



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2022 – 02:10 PM JST

PDB ID : 7EOZ
Title : The structure of rice Defective Pollen Wall (DPW) in the complex with its cofactor NADP
Authors : Yan, L.M.; Wang, W.; Li, G.; Wang, J.
Deposited on : 2021-04-24
Resolution : 3.40 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

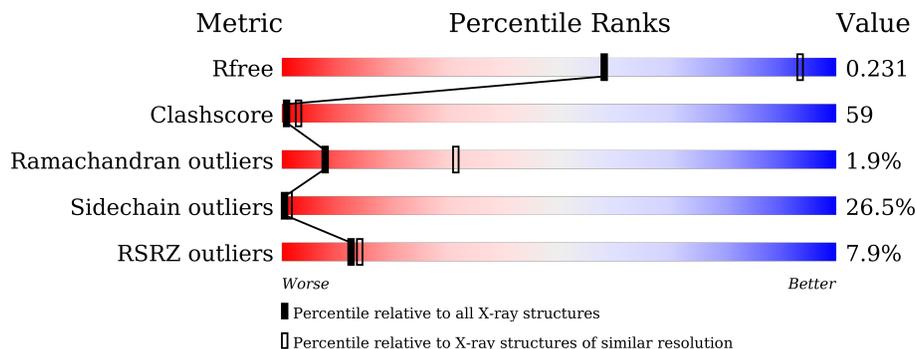
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	532	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 38%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
1	B	532	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 31%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>

2 Entry composition [i](#)

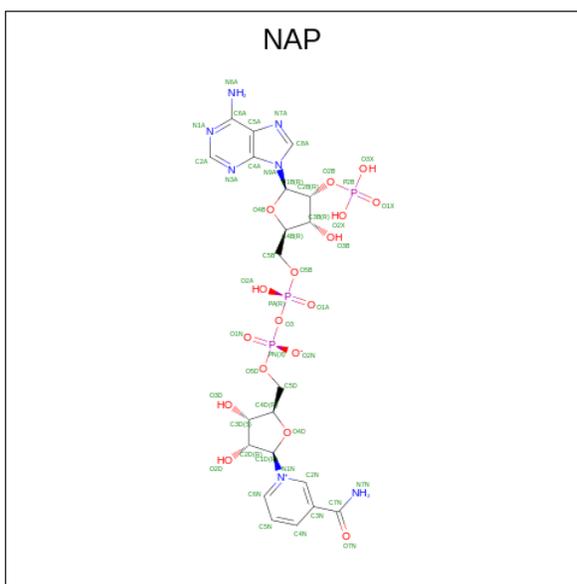
There are 3 unique types of molecules in this entry. The entry contains 7616 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fatty acyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	482	Total 3753	2387	654	694	18	0	0	0
1	B	473	Total 3682	2344	639	681	18	0	0	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



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

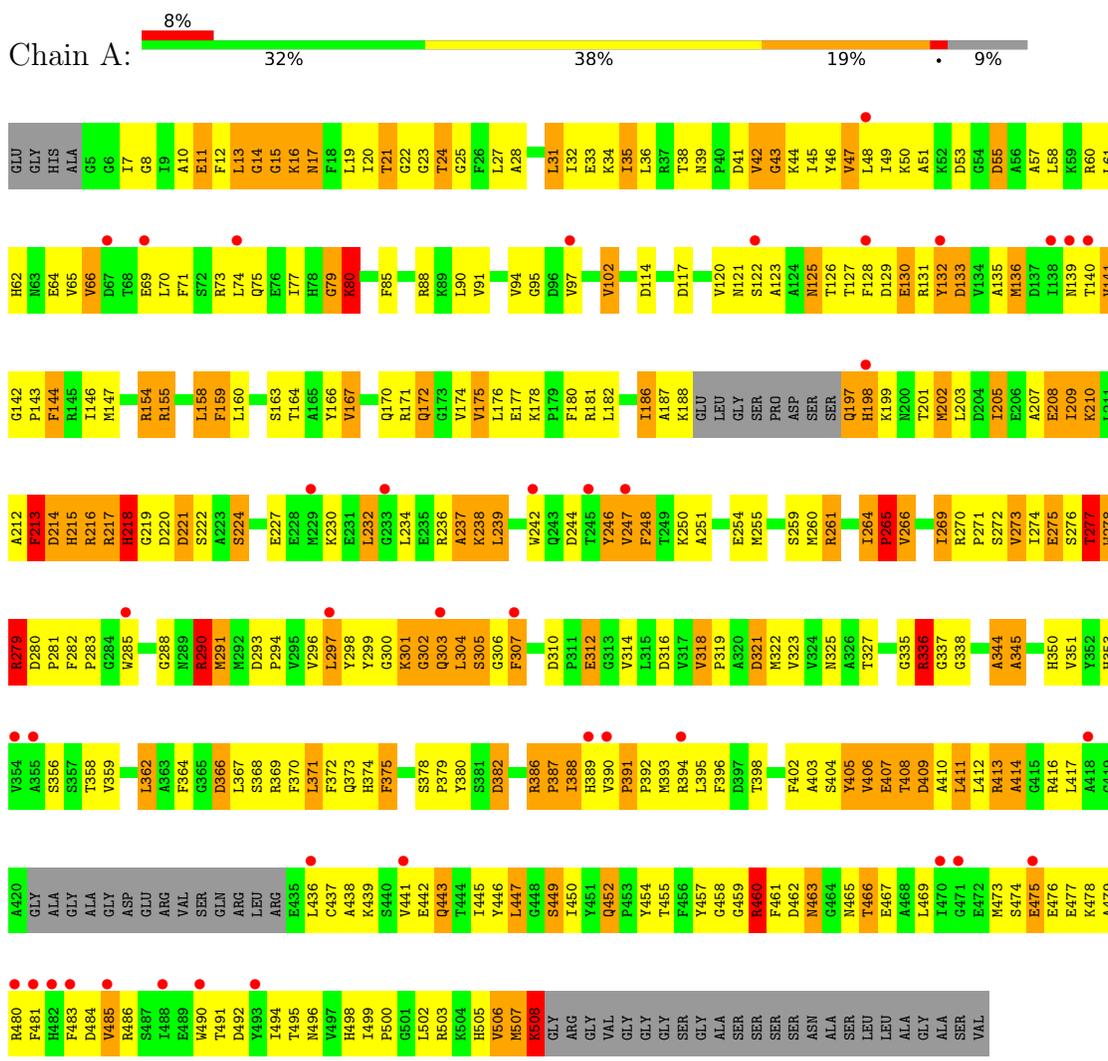
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		
3	B	40	Total	O	0	0
			40	40		

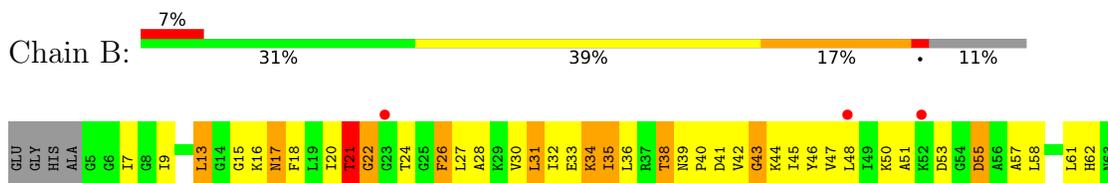
3 Residue-property plots [i](#)

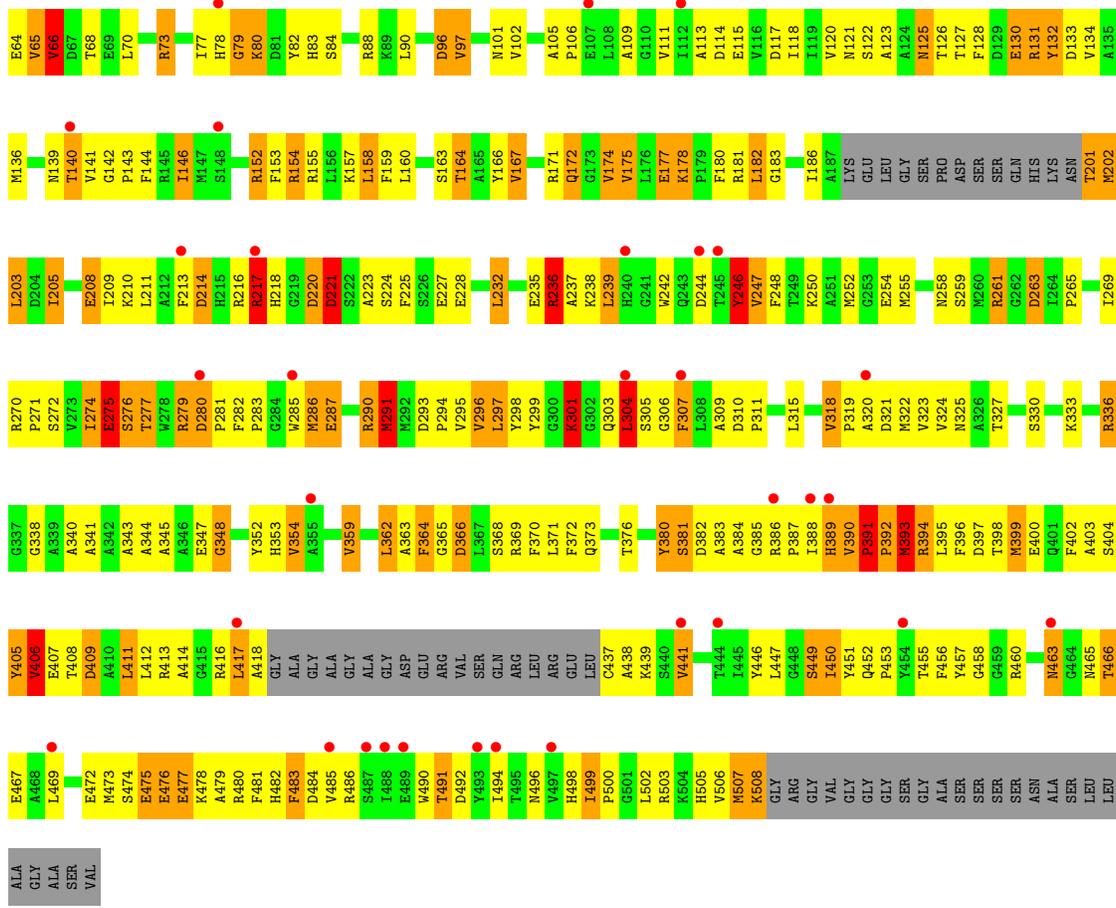
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Fatty acyl-CoA reductase





4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	222.81Å 222.81Å 114.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.45 – 3.40 48.45 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.45-3.40) 97.7 (48.45-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.21 (at 3.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.191 , 0.240 0.217 , 0.231	Depositor DCC
R_{free} test set	2223 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	96.1	Xtrriage
Anisotropy	0.003	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 87.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7616	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP

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	0.80	1/3833 (0.0%)	1.48	56/5180 (1.1%)
1	B	0.85	3/3761 (0.1%)	1.54	69/5085 (1.4%)
All	All	0.83	4/7594 (0.1%)	1.51	125/10265 (1.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	391	PRO	N-CD	15.50	1.69	1.47
1	B	392	PRO	N-CD	10.00	1.61	1.47
1	B	22	GLY	C-O	7.54	1.35	1.23
1	A	23	GLY	C-O	5.85	1.33	1.23

