOH:O	2.00	0.60
1:P:43:GLU:O	1:P:78:LEU:HD13	2.01	0.60
1:P:156:ILE:O	1:P:160:LEU:HD12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:352:PHE:HE1	1:P:354:LEU:HD11	1.66	0.60
2:B:12:VAL:HG22	2:B:18:LEU:HB3	1.81	0.60
2:B:40:GLN:NE2	2:B:86:LEU:HD22	2.16	0.60
2:B:104:ARG:O	2:B:104:ARG:HD3	2.01	0.60
1:P:149:LEU:HD23	1:P:228:ALA:HB3	1.83	0.60
1:P:133:GLU:O	1:P:137:ARG:HG3	2.02	0.60
1:A:145:GLN:HA	1:A:145:GLN:NE2	2.16	0.60
2:B:65:LEU:HD23	2:B:66:HIS:CE1	2.37	0.60
1:A:9:PRO:HD2	1:A:103:GLY:N	2.16	0.60
2:B:59:ASP:O	2:B:72:VAL:HG22	2.02	0.60
1:A:353:THR:HG23	1:A:366:THR:O	2.02	0.59
1:A:132:LEU:O	1:A:136:ARG:HD2	2.01	0.59
1:P:159:GLU:O	1:P:163:THR:HG23	2.03	0.59
1:A:118:THR:HG21	1:A:210:VAL:O	2.02	0.59
1:A:307:ASP:O	1:A:310:ALA:HB3	2.02	0.59
2:B:14:PRO:O	2:B:16:GLU:HG2	2.03	0.59
2:B:62:GLU:HG3	2:B:69:LYS:HG2	1.84	0.59
1:P:12:VAL:HG11	1:P:19:SER:HB2	1.84	0.59
1:P:315:GLU:HG2	1:P:316:LEU:N	2.18	0.59
1:P:355:ILE:HG23	1:P:362:ILE:HG23	1.83	0.59
1:A:55:PHE:HZ	1:A:136:ARG:HG3	1.66	0.59
1:P:119:LEU:HD11	1:P:219:LEU:HD11	1.84	0.59
1:A:56:MET:O	1:A:139:GLN:HG3	2.03	0.58
1:A:400:ARG:HH21	1:A:404:ALA:CA	2.16	0.58
1:A:118:THR:HG22	1:A:119:LEU:HD22	1.84	0.58
1:P:45:PRO:HB2	1:P:66:LEU:HD12	1.85	0.58
1:A:217:VAL:HG11	1:A:225:ARG:HB3	1.85	0.58
1:A:46:TYR:HA	1:A:66:LEU:H	1.68	0.58
1:P:147:ARG:HG3	1:P:170:HIS:ND1	2.19	0.58
1:A:189:LEU:HD22	1:A:366:THR:HG21	1.86	0.58
1:P:162:ALA:HA	1:P:165:ARG:HG2	1.85	0.58
1:A:142:LEU:HD22	1:A:167:ALA:CB	2.33	0.58
1:A:158:LEU:HD22	1:A:197:HIS:CD2	2.39	0.58
1:P:242:ALA:O	1:P:245:ARG:HD3	2.03	0.58
1:P:370:ASN:HD22	1:P:372:ARG:NE	1.96	0.58
1:P:398:ASP:HB3	1:P:401:LYS:HG2	1.85	0.58
1:A:45:PRO:O	1:A:66:LEU:HB2	2.03	0.57
1:A:94:LEU:HD21	1:A:100:LEU:HD11	1.86	0.57
1:A:129:LEU:CD2	1:A:160:LEU:HD22	2.34	0.57
1:P:129:LEU:HD23	1:P:156:ILE:CG2	2.33	0.57
1:P:180:LEU:HD21	1:P:204:LEU:CD2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:210:VAL:HG13	1:P:219:LEU:CD1	2.35	0.57
1:A:189:LEU:O	1:A:193:VAL:HG23	2.05	0.57
1:A:279:ASN:OD1	1:A:281:LEU:HB2	2.05	0.57
1:A:398:ASP:OD2	1:A:401:LYS:HG3	2.03	0.57
1:A:114:ARG:HH21	1:A:235:ILE:HG22	1.70	0.57
1:P:218:VAL:HG12	1:P:226:ILE:CG1	2.34	0.57
1:A:81:THR:HB	1:A:95:SER:HB3	1.85	0.57
1:P:217:VAL:HG22	1:P:225:ARG:CD	2.34	0.57
1:P:373:ASP:O	1:P:376:PRO:HG2	2.04	0.57
1:A:180:LEU:HG	1:A:206:PHE:CE2	2.39	0.57
1:P:174:VAL:HG13	1:P:205:ARG:CB	2.35	0.57
1:A:132:LEU:HD12	1:A:132:LEU:O	2.05	0.57
1:P:287:ARG:HD2	1:P:289:GLU:HB3	1.86	0.56
2:B:91:ILE:HA	2:B:99:LEU:O	2.06	0.56
1:A:208:ARG:HD3	1:A:220:LEU:HD23	1.88	0.56
1:P:49:PRO:HB2	1:P:50:PRO:HD3	1.87	0.56
1:A:235:ILE:HG23	4:A:503:NAI:C8A	2.35	0.56
1:P:156:ILE:HG22	1:P:160:LEU:CD1	2.35	0.56
2:B:92:ARG:HH11	2:B:92:ARG:HB3	1.71	0.56
1:P:56:MET:HE1	1:P:138:ILE:HG21	1.88	0.56
1:P:127:HIS:NE2	1:P:137:ARG:HD3	2.21	0.56
1:P:244:ALA:O	1:P:247:ALA:HB3	2.06	0.56
1:P:44:ARG:HD2	1:P:78:LEU:CD1	2.36	0.56
1:A:162:ALA:O	1:A:165:ARG:HB2	2.06	0.55
1:A:116:LEU:CG	1:A:119:LEU:HD23	2.35	0.55
1:A:208:ARG:HD2	1:A:222:ASP:OD1	2.05	0.55
1:P:129:LEU:HD22	1:P:160:LEU:HD11	1.88	0.55
1:P:149:LEU:HD11	1:P:231:VAL:HG13	1.87	0.55
1:P:338:GLU:HG2	1:P:339:GLU:H	1.70	0.55
1:P:242:ALA:CA	1:P:245:ARG:HD3	2.37	0.55
1:A:55:PHE:CD2	1:A:135:ALA:HB1	2.42	0.55
1:P:94:LEU:HD11	1:P:100:LEU:CD1	2.36	0.55
1:P:129:LEU:CD2	1:P:160:LEU:HD11	2.36	0.55
1:P:171:VAL:O	1:P:172:SER:HB2	2.07	0.55
1:P:175:GLU:OE2	4:P:504:NAI:H1B	2.07	0.55
1:P:304:HIS:HA	1:P:310:ALA:HB3	1.88	0.55
1:A:180:LEU:HD12	1:A:194:ALA:HB2	1.89	0.55
1:P:147:ARG:HG3	1:P:170:HIS:HD1	1.72	0.55
1:P:148:LEU:HD12	1:P:149:LEU:O	2.07	0.55
1:P:119:LEU:CD2	1:P:231:VAL:HG11	2.36	0.55
1:A:119:LEU:HD21	1:A:210:VAL:CG1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:LEU:HG	2:B:19:GLN:O	2.07	0.55
1:P:152:GLY:HA2	1:P:175:GLU:OE2	2.06	0.54
1:P:212:GLY:O	1:P:219:LEU:HA	2.08	0.54
1:A:65:ARG:HG3	1:A:65:ARG:HH11	1.71	0.54
2:B:40:GLN:OE1	2:B:87:LYS:HG3	2.07	0.54
2:B:63:CYS:O	2:B:67:MET:HA	2.07	0.54
1:P:151:VAL:CG1	1:P:235:ILE:HG23	2.37	0.54
1:P:153:GLY:H	1:P:175:GLU:CD	2.15	0.54
1:P:158:LEU:CD1	1:P:180:LEU:HD13	2.35	0.54
2:B:5:LYS:CG	2:B:97:ASP:HB2	2.37	0.54
1:P:55:PHE:CD1	1:P:59:GLY:HA2	2.42	0.54
1:P:122:ALA:HB1	1:P:213:SER:OG	2.08	0.54
1:P:217:VAL:O	1:P:217:VAL:HG12	2.07	0.54
1:A:218:VAL:CB	1:A:226:ILE:HB	2.35	0.54
1:A:82:ALA:HA	1:A:94:LEU:HD12	1.89	0.54
1:A:148:LEU:HB3	1:A:169:VAL:HG11	1.89	0.54
1:P:379:ARG:CZ	1:P:404:ALA:HA	2.37	0.54
1:P:27:ARG:CZ	1:P:35:ILE:HD12	2.38	0.54
1:P:388:ASP:OD2	1:P:390:ALA:HB3	2.08	0.54
1:P:56:MET:HE3	1:P:160:LEU:CD2	2.36	0.54
1:A:400:ARG:HE	1:A:404:ALA:HB2	1.73	0.53
1:P:117:PRO:HA	1:P:120:GLN:HG2	1.90	0.53
1:P:123:THR:HB	1:P:215:ASP:OD2	2.08	0.53
1:P:279:ASN:ND2	1:P:317:PRO:HG2	2.22	0.53
1:P:54:ASP:O	1:P:57:ALA:HB3	2.08	0.53
1:A:297:GLN:O	1:A:301:VAL:HG23	2.08	0.53
1:A:27:ARG:HH21	1:A:35:ILE:HG13	1.72	0.53
1:A:327:ARG:HH21	1:A:369:ASN:HD21	1.57	0.53
1:A:147:ARG:HD2	1:A:227:ALA:O	2.08	0.53
1:P:149:LEU:HD22	1:P:218:VAL:HG11	1.91	0.53
1:P:326:LEU:CD2	1:P:350:PRO:HG2	2.39	0.53
1:P:188:THR:HG21	1:P:339:GLU:OE2	2.08	0.53
1:A:114:ARG:HG3	1:A:236:GLY:O	2.09	0.53
1:P:45:PRO:CB	1:P:66:LEU:HD12	2.39	0.53
1:P:398:ASP:HB3	1:P:401:LYS:CB	2.36	0.53
1:P:218:VAL:HG12	1:P:226:ILE:HG13	1.91	0.53
1:A:98:ARG:HG2	1:A:99:THR:N	2.23	0.52
2:B:3:PHE:HD2	2:B:99:LEU:HB3	1.74	0.52
1:P:25:GLU:OE2	1:P:29:ALA:HB2	2.10	0.52
