



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:42 PM UTC

PDB ID : 1GOS / pdb_00001gos
Title : Human Monoamine Oxidase B
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Deposited on : 2001-10-26
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

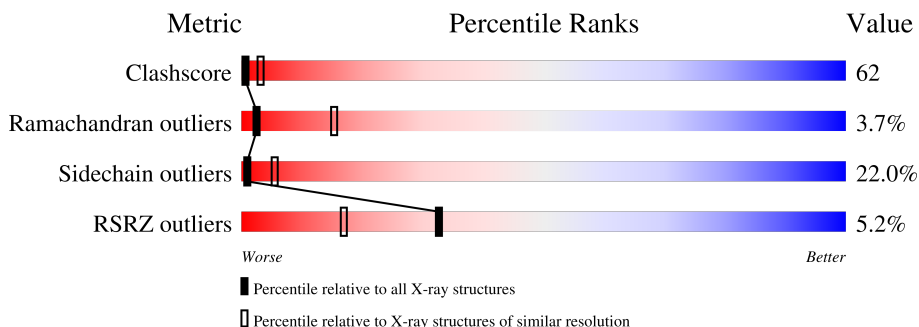
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

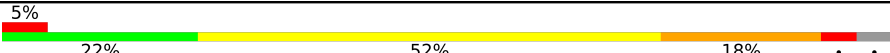
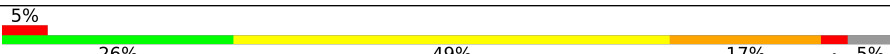
The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	520	
1	B	520	

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
3	NYP	A	601	X	-	X	-
3	NYP	B	601	X	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8020 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 MONOAMINE OXIDASE.

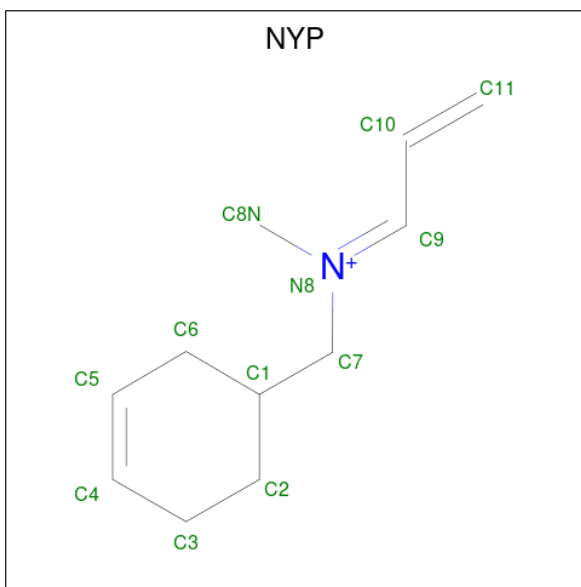
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3958	2531	678	725	24			
1	B	493	Total	C	N	O	S	0	0	0
			3932	2515	674	719	24			

- 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 N-[(E)-METHYL](PHENYL)-N-[(E)-2-PROPENYLIDENE]METHANAMINIUM (CCD ID: NYP) (formula: $C_{11}H_{18}N$).

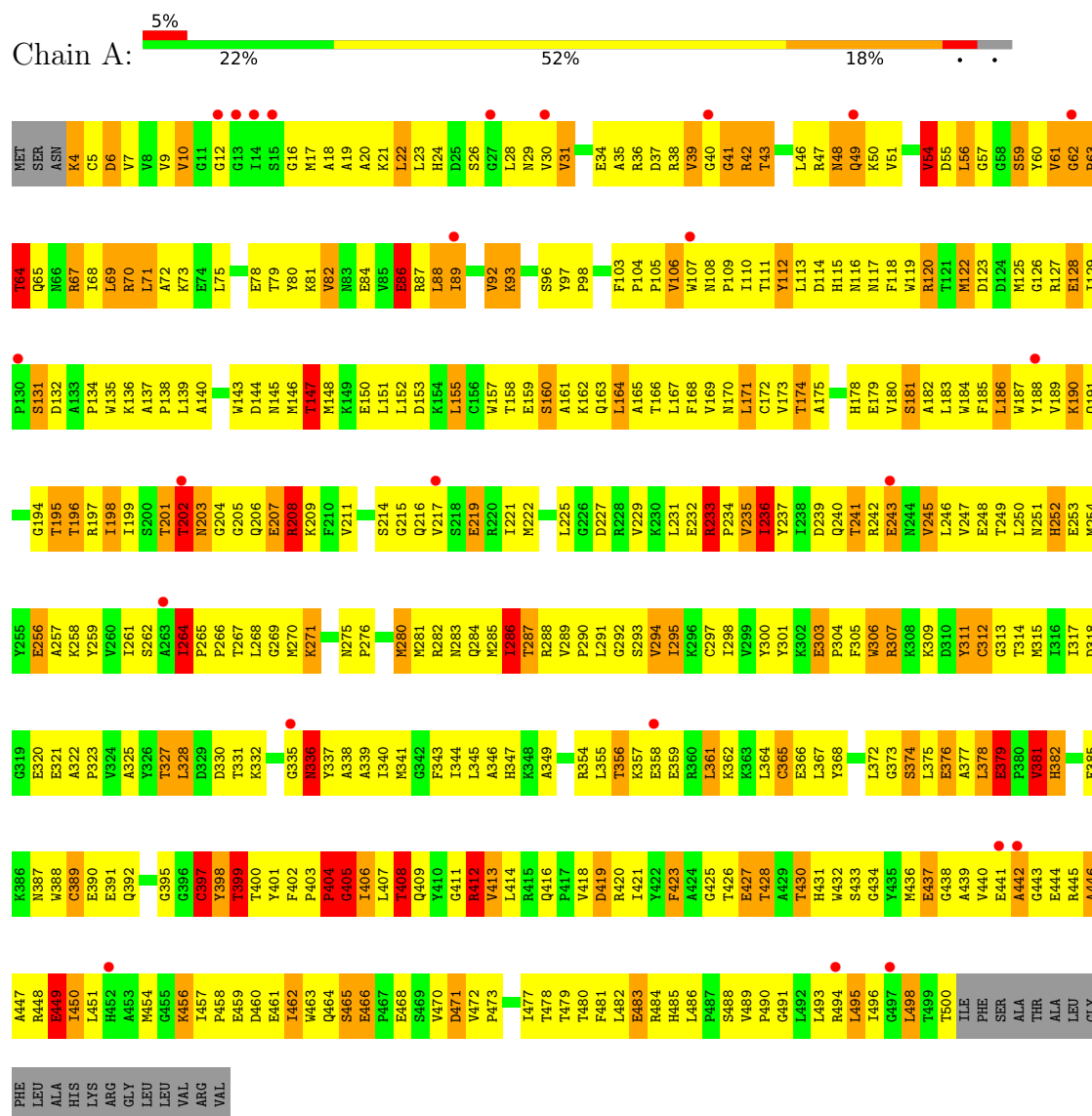


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			12	11	1		
3	B	1	Total	C	N	0	0
			12	11	1		

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: MONOAMINE OXIDASE



• Molecule 1: MONOAMINE OXIDASE



WORLDWIDE
PDB
PROTEIN DATA BANK

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	138.80Å 224.30Å 87.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 40.00 – 3.08	Depositor EDS
% Data completeness (in resolution range)	95.3 (40.00-3.00) 93.5 (40.00-3.08)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.06Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.271 0.253 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8020	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: FAD, NYP

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	0.93	4/4055 (0.1%)	1.59	63/5504 (1.1%)
1	B	1.01	2/4029 (0.0%)	1.58	63/5468 (1.2%)
All	All	0.97	6/8084 (0.1%)	1.59	126/10972 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	B	0	2
All	All	1	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	294	VAL	CA-CB	-7.13	1.47	1.55
1	B	169	VAL	CA-CB	-6.13	1.46	1.54
1	A	406	ILE	CA-CB	-5.46	1.48	1.54
1	A	235	VAL	CA-CB	-5.35	1.48	1.54
1	A	286	ILE	CA-CB	-5.22	1.47	1.54
1	B	173	VAL	CA-CB	-5.02	1.47	1.54

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	ILE	N-CA-C	17.48	126.06	111.90
1	B	406	ILE	N-CA-C	14.07	123.66	111.56
1	A	397	CYS	N-CA-C	12.37	127.58	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	THR	N-CA-C	12.36	128.13	113.18
1	B	397	CYS	N-CA-C	11.05	125.43	108.96
1	B	71	LEU	N-CA-C	-10.57	99.30	111.03
1	B	112	TYR	N-CA-C	-9.94	100.44	111.28
1	A	42	ARG	N-CA-C	-9.86	99.80	113.20
1	B	64	THR	N-CA-C	9.41	124.59	113.20
1	B	5	CYS	O-C-N	9.13	129.96	123.11
1	B	174	THR	N-CA-C	8.83	123.78	112.92
1	A	112	TYR	N-CA-C	-8.54	102.05	111.36
1	A	434	GLY	N-CA-C	-8.54	103.61	114.37
1	A	10	VAL	CA-C-N	-8.42	114.19	122.36
1	A	10	VAL	C-N-CA	-8.42	114.19	122.36
1	B	173	VAL	CA-C-N	-8.25	109.44	122.65
1	B	173	VAL	C-N-CA	-8.25	109.44	122.65
1	B	399	THR	N-CA-C	8.23	119.43	108.07
1	B	335	GLY	N-CA-C	-8.21	103.65	115.64
1	A	54	VAL	CB-CA-C	-8.09	96.41	110.65
1	A	405	GLY	CA-C-N	-8.06	114.84	122.66
1	A	405	GLY	C-N-CA	-8.06	114.84	122.66
1	B	10	VAL	CA-C-N	-7.94	114.66	122.36
1	B	10	VAL	C-N-CA	-7.94	114.66	122.36
1	A	57	GLY	CA-C-N	-7.87	115.41	122.73
1	A	57	GLY	C-N-CA	-7.87	115.41	122.73
1	A	202	THR	CA-C-N	-7.79	109.96	122.66
1	A	202	THR	C-N-CA	-7.79	109.96	122.66
1	B	336	ASN	N-CA-C	7.77	123.08	111.04
1	A	59	SER	N-CA-C	7.68	123.11	113.43
1	A	222	MET	N-CA-C	-7.68	102.91	111.82
1	B	67	ARG	CA-C-N	-7.65	109.55	120.42
1	B	67	ARG	C-N-CA	-7.65	109.55	120.42
1	A	335	GLY	N-CA-C	-7.59	104.73	115.43
1	A	312	CYS	N-CA-C	-7.58	100.32	110.55
1	B	11	GLY	N-CA-C	7.56	124.78	111.25
1	A	236	ILE	CB-CA-C	-7.43	103.37	110.65
1	B	465	SER	N-CA-C	7.42	120.11	110.53
1	A	235	VAL	CB-CA-C	-7.35	100.09	111.26
1	B	5	CYS	CB-CA-C	-7.20	104.00	114.87
1	A	413	VAL	N-CA-C	-7.10	106.57	113.53
1	A	67	ARG	CA-C-N	-7.07	110.39	120.42
1	A	67	ARG	C-N-CA	-7.07	110.39	120.42
1	B	5	CYS	N-CA-C	7.06	116.61	108.49
1	A	71	LEU	N-CA-C	-7.04	103.30	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ASP	N-CA-C	-6.84	104.94	113.55
1	A	465	SER	N-CA-C	6.81	119.74	110.35
1	B	59	SER	N-CA-C	6.77	122.19	113.18
1	B	202	THR	CA-C-N	-6.77	109.47	122.61
1	B	202	THR	C-N-CA	-6.77	109.47	122.61
1	B	173	VAL	CB-CA-C	-6.62	100.44	111.29
1	B	317	ILE	N-CA-C	6.57	117.34	107.75
1	B	227	ASP	N-CA-C	-6.52	105.19	113.01
1	A	317	ILE	N-CA-C	6.47	117.20	107.75
1	B	295	ILE	CB-CA-C	-6.44	101.10	110.63
1	B	54	VAL	CB-CA-C	-6.39	99.41	110.65
1	A	89	ILE	N-CA-C	6.39	117.67	108.48
1	B	312	CYS	N-CA-C	-6.36	101.96	110.55
1	B	362	LYS	N-CA-C	-6.36	103.48	111.11
1	A	62	GLY	N-CA-C	6.33	125.25	112.34
1	B	405	GLY	CA-C-N	-6.29	116.72	123.08
1	B	405	GLY	C-N-CA	-6.29	116.72	123.08
1	B	399	THR	CB-CA-C	-6.27	100.00	114.41
1	A	286	ILE	CB-CA-C	-6.26	101.03	111.29
1	A	106	VAL	N-CA-C	6.25	116.86	108.11
1	B	434	GLY	N-CA-C	-6.20	106.19	114.25
1	A	247	VAL	N-CA-C	-6.17	99.37	108.99
1	B	63	PRO	CA-C-N	-6.15	109.63	121.94
1	B	63	PRO	C-N-CA	-6.15	109.63	121.94
1	B	62	GLY	N-CA-C	6.12	124.83	112.34
1	A	70	ARG	N-CA-C	6.09	117.58	111.07
1	A	63	PRO	CA-C-N	-6.07	109.75	121.58
1	A	63	PRO	C-N-CA	-6.07	109.75	121.58
1	A	203	ASN	N-CA-C	6.05	119.39	112.97
1	B	130	PRO	CA-C-O	-5.94	114.84	121.32
1	A	295	ILE	CB-CA-C	-5.92	102.37	110.77
1	B	18	ALA	N-CA-C	-5.92	104.01	111.11
1	A	92	VAL	N-CA-C	5.89	116.77	108.17
1	A	381	VAL	N-CA-C	-5.88	107.55	113.20
1	A	120	ARG	N-CA-C	-5.83	104.93	111.28
1	B	51	VAL	CB-CA-C	-5.78	104.58	110.88
1	A	264	ILE	N-CA-CB	-5.76	103.15	111.21
1	A	227	ASP	N-CA-C	-5.71	106.16	113.01
1	A	131	SER	N-CA-C	-5.69	104.99	111.14
1	A	186	LEU	N-CA-C	-5.69	104.77	110.97
1	A	208	ARG	N-CA-C	5.65	118.42	109.50
1	B	286	ILE	CB-CA-C	-5.65	102.03	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	PRO	CB-CA-C	-5.64	103.44	111.68
1	B	98	PRO	N-CD-CG	-5.62	94.77	103.20
1	B	156	CYS	CB-CA-C	-5.57	100.91	110.16
1	B	413	VAL	CB-CA-C	-5.57	104.81	110.88
1	B	42	ARG	N-CA-C	-5.50	99.08	110.80
1	B	369	ALA	N-CA-C	-5.50	105.28	111.28
1	B	6	ASP	N-CA-C	5.48	119.94	111.56
1	A	336	ASN	N-CA-C	5.43	122.38	110.80
1	A	404	PRO	CA-C-N	-5.43	109.71	121.17
1	A	404	PRO	C-N-CA	-5.43	109.71	121.17
1	A	399	THR	CB-CA-C	-5.43	99.62	110.42
1	A	423	PHE	N-CA-C	5.42	117.67	108.02
1	B	79	THR	N-CA-CB	-5.39	102.64	110.36
1	A	294	VAL	CB-CA-C	-5.39	103.50	111.80
1	B	392	GLN	CA-C-N	-5.35	114.12	122.73
1	B	392	GLN	C-N-CA	-5.35	114.12	122.73
1	B	488	SER	CA-C-N	-5.32	116.89	120.24
1	B	488	SER	C-N-CA	-5.32	116.89	120.24
1	B	236	ILE	CB-CA-C	-5.30	105.10	110.88
1	A	147	THR	N-CA-CB	-5.29	102.39	110.85
1	B	235	VAL	CB-CA-C	-5.25	103.50	111.33
1	B	173	VAL	N-CA-C	-5.24	98.44	109.34
1	A	233	ARG	CB-CA-C	-5.19	104.06	110.96
1	A	311	TYR	CB-CA-C	-5.16	100.26	109.71
1	B	427	GLU	N-CA-C	-5.13	107.09	113.19
1	B	74	GLU	CA-C-N	-5.12	114.45	122.65
1	B	74	GLU	C-N-CA	-5.12	114.45	122.65
1	B	314	THR	CA-C-N	-5.12	115.51	122.93
1	B	314	THR	C-N-CA	-5.12	115.51	122.93
1	B	131	SER	N-CA-C	-5.11	105.62	111.14
1	A	93	LYS	N-CA-C	-5.10	105.72	112.24
1	A	449	GLU	N-CA-C	-5.06	105.65	111.07
1	A	10	VAL	N-CA-C	5.05	119.47	112.35
1	A	470	VAL	N-CA-C	-5.04	105.51	111.00
1	A	207	GLU	CA-C-N	-5.03	114.77	122.62
1	A	207	GLU	C-N-CA	-5.03	114.77	122.62
1	B	10	VAL	N-CA-C	5.03	119.45	112.35
1	A	335	GLY	CA-C-O	5.01	124.83	119.06
1	A	379	GLU	N-CA-C	5.00	118.92	110.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	64	THR	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	397	CYS	Peptide
1	A	405	GLY	Peptide
1	B	397	CYS	Peptide
1	B	405	GLY	Peptide

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	3958	0	3959	553	0
1	B	3932	0	3931	461	0
2	A	53	0	29	7	0
2	B	53	0	29	4	0
3	A	12	0	16	12	0
3	B	12	0	16	8	0
All	All	8020	0	7980	993	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 62.

