



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:20 PM UTC

PDB ID : 1M8P / pdb_00001m8p
Title : Crystal Structure of P. chrysogenum ATP Sulfurylase in the T-state
Authors : MacRae, I.J.; Segel, I.H.; Fisher, A.J.
Deposited on : 2002-07-25
Resolution : 2.60 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

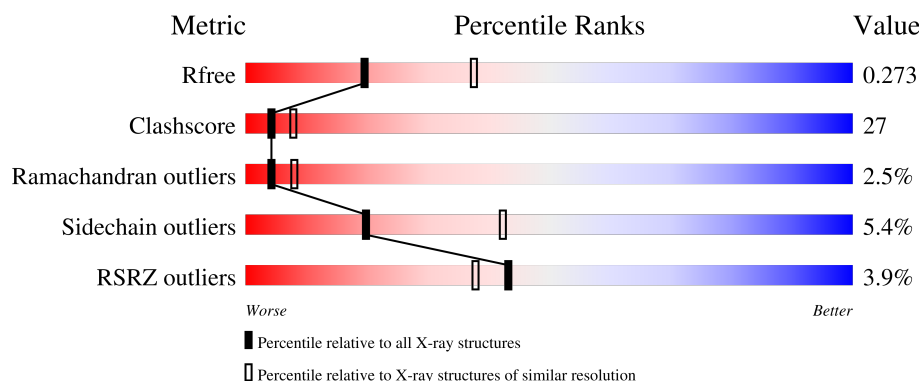
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	573	5% 48% 42% 9%
1	B	573	3% 60% 33% 7%
1	C	573	3% 58% 35% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14054 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.

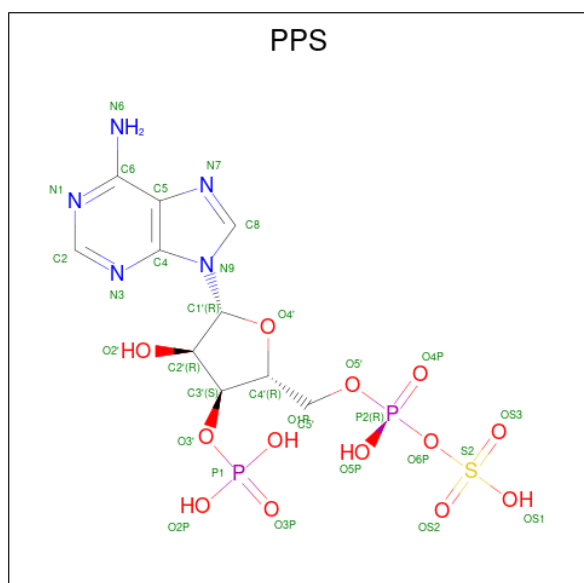
- Molecule 1 is a protein called sulfate adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	0	0	0
			4501	2832	815	841	13			
1	B	573	Total	C	N	O	S	0	0	0
			4501	2832	815	841	13			
1	C	573	Total	C	N	O	S	0	0	0
			4501	2832	815	841	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	369	GLY	-	SEE REMARK 999	UNP Q12650
B	369	GLY	-	SEE REMARK 999	UNP Q12650
C	369	GLY	-	SEE REMARK 999	UNP Q12650

- Molecule 2 is 3'-PHOSPHATE-ADENOSINE-5'-PHOSPHATE SULFATE (CCD ID: PPS) (formula: C₁₀H₁₅N₅O₁₃P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	13	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			31	10	5	13	2	1		
2	C	1	Total	C	N	O	P	S	0	0
			31	10	5	13	2	1		

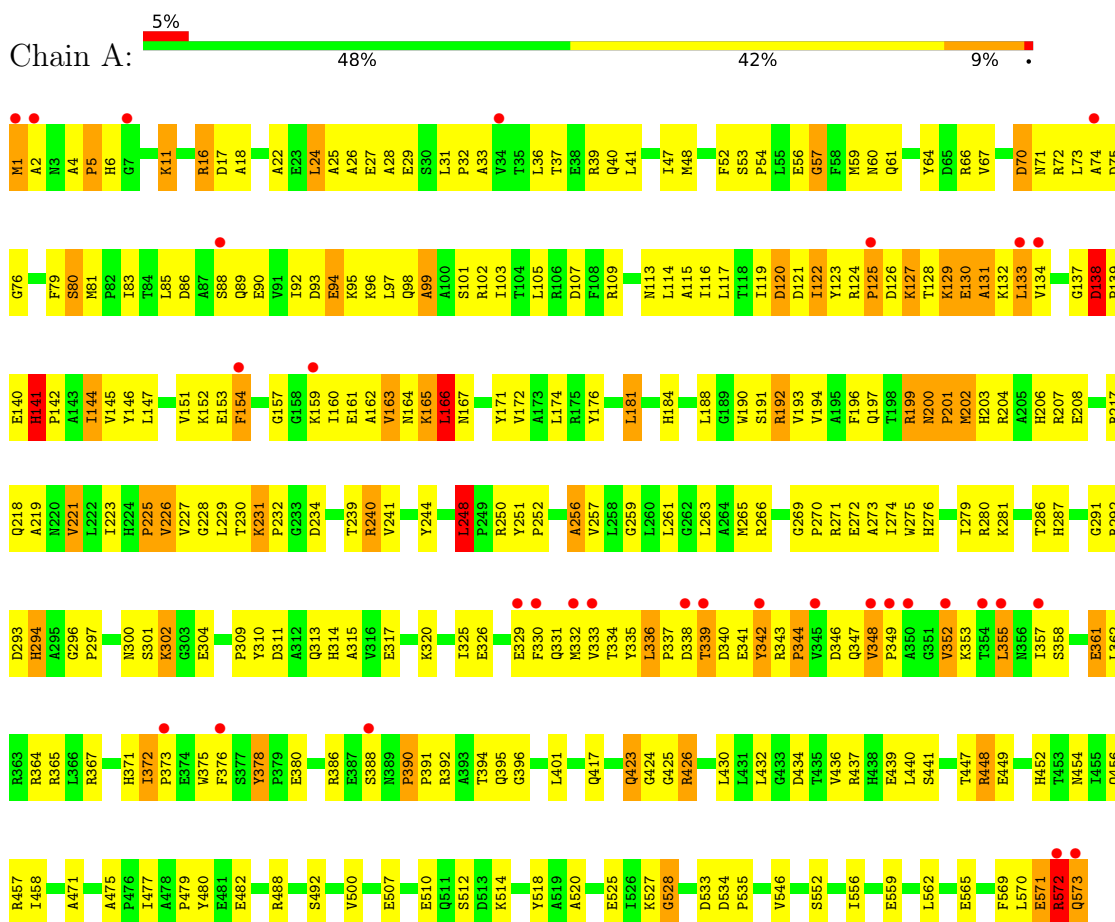
- Molecule 3 is water.

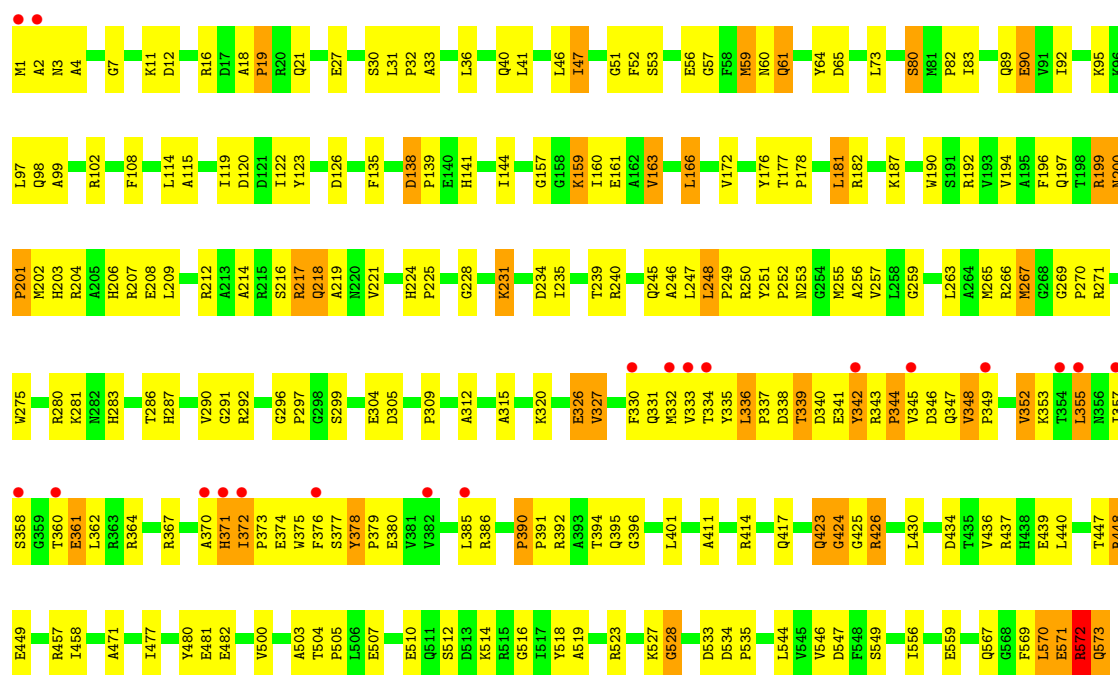
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total	O	0	0
			100	100		
3	B	162	Total	O	0	0
			162	162		
3	C	196	Total	O	0	0
			196	196		

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: sulfate adenylyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.45Å 135.45Å 234.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.33 – 2.60 29.33 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.33-2.60) 99.2 (29.33-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.272 0.218 , 0.273	Depositor DCC
R_{free} test set	3968 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.003 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14054	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8300e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PPS

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	0.63	0/4596	1.17	50/6227 (0.8%)
1	B	0.71	1/4596 (0.0%)	1.17	42/6227 (0.7%)
1	C	0.73	0/4596	1.21	52/6227 (0.8%)
All	All	0.69	1/13788 (0.0%)	1.18	144/18681 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	48	MET	SD-CE	-5.87	1.64	1.79