1:P:114:ARG:HG3	1:P:238:LEU:HD12	1.91	0.52
1:A:172:SER:HA	1:A:203:ASP:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:GLU:HG3	2:B:69:LYS:CG	2.40	0.52
1:P:369:ASN:N	1:P:369:ASN:HD22	2.08	0.52
1:A:361:ARG:HG3	1:A:384:GLY:O	2.09	0.52
1:A:60:ASP:OD2	1:A:63:LYS:HG3	2.10	0.52
1:P:345:VAL:HG22	1:P:352:PHE:CG	2.45	0.52
1:A:254:GLY:HA3	1:A:287:ARG:HD3	1.92	0.52
1:P:124:MET:HG3	1:P:229:ASP:O	2.09	0.52
1:A:129:LEU:HD23	1:A:156:ILE:CG2	2.40	0.52
1:P:129:LEU:HD23	1:P:156:ILE:HG21	1.91	0.52
1:A:64:ILE:HD11	1:A:132:LEU:CD2	2.40	0.51
1:A:375:ALA:HB3	1:A:376:PRO:HD3	1.92	0.51
2:B:9:VAL:HG22	2:B:96:ARG:HG2	1.91	0.51
1:P:347:LEU:HG	1:P:348:ASP:N	2.25	0.51
1:A:158:LEU:HD22	1:A:197:HIS:NE2	2.25	0.51
2:B:94:GLU:HB2	2:B:97:ASP:OD1	2.10	0.51
2:B:94:GLU:HG3	2:B:99:LEU:HD22	1.91	0.51
1:P:124:MET:HB2	1:P:229:ASP:O	2.10	0.51
1:P:398:ASP:CB	1:P:401:LYS:HG2	2.41	0.51
2:B:32:VAL:HG13	2:B:58:GLY:O	2.10	0.51
2:B:19:GLN:O	2:B:20:VAL:HG13	2.11	0.51
1:A:6:LEU:HD21	1:A:31:TYR:CD1	2.46	0.51
1:P:213:SER:HB3	1:P:219:LEU:CD2	2.40	0.51
1:A:263:THR:HG22	1:A:264:THR:H	1.75	0.51
1:P:12:VAL:HG22	1:P:106:VAL:HB	1.91	0.51
1:P:338:GLU:HG2	1:P:339:GLU:N	2.26	0.51
1:A:56:MET:HA	1:A:139:GLN:HG3	1.92	0.51
1:A:56:MET:CE	1:A:56:MET:CA	2.87	0.51
1:A:15:ALA:O	1:A:45:PRO:HB3	2.10	0.51
1:A:203:ASP:CG	1:A:205:ARG:HE	2.19	0.51
2:B:19:GLN:HG2	2:B:20:VAL:N	2.26	0.51
1:P:94:LEU:HD11	1:P:100:LEU:HD11	1.93	0.51
1:P:174:VAL:HG13	1:P:205:ARG:HB2	1.92	0.51
1:P:131:THR:OG1	1:P:134:ASP:HB2	2.10	0.51
1:P:149:LEU:CD1	1:P:231:VAL:HG22	2.41	0.51
1:P:185:ALA:HB1	1:P:189:LEU:HD23	1.92	0.51
1:P:158:LEU:HD21	1:P:180:LEU:HD13	1.93	0.50
1:P:269:TYR:CZ	1:P:305:LEU:HD21	2.46	0.50
1:A:55:PHE:O	1:A:139:GLN:OE1	2.29	0.50
1:A:165:ARG:HE	1:A:201:GLY:C	2.19	0.50
1:A:291:TRP:O	1:A:294:ALA:HB3	2.11	0.50
1:A:327:ARG:HH21	1:A:369:ASN:ND2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:HIS:HB2	5:B:500:FES:S2	2.50	0.50
1:P:210:VAL:HG12	1:P:210:VAL:O	2.11	0.50
1:P:402:LEU:O	1:P:406:VAL:HG23	2.10	0.50
1:A:14:GLY:O	1:A:19:SER:OG	2.30	0.50
1:P:315:GLU:OE1	1:P:316:LEU:O	2.30	0.50
1:P:24:ALA:CA	1:P:71:ALA:HB2	2.41	0.50
1:P:71:ALA:O	1:P:74:VAL:HG23	2.11	0.50
1:P:389:ARG:HG2	1:P:389:ARG:HH11	1.77	0.50
1:A:63:LYS:HG2	2:B:84:GLU:OE2	2.12	0.50
1:P:94:LEU:HD21	1:P:100:LEU:HD12	1.93	0.50
1:P:148:LEU:HD12	1:P:149:LEU:N	2.26	0.50
1:P:276:ARG:HH11	1:P:286:GLU:HA	1.76	0.50
1:A:220:LEU:HB2	1:A:224:THR:HB	1.94	0.50
1:P:119:LEU:HG	1:P:219:LEU:CD2	2.37	0.50
1:P:149:LEU:HD23	1:P:228:ALA:CB	2.42	0.50
1:P:192:PHE:HA	1:P:195:ARG:CD	2.41	0.50
1:A:139:GLN:O	1:A:142:LEU:HB2	2.10	0.50
1:A:249:LEU:HG	1:A:265:CYS:HB2	1.93	0.50
1:P:218:VAL:HG12	1:P:226:ILE:HB	1.93	0.50
1:P:379:ARG:HD3	1:P:403:ALA:HB1	1.92	0.50
1:P:48:ARG:HA	1:P:51:LEU:CD1	2.42	0.50
1:P:144:PRO:O	1:P:168:GLY:O	2.30	0.50
1:P:114:ARG:HB3	1:P:235:ILE:CD1	2.42	0.49
1:P:179:ARG:NH2	1:P:190:ALA:HB2	2.27	0.49
1:A:22:PHE:CE1	1:A:302:ALA:HB2	2.47	0.49
1:A:58:HIS:CD2	1:A:58:HIS:H	2.29	0.49
1:A:196:TYR:CG	1:A:326:LEU:HD11	2.48	0.49
1:P:175:GLU:HG3	1:P:176:THR:N	2.26	0.49
1:P:340:ILE:HD11	1:P:389:ARG:HG3	1.94	0.49
1:A:404:ALA:O	1:A:405:ALA:O	2.29	0.49
1:P:151:VAL:O	1:P:152:GLY:O	2.30	0.49
1:P:195:ARG:HG2	1:P:195:ARG:NH2	2.19	0.49
1:P:331:ALA:HB3	1:P:365:ALA:HB3	1.95	0.49
1:P:353:THR:O	1:P:353:THR:HG22	2.12	0.49
1:A:379:ARG:HG3	1:A:379:ARG:HH11	1.76	0.49
2:B:18:LEU:CD2	2:B:29:ILE:HD12	2.39	0.49
1:P:327:ARG:H	1:P:369:ASN:HD21	1.59	0.49
1:A:61:ALA:HB2	1:A:132:LEU:HD11	1.95	0.49
1:P:347:LEU:HG	1:P:348:ASP:H	1.77	0.49
1:A:20:VAL:CG1	1:A:66:LEU:HD22	2.35	0.49
1:A:351:LYS:O	1:A:351:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:HA	6:A:525:HOH:O	2.12	0.49
1:A:153:GLY:HA3	1:A:175:GLU:OE1	2.13	0.49
1:A:373:ASP:C	1:A:376:PRO:HD2	2.37	0.49
1:A:222:ASP:OD2	1:A:224:THR:OG1	2.30	0.49
1:A:316:LEU:HD23	1:A:381:LEU:HG	1.95	0.49
1:P:149:LEU:CD2	1:P:218:VAL:HG21	2.43	0.49
1:A:63:LYS:HB3	2:B:84:GLU:OE1	2.12	0.48
1:A:340:ILE:HG22	1:A:355:ILE:HD12	1.95	0.48
1:P:151:VAL:HG12	1:P:234:GLY:N	2.23	0.48
1:P:186:PRO:HD2	1:P:189:LEU:HB3	1.94	0.48
1:P:340:ILE:HD11	1:P:389:ARG:CG	2.43	0.48
1:A:138:ILE:HG22	1:A:230:MET:CE	2.44	0.48
1:P:52:SER:HB2	1:P:160:LEU:HG	1.95	0.48
1:P:214:VAL:HG12	1:P:214:VAL:O	2.12	0.48
1:A:340:ILE:CG2	1:A:355:ILE:HD12	2.43	0.48
2:B:62:GLU:HG3	2:B:69:LYS:HE2	1.95	0.48
1:P:398:ASP:OD2	1:P:401:LYS:HG2	2.14	0.48
1:A:171:VAL:O	1:A:202:VAL:HA	2.14	0.48
1:P:373:ASP:OD1	1:P:399:LEU:HD12	2.13	0.48
1:P:241:ASP:O	1:P:245:ARG:HB3	2.14	0.48
1:A:54:ASP:O	1:A:57:ALA:HB3	2.14	0.48
2:B:26:LYS:HE2	6:B:504:HOH:O	2.13	0.48
1:P:149:LEU:CG	1:P:231:VAL:HG22	2.44	0.48
1:P:189:LEU:HD13	1:P:366:THR:CG2	2.37	0.48
1:A:368:VAL:O	1:A:369:ASN:HB2	2.12	0.48
2:B:28:ALA:HB2	2:B:41:ASP:HA	1.94	0.48
1:P:289:GLU:CD	4:P:504:NAI:HO3N	2.22	0.48
1:P:296:ASN:OD1	1:P:315:GLU:OE2	2.31	0.48
1:P:72:PRO:O	1:P:73:GLU:HB2	2.14	0.47
1:A:114:ARG:HG2	1:A:238:LEU:HG	1.96	0.47
1:A:291:TRP:CH2	2:B:81:PRO:HG3	2.49	0.47
1:P:131:THR:O	1:P:134:ASP:HB2	2.15	0.47
1:P:119:LEU:CD1	1:P:219:LEU:HD11	2.43	0.47
1:P:361:ARG:O	1:P:361:ARG:HG2	2.14	0.47
2:B:66:HIS:O	2:B:67:MET:HB2	2.14	0.47
1:P:150:ILE:HG22	1:P:151:VAL:O	2.15	0.47
2:B:76:LYS:HD3	2:B:77:VAL:O	2.14	0.47
1:A:27:ARG:HD2	1:A:72:PRO:O	2.14	0.47
2:B:48:TRP:CD2	2:B:65:LEU:HD13	2.49	0.47
1:P:289:GLU:OE2	4:P:504:NAI:O3D	2.30	0.47