All (993) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:THR:CG2	1:B:208:ARG:HD3	1.66	1.25
1:A:79:THR:CG2	1:A:208:ARG:HD3	1.70	1.20
1:B:175:ALA:HB1	1:B:179:GLU:OE1	1.40	1.19
1:A:82:VAL:HG23	1:A:207:GLU:O	1.43	1.19
1:A:22:LEU:O	1:A:22:LEU:HD12	1.37	1.18
1:A:65:GLN:HB3	1:A:437:GLU:HG3	1.24	1.15
1:B:22:LEU:HD12	1:B:22:LEU:O	1.42	1.15
1:B:82:VAL:HG23	1:B:207:GLU:O	1.45	1.15
1:B:480:THR:HB	1:B:483:GLU:HB2	1.30	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:VAL:HG12	1:B:174:THR:N	1.57	1.12
1:B:88:LEU:N	1:B:88:LEU:HD23	1.49	1.12
1:A:51:VAL:HG11	1:A:54:VAL:HG22	1.32	1.12
1:A:304:PRO:HB2	1:A:307:ARG:HD2	1.28	1.12
1:B:315:MET:HE3	1:B:327:THR:HG21	1.31	1.11
1:B:64:THR:HG22	1:B:432:TRP:HE1	1.03	1.10
1:A:480:THR:HB	1:A:483:GLU:HB2	1.33	1.10
1:A:79:THR:HG21	1:A:208:ARG:HD3	1.31	1.09
1:A:236:ILE:HD11	1:A:250:LEU:HD12	1.32	1.09
1:B:79:THR:HG21	1:B:208:ARG:HD3	1.29	1.08
1:A:171:LEU:HD13	3:A:601:NYP:H3	1.35	1.08
1:B:125:MET:HE2	1:B:186:LEU:CD1	1.85	1.07
1:A:175:ALA:HB1	1:A:179:GLU:OE1	1.56	1.05
1:A:236:ILE:HD13	1:B:236:ILE:HD13	1.33	1.05
1:A:88:LEU:HD23	1:A:88:LEU:N	1.67	1.04
1:B:323:PRO:HD2	1:B:367:LEU:HD22	1.40	1.04
1:A:28:LEU:CD1	1:A:454:MET:HE1	1.88	1.03
1:B:264:ILE:CG2	1:B:268:LEU:HB2	1.89	1.03
1:A:456:LYS:O	1:A:457:ILE:HG13	1.56	1.02
1:B:22:LEU:HD12	1:B:22:LEU:C	1.79	1.00
1:A:304:PRO:HB2	1:A:307:ARG:CD	1.90	1.00
1:B:236:ILE:HD11	1:B:250:LEU:HD12	1.40	1.00
1:B:125:MET:HE2	1:B:186:LEU:HD11	1.38	0.99
1:A:174:THR:CG2	1:A:293:SER:H	1.75	0.99
1:A:233:ARG:NH1	1:A:253:GLU:OE2	1.96	0.99
1:A:327:THR:O	1:A:328:LEU:HD23	1.63	0.99
1:B:249:THR:HG22	1:B:251:ASN:H	1.22	0.99
1:B:65:GLN:HB3	1:B:437:GLU:HG3	1.41	0.98
1:A:64:THR:HG22	1:A:432:TRP:HE1	1.25	0.98
1:A:87:ARG:C	1:A:88:LEU:HD23	1.88	0.98
1:B:249:THR:CG2	1:B:251:ASN:HB2	1.92	0.98
1:A:117:ASN:ND2	1:A:488:SER:HB3	1.80	0.97
1:B:10:VAL:HG22	1:B:235:VAL:HG21	1.45	0.96
1:A:174:THR:CG2	1:A:174:THR:O	2.13	0.96
1:A:67:ARG:N	1:A:437:GLU:OE2	1.98	0.96
1:B:173:VAL:CG1	1:B:174:THR:N	2.29	0.96
1:B:264:ILE:HG23	1:B:268:LEU:HB2	1.45	0.96
1:A:22:LEU:HD12	1:A:22:LEU:C	1.81	0.95
1:B:456:LYS:O	1:B:457:ILE:HG13	1.65	0.95
1:A:28:LEU:HD13	1:A:454:MET:HE1	1.48	0.95
1:A:117:ASN:HD22	1:A:488:SER:HB3	1.29	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:THR:HG21	1:B:208:ARG:CD	1.97	0.95
1:A:264:ILE:HG23	1:A:268:LEU:HB2	1.48	0.94
1:A:201:THR:HG22	1:A:202:THR:N	1.80	0.94
1:B:264:ILE:HG22	1:B:265:PRO:O	1.67	0.93
1:B:243:GLU:O	1:B:420:ARG:NH1	2.01	0.93
1:B:28:LEU:HD13	1:B:454:MET:HE1	1.48	0.93
1:A:270:MET:HG2	1:A:286:ILE:CG2	1.98	0.92
1:B:125:MET:CE	1:B:186:LEU:HD11	1.99	0.92
1:B:64:THR:HG22	1:B:432:TRP:NE1	1.85	0.92
1:B:171:LEU:HD13	3:B:601:NYP:H3	1.50	0.92
1:B:79:THR:CG2	1:B:208:ARG:CD	2.49	0.91
1:A:125:MET:HE2	1:A:186:LEU:HD11	1.50	0.91
1:A:174:THR:CG2	1:A:293:SER:N	2.34	0.91
1:B:67:ARG:N	1:B:437:GLU:OE2	2.03	0.91
1:A:125:MET:CE	1:A:186:LEU:HD11	2.01	0.91
1:B:304:PRO:HB2	1:B:307:ARG:HD2	1.52	0.91
1:A:258:LYS:O	1:A:259:TYR:CG	2.23	0.91
1:B:88:LEU:N	1:B:88:LEU:CD2	2.27	0.90
1:B:87:ARG:C	1:B:88:LEU:HD23	1.96	0.90
1:B:173:VAL:HG12	1:B:174:THR:H	1.32	0.90
1:B:448:ARG:NH1	1:B:464:GLN:HB2	1.87	0.90
1:B:171:LEU:HD22	1:B:171:LEU:O	1.72	0.89
1:A:71:LEU:O	1:A:75:LEU:HD12	1.71	0.89
1:A:448:ARG:NH1	1:A:464:GLN:HB2	1.88	0.89
1:B:49:GLN:HG3	1:B:50:LYS:N	1.87	0.88
1:B:174:THR:CG2	1:B:293:SER:H	1.87	0.88
1:B:51:VAL:HG11	1:B:54:VAL:HG22	1.53	0.88
1:B:249:THR:HG22	1:B:251:ASN:HB2	1.52	0.87
1:A:65:GLN:CB	1:A:437:GLU:HG3	2.04	0.87
1:B:70:ARG:NH2	1:B:444:GLU:OE2	2.07	0.87
1:A:323:PRO:HD2	1:A:367:LEU:HD22	1.56	0.87
1:A:315:MET:H	1:A:327:THR:HG22	1.40	0.87
1:A:174:THR:HG21	1:A:293:SER:N	1.90	0.87
1:B:201:THR:HG22	1:B:202:THR:N	1.87	0.87
1:A:480:THR:O	1:A:481:PHE:C	2.16	0.87
1:A:171:LEU:HD13	3:A:601:NYP:C3	2.04	0.87
1:A:171:LEU:CD1	3:A:601:NYP:H3	2.04	0.86
1:A:249:THR:HG22	1:A:251:ASN:H	1.40	0.86
1:A:327:THR:C	1:A:328:LEU:HD23	2.00	0.86
1:A:49:GLN:HG3	1:A:50:LYS:N	1.89	0.86
1:A:286:ILE:O	1:A:286:ILE:HG22	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LEU:O	1:B:75:LEU:HD12	1.76	0.85
1:A:79:THR:HG21	1:A:208:ARG:CD	2.06	0.85
1:A:79:THR:HG23	1:A:208:ARG:HD3	1.57	0.85
1:A:41:GLY:C	1:A:43:THR:H	1.85	0.85
1:B:216:GLN:HA	1:B:219:GLU:HG3	1.56	0.85
1:A:191:GLN:HE22	1:A:433:SER:N	1.75	0.85
1:B:270:MET:HG2	1:B:286:ILE:CG2	2.07	0.84
1:B:258:LYS:O	1:B:259:TYR:CG	2.30	0.84
1:B:471:ASP:OD1	1:B:471:ASP:N	2.01	0.84
1:A:174:THR:O	1:A:174:THR:HG22	1.78	0.84
1:B:79:THR:HG23	1:B:208:ARG:HD3	1.60	0.84
1:B:268:LEU:O	1:B:271:LYS:HB2	1.78	0.84
1:A:471:ASP:OD1	1:A:471:ASP:N	2.06	0.83
1:A:268:LEU:O	1:A:271:LYS:HB2	1.79	0.83
1:B:425:GLY:O	1:B:428:THR:HB	1.79	0.83
1:B:408:THR:HG22	1:B:409:GLN:HG2	1.61	0.82
1:A:147:THR:HG22	1:A:150:GLU:H	1.45	0.82
1:A:304:PRO:CB	1:A:307:ARG:HD2	2.10	0.82
1:B:270:MET:HG2	1:B:286:ILE:HG22	1.62	0.82
1:A:488:SER:HB2	1:A:490:PRO:HD2	1.61	0.82
1:A:243:GLU:O	1:A:420:ARG:NH1	2.13	0.81
1:B:240:GLN:OE1	1:B:419:ASP:HB3	1.79	0.81
1:B:315:MET:CE	1:B:327:THR:HG21	2.09	0.81
1:B:144:ASP:OD2	1:B:408:THR:HB	1.80	0.81
1:A:88:LEU:N	1:A:88:LEU:CD2	2.45	0.80
1:B:174:THR:CG2	1:B:174:THR:O	2.29	0.80
1:B:173:VAL:CG1	1:B:174:THR:H	1.92	0.79
1:A:264:ILE:CG2	1:A:268:LEU:HB2	2.12	0.79
1:B:327:THR:O	1:B:328:LEU:HD23	1.82	0.79
1:B:289:VAL:O	1:B:289:VAL:HG23	1.79	0.79
1:A:64:THR:HG22	1:A:432:TRP:NE1	1.98	0.79
1:B:65:GLN:CB	1:B:437:GLU:HG3	2.12	0.79
1:A:41:GLY:N	1:A:43:THR:HG22	1.98	0.78
1:A:448:ARG:HD2	1:A:461:GLU:O	1.83	0.78
1:A:258:LYS:O	1:A:259:TYR:CD1	2.36	0.78
1:B:86:GLU:OE2	1:B:86:GLU:N	2.16	0.78
1:A:79:THR:CG2	1:A:208:ARG:CD	2.60	0.78
1:A:251:ASN:O	1:A:252:HIS:HB2	1.83	0.78
1:A:129:ILE:O	1:A:190:LYS:HE2	1.83	0.77
1:B:249:THR:HG21	1:B:251:ASN:HB2	1.66	0.77
1:B:251:ASN:O	1:B:252:HIS:HB2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:THR:O	1:B:481:PHE:C	2.28	0.77
1:A:173:VAL:HG12	1:A:174:THR:H	1.48	0.77
1:A:174:THR:HG22	1:A:293:SER:H	1.48	0.77
1:A:209:LYS:NZ	1:A:330:ASP:OD1	2.17	0.77
1:A:30:VAL:CG1	1:A:31:VAL:N	2.47	0.77
1:B:171:LEU:O	1:B:171:LEU:CD2	2.33	0.76
1:B:125:MET:HE2	1:B:186:LEU:HD13	1.65	0.76
1:A:28:LEU:HD11	1:A:454:MET:HE1	1.65	0.76
1:A:125:MET:HE2	1:A:186:LEU:CD1	2.16	0.76
1:B:47:ARG:NH2	1:B:219:GLU:OE1	2.17	0.76
1:A:265:PRO:HD2	1:A:268:LEU:HD12	1.68	0.76
1:B:174:THR:O	1:B:174:THR:HG23	1.84	0.76
1:A:64:THR:CG2	1:A:432:TRP:HE1	1.98	0.76
1:A:79:THR:HG21	1:A:208:ARG:HH11	1.50	0.76
1:B:92:VAL:HG22	1:B:318:ASP:CB	2.15	0.76
1:A:86:GLU:N	1:A:86:GLU:OE2	2.18	0.75
1:A:315:MET:HE3	1:A:327:THR:HG21	1.67	0.75
1:A:65:GLN:HB3	1:A:437:GLU:CG	2.13	0.75
1:B:174:THR:CG2	1:B:293:SER:N	2.49	0.75
1:A:285:MET:C	1:A:287:THR:H	1.92	0.75
1:B:171:LEU:CD1	3:B:601:NYP:H3	2.15	0.75
1:A:10:VAL:HG22	1:A:235:VAL:HG21	1.69	0.75
1:B:41:GLY:C	1:B:43:THR:H	1.94	0.75
1:B:28:LEU:CD1	1:B:454:MET:HE1	2.17	0.74
1:B:117:ASN:ND2	1:B:488:SER:HB3	2.01	0.74
1:B:174:THR:HG21	1:B:293:SER:N	2.02	0.74
1:A:236:ILE:CD1	1:A:250:LEU:HD12	2.13	0.74
1:B:171:LEU:HD13	3:B:601:NYP:C3	2.17	0.74
1:B:174:THR:HG22	1:B:293:SER:H	1.51	0.74
1:A:267:THR:HG22	1:B:270:MET:HE2	1.67	0.74
1:B:315:MET:H	1:B:327:THR:HG22	1.52	0.74
1:A:288:ARG:NH2	1:B:291:LEU:O	2.20	0.74
1:A:293:SER:HB3	1:A:389:CYS:SG	2.28	0.74
1:A:286:ILE:CG2	1:A:286:ILE:O	2.36	0.74
1:A:275:ASN:HA	1:A:276:PRO:C	2.13	0.74
1:B:253:GLU:OE1	1:B:255:TYR:OH	2.02	0.74
1:B:117:ASN:HD22	1:B:488:SER:CB	2.00	0.73
1:B:64:THR:CG2	1:B:432:TRP:HE1	1.93	0.73
1:A:428:THR:HG23	1:A:445:ARG:HH12	1.53	0.73
1:A:120:ARG:NH2	1:A:486:LEU:O	2.22	0.73
1:B:7:VAL:HG22	1:B:259:TYR:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:MET:CE	1:B:186:LEU:CD1	2.62	0.73
1:A:171:LEU:CD1	3:A:601:NYP:H2	2.18	0.73
1:A:173:VAL:HG12	1:A:174:THR:N	2.02	0.72
1:B:275:ASN:HA	1:B:276:PRO:C	2.13	0.72
1:A:282:ARG:NH2	1:A:423:PHE:CE2	2.57	0.72
1:A:356:THR:OG1	1:A:359:GLU:HG3	1.87	0.72
1:B:54:VAL:CG1	1:B:300:TYR:OH	2.35	0.72
1:A:287:THR:HG23	1:A:287:THR:O	1.88	0.72
1:B:209:LYS:NZ	1:B:330:ASP:OD1	2.22	0.72
1:A:71:LEU:O	1:A:75:LEU:CD1	2.37	0.72
1:B:188:TYR:O	1:B:191:GLN:HG3	1.89	0.72
1:A:22:LEU:C	1:A:22:LEU:CD1	2.59	0.71
1:A:249:THR:CG2	1:A:251:ASN:HB2	2.19	0.71
1:B:78:GLU:O	1:B:211:VAL:HG23	1.89	0.71
1:B:431:HIS:O	1:B:432:TRP:C	2.29	0.71
1:A:249:THR:HG22	1:A:251:ASN:HB2	1.72	0.71
1:A:264:ILE:HG23	1:A:268:LEU:CB	2.19	0.71
1:A:300:TYR:CD2	1:A:339:ALA:HB2	2.25	0.71
1:A:37:ASP:O	1:A:231:LEU:HD13	1.90	0.71
1:B:111:THR:HG23	1:B:158:THR:HG21	1.72	0.71
1:A:43:THR:HG22	1:A:43:THR:O	1.90	0.71
1:A:408:THR:HG22	1:A:409:GLN:HG2	1.71	0.71
2:A:600:FAD:O2A	2:A:600:FAD:O5'	2.07	0.70
2:B:600:FAD:O2A	2:B:600:FAD:O5'	2.07	0.70
1:A:43:THR:O	1:A:43:THR:CG2	2.39	0.70
1:A:240:GLN:OE1	1:A:419:ASP:HB3	1.90	0.70
1:A:174:THR:O	1:A:174:THR:HG23	1.92	0.70
1:A:425:GLY:O	1:A:428:THR:HB	1.91	0.70
1:A:428:THR:CG2	1:A:445:ARG:HH12	2.05	0.70
1:B:22:LEU:C	1:B:22:LEU:CD1	2.56	0.70
1:A:24:HIS:C	1:A:26:SER:H	1.99	0.70
1:B:10:VAL:CG2	1:B:235:VAL:HG21	2.22	0.70
1:B:88:LEU:HD23	1:B:88:LEU:H	1.54	0.70
1:A:117:ASN:HD22	1:A:488:SER:CB	2.03	0.70
1:B:239:ASP:OD1	1:B:241:THR:HB	1.92	0.70
1:B:249:THR:HG22	1:B:251:ASN:N	2.02	0.69
1:B:117:ASN:HD22	1:B:488:SER:HB3	1.56	0.69
1:A:291:LEU:HD23	1:A:400:THR:HA	1.74	0.69
1:A:314:THR:HA	1:A:327:THR:O	1.92	0.69
1:B:198:ILE:HG22	1:B:199:ILE:HG13	1.73	0.69
1:B:445:ARG:HD2	1:B:463:TRP:CZ2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:MET:HE2	1:B:267:THR:HG22	1.75	0.69
1:B:63:PRO:HG2	1:B:204:GLY:HA2	1.73	0.69
1:B:265:PRO:HD2	1:B:268:LEU:HD12	1.74	0.69
1:B:293:SER:HB3	1:B:389:CYS:SG	2.32	0.69
1:A:122:MET:HE1	1:A:185:PHE:HE2	1.58	0.69
1:B:12:GLY:HA3	1:B:34:GLU:OE1	1.93	0.68
1:A:456:LYS:C	1:A:457:ILE:HG13	2.18	0.68
1:B:79:THR:HG21	1:B:208:ARG:HH11	1.58	0.68
1:B:387:ASN:O	1:B:390:GLU:HG2	1.93	0.68
1:B:300:TYR:CD2	1:B:339:ALA:HB2	2.29	0.68
1:A:143:TRP:HA	1:A:146:MET:CE	2.24	0.68
1:A:426:THR:C	1:A:428:THR:H	2.01	0.68
1:B:37:ASP:N	1:B:37:ASP:OD1	2.16	0.68
1:B:406:ILE:O	1:B:407:LEU:C	2.35	0.68
1:A:488:SER:CB	1:A:490:PRO:HD2	2.25	0.68
1:A:109:PRO:C	1:A:111:THR:H	2.02	0.67
1:A:399:THR:HG22	1:A:400:THR:H	1.60	0.67
1:A:54:VAL:HG13	1:A:300:TYR:OH	1.95	0.67
1:B:240:GLN:NE2	1:B:421:ILE:HG13	2.10	0.67
1:A:280:MET:HG3	1:B:389:CYS:HB3	1.76	0.67
1:A:364:LEU:O	1:A:367:LEU:HB3	1.94	0.67
1:B:236:ILE:HG22	1:B:237:TYR:HB2	1.77	0.67
1:A:34:GLU:OE1	2:A:600:FAD:O3B	2.12	0.67
1:A:451:LEU:HB3	1:A:457:ILE:HD12	1.77	0.67
1:B:320:GLU:OE2	1:B:347:HIS:CE1	2.46	0.67
1:A:82:VAL:CG2	1:A:207:GLU:O	2.33	0.67
1:A:37:ASP:OD1	1:A:37:ASP:N	2.28	0.67
1:A:119:TRP:CE3	1:A:195:THR:HG21	2.29	0.67
1:B:92:VAL:HG22	1:B:318:ASP:HB2	1.77	0.67
1:A:315:MET:CE	1:A:327:THR:HG21	2.24	0.67
1:B:428:THR:CG2	1:B:445:ARG:HH12	2.06	0.67