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	ASN	CA-C-N	10.36	132.79	119.84
1	C	200	ASN	C-N-CA	10.36	132.79	119.84
1	A	167	ASN	N-CA-C	9.91	123.42	109.15
1	A	248	LEU	CA-C-N	-9.76	109.62	120.45
1	A	248	LEU	C-N-CA	-9.76	109.62	120.45
1	B	200	ASN	CA-C-N	9.01	131.10	119.84
1	B	200	ASN	C-N-CA	9.01	131.10	119.84
1	C	224	HIS	CA-C-N	-8.49	111.99	120.31
1	C	224	HIS	C-N-CA	-8.49	111.99	120.31
1	A	124	ARG	CA-C-N	8.37	128.38	119.76
1	A	124	ARG	C-N-CA	8.37	128.38	119.76
1	C	326	GLU	N-CA-C	8.31	122.17	108.96
1	B	267	MET	N-CA-C	-8.13	101.03	111.92
1	A	80	SER	N-CA-C	7.87	122.26	113.21
1	A	200	ASN	CA-C-N	7.71	129.48	119.84
1	A	200	ASN	C-N-CA	7.71	129.48	119.84
1	C	231	LYS	N-CA-C	-7.56	98.73	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	LYS	N-CA-C	7.38	120.26	111.33
1	C	199	ARG	N-CA-C	-7.33	102.32	113.89
1	C	32	PRO	N-CA-C	-7.32	99.74	111.38
1	C	7	GLY	N-CA-C	-7.30	105.44	114.92
1	A	120	ASP	N-CA-C	-7.28	105.31	114.56
1	A	221	VAL	N-CA-C	7.27	118.29	108.11
1	C	177	THR	CA-C-N	-7.17	111.40	119.28
1	C	177	THR	C-N-CA	-7.17	111.40	119.28
1	A	64	TYR	N-CA-C	7.11	119.93	111.33
1	A	56	GLU	N-CA-C	6.82	118.45	110.41
1	A	480	TYR	N-CA-C	6.74	120.43	109.59
1	B	228	GLY	N-CA-C	-6.72	102.99	112.60
1	C	228	GLY	N-CA-C	-6.72	102.87	112.55
1	B	61	GLN	N-CA-C	6.71	118.67	111.36
1	A	125	PRO	N-CA-C	6.63	121.48	111.14
1	B	224	HIS	CA-C-N	-6.56	113.22	119.85
1	B	224	HIS	C-N-CA	-6.56	113.22	119.85
1	B	378	TYR	CA-C-N	6.53	128.00	119.84
1	B	378	TYR	C-N-CA	6.53	128.00	119.84
1	A	378	TYR	CA-C-N	6.52	127.99	119.84
1	A	378	TYR	C-N-CA	6.52	127.99	119.84
1	C	120	ASP	N-CA-C	-6.51	102.84	111.24
1	B	36	LEU	N-CA-C	6.50	119.19	110.35
1	C	221	VAL	N-CA-C	6.47	117.44	108.12
1	A	57	GLY	N-CA-C	-6.40	101.35	110.63
1	A	396	GLY	N-CA-C	-6.40	102.55	112.85
1	B	171	TYR	N-CA-C	6.32	120.11	111.39
1	A	256	ALA	N-CA-C	6.30	119.80	109.85
1	C	439	GLU	N-CA-C	6.29	120.16	112.23
1	A	230	THR	N-CA-C	6.27	118.85	109.25
1	C	47	ILE	N-CA-C	-6.25	104.76	110.82
1	A	372	ILE	CA-C-N	6.23	127.62	119.84
1	A	372	ILE	C-N-CA	6.23	127.62	119.84
1	B	119	ILE	N-CA-C	6.20	122.25	109.34
1	C	378	TYR	CA-C-N	6.17	127.55	119.84
1	C	378	TYR	C-N-CA	6.17	127.55	119.84
1	B	480	TYR	N-CA-C	6.16	119.51	109.59
1	C	200	ASN	N-CA-C	6.14	117.67	110.31
1	C	217	ARG	N-CA-C	-6.11	106.18	113.21
1	C	480	TYR	N-CA-C	6.08	119.38	109.59
1	B	48	MET	N-CA-C	6.08	117.91	111.28
1	B	372	ILE	CA-C-N	6.03	127.38	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	372	ILE	C-N-CA	6.03	127.38	119.84
1	B	80	SER	N-CA-C	6.02	120.24	113.02
1	C	372	ILE	CA-C-N	5.99	127.33	119.84
1	C	372	ILE	C-N-CA	5.99	127.33	119.84
1	B	424	GLY	N-CA-C	5.95	127.27	113.18
1	B	221	VAL	N-CA-C	5.88	116.95	108.48
1	B	56	GLU	N-CA-C	5.87	117.95	110.61
1	B	199	ARG	N-CA-C	-5.85	103.71	112.54
1	C	135	PHE	N-CA-C	5.84	121.12	113.30
1	B	439	GLU	N-CA-C	5.82	119.57	112.23
1	A	199	ARG	N-CA-C	-5.79	103.79	112.54
1	B	336	LEU	CA-C-N	5.77	127.06	119.84
1	B	336	LEU	C-N-CA	5.77	127.06	119.84
1	B	570	LEU	N-CA-C	5.75	120.29	113.16
1	C	119	ILE	N-CA-C	5.71	121.22	109.34
1	A	228	GLY	N-CA-C	-5.71	102.84	112.77
1	A	390	PRO	CA-C-N	5.69	126.13	119.99
1	A	390	PRO	C-N-CA	5.69	126.13	119.99
1	B	572	ARG	N-CA-C	5.68	122.89	110.80
1	C	138	ASP	CA-C-N	5.66	125.33	119.56
1	C	138	ASP	C-N-CA	5.66	125.33	119.56
1	C	61	GLN	N-CA-C	5.66	117.53	111.36
1	A	439	GLU	N-CA-C	5.63	119.33	112.23
1	C	336	LEU	CA-C-N	5.63	126.88	119.84
1	C	336	LEU	C-N-CA	5.63	126.88	119.84
1	C	267	MET	N-CA-C	-5.62	104.39	111.92
1	C	424	GLY	N-CA-C	5.61	126.47	113.18
1	A	226	VAL	N-CA-C	5.60	117.96	109.12
1	A	129	LYS	N-CA-C	-5.56	104.91	110.97
1	A	424	GLY	N-CA-C	5.56	126.36	113.18
1	C	73	LEU	N-CA-C	-5.55	102.54	110.59
1	C	572	ARG	N-CA-C	5.54	122.61	110.80
1	B	310	TYR	N-CA-C	5.48	120.65	113.30
1	C	280	ARG	N-CA-C	-5.47	105.47	111.82
1	B	396	GLY	N-CA-C	-5.46	104.06	112.85
1	C	477	ILE	N-CA-C	-5.45	105.53	110.82
1	C	396	GLY	N-CA-C	-5.44	104.09	112.85
1	A	572	ARG	N-CA-C	5.42	122.35	110.80
1	B	154	PHE	N-CA-C	5.42	118.42	109.85
1	A	138	ASP	CA-C-N	5.42	126.61	119.84
1	A	138	ASP	C-N-CA	5.42	126.61	119.84
1	A	471	ALA	N-CA-C	-5.42	99.90	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	59	MET	N-CA-C	5.40	118.64	110.64
1	C	390	PRO	CA-C-N	5.39	125.82	119.99
1	C	390	PRO	C-N-CA	5.39	125.82	119.99
1	B	256	ALA	N-CA-C	5.38	118.36	109.85
1	C	348	VAL	N-CA-C	5.38	113.36	107.60
1	C	30	SER	N-CA-C	5.37	118.29	111.69
1	B	33	ALA	N-CA-C	5.35	117.62	108.90
1	B	348	VAL	N-CA-C	5.32	113.30	107.60
1	C	16	ARG	N-CA-C	5.31	117.49	111.11
1	B	134	VAL	N-CA-C	5.31	116.39	111.45
1	A	348	VAL	N-CA-C	5.30	113.27	107.60
1	C	256	ALA	N-CA-C	5.30	117.74	109.52
1	A	231	LYS	CA-C-N	5.29	126.46	119.84
1	A	231	LYS	C-N-CA	5.29	126.46	119.84
1	A	146	TYR	N-CA-C	-5.29	104.42	112.04
1	A	203	HIS	CA-C-O	5.28	121.00	117.94
1	A	81	MET	CA-C-N	5.25	125.50	119.83
1	A	81	MET	C-N-CA	5.25	125.50	119.83
1	C	141	HIS	CA-C-N	5.25	126.40	119.84
1	C	141	HIS	C-N-CA	5.25	126.40	119.84
1	B	135	PHE	N-CA-C	5.24	119.64	112.88
1	A	559	GLU	N-CA-C	-5.23	105.66	111.36
1	A	201	PRO	N-CA-C	5.23	123.24	112.47
1	A	141	HIS	CA-C-N	5.23	124.68	119.24
1	A	141	HIS	C-N-CA	5.23	124.68	119.24
1	A	336	LEU	CA-C-N	5.20	126.34	119.84
1	A	336	LEU	C-N-CA	5.20	126.34	119.84
1	B	162	ALA	CA-C-N	-5.17	117.86	123.08
1	B	162	ALA	C-N-CA	-5.17	117.86	123.08
1	B	389	ASN	CA-C-N	5.16	125.70	120.38
1	B	389	ASN	C-N-CA	5.16	125.70	120.38
1	B	390	PRO	CA-C-N	5.14	125.54	119.99
1	B	390	PRO	C-N-CA	5.14	125.54	119.99
1	B	32	PRO	N-CA-C	-5.14	103.12	111.14
1	C	327	VAL	CB-CA-C	-5.09	105.12	111.08
1	C	471	ALA	N-CA-C	-5.09	100.22	108.52
1	C	80	SER	N-CA-C	5.09	119.18	112.92
1	C	570	LEU	N-CA-C	5.07	119.45	113.16
1	B	427	SER	N-CA-C	-5.07	102.98	110.48
1	C	201	PRO	N-CA-C	5.07	122.92	112.47
1	A	294	HIS	N-CA-C	-5.05	102.57	110.10
1	C	235	ILE	N-CA-C	5.04	117.34	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	GLN	N-CA-C	5.00	116.73	111.28

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	4501	0	4450	285	0
1	B	4501	0	4450	223	0
1	C	4501	0	4450	224	0
2	A	31	0	11	2	0
2	B	31	0	12	4	0
2	C	31	0	11	2	0
3	A	100	0	0	8	0
3	B	162	0	0	11	0
3	C	196	0	0	14	0
All	All	14054	0	13384	732	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 27.