1:A:165:ARG:HD2	1:A:165:ARG:HA	1.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:LYS:HB3	1:A:386:LYS:HE3	1.50	0.47
2:B:98:VAL:O	2:B:98:VAL:HG12	2.14	0.47
1:P:138:ILE:HD12	1:P:138:ILE:H	1.78	0.47
1:P:331:ALA:HB1	1:P:381:LEU:HD13	1.96	0.47
1:P:404:ALA:O	1:P:405:ALA:HB2	2.14	0.47
1:P:159:GLU:HG2	1:P:322:ASP:O	2.14	0.47
1:A:9:PRO:HD2	1:A:103:GLY:H	1.78	0.47
1:A:17:LEU:HD23	1:A:294:ALA:CB	2.45	0.47
2:B:3:PHE:HB3	2:B:99:LEU:HG	1.96	0.47
2:B:30:PHE:CD2	2:B:56:LEU:HD13	2.50	0.47
1:P:131:THR:H	1:P:134:ASP:HB2	1.80	0.47
1:A:55:PHE:HD2	1:A:56:MET:CE	2.28	0.46
1:A:235:ILE:HG22	1:A:235:ILE:O	2.15	0.46
1:P:155:VAL:HG23	1:P:156:ILE:HG13	1.98	0.46
1:P:385:ALA:C	1:P:387:PRO:HD3	2.40	0.46
1:A:149:LEU:HD22	1:A:218:VAL:HG21	1.97	0.46
2:B:85:PRO:HB2	2:B:107:LEU:CD1	2.46	0.46
1:P:179:ARG:HH21	1:P:190:ALA:HB2	1.81	0.46
1:A:9:PRO:HD2	1:A:102:TYR:HA	1.97	0.46
1:A:211:THR:CG2	1:A:221:ASP:HA	2.45	0.46
1:P:307:ASP:OD2	1:P:309:THR:OG1	2.30	0.46
1:A:393:ALA:O	1:A:395:PRO:HD3	2.16	0.46
1:P:379:ARG:NH1	1:P:404:ALA:HA	2.30	0.46
1:A:54:ASP:OD2	1:A:55:PHE:N	2.49	0.46
1:A:114:ARG:HH21	1:A:235:ILE:CG2	2.28	0.46
1:P:77:LEU:C	1:P:78:LEU:HD23	2.40	0.46
1:P:174:VAL:HG13	1:P:205:ARG:HB3	1.97	0.46
1:P:28:GLN:HE21	1:P:28:GLN:HB3	1.49	0.46
1:P:123:THR:HG21	1:P:215:ASP:HB2	1.98	0.46
1:P:179:ARG:HE	1:P:179:ARG:HB2	1.47	0.46
1:A:211:THR:OG1	1:A:219:LEU:O	2.34	0.46
2:B:40:GLN:HE21	2:B:86:LEU:HD22	1.78	0.46
1:P:119:LEU:CG	1:P:219:LEU:HD11	2.46	0.46
1:A:237:VAL:CG1	4:A:503:NAI:H4D	2.46	0.46
2:B:22:HIS:O	2:B:23:ASP:HB2	2.15	0.46
1:P:155:VAL:CG2	4:P:504:NAI:H2D	2.44	0.46
1:A:123:THR:OG1	1:A:215:ASP:O	2.30	0.46
1:P:341:VAL:HG22	1:P:354:LEU:CD2	2.46	0.46
2:B:61:VAL:O	2:B:61:VAL:HG13	2.16	0.46
1:P:114:ARG:HG3	1:P:238:LEU:CD1	2.46	0.46
1:A:50:PRO:O	1:A:54:ASP:OD2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:TYR:CD2	2:B:102:PHE:HA	2.51	0.45
1:A:215:ASP:N	1:A:215:ASP:OD1	2.49	0.45
2:B:87:LYS:CB	2:B:107:LEU:HD22	2.46	0.45
1:A:71:ALA:HB1	1:A:74:VAL:HG21	1.99	0.45
1:A:116:LEU:HD12	1:A:117:PRO:HD2	1.98	0.45
1:A:291:TRP:O	1:A:294:ALA:N	2.50	0.45
1:A:376:PRO:O	1:A:380:LEU:HD12	2.17	0.45
1:P:191:ASP:OD2	1:P:192:PHE:N	2.50	0.45
1:A:106:VAL:HG11	1:A:271:LEU:HD11	1.99	0.45
1:A:165:ARG:HE	1:A:201:GLY:CA	2.29	0.45
1:A:165:ARG:HE	1:A:201:GLY:HA3	1.80	0.45
1:P:62:GLU:OE1	1:P:62:GLU:N	2.50	0.45
1:P:192:PHE:HA	1:P:195:ARG:CG	2.46	0.45
1:P:218:VAL:CG1	1:P:226:ILE:HD12	2.46	0.45
2:B:21:SER:HB2	2:B:26:LYS:HD3	1.98	0.45
1:P:179:ARG:NH2	1:P:180:LEU:O	2.50	0.45
1:P:245:ARG:HG2	1:P:246:ALA:N	2.28	0.45
1:A:313:TYR:CE2	1:A:315:GLU:HB2	2.52	0.45
1:P:47:ASP:CG	1:P:49:PRO:HD2	2.42	0.45
1:P:110:GLY:N	6:P:522:HOH:O	2.49	0.45
1:P:242:ALA:C	1:P:245:ARG:HH11	2.25	0.45
1:A:58:HIS:O	1:A:60:ASP:N	2.50	0.45
1:A:149:LEU:HD11	1:A:174:VAL:HG23	1.98	0.45
1:A:323:GLN:H	1:A:323:GLN:HG3	1.59	0.45
1:P:28:GLN:OE1	1:P:70:ARG:NH1	2.50	0.45
1:P:158:LEU:HD23	1:P:197:HIS:ND1	2.32	0.45
1:P:244:ALA:CB	1:P:249:LEU:HD22	2.46	0.45
1:P:342:ARG:NH1	1:P:394:ASP:O	2.50	0.45
1:A:55:PHE:HE2	1:A:136:ARG:N	2.15	0.45
1:A:165:ARG:NH2	1:A:200:GLN:O	2.50	0.45
2:B:28:ALA:HB1	2:B:30:PHE:CE1	2.52	0.45
1:P:124:MET:SD	1:P:231:VAL:HG23	2.57	0.45
1:P:207:GLU:O	1:P:208:ARG:NH1	2.50	0.45
1:P:228:ALA:HB1	1:P:230:MET:O	2.17	0.45
1:P:350:PRO:O	1:P:351:LYS:HB2	2.17	0.45
1:P:362:ILE:HD11	1:P:387:PRO:HG2	1.97	0.45
1:A:48:ARG:NH1	3:A:501:FAD:O2A	2.50	0.45
1:P:118:THR:HB	1:P:219:LEU:HD13	1.97	0.45
1:P:175:GLU:HG3	1:P:176:THR:H	1.80	0.45
1:P:273:ASP:OD1	1:P:289:GLU:HA	2.17	0.45
1:A:263:THR:HG22	6:A:505:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:NH2	1:A:73:GLU:O	2.50	0.44
2:B:94:GLU:O	2:B:97:ASP:OD1	2.34	0.44
1:P:111:ALA:O	1:P:130:ARG:NH2	2.50	0.44
1:P:131:THR:H	1:P:134:ASP:CB	2.29	0.44
1:A:151:VAL:HG12	4:A:503:NAI:N1A	2.32	0.44
1:A:175:GLU:OE2	4:A:503:NAI:H1B	2.16	0.44
1:A:221:ASP:OD2	1:A:221:ASP:N	2.50	0.44
1:A:303:ARG:O	1:A:307:ASP:N	2.50	0.44
2:B:91:ILE:HG23	2:B:91:ILE:O	2.16	0.44
1:P:149:LEU:CD1	1:P:231:VAL:HG13	2.47	0.44
1:A:327:ARG:HE	1:A:327:ARG:N	2.11	0.44
2:B:5:LYS:HB3	2:B:5:LYS:HE3	1.58	0.44
1:A:107:LEU:O	1:A:270:ALA:HA	2.18	0.44
1:A:116:LEU:HD22	1:A:233:VAL:HG22	1.98	0.44
2:B:22:HIS:ND1	2:B:25:GLN:OE1	2.50	0.44
1:P:149:LEU:HD11	1:P:231:VAL:CG2	2.44	0.44
1:P:156:ILE:HG22	1:P:160:LEU:HD12	1.99	0.44
1:P:282:SER:O	1:P:284:ARG:NH1	2.50	0.44
1:A:36:THR:OG1	1:A:75:GLU:OE1	2.32	0.44
1:A:83:GLN:NE2	1:A:95:SER:HA	2.33	0.44
1:P:29:ALA:CB	1:P:306:VAL:HG21	2.47	0.44
1:P:83:GLN:O	1:P:84:SER:HB3	2.17	0.44
1:A:197:HIS:HB3	1:A:202:VAL:HG11	2.00	0.44
1:A:307:ASP:HA	1:A:308:PRO:HD3	1.72	0.44
2:B:87:LYS:HE3	2:B:105:ALA:HB1	1.98	0.44
1:P:205:ARG:HG2	1:P:205:ARG:HH11	1.82	0.44
1:P:156:ILE:HG22	1:P:160:LEU:HD11	1.98	0.44
1:P:363:VAL:C	1:P:381:LEU:HD21	2.42	0.44
1:A:241:ASP:O	1:A:244:ALA:HB3	2.17	0.44
1:P:278:ARG:HG2	1:P:278:ARG:HH11	1.82	0.44
1:P:340:ILE:HD12	1:P:357:LEU:HD11	1.99	0.44
1:A:143:ARG:NH2	1:A:145:GLN:O	2.50	0.43
1:A:83:GLN:OE1	1:A:95:SER:N	2.51	0.43
1:A:90:HIS:NE2	1:A:267:ASP:OD1	2.50	0.43
1:A:98:ARG:HD3	1:A:100:LEU:CD2	2.48	0.43
1:A:146:SER:O	1:A:169:VAL:HG13	2.18	0.43
1:P:40:ASP:HA	1:P:80:VAL:O	2.18	0.43
1:P:46:TYR:HB2	1:P:64:ILE:O	2.17	0.43
1:P:129:LEU:HD22	1:P:160:LEU:HD21	2.01	0.43
1:P:217:VAL:HG22	1:P:225:ARG:NE	2.33	0.43
1:A:164:ALA:HB3	1:A:171:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:VAL:HG22	1:A:219:LEU:HG	2.00	0.43