1:A:126:GLY:C	1:A:128:GLU:H	2.02	0.66
1:A:448:ARG:NH1	1:A:462:ILE:O	2.28	0.66
1:B:220:ARG:HA	1:B:223:ASP:OD2	1.95	0.66
1:A:86:GLU:HG2	1:A:312:CYS:HB3	1.77	0.66
1:A:431:HIS:CD2	1:A:432:TRP:CD1	2.84	0.66
1:B:54:VAL:HG13	1:B:300:TYR:OH	1.95	0.66
1:B:456:LYS:O	1:B:457:ILE:CG1	2.40	0.66
1:B:41:GLY:C	1:B:43:THR:N	2.51	0.66
1:A:445:ARG:HD2	1:A:463:TRP:CZ2	2.31	0.66
1:B:291:LEU:HD23	1:B:400:THR:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:VAL:HG11	1:A:54:VAL:CG2	2.19	0.66
1:A:233:ARG:NH1	1:A:253:GLU:CD	2.53	0.66
1:B:182:ALA:O	1:B:183:LEU:C	2.38	0.66
1:B:337:TYR:O	1:B:338:ALA:C	2.35	0.66
1:A:264:ILE:HG22	1:A:265:PRO:O	1.96	0.65
1:A:285:MET:HE1	1:A:414:LEU:HD23	1.78	0.65
1:B:264:ILE:HG23	1:B:268:LEU:CB	2.23	0.65
1:B:70:ARG:HH22	1:B:444:GLU:CD	2.04	0.65
1:A:304:PRO:CB	1:A:307:ARG:CD	2.71	0.65
1:A:343:PHE:HB3	1:A:345:LEU:HD21	1.78	0.65
1:A:51:VAL:CG1	1:A:54:VAL:HG22	2.19	0.65
1:A:275:ASN:OD1	1:A:276:PRO:HA	1.97	0.65
1:A:399:THR:CG2	1:A:400:THR:H	2.08	0.65
1:A:270:MET:HG2	1:A:286:ILE:HG22	1.78	0.65
1:B:30:VAL:CG1	1:B:31:VAL:N	2.59	0.65
1:A:4:LYS:HB2	1:A:256:GLU:HG3	1.78	0.65
1:B:286:ILE:HG22	1:B:286:ILE:O	1.96	0.65
1:B:43:THR:O	1:B:43:THR:HG22	1.97	0.65
1:B:428:THR:HG23	1:B:445:ARG:HH12	1.61	0.65
1:A:41:GLY:C	1:A:43:THR:N	2.51	0.65
1:A:174:THR:HG22	1:A:292:GLY:CA	2.27	0.65
1:A:236:ILE:HG22	1:A:237:TYR:HB2	1.79	0.65
1:A:168:PHE:O	1:A:168:PHE:CG	2.50	0.64
1:A:191:GLN:HE22	1:A:433:SER:CA	2.09	0.64
1:A:491:GLY:O	1:A:494:ARG:HG2	1.96	0.64
1:B:65:GLN:HB3	1:B:437:GLU:CG	2.22	0.64
1:B:134:PRO:HG2	1:B:407:LEU:HD21	1.78	0.64
1:A:47:ARG:NH2	1:A:219:GLU:OE1	2.28	0.64
1:B:264:ILE:CG2	1:B:268:LEU:CB	2.73	0.64
1:B:304:PRO:CB	1:B:307:ARG:HD2	2.27	0.64
1:A:291:LEU:HD12	1:A:395:GLY:C	2.23	0.64
1:A:456:LYS:O	1:A:457:ILE:CG1	2.39	0.64
1:B:387:ASN:OD1	1:B:389:CYS:HB2	1.97	0.64
1:B:448:ARG:NH1	1:B:462:ILE:O	2.30	0.64
1:A:216:GLN:HA	1:A:219:GLU:HG3	1.80	0.64
1:A:144:ASP:OD2	1:A:408:THR:HB	1.96	0.64
1:A:174:THR:CG2	1:A:292:GLY:HA3	2.28	0.64
1:B:323:PRO:HD2	1:B:367:LEU:CD2	2.25	0.64
1:B:233:ARG:NH1	1:B:253:GLU:OE2	2.30	0.64
1:A:287:THR:HG22	1:A:288:ARG:HG3	1.79	0.64
1:B:126:GLY:C	1:B:128:GLU:H	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLU:HB2	1:A:312:CYS:N	2.13	0.64
1:A:236:ILE:HG22	1:A:237:TYR:CB	2.28	0.64
1:A:248:GLU:OE2	1:B:252:HIS:NE2	2.30	0.64
1:B:426:THR:C	1:B:428:THR:H	2.05	0.63
1:B:400:THR:OG1	1:B:427:GLU:OE1	2.10	0.63
1:B:456:LYS:C	1:B:457:ILE:HG13	2.22	0.63
1:A:89:ILE:CG2	1:A:96:SER:HB3	2.29	0.63
1:A:267:THR:HG22	1:B:270:MET:CE	2.29	0.63
1:A:315:MET:N	1:A:327:THR:HG22	2.12	0.63
1:A:381:VAL:HG13	1:A:381:VAL:O	1.99	0.63
1:B:216:GLN:CA	1:B:219:GLU:HG3	2.27	0.63
1:A:171:LEU:HD13	3:A:601:NYP:C2	2.29	0.63
1:B:448:ARG:HD2	1:B:461:GLU:O	1.98	0.63
1:B:147:THR:HG22	1:B:150:GLU:H	1.64	0.63
1:A:446:ALA:O	1:A:449:GLU:HB2	1.99	0.62
1:B:36:ARG:NH1	1:B:391:GLU:OE1	2.32	0.62
1:A:270:MET:HG2	1:A:286:ILE:HG21	1.81	0.62
1:A:12:GLY:HA3	1:A:34:GLU:OE1	1.99	0.62
1:A:236:ILE:CD1	1:B:236:ILE:HD13	2.20	0.62
1:A:30:VAL:HG12	1:A:31:VAL:N	2.14	0.62
1:A:289:VAL:HG23	1:A:289:VAL:O	1.99	0.62
1:A:41:GLY:H	1:A:43:THR:HG22	1.63	0.62
1:A:285:MET:C	1:A:287:THR:N	2.53	0.62
1:A:171:LEU:HD13	3:A:601:NYP:H2	1.82	0.62
1:A:258:LYS:O	1:A:259:TYR:CD2	2.52	0.62
1:A:489:VAL:N	1:A:490:PRO:CD	2.62	0.62
1:B:191:GLN:HE22	1:B:433:SER:N	1.96	0.62
1:B:428:THR:HG23	1:B:428:THR:O	2.00	0.62
1:B:285:MET:C	1:B:287:THR:H	2.08	0.62
1:B:249:THR:HG22	1:B:251:ASN:CB	2.28	0.62
1:B:291:LEU:HD22	1:B:399:THR:C	2.24	0.62
1:A:240:GLN:NE2	1:A:418:VAL:O	2.23	0.62
1:A:252:HIS:CE1	1:B:248:GLU:OE2	2.52	0.61
1:B:92:VAL:HG22	1:B:318:ASP:HB3	1.82	0.61
1:B:171:LEU:CD2	1:B:171:LEU:C	2.70	0.61
1:B:343:PHE:HB3	1:B:345:LEU:HD21	1.82	0.61
1:B:21:LYS:O	1:B:22:LEU:C	2.39	0.61
1:B:171:LEU:HD22	1:B:171:LEU:C	2.25	0.61
1:A:178:HIS:CE1	1:B:145:ASN:OD1	2.53	0.61
1:A:287:THR:HG23	1:B:290:PRO:HB3	1.83	0.61
1:A:438:GLY:O	1:A:439:ALA:C	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:MET:CE	1:A:186:LEU:CD1	2.76	0.61
1:B:320:GLU:OE2	1:B:347:HIS:NE2	2.33	0.61
1:A:24:HIS:C	1:A:26:SER:N	2.54	0.61
1:A:46:LEU:HB3	1:A:54:VAL:HG23	1.82	0.61
1:A:191:GLN:NE2	1:A:433:SER:N	2.48	0.61
1:B:34:GLU:OE1	2:B:600:FAD:O3B	2.19	0.61
1:B:54:VAL:HG11	1:B:300:TYR:OH	2.00	0.61
1:A:151:LEU:O	1:A:155:LEU:HB2	2.01	0.60
1:B:48:ASN:C	1:B:48:ASN:OD1	2.44	0.60
1:A:168:PHE:CE1	1:A:199:ILE:HD11	2.36	0.60
1:A:55:ASP:OD2	1:A:59:SER:OG	2.18	0.60
1:B:258:LYS:O	1:B:259:TYR:CD2	2.54	0.60
1:B:446:ALA:O	1:B:449:GLU:N	2.33	0.60
1:A:48:ASN:OD1	1:A:48:ASN:C	2.43	0.60
1:A:291:LEU:HD22	1:A:399:THR:C	2.26	0.60
1:B:24:HIS:C	1:B:26:SER:H	2.09	0.60
1:A:79:THR:HG22	1:A:80:TYR:N	2.15	0.60
1:A:209:LYS:CE	1:A:330:ASP:OD1	2.50	0.59
1:A:5:CYS:SG	1:A:6:ASP:N	2.75	0.59
1:A:75:LEU:HD12	1:A:75:LEU:N	2.17	0.59
1:A:171:LEU:HD11	3:A:601:NYP:H2	1.84	0.59
1:A:173:VAL:CG1	1:A:174:THR:H	2.16	0.59
1:A:28:LEU:HD11	1:A:454:MET:CE	2.32	0.59
1:B:71:LEU:O	1:B:75:LEU:CD1	2.49	0.59
1:A:114:ASP:O	1:A:115:HIS:C	2.43	0.59
1:A:320:GLU:C	1:A:322:ALA:H	2.10	0.59
1:A:458:PRO:O	1:A:459:GLU:C	2.46	0.59
1:A:86:GLU:CD	1:A:86:GLU:H	2.08	0.59
1:B:6:ASP:HB2	1:B:29:ASN:HB2	1.83	0.59
1:A:68:ILE:HD12	1:A:436:MET:HB3	1.85	0.59
1:A:406:ILE:O	1:A:407:LEU:C	2.45	0.59
1:A:426:THR:HG23	1:A:427:GLU:N	2.16	0.59
1:B:313:GLY:O	1:B:327:THR:CG2	2.50	0.59
1:B:63:PRO:HG2	1:B:204:GLY:CA	2.32	0.59
1:B:67:ARG:NH2	1:B:466:GLU:HG2	2.17	0.59
1:A:365:CYS:O	1:A:366:GLU:C	2.45	0.59
1:A:378:LEU:N	1:A:378:LEU:HD23	2.16	0.59
1:B:285:MET:HE1	1:B:414:LEU:HD23	1.84	0.59
1:A:79:THR:CG2	1:A:80:TYR:N	2.66	0.58
1:B:307:ARG:O	1:B:310:ASP:N	2.32	0.58
1:B:68:ILE:HG22	1:B:437:GLU:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:HIS:C	1:B:26:SER:N	2.59	0.58
1:A:172:CYS:SG	3:A:601:NYP:H5	2.44	0.58
1:A:252:HIS:ND1	1:B:252:HIS:CE1	2.72	0.58
1:B:346:ALA:O	1:B:347:HIS:C	2.45	0.58
1:A:6:ASP:HB2	1:A:29:ASN:O	2.03	0.58
1:B:159:GLU:O	1:B:160:SER:C	2.45	0.58
1:A:41:GLY:H	1:A:43:THR:CG2	2.14	0.58
1:B:232:GLU:C	1:B:234:PRO:HD3	2.29	0.58
1:A:7:VAL:HG22	1:A:259:TYR:HB2	1.84	0.58
1:B:79:THR:HG23	1:B:208:ARG:CD	2.25	0.58
1:B:206:GLN:NE2	3:B:601:NYP:H8N1	2.19	0.58
1:A:30:VAL:HG13	1:A:31:VAL:N	2.18	0.58
1:A:405:GLY:C	1:A:406:ILE:HG13	2.29	0.58
1:A:431:HIS:O	1:A:432:TRP:C	2.45	0.58
1:B:233:ARG:CD	1:B:251:ASN:HD22	2.17	0.58
1:A:30:VAL:O	1:A:31:VAL:HG23	2.04	0.57
1:B:388:TRP:O	1:B:389:CYS:C	2.46	0.57
1:A:62:GLY:O	1:A:63:PRO:C	2.47	0.57
1:A:413:VAL:HG12	1:A:413:VAL:O	2.04	0.57
1:B:489:VAL:N	1:B:490:PRO:CD	2.67	0.57
1:A:269:GLY:C	1:A:271:LYS:H	2.11	0.57
1:A:285:MET:O	1:A:287:THR:N	2.38	0.57
1:B:87:ARG:C	1:B:88:LEU:CD2	2.71	0.57
1:B:346:ALA:O	1:B:349:ALA:N	2.36	0.57
1:A:119:TRP:HE3	1:A:195:THR:HG21	1.67	0.57
1:A:482:LEU:O	1:A:486:LEU:HG	2.04	0.57
1:A:297:CYS:C	1:A:298:ILE:HD12	2.30	0.57
1:A:134:PRO:HD2	1:A:135:TRP:CE3	2.40	0.57
1:A:215:GLY:O	1:A:219:GLU:HG2	2.04	0.57
1:A:240:GLN:CD	1:A:419:ASP:HB3	2.29	0.57
1:B:157:TRP:CZ2	1:B:490:PRO:HG3	2.40	0.57
1:A:21:LYS:O	1:A:22:LEU:C	2.46	0.57
1:B:85:VAL:HB	1:B:86:GLU:OE2	2.04	0.57
1:B:126:GLY:C	1:B:128:GLU:N	2.60	0.57
1:A:236:ILE:HD13	1:B:236:ILE:CD1	2.23	0.56
1:A:337:TYR:O	1:A:338:ALA:C	2.47	0.56
1:B:60:TYR:OH	1:B:341:MET:HE2	2.05	0.56
1:A:23:LEU:O	1:A:26:SER:HB3	2.05	0.56
1:A:92:VAL:O	1:A:93:LYS:HB2	2.05	0.56
1:A:126:GLY:O	1:A:190:LYS:HD3	2.06	0.56
1:B:249:THR:CG2	1:B:251:ASN:CB	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:MET:CE	1:B:414:LEU:HD23	2.35	0.56
1:A:10:VAL:CG2	1:A:235:VAL:HG21	2.33	0.56
1:B:458:PRO:O	1:B:459:GLU:C	2.47	0.56
1:A:291:LEU:HD22	1:A:399:THR:O	2.05	0.56
1:B:290:PRO:O	1:B:400:THR:HA	2.06	0.56
1:A:38:ARG:NH2	1:A:41:GLY:O	2.37	0.56
1:B:446:ALA:O	1:B:447:ALA:C	2.47	0.56
1:B:38:ARG:NH2	1:B:41:GLY:O	2.39	0.56
1:B:236:ILE:HG22	1:B:237:TYR:CB	2.36	0.56
1:B:287:THR:HG23	1:B:287:THR:O	2.05	0.56
1:A:40:GLY:C	1:A:43:THR:HG22	2.31	0.56
1:B:167:LEU:O	1:B:168:PHE:C	2.46	0.56
1:B:428:THR:CG2	1:B:428:THR:O	2.52	0.56
1:A:40:GLY:CA	1:A:43:THR:HG22	2.36	0.55
1:B:17:MET:O	1:B:18:ALA:C	2.48	0.55
1:B:430:THR:HB	1:B:441:GLU:OE2	2.06	0.55
1:B:426:THR:HB	1:B:439:ALA:HB2	1.88	0.55
1:A:119:TRP:CE3	1:A:195:THR:CG2	2.88	0.55
1:A:80:TYR:CE2	1:A:209:LYS:HB2	2.41	0.55
1:A:126:GLY:C	1:A:128:GLU:N	2.58	0.55
1:A:481:PHE:O	1:A:485:HIS:HD2	1.89	0.55
1:A:290:PRO:HB3	1:B:287:THR:HG23	1.87	0.55
1:B:65:GLN:CA	1:B:437:GLU:HG3	2.37	0.55
1:B:82:VAL:CG2	1:B:207:GLU:O	2.36	0.55
1:B:240:GLN:CD	1:B:419:ASP:HB3	2.32	0.55
1:A:109:PRO:C	1:A:111:THR:N	2.65	0.55
1:A:174:THR:CG2	1:A:292:GLY:CA	2.84	0.55
1:A:236:ILE:O	1:A:236:ILE:CG2	2.48	0.55
1:A:252:HIS:CE1	1:B:252:HIS:ND1	2.75	0.55
1:B:303:GLU:CB	1:B:304:PRO:CD	2.84	0.55
1:A:188:TYR:O	1:A:191:GLN:HG3	2.06	0.55
1:A:291:LEU:HD12	1:A:395:GLY:CA	2.37	0.55
1:A:309:LYS:NZ	1:A:373:GLY:O	2.40	0.55
1:B:442:ALA:O	1:B:443:GLY:C	2.50	0.55
1:A:78:GLU:O	1:A:211:VAL:HG23	2.07	0.55
1:A:216:GLN:O	1:A:217:VAL:C	2.47	0.55
1:A:239:ASP:OD1	1:A:241:THR:HB	2.07	0.55
1:B:110:ILE:HG22	1:B:110:ILE:O	2.07	0.55
1:B:444:GLU:HB3	1:B:448:ARG:HH21	1.71	0.55
1:A:387:ASN:O	1:A:390:GLU:HG2	2.06	0.54
1:B:41:GLY:N	1:B:43:THR:HG22	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:VAL:CG2	1:B:318:ASP:HB2	2.36	0.54
1:A:173:VAL:CG1	1:A:174:THR:N	2.68	0.54
1:A:291:LEU:HD12	1:A:395:GLY:HA3	1.89	0.54
1:A:295:ILE:HG12	1:A:387:ASN:HB2	1.88	0.54
1:A:301:TYR:O	1:A:338:ALA:HB3	2.07	0.54
1:A:303:GLU:CB	1:A:304:PRO:CD	2.85	0.54
1:B:171:LEU:CD1	3:B:601:NYP:H2	2.37	0.54
1:B:392:GLN:HG2	1:B:393:TYR:CE1	2.43	0.54
1:A:266:PRO:O	1:A:267:THR:C	2.51	0.54
1:B:287:THR:HG22	1:B:288:ARG:HG3	1.89	0.54
1:A:171:LEU:HA	1:A:345:LEU:HD13	1.88	0.54
1:A:446:ALA:O	1:A:447:ALA:C	2.50	0.54
1:B:332:LYS:HB3	1:B:333:PRO:CD	2.36	0.54
1:A:28:LEU:CD1	1:A:454:MET:CE	2.76	0.54
1:A:196:THR:O	1:A:197:ARG:C	2.49	0.54
1:A:209:LYS:HZ1	1:A:330:ASP:CG	2.15	0.54
1:A:430:THR:HB	1:A:441:GLU:OE2	2.06	0.54
1:B:198:ILE:CG2	1:B:199:ILE:N	2.69	0.54
1:B:249:THR:C	1:B:251:ASN:N	2.63	0.54
1:A:16:GLY:O	1:A:19:ALA:N	2.40	0.54
1:B:258:LYS:O	1:B:259:TYR:CD1	2.61	0.54
1:B:315:MET:N	1:B:327:THR:HG22	2.22	0.54
1:A:147:THR:HG22	1:A:147:THR:O	2.05	0.54
1:A:271:LYS:HD3	1:B:270:MET:O	2.07	0.54
1:A:204:GLY:O	1:A:205:GLY:C	2.51	0.53
1:A:480:THR:O	1:A:482:LEU:N	2.41	0.53
1:B:167:LEU:C	1:B:169:VAL:N	2.66	0.53
1:B:280:MET:O	1:B:281:MET:C	2.48	0.53
1:A:92:VAL:HG22	1:A:318:ASP:HB2	1.91	0.53
1:A:171:LEU:HA	1:A:345:LEU:CD1	2.39	0.53
1:B:120:ARG:NH2	1:B:486:LEU:O	2.38	0.53
1:B:198:ILE:HG22	1:B:199:ILE:N	2.23	0.53
1:B:426:THR:C	1:B:428:THR:N	2.63	0.53
1:A:305:PHE:CE1	1:A:306:TRP:HZ3	2.26	0.53
1:B:285:MET:O	1:B:287:THR:N	2.42	0.53
1:A:269:GLY:C	1:A:271:LYS:N	2.62	0.53