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	ASP	CB-CA-C	20.62	151.64	110.40
1	B	301	LYS	CB-CA-C	-17.67	75.05	110.40
1	A	278	TRP	CB-CA-C	-17.48	75.45	110.40
1	B	217	ARG	CB-CA-C	-16.29	77.82	110.40
1	A	304	LEU	N-CA-CB	-15.96	78.49	110.40
1	A	213	PHE	N-CA-C	15.65	153.26	111.00
1	A	414	ALA	CB-CA-C	-15.55	86.78	110.10
1	B	275	GLU	CB-CA-C	15.07	140.55	110.40
1	A	336	ARG	CB-CA-C	-14.83	80.73	110.40
1	A	406	VAL	CB-CA-C	-14.64	83.58	111.40
1	B	392	PRO	N-CA-C	-14.35	74.80	112.10
1	B	382	ASP	N-CA-C	-13.87	73.56	111.00
1	A	15	GLY	N-CA-C	-13.62	79.05	113.10
1	B	66	VAL	N-CA-C	-13.50	74.56	111.00
1	B	393	MET	N-CA-CB	-13.42	86.44	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	PRO	CB-CA-C	-13.33	78.67	112.00
1	B	383	ALA	CB-CA-C	13.03	129.65	110.10
1	A	508	LYS	N-CA-CB	12.70	133.46	110.60
1	B	276	SER	N-CA-CB	-12.53	91.70	110.50
1	A	213	PHE	CB-CA-C	-12.31	85.78	110.40
1	A	387	PRO	CB-CA-C	-12.07	81.81	112.00
1	B	391	PRO	N-CA-C	-11.95	81.02	112.10
1	A	44	LYS	N-CA-CB	-11.36	90.15	110.60
1	B	383	ALA	N-CA-CB	-11.24	94.36	110.10
1	A	266	VAL	N-CA-CB	-11.22	86.81	111.50
1	B	347	GLU	CB-CA-C	-11.09	88.22	110.40
1	B	213	PHE	CB-CA-C	-10.77	88.87	110.40
1	B	291	MET	N-CA-CB	-10.74	91.26	110.60
1	A	303	GLN	CB-CA-C	-10.74	88.92	110.40
1	B	96	ASP	N-CA-C	-10.51	82.63	111.00
1	A	344	ALA	CB-CA-C	-10.50	94.34	110.10
1	A	507	MET	CB-CA-C	10.50	131.40	110.40
1	A	279	ARG	N-CA-C	10.49	139.32	111.00
1	A	410	ALA	N-CA-CB	-10.24	95.76	110.10
1	B	482	HIS	N-CA-CB	-10.22	92.20	110.60
1	B	218	HIS	N-CA-CB	-9.93	92.73	110.60
1	B	382	ASP	CB-CA-C	9.86	130.13	110.40
1	A	345	ALA	N-CA-CB	-9.76	96.44	110.10
1	A	13	LEU	N-CA-C	-9.70	84.81	111.00
1	A	409	ASP	CB-CA-C	9.65	129.70	110.40
1	B	65	VAL	CB-CA-C	-9.65	93.06	111.40
1	A	336	ARG	N-CA-C	-9.54	85.23	111.00
1	B	79	GLY	N-CA-C	9.45	136.73	113.10
1	A	44	LYS	N-CA-C	9.44	136.48	111.00
1	B	290	ARG	CB-CA-C	9.41	129.21	110.40
1	A	388	ILE	N-CA-C	9.14	135.68	111.00
1	A	303	GLN	N-CA-C	9.14	135.67	111.00
1	B	381	SER	CB-CA-C	9.08	127.35	110.10
1	A	460	ARG	N-CA-C	-9.07	86.50	111.00
1	B	390	VAL	C-N-CD	-8.86	101.10	120.60
1	B	392	PRO	CB-CA-C	8.83	134.07	112.00
1	A	55	ASP	CB-CA-C	8.83	128.05	110.40
1	B	481	PHE	N-CA-C	-8.74	87.40	111.00
1	A	507	MET	N-CA-C	-8.70	87.51	111.00
1	B	304	LEU	N-CA-C	8.62	134.28	111.00
1	A	215	HIS	CB-CA-C	8.48	127.36	110.40
1	B	406	VAL	CB-CA-C	-8.44	95.37	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	ARG	CB-CA-C	8.39	127.17	110.40
1	A	463	ASN	CB-CA-C	8.25	126.90	110.40
1	A	277	THR	CB-CA-C	-8.22	89.40	111.60
1	B	381	SER	N-CA-CB	-8.19	98.22	110.50
1	B	304	LEU	N-CA-CB	-8.12	94.16	110.40
1	B	384	ALA	N-CA-CB	-8.00	98.91	110.10
1	B	213	PHE	N-CA-C	7.97	132.53	111.00
1	B	55	ASP	CB-CA-C	7.88	126.17	110.40
1	B	348	GLY	N-CA-C	7.87	132.79	113.10
1	B	172	GLN	N-CA-C	7.81	132.09	111.00
1	B	221	ASP	N-CA-CB	-7.78	96.60	110.60
1	A	388	ILE	N-CA-CB	-7.58	93.36	110.80
1	B	276	SER	N-CA-C	7.46	131.14	111.00
1	B	391	PRO	CA-N-CD	-7.40	101.14	111.50
1	B	236	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	481	PHE	CB-CA-C	-7.15	96.10	110.40
1	A	214	ASP	N-CA-CB	-7.07	97.88	110.60
1	A	14	GLY	N-CA-C	-7.00	95.60	113.10
1	B	385	GLY	N-CA-C	6.98	130.55	113.10
1	A	238	LYS	CB-CA-C	-6.89	96.63	110.40
1	A	414	ALA	N-CA-C	6.88	129.57	111.00
1	B	178	LYS	CB-CA-C	6.88	124.16	110.40
1	A	79	GLY	N-CA-C	6.83	130.17	113.10
1	A	265	PRO	N-CA-C	6.83	129.85	112.10
1	A	273	VAL	N-CA-C	6.76	129.25	111.00
1	B	66	VAL	CB-CA-C	6.73	124.19	111.40
1	B	174	VAL	N-CA-C	6.73	129.16	111.00
1	A	239	LEU	N-CA-CB	-6.70	97.01	110.40
1	A	43	GLY	N-CA-C	-6.66	96.46	113.10
1	A	47	VAL	N-CA-C	6.64	128.92	111.00
1	A	338	GLY	N-CA-C	-6.63	96.52	113.10
1	B	80	LYS	N-CA-C	-6.59	93.20	111.00
1	B	65	VAL	N-CA-CB	-6.59	97.01	111.50
1	B	65	VAL	N-CA-C	6.52	128.62	111.00
1	A	141	VAL	CB-CA-C	-6.48	99.09	111.40
1	B	363	ALA	CB-CA-C	6.40	119.70	110.10
1	B	220	ASP	CB-CA-C	-6.36	97.67	110.40
1	B	364	PHE	CB-CA-C	-6.26	97.87	110.40
1	A	345	ALA	N-CA-C	6.25	127.89	111.00
1	B	13	LEU	N-CA-C	-6.12	94.49	111.00
1	B	336	ARG	N-CA-C	-6.09	94.54	111.00
1	B	449	SER	CB-CA-C	-6.00	98.70	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	PHE	N-CA-CB	5.99	121.38	110.60
1	B	238	LYS	CB-CA-C	-5.93	98.54	110.40
1	B	364	PHE	N-CA-C	-5.92	95.02	111.00
1	A	303	GLN	N-CA-CB	5.88	121.19	110.60
1	B	392	PRO	CA-N-CD	-5.88	103.26	111.50
1	B	463	ASN	CB-CA-C	5.77	121.94	110.40
1	B	140	THR	N-CA-CB	-5.75	99.37	110.30
1	B	380	TYR	CB-CA-C	-5.75	98.90	110.40
1	A	275	GLU	CB-CA-C	5.74	121.88	110.40
1	B	214	ASP	N-CA-C	-5.70	95.62	111.00
1	B	15	GLY	N-CA-C	-5.69	98.88	113.10
1	B	21	THR	CB-CA-C	5.66	126.88	111.60
1	A	290	ARG	N-CA-CB	-5.48	100.74	110.60
1	B	97	VAL	N-CA-CB	-5.48	99.45	111.50
1	B	172	GLN	CB-CA-C	-5.42	99.56	110.40
1	A	382	ASP	CB-CA-C	-5.38	99.64	110.40
1	B	507	MET	CB-CA-C	5.29	120.97	110.40
1	A	302	GLY	N-CA-C	5.25	126.23	113.10
1	A	80	LYS	N-CA-C	-5.22	96.89	111.00
1	A	350	HIS	CB-CA-C	5.20	120.80	110.40
1	B	275	GLU	N-CA-C	-5.17	97.05	111.00
1	A	264	ILE	CB-CA-C	-5.08	101.45	111.60
1	A	508	LYS	N-CA-C	-5.08	97.29	111.00
1	B	366	ASP	N-CA-C	-5.07	97.30	111.00
1	B	246	TYR	CB-CG-CD2	5.04	124.03	121.00
1	B	287	GLU	N-CA-C	5.03	124.57	111.00

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	3753	0	3712	476	2
1	B	3682	0	3639	436	2
2	A	48	0	25	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	0	25	3	0
3	A	45	0	0	36	0
3	B	40	0	0	30	0
All	All	7616	0	7401	887	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