1:P:107:LEU:HD13	1:P:244:ALA:HB2	1.99	0.43
1:A:159:GLU:OE2	1:A:321:SER:HA	2.18	0.43
1:A:222:ASP:CG	1:A:224:THR:HG1	2.26	0.43
1:P:155:VAL:HG23	1:P:156:ILE:N	2.33	0.43
1:P:317:PRO:O	1:P:318:TRP:HB3	2.19	0.43
1:A:342:ARG:O	1:A:352:PHE:HB2	2.18	0.43
2:B:103:SER:O	2:B:105:ALA:N	2.51	0.43
1:A:81:THR:O	1:A:95:SER:N	2.50	0.43
1:A:86:ASP:HA	1:A:87:PRO:HD2	1.84	0.43
1:A:124:MET:HE3	1:A:213:SER:HB2	1.99	0.43
2:B:38:ALA:CB	2:B:91:ILE:HD12	2.44	0.43
2:B:92:ARG:HB2	2:B:99:LEU:CB	2.49	0.43
1:P:8:ALA:HB1	1:P:9:PRO:HA	1.99	0.43
1:P:326:LEU:HD21	1:P:350:PRO:HG2	2.01	0.43
1:A:27:ARG:C	1:A:29:ALA:H	2.26	0.43
1:A:86:ASP:O	1:A:90:HIS:N	2.52	0.43
1:A:153:GLY:HA3	1:A:180:LEU:CD2	2.49	0.43
1:P:31:TYR:CZ	1:P:33:GLY:HA3	2.53	0.43
1:P:124:MET:HE1	1:P:213:SER:HB2	2.01	0.43
1:P:361:ARG:O	1:P:363:VAL:HG13	2.17	0.43
1:A:217:VAL:CG1	1:A:225:ARG:HB3	2.49	0.43
1:A:177:GLN:CD	1:A:178:PRO:HD2	2.44	0.43
1:A:203:ASP:OD1	1:A:205:ARG:NH2	2.49	0.43
2:B:20:VAL:O	2:B:27:VAL:N	2.51	0.43
1:P:65:ARG:H	1:P:65:ARG:HD3	1.82	0.43
1:P:138:ILE:HD12	1:P:138:ILE:N	2.34	0.43
1:P:191:ASP:OD2	1:P:195:ARG:NH2	2.52	0.43
1:P:327:ARG:HG2	1:P:327:ARG:HH11	1.83	0.43
1:P:339:GLU:OE2	1:P:354:LEU:HD22	2.18	0.43
1:P:398:ASP:HB3	1:P:401:LYS:CG	2.46	0.43
1:P:116:LEU:HD12	1:P:117:PRO:HD2	2.01	0.42
1:P:131:THR:N	1:P:134:ASP:HB2	2.34	0.42
1:P:179:ARG:NH2	1:P:181:MET:O	2.51	0.42
1:P:349:ALA:N	1:P:350:PRO:HD3	2.34	0.42
1:A:117:PRO:O	1:A:120:GLN:HB2	2.18	0.42
1:P:155:VAL:HG21	4:P:504:NAI:C2D	2.47	0.42
1:P:279:ASN:HA	1:P:280:PRO:HD3	1.74	0.42
1:P:347:LEU:HD23	1:P:347:LEU:H	1.84	0.42
1:A:118:THR:HG23	1:A:212:GLY:HA2	2.02	0.42
1:A:218:VAL:HG12	1:A:219:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:VAL:HG13	4:A:503:NAI:H4D	2.00	0.42
1:P:247:ALA:HB3	1:P:249:LEU:HD13	2.01	0.42
1:A:65:ARG:NH2	1:A:66:LEU:O	2.50	0.42
1:A:69:LYS:HB3	1:A:69:LYS:NZ	2.34	0.42
1:A:196:TYR:O	1:A:200:GLN:HG2	2.19	0.42
1:A:291:TRP:CZ2	2:B:81:PRO:HG3	2.54	0.42
1:P:114:ARG:NE	1:P:235:ILE:HD12	2.34	0.42
1:P:186:PRO:HA	1:P:334:ALA:HB1	2.01	0.42
1:A:116:LEU:HD12	1:A:116:LEU:HA	1.85	0.42
2:B:84:GLU:HA	2:B:85:PRO:HD3	1.88	0.42
1:P:27:ARG:NH2	1:P:73:GLU:O	2.49	0.42
1:P:149:LEU:CD2	1:P:231:VAL:HG22	2.47	0.42
1:P:202:VAL:O	1:P:202:VAL:HG12	2.19	0.42
1:A:49:PRO:HB2	1:A:50:PRO:HD3	2.02	0.42
2:B:18:LEU:HD23	2:B:18:LEU:O	2.19	0.42
1:P:52:SER:O	1:P:163:THR:HG21	2.20	0.42
1:A:56:MET:HA	1:A:139:GLN:CG	2.50	0.42
1:A:67:ASP:OD1	1:A:69:LYS:HB2	2.20	0.42
1:A:138:ILE:HG12	1:A:138:ILE:H	1.46	0.42
1:P:127:HIS:O	1:P:233:VAL:HG23	2.20	0.42
1:A:6:LEU:HB2	1:A:305:LEU:CD2	2.47	0.42
1:A:112:ALA:O	1:A:237:VAL:HA	2.20	0.42
1:A:192:PHE:CE1	1:A:347:LEU:HD23	2.54	0.42
1:P:54:ASP:O	1:P:57:ALA:N	2.50	0.42
1:P:96:ASP:OD1	1:P:98:ARG:HB3	2.19	0.42
1:A:55:PHE:HB3	1:A:56:MET:HE3	2.00	0.42
1:A:193:VAL:O	1:A:196:TYR:HB3	2.20	0.42
2:B:6:ALA:O	2:B:7:CYS:HB3	2.19	0.42
1:P:112:ALA:HA	1:P:113:PRO:HD3	1.81	0.42
1:A:148:LEU:HA	1:A:230:MET:O	2.20	0.42
1:A:357:LEU:N	1:A:357:LEU:HD12	2.34	0.42
1:P:167:ALA:HB3	1:P:169:VAL:HG23	2.00	0.42
1:P:219:LEU:H	1:P:219:LEU:HG	1.45	0.42
1:A:56:MET:C	1:A:139:GLN:HG3	2.45	0.41
1:A:193:VAL:HG12	1:A:197:HIS:CD2	2.54	0.41
2:B:92:ARG:HD3	2:B:99:LEU:HD23	2.02	0.41
1:P:192:PHE:HA	1:P:195:ARG:NE	2.35	0.41
1:A:56:MET:CE	1:A:56:MET:N	2.83	0.41
1:A:183:ARG:NH2	4:A:503:NAI:O2D	2.53	0.41
1:A:364:GLY:O	1:A:365:ALA:HB2	2.20	0.41
1:P:48:ARG:HA	1:P:51:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:276:ARG:NH1	1:P:286:GLU:HA	2.35	0.41
1:A:9:PRO:HD2	1:A:102:TYR:C	2.45	0.41
1:A:83:GLN:HE22	1:A:95:SER:HA	1.84	0.41
1:A:181:MET:HE2	1:A:185:ALA:HB2	2.02	0.41
1:A:25:GLU:O	1:A:29:ALA:HB3	2.20	0.41
1:A:126:VAL:HA	1:A:231:VAL:O	2.20	0.41
1:P:147:ARG:HB3	1:P:148:LEU:H	1.54	0.41
1:P:210:VAL:O	1:P:211:THR:OG1	2.36	0.41
1:A:379:ARG:HG3	1:A:379:ARG:NH1	2.34	0.41
2:B:85:PRO:HB2	2:B:107:LEU:HD11	2.03	0.41
1:P:151:VAL:HG13	1:P:152:GLY:N	2.32	0.41
1:P:161:ALA:O	1:P:164:ALA:HB3	2.21	0.41
1:P:272:GLY:N	1:P:297:GLN:HE22	2.13	0.41
1:A:112:ALA:O	1:A:238:LEU:N	2.50	0.41
1:P:202:VAL:O	1:P:204:LEU:N	2.53	0.41
1:A:116:LEU:CD2	1:A:119:LEU:HD23	2.51	0.41
1:A:106:VAL:CG1	1:A:271:LEU:HD11	2.51	0.41
1:A:124:MET:CE	1:A:213:SER:HB2	2.50	0.41
1:A:70:ARG:H	1:A:70:ARG:HG3	1.34	0.41
2:B:21:SER:HB2	2:B:26:LYS:CD	2.51	0.41
2:B:28:ALA:O	2:B:38:ALA:HA	2.21	0.41
2:B:65:LEU:HD23	2:B:66:HIS:NE2	2.34	0.41
1:P:355:ILE:CG2	1:P:362:ILE:HG23	2.51	0.41
1:P:344:GLU:N	1:P:351:LYS:O	2.49	0.41
1:P:402:LEU:HD22	1:P:406:VAL:CG2	2.44	0.41
1:A:27:ARG:O	1:A:30:GLY:N	2.50	0.40
1:A:153:GLY:HA3	1:A:180:LEU:HD23	2.03	0.40
1:P:307:ASP:OD2	1:P:308:PRO:HD2	2.21	0.40
2:B:59:ASP:C	2:B:72:VAL:HG22	2.46	0.40
1:P:74:VAL:HB	1:P:76:TRP:CE2	2.56	0.40
1:P:158:LEU:HD23	1:P:197:HIS:CE1	2.56	0.40
1:P:44:ARG:HA	1:P:78:LEU:CD1	2.51	0.40
1:A:114:ARG:O	1:A:115:ALA:O	2.40	0.40
1:A:160:LEU:HD23	1:A:232:VAL:HG11	2.03	0.40
1:A:306:VAL:O	1:A:306:VAL:HG12	2.21	0.40
1:P:151:VAL:HG11	1:P:233:VAL:CG1	2.51	0.40
1:A:208:ARG:NH1	1:A:208:ARG:HG2	2.36	0.40
1:P:119:LEU:HG	1:P:219:LEU:HD11	2.04	0.40
1:P:148:LEU:HD11	1:P:150:ILE:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/408 (98%)	344 (86%)	46 (12%)	10 (2%)	4	1
1	P	399/408 (98%)	331 (83%)	51 (13%)	17 (4%)	2	0
2	B	104/109 (95%)	87 (84%)	14 (14%)	3 (3%)	3	0
All	All	903/925 (98%)	762 (84%)	111 (12%)	30 (3%)	3	0