All (732) 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:59:MET:HE1	1:B:82:PRO:HA	1.33	1.10
1:C:337:PRO:HD2	1:C:353:LYS:HB2	1.34	1.08
1:A:337:PRO:HD2	1:A:353:LYS:HB2	1.36	1.05
1:B:337:PRO:HD2	1:B:353:LYS:HB2	1.37	1.04
1:B:199:ARG:HD2	1:B:265:MET:HE1	1.39	1.03
1:B:423:GLN:HE21	1:B:425:GLY:H	1.08	0.99
1:C:481:GLU:HG3	3:C:647:HOH:O	1.61	0.99
1:B:423:GLN:NE2	1:B:425:GLY:H	1.61	0.99
1:B:48:MET:CE	1:B:115:ALA:HB2	1.93	0.98
1:C:358:SER:HB3	1:C:361:GLU:HB2	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HG2	1:B:2:ALA:H	1.31	0.96
1:A:358:SER:HB3	1:A:361:GLU:HB2	1.50	0.94
1:B:358:SER:HB3	1:B:361:GLU:HB2	1.50	0.94
1:A:192:ARG:HA	1:A:286:THR:HG21	1.50	0.93
1:A:423:GLN:NE2	1:A:425:GLY:H	1.65	0.93
1:C:423:GLN:NE2	1:C:425:GLY:H	1.68	0.91
1:A:92:ILE:HA	1:A:97:LEU:HD12	1.53	0.90
1:B:231:LYS:HB2	1:B:234:ASP:HB2	1.53	0.89
1:A:401:LEU:HD23	1:A:500:VAL:HB	1.51	0.89
1:B:401:LEU:HD23	1:B:500:VAL:HB	1.53	0.89
1:C:337:PRO:HD2	1:C:353:LYS:CB	2.03	0.89
1:C:200:ASN:HB3	1:C:201:PRO:HD2	1.54	0.88
1:B:192:ARG:HH11	1:B:192:ARG:HB2	1.39	0.87
1:C:401:LEU:HD23	1:C:500:VAL:HB	1.55	0.86
1:B:337:PRO:HD2	1:B:353:LYS:CB	2.05	0.86
1:A:423:GLN:HE21	1:A:425:GLY:H	1.17	0.86
1:A:337:PRO:HD2	1:A:353:LYS:CB	2.05	0.86
1:C:114:LEU:HD13	1:C:166:LEU:HD22	1.55	0.85
1:A:300:ASN:HD21	1:A:304:GLU:HB2	1.41	0.85
1:A:1:MET:HE1	1:A:5:PRO:HD3	1.58	0.85
1:C:208:GLU:O	1:C:212:ARG:HG2	1.75	0.85
1:A:60:ASN:HB2	1:A:121:ASP:OD2	1.77	0.85
1:A:11:LYS:HD3	1:A:54:PRO:HA	1.57	0.84
1:C:373:PRO:HB3	1:C:375:TRP:NE1	1.93	0.84
1:A:300:ASN:ND2	1:A:304:GLU:HB2	1.92	0.83
1:C:423:GLN:HE21	1:C:425:GLY:H	1.21	0.83
1:A:165:LYS:O	1:A:166:LEU:HB3	1.77	0.83
1:B:202:MET:N	3:B:610:HOH:O	2.12	0.82
1:B:159:LYS:NZ	3:B:578:HOH:O	2.12	0.82
1:C:59:MET:HE3	1:C:64:TYR:HA	1.61	0.82
1:B:286:THR:OG1	1:B:287:HIS:HD2	1.64	0.81
1:B:200:ASN:HB3	1:B:201:PRO:HD2	1.63	0.80
1:C:11:LYS:HE2	1:C:56:GLU:OE2	1.81	0.80
1:C:61:GLN:HG3	1:C:123:TYR:CD1	2.16	0.80
1:A:48:MET:HE3	1:A:162:ALA:HA	1.64	0.79
1:B:373:PRO:HB3	1:B:375:TRP:NE1	1.97	0.78
1:A:31:LEU:HD22	1:A:102:ARG:HB3	1.65	0.78
1:C:192:ARG:NH1	1:C:217:ARG:O	2.17	0.78
1:C:200:ASN:HB3	1:C:201:PRO:CD	2.14	0.77
1:B:61:GLN:HG3	1:B:123:TYR:CG	2.21	0.76
1:A:373:PRO:HB3	1:A:375:TRP:NE1	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ALA:HB2	1:A:147:LEU:HD23	1.65	0.76
1:A:199:ARG:HB3	1:A:265:MET:HE1	1.68	0.74
1:A:37:THR:OG1	1:A:40:GLN:HG3	1.87	0.74
1:A:344:PRO:HB2	1:A:347:GLN:HG2	1.69	0.74
1:B:61:GLN:HG3	1:B:123:TYR:CD2	2.22	0.74
1:A:401:LEU:CD2	1:A:500:VAL:HB	2.18	0.73
1:B:423:GLN:NE2	1:B:425:GLY:N	2.36	0.73
1:C:570:LEU:O	1:C:572:ARG:N	2.21	0.73
1:C:59:MET:HE1	1:C:82:PRO:HA	1.70	0.73
1:A:204:ARG:HD3	1:A:378:TYR:CZ	2.24	0.73
1:B:300:ASN:ND2	1:B:304:GLU:HB2	2.04	0.72
1:C:336:LEU:HD22	1:C:352:VAL:HG11	1.70	0.72
1:B:48:MET:HE3	1:B:115:ALA:HB2	1.70	0.72
1:A:59:MET:HE1	1:A:67:VAL:HG21	1.71	0.72
1:C:12:ASP:HB3	3:C:663:HOH:O	1.89	0.72
1:B:401:LEU:CD2	1:B:500:VAL:HB	2.19	0.72
1:B:117:LEU:C	1:B:117:LEU:HD23	2.14	0.71
1:B:357:ILE:HD11	1:B:373:PRO:HG2	1.72	0.71
1:A:147:LEU:HA	1:A:151:VAL:CG2	2.21	0.71
1:C:392:ARG:HG3	1:C:392:ARG:HH11	1.55	0.71
1:A:60:ASN:HA	1:A:157:GLY:HA3	1.71	0.70
1:B:344:PRO:HB2	1:B:347:GLN:HG2	1.73	0.70
1:C:286:THR:OG1	1:C:287:HIS:HD2	1.74	0.70
1:A:47:ILE:HD11	1:A:83:ILE:HG21	1.73	0.70
1:A:423:GLN:NE2	1:A:425:GLY:N	2.38	0.70
1:A:570:LEU:O	1:A:572:ARG:N	2.23	0.70
1:C:204:ARG:HB3	1:C:376:PHE:O	1.91	0.70
1:C:331:GLN:HE21	1:C:344:PRO:HB3	1.57	0.70
1:C:33:ALA:O	1:C:95:LYS:HE2	1.92	0.70
1:A:140:GLU:OE2	1:A:300:ASN:HB2	1.92	0.69
1:B:247:LEU:O	1:B:247:LEU:HD12	1.92	0.69
1:B:331:GLN:HE21	1:B:344:PRO:HB3	1.56	0.69
1:C:344:PRO:HB2	1:C:347:GLN:HG2	1.73	0.69
1:A:131:ALA:O	1:A:144:ILE:HD11	1.93	0.69
1:A:28:ALA:HA	1:A:31:LEU:HD12	1.74	0.69
1:A:202:MET:HA	1:A:206:HIS:ND1	2.08	0.69
1:A:331:GLN:HE21	1:A:344:PRO:HB3	1.58	0.69
1:A:352:VAL:O	1:A:353:LYS:HG2	1.93	0.69
1:B:1:MET:HG2	1:B:2:ALA:N	2.04	0.69
1:C:357:ILE:HD11	1:C:373:PRO:HG2	1.74	0.69
1:C:3:ASN:HA	3:C:634:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:MET:CE	1:A:67:VAL:HG21	2.24	0.68
1:A:102:ARG:HH11	1:A:116:ILE:HG21	1.58	0.68
1:C:401:LEU:CD2	1:C:500:VAL:HB	2.22	0.68
1:A:357:ILE:HD11	1:A:373:PRO:HG2	1.74	0.68
1:B:570:LEU:O	1:B:572:ARG:N	2.27	0.68
1:C:449:GLU:HG3	3:C:677:HOH:O	1.93	0.68
1:B:336:LEU:HD22	1:B:352:VAL:HG11	1.76	0.68
1:B:395:GLN:O	1:B:426:ARG:NH1	2.27	0.68
1:C:528:GLY:HA2	1:C:533:ASP:HB2	1.75	0.68
1:A:129:LYS:HE2	1:A:133:LEU:HD11	1.76	0.67
1:B:200:ASN:HB3	1:B:201:PRO:CD	2.24	0.67
1:C:345:VAL:CG1	3:C:693:HOH:O	2.42	0.67
1:A:392:ARG:HG3	1:A:392:ARG:HH11	1.57	0.67
1:B:372:ILE:HG13	1:B:386:ARG:HH22	1.58	0.67
1:C:4:ALA:O	1:C:281:LYS:HE2	1.93	0.67
1:C:204:ARG:CZ	1:C:342:TYR:OH	2.42	0.67
1:A:313:GLN:HB3	1:A:329:GLU:HG2	1.75	0.67
1:A:565:GLU:HG2	3:A:655:HOH:O	1.93	0.67
1:C:423:GLN:NE2	1:C:425:GLY:N	2.41	0.67
1:A:90:GLU:O	1:A:94:GLU:HB2	1.93	0.67
1:B:528:GLY:HA2	1:B:533:ASP:HB2	1.77	0.67
1:A:193:VAL:H	1:A:286:THR:HG23	1.58	0.67
1:C:337:PRO:HG3	1:C:355:LEU:HD12	1.77	0.67
1:A:344:PRO:HD2	1:A:347:GLN:HG3	1.77	0.67
1:C:217:ARG:HH11	1:C:217:ARG:HG2	1.58	0.67
1:B:352:VAL:O	1:B:353:LYS:HG2	1.94	0.66
1:A:527:LYS:HG2	1:A:528:GLY:N	2.11	0.66
1:B:231:LYS:HB2	1:B:234:ASP:CB	2.22	0.66
1:B:449:GLU:HG3	3:B:623:HOH:O	1.95	0.66
1:A:426:ARG:NH2	1:A:569:PHE:O	2.28	0.66
1:A:337:PRO:HG3	1:A:355:LEU:HD12	1.77	0.66
1:B:333:VAL:HB	1:B:343:ARG:C	2.21	0.66
1:A:572:ARG:HD2	1:B:253:ASN:HB3	1.78	0.66
1:C:352:VAL:O	1:C:353:LYS:HG2	1.95	0.66
1:A:199:ARG:HH11	1:A:265:MET:HE1	1.61	0.66
1:C:196:PHE:CE2	1:C:202:MET:HE3	2.31	0.65
1:C:212:ARG:HH21	1:C:342:TYR:HB2	1.61	0.65
1:A:221:VAL:HB	1:A:256:ALA:HB2	1.78	0.65
1:B:313:GLN:HG3	3:B:584:HOH:O	1.95	0.65
1:A:33:ALA:O	1:A:95:LYS:HE2	1.97	0.65
1:C:320:LYS:HE3	1:C:326:GLU:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:GLU:O	1:B:94:GLU:HB2	1.96	0.65
1:C:57:GLY:HA2	1:C:160:ILE:HG12	1.78	0.65
1:C:59:MET:CE	1:C:64:TYR:HA	2.27	0.65
1:A:131:ALA:HB1	1:A:144:ILE:HG13	1.79	0.65
1:A:336:LEU:HD22	1:A:352:VAL:HG11	1.77	0.65
1:C:333:VAL:HB	1:C:343:ARG:C	2.21	0.65
1:A:302:LYS:HE3	1:A:304:GLU:OE2	1.97	0.64
1:C:291:GLY:HA3	1:C:330:PHE:CE2	2.32	0.64
1:C:57:GLY:HA2	1:C:160:ILE:CG1	2.27	0.64
1:A:395:GLN:O	1:A:426:ARG:NH1	2.31	0.64
1:B:337:PRO:HG3	1:B:355:LEU:HD12	1.80	0.64
1:C:372:ILE:HG13	1:C:386:ARG:HH22	1.62	0.64
1:A:27:GLU:OE2	1:A:102:ARG:HD3	1.97	0.64
1:A:343:ARG:HB3	1:A:347:GLN:HB2	1.81	0.63
1:A:231:LYS:HB2	1:A:234:ASP:HB2	1.79	0.63
1:C:115:ALA:HA	1:C:163:VAL:HG13	1.81	0.63
1:C:395:GLN:O	1:C:426:ARG:NH1	2.30	0.63
1:B:546:VAL:HG11	1:B:556:ILE:CG2	2.29	0.63
1:B:549:SER:O	3:B:716:HOH:O	2.15	0.63
1:B:527:LYS:HG2	1:B:528:GLY:N	2.12	0.63
1:C:331:GLN:NE2	1:C:344:PRO:HB3	2.15	0.62
1:A:333:VAL:HB	1:A:343:ARG:C	2.25	0.62
1:B:392:ARG:HG3	1:B:392:ARG:HH11	1.65	0.62
1:C:343:ARG:HB3	1:C:347:GLN:HB2	1.82	0.62
1:C:527:LYS:HG2	1:C:528:GLY:N	2.14	0.62
1:C:546:VAL:HG11	1:C:556:ILE:HD13	1.81	0.62
1:B:331:GLN:NE2	1:B:344:PRO:HB3	2.14	0.62
1:C:344:PRO:HD2	1:C:347:GLN:HG3	1.81	0.62
1:B:55:LEU:HD12	1:B:56:GLU:N	2.14	0.62
1:A:272:GLU:O	1:A:275:TRP:HB3	2.00	0.62
1:B:207:ARG:O	1:B:211:VAL:HG23	2.00	0.62
1:B:344:PRO:HD2	1:B:347:GLN:HG3	1.82	0.62
1:C:159:LYS:NZ	3:C:578:HOH:O	2.32	0.61
1:B:55:LEU:HD11	1:B:57:GLY:O	2.00	0.61
1:B:343:ARG:HB3	1:B:347:GLN:HB2	1.82	0.61
1:C:434:ASP:HB3	2:C:576:PPS:O3P	1.99	0.61
1:A:372:ILE:HG13	1:A:386:ARG:HH22	1.65	0.61
1:A:528:GLY:HA2	1:A:533:ASP:HB2	1.82	0.61
1:B:300:ASN:HD21	1:B:304:GLU:HB2	1.65	0.61
1:B:534:ASP:OD2	1:B:535:PRO:HD2	2.01	0.61
1:C:60:ASN:HA	1:C:157:GLY:HA3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:ILE:HG13	1:C:386:ARG:NH2	2.15	0.61
1:B:209:LEU:CD1	1:B:330:PHE:HB2	2.32	0.60
1:A:147:LEU:HA	1:A:151:VAL:HG23	1.81	0.60
1:C:345:VAL:HG13	3:C:693:HOH:O	2.00	0.60
1:C:426:ARG:NH2	1:C:569:PHE:O	2.34	0.60
1:A:199:ARG:HH11	1:A:265:MET:CE	2.15	0.60