All (887) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:HIS:CD2	1:B:216:ARG:HG2	1.26	1.69
1:B:306:GLY:HA2	1:B:393:MET:CE	1.26	1.59
1:B:446:TYR:CE1	1:B:450:ILE:HD11	1.43	1.51
1:B:446:TYR:HE1	1:B:450:ILE:CD1	1.25	1.50
1:A:215:HIS:CD2	1:B:216:ARG:CG	1.94	1.47
1:A:294:PRO:O	1:A:298:TYR:CD2	1.69	1.45
1:A:299:TYR:HA	1:A:304:LEU:CD2	1.48	1.42
1:A:306:GLY:HA2	1:A:393:MET:CE	1.46	1.42
1:A:409:ASP:OD2	1:A:438:ALA:CB	1.67	1.41
1:B:372:PHE:CD1	1:B:390:VAL:CG1	2.01	1.41
1:B:372:PHE:CD1	1:B:390:VAL:HG12	1.57	1.40
1:A:79:GLY:O	1:A:80:LYS:CE	1.72	1.37
1:B:306:GLY:CA	1:B:393:MET:CE	2.03	1.34
1:B:391:PRO:N	1:B:391:PRO:CD	1.69	1.32
1:A:187:ALA:HB2	3:A:739:HOH:O	1.18	1.32
1:A:79:GLY:O	1:A:80:LYS:HE3	1.28	1.31
1:A:215:HIS:NE2	1:B:216:ARG:NE	1.72	1.31
1:A:299:TYR:CA	1:A:304:LEU:HD22	1.61	1.30
1:A:175:VAL:HG23	1:A:460:ARG:O	1.32	1.30
1:B:446:TYR:CE1	1:B:450:ILE:CD1	2.08	1.30
1:A:65:VAL:O	1:A:71:PHE:CD2	1.86	1.29
1:B:276:SER:OG	1:B:286:MET:HG3	1.31	1.26
1:A:409:ASP:OD2	1:A:438:ALA:HB2	1.13	1.25
1:A:215:HIS:NE2	1:B:216:ARG:CD	1.99	1.25
1:B:451:TYR:O	1:B:455:THR:CG2	1.84	1.25
1:A:306:GLY:CA	1:A:393:MET:CE	2.14	1.24
1:A:298:TYR:O	1:A:304:LEU:CD2	1.87	1.23
1:B:306:GLY:CA	1:B:393:MET:HE1	1.64	1.22
1:A:394:ARG:HD2	1:A:405:TYR:OH	1.39	1.21
1:B:64:GLU:O	1:B:68:THR:HG21	1.40	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:TYR:O	1:B:387:PRO:HD2	1.05	1.21
1:A:306:GLY:CA	1:A:393:MET:HE1	1.71	1.20
1:B:271:PRO:HA	3:B:705:HOH:O	1.40	1.20
1:B:62:HIS:HA	1:B:66:VAL:CG2	1.73	1.18
1:B:380:TYR:O	1:B:387:PRO:CD	1.93	1.16
1:B:451:TYR:O	1:B:455:THR:HG23	1.02	1.16
1:B:306:GLY:HA2	1:B:393:MET:HE3	1.26	1.16
1:B:275:GLU:OE2	1:B:293:ASP:OD2	1.62	1.15
1:B:365:GLY:O	1:B:369:ARG:NH2	1.79	1.15
1:B:372:PHE:CE1	1:B:390:VAL:CG1	2.31	1.14
1:A:215:HIS:CD2	1:B:216:ARG:HE	1.66	1.14
1:B:306:GLY:HA2	1:B:393:MET:HE2	1.29	1.14
1:A:47:VAL:HG12	1:A:47:VAL:O	1.47	1.12
1:A:299:TYR:N	1:A:304:LEU:HD22	1.64	1.12
1:A:146:ILE:HG23	3:A:743:HOH:O	1.51	1.11
1:B:275:GLU:OE2	1:B:293:ASP:CG	1.87	1.11
1:B:372:PHE:O	1:B:376:THR:HG23	1.48	1.11
1:B:290:ARG:O	1:B:294:PRO:CD	1.99	1.11
1:A:62:HIS:HA	1:A:66:VAL:CG2	1.80	1.09
1:A:344:ALA:O	1:B:345:ALA:HB2	1.51	1.09
1:A:321:ASP:O	1:A:325:ASN:ND2	1.84	1.08
1:B:279:ARG:O	1:B:279:ARG:CG	2.00	1.08
1:A:299:TYR:CD1	1:A:304:LEU:HD13	1.88	1.08
1:A:300:GLY:HA2	1:A:375:PHE:CE2	1.88	1.08
1:B:372:PHE:CE1	1:B:390:VAL:HG12	1.88	1.08
1:A:215:HIS:CD2	1:B:216:ARG:NE	2.20	1.07
1:A:345:ALA:HA	1:B:345:ALA:HA	1.36	1.07
1:B:275:GLU:OE2	1:B:293:ASP:OD1	1.72	1.07
1:A:299:TYR:HA	1:A:304:LEU:HD22	1.14	1.07
1:B:279:ARG:O	1:B:279:ARG:HG3	1.32	1.07
1:A:391:PRO:HB2	1:A:392:PRO:HD2	1.29	1.06
1:A:294:PRO:HB2	3:A:726:HOH:O	1.53	1.06
1:A:353:HIS:O	1:A:466:THR:HG21	1.53	1.06
1:A:304:LEU:HD12	1:A:304:LEU:O	1.55	1.05
1:B:34:LYS:O	1:B:38:THR:HG22	1.52	1.05
1:B:304:LEU:O	3:B:701:HOH:O	1.72	1.05
1:B:62:HIS:HA	1:B:66:VAL:HG23	1.08	1.05
1:B:290:ARG:O	1:B:294:PRO:HD3	1.57	1.05
1:A:24:THR:HG22	2:A:601:NAP:O1X	1.56	1.04
1:B:280:ASP:HB3	1:B:281:PRO:CD	1.86	1.04
1:A:65:VAL:O	1:A:71:PHE:CE2	2.09	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLY:CA	1:A:375:PHE:CE2	2.40	1.03
1:B:172:GLN:HE21	1:B:458:GLY:HA3	1.20	1.03
1:A:306:GLY:N	1:A:393:MET:HE1	1.74	1.03
1:A:79:GLY:O	1:A:80:LYS:HE2	1.55	1.02
1:A:306:GLY:HA2	1:A:393:MET:HE2	1.07	1.02
1:B:277:THR:HG21	1:B:281:PRO:HD2	1.41	1.02
1:A:214:ASP:O	1:B:214:ASP:OD1	1.75	1.02
1:A:270:ARG:NH1	1:A:351:VAL:HG11	1.75	1.02
1:B:290:ARG:N	3:B:703:HOH:O	1.93	1.01
1:A:274:ILE:CD1	1:A:323:VAL:HG21	1.90	1.01
1:A:298:TYR:C	1:A:304:LEU:HD22	1.81	1.00
1:B:372:PHE:CE1	1:B:390:VAL:HG11	1.96	1.00
1:B:452:GLN:HB3	1:B:453:PRO:HD3	1.41	1.00
1:A:305:SER:O	1:A:393:MET:HE3	1.61	1.00
1:B:64:GLU:O	1:B:68:THR:CG2	2.09	0.99
1:A:302:GLY:O	1:A:304:LEU:HD23	1.61	0.99
1:B:330:SER:HA	3:B:727:HOH:O	1.61	0.99
1:A:507:MET:O	1:A:508:LYS:HD2	1.60	0.99
1:B:354:VAL:H	1:B:466:THR:HG21	1.24	0.99
1:A:299:TYR:HD1	1:A:304:LEU:CD1	1.76	0.99
1:B:62:HIS:CA	1:B:66:VAL:HG23	1.93	0.99
1:A:146:ILE:CG2	3:A:743:HOH:O	2.09	0.99
1:A:215:HIS:CG	1:B:216:ARG:HG2	1.98	0.98
1:A:391:PRO:HB2	1:A:392:PRO:CD	1.93	0.98
1:B:299:TYR:OH	1:B:372:PHE:HA	1.64	0.98
1:B:174:VAL:HG12	1:B:174:VAL:O	1.64	0.97
1:B:370:PHE:CE1	1:B:491:THR:HA	1.98	0.97
1:A:299:TYR:CB	1:A:304:LEU:HD13	1.94	0.97
1:B:406:VAL:HG13	1:B:441:VAL:HG11	1.46	0.97
1:A:65:VAL:O	1:A:71:PHE:HD2	1.40	0.96
1:B:393:MET:HE3	1:B:393:MET:HA	1.48	0.96
1:B:372:PHE:CD1	1:B:390:VAL:HG11	1.99	0.95
1:B:261:ARG:HH11	1:B:261:ARG:HG3	1.29	0.95
1:B:390:VAL:C	1:B:391:PRO:CD	2.35	0.95
1:A:394:ARG:HD2	1:A:405:TYR:HH	1.23	0.94
1:A:201:THR:HG22	3:A:730:HOH:O	1.64	0.94
1:B:167:VAL:O	1:B:242:TRP:HZ3	1.49	0.94
1:B:499:ILE:O	1:B:503:ARG:HG3	1.68	0.94
1:A:205:ILE:HD12	1:A:205:ILE:N	1.83	0.94
1:A:215:HIS:HD2	1:B:216:ARG:CG	1.77	0.94
1:B:295:VAL:HA	1:B:298:TYR:HD2	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ASP:OD1	1:B:221:ASP:N	1.99	0.93
1:B:365:GLY:O	1:B:369:ARG:CZ	2.16	0.93
1:B:372:PHE:HD1	1:B:390:VAL:CG1	1.58	0.93
1:B:61:LEU:O	1:B:66:VAL:HG22	1.68	0.93
1:B:290:ARG:CA	3:B:703:HOH:O	2.16	0.92
1:A:407:GLU:O	1:A:411:LEU:HB2	1.68	0.92
1:A:215:HIS:CD2	1:B:216:ARG:CD	2.44	0.92
1:A:394:ARG:CD	1:A:405:TYR:OH	2.17	0.92
1:A:215:HIS:NE2	1:B:216:ARG:HG2	1.85	0.92
1:B:143:PRO:HA	1:B:146:ILE:HD12	1.52	0.92
1:B:220:ASP:O	1:B:220:ASP:CG	2.04	0.92
1:B:446:TYR:HE1	1:B:450:ILE:HD12	1.35	0.91
1:A:14:GLY:O	1:A:41:ASP:O	1.89	0.91
1:A:38:THR:HB	3:A:736:HOH:O	1.70	0.91
1:A:47:VAL:N	3:A:702:HOH:O	2.02	0.91
1:A:164:THR:O	1:A:270:ARG:HG2	1.71	0.91
1:A:294:PRO:O	1:A:298:TYR:HD2	1.30	0.90
1:A:299:TYR:CD1	1:A:304:LEU:CD1	2.52	0.90
1:B:368:SER:HB2	1:B:393:MET:HB3	1.54	0.90
1:A:186:ILE:HG13	1:A:242:TRP:CH2	2.07	0.90
1:B:280:ASP:HB3	1:B:281:PRO:HD3	1.54	0.90
1:A:205:ILE:HD12	1:A:205:ILE:H	1.37	0.89
1:A:62:HIS:HA	1:A:66:VAL:HG23	1.53	0.89
1:A:277:THR:HG21	1:A:281:PRO:HD2	1.53	0.89
1:B:205:ILE:N	1:B:205:ILE:HD12	1.87	0.89
1:A:300:GLY:HA2	1:A:375:PHE:CD2	2.08	0.88
1:B:408:THR:HG23	1:B:412:LEU:HD13	1.55	0.88
1:A:50:LYS:HA	3:A:710:HOH:O	1.74	0.88
1:B:496:ASN:O	1:B:500:PRO:HG2	1.73	0.87
1:A:299:TYR:HA	1:A:304:LEU:HD21	1.56	0.87
1:B:167:VAL:O	1:B:242:TRP:CZ3	2.28	0.87
1:A:294:PRO:O	1:A:298:TYR:CE2	2.28	0.87
1:A:182:LEU:HD21	1:A:205:ILE:HG12	1.57	0.86
1:B:79:GLY:O	3:B:702:HOH:O	1.92	0.86
1:B:372:PHE:HD1	1:B:390:VAL:HG12	1.07	0.86
1:A:182:LEU:HD21	1:A:205:ILE:CG1	2.06	0.86
1:A:171:ARG:NH1	1:A:186:ILE:HD13	1.89	0.86
1:A:46:TYR:O	1:A:91:VAL:O	1.92	0.86
1:A:345:ALA:CA	1:B:345:ALA:HA	2.04	0.85
1:B:33:GLU:O	3:B:704:HOH:O	1.94	0.85
1:B:182:LEU:HD21	1:B:205:ILE:HG12	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:PHE:CE1	1:A:491:THR:HA	2.12	0.85
1:B:304:LEU:O	1:B:304:LEU:HD23	1.76	0.85
1:B:276:SER:OG	1:B:286:MET:CG	2.23	0.85
1:B:306:GLY:C	1:B:393:MET:HE1	1.98	0.85
1:A:65:VAL:HG13	1:A:71:PHE:CE2	2.11	0.84
1:A:406:VAL:HG12	1:A:406:VAL:O	1.74	0.84
1:B:62:HIS:O	1:B:66:VAL:O	1.95	0.84
1:B:403:ALA:O	1:B:406:VAL:HG22	1.76	0.84
1:B:446:TYR:CZ	1:B:450:ILE:HD11	2.11	0.84
1:A:344:ALA:C	1:B:345:ALA:HB2	1.95	0.84
1:A:409:ASP:OD2	1:A:438:ALA:CA	2.26	0.84
1:A:298:TYR:O	1:A:304:LEU:HD23	1.75	0.84
1:A:187:ALA:CB	3:A:739:HOH:O	1.89	0.84
1:A:7:ILE:HG23	1:A:477:GLU:OE1	1.78	0.84
1:A:298:TYR:C	1:A:304:LEU:CD2	2.42	0.84
1:A:299:TYR:CG	1:A:304:LEU:HD13	2.12	0.83
1:B:293:ASP:HB3	1:B:502:LEU:HD11	1.59	0.83
1:B:205:ILE:HD12	1:B:205:ILE:H	1.42	0.83
1:A:274:ILE:HD12	1:A:323:VAL:HG21	1.61	0.83
1:A:299:TYR:HA	1:A:304:LEU:CG	2.07	0.83
1:A:382:ASP:OD2	1:A:386:ARG:HG3	1.79	0.83
1:B:236:ARG:HH11	1:B:236:ARG:HG3	1.42	0.83
1:A:388:ILE:HG23	1:A:390:VAL:HG13	1.61	0.83
1:A:182:LEU:HD23	1:A:182:LEU:O	1.79	0.82
1:B:295:VAL:HA	1:B:298:TYR:CD2	2.13	0.82
1:A:463:ASN:O	1:A:466:THR:HG23	1.78	0.82
1:B:287:GLU:O	1:B:505:HIS:CE1	2.33	0.82
1:A:215:HIS:CD2	1:B:216:ARG:HG3	2.13	0.82
1:A:299:TYR:CA	1:A:304:LEU:CD2	2.30	0.81
1:A:375:PHE:HB3	1:A:390:VAL:HG21	1.59	0.81
1:B:404:SER:O	1:B:407:GLU:OE1	1.97	0.81
1:A:47:VAL:O	1:A:47:VAL:CG1	2.22	0.81
1:A:304:LEU:O	1:A:304:LEU:CD1	2.29	0.81
1:B:397:ASP:HB2	3:B:708:HOH:O	1.80	0.81
1:A:368:SER:HB2	1:A:393:MET:HB3	1.60	0.81
1:A:273:VAL:HG12	1:A:273:VAL:O	1.80	0.80
1:A:180:PHE:CE2	1:A:242:TRP:HH2	2.00	0.80
1:B:280:ASP:HB2	1:B:321:ASP:CB	2.11	0.80
1:A:302:GLY:O	1:A:304:LEU:CD2	2.30	0.80
1:A:261:ARG:HG3	1:A:261:ARG:HH11	1.45	0.80
1:A:299:TYR:HA	1:A:304:LEU:CD1	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ARG:HH11	1:A:351:VAL:HG11	1.47	0.79
1:A:393:MET:N	3:A:703:HOH:O	2.15	0.79
1:B:407:GLU:N	1:B:407:GLU:OE2	2.15	0.79
1:B:287:GLU:O	1:B:505:HIS:NE2	2.16	0.79
1:B:388:ILE:O	1:B:390:VAL:HG23	1.82	0.79
1:A:215:HIS:NE2	1:B:216:ARG:HD3	1.95	0.79
1:B:299:TYR:CE2	1:B:371:LEU:HB3	2.18	0.78
1:A:298:TYR:O	1:A:304:LEU:HD21	1.83	0.78
1:A:364:PHE:HB3	3:A:732:HOH:O	1.82	0.78
1:B:280:ASP:CB	1:B:281:PRO:CD	2.62	0.78
1:B:399:MET:O	1:B:399:MET:HG3	1.83	0.77
1:B:301:LYS:O	1:B:303:GLN:HG2	1.84	0.77
1:A:65:VAL:CG1	1:A:71:PHE:CE2	2.67	0.77
1:B:299:TYR:OH	1:B:372:PHE:CA	2.33	0.77
1:B:446:TYR:CE1	1:B:450:ILE:CG1	2.67	0.77
1:B:306:GLY:N	1:B:393:MET:HE1	2.00	0.77
1:B:322:MET:HE1	1:B:485:VAL:HA	1.67	0.77
1:B:180:PHE:CE2	1:B:242:TRP:HH2	2.03	0.77
1:B:274:ILE:HD13	1:B:323:VAL:HG21	1.66	0.77
1:B:412:LEU:C	1:B:414:ALA:H	1.88	0.76
1:B:310:ASP:N	1:B:456:PHE:CE1	2.53	0.76
1:A:172:GLN:HG3	1:A:458:GLY:HA3	1.66	0.76
1:A:299:TYR:HD1	1:A:304:LEU:HD13	1.33	0.76
1:A:405:TYR:C	1:A:407:GLU:H	1.89	0.76
1:B:177:GLU:OE1	1:B:465:ASN:N	2.18	0.75
1:B:132:TYR:OH	1:B:208:GLU:HG3	1.87	0.75
1:A:280:ASP:HB3	1:A:281:PRO:HD3	1.67	0.74
1:A:306:GLY:CA	1:A:393:MET:HE2	1.95	0.74
1:A:409:ASP:OD2	1:A:438:ALA:HB1	1.84	0.74
1:A:22:GLY:N	3:A:704:HOH:O	2.20	0.74
1:A:299:TYR:HB2	1:A:304:LEU:HD13	1.67	0.74
1:A:390:VAL:HG22	3:A:719:HOH:O	1.88	0.74
1:B:280:ASP:HB3	1:B:281:PRO:HD2	1.70	0.74
1:A:322:MET:HE1	1:A:485:VAL:HA	1.68	0.74
1:A:33:GLU:HG3	1:A:70:LEU:CD2	2.18	0.74
1:A:70:LEU:O	1:A:70:LEU:HD23	1.88	0.73
1:B:295:VAL:CA	1:B:298:TYR:HD2	2.01	0.73
1:B:354:VAL:HB	3:B:705:HOH:O	1.88	0.73
1:B:386:ARG:HD3	1:B:388:ILE:HD11	1.70	0.73
1:B:407:GLU:O	1:B:411:LEU:HB2	1.87	0.73
1:B:310:ASP:N	1:B:456:PHE:HE1	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLY:HA3	1:A:375:PHE:CE2	2.23	0.72
1:A:62:HIS:HA	1:A:66:VAL:HG21	1.70	0.72
1:B:405:TYR:HD1	1:B:405:TYR:O	1.71	0.72
1:A:301:LYS:O	1:A:304:LEU:HD21	1.88	0.72
1:B:280:ASP:HB2	1:B:321:ASP:HB2	1.69	0.72
1:B:291:MET:HE2	1:B:291:MET:HA	1.71	0.72
1:B:275:GLU:CG	1:B:498:HIS:CE1	2.73	0.72
1:B:274:ILE:HG13	2:B:601:NAP:O7N	1.88	0.71
1:A:158:LEU:HD23	1:A:265:PRO:O	1.89	0.71
1:A:65:VAL:HG13	1:A:71:PHE:HE2	1.55	0.71
1:B:275:GLU:HG2	1:B:498:HIS:CE1	2.25	0.71
1:A:353:HIS:O	1:A:466:THR:CG2	2.35	0.71
1:A:130:GLU:OE1	1:A:131:ARG:N	2.24	0.71
1:B:290:ARG:O	1:B:294:PRO:HD2	1.89	0.71
1:B:496:ASN:C	1:B:500:PRO:HG2	2.11	0.71
1:A:133:ASP:OD1	1:A:133:ASP:N	2.22	0.71
1:B:305:SER:O	1:B:393:MET:HE3	1.90	0.71
1:A:405:TYR:O	1:A:408:THR:OG1	2.09	0.71
1:B:372:PHE:CD1	1:B:390:VAL:HG13	2.24	0.71
1:A:270:ARG:NH1	1:A:351:VAL:CG1	2.53	0.70
1:A:16:LYS:H	1:A:43:GLY:H	1.39	0.70
1:A:215:HIS:NE2	1:B:216:ARG:CG	2.30	0.70
1:A:13:LEU:HD13	1:A:35:ILE:CG2	2.22	0.70
1:B:388:ILE:O	1:B:388:ILE:HG22	1.91	0.70
1:A:217:ARG:O	1:A:220:ASP:N	2.21	0.70
1:B:299:TYR:CD2	1:B:371:LEU:HB3	2.27	0.70
1:B:36:LEU:N	3:B:704:HOH:O	2.25	0.70
1:B:220:ASP:OD1	1:B:220:ASP:C	2.28	0.69
1:B:366:ASP:O	1:B:370:PHE:CD2	2.45	0.69
1:B:232:LEU:HD22	1:B:232:LEU:O	1.92	0.69
1:B:88:ARG:NH1	3:B:707:HOH:O	2.25	0.69
1:B:298:TYR:HA	1:B:303:GLN:HG3	1.73	0.69
1:A:171:ARG:CZ	1:A:186:ILE:CD1	2.70	0.69
1:A:380:TYR:HD2	3:A:728:HOH:O	1.75	0.69
1:A:48:LEU:HD11	1:A:95:GLY:HA3	1.73	0.69
1:B:22:GLY:HA3	1:B:28:ALA:HB3	1.74	0.69
1:A:114:ASP:OD1	1:A:154:ARG:NH1	2.26	0.69
1:A:290:ARG:N	3:A:706:HOH:O	2.25	0.69
1:A:8:GLY:O	1:A:11:GLU:HG2	1.92	0.69
1:A:171:ARG:NH1	1:A:186:ILE:CD1	2.56	0.68
1:A:215:HIS:HD2	1:B:216:ARG:HG3	1.52	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ARG:CZ	1:A:386:ARG:HB2	2.23	0.68
1:B:180:PHE:HE2	1:B:242:TRP:HH2	1.39	0.68
1:B:449:SER:OG	1:B:450:ILE:N	2.24	0.68
1:B:21:THR:HB	1:B:123:ALA:HB2	1.76	0.68
1:B:306:GLY:C	1:B:393:MET:CE	2.58	0.68
1:A:374:HIS:ND1	1:A:495:THR:O	2.24	0.68
1:A:392:PRO:CA	3:A:703:HOH:O	2.42	0.68
1:B:446:TYR:CD1	1:B:450:ILE:HG13	2.29	0.68
1:A:408:THR:O	1:A:412:LEU:N	2.26	0.67
1:B:406:VAL:HG12	1:B:441:VAL:HG21	1.75	0.67
1:A:142:GLY:O	1:A:146:ILE:HD12	1.94	0.67
1:A:382:ASP:OD2	1:A:386:ARG:CG	2.41	0.67
1:B:417:LEU:C	1:B:417:LEU:HD22	2.14	0.67
1:B:417:LEU:HD13	1:B:417:LEU:H	1.60	0.67
1:A:276:SER:HG	1:A:498:HIS:HD1	1.42	0.67
1:A:345:ALA:HA	1:B:345:ALA:CA	2.20	0.67
1:A:386:ARG:HG3	1:A:386:ARG:O	1.94	0.67
1:B:275:GLU:HG2	1:B:498:HIS:NE2	2.09	0.67
1:A:475:GLU:N	1:A:475:GLU:CD	2.48	0.67