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	GLY
1	A	115	ALA
1	A	405	ALA
2	B	104	ARG
1	P	148	LEU
1	P	152	GLY
1	P	171	VAL
1	P	172	SER
1	P	202	VAL
1	P	210	VAL
1	P	405	ALA
1	A	215	ASP
1	P	164	ALA
1	A	43	GLU
1	A	144	PRO
1	P	252	ASP
1	A	54	ASP
1	A	199	ALA
1	A	292	SER
2	B	23	ASP
2	B	103	SER
1	P	147	ARG
1	P	203	ASP
1	P	216	GLY

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Mol	Chain	Res	Type
1	P	144	PRO
1	A	365	ALA
1	P	84	SER
1	P	130	ARG
1	P	217	VAL
1	P	223	GLY

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	302/307 (98%)	224 (74%)	78 (26%)	0	0
1	P	303/307 (99%)	232 (77%)	71 (23%)	1	0
2	B	89/92 (97%)	64 (72%)	25 (28%)	0	0
All	All	694/706 (98%)	520 (75%)	174 (25%)	0	0

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	19	SER
1	A	21	SER
1	A	32	GLN
1	A	34	LEU
1	A	43	GLU
1	A	44	ARG
1	A	49	PRO
1	A	52	SER
1	A	56	MET
1	A	58	HIS
1	A	64	ILE
1	A	65	ARG
1	A	66	LEU
1	A	67	ASP
1	A	68	CYS

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Mol	Chain	Res	Type
1	A	69	LYS
1	A	70	ARG
1	A	73	GLU
1	A	83	GLN
1	A	88	GLN
1	A	92	VAL
1	A	94	LEU
1	A	98	ARG
1	A	109	THR
1	A	114	ARG
1	A	116	LEU
1	A	118	THR
1	A	120	GLN
1	A	123	THR
1	A	124	MET
1	A	127	HIS
1	A	128	THR
1	A	130	ARG
1	A	132	LEU
1	A	137	ARG
1	A	138	ILE
1	A	143	ARG
1	A	145	GLN
1	A	147	ARG
1	A	148	LEU
1	A	155	VAL
1	A	163	THR
1	A	165	ARG
1	A	200	GLN
1	A	202	VAL
1	A	209	SER
1	A	214	VAL
1	A	215	ASP
1	A	219	LEU
1	A	221	ASP
1	A	226	ILE
1	A	229	ASP
1	A	230	MET
1	A	238	LEU
1	A	262	ARG
1	A	263	THR
1	A	271	LEU

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Mol	Chain	Res	Type
1	A	274	VAL
1	A	288	ILE
1	A	292	SER
1	A	315	GLU
1	A	323	GLN
1	A	327	ARG
1	A	335	SER
1	A	338	GLU
1	A	345	VAL
1	A	347	LEU
1	A	355	ILE
1	A	362	ILE
1	A	370	ASN
1	A	379	ARG
1	A	380	LEU
1	A	386	LYS
1	A	389	ARG
1	A	392	LEU
1	A	398	ASP
1	A	401	LYS
2	B	2	THR
2	B	4	THR
2	B	5	LYS
2	B	18	LEU
2	B	20	VAL
2	B	21	SER
2	B	25	GLN
2	B	32	VAL
2	B	40	GLN
2	B	41	ASP
2	B	42	GLN
2	B	47	GLU
2	B	51	SER
2	B	52	GLU
2	B	56	LEU
2	B	72	VAL
2	B	76	LYS
2	B	78	LYS
2	B	79	SER
2	B	83	CYS
2	B	87	LYS
2	B	92	ARG

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Mol	Chain	Res	Type
2	B	99	LEU
2	B	100	VAL
2	B	107	LEU
1	P	6	LEU
1	P	10	VAL
1	P	19	SER
1	P	23	VAL
1	P	26	LEU
1	P	28	GLN
1	P	32	GLN
1	P	36	THR
1	P	41	GLU
1	P	53	LYS
1	P	62	GLU
1	P	63	LYS
1	P	65	ARG
1	P	69	LYS
1	P	70	ARG
1	P	78	LEU
1	P	94	LEU
1	P	104	THR
1	P	120	GLN
1	P	123	THR
1	P	124	MET
1	P	137	ARG
1	P	139	GLN
1	P	142	LEU
1	P	143	ARG
1	P	145	GLN
1	P	147	ARG
1	P	148	LEU
1	P	151	VAL
1	P	156	ILE
1	P	165	ARG
1	P	171	VAL
1	P	172	SER
1	P	174	VAL
1	P	175	GLU
1	P	179	ARG
1	P	182	SER
1	P	188	THR
1	P	193	VAL

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Mol	Chain	Res	Type
1	P	195	ARG
1	P	204	LEU
1	P	205	ARG
1	P	209	SER
1	P	215	ASP
1	P	218	VAL
1	P	219	LEU
1	P	220	LEU
1	P	221	ASP
1	P	224	THR
1	P	226	ILE
1	P	230	MET
1	P	233	VAL
1	P	235	ILE
1	P	245	ARG
1	P	278	ARG
1	P	281	LEU
1	P	288	ILE
1	P	333	LEU
1	P	335	SER
1	P	339	GLU
1	P	344	GLU
1	P	347	LEU
1	P	353	THR
1	P	357	LEU
1	P	361	ARG
1	P	369	ASN
1	P	372	ARG
1	P	381	LEU
1	P	400	ARG
1	P	401	LYS
1	P	402	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	58	HIS
1	A	139	GLN
1	A	145	GLN
1	A	197	HIS
1	A	200	GLN

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Mol	Chain	Res	Type
1	A	240	ASN
1	A	297	GLN
1	A	358	GLN
1	A	370	ASN
1	P	32	GLN
1	P	139	GLN
1	P	145	GLN
1	P	200	GLN
1	P	240	ASN
1	P	277	GLN
1	P	296	ASN
1	P	297	GLN
1	P	369	ASN
1	P	370	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	NAI	P	504	-	38,38,48	1.36	5 (13%)	53,58,73	1.75	12 (22%)
3	FAD	A	501	-	58,58,58	1.15	6 (10%)	85,89,89	1.00	4 (4%)
4	NAI	A	503	-	38,38,48	1.35	5 (13%)	53,58,73	1.78	12 (22%)
5	FES	B	500	2	0,4,4	-	-	-	-	-
3	FAD	P	502	-	58,58,58	1.13	4 (6%)	85,89,89	1.08	4 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAI	P	504	-	-	5/22/51/72	0/4/4/5
3	FAD	A	501	-	-	6/34/50/50	0/6/6/6
4	NAI	A	503	-	-	5/22/51/72	0/4/4/5
5	FES	B	500	2	-	-	0/1/1/1
3	FAD	P	502	-	-	2/34/50/50	0/6/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	502	FAD	C4X-N5	4.68	1.40	1.30
3	A	501	FAD	C4X-N5	4.62	1.40	1.30
4	P	504	NAI	PA-O3	4.36	1.64	1.59
4	A	503	NAI	PA-O3	4.13	1.64	1.59
4	A	503	NAI	C2A-N1A	3.07	1.39	1.33
4	P	504	NAI	C2A-N1A	3.03	1.39	1.33
4	P	504	NAI	C2A-N3A	3.02	1.39	1.33
4	A	503	NAI	C2A-N3A	2.98	1.39	1.33
3	A	501	FAD	C6-C7	-2.91	1.35	1.39
3	P	502	FAD	C4A-N3A	2.74	1.39	1.34
4	P	504	NAI	PN-O3	2.64	1.62	1.59
3	P	502	FAD	C5A-C4A	-2.56	1.34	1.39
3	P	502	FAD	C6-C7	-2.40	1.36	1.39
3	A	501	FAD	C9-C8	2.37	1.42	1.39
4	A	503	NAI	C8A-N7A	2.28	1.36	1.31
4	P	504	NAI	C8A-N7A	2.27	1.36	1.31
4	A	503	NAI	PN-O3	2.24	1.61	1.59
3	A	501	FAD	C5A-C4A	-2.23	1.35	1.39
3	A	501	FAD	C4A-N3A	2.15	1.38	1.34
3	A	501	FAD	P-O3P	2.06	1.61	1.59