1:A:331:GLN:NE2	1:A:344:PRO:HB3	2.16	0.59
1:C:546:VAL:HG11	1:C:556:ILE:CG2	2.32	0.59
1:A:27:GLU:O	1:A:31:LEU:HG	2.03	0.59
1:C:204:ARG:HD3	1:C:378:TYR:CZ	2.37	0.59
1:A:192:ARG:CD	1:A:218:GLN:O	2.51	0.59
1:B:372:ILE:HG13	1:B:386:ARG:NH2	2.16	0.59
1:C:1:MET:HE2	1:C:182:ARG:HH11	1.67	0.59
1:A:131:ALA:HB1	1:A:144:ILE:CG1	2.33	0.59
1:B:250:ARG:NH2	1:B:380:GLU:OE2	2.35	0.59
1:A:165:LYS:O	1:A:166:LEU:CB	2.45	0.59
1:C:199:ARG:HH11	1:C:265:MET:HE3	1.67	0.59
1:B:339:THR:HG22	1:B:341:GLU:OE2	2.03	0.58
1:C:18:ALA:HB3	1:C:19:PRO:HD3	1.86	0.58
1:C:187:LYS:HE3	3:C:758:HOH:O	2.01	0.58
1:A:122:ILE:HG22	1:A:122:ILE:O	2.03	0.58
1:A:263:LEU:HD11	1:A:275:TRP:CH2	2.38	0.58
1:A:546:VAL:HG11	1:A:556:ILE:HD13	1.85	0.58
1:C:330:PHE:CD1	1:C:330:PHE:C	2.81	0.58
1:A:102:ARG:NH1	1:A:116:ILE:HG21	2.17	0.58
1:A:226:VAL:O	1:A:240:ARG:NH2	2.37	0.58
2:A:574:PPS:H5'2	2:A:574:PPS:N3	2.19	0.58
1:C:392:ARG:HG3	1:C:392:ARG:NH1	2.18	0.58
1:B:55:LEU:HD12	1:B:56:GLU:H	1.69	0.58
1:C:138:ASP:O	1:C:144:ILE:HD12	2.04	0.58
1:C:373:PRO:HB3	1:C:375:TRP:CD1	2.39	0.58
1:A:123:TYR:O	1:A:154:PHE:HB3	2.04	0.57
1:A:272:GLU:HG3	1:A:275:TRP:HE3	1.69	0.57
1:B:546:VAL:HG11	1:B:556:ILE:HD13	1.86	0.57
1:A:73:LEU:HG	1:A:79:PHE:CB	2.34	0.57
1:A:572:ARG:NH2	3:A:651:HOH:O	2.37	0.57
1:B:240:ARG:HD2	1:B:244:TYR:CE1	2.38	0.57
1:A:144:ILE:HG22	1:A:145:VAL:N	2.19	0.57
1:B:194:VAL:HG22	1:B:287:HIS:HB2	1.87	0.57
1:C:231:LYS:HB2	1:C:234:ASP:HB2	1.85	0.57
1:A:344:PRO:HD2	1:A:347:GLN:CG	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ARG:HG3	1:A:392:ARG:NH1	2.20	0.57
1:A:125:PRO:HD2	1:A:154:PHE:HA	1.87	0.57
1:A:250:ARG:HD2	1:A:378:TYR:CE2	2.40	0.57
1:A:147:LEU:HA	1:A:151:VAL:HG21	1.85	0.57
1:A:330:PHE:CD1	1:A:330:PHE:C	2.83	0.57
1:C:570:LEU:O	1:C:571:GLU:C	2.48	0.57
1:A:140:GLU:CD	1:A:300:ASN:HB2	2.30	0.56
1:C:59:MET:HB2	1:C:83:ILE:O	2.05	0.56
1:B:48:MET:HE2	1:B:115:ALA:HB2	1.85	0.56
1:A:192:ARG:HA	1:A:286:THR:CG2	2.29	0.56
1:B:330:PHE:CD1	1:B:330:PHE:C	2.83	0.56
1:C:546:VAL:CG1	1:C:556:ILE:HD13	2.35	0.56
1:A:129:LYS:HG2	1:A:133:LEU:HD11	1.87	0.56
1:A:287:HIS:ND1	1:A:326:GLU:HB2	2.20	0.56
1:C:339:THR:HG22	1:C:341:GLU:OE2	2.06	0.56
1:B:201:PRO:O	1:B:202:MET:HB2	2.06	0.56
1:A:194:VAL:HG22	1:A:287:HIS:HB2	1.87	0.56
1:A:204:ARG:HD3	1:A:378:TYR:OH	2.06	0.56
1:B:199:ARG:HH11	1:B:265:MET:HE1	1.69	0.56
1:A:127:LYS:HZ1	1:A:152:LYS:C	2.14	0.56
1:A:546:VAL:HG11	1:A:556:ILE:CG2	2.36	0.56
1:B:57:GLY:HA2	1:B:160:ILE:HG12	1.87	0.56
1:B:199:ARG:HH11	1:B:265:MET:CE	2.18	0.56
1:B:18:ALA:O	1:B:21:GLN:HB2	2.06	0.55
1:A:423:GLN:HE22	1:A:425:GLY:HA3	1.70	0.55
1:C:214:ALA:HB1	1:C:219:ALA:O	2.06	0.55
1:B:451:ARG:NH2	2:B:575:PPS:N1	2.51	0.55
1:C:417:GLN:OE1	1:C:430:LEU:HD22	2.07	0.55
1:A:207:ARG:O	1:A:207:ARG:HD3	2.07	0.55
1:A:339:THR:HG22	1:A:341:GLU:OE2	2.06	0.55
1:A:86:ASP:OD2	1:A:152:LYS:HG2	2.06	0.55
1:A:527:LYS:HG2	1:A:528:GLY:H	1.70	0.55
1:C:336:LEU:HD22	1:C:352:VAL:CG1	2.35	0.55
1:A:140:GLU:O	1:A:141:HIS:C	2.50	0.55
1:C:336:LEU:O	1:C:340:ASP:N	2.31	0.55
1:B:159:LYS:N	1:B:159:LYS:HE2	2.21	0.55
1:A:190:TRP:CZ3	1:A:257:VAL:HG23	2.43	0.54
1:A:192:ARG:HD3	1:A:218:GLN:O	2.07	0.54
1:A:546:VAL:CG1	1:A:556:ILE:HD13	2.38	0.54
1:C:27:GLU:O	1:C:31:LEU:HG	2.08	0.54
1:B:21:GLN:NE2	1:B:163:VAL:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:VAL:CG1	1:B:556:ILE:HD13	2.37	0.54
1:B:52:PHE:O	1:B:53:SER:C	2.51	0.54
1:C:199:ARG:HB3	1:C:265:MET:CE	2.38	0.54
1:B:286:THR:OG1	1:B:287:HIS:CD2	2.53	0.54
1:A:570:LEU:O	1:A:571:GLU:C	2.51	0.54
1:B:80:SER:HB2	1:B:271:ARG:HD3	1.90	0.54
1:B:123:TYR:CE1	1:B:155:TYR:HB2	2.43	0.54
1:C:201:PRO:O	1:C:202:MET:HB2	2.06	0.54
1:B:373:PRO:HB3	1:B:375:TRP:CD1	2.42	0.53
1:B:185:PHE:O	1:B:190:TRP:HB2	2.08	0.53
1:A:292:ARG:NH2	1:A:309:PRO:HB3	2.23	0.53
1:A:331:GLN:O	1:A:331:GLN:HG3	2.08	0.53
1:A:372:ILE:HG13	1:A:386:ARG:NH2	2.22	0.53
1:B:331:GLN:O	1:B:331:GLN:HG3	2.08	0.53
1:B:192:ARG:HH11	1:B:192:ARG:CB	2.17	0.53
1:B:60:ASN:HB2	1:B:121:ASP:OD2	2.07	0.53
1:B:199:ARG:NH1	1:B:265:MET:CE	2.71	0.53
1:B:432:LEU:HD23	1:B:475:ALA:HB3	1.89	0.53
1:C:204:ARG:HD3	1:C:378:TYR:CE1	2.44	0.53
1:B:209:LEU:HD11	1:B:330:PHE:HB2	1.89	0.53
1:C:212:ARG:NH2	1:C:342:TYR:CD1	2.77	0.53
1:C:344:PRO:HD2	1:C:347:GLN:CG	2.38	0.53
1:A:344:PRO:C	1:A:346:ASP:H	2.16	0.53
1:B:176:TYR:CD2	1:B:181:LEU:HD13	2.43	0.53
1:B:214:ALA:HB1	1:B:219:ALA:O	2.09	0.53
1:B:570:LEU:O	1:B:571:GLU:C	2.51	0.53
1:B:18:ALA:HB3	1:B:19:PRO:HD3	1.91	0.53
1:B:101:SER:HB2	1:B:119:ILE:HD12	1.90	0.53
1:B:223:ILE:HG22	1:B:225:PRO:HD3	1.90	0.53
1:B:423:GLN:HE21	1:B:425:GLY:N	1.91	0.53
1:B:426:ARG:NH2	1:B:569:PHE:O	2.42	0.52
1:A:336:LEU:HB2	1:A:339:THR:HB	1.90	0.52
1:B:507:GLU:CD	1:B:507:GLU:H	2.17	0.52
1:C:214:ALA:HB3	1:C:255:MET:HE2	1.91	0.52
1:A:176:TYR:CG	1:A:181:LEU:HD13	2.45	0.52
1:B:107:ASP:HB2	1:B:114:LEU:HD11	1.92	0.52
1:C:250:ARG:NE	1:C:378:TYR:CD2	2.77	0.52
1:A:22:ALA:O	1:A:25:ALA:HB3	2.09	0.52
1:A:114:LEU:C	1:A:163:VAL:HG13	2.33	0.52
1:C:331:GLN:O	1:C:331:GLN:HG3	2.08	0.52
1:C:336:LEU:HB2	1:C:339:THR:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:TYR:CD1	1:C:342:TYR:N	2.77	0.52
1:A:275:TRP:O	1:A:279:ILE:HG13	2.10	0.52
1:B:527:LYS:HG2	1:B:528:GLY:H	1.73	0.52
1:A:281:LYS:HB2	1:A:325:ILE:HD12	1.92	0.52
1:B:2:ALA:HA	3:B:617:HOH:O	2.09	0.52
1:B:90:GLU:OE1	1:B:90:GLU:N	2.35	0.52
1:B:272:GLU:HG2	1:B:276:HIS:NE2	2.24	0.52
1:A:373:PRO:HB3	1:A:375:TRP:CD1	2.45	0.52
1:C:336:LEU:HD11	1:C:343:ARG:HD2	1.92	0.52
1:B:297:PRO:HB2	1:B:306:PHE:CD1	2.44	0.52
1:B:336:LEU:HD22	1:B:352:VAL:CG1	2.40	0.52
1:A:291:GLY:HA3	1:A:330:PHE:CE2	2.44	0.51
1:A:423:GLN:HE21	1:A:425:GLY:N	1.98	0.51
1:A:107:ASP:HB2	1:A:114:LEU:HD11	1.92	0.51
1:C:194:VAL:HA	1:C:287:HIS:HB2	1.93	0.51
1:A:132:LYS:HA	1:A:137:GLY:HA2	1.92	0.51
1:B:546:VAL:HG11	1:B:556:ILE:HG23	1.92	0.51
1:C:207:ARG:O	1:C:207:ARG:HD3	2.10	0.51
1:A:140:GLU:CD	1:A:301:SER:H	2.18	0.51
1:A:92:ILE:HD11	1:A:154:PHE:CD1	2.45	0.51
1:A:441:SER:OG	1:A:454:ASN:ND2	2.43	0.51
1:C:423:GLN:HE22	1:C:425:GLY:HA3	1.76	0.51
1:B:57:GLY:HA2	1:B:160:ILE:CG1	2.40	0.51
1:B:93:ASP:O	1:B:95:LYS:N	2.44	0.51
1:C:212:ARG:NH2	1:C:342:TYR:HB2	2.24	0.51
1:C:516:GLY:HA2	3:C:595:HOH:O	2.10	0.51
1:B:339:THR:HG22	1:B:341:GLU:CD	2.36	0.51
1:A:342:TYR:CD1	1:A:342:TYR:N	2.78	0.51
1:A:346:ASP:C	1:A:348:VAL:H	2.19	0.51
1:A:507:GLU:CD	1:A:507:GLU:H	2.16	0.51
1:B:102:ARG:NH2	1:B:161:GLU:OE1	2.44	0.51
1:B:121:ASP:OD1	1:B:123:TYR:CD2	2.64	0.51
1:B:166:LEU:HD12	1:B:166:LEU:H	1.76	0.51
1:B:344:PRO:HD2	1:B:347:GLN:CG	2.39	0.51
1:B:342:TYR:N	1:B:342:TYR:CD1	2.78	0.50
1:A:86:ASP:HB2	1:A:152:LYS:HB2	1.94	0.50
1:B:60:ASN:HA	1:B:157:GLY:HA3	1.93	0.50
1:A:200:ASN:HB3	1:A:201:PRO:HD2	1.93	0.50
1:B:346:ASP:C	1:B:348:VAL:H	2.18	0.50
1:A:114:LEU:O	1:A:163:VAL:HG13	2.11	0.50
1:B:59:MET:CE	1:B:82:PRO:HA	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ARG:HG3	1:B:392:ARG:NH1	2.27	0.50
1:B:477:ILE:HG22	1:B:479:PRO:HG3	1.93	0.50
1:A:330:PHE:HD1	1:A:332:MET:H	1.59	0.50
1:B:95:LYS:O	1:B:96:LYS:HB2	2.11	0.50
1:B:425:GLY:HA2	1:B:573:GLN:HE22	1.77	0.50
1:C:3:ASN:ND2	3:C:634:HOH:O	2.44	0.50
1:C:204:ARG:NH1	1:C:204:ARG:HG2	2.26	0.50
1:A:119:ILE:HG22	1:A:120:ASP:N	2.26	0.50
1:A:534:ASP:OD2	1:A:535:PRO:HD2	2.12	0.50
1:B:552:SER:O	1:B:556:ILE:HG13	2.11	0.50
1:C:1:MET:HE2	1:C:182:ARG:NH1	2.27	0.50
1:C:216:SER:C	1:C:218:GLN:H	2.18	0.50
1:C:346:ASP:C	1:C:348:VAL:H	2.18	0.50
1:A:57:GLY:HA3	1:A:159:LYS:HA	1.93	0.50
1:C:339:THR:HG22	1:C:341:GLU:CD	2.37	0.50
1:A:73:LEU:HG	1:A:79:PHE:HB2	1.93	0.50
1:B:337:PRO:HG2	1:B:355:LEU:HG	1.94	0.50
1:C:61:GLN:HG3	1:C:123:TYR:CE1	2.47	0.50
1:C:225:PRO:HD2	1:C:259:GLY:O	2.12	0.50
1:A:417:GLN:OE1	1:A:430:LEU:HD22	2.12	0.50
1:C:178:PRO:HG3	1:C:283:HIS:CE1	2.46	0.50
1:C:330:PHE:HD1	1:C:332:MET:H	1.60	0.50
1:C:344:PRO:C	1:C:346:ASP:H	2.20	0.50
1:A:270:PRO:HG3	1:A:311:ASP:C	2.37	0.49
1:A:436:VAL:HG11	1:A:458:ILE:HD11	1.94	0.49