1:A:380:TYR:CD2	3:A:728:HOH:O	2.48	0.67
1:A:277:THR:OG1	1:A:285:TRP:HB3	1.95	0.67
1:B:261:ARG:HG3	1:B:261:ARG:NH1	2.02	0.67
1:A:16:LYS:O	1:A:43:GLY:CA	2.43	0.67
1:B:321:ASP:O	1:B:325:ASN:ND2	2.27	0.67
1:B:393:MET:CE	1:B:393:MET:HA	2.24	0.67
1:A:294:PRO:CB	3:A:726:HOH:O	2.25	0.66
1:B:261:ARG:O	1:B:261:ARG:HG2	1.93	0.66
1:A:305:SER:O	1:A:393:MET:CE	2.42	0.66
1:B:322:MET:CE	1:B:485:VAL:HA	2.25	0.66
1:B:141:VAL:O	1:B:144:PHE:HB3	1.95	0.66
1:B:236:ARG:HG3	1:B:236:ARG:NH1	2.08	0.66
1:B:396:PHE:CZ	1:B:405:TYR:HD2	2.13	0.66
1:B:304:LEU:HD23	1:B:304:LEU:C	2.15	0.66
1:A:158:LEU:CD2	1:A:265:PRO:O	2.44	0.66
1:B:174:VAL:O	1:B:174:VAL:CG1	2.37	0.66
1:B:494:ILE:O	1:B:499:ILE:HG13	1.96	0.66
1:A:164:THR:HG22	2:A:601:NAP:H5N	1.78	0.66
1:A:136:MET:HA	1:A:140:THR:HG22	1.77	0.66
1:A:216:ARG:H	1:A:216:ARG:HE	1.44	0.66
1:A:306:GLY:N	1:A:393:MET:CE	2.46	0.66
1:A:48:LEU:CD1	1:A:95:GLY:HA3	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:HD13	1:B:35:ILE:CG2	2.26	0.65
1:B:223:ALA:O	1:B:227:GLU:N	2.26	0.65
1:A:31:LEU:HD22	1:A:35:ILE:HD11	1.77	0.65
1:A:303:GLN:OE1	1:A:303:GLN:O	2.14	0.65
1:B:330:SER:HB3	3:B:718:HOH:O	1.95	0.65
1:A:13:LEU:O	1:A:39:ASN:ND2	2.30	0.65
1:A:163:SER:O	1:A:270:ARG:HA	1.96	0.65
1:A:28:ALA:O	1:A:31:LEU:HB3	1.97	0.65
1:B:125:ASN:HD22	1:B:125:ASN:C	2.01	0.64
1:B:139:ASN:O	1:B:143:PRO:HG3	1.97	0.64
1:B:172:GLN:O	1:B:458:GLY:O	2.15	0.64
1:B:408:THR:O	1:B:412:LEU:HB2	1.97	0.64
1:A:13:LEU:HD13	1:A:35:ILE:HG23	1.79	0.64
1:A:271:PRO:HB2	1:A:274:ILE:HD11	1.80	0.64
1:B:393:MET:HE3	1:B:393:MET:CA	2.27	0.64
1:B:417:LEU:CD1	1:B:417:LEU:N	2.60	0.64
1:A:214:ASP:O	1:B:214:ASP:CG	2.35	0.64
1:B:272:SER:OG	1:B:318:VAL:HG22	1.96	0.64
1:A:236:ARG:O	1:A:237:ALA:C	2.36	0.64
1:A:366:ASP:O	1:A:370:PHE:CD2	2.51	0.64
1:A:379:PRO:HB2	1:A:388:ILE:HG22	1.80	0.64
1:B:33:GLU:C	3:B:704:HOH:O	2.33	0.64
1:A:171:ARG:CZ	1:A:186:ILE:HD11	2.29	0.64
1:B:296:VAL:HG11	1:B:499:ILE:HD13	1.80	0.64
1:A:205:ILE:H	1:A:205:ILE:CD1	2.07	0.63
1:B:61:LEU:O	1:B:66:VAL:CG2	2.46	0.63
1:A:24:THR:CG2	2:A:601:NAP:O1X	2.42	0.63
1:B:220:ASP:O	1:B:220:ASP:OD1	2.16	0.63
1:B:280:ASP:CB	1:B:281:PRO:HD3	2.26	0.63
1:A:271:PRO:HG2	2:A:601:NAP:H6N	1.81	0.63
1:A:396:PHE:CZ	1:A:405:TYR:CE1	2.86	0.63
1:A:396:PHE:HZ	1:A:405:TYR:CE1	2.17	0.63
1:B:309:ALA:O	1:B:311:PRO:HD3	1.99	0.63
1:A:163:SER:O	1:A:271:PRO:HD2	1.99	0.63
1:A:17:ASN:N	1:A:17:ASN:HD22	1.96	0.63
1:A:270:ARG:HH11	1:A:351:VAL:CG1	2.10	0.63
1:B:73:ARG:HG3	1:B:73:ARG:HH11	1.63	0.63
1:A:254:GLU:HG2	3:A:727:HOH:O	1.99	0.63
1:B:368:SER:HB2	1:B:393:MET:CB	2.28	0.63
1:A:45:ILE:HG22	1:A:47:VAL:HG23	1.81	0.62
1:A:141:VAL:HG12	1:A:141:VAL:O	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ILE:HG12	3:A:743:HOH:O	1.99	0.62
1:A:167:VAL:O	1:A:242:TRP:CZ3	2.52	0.62
1:A:164:THR:HG23	1:A:246:TYR:OH	1.98	0.62
1:B:446:TYR:CE1	1:B:450:ILE:HD12	2.19	0.62
1:B:126:THR:O	1:B:290:ARG:NH1	2.32	0.62
1:B:478:LYS:HG2	3:B:732:HOH:O	1.99	0.62
1:B:182:LEU:HD13	1:B:182:LEU:O	2.00	0.62
1:A:310:ASP:OD1	1:A:310:ASP:C	2.36	0.62
1:B:114:ASP:OD1	1:B:154:ARG:NH1	2.32	0.62
1:A:167:VAL:HG11	1:A:270:ARG:HE	1.63	0.62
1:A:177:GLU:HG2	1:A:353:HIS:CD2	2.34	0.62
1:B:232:LEU:HD22	1:B:232:LEU:C	2.20	0.62
1:A:140:THR:O	1:A:143:PRO:HG2	2.00	0.62
1:B:297:LEU:O	1:B:301:LYS:HG3	1.99	0.62
1:A:16:LYS:O	1:A:43:GLY:N	2.32	0.62
1:A:154:ARG:HG3	1:A:154:ARG:HH11	1.65	0.62
1:B:277:THR:CG2	1:B:321:ASP:HB3	2.29	0.62
1:A:164:THR:HG22	2:A:601:NAP:C5N	2.30	0.61
1:A:167:VAL:O	1:A:242:TRP:HZ3	1.83	0.61
1:A:88:ARG:NH1	3:A:708:HOH:O	2.33	0.61
1:A:50:LYS:HD2	2:A:601:NAP:C6A	2.31	0.61
1:A:269:ILE:CD1	1:A:327:THR:HA	2.31	0.61
1:B:24:THR:HG23	1:B:24:THR:O	2.00	0.61
1:A:216:ARG:HD2	1:A:216:ARG:N	2.16	0.61
1:A:298:TYR:O	1:A:302:GLY:O	2.18	0.61
1:A:299:TYR:CA	1:A:304:LEU:HD13	2.29	0.61
1:A:492:ASP:O	1:A:496:ASN:HB2	2.00	0.61
1:B:96:ASP:O	1:B:102:VAL:O	2.18	0.61
1:A:51:ALA:CB	1:A:57:ALA:HB2	2.30	0.61
1:A:409:ASP:CG	1:A:438:ALA:HB2	2.13	0.61
1:A:177:GLU:OE1	1:A:465:ASN:N	2.27	0.61
1:B:409:ASP:OD2	1:B:437:CYS:O	2.19	0.61
1:A:305:SER:C	1:A:393:MET:CE	2.69	0.60
1:A:475:GLU:CD	1:A:475:GLU:H	2.03	0.60
1:B:394:ARG:HB3	1:B:396:PHE:HE1	1.66	0.60
1:A:80:LYS:HE2	1:A:80:LYS:HA	1.83	0.60
1:B:318:VAL:HG12	1:B:319:PRO:HD2	1.82	0.60
1:B:452:GLN:HB3	1:B:453:PRO:CD	2.23	0.60
1:A:449:SER:O	1:A:452:GLN:HB3	2.01	0.60
1:B:307:PHE:HA	1:B:402:PHE:HE1	1.67	0.60
1:B:372:PHE:O	1:B:376:THR:CG2	2.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:THR:HG22	1:B:390:VAL:HG11	1.82	0.60
1:B:502:LEU:O	1:B:506:VAL:HG12	2.01	0.60
1:A:62:HIS:O	1:A:66:VAL:HG23	2.02	0.60
1:A:242:TRP:CD1	1:A:248:PHE:CD1	2.89	0.60
1:A:7:ILE:HG22	1:A:473:MET:HA	1.84	0.60
1:A:393:MET:HE3	1:A:394:ARG:H	1.67	0.60
1:A:370:PHE:CZ	1:A:491:THR:HA	2.37	0.60
1:B:40:PRO:HB3	3:B:721:HOH:O	2.02	0.60
1:B:274:ILE:CD1	1:B:323:VAL:HG21	2.31	0.60
1:B:406:VAL:N	1:B:407:GLU:OE2	2.35	0.60
1:B:208:GLU:OE2	1:B:208:GLU:HA	2.01	0.59
1:A:476:GLU:O	1:A:479:ALA:HB3	2.02	0.59
1:B:299:TYR:HE2	1:B:371:LEU:C	2.05	0.59
1:A:12:PHE:O	1:A:14:GLY:N	2.35	0.59
1:A:216:ARG:H	1:A:216:ARG:NE	1.99	0.59
1:B:403:ALA:O	1:B:406:VAL:CG2	2.50	0.59
1:A:131:ARG:HA	1:A:230:LYS:HA	1.85	0.59
1:A:499:ILE:N	1:A:500:PRO:CD	2.65	0.59
1:B:417:LEU:H	1:B:417:LEU:CD1	2.16	0.59
1:A:62:HIS:CA	1:A:66:VAL:HG23	2.31	0.59
1:A:369:ARG:HG2	1:A:373:GLN:OE1	2.03	0.59
1:B:396:PHE:CZ	1:B:405:TYR:CD2	2.90	0.59
1:B:405:TYR:O	1:B:405:TYR:CD1	2.55	0.59
1:B:446:TYR:CE1	1:B:450:ILE:HG13	2.37	0.59
1:A:186:ILE:O	1:A:186:ILE:HG22	2.02	0.59
1:A:446:TYR:CE1	1:A:450:ILE:CD1	2.86	0.59
1:A:182:LEU:HD12	1:A:259:SER:OG	2.03	0.59
1:B:499:ILE:N	1:B:500:PRO:CD	2.66	0.59
1:A:65:VAL:HG13	1:A:71:PHE:CZ	2.37	0.59
1:B:274:ILE:HG13	2:B:601:NAP:C7N	2.33	0.59
1:A:34:LYS:NZ	1:A:325:ASN:OD1	2.35	0.58
1:A:216:ARG:N	1:A:216:ARG:CD	2.66	0.58
1:B:395:LEU:C	1:B:396:PHE:CD1	2.77	0.58
1:B:406:VAL:CG1	1:B:441:VAL:HG11	2.28	0.58
1:B:391:PRO:C	1:B:392:PRO:O	2.24	0.58
1:B:446:TYR:HE1	1:B:450:ILE:HD11	0.79	0.58
1:A:21:THR:C	3:A:704:HOH:O	2.42	0.58
1:A:271:PRO:HG2	2:A:601:NAP:C6N	2.33	0.58
1:A:345:ALA:HB2	1:B:344:ALA:C	2.24	0.58
1:A:438:ALA:HB1	1:A:441:VAL:HG23	1.85	0.58
1:B:73:ARG:HH11	1:B:73:ARG:CG	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ARG:C	3:B:703:HOH:O	2.34	0.58
1:B:105:ALA:HB1	1:B:106:PRO:HD2	1.86	0.58
1:A:221:ASP:N	1:A:221:ASP:OD1	2.37	0.58
1:B:34:LYS:O	1:B:38:THR:CG2	2.40	0.58
1:A:164:THR:HB	1:A:166:TYR:H	1.68	0.57
1:A:207:ALA:HA	1:A:210:LYS:HD3	1.85	0.57
1:A:217:ARG:HB2	1:A:220:ASP:HB3	1.85	0.57
1:A:404:SER:O	1:A:407:GLU:OE1	2.22	0.57
1:B:254:GLU:OE1	1:B:270:ARG:NH2	2.32	0.57
1:A:393:MET:CE	1:A:394:ARG:H	2.17	0.57
1:B:236:ARG:HH11	1:B:236:ARG:CG	2.17	0.57
1:A:299:TYR:CA	1:A:304:LEU:CD1	2.81	0.57
1:B:412:LEU:C	1:B:414:ALA:N	2.56	0.57
1:A:146:ILE:CG1	3:A:743:HOH:O	2.52	0.57
1:A:274:ILE:HB	2:A:601:NAP:O7N	2.05	0.57
1:B:164:THR:HG23	1:B:246:TYR:OH	2.05	0.57
1:B:205:ILE:H	1:B:205:ILE:CD1	2.07	0.57
1:A:232:LEU:HD12	1:A:232:LEU:O	2.05	0.57
1:B:285:TRP:CZ2	1:B:287:GLU:HG3	2.39	0.57
1:B:306:GLY:N	1:B:393:MET:CE	2.63	0.57
1:B:452:GLN:CB	1:B:453:PRO:HD3	2.20	0.57
1:A:62:HIS:CD2	1:A:66:VAL:HG21	2.39	0.56
1:B:164:THR:HB	1:B:166:TYR:H	1.69	0.56
1:B:295:VAL:O	1:B:298:TYR:N	2.38	0.56
1:A:299:TYR:CE2	1:A:371:LEU:HB3	2.40	0.56
1:B:277:THR:HG23	1:B:321:ASP:HB3	1.86	0.56
1:A:216:ARG:NE	1:A:216:ARG:HA	2.20	0.56
1:A:300:GLY:HA3	1:A:375:PHE:CZ	2.40	0.56
1:A:364:PHE:CB	3:A:732:HOH:O	2.47	0.56
1:B:370:PHE:CZ	1:B:491:THR:HA	2.40	0.56
1:A:144:PHE:CD1	1:A:260:MET:CE	2.89	0.56
1:A:293:ASP:N	1:A:294:PRO:HD2	2.21	0.56
1:B:398:THR:HG23	3:B:708:HOH:O	2.06	0.56
1:A:141:VAL:O	1:A:141:VAL:CG1	2.53	0.56
1:A:232:LEU:HD12	1:A:232:LEU:C	2.25	0.56
1:A:446:TYR:CE1	1:A:450:ILE:HD11	2.41	0.56
1:B:26:PHE:O	1:B:30:VAL:HG23	2.06	0.56
1:B:463:ASN:ND2	1:B:467:GLU:OE1	2.39	0.56
1:B:136:MET:HA	1:B:140:THR:HG22	1.88	0.56
1:B:294:PRO:HB2	1:B:298:TYR:HE2	1.70	0.56
1:B:395:LEU:C	1:B:396:PHE:HD1	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:TYR:C	1:A:407:GLU:N	2.58	0.56
1:B:217:ARG:HD3	1:B:225:PHE:CD1	2.41	0.56
1:B:263:ASP:OD1	1:B:263:ASP:N	2.39	0.56
1:B:279:ARG:HA	1:B:283:PRO:HG3	1.87	0.56
1:B:62:HIS:CA	1:B:66:VAL:CG2	2.64	0.56
1:B:22:GLY:HA3	1:B:28:ALA:CB	2.36	0.55
1:B:201:THR:O	1:B:201:THR:OG1	2.22	0.55
1:A:217:ARG:O	1:A:219:GLY:N	2.38	0.55
1:A:409:ASP:OD2	1:A:438:ALA:HA	2.04	0.55
1:B:296:VAL:CG1	1:B:499:ILE:HD13	2.37	0.55
1:A:278:TRP:H	1:A:321:ASP:HB2	1.72	0.55
1:A:390:VAL:HG23	1:A:390:VAL:O	2.05	0.55
1:A:159:PHE:O	1:A:266:VAL:HA	2.07	0.55
1:B:143:PRO:HA	1:B:146:ILE:CD1	2.33	0.55
1:A:65:VAL:HG12	1:A:71:PHE:CE2	2.42	0.55
1:B:13:LEU:HD13	1:B:35:ILE:HG23	1.87	0.55
1:B:48:LEU:HD21	1:B:96:ASP:O	2.07	0.55
1:A:70:LEU:HD23	1:A:70:LEU:C	2.25	0.55
1:A:131:ARG:HD3	1:A:133:ASP:OD1	2.07	0.55
1:A:17:ASN:N	1:A:17:ASN:ND2	2.54	0.55
1:A:216:ARG:HE	1:A:216:ARG:HA	1.72	0.55
1:A:276:SER:HA	1:A:285:TRP:O	2.07	0.55
1:A:386:ARG:CZ	1:A:386:ARG:CB	2.85	0.55
1:A:496:ASN:O	1:A:500:PRO:HG2	2.06	0.55
1:B:291:MET:CE	1:B:291:MET:CA	2.85	0.55
1:B:172:GLN:O	1:B:458:GLY:C	2.45	0.54
1:B:365:GLY:O	1:B:369:ARG:NH1	2.40	0.54
1:B:475:GLU:OE2	1:B:476:GLU:N	2.40	0.54
1:B:17:ASN:N	1:B:17:ASN:ND2	2.55	0.54
1:B:291:MET:HE2	1:B:291:MET:CA	2.37	0.54
1:B:13:LEU:HD13	1:B:35:ILE:HG22	1.88	0.54
1:B:242:TRP:CD1	1:B:248:PHE:CD1	2.96	0.54
1:B:338:GLY:HA3	1:B:341:ALA:HB3	1.89	0.54
1:B:180:PHE:HE2	1:B:242:TRP:CH2	2.24	0.54
1:B:393:MET:CE	1:B:393:MET:CA	2.85	0.54
1:B:307:PHE:HA	1:B:402:PHE:CE1	2.43	0.54
1:B:484:ASP:OD1	1:B:486:ARG:HB2	2.07	0.54
1:B:452:GLN:N	1:B:453:PRO:CD	2.71	0.54
1:A:166:TYR:CE2	1:A:272:SER:HB2	2.43	0.53
1:A:244:ASP:OD1	1:A:247:VAL:HG22	2.08	0.53
1:B:65:VAL:HG12	1:B:65:VAL:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ARG:O	1:A:413:ARG:HD3	2.09	0.53
1:B:277:THR:CG2	1:B:281:PRO:HD2	2.28	0.53
1:A:21:THR:HB	1:A:123:ALA:HB2	1.90	0.53
1:B:180:PHE:CE2	1:B:242:TRP:CH2	2.91	0.53
1:B:372:PHE:HD1	1:B:390:VAL:HG13	1.63	0.53
1:B:417:LEU:HD13	1:B:417:LEU:N	2.20	0.53
1:A:13:LEU:HD13	1:A:35:ILE:HG22	1.91	0.53
1:B:244:ASP:OD1	1:B:247:VAL:HG22	2.09	0.53
1:A:175:VAL:CG2	1:A:460:ARG:O	2.28	0.53
1:B:78:HIS:HB2	1:B:82:TYR:HB2	1.90	0.53
1:A:85:PHE:N	3:A:708:HOH:O	2.41	0.52
1:B:457:TYR:O	1:B:460:ARG:NH2	2.37	0.52
1:B:507:MET:O	1:B:508:LYS:HD2	2.09	0.52
1:A:391:PRO:CB	1:A:392:PRO:CD	2.70	0.52
1:A:392:PRO:HA	3:A:703:HOH:O	2.05	0.52
1:B:306:GLY:CA	1:B:393:MET:HE2	2.07	0.52
1:A:61:LEU:O	1:A:65:VAL:HB	2.10	0.52
1:B:286:MET:C	1:B:286:MET:HE3	2.29	0.52
1:A:345:ALA:N	1:B:345:ALA:N	2.57	0.52
1:B:291:MET:O	1:B:451:TYR:HE2	1.93	0.52
1:A:21:THR:OG1	1:A:121:ASN:HA	2.10	0.52
1:A:358:THR:HG21	1:A:462:ASP:HA	1.92	0.52
1:B:62:HIS:HA	1:B:66:VAL:HG21	1.81	0.52
1:B:404:SER:O	1:B:404:SER:OG	2.21	0.52
1:A:310:ASP:OD1	1:A:312:GLU:N	2.40	0.52
1:B:73:ARG:HG3	1:B:73:ARG:NH1	2.24	0.52
1:B:163:SER:O	1:B:271:PRO:HD2	2.09	0.52
1:A:21:THR:CA	3:A:704:HOH:O	2.57	0.52
1:A:506:VAL:O	1:A:506:VAL:CG2	2.57	0.52
1:B:182:LEU:HD11	1:B:205:ILE:HD11	1.91	0.52
1:A:79:GLY:C	1:A:80:LYS:CE	2.73	0.52
1:A:254:GLU:OE1	1:A:270:ARG:NH2	2.42	0.52
1:A:484:ASP:OD1	1:A:486:ARG:HB2	2.09	0.52
1:B:17:ASN:HD22	1:B:17:ASN:H	1.58	0.52
1:A:322:MET:CE	1:A:485:VAL:HA	2.37	0.52
1:A:49:ILE:HG22	1:A:50:LYS:O	2.10	0.51
1:A:144:PHE:CD1	1:A:260:MET:HE3	2.46	0.51
1:A:306:GLY:C	1:A:393:MET:HE1	2.30	0.51
1:A:406:VAL:O	1:A:406:VAL:CG1	2.36	0.51
1:B:32:ILE:O	3:B:704:HOH:O	2.18	0.51
1:B:304:LEU:HD22	1:B:304:LEU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:VAL:O	1:A:506:VAL:HG22	2.11	0.51
1:B:16:LYS:O	1:B:43:GLY:N	2.43	0.51
1:A:318:VAL:HG12	1:A:319:PRO:HD2	1.92	0.51
1:B:275:GLU:HG2	1:B:498:HIS:CD2	2.45	0.51
1:B:17:ASN:N	1:B:17:ASN:HD22	2.08	0.51
1:A:386:ARG:CB	1:A:386:ARG:NH1	2.73	0.51
1:B:364:PHE:O	1:B:395:LEU:CD1	2.58	0.51
1:B:417:LEU:HD22	1:B:418:ALA:HB2	1.92	0.51
1:A:19:LEU:HA	3:A:702:HOH:O	2.11	0.51
1:A:51:ALA:N	3:A:710:HOH:O	2.43	0.51
1:A:158:LEU:HB2	1:A:335:GLY:HA3	1.93	0.51
1:A:217:ARG:O	1:A:218:HIS:C	2.47	0.51
1:A:299:TYR:HD1	1:A:304:LEU:HD12	1.70	0.51
1:B:390:VAL:N	1:B:391:PRO:HD3	2.25	0.51
1:A:125:ASN:C	1:A:125:ASN:HD22	2.14	0.51
1:A:141:VAL:O	1:A:144:PHE:HB3	2.11	0.51
1:B:82:TYR:CD2	1:B:83:HIS:HD2	2.28	0.51
1:B:139:ASN:O	1:B:143:PRO:CG	2.59	0.51
1:B:476:GLU:O	1:B:479:ALA:HB3	2.11	0.51
1:A:227:GLU:O	1:A:230:LYS:N	2.44	0.50
1:B:125:ASN:HD21	1:B:130:GLU:HG2	1.76	0.50
1:A:244:ASP:OD2	1:A:454:TYR:OH	2.16	0.50
1:A:364:PHE:CZ	1:A:455:THR:HA	2.46	0.50
1:B:275:GLU:HG3	1:B:498:HIS:CE1	2.44	0.50
1:A:499:ILE:N	1:A:500:PRO:HD2	2.27	0.50
1:B:463:ASN:O	1:B:466:THR:HG23	2.12	0.50
1:A:143:PRO:HA	1:A:146:ILE:HD13	1.94	0.50
1:B:340:ALA:HB2	3:B:738:HOH:O	2.10	0.50
1:B:452:GLN:N	1:B:453:PRO:HD2	2.25	0.50
1:B:369:ARG:HG2	1:B:373:GLN:HE21	1.75	0.50
1:B:396:PHE:CD1	1:B:396:PHE:N	2.79	0.50
1:A:135:ALA:O	1:A:139:ASN:HB2	2.12	0.50