1:A:346:ALA:O	1:A:347:HIS:C	2.50	0.53
1:B:62:GLY:O	1:B:63:PRO:C	2.50	0.53
1:B:405:GLY:C	1:B:406:ILE:HG13	2.33	0.53
1:B:437:GLU:O	1:B:438:GLY:C	2.52	0.53
1:B:304:PRO:HB2	1:B:307:ARG:CD	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:THR:OG1	1:B:338:ALA:HA	2.09	0.53
1:A:236:ILE:O	1:A:236:ILE:HG23	2.08	0.53
1:B:413:VAL:O	1:B:413:VAL:HG12	2.07	0.53
1:A:251:ASN:O	1:A:252:HIS:CB	2.51	0.53
1:A:168:PHE:O	1:A:168:PHE:CD1	2.62	0.52
1:A:215:GLY:O	1:A:216:GLN:C	2.51	0.52
1:B:64:THR:HG23	1:B:64:THR:O	2.08	0.52
1:B:365:CYS:O	1:B:368:TYR:N	2.43	0.52
1:A:167:LEU:HD11	1:A:325:ALA:HB1	1.91	0.52
1:A:174:THR:HG22	1:A:293:SER:N	2.14	0.52
1:B:40:GLY:CA	1:B:43:THR:HG22	2.39	0.52
1:A:198:ILE:HG22	1:A:199:ILE:HG13	1.90	0.52
1:A:258:LYS:C	1:A:259:TYR:CG	2.87	0.52
1:A:36:ARG:NH1	1:A:391:GLU:OE1	2.43	0.52
1:B:41:GLY:H	1:B:43:THR:CG2	2.23	0.52
1:B:368:TYR:O	1:B:372:LEU:HB2	2.09	0.52
1:B:431:HIS:O	1:B:433:SER:N	2.42	0.52
1:B:49:GLN:CG	1:B:50:LYS:N	2.67	0.52
1:A:122:MET:HE1	1:A:185:PHE:CE2	2.43	0.52
1:B:481:PHE:O	1:B:485:HIS:HD2	1.93	0.52
1:B:336:ASN:HB3	1:B:337:TYR:HD1	1.74	0.52
1:A:110:ILE:O	1:A:110:ILE:HG22	2.10	0.52
1:A:275:ASN:OD1	1:A:276:PRO:CA	2.58	0.52
1:A:285:MET:CE	1:A:414:LEU:HA	2.40	0.52
1:A:480:THR:O	1:A:483:GLU:N	2.43	0.52
1:B:114:ASP:O	1:B:115:HIS:C	2.52	0.52
1:A:361:LEU:O	1:A:362:LYS:C	2.53	0.52
1:B:30:VAL:HG12	1:B:31:VAL:N	2.25	0.52
1:B:202:THR:O	1:B:207:GLU:OE1	2.27	0.52
1:A:137:ALA:O	1:A:138:PRO:C	2.51	0.51
1:A:249:THR:HG21	1:A:251:ASN:HB2	1.92	0.51
1:A:264:ILE:CG2	1:A:268:LEU:CB	2.84	0.51
1:A:413:VAL:O	1:A:414:LEU:C	2.54	0.51
1:A:485:HIS:O	1:A:486:LEU:C	2.50	0.51
1:A:388:TRP:O	1:A:390:GLU:N	2.43	0.51
1:A:236:ILE:HD11	1:A:250:LEU:CD1	2.23	0.51
1:A:337:TYR:CD1	1:A:337:TYR:N	2.77	0.51
1:B:40:GLY:HA3	1:B:43:THR:HG22	1.92	0.51
1:B:91:HIS:HA	1:B:95:LYS:O	2.11	0.51
1:B:194:GLY:O	1:B:195:THR:C	2.53	0.51
1:A:320:GLU:OE2	1:A:347:HIS:CE1	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ALA:O	1:A:183:LEU:C	2.50	0.51
1:A:269:GLY:O	1:A:271:LYS:N	2.43	0.51
1:A:293:SER:CB	1:A:389:CYS:SG	2.98	0.51
1:A:134:PRO:HG2	1:A:407:LEU:HD21	1.92	0.51
1:A:313:GLY:O	1:A:327:THR:CG2	2.59	0.51
1:B:285:MET:CE	1:B:414:LEU:HA	2.41	0.51
1:B:387:ASN:OD1	1:B:387:ASN:C	2.53	0.51
1:A:246:LEU:HD23	1:A:256:GLU:HB3	1.91	0.51
1:B:189:VAL:HG12	1:B:194:GLY:HA2	1.92	0.51
1:A:54:VAL:CG1	1:A:300:TYR:OH	2.58	0.51
1:A:64:THR:HG23	1:A:64:THR:O	2.10	0.51
1:A:291:LEU:O	1:B:288:ARG:NH2	2.44	0.51
1:B:6:ASP:HB2	1:B:29:ASN:O	2.11	0.51
1:B:171:LEU:HD13	3:B:601:NYP:C2	2.41	0.51
1:B:196:THR:O	1:B:197:ARG:C	2.53	0.51
1:B:375:LEU:O	1:B:376:GLU:C	2.52	0.51
1:A:400:THR:OG1	1:A:427:GLU:OE1	2.23	0.51
1:A:426:THR:HG23	1:A:427:GLU:HG2	1.92	0.51
1:A:459:GLU:O	1:A:462:ILE:HG13	2.10	0.51
1:B:270:MET:CG	1:B:286:ILE:HG22	2.37	0.51
1:B:285:MET:C	1:B:287:THR:N	2.68	0.51
1:B:309:LYS:NZ	1:B:373:GLY:O	2.44	0.51
1:A:17:MET:O	1:A:18:ALA:C	2.53	0.50
1:A:440:VAL:O	1:A:441:GLU:C	2.53	0.50
1:B:241:THR:HG22	1:B:242:ARG:HG3	1.93	0.50
1:A:327:THR:HA	1:A:341:MET:O	2.10	0.50
1:A:389:CYS:HB3	1:B:280:MET:HG3	1.94	0.50
1:B:313:GLY:O	1:B:327:THR:HG22	2.11	0.50
1:A:285:MET:CE	1:A:414:LEU:HD23	2.41	0.50
1:A:320:GLU:C	1:A:322:ALA:N	2.69	0.50
1:B:54:VAL:CG1	1:B:300:TYR:HH	2.25	0.50
1:B:282:ARG:NH2	1:B:423:PHE:CE2	2.80	0.50
1:A:111:THR:HG23	1:A:158:THR:HG21	1.93	0.50
1:B:117:ASN:ND2	1:B:488:SER:CB	2.67	0.50
1:B:151:LEU:O	1:B:155:LEU:HB2	2.12	0.50
1:A:365:CYS:O	1:A:368:TYR:N	2.45	0.50
1:B:275:ASN:CA	1:B:276:PRO:C	2.84	0.50
1:A:426:THR:C	1:A:428:THR:N	2.61	0.50
1:B:168:PHE:CE1	1:B:172:CYS:SG	3.05	0.50
1:A:290:PRO:O	1:A:400:THR:HA	2.11	0.50
1:B:86:GLU:H	1:B:86:GLU:CD	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:VAL:O	1:B:382:HIS:HB2	2.12	0.50
1:A:6:ASP:OD2	1:A:28:LEU:HD22	2.12	0.50
1:A:88:LEU:O	1:A:98:PRO:HA	2.12	0.50
1:A:144:ASP:OD2	1:A:408:THR:CB	2.60	0.50
1:A:364:LEU:HB3	1:A:368:TYR:CE1	2.46	0.50
1:A:134:PRO:HG3	1:A:187:TRP:CD1	2.47	0.49
1:A:188:TYR:O	1:A:189:VAL:C	2.55	0.49
1:B:137:ALA:O	1:B:138:PRO:C	2.55	0.49
1:A:328:LEU:HB2	1:A:341:MET:HE3	1.93	0.49
1:A:336:ASN:HB3	1:A:337:TYR:HD1	1.77	0.49
1:A:448:ARG:NH1	1:A:464:GLN:CB	2.69	0.49
1:B:109:PRO:C	1:B:111:THR:H	2.19	0.49
1:A:79:THR:HG23	1:A:208:ARG:CD	2.35	0.49
1:A:167:LEU:C	1:A:169:VAL:N	2.69	0.49
1:B:86:GLU:N	1:B:86:GLU:CD	2.69	0.49
1:B:282:ARG:O	1:B:285:MET:N	2.45	0.49
1:A:169:VAL:O	1:A:170:ASN:C	2.54	0.49
1:A:291:LEU:HD23	1:A:400:THR:CA	2.43	0.49
1:A:411:GLY:O	1:A:413:VAL:N	2.45	0.49
1:B:75:LEU:HD12	1:B:75:LEU:N	2.26	0.49
1:B:167:LEU:HD11	1:B:325:ALA:HB1	1.93	0.49
1:B:327:THR:HA	1:B:341:MET:O	2.12	0.49
1:A:60:TYR:OH	1:A:341:MET:HE2	2.13	0.49
1:B:236:ILE:CD1	1:B:250:LEU:HD12	2.28	0.49
1:A:89:ILE:HG23	1:A:96:SER:HB3	1.94	0.49
1:A:159:GLU:O	1:A:160:SER:C	2.55	0.49
1:A:446:ALA:O	1:A:449:GLU:N	2.43	0.49
1:A:306:TRP:CZ3	1:A:340:ILE:HD11	2.48	0.49
1:B:119:TRP:O	1:B:120:ARG:C	2.54	0.49
1:B:171:LEU:HD13	3:B:601:NYP:H2	1.94	0.49
1:A:68:ILE:HG22	1:A:437:GLU:HG2	1.95	0.49
1:A:148:MET:O	1:A:152:LEU:HG	2.13	0.49
1:B:134:PRO:HD2	1:B:135:TRP:CZ3	2.48	0.49
1:B:151:LEU:O	1:B:152:LEU:C	2.54	0.49
1:A:92:VAL:HG22	1:A:318:ASP:CB	2.43	0.49
1:B:426:THR:OG1	1:B:434:GLY:N	2.38	0.49
1:A:67:ARG:NH2	1:A:466:GLU:HG2	2.28	0.49
1:B:148:MET:HE3	1:B:148:MET:CA	2.43	0.49
1:B:337:TYR:CD1	1:B:337:TYR:N	2.80	0.49
1:A:55:ASP:OD2	1:A:59:SER:CB	2.61	0.48
1:A:443:GLY:O	1:A:446:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ARG:HH12	1:A:464:GLN:HB2	1.76	0.48
1:A:86:GLU:HB2	1:A:311:TYR:C	2.38	0.48
1:A:239:ASP:OD1	1:A:239:ASP:C	2.56	0.48
1:A:388:TRP:O	1:A:389:CYS:C	2.55	0.48
1:B:8:VAL:O	1:B:260:VAL:HA	2.12	0.48
1:B:392:GLN:HG2	1:B:393:TYR:CD1	2.48	0.48
1:A:171:LEU:O	1:A:171:LEU:HD22	2.14	0.48
1:A:426:THR:O	1:A:428:THR:N	2.46	0.48
1:B:79:THR:HG23	1:B:208:ARG:CB	2.44	0.48
1:B:215:GLY:O	1:B:219:GLU:HG2	2.13	0.48
1:B:216:GLN:O	1:B:217:VAL:C	2.55	0.48
1:A:42:ARG:CZ	2:A:600:FAD:H5'1	2.43	0.48
1:A:445:ARG:NE	1:A:449:GLU:OE2	2.45	0.48
1:B:184:TRP:O	1:B:185:PHE:C	2.55	0.48
1:B:471:ASP:C	1:B:473:PRO:HD3	2.37	0.48
1:A:240:GLN:NE2	1:A:421:ILE:HG13	2.28	0.48
1:A:270:MET:CG	1:A:286:ILE:CG2	2.84	0.48
1:A:443:GLY:O	1:A:444:GLU:C	2.55	0.48
1:B:75:LEU:HD21	1:B:221:ILE:HG12	1.94	0.48
1:A:438:GLY:O	1:A:440:VAL:N	2.46	0.48
1:A:471:ASP:C	1:A:473:PRO:HD3	2.39	0.48
2:A:600:FAD:H9	2:A:600:FAD:O2'	2.13	0.48
1:A:97:TYR:CD1	1:A:97:TYR:N	2.82	0.48
1:A:153:ASP:HA	1:A:162:LYS:HE2	1.95	0.48
1:B:43:THR:O	1:B:43:THR:CG2	2.56	0.48
1:B:157:TRP:CE2	1:B:490:PRO:HG3	2.49	0.48
1:A:161:ALA:O	1:A:162:LYS:C	2.56	0.48
1:A:246:LEU:CD2	1:A:256:GLU:HB3	2.44	0.48
1:A:264:ILE:HG21	1:A:268:LEU:C	2.39	0.48
1:A:320:GLU:OE2	1:A:347:HIS:NE2	2.47	0.48
1:A:385:GLU:O	1:A:385:GLU:HG3	2.13	0.48
1:B:138:PRO:O	1:B:139:LEU:HD23	2.13	0.48
1:A:6:ASP:CB	1:A:29:ASN:O	2.62	0.48
1:A:42:ARG:NH2	2:A:600:FAD:O3P	2.42	0.48
1:B:51:VAL:O	1:B:51:VAL:HG12	2.10	0.48
1:A:184:TRP:CZ2	1:A:401:TYR:HA	2.49	0.47
1:A:198:ILE:HG22	1:A:199:ILE:N	2.28	0.47
1:A:362:LYS:O	1:A:366:GLU:HG3	2.12	0.47
1:B:4:LYS:HB2	1:B:256:GLU:HG3	1.96	0.47
1:B:448:ARG:NH1	1:B:464:GLN:CB	2.70	0.47
1:B:448:ARG:HH12	1:B:464:GLN:HB2	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLN:CA	1:A:437:GLU:HG3	2.43	0.47
1:A:300:TYR:CE2	1:A:339:ALA:HB2	2.49	0.47
1:A:206:GLN:NE2	3:A:601:NYP:H8N1	2.29	0.47
1:A:250:LEU:HD21	1:B:237:TYR:CE1	2.49	0.47
1:B:6:ASP:O	1:B:257:ALA:HB1	2.14	0.47
1:B:258:LYS:C	1:B:259:TYR:CG	2.90	0.47
1:A:442:ALA:O	1:A:443:GLY:C	2.56	0.47
1:A:374:SER:O	1:A:375:LEU:C	2.56	0.47
1:A:30:VAL:HG13	1:A:31:VAL:H	1.80	0.47
1:A:117:ASN:O	1:A:118:PHE:C	2.56	0.47
1:A:134:PRO:HG3	1:A:187:TRP:NE1	2.30	0.47
1:A:143:TRP:HA	1:A:146:MET:HE3	1.96	0.47
1:A:377:ALA:C	1:A:379:GLU:H	2.23	0.47
1:A:459:GLU:O	1:A:460:ASP:C	2.57	0.47
1:B:119:TRP:CE3	1:B:195:THR:HG21	2.50	0.47
1:A:70:ARG:O	1:A:70:ARG:HG2	2.07	0.47
1:A:135:TRP:CH2	1:A:412:ARG:HA	2.50	0.47
1:A:264:ILE:O	1:A:265:PRO:C	2.57	0.47
1:A:284:GLN:O	1:A:287:THR:HG22	2.15	0.47
1:B:184:TRP:CZ2	1:B:401:TYR:HA	2.48	0.47
1:B:489:VAL:HB	1:B:490:PRO:HD3	1.96	0.47
1:B:125:MET:HE1	1:B:186:LEU:HD11	1.91	0.47
1:B:270:MET:HG2	1:B:286:ILE:HG21	1.94	0.47
1:B:413:VAL:O	1:B:413:VAL:CG1	2.63	0.47
1:A:69:LEU:O	1:A:72:ALA:HB3	2.15	0.47
1:A:70:ARG:HH22	1:A:444:GLU:CD	2.22	0.47
1:A:249:THR:HG22	1:A:251:ASN:CB	2.43	0.47
1:A:355:LEU:HB3	1:A:359:GLU:HB2	1.97	0.47
1:A:444:GLU:HB3	1:A:448:ARG:HH21	1.80	0.47
1:A:495:LEU:HD12	1:A:495:LEU:HA	1.62	0.47
1:A:270:MET:CG	1:A:286:ILE:HG22	2.46	0.46
1:A:280:MET:HE3	1:A:280:MET:HB3	1.39	0.46
1:B:358:GLU:H	1:B:358:GLU:HG2	1.33	0.46
1:A:171:LEU:O	1:A:171:LEU:CD2	2.63	0.46
1:A:291:LEU:CD2	1:A:399:THR:O	2.64	0.46
1:B:147:THR:O	1:B:148:MET:C	2.56	0.46
1:B:282:ARG:CZ	1:B:423:PHE:CZ	2.99	0.46
1:B:407:LEU:HD12	1:B:407:LEU:HA	1.32	0.46
1:B:446:ALA:O	1:B:449:GLU:HB2	2.15	0.46
1:A:115:HIS:O	1:A:116:ASN:C	2.57	0.46
1:A:171:LEU:CD2	1:A:171:LEU:C	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:GLY:C	1:A:413:VAL:H	2.24	0.46
1:B:51:VAL:O	1:B:51:VAL:CG1	2.59	0.46
1:B:381:VAL:O	1:B:381:VAL:HG13	2.14	0.46
1:A:181:SER:O	1:A:182:ALA:C	2.57	0.46
1:A:298:ILE:HD12	1:A:298:ILE:N	2.30	0.46
1:B:171:LEU:HA	1:B:171:LEU:HD23	1.64	0.46
1:B:171:LEU:HA	1:B:345:LEU:CD1	2.45	0.46
1:B:495:LEU:HD12	1:B:495:LEU:HA	1.62	0.46
1:B:233:ARG:HD2	1:B:251:ASN:HD22	1.80	0.46
1:A:191:GLN:NE2	1:A:433:SER:HB3	2.31	0.46
1:A:275:ASN:CA	1:A:276:PRO:C	2.87	0.46
1:A:285:MET:HE1	1:A:414:LEU:HA	1.98	0.46
1:B:275:ASN:OD1	1:B:276:PRO:HA	2.16	0.46
1:B:97:TYR:CD1	1:B:97:TYR:N	2.84	0.46
1:B:113:LEU:HD23	1:B:113:LEU:HA	1.79	0.46
1:B:141:GLU:O	1:B:142:GLU:C	2.56	0.46
1:B:168:PHE:CD1	1:B:168:PHE:O	2.69	0.46
1:B:365:CYS:O	1:B:366:GLU:C	2.59	0.46
1:A:56:LEU:HA	1:A:56:LEU:HD23	1.22	0.46
1:B:184:TRP:O	1:B:187:TRP:HB3	2.16	0.46
1:A:165:ALA:O	1:A:166:THR:C	2.58	0.46
1:A:184:TRP:O	1:A:185:PHE:C	2.55	0.46
1:A:388:TRP:C	1:A:390:GLU:N	2.74	0.46
3:A:601:NYP:H8N1	3:A:601:NYP:H6	1.97	0.46
1:A:9:VAL:HG22	1:A:261:ILE:HB	1.98	0.46
1:A:320:GLU:O	1:A:322:ALA:N	2.49	0.46
1:A:373:GLY:C	1:A:374:SER:OG	2.59	0.46
1:A:445:ARG:HD2	1:A:463:TRP:CH2	2.51	0.46
1:B:233:ARG:HA	1:B:233:ARG:HD3	1.66	0.46
1:B:236:ILE:HD11	1:B:250:LEU:CD1	2.28	0.46
1:A:113:LEU:CD2	1:A:486:LEU:HB3	2.46	0.45
1:A:451:LEU:CB	1:A:457:ILE:HD12	2.44	0.45
1:B:54:VAL:HG13	1:B:300:TYR:HH	1.81	0.45
1:B:174:THR:HG22	1:B:293:SER:N	2.20	0.45
1:B:174:THR:HG22	1:B:292:GLY:CA	2.46	0.45
1:B:282:ARG:O	1:B:283:ASN:C	2.59	0.45
1:B:413:VAL:O	1:B:414:LEU:C	2.58	0.45
1:A:71:LEU:O	1:A:72:ALA:C	2.58	0.45
1:A:169:VAL:C	1:A:171:LEU:N	2.72	0.45
1:A:437:GLU:O	1:A:438:GLY:C	2.58	0.45
1:B:233:ARG:NH1	1:B:253:GLU:CD	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:LEU:O	1:A:376:GLU:C	2.57	0.45