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	NAI	N3A-C2A-N1A	-5.71	119.94	128.58
4	P	504	NAI	N3A-C2A-N1A	-5.65	120.02	128.58
4	A	503	NAI	C5A-C4A-N3A	-4.44	120.61	126.72
4	P	504	NAI	C5A-C4A-N3A	-4.42	120.64	126.72
4	A	503	NAI	N9A-C8A-N7A	-4.19	107.99	113.94
4	P	504	NAI	N9A-C8A-N7A	-4.08	108.15	113.94
3	A	501	FAD	O4B-C1B-C2B	-3.93	98.21	106.62
4	A	503	NAI	C5A-N7A-C8A	3.47	108.91	103.45
4	A	503	NAI	C2A-N3A-C4A	3.43	120.21	111.83
4	P	504	NAI	C5A-N7A-C8A	3.37	108.74	103.45
4	P	504	NAI	C2A-N3A-C4A	3.36	120.03	111.83
3	P	502	FAD	C4X-C10-N10	3.29	121.19	116.48
4	A	503	NAI	N3A-C4A-N9A	3.28	132.75	127.17
4	P	504	NAI	N3A-C4A-N9A	3.11	132.45	127.17
3	P	502	FAD	O4B-C1B-N9A	2.76	113.38	108.09
3	A	501	FAD	C2B-C3B-C4B	-2.73	97.33	102.61
3	P	502	FAD	O3'-C3'-C2'	-2.65	102.91	108.93
4	A	503	NAI	O2A-PA-O3	2.64	114.42	107.27
3	P	502	FAD	O4B-C1B-C2B	-2.56	101.13	106.62
4	P	504	NAI	O2A-PA-O3	2.56	114.20	107.27
4	A	503	NAI	C4A-N9A-C8A	2.44	108.30	105.74
4	P	504	NAI	C4A-N9A-C8A	2.28	108.14	105.74
4	A	503	NAI	O1N-PN-O2N	2.28	123.04	112.44
3	A	501	FAD	C4X-C10-N10	2.27	119.73	116.48
4	P	504	NAI	O1N-PN-O2N	2.21	122.73	112.44
3	A	501	FAD	O2B-C2B-C3B	2.19	118.83	111.82
4	A	503	NAI	C4A-C5A-N7A	-2.14	108.13	110.58
4	P	504	NAI	O3-PA-O1A	-2.12	104.32	110.70
4	P	504	NAI	C4A-C5A-N7A	-2.09	108.19	110.58
4	A	503	NAI	O3-PA-O1A	-2.07	104.47	110.70
4	A	503	NAI	C1D-O4D-C4D	2.07	112.64	108.06
4	P	504	NAI	C1D-O4D-C4D	2.02	112.51	108.06

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	FAD	O4'-C4'-C5'-O5'
3	A	501	FAD	C5'-O5'-P-O2P
3	P	502	FAD	N10-C1'-C2'-O2'
3	P	502	FAD	C5'-O5'-P-O3P

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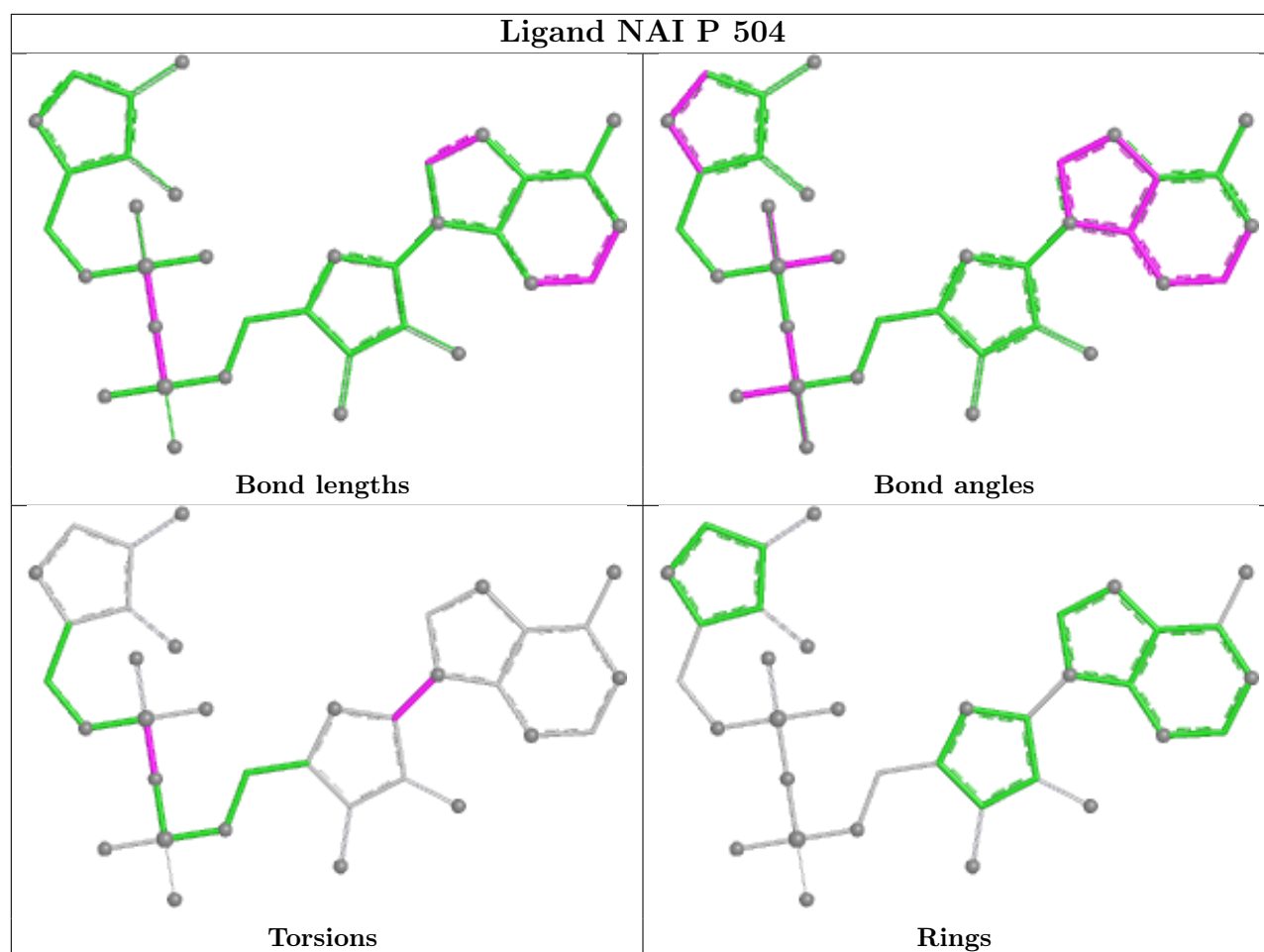
Mol	Chain	Res	Type	Atoms
3	A	501	FAD	C3'-C4'-C5'-O5'
3	A	501	FAD	C3B-C4B-C5B-O5B
4	A	503	NAI	C2B-C1B-N9A-C8A
4	P	504	NAI	C2B-C1B-N9A-C8A
4	P	504	NAI	PA-O3-PN-O2N
3	A	501	FAD	O4B-C4B-C5B-O5B
3	A	501	FAD	C5'-O5'-P-O1P
4	A	503	NAI	PA-O3-PN-O2N
4	P	504	NAI	PA-O3-PN-O1N
4	A	503	NAI	O4B-C1B-N9A-C8A
4	P	504	NAI	O4B-C1B-N9A-C8A
4	A	503	NAI	PA-O3-PN-O1N
4	A	503	NAI	C2B-C1B-N9A-C4A
4	P	504	NAI	C2B-C1B-N9A-C4A