1:B:43:ASP:O	1:B:47:ILE:HG13	2.11	0.49
1:B:65:ASP:O	1:B:69:GLU:HG2	2.12	0.49
1:B:344:PRO:C	1:B:346:ASP:H	2.20	0.49
1:A:160:ILE:CG2	1:A:161:GLU:N	2.74	0.49
1:A:36:LEU:HB3	1:A:40:GLN:HB2	1.95	0.49
1:A:261:LEU:HD23	1:A:280:ARG:NH2	2.27	0.49
1:A:336:LEU:HD11	1:A:343:ARG:HD2	1.94	0.49
1:B:336:LEU:HB2	1:B:339:THR:HB	1.92	0.49
1:B:417:GLN:OE1	1:B:430:LEU:HD22	2.12	0.49
1:C:299:SER:HB2	1:C:304:GLU:O	2.11	0.49
1:A:388:SER:HB3	3:A:642:HOH:O	2.11	0.49
1:A:361:GLU:O	1:A:365:ARG:HG3	2.12	0.49
1:B:92:ILE:HG23	1:B:97:LEU:HB2	1.95	0.49
1:B:336:LEU:HD11	1:B:343:ARG:HD2	1.95	0.49
1:B:360:THR:O	1:B:364:ARG:HB2	2.12	0.49
1:A:126:ASP:O	1:A:128:THR:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:THR:HG22	1:A:341:GLU:CD	2.38	0.49
1:A:339:THR:O	1:A:340:ASP:HB3	2.13	0.49
1:A:546:VAL:HG11	1:A:556:ILE:HG23	1.95	0.49
1:A:93:ASP:O	1:A:96:LYS:N	2.43	0.49
1:A:129:LYS:O	1:A:130:GLU:C	2.55	0.49
1:A:364:ARG:HA	1:A:367:ARG:HD3	1.95	0.49
1:C:320:LYS:CE	1:C:326:GLU:HG2	2.43	0.49
1:A:98:GLN:O	1:A:99:ALA:C	2.56	0.49
1:A:204:ARG:HD3	1:A:378:TYR:CE1	2.47	0.49
1:A:317:GLU:HA	1:A:320:LYS:HB2	1.95	0.49
1:A:336:LEU:HD22	1:A:352:VAL:CG1	2.42	0.49
1:A:447:THR:O	1:A:448:ARG:C	2.55	0.49
1:C:115:ALA:HB1	1:C:161:GLU:O	2.13	0.49
1:B:528:GLY:O	1:B:534:ASP:HB2	2.12	0.49
1:A:134:VAL:HG22	1:A:271:ARG:NH1	2.28	0.49
1:B:108:PHE:CD1	1:B:108:PHE:C	2.91	0.49
1:C:90:GLU:CD	1:C:90:GLU:H	2.21	0.49
1:C:270:PRO:HB3	1:C:315:ALA:HB2	1.94	0.48
1:A:6:HIS:HB3	1:A:53:SER:O	2.12	0.48
1:A:115:ALA:HA	1:A:163:VAL:HG12	1.94	0.48
1:B:90:GLU:H	1:B:90:GLU:CD	2.20	0.48
1:C:159:LYS:HE2	1:C:159:LYS:N	2.29	0.48
2:C:576:PPS:H5'2	2:C:576:PPS:N3	2.29	0.48
1:A:184:HIS:NE2	1:A:188:LEU:HD11	2.28	0.48
1:A:362:LEU:HD22	1:A:376:PHE:CE2	2.48	0.48
1:B:339:THR:O	1:B:340:ASP:HB3	2.14	0.48
1:A:39:ARG:HD2	3:A:626:HOH:O	2.13	0.48
1:A:449:GLU:HG3	3:A:657:HOH:O	2.13	0.48
1:B:59:MET:CE	1:B:83:ILE:H	2.26	0.48
1:B:330:PHE:HD1	1:B:332:MET:H	1.60	0.48
1:C:337:PRO:HG2	1:C:355:LEU:HG	1.94	0.48
1:C:425:GLY:HA2	1:C:573:GLN:HE22	1.78	0.48
1:A:11:LYS:HD2	1:A:11:LYS:N	2.29	0.48
1:A:71:ASN:OD1	1:A:80:SER:HB3	2.13	0.48
1:B:90:GLU:O	1:B:94:GLU:N	2.43	0.48
1:B:272:GLU:HG3	1:B:275:TRP:HE3	1.77	0.48
1:B:547:ASP:OD1	1:B:549:SER:HB2	2.13	0.48
1:C:207:ARG:NE	1:C:250:ARG:O	2.42	0.48
1:A:336:LEU:O	1:A:340:ASP:N	2.31	0.48
1:C:339:THR:O	1:C:340:ASP:HB3	2.14	0.48
1:C:534:ASP:OD2	1:C:535:PRO:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:MET:CE	1:A:162:ALA:HA	2.40	0.48
1:A:171:TYR:CD1	1:A:241:VAL:HG11	2.48	0.48
1:A:172:VAL:HG22	3:A:622:HOH:O	2.13	0.48
1:A:197:GLN:HE22	1:A:226:VAL:HG21	1.79	0.48
1:B:98:GLN:O	1:B:99:ALA:C	2.55	0.48
1:B:423:GLN:HE22	1:B:425:GLY:HA3	1.78	0.48
1:C:527:LYS:HG2	1:C:528:GLY:H	1.79	0.48
1:A:171:TYR:CE1	1:A:241:VAL:HG11	2.49	0.48
1:B:11:LYS:N	1:B:11:LYS:HD2	2.27	0.48
1:A:392:ARG:HD2	1:A:569:PHE:CZ	2.49	0.48
1:B:21:GLN:HA	3:B:630:HOH:O	2.14	0.48
1:B:336:LEU:O	1:B:340:ASP:N	2.33	0.48
1:C:202:MET:HA	1:C:206:HIS:ND1	2.28	0.48
1:C:207:ARG:HD3	1:C:207:ARG:C	2.39	0.48
1:A:126:ASP:C	1:A:128:THR:H	2.22	0.47
1:B:115:ALA:HA	1:B:163:VAL:HG13	1.95	0.47
1:B:121:ASP:OD1	1:B:123:TYR:HD2	1.97	0.47
1:B:302:LYS:HE3	1:B:304:GLU:OE2	2.13	0.47
1:C:330:PHE:CD1	1:C:330:PHE:O	2.67	0.47
1:C:378:TYR:HB3	1:C:380:GLU:OE1	2.13	0.47
1:C:392:ARG:HD2	1:C:569:PHE:CZ	2.50	0.47
1:C:423:GLN:HE21	1:C:425:GLY:N	2.02	0.47
1:A:101:SER:HB2	1:A:119:ILE:HD12	1.95	0.47
1:B:378:TYR:HB3	1:B:380:GLU:OE1	2.14	0.47
1:C:364:ARG:HA	1:C:367:ARG:HD3	1.96	0.47
1:C:114:LEU:HD13	1:C:166:LEU:CD2	2.37	0.47
1:C:199:ARG:HB3	1:C:265:MET:HE1	1.96	0.47
1:C:290:VAL:HG23	1:C:327:VAL:HG13	1.96	0.47
1:C:448:ARG:NH1	1:C:482:GLU:OE1	2.47	0.47
1:A:199:ARG:NH1	1:A:265:MET:CE	2.78	0.47
1:A:432:LEU:HD23	1:A:475:ALA:HB3	1.95	0.47
1:B:286:THR:HG1	1:B:287:HIS:HD2	1.59	0.47
1:B:357:ILE:HB	1:B:376:PHE:CE1	2.50	0.47
1:C:80:SER:HB2	1:C:271:ARG:HD3	1.97	0.47
1:C:208:GLU:O	1:C:209:LEU:C	2.56	0.47
1:C:208:GLU:O	1:C:212:ARG:CG	2.57	0.47
1:A:47:ILE:HD11	1:A:83:ILE:CG2	2.43	0.47
1:A:48:MET:HE1	1:A:114:LEU:O	2.14	0.47
1:A:488:ARG:O	1:A:492:SER:OG	2.29	0.47
1:B:263:LEU:HD11	1:B:275:TRP:CH2	2.49	0.47
1:C:61:GLN:NE2	1:C:65:ASP:OD2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:VAL:CG2	1:C:327:VAL:HG13	2.45	0.47
1:C:1:MET:CG	1:C:2:ALA:N	2.78	0.47
1:C:546:VAL:HG21	1:C:556:ILE:HG23	1.97	0.47
1:B:122:ILE:O	1:B:122:ILE:HG22	2.15	0.47
1:B:190:TRP:CH2	1:B:257:VAL:HG23	2.50	0.47
1:B:127:LYS:HD3	1:B:147:LEU:O	2.14	0.46
1:B:448:ARG:NH1	1:B:482:GLU:OE1	2.47	0.46
1:C:360:THR:O	1:C:364:ARG:HB2	2.15	0.46
1:C:414:ARG:NH2	3:C:754:HOH:O	2.39	0.46
1:A:251:TYR:O	1:A:252:PRO:C	2.57	0.46
1:A:388:SER:CB	3:A:642:HOH:O	2.63	0.46
1:B:117:LEU:C	1:B:117:LEU:CD2	2.86	0.46
1:B:274:ILE:HD11	1:B:315:ALA:HB1	1.96	0.46
1:B:361:GLU:O	1:B:365:ARG:HG3	2.15	0.46
1:B:519:ALA:HB3	3:B:674:HOH:O	2.15	0.46
1:C:546:VAL:HG11	1:C:556:ILE:HG23	1.97	0.46
1:A:138:ASP:OD2	1:A:138:ASP:C	2.59	0.46
1:B:48:MET:HG2	1:B:162:ALA:HB2	1.96	0.46
1:C:206:HIS:O	1:C:209:LEU:HB3	2.15	0.46
1:B:364:ARG:HA	1:B:367:ARG:HD3	1.96	0.46
1:A:171:TYR:HB3	1:A:174:LEU:HD12	1.97	0.46
1:B:452:HIS:O	1:B:456:GLN:HG3	2.16	0.46
1:C:98:GLN:O	1:C:99:ALA:C	2.57	0.46
1:C:203:HIS:HE1	1:C:385:LEU:CD1	2.29	0.46
1:A:5:PRO:O	1:A:281:LYS:HE3	2.16	0.46
1:A:40:GLN:NE2	1:A:85:LEU:HD12	2.30	0.46
1:A:208:GLU:OE2	1:A:208:GLU:HA	2.15	0.46
1:A:378:TYR:HB3	1:A:380:GLU:OE1	2.16	0.46
1:B:40:GLN:NE2	1:B:85:LEU:HD12	2.30	0.46
1:B:44:LEU:HD11	1:B:48:MET:HE3	1.96	0.46
1:B:316:VAL:O	1:B:320:LYS:HB2	2.15	0.46
1:A:1:MET:SD	1:A:4:ALA:HA	2.56	0.46
1:A:225:PRO:HD2	1:A:259:GLY:O	2.15	0.46
1:A:117:LEU:C	1:A:117:LEU:HD23	2.41	0.46
1:A:217:ARG:HH11	1:A:217:ARG:HG2	1.81	0.46
1:C:266:ARG:O	1:C:267:MET:HB2	2.16	0.46
1:C:362:LEU:HD22	1:C:376:PHE:CE2	2.50	0.46
1:B:546:VAL:HG11	1:B:556:ILE:HG21	1.96	0.46
1:A:372:ILE:HA	1:A:373:PRO:HD3	1.82	0.45
1:B:447:THR:O	1:B:448:ARG:C	2.59	0.45
1:C:176:TYR:HB2	1:C:181:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HD23	1:A:116:ILE:HD12	1.98	0.45
1:A:113:ASN:O	1:A:164:ASN:HB2	2.17	0.45
1:C:263:LEU:HD11	1:C:275:TRP:CH2	2.51	0.45
1:C:312:ALA:HB3	3:C:620:HOH:O	2.16	0.45
1:A:109:ARG:NE	1:A:229:LEU:HD13	2.31	0.45
1:A:119:ILE:CG2	1:A:120:ASP:N	2.79	0.45
1:A:292:ARG:CZ	1:A:292:ARG:HB3	2.46	0.45
1:A:357:ILE:HB	1:A:376:PHE:CE1	2.51	0.45
1:B:392:ARG:HD2	1:B:569:PHE:CZ	2.52	0.45
1:C:59:MET:CE	1:C:82:PRO:HA	2.42	0.45
1:C:333:VAL:HG23	1:C:342:TYR:HB3	1.99	0.45
1:A:98:GLN:HA	1:A:122:ILE:HD12	1.98	0.45
1:C:231:LYS:HB2	1:C:234:ASP:CB	2.46	0.45
1:A:72:ARG:NH1	1:A:76:GLY:O	2.48	0.45
1:B:88:SER:O	1:B:92:ILE:HG13	2.17	0.45
1:B:93:ASP:O	1:B:94:GLU:C	2.59	0.45
1:C:447:THR:O	1:C:448:ARG:C	2.59	0.45
1:A:349:PRO:O	1:A:352:VAL:HG23	2.17	0.45
1:B:64:TYR:OH	1:B:130:GLU:OE1	2.32	0.45
1:B:441:SER:OG	1:B:454:ASN:ND2	2.48	0.45
1:C:546:VAL:CG1	1:C:556:ILE:CD1	2.94	0.45
1:A:36:LEU:HD21	1:A:105:LEU:HD22	1.98	0.45
1:A:66:ARG:O	1:A:70:ASP:HB2	2.16	0.45
1:A:313:GLN:HB3	1:A:329:GLU:CG	2.43	0.45
1:B:370:ALA:O	1:B:371:HIS:C	2.60	0.45
1:C:349:PRO:O	1:C:352:VAL:HG23	2.16	0.45
1:A:330:PHE:CD1	1:A:330:PHE:O	2.69	0.45
1:C:249:PRO:C	1:C:251:TYR:H	2.25	0.45
1:A:73:LEU:HG	1:A:79:PHE:HB3	1.99	0.45
1:A:240:ARG:NH1	1:A:244:TYR:OH	2.50	0.45
1:A:291:GLY:CA	1:A:330:PHE:CE2	3.00	0.45
1:C:357:ILE:HB	1:C:376:PHE:CE1	2.52	0.45
1:C:507:GLU:CD	1:C:507:GLU:H	2.24	0.45
1:B:362:LEU:HD22	1:B:376:PHE:CE2	2.52	0.44
1:C:203:HIS:N	1:C:206:HIS:ND1	2.47	0.44
1:B:330:PHE:CD1	1:B:330:PHE:O	2.70	0.44
1:B:477:ILE:CG2	1:B:479:PRO:HG3	2.46	0.44
1:A:88:SER:O	1:A:92:ILE:HG13	2.16	0.44
1:A:331:GLN:O	1:A:332:MET:C	2.60	0.44
1:C:204:ARG:HG2	1:C:204:ARG:HH11	1.83	0.44
1:C:214:ALA:HB3	1:C:255:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ARG:HH21	1:C:379:PRO:HD2	1.82	0.44
1:C:392:ARG:NH1	1:C:567:GLN:O	2.50	0.44
1:A:36:LEU:HD22	1:A:85:LEU:HD13	1.99	0.44
1:A:423:GLN:NE2	1:A:425:GLY:HA3	2.32	0.44
1:A:52:PHE:O	1:A:53:SER:C	2.60	0.44