1:B:480:THR:O	1:B:484:ARG:HG2	2.16	0.45
1:A:80:TYR:O	1:A:80:TYR:CG	2.70	0.45
1:A:104:PRO:HA	1:A:105:PRO:HD3	1.86	0.45
1:A:178:HIS:CG	1:B:145:ASN:HB3	2.51	0.45
1:A:189:VAL:HG12	1:A:194:GLY:HA2	1.99	0.45
1:A:358:GLU:H	1:A:358:GLU:HG2	1.21	0.45
1:B:75:LEU:HD12	1:B:75:LEU:H	1.81	0.45
1:B:167:LEU:O	1:B:169:VAL:N	2.49	0.45
1:B:174:THR:CG2	1:B:292:GLY:HA3	2.46	0.45
1:B:280:MET:HG2	1:B:281:MET:N	2.27	0.45
1:B:304:PRO:O	1:B:305:PHE:C	2.59	0.45
1:A:23:LEU:O	1:A:26:SER:CB	2.64	0.45
1:A:343:PHE:HB3	1:A:345:LEU:CD2	2.46	0.45
1:B:375:LEU:HD23	1:B:375:LEU:HA	1.65	0.45
1:B:411:GLY:C	1:B:413:VAL:H	2.23	0.45
1:A:173:VAL:HG21	1:A:184:TRP:CZ3	2.51	0.45
1:A:450:ILE:O	1:A:451:LEU:C	2.60	0.45
1:A:457:ILE:HA	1:A:458:PRO:HD3	1.81	0.45
1:B:30:VAL:HG13	1:B:31:VAL:N	2.31	0.45
1:B:456:LYS:HE2	1:B:456:LYS:HB3	1.85	0.45
1:A:19:ALA:O	1:A:20:ALA:C	2.57	0.45
1:A:489:VAL:O	1:A:493:LEU:HG	2.16	0.45
1:B:207:GLU:HG2	1:B:208:ARG:HG2	1.98	0.45
1:B:266:PRO:O	1:B:267:THR:C	2.57	0.45
1:A:164:LEU:O	1:A:164:LEU:HD12	2.17	0.45
1:A:216:GLN:CA	1:A:219:GLU:HG3	2.46	0.45
1:A:498:LEU:HD12	1:A:498:LEU:O	2.17	0.45
1:B:41:GLY:H	1:B:43:THR:HG22	1.82	0.45
1:B:134:PRO:HD2	1:B:135:TRP:CE3	2.51	0.45
1:A:42:ARG:HB3	2:A:600:FAD:C8M	2.47	0.45
1:A:480:THR:CB	1:A:483:GLU:HB2	2.24	0.45
1:B:79:THR:CG2	1:B:208:ARG:HH11	2.27	0.45
1:B:168:PHE:CE1	1:B:199:ILE:HD11	2.52	0.45
1:B:442:ALA:O	1:B:445:ARG:N	2.50	0.45
1:A:134:PRO:HD2	1:A:135:TRP:CZ3	2.52	0.44
1:A:291:LEU:CD2	1:A:399:THR:C	2.90	0.44
1:B:86:GLU:HG2	1:B:312:CYS:HB3	1.99	0.44
1:B:163:GLN:O	1:B:164:LEU:C	2.55	0.44
1:B:457:ILE:HG23	1:B:458:PRO:HD2	1.99	0.44
1:B:490:PRO:O	1:B:491:GLY:C	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLN:NE2	1:A:433:SER:H	2.14	0.44
1:A:387:ASN:OD1	1:A:389:CYS:HB2	2.17	0.44
1:A:407:LEU:HA	1:A:407:LEU:HD12	1.63	0.44
1:A:436:MET:O	1:A:437:GLU:C	2.59	0.44
1:A:458:PRO:C	1:A:460:ASP:N	2.75	0.44
1:B:144:ASP:OD2	1:B:408:THR:CB	2.59	0.44
1:B:161:ALA:O	1:B:162:LYS:C	2.58	0.44
1:B:291:LEU:HD23	1:B:400:THR:CA	2.45	0.44
1:A:134:PRO:C	1:A:136:LYS:H	2.24	0.44
1:A:168:PHE:CD1	1:A:199:ILE:HD11	2.52	0.44
1:A:298:ILE:HG21	1:A:300:TYR:CZ	2.52	0.44
1:A:413:VAL:O	1:A:413:VAL:CG1	2.61	0.44
1:B:86:GLU:HG2	1:B:312:CYS:CA	2.47	0.44
1:B:165:ALA:O	1:B:166:THR:C	2.61	0.44
1:B:457:ILE:HG23	1:B:461:GLU:HB2	1.99	0.44
1:A:280:MET:HG2	1:A:281:MET:N	2.32	0.44
1:B:139:LEU:HD23	1:B:139:LEU:HA	1.42	0.44
1:B:202:THR:HG22	1:B:203:ASN:N	2.31	0.44
1:B:291:LEU:HD22	1:B:399:THR:O	2.17	0.44
1:B:445:ARG:CD	1:B:463:TRP:CZ2	2.99	0.44
1:A:191:GLN:NE2	1:A:433:SER:O	2.51	0.44
1:B:79:THR:HG22	1:B:80:TYR:N	2.32	0.44
1:B:119:TRP:CE3	1:B:195:THR:CG2	3.00	0.44
1:B:122:MET:HE1	1:B:185:PHE:HE2	1.82	0.44
1:A:54:VAL:HG13	1:A:300:TYR:HH	1.82	0.44
1:A:157:TRP:CE2	1:A:490:PRO:HG3	2.52	0.44
1:A:300:TYR:HD2	1:A:339:ALA:HB2	1.79	0.44
1:A:303:GLU:CB	1:A:304:PRO:HD2	2.48	0.44
1:B:291:LEU:CD2	1:B:399:THR:C	2.90	0.44
1:A:6:ASP:HB2	1:A:29:ASN:HB2	1.99	0.44
1:A:249:THR:CG2	1:A:251:ASN:CB	2.93	0.44
1:A:282:ARG:CZ	1:A:423:PHE:CZ	3.01	0.44
1:A:468:GLU:OE2	1:A:473:PRO:HA	2.17	0.44
1:A:145:ASN:OD1	1:B:178:HIS:CE1	2.71	0.44
1:A:480:THR:HG22	1:A:482:LEU:H	1.83	0.44
1:B:249:THR:O	1:B:252:HIS:N	2.42	0.44
1:B:378:LEU:HD22	1:B:378:LEU:HA	1.83	0.44
1:A:202:THR:HG22	1:A:203:ASN:N	2.33	0.43
1:A:249:THR:C	1:A:251:ASN:N	2.75	0.43
1:A:287:THR:CG2	1:A:288:ARG:HG3	2.46	0.43
1:A:304:PRO:O	1:A:307:ARG:HD2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:VAL:O	1:A:382:HIS:HB2	2.18	0.43
1:A:445:ARG:CD	1:A:463:TRP:CH2	3.00	0.43
1:A:61:VAL:O	1:A:61:VAL:HG12	2.14	0.43
1:A:75:LEU:HD21	1:A:221:ILE:HG12	1.99	0.43
3:A:601:NYP:H6	3:A:601:NYP:C8N	2.49	0.43
1:B:66:ASN:ND2	1:B:468:GLU:HA	2.33	0.43
1:B:139:LEU:O	1:B:140:ALA:C	2.58	0.43
1:B:191:GLN:NE2	1:B:433:SER:HB3	2.32	0.43
1:B:260:VAL:O	1:B:421:ILE:HA	2.18	0.43
1:B:281:MET:O	1:B:282:ARG:C	2.59	0.43
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.67	0.43
1:A:207:GLU:HG2	1:A:208:ARG:HG2	1.99	0.43
1:A:233:ARG:HA	1:A:233:ARG:HD3	1.77	0.43
1:A:295:ILE:HG22	1:A:297:CYS:SG	2.58	0.43
1:A:184:TRP:O	1:A:187:TRP:HB3	2.17	0.43
1:A:269:GLY:O	1:A:270:MET:C	2.61	0.43
1:A:356:THR:O	1:A:357:LYS:C	2.60	0.43
1:B:431:HIS:C	1:B:433:SER:N	2.76	0.43
1:A:23:LEU:O	1:A:26:SER:N	2.49	0.43
1:A:23:LEU:HD23	1:A:23:LEU:HA	1.84	0.43
1:A:35:ALA:HB1	1:A:234:PRO:HG3	2.00	0.43
1:A:42:ARG:HA	1:A:388:TRP:CZ3	2.54	0.43
1:A:79:THR:CG2	1:A:208:ARG:HH11	2.24	0.43
1:A:167:LEU:C	1:A:169:VAL:H	2.26	0.43
1:A:214:SER:O	1:A:215:GLY:C	2.61	0.43
1:A:267:THR:CG2	1:B:270:MET:HE2	2.44	0.43
1:A:362:LYS:HG2	1:A:366:GLU:OE2	2.19	0.43
1:B:215:GLY:O	1:B:216:GLN:C	2.60	0.43
1:B:241:THR:HG22	1:B:242:ARG:N	2.32	0.43
1:A:70:ARG:NH2	1:A:444:GLU:OE2	2.51	0.43
1:A:171:LEU:CD1	3:A:601:NYP:C2	2.90	0.43
1:A:372:LEU:HD23	1:A:372:LEU:HA	1.59	0.43
1:B:79:THR:CG2	1:B:80:TYR:N	2.81	0.43
1:A:139:LEU:O	1:A:140:ALA:C	2.62	0.43
1:B:79:THR:HG23	1:B:208:ARG:HB3	1.99	0.43
1:B:195:THR:O	1:B:196:THR:C	2.58	0.43
1:B:344:ILE:HG22	1:B:349:ALA:HA	2.01	0.43
1:A:438:GLY:O	1:A:441:GLU:N	2.52	0.43
1:B:438:GLY:O	1:B:439:ALA:C	2.59	0.43
1:A:49:GLN:CG	1:A:50:LYS:N	2.74	0.43
1:A:157:TRP:CZ2	1:A:490:PRO:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:VAL:O	1:B:61:VAL:HG12	2.17	0.43
1:B:108:ASN:OD1	1:B:108:ASN:C	2.60	0.43
1:A:280:MET:O	1:A:281:MET:C	2.62	0.43
1:A:331:THR:OG1	1:A:338:ALA:HA	2.19	0.43
1:A:174:THR:HG21	1:A:292:GLY:C	2.42	0.42
1:A:267:THR:HG22	1:A:267:THR:O	2.18	0.42
1:A:332:LYS:HA	1:A:332:LYS:HD3	1.78	0.42
1:B:430:THR:O	1:B:430:THR:HG22	2.19	0.42
1:B:480:THR:HG22	1:B:482:LEU:H	1.83	0.42
1:A:346:ALA:O	1:A:349:ALA:N	2.52	0.42
1:A:480:THR:O	1:A:484:ARG:HG2	2.19	0.42
1:A:235:VAL:CG1	1:A:236:ILE:N	2.78	0.42
1:A:252:HIS:HE1	1:B:248:GLU:OE2	2.00	0.42
1:A:258:LYS:C	1:A:259:TYR:CD1	2.97	0.42
1:B:38:ARG:HH11	1:B:38:ARG:HD3	1.65	0.42
1:B:171:LEU:HD11	3:B:601:NYP:H2	2.02	0.42
1:B:236:ILE:HD12	1:B:250:LEU:HA	2.01	0.42
1:A:163:GLN:O	1:A:164:LEU:C	2.60	0.42
1:A:233:ARG:HH12	1:A:253:GLU:CD	2.22	0.42
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.47	0.42
1:B:445:ARG:HD3	1:B:463:TRP:CH2	2.54	0.42
2:B:600:FAD:HM82	2:B:600:FAD:HM71	1.57	0.42
1:A:6:ASP:C	1:A:257:ALA:HB1	2.44	0.42
1:A:24:HIS:C	1:A:24:HIS:CD2	2.97	0.42
1:B:249:THR:O	1:B:250:LEU:C	2.62	0.42
1:B:314:THR:HA	1:B:327:THR:O	2.20	0.42
1:B:317:ILE:HD13	1:B:371:VAL:HG21	2.01	0.42
1:A:68:ILE:O	1:A:69:LEU:C	2.61	0.42
1:A:315:MET:HE1	1:A:368:TYR:CD2	2.54	0.42
1:B:23:LEU:O	1:B:26:SER:CB	2.68	0.42
1:B:46:LEU:HB3	1:B:54:VAL:HG23	2.02	0.42
1:B:51:VAL:HG22	1:B:300:TYR:CE1	2.55	0.42
1:B:427:GLU:H	1:B:427:GLU:HG2	1.10	0.42
1:B:440:VAL:O	1:B:441:GLU:C	2.62	0.42
1:A:457:ILE:HG23	1:A:461:GLU:HB2	2.02	0.42
1:B:236:ILE:HD13	1:B:236:ILE:HG21	1.65	0.42
1:B:286:ILE:HG21	1:B:286:ILE:HD13	1.50	0.42
1:A:55:ASP:OD2	1:A:59:SER:HB2	2.20	0.42
1:A:198:ILE:CG2	1:A:199:ILE:N	2.79	0.42
1:B:19:ALA:O	1:B:20:ALA:C	2.60	0.42
1:B:88:LEU:O	1:B:98:PRO:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:GLU:HG2	1:B:219:GLU:H	1.56	0.42
1:B:332:LYS:HB3	1:B:333:PRO:HD2	2.02	0.42
1:B:426:THR:O	1:B:428:THR:N	2.53	0.42
1:B:491:GLY:O	1:B:492:LEU:C	2.63	0.42
1:A:79:THR:HG23	1:A:208:ARG:CB	2.49	0.42
1:A:143:TRP:O	1:A:182:ALA:HB3	2.19	0.42
1:A:313:GLY:O	1:A:327:THR:HG23	2.20	0.42
1:A:447:ALA:O	1:A:448:ARG:C	2.63	0.42
1:B:457:ILE:HA	1:B:458:PRO:HD3	1.83	0.42
1:B:119:TRP:HE3	1:B:195:THR:HG21	1.86	0.41
1:B:485:HIS:O	1:B:486:LEU:C	2.62	0.41
1:A:445:ARG:HH11	1:A:445:ARG:HD3	1.68	0.41
1:B:68:ILE:O	1:B:69:LEU:C	2.62	0.41
1:A:67:ARG:HG3	1:A:437:GLU:OE2	2.21	0.41
1:A:167:LEU:O	1:A:168:PHE:C	2.61	0.41
1:A:237:TYR:CE1	1:B:250:LEU:HD21	2.56	0.41
1:A:267:THR:HG21	1:B:287:THR:OG1	2.21	0.41
1:A:282:ARG:O	1:A:283:ASN:C	2.62	0.41
1:B:355:LEU:HB3	1:B:359:GLU:HB2	2.02	0.41
1:B:303:GLU:HB3	1:B:304:PRO:CD	2.48	0.41
1:B:416:GLN:HA	1:B:417:PRO:HD3	1.81	0.41
1:B:459:GLU:O	1:B:460:ASP:C	2.63	0.41
1:A:84:GLU:OE2	1:A:201:THR:HB	2.20	0.41
1:A:151:LEU:O	1:A:151:LEU:HD12	2.21	0.41
1:A:402:PHE:HZ	1:A:414:LEU:HD11	1.84	0.41
1:A:414:LEU:HD23	1:A:414:LEU:HA	1.94	0.41
1:B:303:GLU:HB3	1:B:304:PRO:HD3	2.03	0.41
1:B:327:THR:C	1:B:328:LEU:HD23	2.45	0.41
1:A:41:GLY:HA3	2:A:600:FAD:O2A	2.21	0.41
1:A:79:THR:HG23	1:A:208:ARG:HB3	2.03	0.41
1:A:165:ALA:O	1:A:168:PHE:HB3	2.20	0.41
1:A:250:LEU:HD21	1:B:237:TYR:CD1	2.55	0.41
1:B:388:TRP:O	1:B:390:GLU:N	2.53	0.41
1:A:103:PHE:HA	1:A:104:PRO:HD3	1.75	0.41
1:A:167:LEU:O	1:A:169:VAL:N	2.54	0.41
1:B:42:ARG:NH2	2:B:600:FAD:O3P	2.53	0.41
1:B:191:GLN:HE22	1:B:433:SER:CA	2.33	0.41
1:A:89:ILE:HG21	1:A:96:SER:HB3	2.01	0.41
1:A:174:THR:HG22	1:A:292:GLY:HA3	1.91	0.41
1:A:304:PRO:HB2	1:A:307:ARG:HD3	1.93	0.41
1:B:66:ASN:CG	1:B:468:GLU:HA	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:VAL:CG1	1:B:93:LYS:N	2.84	0.41
1:B:97:TYR:HA	1:B:98:PRO:HD3	1.70	0.41
1:B:451:LEU:HB3	1:B:457:ILE:HD12	2.02	0.41
1:A:16:GLY:O	1:A:20:ALA:N	2.40	0.41
1:A:108:ASN:O	1:A:112:TYR:N	2.54	0.41
1:A:225:LEU:HD23	1:A:225:LEU:HA	1.62	0.41
1:A:245:VAL:O	1:A:256:GLU:HA	2.21	0.41
1:A:286:ILE:HG21	1:A:286:ILE:HD13	1.64	0.41
1:A:392:GLN:O	1:A:392:GLN:HG3	2.20	0.41
1:A:418:VAL:O	1:A:418:VAL:HG12	2.20	0.41
1:B:46:LEU:HA	1:B:46:LEU:HD12	1.75	0.41
1:B:245:VAL:HG23	1:B:257:ALA:O	2.21	0.41
1:B:341:MET:HE3	1:B:341:MET:HB3	1.97	0.41
1:B:376:GLU:C	1:B:378:LEU:N	2.77	0.41
1:B:388:TRP:CD1	1:B:388:TRP:H	2.37	0.41
1:B:480:THR:CB	1:B:483:GLU:HB2	2.23	0.41
1:A:92:VAL:HG12	1:A:93:LYS:HG3	2.03	0.41
1:A:151:LEU:HD12	1:A:151:LEU:C	2.44	0.41
1:A:209:LYS:NZ	1:A:330:ASP:CG	2.77	0.41
1:A:242:ARG:HB3	1:A:243:GLU:H	1.67	0.41
1:B:387:ASN:O	1:B:387:ASN:CG	2.61	0.41
1:A:271:LYS:HD3	1:A:271:LYS:HA	1.95	0.40
1:B:39:VAL:O	1:B:39:VAL:HG13	2.21	0.40
1:B:174:THR:O	1:B:174:THR:HG22	2.17	0.40
1:B:356:THR:HG1	1:B:359:GLU:HG3	1.86	0.40
1:A:75:LEU:CD2	1:A:221:ILE:HG12	2.51	0.40
1:A:344:ILE:HG22	1:A:349:ALA:HA	2.04	0.40
1:A:403:PRO:O	1:A:404:PRO:C	2.64	0.40
1:B:73:LYS:O	1:B:74:GLU:C	2.65	0.40
1:B:109:PRO:C	1:B:111:THR:N	2.80	0.40
1:B:436:MET:O	1:B:437:GLU:C	2.63	0.40
1:A:108:ASN:O	1:A:111:THR:HB	2.22	0.40
1:A:252:HIS:ND1	1:B:252:HIS:ND1	2.69	0.40
1:B:203:ASN:CG	1:B:203:ASN:O	2.62	0.40
1:B:269:GLY:C	1:B:271:LYS:N	2.77	0.40
1:A:28:LEU:HA	1:A:28:LEU:HD23	1.51	0.40
1:A:175:ALA:CB	1:A:179:GLU:OE1	2.47	0.40
1:A:407:LEU:O	1:A:411:GLY:HA3	2.20	0.40
1:B:126:GLY:O	1:B:128:GLU:N	2.55	0.40
1:B:269:GLY:C	1:B:271:LYS:H	2.30	0.40
1:B:286:ILE:CG2	1:B:286:ILE:O	2.65	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	495/520 (95%)	391 (79%)	83 (17%)	21 (4%)	2	13
1	B	491/520 (94%)	400 (82%)	76 (16%)	15 (3%)	3	19
All	All	986/1040 (95%)	791 (80%)	159 (16%)	36 (4%)	2	15