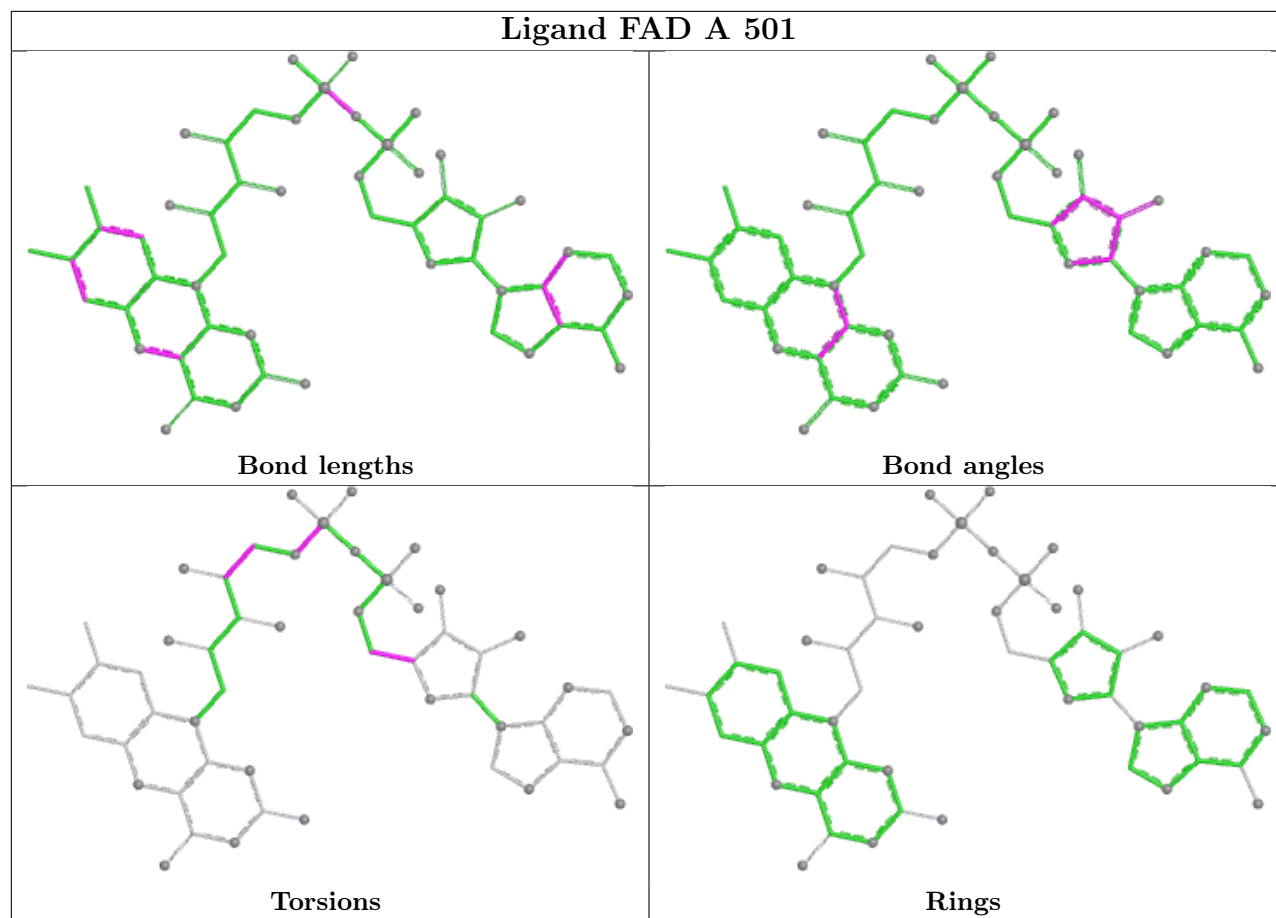
There are no ring outliers.

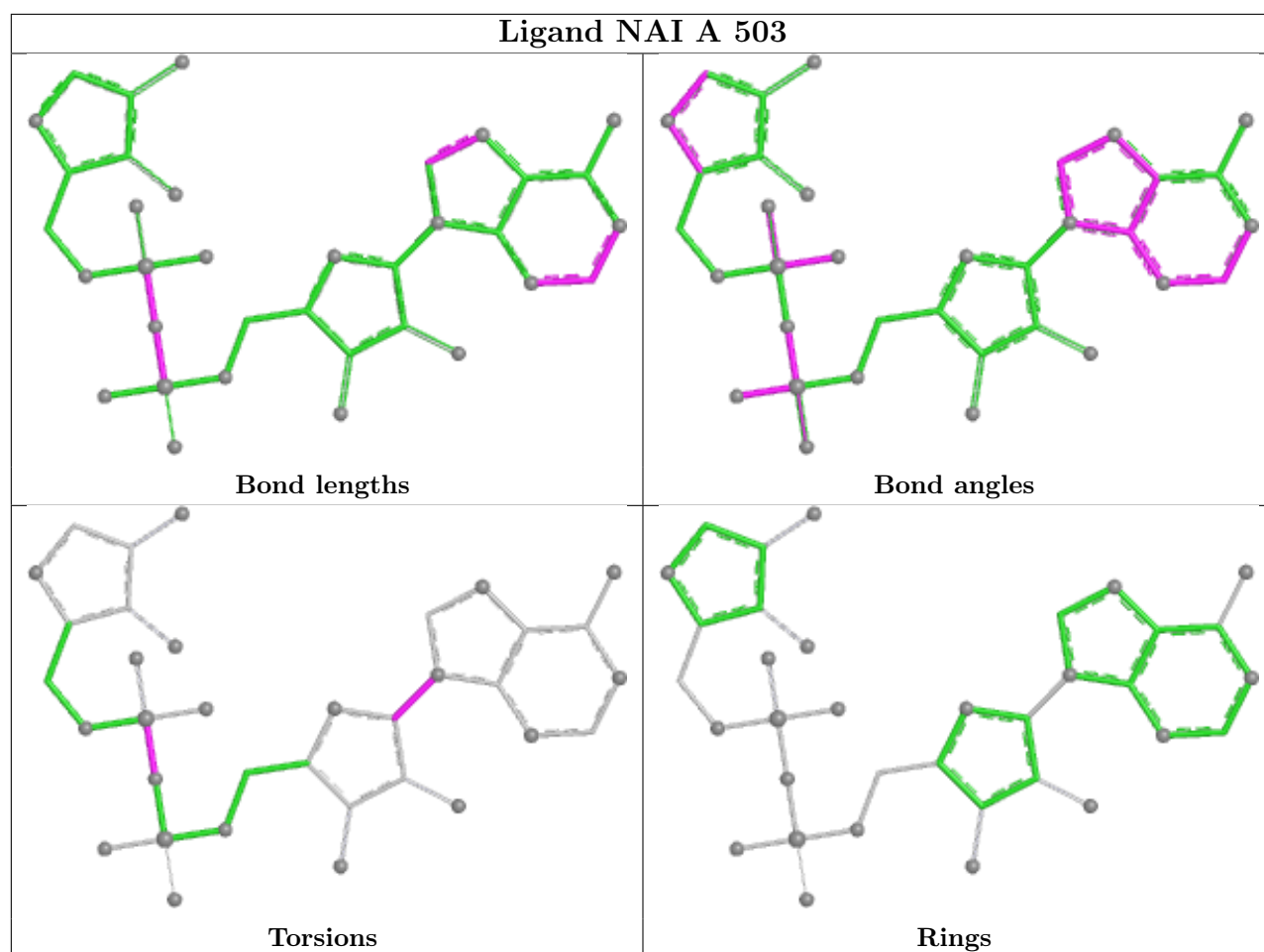
4 monomers are involved in 17 short contacts:

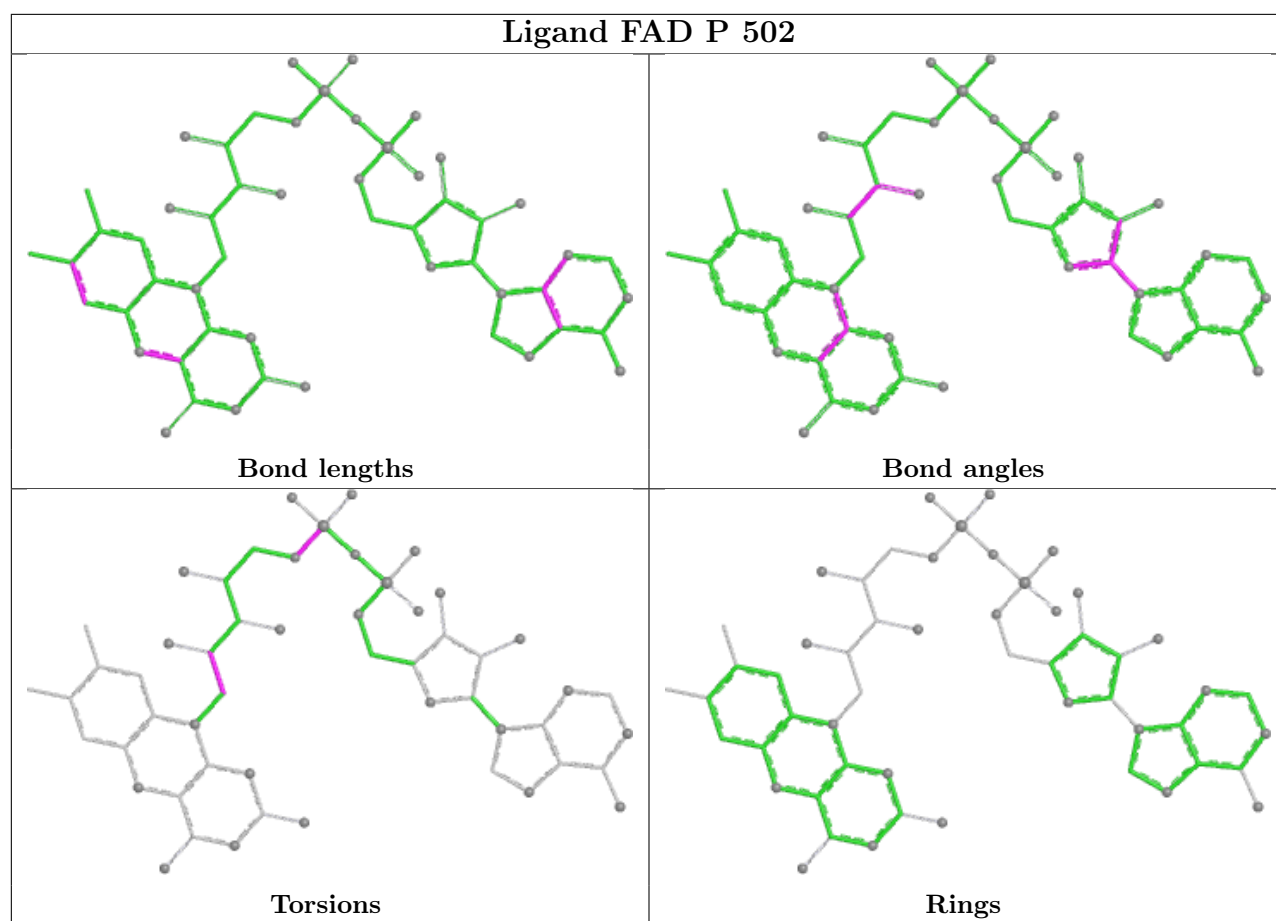
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	504	NAI	6	0
3	A	501	FAD	1	0
4	A	503	NAI	8	0
5	B	500	FES	2	0