1:A:95:LYS:O	1:A:96:LYS:HB2	2.18	0.44
1:A:109:ARG:HD3	1:A:229:LEU:HD13	1.99	0.44
1:A:196:PHE:CE2	1:A:202:MET:HE3	2.53	0.44
1:A:344:PRO:C	1:A:346:ASP:N	2.75	0.44
1:C:411:ALA:HA	3:C:750:HOH:O	2.17	0.44
1:A:204:ARG:HD2	1:A:204:ARG:O	2.17	0.44
1:B:443:GLU:HB2	3:B:654:HOH:O	2.16	0.44
1:C:255:MET:O	1:C:255:MET:HG2	2.17	0.44
1:A:337:PRO:HG3	1:A:355:LEU:CD1	2.47	0.44
1:A:423:GLN:NE2	1:A:425:GLY:CA	2.81	0.44
1:A:434:ASP:HB3	2:A:574:PPS:O3P	2.18	0.44
1:A:133:LEU:N	1:A:133:LEU:HD23	2.33	0.44
1:C:197:GLN:HE22	1:C:265:MET:CE	2.31	0.44
1:A:141:HIS:HA	1:A:142:PRO:HD3	1.86	0.44
1:A:190:TRP:CH2	1:A:257:VAL:HG23	2.52	0.44
1:A:207:ARG:HD3	1:A:207:ARG:C	2.43	0.44
1:A:226:VAL:HG12	1:A:227:VAL:N	2.33	0.44
1:B:437:ARG:HD2	1:B:437:ARG:HA	1.87	0.44
1:C:190:TRP:CZ3	1:C:257:VAL:HG23	2.52	0.44
1:C:510:GLU:HG2	1:C:518:TYR:CG	2.53	0.44
1:C:546:VAL:HG11	1:C:556:ILE:HG21	2.00	0.44
1:A:448:ARG:NH1	1:A:482:GLU:OE1	2.50	0.43
1:B:20:ARG:O	1:B:21:GLN:C	2.61	0.43
1:C:217:ARG:HG2	1:C:217:ARG:NH1	2.31	0.43
1:C:510:GLU:HG2	1:C:518:TYR:CD2	2.53	0.43
1:A:31:LEU:HD22	1:A:102:ARG:O	2.17	0.43
1:A:333:VAL:HG23	1:A:342:TYR:HB3	2.00	0.43
1:B:451:ARG:HH12	2:B:575:PPS:C2	2.31	0.43
1:C:52:PHE:O	1:C:53:SER:C	2.60	0.43
1:A:26:ALA:O	1:A:29:GLU:HB2	2.18	0.43
1:A:292:ARG:HH21	1:A:309:PRO:HB3	1.82	0.43
1:A:520:ALA:HB1	1:A:525:GLU:HB2	2.00	0.43
1:A:528:GLY:O	1:A:534:ASP:HB2	2.19	0.43
1:C:204:ARG:NH2	1:C:342:TYR:OH	2.50	0.43
1:C:296:GLY:HA2	1:C:297:PRO:HD3	1.81	0.43
1:A:176:TYR:CB	1:A:181:LEU:HD13	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:HIS:O	1:A:317:GLU:HG2	2.18	0.43
1:B:81:MET:SD	1:B:82:PRO:HD2	2.58	0.43
1:C:390:PRO:HA	1:C:391:PRO:HD3	1.80	0.43
1:A:274:ILE:HD11	1:A:315:ALA:O	2.19	0.43
1:A:452:HIS:O	1:A:456:GLN:HG3	2.18	0.43
1:B:44:LEU:HA	1:B:47:ILE:HD12	2.01	0.43
1:B:250:ARG:HA	1:B:250:ARG:HD3	1.72	0.43
1:C:138:ASP:HA	1:C:139:PRO:HD3	1.79	0.43
1:C:252:PRO:O	1:C:253:ASN:C	2.61	0.43
1:C:370:ALA:O	1:C:371:HIS:C	2.61	0.43
1:A:16:ARG:O	1:A:18:ALA:N	2.51	0.43
1:A:337:PRO:HG2	1:A:355:LEU:HG	2.00	0.43
1:A:572:ARG:HD2	1:B:253:ASN:OD1	2.19	0.43
1:B:202:MET:HA	1:B:206:HIS:ND1	2.33	0.43
1:B:214:ALA:HB2	1:B:221:VAL:CG2	2.49	0.43
1:C:334:THR:OG1	1:C:335:TYR:N	2.52	0.43
1:A:562:LEU:HA	1:A:562:LEU:HD23	1.79	0.43
1:A:192:ARG:HG3	1:A:219:ALA:HA	2.00	0.43
1:B:138:ASP:HA	1:B:139:PRO:HD3	1.88	0.43
1:C:217:ARG:O	1:C:218:GLN:C	2.62	0.43
1:A:193:VAL:H	1:A:286:THR:CG2	2.29	0.43
1:A:390:PRO:HA	1:A:391:PRO:HD3	1.80	0.43
1:A:425:GLY:HA2	1:A:573:GLN:HE22	1.84	0.43
1:A:16:ARG:C	1:A:18:ALA:H	2.26	0.42
1:A:71:ASN:OD1	1:A:80:SER:CB	2.67	0.42
1:B:103:ILE:O	1:B:116:ILE:HA	2.19	0.42
1:B:349:PRO:O	1:B:352:VAL:HG23	2.19	0.42
1:C:36:LEU:HB3	1:C:40:GLN:HB2	2.00	0.42
1:C:544:LEU:HD11	1:C:559:GLU:OE2	2.19	0.42
1:A:74:ALA:O	1:A:76:GLY:N	2.50	0.42
1:A:302:LYS:HG3	1:A:304:GLU:OE2	2.19	0.42
1:A:546:VAL:CG1	1:A:556:ILE:CD1	2.97	0.42
1:C:202:MET:HB3	1:C:247:LEU:HD22	2.01	0.42
1:C:251:TYR:O	1:C:252:PRO:C	2.61	0.42
1:C:512:SER:O	1:C:514:LYS:HG3	2.18	0.42
1:A:119:ILE:HG22	1:A:121:ASP:N	2.34	0.42
1:A:137:GLY:O	1:A:138:ASP:C	2.62	0.42
1:B:272:GLU:HG2	1:B:276:HIS:CD2	2.54	0.42
1:C:212:ARG:NH2	1:C:342:TYR:HD1	2.17	0.42
1:B:432:LEU:HD23	1:B:432:LEU:HA	1.74	0.42
1:C:331:GLN:O	1:C:332:MET:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:NH1	1:A:266:ARG:HG3	2.34	0.42
1:A:572:ARG:HD2	1:B:253:ASN:CB	2.48	0.42
1:B:313:GLN:CD	1:B:329:GLU:HG2	2.45	0.42
1:B:337:PRO:CD	1:B:353:LYS:CB	2.89	0.42
1:B:512:SER:O	1:B:514:LYS:HG3	2.20	0.42
1:C:1:MET:HG3	1:C:2:ALA:H	1.83	0.42
1:B:331:GLN:O	1:B:332:MET:C	2.61	0.42
1:A:89:GLN:HA	1:A:92:ILE:HD12	2.02	0.42
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.76	0.42
1:A:273:ALA:O	1:A:276:HIS:HB2	2.20	0.42
1:B:41:LEU:HA	1:B:41:LEU:HD23	1.65	0.42
1:B:562:LEU:HD23	1:B:562:LEU:HA	1.78	0.42
1:C:102:ARG:NH2	1:C:161:GLU:OE1	2.52	0.42
1:B:192:ARG:HD2	1:B:217:ARG:O	2.20	0.42
1:B:272:GLU:O	1:B:275:TRP:HB3	2.19	0.42
1:C:204:ARG:H	1:C:377:SER:HA	1.84	0.42
1:A:292:ARG:O	1:A:293:ASP:HB2	2.19	0.42
1:B:192:ARG:HB3	1:B:219:ALA:HB2	2.02	0.42
1:B:250:ARG:HG3	1:B:378:TYR:CD2	2.55	0.42
1:B:299:SER:HA	1:B:304:GLU:O	2.19	0.42
1:B:451:ARG:HH12	2:B:575:PPS:H2	1.85	0.42
1:C:36:LEU:HB2	1:C:41:LEU:HG	2.02	0.42
1:A:138:ASP:HA	1:A:139:PRO:HD3	1.78	0.42
1:B:333:VAL:HG23	1:B:342:TYR:HB3	2.01	0.42
1:B:397:PHE:CD1	1:B:397:PHE:C	2.98	0.42
1:C:27:GLU:HG2	1:C:31:LEU:HD11	2.02	0.42
1:C:299:SER:HB3	1:C:305:ASP:OD1	2.20	0.42
1:A:140:GLU:O	1:A:145:VAL:HG23	2.19	0.41
1:A:197:GLN:HG2	1:A:294:HIS:CE1	2.54	0.41
1:B:48:MET:HE1	1:B:114:LEU:O	2.20	0.41
1:B:213:ALA:O	1:B:214:ALA:C	2.61	0.41
1:C:108:PHE:CD1	1:C:108:PHE:C	2.98	0.41
1:A:74:ALA:C	1:A:76:GLY:H	2.28	0.41
1:B:546:VAL:HG21	1:B:556:ILE:HG23	2.02	0.41
1:C:57:GLY:HA2	1:C:160:ILE:HG13	2.01	0.41
1:C:89:GLN:HB3	1:C:90:GLU:OE1	2.19	0.41
1:C:440:LEU:O	1:C:457:ARG:NH1	2.40	0.41
1:A:223:ILE:HD11	1:A:251:TYR:CE1	2.55	0.41
1:A:477:ILE:CG2	1:A:479:PRO:HG3	2.50	0.41
1:A:565:GLU:CB	3:A:655:HOH:O	2.68	0.41
1:C:98:GLN:HA	1:C:122:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ARG:HD2	3:B:622:HOH:O	2.20	0.41
1:C:204:ARG:HB3	1:C:376:PHE:C	2.45	0.41
1:A:36:LEU:HD11	1:A:105:LEU:HB3	2.03	0.41
1:A:334:THR:OG1	1:A:335:TYR:N	2.53	0.41
1:A:477:ILE:HG22	1:A:479:PRO:HG3	2.02	0.41
1:B:337:PRO:HG3	1:B:355:LEU:CD1	2.49	0.41
1:A:362:LEU:HD22	1:A:376:PHE:HE2	1.85	0.41
1:B:199:ARG:CD	1:B:265:MET:HE1	2.29	0.41
1:B:217:ARG:HG2	1:B:217:ARG:HH11	1.85	0.41
1:B:501:HIS:CE1	1:B:539:PRO:HD2	2.55	0.41
1:C:47:ILE:HG13	1:C:52:PHE:HD1	1.86	0.41
1:C:345:VAL:HG11	3:C:693:HOH:O	2.17	0.41
1:A:31:LEU:CD2	1:A:102:ARG:HB3	2.45	0.41
1:A:109:ARG:HH21	1:A:166:LEU:CD1	2.34	0.41
1:C:92:ILE:HA	1:C:97:LEU:HD12	2.02	0.41
1:C:337:PRO:HG3	1:C:355:LEU:CD1	2.47	0.41
1:A:510:GLU:HG2	1:A:518:TYR:CD2	2.56	0.41
1:B:313:GLN:NE2	1:B:329:GLU:HG2	2.35	0.41
1:C:519:ALA:C	1:C:523:ARG:NH1	2.79	0.41
1:A:90:GLU:O	1:A:94:GLU:CB	2.64	0.41
1:A:117:LEU:HA	1:A:160:ILE:HD13	2.02	0.41
1:A:153:GLU:HG2	1:A:154:PHE:CD2	2.55	0.41
1:A:440:LEU:O	1:A:457:ARG:HD3	2.21	0.41
1:B:131:ALA:HB1	1:B:144:ILE:CD1	2.50	0.41
1:B:392:ARG:NH1	1:B:567:GLN:O	2.52	0.41
1:C:18:ALA:O	1:C:19:PRO:C	2.64	0.41
1:C:199:ARG:HB3	1:C:265:MET:HE3	2.02	0.41
1:C:203:HIS:NE2	1:C:362:LEU:HD21	2.36	0.41
1:C:423:GLN:NE2	1:C:425:GLY:HA3	2.36	0.41
1:C:436:VAL:HG11	1:C:458:ILE:HD11	2.02	0.41
1:C:547:ASP:OD1	1:C:549:SER:HB2	2.21	0.41
1:A:48:MET:HE2	1:A:162:ALA:HB1	2.02	0.41
1:A:309:PRO:C	1:A:310:TYR:CD1	2.99	0.41
1:B:86:ASP:HA	1:B:154:PHE:O	2.21	0.41
1:C:18:ALA:O	1:C:21:GLN:HB2	2.20	0.41
1:C:245:GLN:O	1:C:248:LEU:HB2	2.21	0.41
1:A:103:ILE:O	1:A:116:ILE:HA	2.21	0.40
1:A:129:LYS:CE	1:A:133:LEU:HD11	2.48	0.40
1:A:296:GLY:HA2	1:A:297:PRO:HD3	1.88	0.40
1:A:552:SER:O	1:A:556:ILE:HG13	2.21	0.40
1:B:59:MET:HE3	1:B:64:TYR:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:575:PPS:H5'2	2:B:575:PPS:N3	2.35	0.40
1:C:46:LEU:O	1:C:51:GLY:N	2.54	0.40
1:C:246:ALA:O	1:C:249:PRO:HD2	2.21	0.40
1:C:504:THR:HA	1:C:505:PRO:HD3	1.96	0.40
1:A:126:ASP:C	1:A:128:THR:N	2.80	0.40
1:B:209:LEU:HD13	1:B:330:PHE:HB2	2.03	0.40
1:C:250:ARG:HG3	1:C:378:TYR:CD2	2.56	0.40
1:A:32:PRO:HB3	1:A:95:LYS:HB3	2.03	0.40
1:A:200:ASN:HB3	1:A:201:PRO:CD	2.51	0.40
1:B:92:ILE:HD13	1:B:122:ILE:HG21	2.04	0.40
1:B:199:ARG:NH1	1:B:265:MET:HE1	2.35	0.40
1:C:41:LEU:HD22	1:C:166:LEU:HD13	2.02	0.40
1:C:269:GLY:HA3	1:C:270:PRO:HD3	1.91	0.40
1:C:372:ILE:HA	1:C:373:PRO:HD3	1.84	0.40
1:A:109:ARG:CD	1:A:229:LEU:HD13	2.51	0.40
1:A:512:SER:O	1:A:514:LYS:HG3	2.21	0.40
1:B:312:ALA:HB3	3:B:584:HOH:O	2.21	0.40
1:B:344:PRO:C	1:B:346:ASP:N	2.78	0.40
1:C:292:ARG:HA	1:C:309:PRO:O	2.21	0.40
1:C:344:PRO:C	1:C:346:ASP:N	2.79	0.40
1:C:374:GLU:HG3	1:C:379:PRO:HD3	2.04	0.40
1:B:506:LEU:O	1:B:507:GLU:C	2.65	0.40
1:C:333:VAL:HB	1:C:343:ARG:O	2.21	0.40
1:C:528:GLY:O	1:C:534:ASP:HB2	2.22	0.40
1:C:546:VAL:HG11	1:C:556:ILE:CD1	2.51	0.40