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	CYS
1	B	286	ILE
1	B	442	ALA
1	B	446	ALA
1	A	252	HIS
1	A	286	ILE
1	A	398	TYR
1	A	446	ALA
1	A	496	ILE
1	B	132	ASP
1	B	195	THR
1	B	252	HIS
1	A	122	MET
1	A	132	ASP
1	A	321	GLU
1	A	365	CYS
1	A	408	THR
1	B	398	TYR
1	A	419	ASP
1	A	442	ALA
1	B	212	GLY
1	B	365	CYS

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Mol	Chain	Res	Type
1	B	408	THR
1	B	412	ARG
1	A	86	GLU
1	A	127	ARG
1	A	382	HIS
1	A	404	PRO
1	A	412	ARG
1	B	110	ILE
1	B	419	ASP
1	A	336	ASN
1	B	114	ASP
1	B	389	CYS
1	A	41	GLY
1	A	39	VAL

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	426/444 (96%)	334 (78%)	92 (22%)	1	6
1	B	423/444 (95%)	328 (78%)	95 (22%)	1	5
All	All	849/888 (96%)	662 (78%)	187 (22%)	1	5

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	6	ASP
1	A	22	LEU
1	A	31	VAL
1	A	39	VAL
1	A	43	THR
1	A	48	ASN
1	A	49	GLN
1	A	54	VAL