1:A:402:PHE:O	1:A:405:TYR:HB2	2.11	0.50
1:A:36:LEU:HD11	1:A:90:LEU:HD21	1.94	0.50
1:A:386:ARG:NH1	1:A:386:ARG:HB3	2.26	0.50
1:A:97:VAL:HA	1:A:102:VAL:HG12	1.94	0.50
1:A:496:ASN:C	1:A:500:PRO:HG2	2.32	0.50
1:B:282:PHE:CD1	1:B:282:PHE:C	2.85	0.50
1:A:307:PHE:HA	1:A:402:PHE:HE1	1.77	0.50
1:A:125:ASN:C	1:A:125:ASN:ND2	2.65	0.49
1:A:215:HIS:O	1:A:218:HIS:ND1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:CB	2:A:601:NAP:O7N	2.60	0.49
1:B:130:GLU:OE1	1:B:131:ARG:N	2.42	0.49
1:A:273:VAL:HB	1:A:316:ASP:O	2.11	0.49
1:A:499:ILE:O	1:A:503:ARG:HG3	2.12	0.49
1:A:394:ARG:NH1	1:A:405:TYR:OH	2.43	0.49
1:A:502:LEU:O	1:A:506:VAL:HG12	2.12	0.49
1:B:164:THR:CG2	1:B:246:TYR:OH	2.60	0.49
1:A:378:SER:O	1:A:378:SER:OG	2.20	0.49
1:B:45:ILE:HG22	1:B:47:VAL:HG22	1.94	0.49
1:B:372:PHE:C	1:B:376:THR:HG23	2.27	0.49
1:A:293:ASP:HB3	1:A:502:LEU:HD11	1.94	0.49
1:A:12:PHE:HD2	1:A:13:LEU:HD23	1.78	0.49
1:A:65:VAL:CG1	1:A:71:PHE:HE2	2.17	0.48
1:A:396:PHE:CE2	1:A:405:TYR:CD1	3.01	0.48
1:B:293:ASP:N	1:B:294:PRO:HD2	2.27	0.48
1:A:216:ARG:H	1:A:216:ARG:CD	2.26	0.48
1:B:205:ILE:N	1:B:205:ILE:CD1	2.60	0.48
1:B:235:GLU:O	1:B:239:LEU:HB2	2.12	0.48
1:B:399:MET:O	1:B:399:MET:CG	2.59	0.48
1:A:102:VAL:CG1	1:A:146:ILE:HG13	2.43	0.48
1:B:362:LEU:HD12	1:B:490:TRP:HB3	1.95	0.48
1:A:142:GLY:N	1:A:143:PRO:HD2	2.28	0.48
1:A:217:ARG:C	1:A:219:GLY:N	2.65	0.48
1:A:102:VAL:HG11	1:A:146:ILE:HG13	1.95	0.48
1:A:316:ASP:HA	3:A:716:HOH:O	2.14	0.48
1:B:261:ARG:HH22	1:B:348:GLY:HA2	1.78	0.48
1:B:449:SER:O	1:B:450:ILE:C	2.52	0.48
1:A:182:LEU:CD2	1:A:205:ILE:HD11	2.44	0.48
1:A:494:ILE:O	1:A:499:ILE:HG13	2.14	0.48
1:A:505:HIS:O	1:A:507:MET:O	2.32	0.48
1:B:51:ALA:CB	1:B:57:ALA:HB2	2.43	0.48
1:B:304:LEU:N	1:B:304:LEU:CD2	2.77	0.48
1:B:31:LEU:HD22	1:B:35:ILE:HD11	1.96	0.48
1:B:265:PRO:CG	3:B:731:HOH:O	2.61	0.48
1:A:409:ASP:O	1:A:413:ARG:HB2	2.14	0.48
1:B:35:ILE:HA	1:B:38:THR:HG23	1.95	0.48
1:B:280:ASP:CB	1:B:321:ASP:CB	2.89	0.48
1:B:290:ARG:O	1:B:294:PRO:CG	2.59	0.48
1:A:16:LYS:O	1:A:43:GLY:HA3	2.14	0.47
1:A:155:ARG:O	1:A:155:ARG:HG2	2.13	0.47
1:A:261:ARG:HH11	1:A:261:ARG:CG	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ILE:CG2	1:A:390:VAL:HG13	2.40	0.47
1:B:269:ILE:CD1	1:B:327:THR:HA	2.44	0.47
1:B:298:TYR:HB3	1:B:303:GLN:HB2	1.96	0.47
1:A:144:PHE:CE1	1:A:260:MET:CE	2.96	0.47
1:B:310:ASP:OD1	1:B:310:ASP:C	2.51	0.47
1:A:28:ALA:O	1:A:31:LEU:CB	2.62	0.47
1:A:126:THR:HB	1:A:290:ARG:NH1	2.30	0.47
1:A:182:LEU:HD21	1:A:205:ILE:CD1	2.45	0.47
1:A:278:TRP:CE3	1:A:279:ARG:HG2	2.48	0.47
1:A:396:PHE:HZ	1:A:405:TYR:HE1	1.58	0.47
1:B:131:ARG:HD2	1:B:134:VAL:HG23	1.95	0.47
1:B:133:ASP:N	1:B:133:ASP:OD1	2.47	0.47
1:A:305:SER:C	1:A:393:MET:HE1	2.29	0.47
1:B:301:LYS:NZ	1:B:380:TYR:CZ	2.83	0.47
1:A:197:GLN:CA	1:A:197:GLN:HE21	2.28	0.47
1:A:261:ARG:O	1:A:261:ARG:HG2	2.14	0.47
1:B:18:PHE:HA	1:B:118:ILE:O	2.14	0.47
1:B:293:ASP:OD2	1:B:502:LEU:HD12	2.15	0.47
1:A:414:ALA:C	1:A:416:ARG:H	2.17	0.47
1:A:386:ARG:HA	1:A:387:PRO:HD2	1.54	0.47
1:B:252:MET:O	1:B:255:MET:HB2	2.14	0.47
1:B:380:TYR:CD2	1:B:381:SER:O	2.68	0.47
1:A:31:LEU:O	1:A:35:ILE:HG13	2.15	0.47
1:B:136:MET:O	1:B:140:THR:HG22	2.15	0.47
1:A:126:THR:O	1:A:290:ARG:NH1	2.45	0.47
1:B:21:THR:OG1	1:B:121:ASN:HA	2.16	0.47
1:B:280:ASP:CB	1:B:321:ASP:HB2	2.40	0.47
1:B:389:HIS:N	1:B:389:HIS:ND1	2.62	0.47
1:A:136:MET:O	1:A:140:THR:HG22	2.15	0.46
1:A:215:HIS:NE2	1:B:216:ARG:CZ	2.68	0.46
1:B:26:PHE:CD1	1:B:26:PHE:C	2.85	0.46
1:A:378:SER:HA	1:A:379:PRO:HD2	1.78	0.46
1:B:272:SER:OG	1:B:318:VAL:CG2	2.63	0.46
1:B:354:VAL:O	3:B:705:HOH:O	2.20	0.46
1:B:380:TYR:O	1:B:387:PRO:CG	2.62	0.46
1:A:269:ILE:HD13	1:A:327:THR:HA	1.97	0.46
1:A:304:LEU:H	1:A:304:LEU:HG	0.79	0.46
1:A:345:ALA:CA	1:B:345:ALA:CA	2.84	0.46
1:B:291:MET:O	1:B:451:TYR:CE2	2.68	0.46
1:A:368:SER:CB	1:A:393:MET:HB3	2.37	0.46
1:A:375:PHE:HD1	1:A:375:PHE:HA	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LEU:HD22	1:B:159:PHE:N	2.29	0.46
1:B:406:VAL:CG1	1:B:441:VAL:HG21	2.43	0.46
1:A:380:TYR:HD1	1:A:380:TYR:O	1.98	0.46
1:B:261:ARG:NH1	1:B:261:ARG:CG	2.73	0.46
1:B:295:VAL:C	1:B:297:LEU:N	2.69	0.46
1:B:45:ILE:HG22	1:B:47:VAL:CG2	2.46	0.46
1:B:142:GLY:N	1:B:143:PRO:HD2	2.30	0.46
1:B:307:PHE:N	1:B:393:MET:HE2	2.31	0.46
1:A:344:ALA:O	1:B:345:ALA:CB	2.43	0.46
1:A:498:HIS:C	1:A:500:PRO:HD2	2.36	0.46
1:B:296:VAL:HG13	1:B:371:LEU:HD22	1.98	0.46
1:A:34:LYS:CD	1:A:38:THR:HG23	2.46	0.46
1:B:101:ASN:OD1	1:B:152:ARG:NH2	2.49	0.46
1:B:386:ARG:HH11	1:B:388:ILE:HD11	1.80	0.46
1:A:199:LYS:HG2	3:A:739:HOH:O	2.15	0.45
1:A:443:GLN:O	1:A:447:LEU:HB2	2.15	0.45
1:B:106:PRO:HA	1:B:109:ALA:HB3	1.98	0.45
1:A:216:ARG:HE	1:A:216:ARG:N	2.10	0.45
1:B:172:GLN:HE21	1:B:458:GLY:CA	2.09	0.45
1:B:277:THR:OG1	1:B:285:TRP:HB3	2.15	0.45
1:A:132:TYR:CD2	1:A:212:ALA:HB2	2.51	0.45
1:B:277:THR:HG22	1:B:321:ASP:HB3	1.99	0.45
1:A:379:PRO:CB	1:A:388:ILE:HG22	2.46	0.45
1:B:307:PHE:CA	1:B:402:PHE:HE1	2.28	0.45
1:B:352:TYR:CE1	3:B:729:HOH:O	2.56	0.45
1:A:403:ALA:O	1:A:406:VAL:HG23	2.16	0.45
1:B:282:PHE:CD1	1:B:282:PHE:O	2.70	0.45
1:A:80:LYS:HE2	1:A:80:LYS:CA	2.46	0.45
1:A:158:LEU:HD22	1:A:159:PHE:N	2.31	0.45
1:A:202:MET:HA	3:A:714:HOH:O	2.15	0.45
1:A:216:ARG:N	1:A:216:ARG:NE	2.64	0.45
1:B:7:ILE:O	1:B:9:ILE:HG13	2.17	0.45
1:A:129:ASP:OD1	1:A:129:ASP:O	2.34	0.45
1:A:180:PHE:CE2	1:A:242:TRP:CH2	2.92	0.45
1:A:380:TYR:O	1:A:380:TYR:CD1	2.70	0.45
1:A:446:TYR:CE1	1:A:450:ILE:HD12	2.51	0.45
1:B:21:THR:HG1	1:B:121:ASN:HA	1.82	0.45
1:A:10:ALA:HA	3:A:736:HOH:O	2.15	0.45
1:A:70:LEU:CD2	1:A:70:LEU:C	2.85	0.45
1:B:217:ARG:HH12	1:B:228:GLU:CD	2.20	0.45
1:B:297:LEU:HA	1:B:297:LEU:HD22	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLY:H	1:A:505:HIS:CE1	2.34	0.45
1:A:261:ARG:HG3	1:A:261:ARG:NH1	2.22	0.45
1:A:299:TYR:CG	1:A:299:TYR:O	2.70	0.45
1:B:26:PHE:O	1:B:26:PHE:CD1	2.70	0.45
1:A:207:ALA:HA	1:A:210:LYS:CD	2.46	0.44
1:A:236:ARG:O	1:A:238:LYS:N	2.49	0.44
1:B:474:SER:OG	1:B:477:GLU:HB2	2.18	0.44
1:B:502:LEU:O	1:B:502:LEU:HD23	2.17	0.44
1:A:372:PHE:HB2	1:A:392:PRO:HA	1.99	0.44
1:B:125:ASN:C	1:B:125:ASN:ND2	2.67	0.44
1:A:136:MET:CA	1:A:140:THR:HG22	2.47	0.44
1:A:374:HIS:CD2	1:A:374:HIS:C	2.90	0.44
1:A:406:VAL:HG13	1:A:441:VAL:HG21	1.98	0.44
1:B:39:ASN:OD1	1:B:41:ASP:HB2	2.18	0.44
1:B:36:LEU:HD11	1:B:90:LEU:HD21	2.00	0.44
1:B:258:ASN:HA	1:B:261:ARG:HD3	1.99	0.44
1:B:298:TYR:HB3	1:B:303:GLN:CB	2.48	0.44
1:A:33:GLU:HG3	1:A:70:LEU:HD22	1.99	0.44
1:A:264:ILE:HG22	1:A:265:PRO:N	2.32	0.44
1:A:282:PHE:O	1:A:282:PHE:CD1	2.70	0.44
1:A:374:HIS:CD2	1:A:374:HIS:O	2.70	0.44
1:A:325:ASN:HB3	1:A:481:PHE:HB3	1.99	0.44
1:A:132:TYR:OH	1:A:208:GLU:HG3	2.18	0.44
1:A:213:PHE:HA	1:A:216:ARG:HG2	2.00	0.44
1:A:297:LEU:HD22	1:A:297:LEU:HA	1.74	0.44
1:B:46:TYR:O	3:B:706:HOH:O	2.21	0.44
1:A:336:ARG:C	1:A:337:GLY:O	2.54	0.44
1:A:457:TYR:CE2	1:A:459:GLY:HA3	2.53	0.44
1:B:154:ARG:HH11	1:B:154:ARG:HG3	1.83	0.44
1:A:32:ILE:O	1:A:33:GLU:C	2.56	0.44
1:A:389:HIS:O	1:A:389:HIS:CD2	2.70	0.44
1:B:126:THR:HB	1:B:290:ARG:NH1	2.33	0.44
1:B:286:MET:HE3	1:B:287:GLU:N	2.32	0.44
1:B:305:SER:C	1:B:393:MET:HE3	2.37	0.44
1:B:330:SER:CB	3:B:718:HOH:O	2.59	0.44
1:A:15:GLY:O	1:A:16:LYS:HG2	2.17	0.43
1:B:202:MET:HE3	1:B:202:MET:HB3	1.88	0.43
1:B:295:VAL:C	1:B:297:LEU:H	2.20	0.43
1:A:16:LYS:H	1:A:43:GLY:N	2.12	0.43
1:A:171:ARG:NH2	1:A:180:PHE:CZ	2.86	0.43
1:A:182:LEU:HA	1:A:255:MET:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:PHE:HA	1:A:402:PHE:CE1	2.53	0.43
1:A:463:ASN:O	1:A:466:THR:CG2	2.58	0.43
1:B:21:THR:C	3:B:719:HOH:O	2.55	0.43
1:B:157:LYS:O	1:B:265:PRO:HG2	2.18	0.43
1:B:181:ARG:O	1:B:183:GLY:N	2.51	0.43
1:B:203:LEU:HA	1:B:203:LEU:HD23	1.69	0.43
1:B:388:ILE:HG22	1:B:390:VAL:HG23	1.98	0.43
1:A:170:GLN:O	1:A:172:GLN:OE1	2.35	0.43
1:A:278:TRP:CG	1:A:278:TRP:O	2.45	0.43
1:B:115:GLU:O	1:B:155:ARG:NE	2.50	0.43
1:A:374:HIS:O	1:A:374:HIS:CG	2.70	0.43
1:A:364:PHE:CE2	1:A:455:THR:HA	2.54	0.43
1:B:446:TYR:CD1	1:B:446:TYR:C	2.92	0.43
1:A:7:ILE:CG2	1:A:473:MET:HA	2.49	0.43
1:B:372:PHE:HE1	1:B:390:VAL:CG1	2.15	0.43
1:A:61:LEU:O	1:A:66:VAL:HG22	2.18	0.43
1:A:314:VAL:HG23	1:A:460:ARG:NH1	2.34	0.43
1:B:417:LEU:HD22	1:B:417:LEU:O	2.19	0.43
1:A:271:PRO:HG2	1:A:271:PRO:O	2.19	0.43
1:A:395:LEU:HD13	3:A:732:HOH:O	2.17	0.43
1:B:304:LEU:HD22	1:B:304:LEU:N	2.33	0.43
1:A:79:GLY:C	1:A:80:LYS:HE2	2.33	0.43
1:A:164:THR:HB	1:A:166:TYR:N	2.34	0.43
1:A:222:SER:OG	1:A:224:SER:HB3	2.19	0.43
1:B:80:LYS:HA	3:B:702:HOH:O	2.17	0.43
1:B:236:ARG:O	1:B:237:ALA:C	2.56	0.43
1:A:60:ARG:O	1:A:64:GLU:HG3	2.19	0.42
1:A:71:PHE:HD1	1:A:74:LEU:HD12	1.82	0.42
1:A:382:ASP:OD1	1:A:382:ASP:C	2.57	0.42
1:B:113:ALA:O	1:B:153:PHE:HA	2.18	0.42
1:B:305:SER:O	1:B:393:MET:HA	2.18	0.42
1:A:277:THR:O	1:A:283:PRO:HA	2.19	0.42
1:B:28:ALA:O	1:B:31:LEU:CB	2.68	0.42
1:B:28:ALA:O	1:B:31:LEU:HB3	2.19	0.42
1:A:242:TRP:CD1	1:A:248:PHE:HD1	2.34	0.42
1:A:290:ARG:CG	1:A:290:ARG:HH11	2.33	0.42
1:A:307:PHE:O	1:A:395:LEU:HA	2.19	0.42
1:B:21:THR:CA	3:B:719:HOH:O	2.67	0.42
1:A:42:VAL:HB	1:A:43:GLY:O	2.19	0.42
1:A:167:VAL:HG22	1:A:251:ALA:HB2	2.02	0.42
1:A:182:LEU:CD2	1:A:205:ILE:CG1	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:VAL:C	1:A:71:PHE:CE2	2.89	0.42
1:A:205:ILE:N	1:A:205:ILE:CD1	2.58	0.42
1:B:227:GLU:O	1:B:228:GLU:C	2.57	0.42
1:A:213:PHE:CD1	1:A:213:PHE:C	2.93	0.42
1:B:473:MET:HB3	1:B:477:GLU:HB3	2.01	0.42
1:A:274:ILE:N	2:A:601:NAP:O7N	2.52	0.42
1:A:128:PHE:CE2	1:A:291:MET:SD	3.13	0.42
1:A:146:ILE:HG22	1:A:159:PHE:HE2	1.85	0.42
1:A:187:ALA:HB1	1:A:199:LYS:HD3	2.02	0.42
1:A:478:LYS:HB3	3:A:735:HOH:O	2.18	0.42
1:A:492:ASP:OD1	1:A:492:ASP:C	2.58	0.42
1:B:203:LEU:HD23	3:B:710:HOH:O	2.18	0.42
1:B:352:TYR:CD1	3:B:729:HOH:O	2.73	0.42
1:A:319:PRO:HG2	1:A:322:MET:HG3	2.00	0.42
1:B:20:ILE:HG12	1:B:120:VAL:HB	2.02	0.42
1:B:31:LEU:HA	1:B:324:VAL:HG13	2.02	0.42
1:B:174:VAL:HA	1:B:460:ARG:O	2.20	0.42
1:A:61:LEU:HD11	1:A:90:LEU:HD13	2.01	0.42
1:A:65:VAL:CG1	1:A:71:PHE:CZ	2.99	0.42
1:A:396:PHE:CD2	1:A:402:PHE:HA	2.54	0.42
1:A:414:ALA:C	1:A:416:ARG:N	2.71	0.42
1:B:26:PHE:CZ	1:B:320:ALA:HB2	2.55	0.41
1:B:315:LEU:HD12	1:B:315:LEU:HA	1.89	0.41
1:B:396:PHE:HD1	1:B:396:PHE:N	2.18	0.41
1:A:45:ILE:HG22	1:A:47:VAL:CG2	2.49	0.41
1:B:437:CYS:SG	1:B:438:ALA:N	2.90	0.41
1:A:79:GLY:O	1:A:80:LYS:CD	2.60	0.41
1:A:186:ILE:HG13	1:A:242:TRP:CZ3	2.55	0.41
1:A:209:ILE:O	1:A:212:ALA:O	2.38	0.41
1:A:392:PRO:C	3:A:703:HOH:O	2.49	0.41
1:B:13:LEU:O	1:B:39:ASN:ND2	2.54	0.41
2:B:601:NAP:H2N	2:B:601:NAP:H2D	1.81	0.41
1:A:20:ILE:HA	1:A:120:VAL:O	2.19	0.41
1:A:24:THR:O	1:A:25:GLY:C	2.59	0.41
1:A:65:VAL:O	1:A:71:PHE:HE2	1.88	0.41
1:A:159:PHE:C	1:A:159:PHE:CD1	2.94	0.41
1:A:216:ARG:NE	1:A:216:ARG:CA	2.83	0.41
1:B:61:LEU:O	1:B:65:VAL:HB	2.21	0.41
1:B:65:VAL:C	1:B:66:VAL:O	2.40	0.41
1:B:182:LEU:HB2	1:B:259:SER:OG	2.20	0.41
1:B:333:LYS:HE3	1:B:472:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LEU:HD12	1:A:490:TRP:HB3	2.01	0.41
1:B:182:LEU:HD11	1:B:205:ILE:CD1	2.50	0.41
1:B:171:ARG:HD2	1:B:175:VAL:CG1	2.50	0.41
1:B:232:LEU:C	1:B:232:LEU:CD2	2.88	0.41
1:B:239:LEU:HD13	1:B:239:LEU:O	2.20	0.41
1:A:7:ILE:CG2	1:A:477:GLU:OE1	2.61	0.41
1:A:396:PHE:HE2	1:A:405:TYR:CD1	2.38	0.41
1:B:182:LEU:HD21	1:B:205:ILE:CG1	2.41	0.41
1:A:164:THR:CG2	1:A:246:TYR:OH	2.66	0.41
1:A:213:PHE:HA	1:A:216:ARG:CD	2.51	0.41
1:A:264:ILE:HA	1:A:265:PRO:HD3	1.88	0.41
1:A:274:ILE:HD13	1:A:323:VAL:HG21	1.90	0.41
1:B:136:MET:CE	1:B:209:ILE:HG13	2.51	0.41
1:B:340:ALA:CB	3:B:738:HOH:O	2.68	0.41
1:B:340:ALA:HA	1:B:343:ALA:HB3	2.02	0.41
1:B:483:PHE:N	1:B:483:PHE:CD1	2.89	0.41
1:A:396:PHE:HD2	1:A:402:PHE:HA	1.86	0.41
1:A:278:TRP:O	1:A:279:ARG:HG2	2.20	0.40
1:B:127:THR:HB	1:B:130:GLU:HG2	2.03	0.40
1:B:286:MET:HE2	1:B:286:MET:HB3	1.61	0.40
1:A:47:VAL:O	1:A:48:LEU:C	2.60	0.40
1:A:380:TYR:CD1	1:A:380:TYR:C	2.94	0.40
1:B:287:GLU:HA	1:B:505:HIS:CD2	2.56	0.40
1:A:198:HIS:ND1	1:A:198:HIS:N	2.69	0.40
1:A:404:SER:O	1:A:407:GLU:CD	2.59	0.40
1:A:406:VAL:C	1:A:408:THR:H	2.23	0.40
1:A:474:SER:O	1:A:477:GLU:N	2.53	0.40
1:B:62:HIS:O	1:B:66:VAL:HG23	2.21	0.40
1:B:285:TRP:CZ2	1:B:287:GLU:CG	3.04	0.40
1:B:305:SER:C	1:B:393:MET:CE	2.89	0.40
1:B:364:PHE:O	1:B:395:LEU:HD13	2.22	0.40
1:A:208:GLU:OE2	1:A:208:GLU:HA	2.22	0.40
1:B:182:LEU:CD1	1:B:205:ILE:HD11	2.52	0.40
1:B:492:ASP:C	1:B:492:ASP:OD1	2.60	0.40
1:A:212:ALA:O	1:A:213:PHE:CD1	2.74	0.40
1:B:7:ILE:O	1:B:7:ILE:CG1	2.69	0.40
1:B:295:VAL:O	1:B:297:LEU:N	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:LEU:CB	1:B:303:GLN:OE1[5_554]	1.82	0.38
1:A:416:ARG:NH2	1:B:437:CYS:O[5_554]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/532 (90%)	375 (79%)	91 (19%)	10 (2%)	7	30
1	B	467/532 (88%)	391 (84%)	68 (15%)	8 (2%)	9	34
All	All	943/1064 (89%)	766 (81%)	159 (17%)	18 (2%)	8	31