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	402/408 (98%)	0.15	4 (0%) 79 82	18, 36, 65, 90	0
1	P	401/408 (98%)	0.18	6 (1%) 72 75	14, 37, 68, 110	0
2	B	106/109 (97%)	0.35	1 (0%) 81 83	26, 47, 70, 80	2 (1%)
All	All	909/925 (98%)	0.19	11 (1%) 76 79	14, 38, 68, 110	2 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	226	ILE	3.4
1	A	185	ALA	3.0
1	P	171	VAL	3.0
1	A	385	ALA	2.9
2	B	55	TYR	2.8
1	P	174	VAL	2.7
1	A	406	VAL	2.6
1	P	201	GLY	2.3
1	P	122	ALA	2.2
1	P	64	ILE	2.1
1	A	188	THR	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 ⓘ

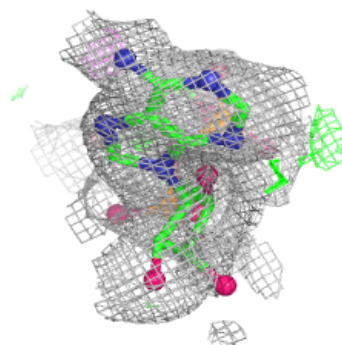
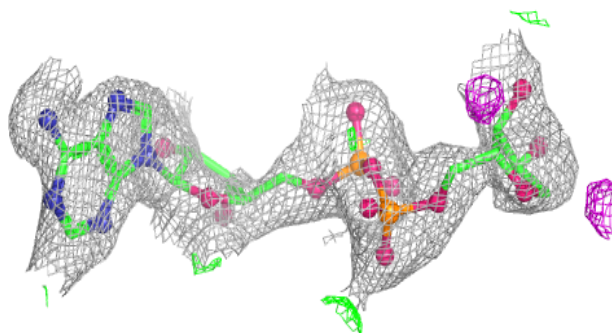
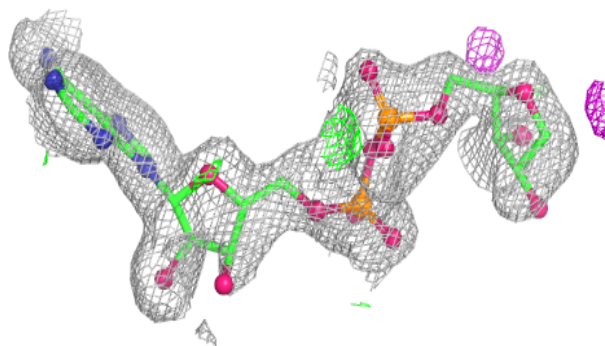
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAI	P	504	35/44	0.96	0.08	32,51,69,93	0
3	FAD	P	502	53/53	0.97	0.07	16,30,39,62	0
4	NAI	A	503	35/44	0.97	0.10	27,44,73,98	0
3	FAD	A	501	53/53	0.97	0.07	15,32,50,66	0
5	FES	B	500	4/4	0.99	0.03	34,35,37,37	0

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

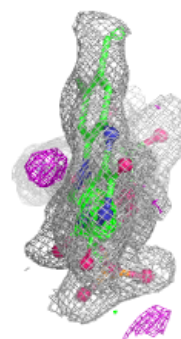
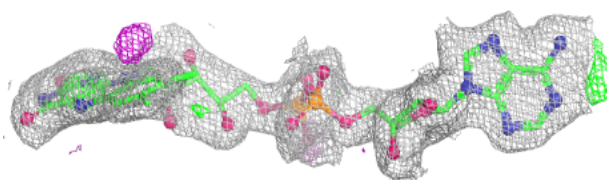
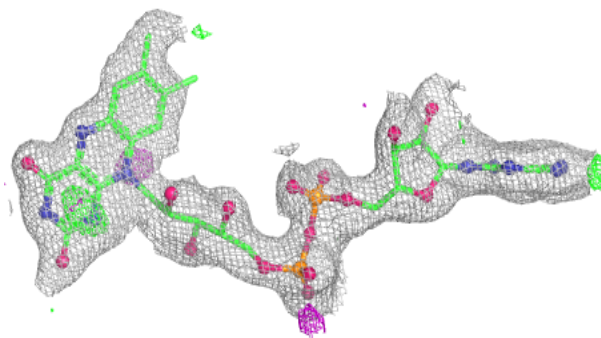
Electron density around NAI P 504:

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

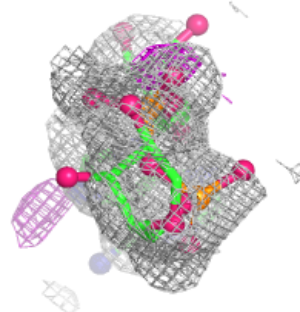
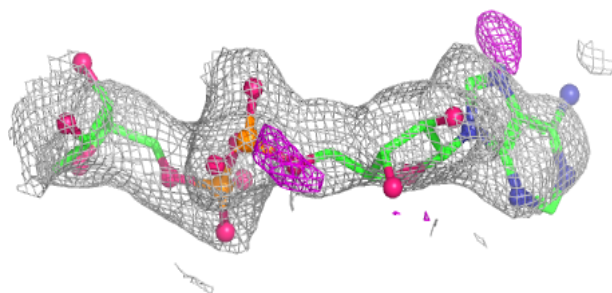
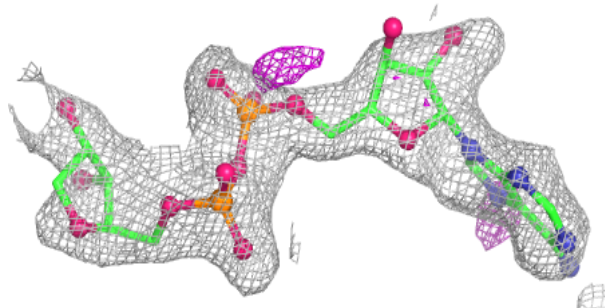


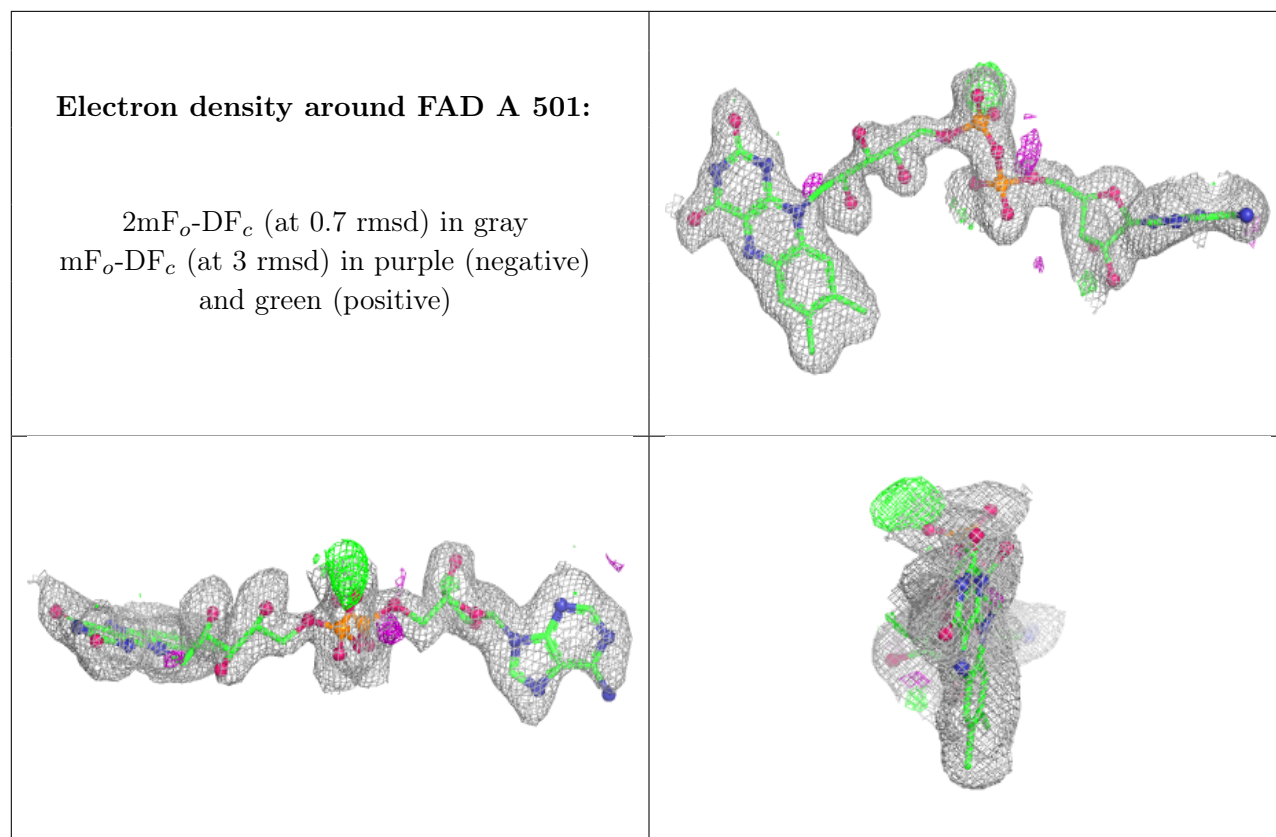
Electron density around FAD P 502:

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

**Electron density around NAI A 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.