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Mol	Chain	Res	Type
1	A	56	LEU
1	A	61	VAL
1	A	64	THR
1	A	69	LEU
1	A	73	LYS
1	A	81	LYS
1	A	82	VAL
1	A	86	GLU
1	A	88	LEU
1	A	106	VAL
1	A	107	TRP
1	A	128	GLU
1	A	131	SER
1	A	147	THR
1	A	155	LEU
1	A	160	SER
1	A	164	LEU
1	A	171	LEU
1	A	174	THR
1	A	180	VAL
1	A	181	SER
1	A	190	LYS
1	A	195	THR
1	A	196	THR
1	A	198	ILE
1	A	201	THR
1	A	202	THR
1	A	208	ARG
1	A	219	GLU
1	A	229	VAL
1	A	232	GLU
1	A	233	ARG
1	A	236	ILE
1	A	241	THR
1	A	243	GLU
1	A	245	VAL
1	A	254	MET
1	A	256	GLU
1	A	262	SER
1	A	264	ILE
1	A	271	LYS
1	A	280	MET

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Mol	Chain	Res	Type
1	A	287	THR
1	A	294	VAL
1	A	303	GLU
1	A	306	TRP
1	A	307	ARG
1	A	327	THR
1	A	328	LEU
1	A	354	ARG
1	A	356	THR
1	A	361	LEU
1	A	374	SER
1	A	376	GLU
1	A	378	LEU
1	A	379	GLU
1	A	381	VAL
1	A	397	CYS
1	A	398	TYR
1	A	399	THR
1	A	404	PRO
1	A	408	THR
1	A	412	ARG
1	A	416	GLN
1	A	427	GLU
1	A	428	THR
1	A	430	THR
1	A	437	GLU
1	A	449	GLU
1	A	450	ILE
1	A	456	LYS
1	A	462	ILE
1	A	465	SER
1	A	466	GLU
1	A	471	ASP
1	A	472	VAL
1	A	477	ILE
1	A	478	THR
1	A	479	THR
1	A	483	GLU
1	A	495	LEU
1	A	498	LEU
1	A	500	THR
1	B	4	LYS

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Mol	Chain	Res	Type
1	B	6	ASP
1	B	8	VAL
1	B	17	MET
1	B	22	LEU
1	B	26	SER
1	B	30	VAL
1	B	31	VAL
1	B	39	VAL
1	B	43	THR
1	B	48	ASN
1	B	49	GLN
1	B	54	VAL
1	B	61	VAL
1	B	64	THR
1	B	69	LEU
1	B	70	ARG
1	B	73	LYS
1	B	79	THR
1	B	82	VAL
1	B	84	GLU
1	B	86	GLU
1	B	88	LEU
1	B	106	VAL
1	B	107	TRP
1	B	128	GLU
1	B	131	SER
1	B	147	THR
1	B	155	LEU
1	B	160	SER
1	B	164	LEU
1	B	171	LEU
1	B	174	THR
1	B	180	VAL
1	B	181	SER
1	B	190	LYS
1	B	195	THR
1	B	196	THR
1	B	198	ILE
1	B	201	THR
1	B	202	THR
1	B	208	ARG
1	B	219	GLU

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Mol	Chain	Res	Type
1	B	232	GLU
1	B	233	ARG
1	B	236	ILE
1	B	241	THR
1	B	243	GLU
1	B	245	VAL
1	B	254	MET
1	B	256	GLU
1	B	262	SER
1	B	271	LYS
1	B	280	MET
1	B	287	THR
1	B	294	VAL
1	B	303	GLU
1	B	306	TRP
1	B	321	GLU
1	B	327	THR
1	B	328	LEU
1	B	337	TYR
1	B	341	MET
1	B	354	ARG
1	B	356	THR
1	B	361	LEU
1	B	364	LEU
1	B	370	LYS
1	B	374	SER
1	B	376	GLU
1	B	378	LEU
1	B	379	GLU
1	B	381	VAL
1	B	397	CYS
1	B	398	TYR
1	B	399	THR
1	B	408	THR
1	B	416	GLN
1	B	427	GLU
1	B	428	THR
1	B	430	THR
1	B	437	GLU
1	B	441	GLU
1	B	456	LYS
1	B	462	ILE

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Mol	Chain	Res	Type
1	B	465	SER
1	B	466	GLU
1	B	469	SER
1	B	470	VAL
1	B	471	ASP
1	B	472	VAL
1	B	477	ILE
1	B	478	THR
1	B	479	THR
1	B	495	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	83	ASN
1	A	90	HIS
1	A	116	ASN
1	A	191	GLN
1	A	206	GLN
1	A	431	HIS
1	A	452	HIS
1	A	485	HIS
1	B	24	HIS
1	B	90	HIS
1	B	178	HIS
1	B	191	GLN
1	B	206	GLN
1	B	251	ASN
1	B	431	HIS
1	B	485	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	600	1,3	58,58,58	1.27	9 (15%)	85,89,89	2.05	26 (30%)
3	NYP	B	601	2	9,12,12	3.55	8 (88%)	9,14,14	3.72	5 (55%)
2	FAD	B	600	1,3	58,58,58	1.23	6 (10%)	85,89,89	2.19	29 (34%)
3	NYP	A	601	2	9,12,12	3.40	8 (88%)	9,14,14	3.79	5 (55%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	600	1,3	-	8/34/50/50	0/6/6/6
3	NYP	B	601	2	1/1/2/6	3/4/15/15	0/1/1/1
2	FAD	B	600	1,3	-	6/34/50/50	0/6/6/6
3	NYP	A	601	2	1/1/2/6	3/4/15/15	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	NYP	C9-N8	5.44	1.33	1.30
3	A	601	NYP	C2-C3	-5.17	1.40	1.52
3	B	601	NYP	C2-C3	-4.97	1.40	1.52
3	A	601	NYP	C2-C1	-4.60	1.39	1.52
3	A	601	NYP	C6-C5	-4.43	1.40	1.49
3	B	601	NYP	C6-C5	-4.31	1.40	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	NYP	C2-C1	-4.08	1.40	1.52
3	A	601	NYP	C9-N8	3.64	1.32	1.30
2	B	600	FAD	C4X-N5	3.43	1.38	1.30
2	A	600	FAD	C4X-N5	3.37	1.38	1.30
2	B	600	FAD	C5A-N7A	-3.21	1.33	1.39
2	B	600	FAD	C2A-N3A	3.08	1.39	1.33
2	A	600	FAD	C2A-N1A	2.89	1.39	1.33
2	A	600	FAD	C5A-N7A	-2.87	1.33	1.39
2	A	600	FAD	C2A-N3A	2.77	1.38	1.33
3	A	601	NYP	C9-C10	2.77	1.50	1.42
3	B	601	NYP	C9-C10	2.76	1.50	1.42
3	B	601	NYP	C5-C4	2.54	1.40	1.32
2	A	600	FAD	C9A-N10	-2.51	1.36	1.41
2	B	600	FAD	C2A-N1A	2.50	1.38	1.33
2	B	600	FAD	C10-N1	2.48	1.38	1.33
3	A	601	NYP	C7-C1	-2.32	1.50	1.52
3	B	601	NYP	C7-C1	-2.31	1.50	1.52
2	A	600	FAD	C10-N1	2.26	1.37	1.33
2	A	600	FAD	C8A-N7A	2.25	1.36	1.31
3	A	601	NYP	C3-C4	-2.23	1.40	1.48
2	B	600	FAD	C9A-N10	-2.23	1.37	1.41
3	A	601	NYP	C5-C4	2.23	1.39	1.32
3	B	601	NYP	C3-C4	-2.12	1.41	1.48
2	A	600	FAD	O2'-C2'	-2.04	1.39	1.43
2	A	600	FAD	C4X-C10	-2.02	1.38	1.44

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	NYP	C2-C1-C6	7.51	121.52	109.33
3	A	601	NYP	C2-C1-C6	6.98	120.67	109.33
2	B	600	FAD	C5A-C4A-N3A	-6.94	117.16	126.72
2	B	600	FAD	O4B-C1B-C2B	-5.83	94.13	106.62
2	A	600	FAD	C5A-C4A-N3A	-5.77	118.78	126.72
3	A	601	NYP	C8N-N8-C7	5.42	124.48	115.78
2	B	600	FAD	N3A-C4A-N9A	5.24	136.07	127.17
2	A	600	FAD	C9A-C5X-N5	-5.04	117.10	122.45
3	B	601	NYP	C3-C2-C1	4.99	120.06	112.14
2	A	600	FAD	O2P-P-O3P	4.93	120.60	107.27
2	A	600	FAD	N3A-C2A-N1A	-4.90	121.16	128.58
2	B	600	FAD	C9A-C5X-N5	-4.70	117.46	122.45
3	A	601	NYP	C3-C2-C1	4.68	119.56	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	NYP	C8N-N8-C7	4.66	123.26	115.78
2	A	600	FAD	C5X-C9A-N10	4.30	121.86	117.97
2	B	600	FAD	C6A-C5A-C4A	4.03	122.69	117.18
2	B	600	FAD	N3A-C2A-N1A	-3.97	122.58	128.58
2	A	600	FAD	O3'-C3'-C2'	-3.91	100.04	108.93
2	A	600	FAD	N3A-C4A-N9A	3.91	133.81	127.17
2	B	600	FAD	C5A-C6A-N6A	-3.90	113.63	123.29
2	A	600	FAD	C2A-N3A-C4A	3.54	120.48	111.83
2	A	600	FAD	C6A-C5A-C4A	3.53	122.00	117.18
2	A	600	FAD	C9-C9A-N10	-3.52	117.12	121.85
2	B	600	FAD	C2A-N3A-C4A	3.50	120.38	111.83
2	A	600	FAD	C4-N3-C2	-3.41	119.58	125.64
3	A	601	NYP	C2-C3-C4	3.40	120.28	112.37
2	B	600	FAD	O3'-C3'-C2'	-3.35	101.31	108.93
2	B	600	FAD	C10-C4X-N5	-3.33	118.00	124.81
2	A	600	FAD	O5'-P-O1P	3.17	121.51	108.94
2	B	600	FAD	C7M-C7-C8	-3.10	114.43	120.76
2	B	600	FAD	N6A-C6A-N1A	3.10	125.28	118.38
2	B	600	FAD	C5'-C4'-C3'	2.97	117.81	112.22
3	A	601	NYP	C11-C10-C9	-2.83	116.85	122.33
2	A	600	FAD	C5A-C6A-N6A	-2.81	116.33	123.29
2	A	600	FAD	N9A-C8A-N7A	-2.76	110.02	113.94
2	B	600	FAD	O2A-PA-O3P	-2.75	99.83	107.27
2	A	600	FAD	C10-C4X-N5	-2.75	119.19	124.81
2	A	600	FAD	C4X-C4-N3	2.69	120.09	113.25
3	B	601	NYP	C2-C3-C4	2.59	118.40	112.37
2	B	600	FAD	C4-C4X-N5	2.58	121.77	118.21
2	B	600	FAD	O2-C2-N3	2.57	123.51	118.58
2	B	600	FAD	C4-N3-C2	-2.56	121.10	125.64
2	A	600	FAD	O4-C4-C4X	-2.54	119.83	126.53
2	A	600	FAD	C5B-C4B-C3B	-2.44	106.42	115.21
2	B	600	FAD	C4X-C4-N3	2.42	119.40	113.25
2	A	600	FAD	O2-C2-N1	-2.40	117.81	121.80
2	B	600	FAD	N9A-C8A-N7A	-2.37	110.57	113.94
2	A	600	FAD	C5A-N7A-C8A	2.35	107.14	103.45
2	A	600	FAD	O3P-P-O1P	-2.33	103.69	110.70
2	B	600	FAD	C5A-N7A-C8A	2.33	107.11	103.45
3	B	601	NYP	C11-C10-C9	-2.33	117.82	122.33
2	B	600	FAD	C10-N1-C2	2.32	121.86	116.85
2	B	600	FAD	C9-C9A-N10	-2.30	118.76	121.85
2	B	600	FAD	O2P-P-O3P	2.23	113.29	107.27
2	B	600	FAD	C6A-C5A-N7A	-2.22	127.82	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	C5X-C9A-N10	2.15	119.91	117.97
2	B	600	FAD	C5B-C4B-C3B	-2.14	107.51	115.21
2	A	600	FAD	O2B-C2B-C1B	2.13	117.45	110.10
2	B	600	FAD	C4X-C10-N1	-2.13	119.36	124.59
2	A	600	FAD	O4B-C1B-C2B	-2.13	102.06	106.62
2	A	600	FAD	O4B-C1B-N9A	2.13	112.17	108.09
2	B	600	FAD	C7M-C7-C6	2.09	123.26	119.57
2	A	600	FAD	C3B-C2B-C1B	-2.03	97.63	101.46
2	A	600	FAD	N6A-C6A-N1A	2.02	122.88	118.38
2	B	600	FAD	O2-C2-N1	-2.02	118.45	121.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	NYP	C1
3	B	601	NYP	C1

All (20) torsion outliers are listed below:

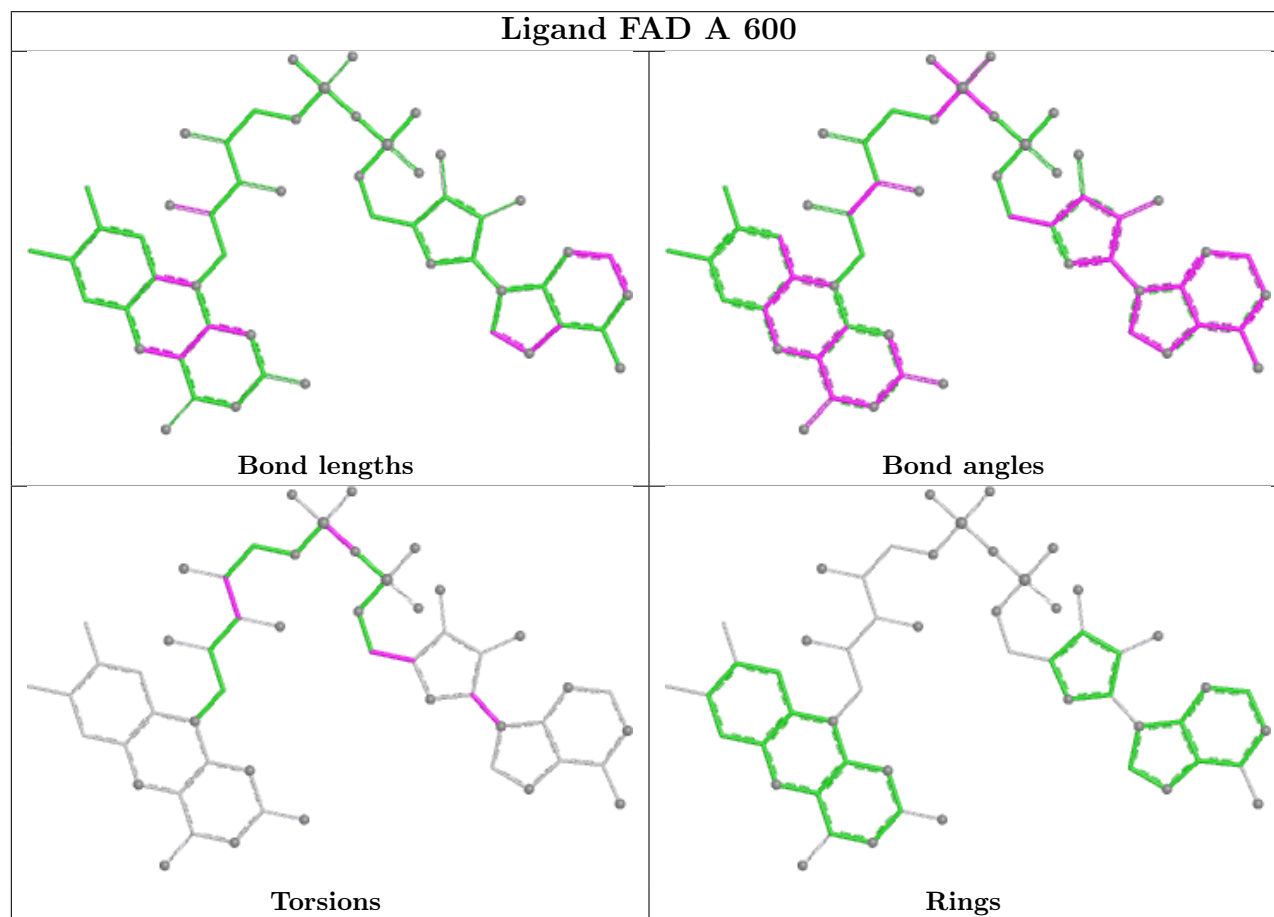
Mol	Chain	Res	Type	Atoms
2	A	600	FAD	O3'-C3'-C4'-O4'
2	A	600	FAD	O3'-C3'-C4'-C5'
3	A	601	NYP	C1-C7-N8-C8N
3	A	601	NYP	C2-C1-C7-N8
3	A	601	NYP	C6-C1-C7-N8
3	B	601	NYP	C2-C1-C7-N8
3	B	601	NYP	C6-C1-C7-N8
2	A	600	FAD	C2'-C3'-C4'-O4'
2	A	600	FAD	C3B-C4B-C5B-O5B
2	B	600	FAD	C3B-C4B-C5B-O5B
2	A	600	FAD	O4B-C4B-C5B-O5B
2	B	600	FAD	O4B-C4B-C5B-O5B
2	B	600	FAD	O3'-C3'-C4'-C5'
2	B	600	FAD	O3'-C3'-C4'-O4'
2	A	600	FAD	C2'-C3'-C4'-C5'
2	B	600	FAD	C2'-C3'-C4'-O4'
2	A	600	FAD	PA-O3P-P-O5'
2	A	600	FAD	C2B-C1B-N9A-C8A
3	B	601	NYP	C1-C7-N8-C8N
2	B	600	FAD	C2B-C1B-N9A-C8A

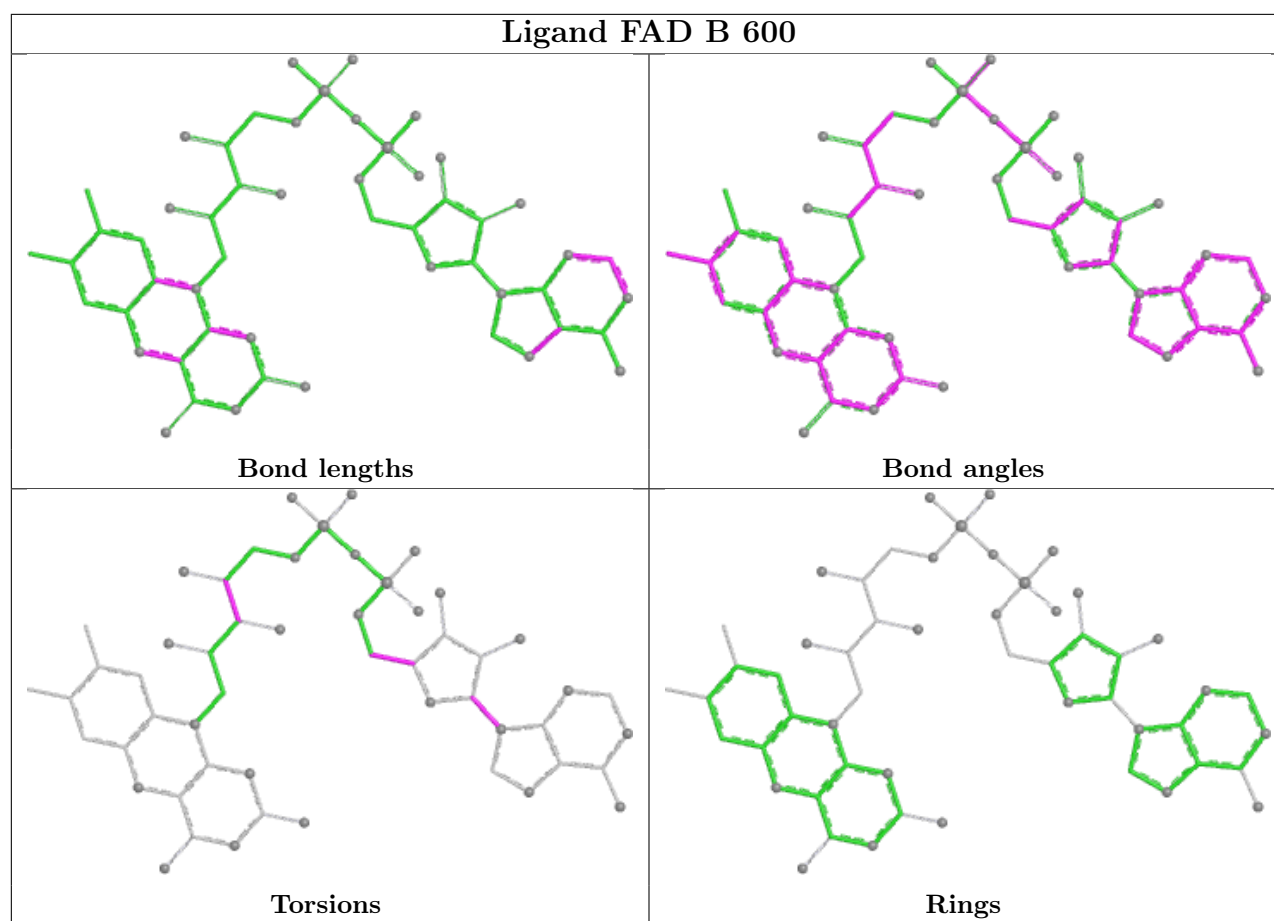
There are no ring outliers.

4 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	7	0
3	B	601	NYP	8	0
2	B	600	FAD	4	0
3	A	601	NYP	12	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	497/520 (95%)	0.71	24 (4%)	35	19	27, 44, 74, 100	0
1	B	493/520 (94%)	0.53	27 (5%)	30	15	27, 44, 73, 91	0
All	All	990/1040 (95%)	0.62	51 (5%)	33	17	27, 44, 74, 100	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	GLY	4.3
1	A	497	GLY	3.8
1	B	4	LYS	3.8
1	B	107	TRP	3.3
1	B	318	ASP	3.3
1	B	244	ASN	3.0
1	B	251	ASN	3.0
1	A	107	TRP	2.9
1	A	13	GLY	2.9
1	A	202	THR	2.9
1	B	243	GLU	2.8
1	A	40	GLY	2.7
1	B	466	GLU	2.7
1	A	14	ILE	2.7
1	B	443	GLY	2.6
1	A	62	GLY	2.6
1	A	12	GLY	2.6
1	B	227	ASP	2.5
1	B	15	SER	2.5
1	B	218	SER	2.5
1	A	130	PRO	2.5
1	A	30	VAL	2.4
1	A	217	VAL	2.4
1	B	160	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	250	LEU	2.4
1	B	158	THR	2.3
1	B	495	LEU	2.3
1	B	95	LYS	2.3
1	A	188	TYR	2.3
1	B	301	TYR	2.3
1	A	442	ALA	2.2
1	B	97	TYR	2.2
1	A	243	GLU	2.2
1	B	309	LYS	2.2
1	B	39	VAL	2.2
1	A	15	SER	2.2
1	A	49	GLN	2.2
1	B	246	LEU	2.2
1	B	11	GLY	2.2
1	B	49	GLN	2.2
1	A	452	HIS	2.1
1	A	89	ILE	2.1
1	B	254	MET	2.1
1	A	494	ARG	2.1
1	A	335	GLY	2.1
1	A	263	ALA	2.1
1	B	475	GLN	2.0
1	B	370	LYS	2.0
1	B	103	PHE	2.0
1	A	358	GLU	2.0
1	A	441	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

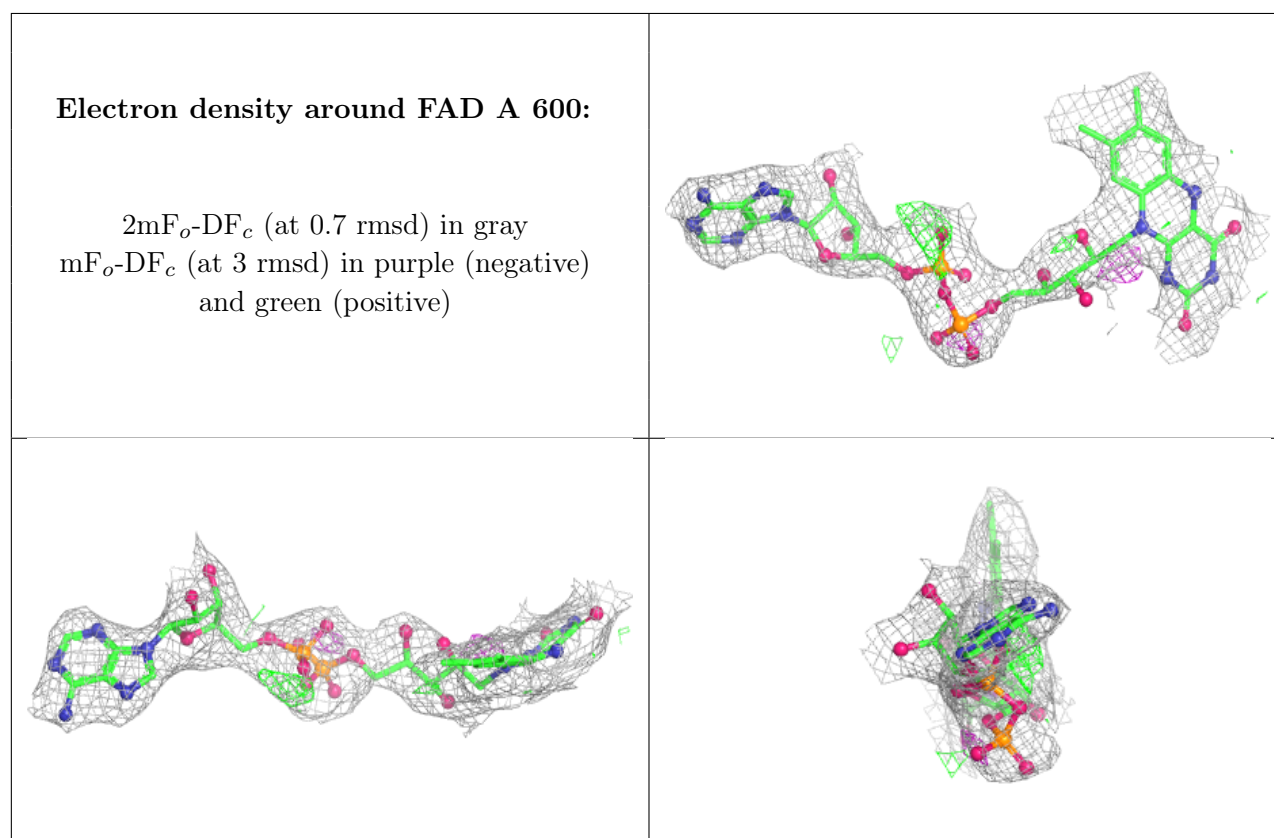
6.4 Ligands [i](#)

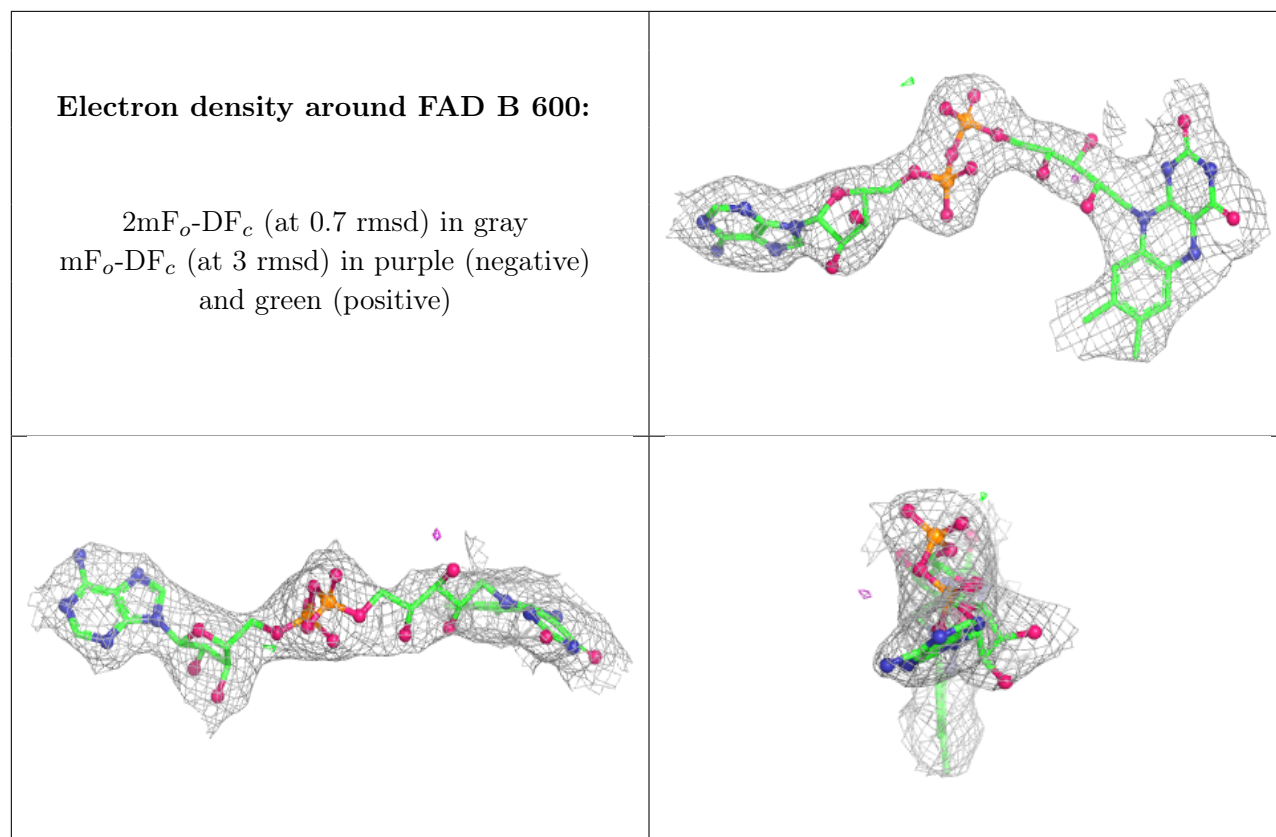
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NYP	B	601	12/12	0.79	0.16	46,53,58,58	0
3	NYP	A	601	12/12	0.82	0.17	46,53,58,59	0
2	FAD	A	600	53/53	0.85	0.14	24,35,45,49	0
2	FAD	B	600	53/53	0.93	0.10	23,35,45,50	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.