There are no symmetry-related clashes.

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	571/573 (100%)	492 (86%)	56 (10%)	23 (4%)	2 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	571/573 (100%)	513 (90%)	47 (8%)	11 (2%)	6	13
1	C	571/573 (100%)	517 (90%)	46 (8%)	8 (1%)	9	19
All	All	1713/1719 (100%)	1522 (89%)	149 (9%)	42 (2%)	4	8

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	75	ASP
1	A	571	GLU
1	B	571	GLU
1	C	571	GLU
1	A	2	ALA
1	A	16	ARG
1	A	94	GLU
1	A	127	LYS
1	A	138	ASP
1	A	166	LEU
1	A	202	MET
1	A	352	VAL
1	A	572	ARG
1	B	94	GLU
1	B	352	VAL
1	B	371	HIS
1	C	352	VAL
1	C	371	HIS
1	C	572	ARG
1	A	131	ALA
1	A	232	PRO
1	A	269	GLY
1	A	371	HIS
1	A	528	GLY
1	B	202	MET
1	B	528	GLY
1	B	572	ARG
1	A	5	PRO
1	A	99	ALA
1	A	130	GLU
1	A	141	HIS
1	C	424	GLY
1	C	528	GLY

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Mol	Chain	Res	Type
1	B	347	GLN
1	B	503	ALA
1	C	503	ALA
1	B	269	GLY
1	B	344	PRO
1	C	344	PRO
1	A	122	ILE
1	A	344	PRO

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	472/474 (100%)	443 (94%)	29 (6%)	17	37
1	B	472/474 (100%)	448 (95%)	24 (5%)	21	45
1	C	472/474 (100%)	449 (95%)	23 (5%)	22	47
All	All	1416/1422 (100%)	1340 (95%)	76 (5%)	20	42

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	11	LYS
1	A	24	LEU
1	A	41	LEU
1	A	70	ASP
1	A	133	LEU
1	A	144	ILE
1	A	154	PHE
1	A	163	VAL
1	A	166	LEU
1	A	181	LEU
1	A	191	SER
1	A	192	ARG
1	A	225	PRO

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Mol	Chain	Res	Type
1	A	239	THR
1	A	240	ARG
1	A	248	LEU
1	A	302	LYS
1	A	338	ASP
1	A	339	THR
1	A	342	TYR
1	A	355	LEU
1	A	361	GLU
1	A	394	THR
1	A	423	GLN
1	A	426	ARG
1	A	437	ARG
1	A	448	ARG
1	A	573	GLN
1	B	3	ASN
1	B	11	LYS
1	B	14	LEU
1	B	90	GLU
1	B	163	VAL
1	B	181	LEU
1	B	192	ARG
1	B	199	ARG
1	B	209	LEU
1	B	240	ARG
1	B	248	LEU
1	B	252	PRO
1	B	338	ASP
1	B	339	THR
1	B	342	TYR
1	B	355	LEU
1	B	361	GLU
1	B	394	THR
1	B	423	GLN
1	B	426	ARG
1	B	437	ARG
1	B	448	ARG
1	B	507	GLU
1	B	573	GLN
1	C	19	PRO
1	C	90	GLU
1	C	126	ASP

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Mol	Chain	Res	Type
1	C	159	LYS
1	C	163	VAL
1	C	166	LEU
1	C	172	VAL
1	C	181	LEU
1	C	218	GLN
1	C	239	THR
1	C	240	ARG
1	C	248	LEU
1	C	338	ASP
1	C	339	THR
1	C	342	TYR
1	C	355	LEU
1	C	361	GLU
1	C	394	THR
1	C	423	GLN
1	C	426	ARG
1	C	437	ARG
1	C	448	ARG
1	C	573	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	61	GLN
1	A	77	ASN
1	A	167	ASN
1	A	220	ASN
1	A	331	GLN
1	A	356	ASN
1	A	423	GLN
1	A	438	HIS
1	A	454	ASN
1	A	456	GLN
1	B	3	ASN
1	B	167	ASN
1	B	184	HIS
1	B	220	ASN
1	B	287	HIS
1	B	313	GLN
1	B	331	GLN

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Mol	Chain	Res	Type
1	B	423	GLN
1	B	454	ASN
1	B	456	GLN
1	B	551	GLN
1	B	573	GLN
1	C	3	ASN
1	C	89	GLN
1	C	167	ASN
1	C	220	ASN
1	C	287	HIS
1	C	331	GLN
1	C	423	GLN
1	C	454	ASN
1	C	456	GLN
1	C	558	HIS
1	C	573	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	PPS	B	575	-	33,33,33	1.34	5 (15%)	49,52,52	1.38	6 (12%)
2	PPS	A	574	-	33,33,33	1.21	3 (9%)	49,52,52	1.30	4 (8%)
2	PPS	C	576	-	33,33,33	1.30	4 (12%)	49,52,52	1.37	5 (10%)

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	PPS	B	575	-	-	5/15/37/37	0/3/3/3
2	PPS	A	574	-	-	2/15/37/37	0/3/3/3
2	PPS	C	576	-	-	1/15/37/37	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	576	PPS	O4'-C1'	3.13	1.49	1.42
2	C	576	PPS	C2-N1	2.97	1.39	1.33
2	B	575	PPS	C4-N3	2.85	1.39	1.34
2	B	575	PPS	C2-N1	2.63	1.38	1.33
2	C	576	PPS	P2-O6P	2.60	1.66	1.59
2	B	575	PPS	O4'-C1'	2.58	1.48	1.42
2	A	574	PPS	O4'-C1'	2.54	1.47	1.42
2	A	574	PPS	C4-N3	2.47	1.39	1.34
2	A	574	PPS	C2-N1	2.38	1.38	1.33
2	B	575	PPS	O5'-C5'	-2.15	1.36	1.44
2	C	576	PPS	C4-N3	2.10	1.38	1.34
2	B	575	PPS	C2'-C3'	2.01	1.57	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	576	PPS	O4'-C1'-N9	3.16	114.15	108.09
2	A	574	PPS	C2'-C3'-C4'	-2.95	98.08	103.24
2	C	576	PPS	O2P-P1-O1P	2.72	118.00	107.80
2	A	574	PPS	O2P-P1-O1P	2.63	117.67	107.80
2	B	575	PPS	C2'-C3'-C4'	-2.62	98.65	103.24
2	B	575	PPS	N9-C8-N7	2.56	117.57	113.94
2	B	575	PPS	O2P-P1-O1P	2.41	116.82	107.80
2	C	576	PPS	O3'-C3'-C2'	-2.37	103.16	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	575	PPS	O6P-P2-O4P	-2.34	103.67	110.70
2	C	576	PPS	N9-C8-N7	2.34	117.25	113.94
2	C	576	PPS	C2-N3-C4	-2.32	106.17	111.83
2	A	574	PPS	C2-N3-C4	-2.11	106.69	111.83
2	B	575	PPS	O4'-C1'-N9	2.10	112.13	108.09
2	B	575	PPS	C2-N3-C4	-2.10	106.71	111.83
2	A	574	PPS	N9-C8-N7	2.07	116.88	113.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	575	PPS	C3'-C4'-C5'-O5'
2	B	575	PPS	O4'-C4'-C5'-O5'
2	B	575	PPS	C2'-C3'-O3'-P1
2	B	575	PPS	O4'-C1'-N9-C8
2	A	574	PPS	C2'-C3'-O3'-P1
2	B	575	PPS	C2'-C1'-N9-C8
2	A	574	PPS	O4'-C1'-N9-C8
2	C	576	PPS	O4'-C1'-N9-C8

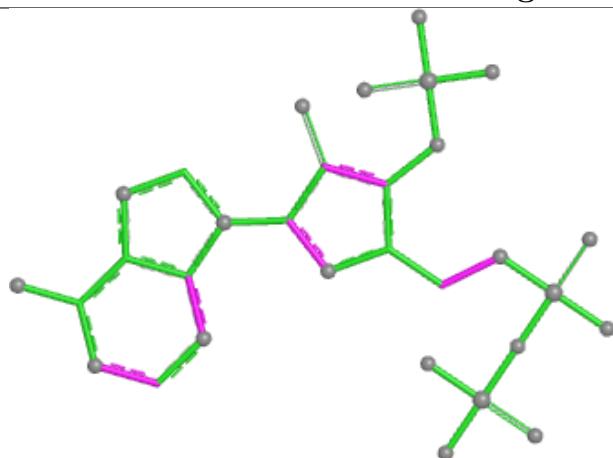
There are no ring outliers.

3 monomers are involved in 8 short contacts:

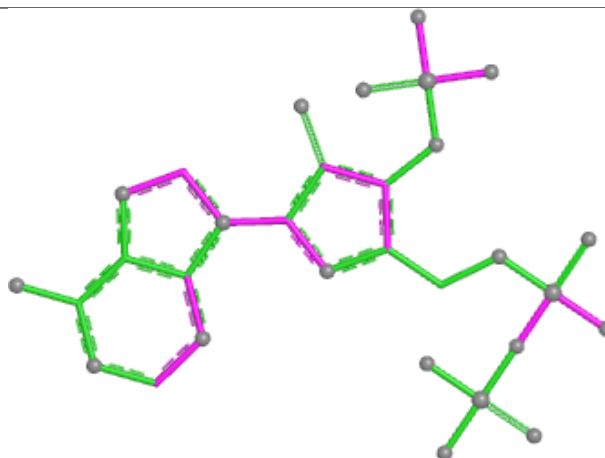
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	575	PPS	4	0
2	A	574	PPS	2	0
2	C	576	PPS	2	0