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	280	ASP
1	B	296	VAL
1	A	442	GLU
1	A	75	GLN
1	A	144	PHE
1	A	296	VAL
1	B	182	LEU
1	A	237	ALA
1	B	224	SER
1	A	218	HIS
1	A	248	PHE
1	A	321	ASP
1	B	491	THR
1	A	391	PRO
1	B	43	GLY
1	B	359	VAL
1	A	359	VAL
1	B	354	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	391/422 (93%)	283 (72%)	108 (28%)	0	1
1	B	384/422 (91%)	287 (75%)	97 (25%)	0	2
All	All	775/844 (92%)	570 (74%)	205 (26%)	0	1

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	16	LYS
1	A	17	ASN
1	A	21	THR
1	A	24	THR
1	A	27	LEU
1	A	31	LEU
1	A	35	ILE
1	A	42	VAL
1	A	53	ASP
1	A	55	ASP
1	A	58	LEU
1	A	66	VAL
1	A	69	GLU
1	A	73	ARG
1	A	77	ILE
1	A	80	LYS
1	A	94	VAL
1	A	102	VAL
1	A	117	ASP
1	A	122	SER
1	A	125	ASN
1	A	127	THR
1	A	130	GLU
1	A	132	TYR
1	A	133	ASP
1	A	136	MET