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

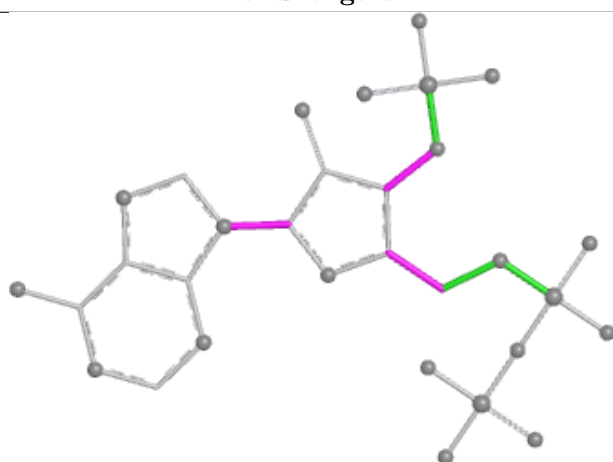
Ligand PPS B 575



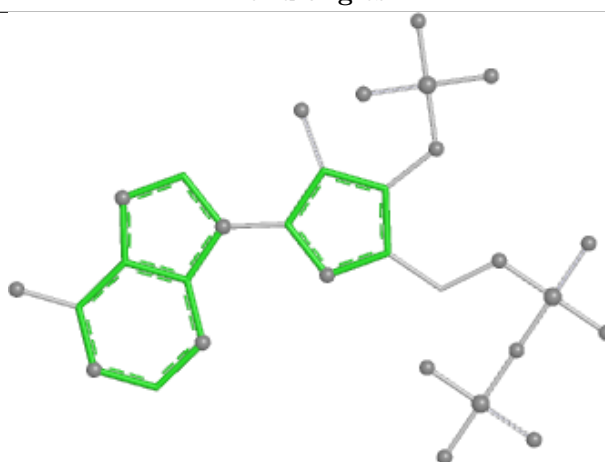
Bond lengths



Bond angles

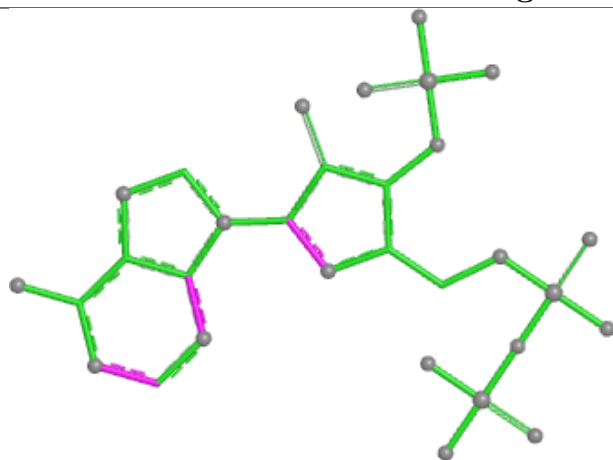


Torsions

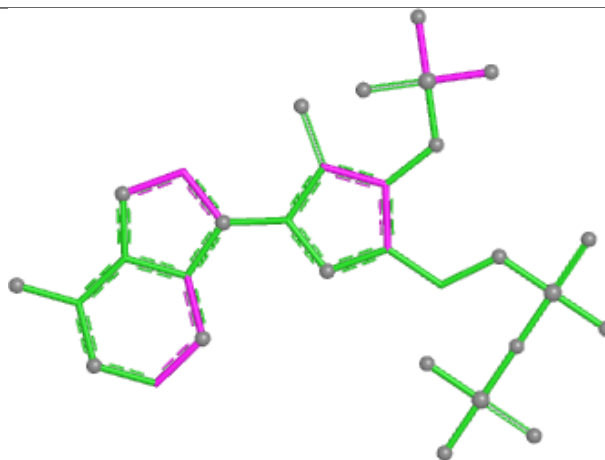


Rings

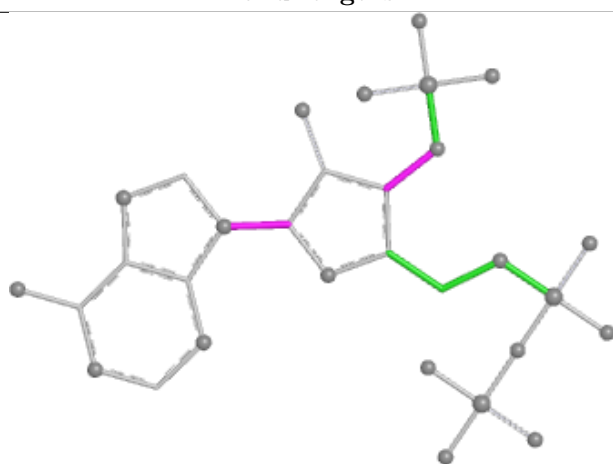
Ligand PPS A 574



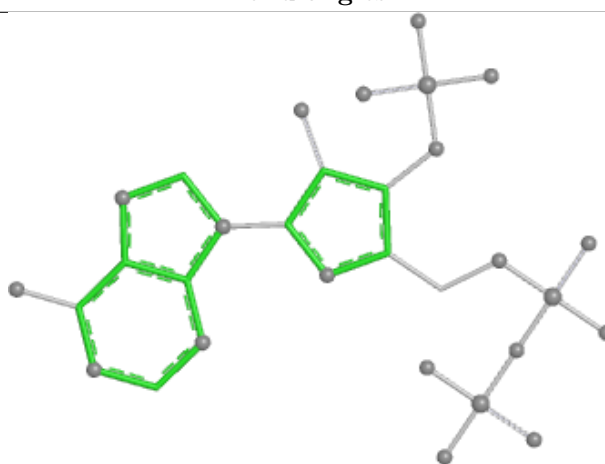
Bond lengths



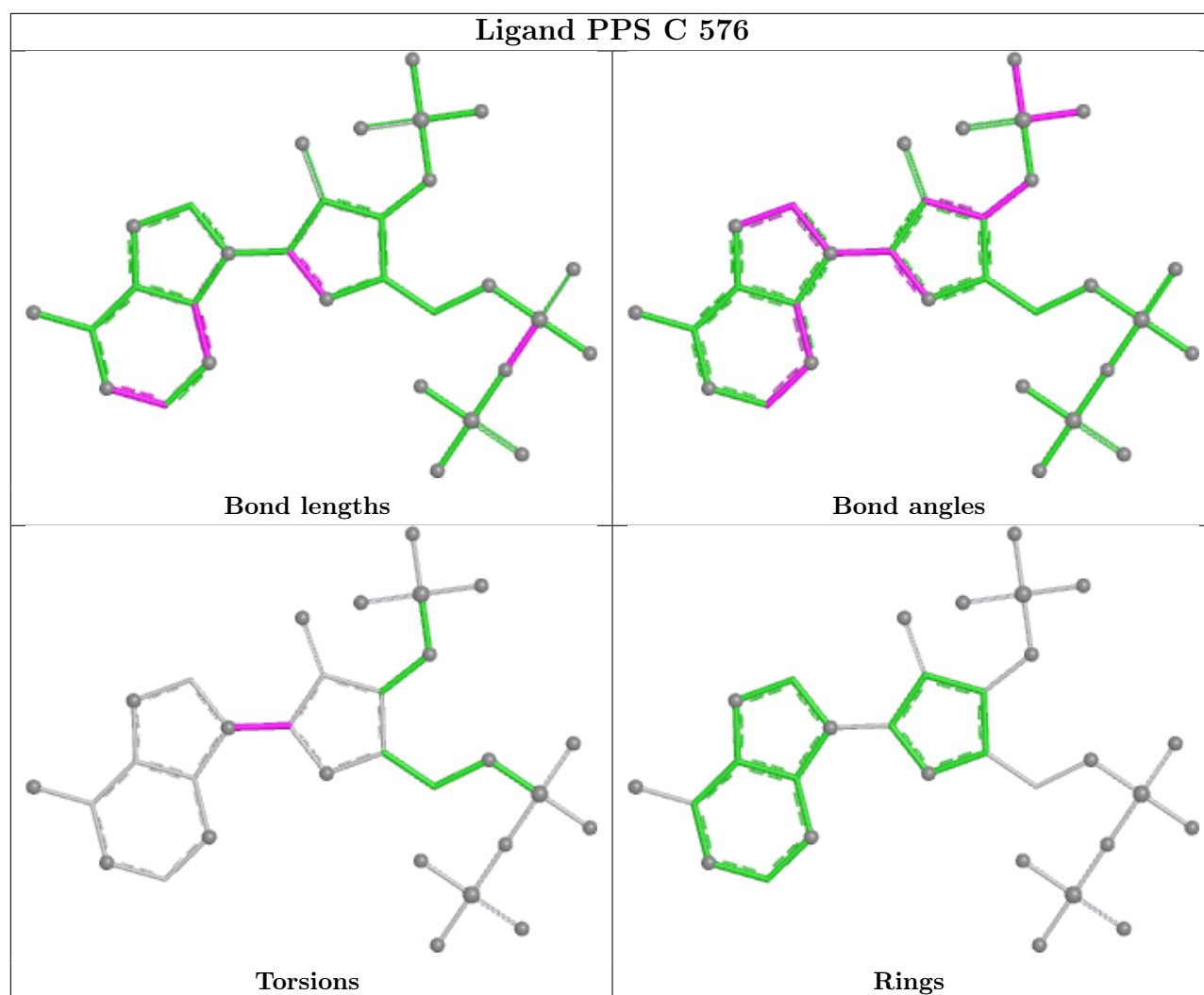
Bond angles



Torsions



Rings



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	573/573 (100%)	0.25	31 (5%) 31 26	30, 75, 129, 165	0
1	B	573/573 (100%)	-0.11	16 (2%) 55 49	30, 59, 102, 157	0
1	C	573/573 (100%)	-0.25	20 (3%) 47 41	29, 53, 122, 168	0
All	All	1719/1719 (100%)	-0.04	67 (3%) 43 38	29, 60, 119, 168	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	345	VAL	4.6
1	A	573	GLN	4.0
1	A	345	VAL	3.8
1	C	333	VAL	3.5
1	B	333	VAL	3.4
1	B	535	PRO	3.2
1	A	342	TYR	3.2
1	B	345	VAL	3.0
1	B	573	GLN	2.9
1	C	370	ALA	2.9
1	C	342	TYR	2.9
1	A	34	VAL	2.9
1	B	355	LEU	2.8
1	C	334	THR	2.8
1	A	134	VAL	2.7
1	A	154	PHE	2.7
1	B	344	PRO	2.7
1	A	332	MET	2.7
1	B	366	LEU	2.6
1	A	350	ALA	2.6
1	A	354	THR	2.6
1	A	357	ILE	2.6
1	C	2	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	330	PHE	2.6
1	A	7	GLY	2.6
1	A	349	PRO	2.5
1	A	2	ALA	2.5
1	A	133	LEU	2.5
1	A	355	LEU	2.5
1	B	524	GLY	2.5
1	A	333	VAL	2.5
1	C	372	ILE	2.5
1	A	352	VAL	2.5
1	C	357	ILE	2.4
1	B	350	ALA	2.4
1	B	354	THR	2.4
1	A	388	SER	2.4
1	C	376	PHE	2.4
1	C	332	MET	2.3
1	C	349	PRO	2.3
1	A	339	THR	2.3
1	B	330	PHE	2.3
1	A	373	PRO	2.3
1	C	360	THR	2.3
1	C	355	LEU	2.3
1	A	330	PHE	2.2
1	B	523	ARG	2.2
1	B	351	GLY	2.2
1	A	1	MET	2.2
1	A	88	SER	2.2
1	B	362	LEU	2.2
1	A	159	LYS	2.2
1	C	1	MET	2.2
1	A	348	VAL	2.2
1	C	358	SER	2.2
1	B	526	ILE	2.2
1	C	371	HIS	2.2
1	B	432	LEU	2.1
1	A	74	ALA	2.1
1	A	329	GLU	2.1
1	A	572	ARG	2.1
1	A	125	PRO	2.1
1	A	376	PHE	2.1
1	C	385	LEU	2.0
1	A	338	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	354	THR	2.0
1	C	382	VAL	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](#)

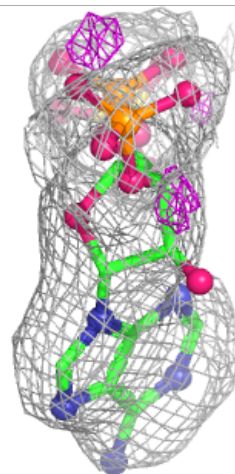
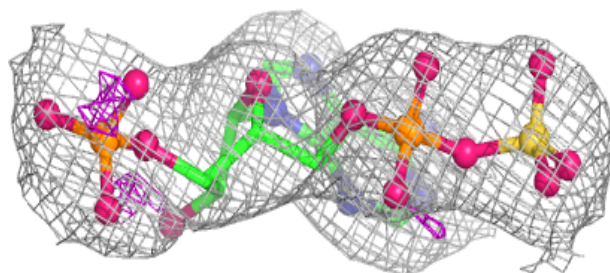
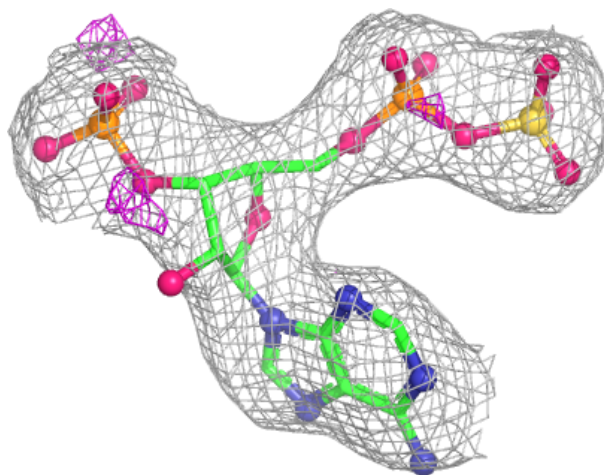
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PPS	A	574	31/31	0.94	0.08	59,72,103,111	0
2	PPS	B	575	31/31	0.95	0.07	50,68,96,97	0
2	PPS	C	576	31/31	0.97	0.06	41,59,89,98	0

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

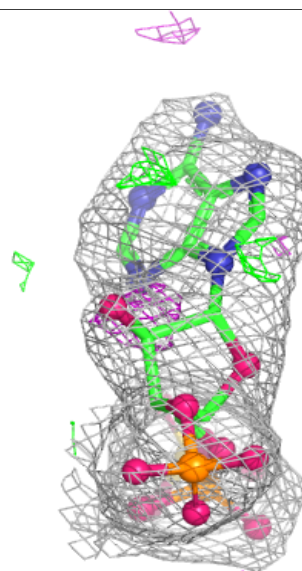
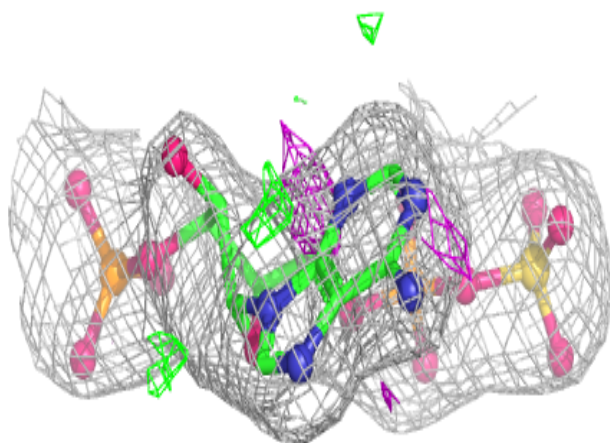
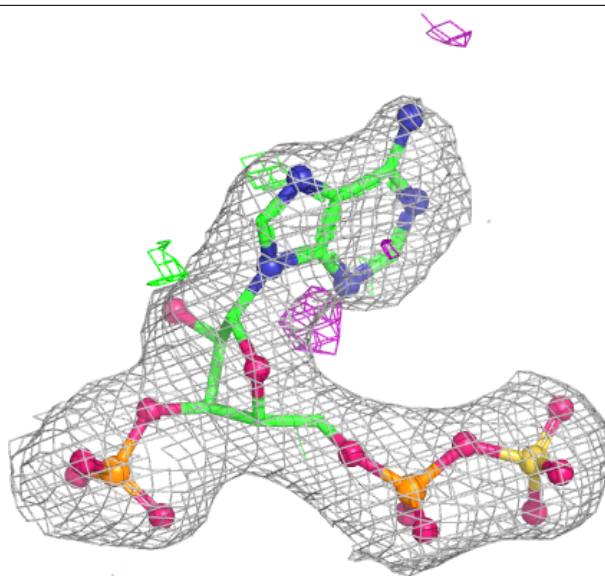
Electron density around PPS A 574:

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



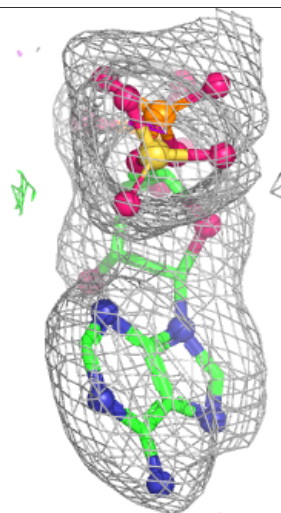
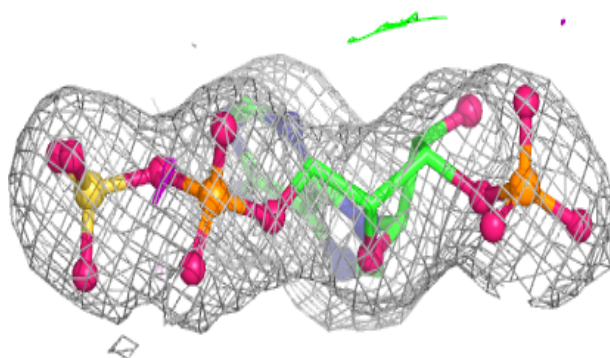
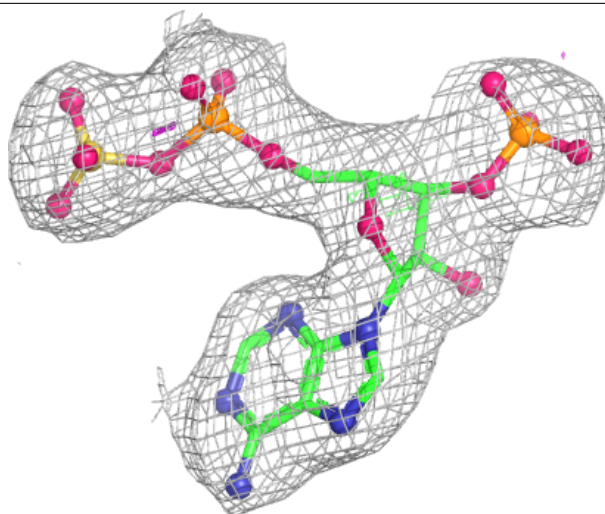
Electron density around PPS B 575:

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



Electron density around PPS C 576:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.