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Mol	Chain	Res	Type
1	A	147	MET
1	A	154	ARG
1	A	155	ARG
1	A	158	LEU
1	A	159	PHE
1	A	160	LEU
1	A	167	VAL
1	A	172	GLN
1	A	174	VAL
1	A	175	VAL
1	A	176	LEU
1	A	178	LYS
1	A	181	ARG
1	A	186	ILE
1	A	188	LYS
1	A	197	GLN
1	A	198	HIS
1	A	202	MET
1	A	203	LEU
1	A	205	ILE
1	A	208	GLU
1	A	209	ILE
1	A	210	LYS
1	A	213	PHE
1	A	216	ARG
1	A	217	ARG
1	A	218	HIS
1	A	221	ASP
1	A	224	SER
1	A	232	LEU
1	A	234	LEU
1	A	239	LEU
1	A	246	TYR
1	A	247	VAL
1	A	250	LYS
1	A	261	ARG
1	A	265	PRO
1	A	269	ILE
1	A	275	GLU
1	A	277	THR
1	A	279	ARG
1	A	290	ARG

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Mol	Chain	Res	Type
1	A	291	MET
1	A	297	LEU
1	A	301	LYS
1	A	305	SER
1	A	307	PHE
1	A	312	GLU
1	A	318	VAL
1	A	336	ARG
1	A	356	SER
1	A	362	LEU
1	A	366	ASP
1	A	367	LEU
1	A	371	LEU
1	A	375	PHE
1	A	386	ARG
1	A	398	THR
1	A	405	TYR
1	A	407	GLU
1	A	408	THR
1	A	411	LEU
1	A	413	ARG
1	A	436	LEU
1	A	437	CYS
1	A	439	LYS
1	A	443	GLN
1	A	445	ILE
1	A	447	LEU
1	A	449	SER
1	A	452	GLN
1	A	460	ARG
1	A	466	THR
1	A	467	GLU
1	A	469	LEU
1	A	475	GLU
1	A	480	ARG
1	A	483	PHE
1	A	485	VAL
1	A	506	VAL
1	A	508	LYS
1	B	17	ASN
1	B	21	THR
1	B	26	PHE

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Mol	Chain	Res	Type
1	B	27	LEU
1	B	31	LEU
1	B	34	LYS
1	B	35	ILE
1	B	38	THR
1	B	42	VAL
1	B	44	LYS
1	B	50	LYS
1	B	53	ASP
1	B	55	ASP
1	B	58	LEU
1	B	66	VAL
1	B	70	LEU
1	B	73	ARG
1	B	77	ILE
1	B	84	SER
1	B	97	VAL
1	B	111	VAL
1	B	117	ASP
1	B	122	SER
1	B	125	ASN
1	B	128	PHE
1	B	130	GLU
1	B	131	ARG
1	B	132	TYR
1	B	146	ILE
1	B	152	ARG
1	B	154	ARG
1	B	158	LEU
1	B	160	LEU
1	B	164	THR
1	B	167	VAL
1	B	175	VAL
1	B	177	GLU
1	B	178	LYS
1	B	186	ILE
1	B	201	THR
1	B	202	MET
1	B	203	LEU
1	B	205	ILE
1	B	208	GLU
1	B	210	LYS

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Mol	Chain	Res	Type
1	B	211	LEU
1	B	217	ARG
1	B	221	ASP
1	B	232	LEU
1	B	236	ARG
1	B	239	LEU
1	B	246	TYR
1	B	247	VAL
1	B	250	LYS
1	B	261	ARG
1	B	263	ASP
1	B	274	ILE
1	B	275	GLU
1	B	277	THR
1	B	279	ARG
1	B	286	MET
1	B	291	MET
1	B	297	LEU
1	B	301	LYS
1	B	304	LEU
1	B	307	PHE
1	B	318	VAL
1	B	336	ARG
1	B	353	HIS
1	B	359	VAL
1	B	362	LEU
1	B	389	HIS
1	B	391	PRO
1	B	393	MET
1	B	394	ARG
1	B	399	MET
1	B	400	GLU
1	B	405	TYR
1	B	406	VAL
1	B	409	ASP
1	B	411	LEU
1	B	413	ARG
1	B	416	ARG
1	B	417	LEU
1	B	439	LYS
1	B	441	VAL
1	B	447	LEU

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Mol	Chain	Res	Type
1	B	450	ILE
1	B	466	THR
1	B	469	LEU
1	B	475	GLU
1	B	476	GLU
1	B	477	GLU
1	B	480	ARG
1	B	483	PHE
1	B	499	ILE
1	B	508	LYS

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	17	ASN
1	A	62	HIS
1	A	125	ASN
1	A	170	GLN
1	A	197	GLN
1	A	303	GLN
1	A	350	HIS
1	A	353	HIS
1	A	389	HIS
1	A	401	GLN
1	A	443	GLN
1	A	465	ASN
1	A	505	HIS
1	B	17	ASN
1	B	83	HIS
1	B	125	ASN
1	B	172	GLN
1	B	373	GLN
1	B	463	ASN
1	B	465	ASN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	NAP	B	601	-	45,52,52	1.10	2 (4%)	56,80,80	1.81	15 (26%)
2	NAP	A	601	-	45,52,52	0.98	3 (6%)	56,80,80	1.69	10 (17%)

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	NAP	B	601	-	-	21/31/67/67	0/5/5/5
2	NAP	A	601	-	-	15/31/67/67	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAP	C2N-N1N	5.35	1.41	1.35
2	A	601	NAP	C2N-N1N	4.08	1.39	1.35
2	A	601	NAP	O4D-C1D	2.85	1.45	1.41
2	B	601	NAP	P2B-O2B	2.28	1.63	1.59
2	A	601	NAP	C8A-N7A	-2.10	1.31	1.34

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAP	C6N-N1N-C2N	-6.18	116.34	121.97
2	B	601	NAP	O2X-P2B-O2B	4.53	126.30	105.99
2	B	601	NAP	O2B-P2B-O1X	-4.18	93.25	109.39
2	A	601	NAP	O2B-P2B-O1X	-4.02	93.88	109.39
2	B	601	NAP	C6N-N1N-C2N	-3.92	118.40	121.97
2	B	601	NAP	O3B-C3B-C2B	3.83	122.05	111.17
2	B	601	NAP	C3N-C2N-N1N	-3.76	116.75	120.43
2	A	601	NAP	C5N-C4N-C3N	-3.61	116.08	120.34
2	B	601	NAP	C3B-C2B-C1B	-3.36	96.57	102.89
2	A	601	NAP	O2X-P2B-O2B	3.29	120.74	105.99
2	A	601	NAP	C3B-C2B-C1B	-2.98	97.28	102.89
2	A	601	NAP	C3N-C2N-N1N	-2.94	117.56	120.43
2	A	601	NAP	PN-O3-PA	-2.76	123.34	132.83
2	B	601	NAP	O3B-C3B-C4B	-2.72	103.17	111.05
2	B	601	NAP	C5N-C4N-C3N	-2.71	117.14	120.34
2	B	601	NAP	C2N-C3N-C4N	-2.58	115.33	118.26
2	A	601	NAP	O2B-C2B-C3B	2.53	120.86	111.68
2	A	601	NAP	O3B-C3B-C2B	2.37	117.89	111.17
2	B	601	NAP	O2N-PN-O1N	2.32	123.69	112.24
2	A	601	NAP	O2N-PN-O1N	2.27	123.45	112.24
2	B	601	NAP	O2A-PA-O1A	2.17	122.95	112.24
2	B	601	NAP	C2B-C3B-C4B	-2.15	97.32	101.99
2	B	601	NAP	O2B-C2B-C3B	2.08	119.21	111.68
2	B	601	NAP	O3X-P2B-O2B	-2.06	96.75	105.99
2	B	601	NAP	C3N-C7N-N7N	2.03	120.19	117.75

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAP	C5B-O5B-PA-O3
2	A	601	NAP	O4B-C4B-C5B-O5B
2	A	601	NAP	C3B-C4B-C5B-O5B
2	A	601	NAP	C5D-O5D-PN-O3
2	A	601	NAP	C5D-O5D-PN-O2N
2	A	601	NAP	O4D-C1D-N1N-C2N
2	A	601	NAP	C2N-C3N-C7N-O7N
2	A	601	NAP	C2N-C3N-C7N-N7N
2	B	601	NAP	C5B-O5B-PA-O2A
2	B	601	NAP	C3B-C4B-C5B-O5B
2	B	601	NAP	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
2	B	601	NAP	C5D-O5D-PN-O2N
2	B	601	NAP	O4D-C1D-N1N-C2N
2	B	601	NAP	O4D-C1D-N1N-C6N
2	B	601	NAP	C2D-C1D-N1N-C6N
2	A	601	NAP	C4N-C3N-C7N-O7N
2	A	601	NAP	C4N-C3N-C7N-N7N
2	A	601	NAP	O4D-C4D-C5D-O5D
2	B	601	NAP	O4D-C4D-C5D-O5D
2	B	601	NAP	C4N-C3N-C7N-O7N
2	B	601	NAP	C4N-C3N-C7N-N7N
2	B	601	NAP	C2N-C3N-C7N-O7N
2	B	601	NAP	O4B-C4B-C5B-O5B
2	B	601	NAP	C3D-C4D-C5D-O5D
2	A	601	NAP	C3D-C4D-C5D-O5D
2	B	601	NAP	C2N-C3N-C7N-N7N
2	B	601	NAP	C4B-C5B-O5B-PA
2	B	601	NAP	C5B-O5B-PA-O3
2	B	601	NAP	PN-O3-PA-O1A
2	A	601	NAP	C5B-O5B-PA-O1A
2	B	601	NAP	C5B-O5B-PA-O1A
2	B	601	NAP	PA-O3-PN-O2N
2	A	601	NAP	C2B-O2B-P2B-O1X
2	A	601	NAP	C1B-C2B-O2B-P2B
2	B	601	NAP	C2D-C1D-N1N-C2N
2	B	601	NAP	PA-O3-PN-O1N

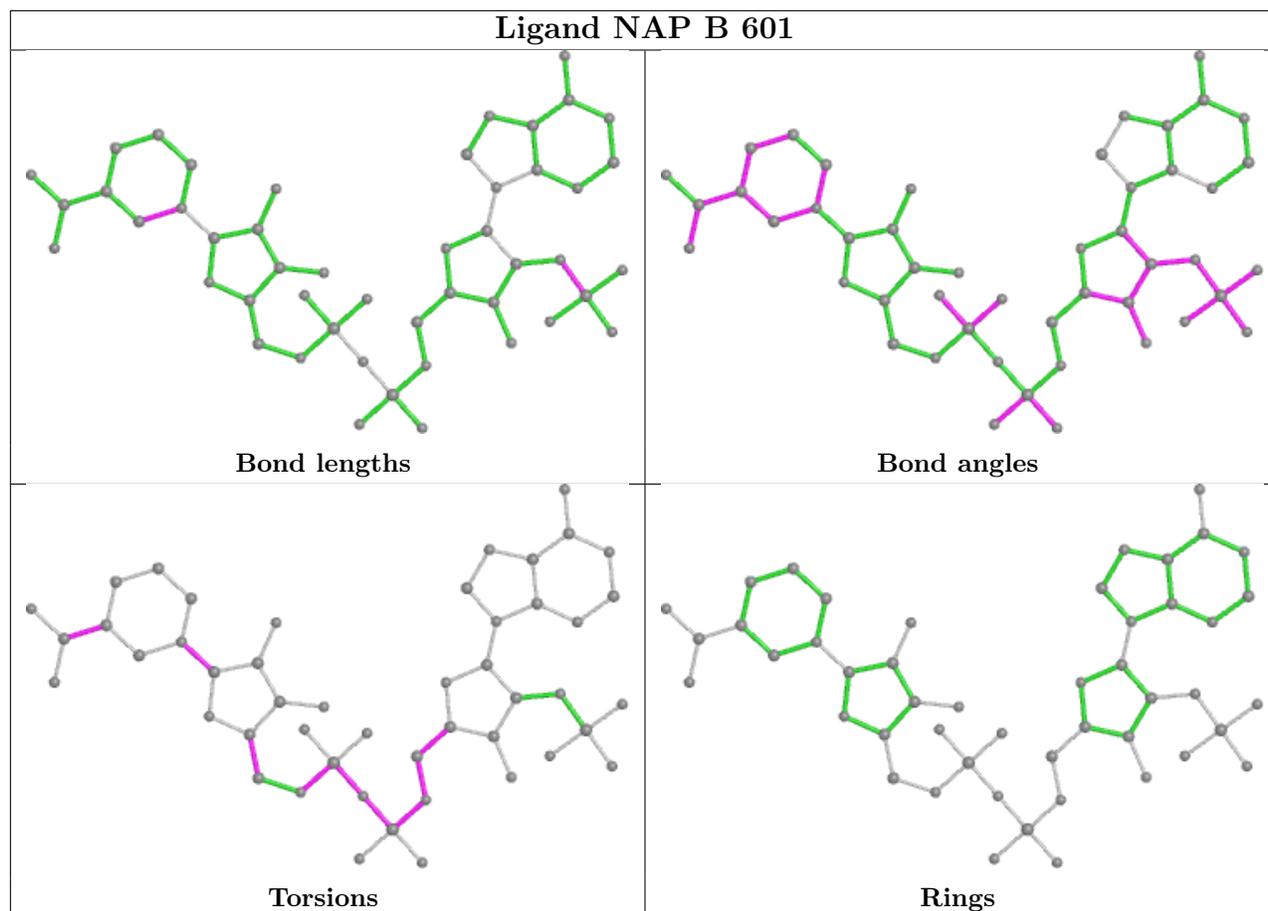
There are no ring outliers.

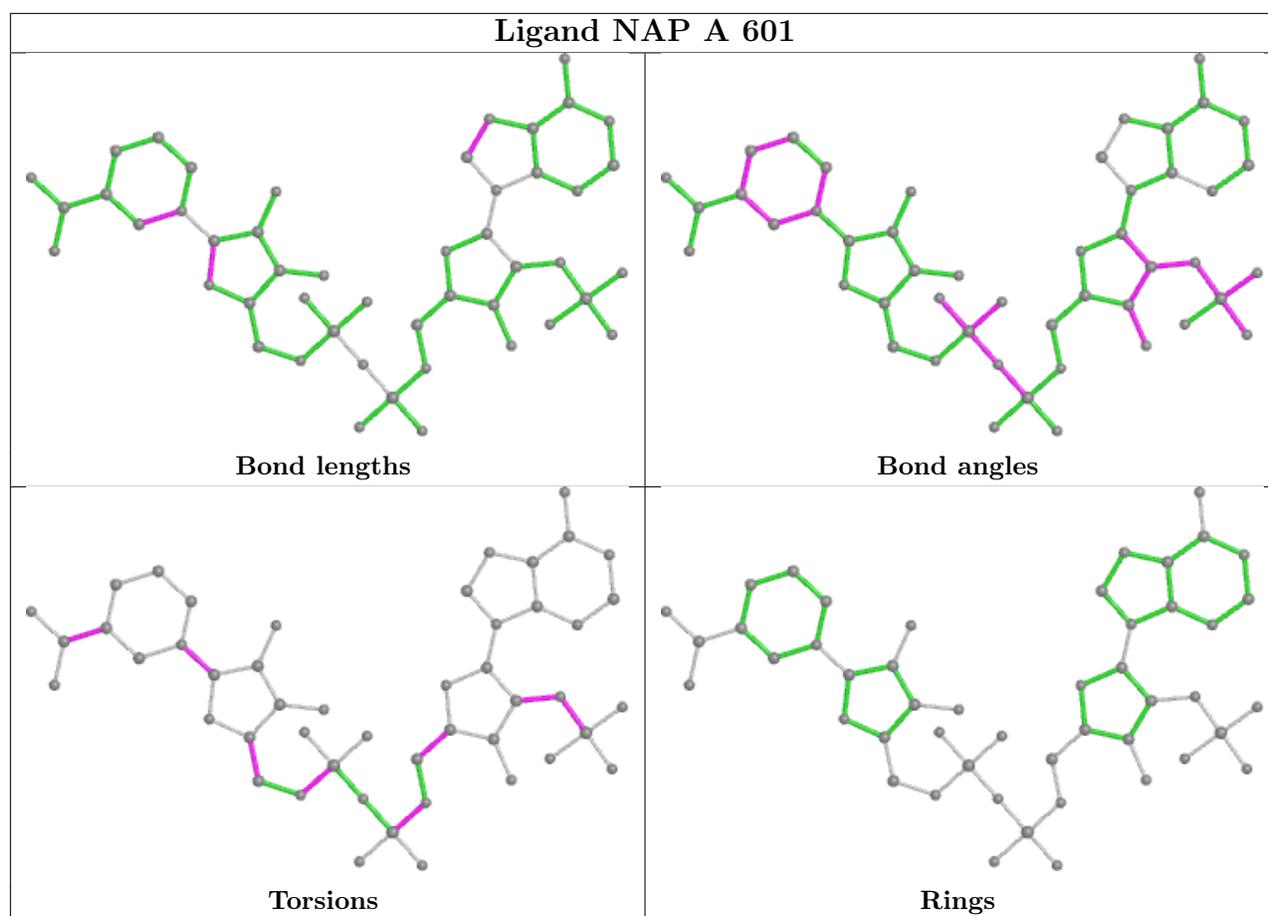
2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	NAP	3	0
2	A	601	NAP	10	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	482/532 (90%)	0.79	40 (8%) 11 13	30, 97, 152, 190	0
1	B	473/532 (88%)	0.80	35 (7%) 14 16	60, 95, 144, 195	0
All	All	955/1064 (89%)	0.79	75 (7%) 12 14	30, 96, 149, 195	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	GLN	4.4
1	B	488	ILE	4.3
1	B	280	ASP	3.8
1	A	390	VAL	3.8
1	A	490	TRP	3.8
1	A	307	PHE	3.4
1	A	389	HIS	3.4
1	A	74	LEU	3.4
1	B	307	PHE	3.4
1	B	355	ALA	3.3
1	A	488	ILE	3.3
1	B	386	ARG	3.2
1	B	245	THR	3.0
1	A	69	GLU	3.0
1	B	469	LEU	2.9
1	B	489	GLU	2.8
1	A	482	HIS	2.7
1	A	48	LEU	2.6
1	B	487	SER	2.6
1	A	285	TRP	2.6
1	B	444	THR	2.5
1	A	493	TYR	2.5
1	B	493	TYR	2.5
1	A	418	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	148	SER	2.5
1	B	285	TRP	2.4
1	A	481	PHE	2.4
1	A	67	ASP	2.4
1	A	247	VAL	2.4
1	B	388	ILE	2.4
1	B	389	HIS	2.4
1	A	470	ILE	2.4
1	A	441	VAL	2.3
1	B	78	HIS	2.3
1	A	394	ARG	2.3
1	B	485	VAL	2.3
1	A	471	GLY	2.3
1	A	139	ASN	2.3
1	A	138	ILE	2.3
1	B	140	THR	2.3
1	B	441	VAL	2.3
1	B	23	GLY	2.2
1	A	122	SER	2.2
1	B	417	LEU	2.2
1	A	97	VAL	2.2
1	A	233	GLY	2.2
1	A	132	TYR	2.2
1	A	355	ALA	2.2
1	B	52	LYS	2.2
1	B	244	ASP	2.2
1	B	240	HIS	2.2
1	A	475	GLU	2.1
1	A	480	ARG	2.1
1	A	485	VAL	2.1
1	B	494	ILE	2.1
1	B	304	LEU	2.1
1	A	245	THR	2.1
1	A	297	LEU	2.1
1	A	354	VAL	2.1
1	B	213	PHE	2.1
1	B	463	ASN	2.1
1	B	107	GLU	2.1
1	B	217	ARG	2.0
1	A	483	PHE	2.0
1	A	198	HIS	2.0
1	B	320	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	436	LEU	2.0
1	A	242	TRP	2.0
1	A	128	PHE	2.0
1	B	497	VAL	2.0
1	B	112	ILE	2.0
1	A	140	THR	2.0
1	A	229	MET	2.0
1	B	48	LEU	2.0
1	B	454	TYR	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 [\(i\)](#)

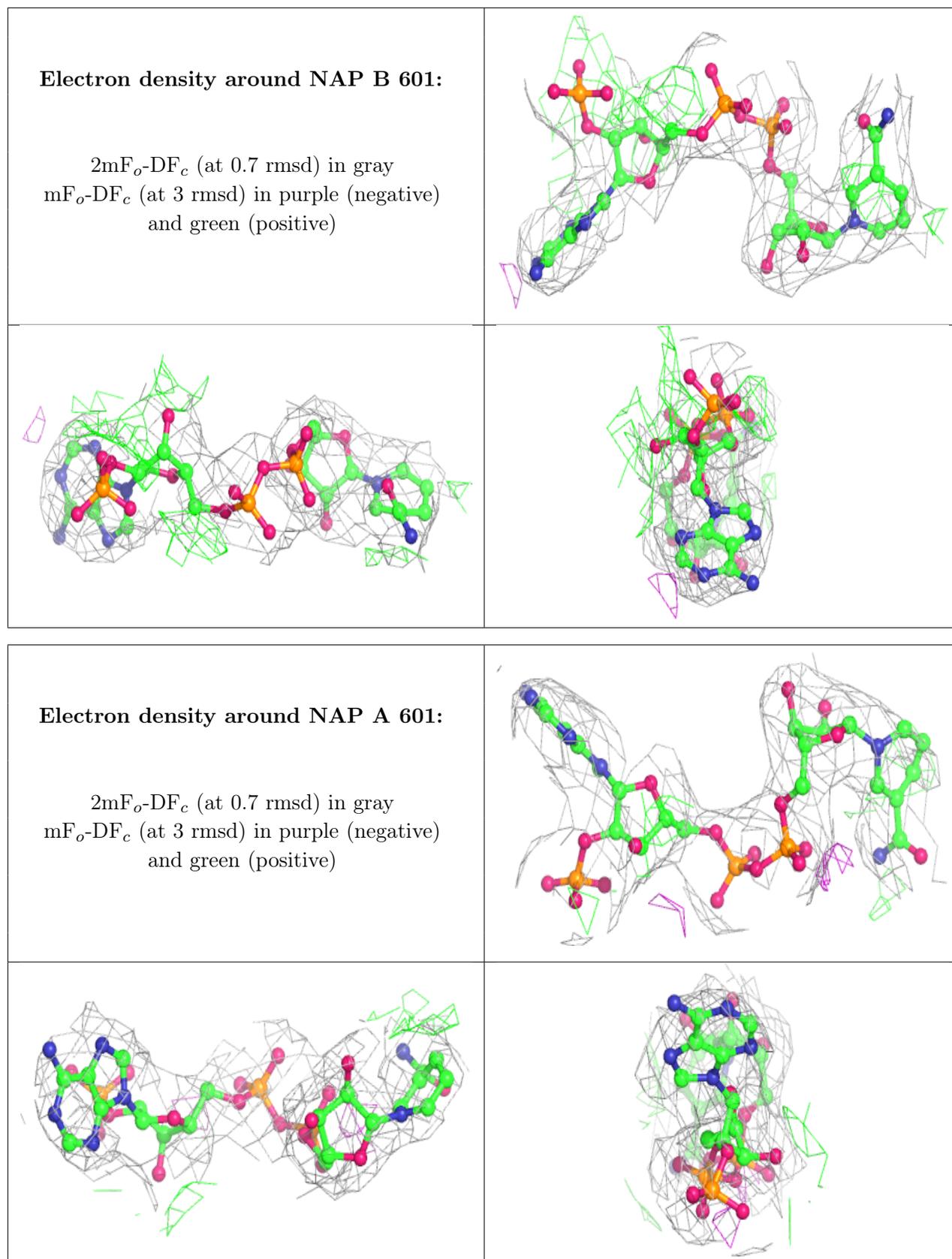
There are no monosaccharides in this entry.

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
2	NAP	B	601	48/48	0.94	0.30	55,81,112,122	0
2	NAP	A	601	48/48	0.95	0.30	65,80,113,136	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.