Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2023 – 07:55 PM EDT

PDB ID	:	3A5C
Title	:	Inter-subunit interaction and quaternary rearrangement defined by the central stalk of prokaryotic V1-ATPase
Authors	:	Numoto, N.; Hasegawa, Y.; Takeda, K.; Miki, K.
Deposited on	:	2009-08-06
Resolution	:	4.51 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:

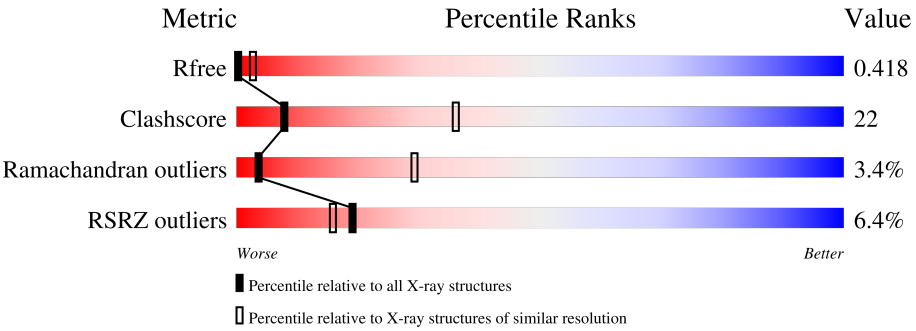
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.51 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	1056 (5.22-3.80)
Clashscore	141614	1124 (5.22-3.80)
Ramachandran outliers	138981	1070 (5.22-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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 <=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	578	8% 83% 12%
1	B	578	2% 85% 11%
1	C	578	8% 84% 11%
1	I	578	11% 81% 13%
1	J	578	2% 84% 11%
1	K	578	8% 83% 12%

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Mol	Chain	Length	Quality of chain
2	D	478	5% 83% 9% 6%
2	E	478	6% 81% 11% 6%
2	F	478	8% 83% 10% 6%
2	L	478	4% 83% 10% 6%
2	M	478	5% 83% 10% 6%
2	N	478	10% 82% 11% 6%
3	G	223	24% 23% 7% 42%
3	O	223	23% 24% 8% 42%
4	H	104	5% 79% 18%
4	P	104	7% 77% 16% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ADP	K	600	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 32188 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 V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	561	Total 2752	C 1630	N 561	O 561	0	0	0
1	B	561	Total 2752	C 1630	N 561	O 561	0	0	0
1	C	561	Total 2752	C 1630	N 561	O 561	0	0	0
1	I	561	Total 2752	C 1630	N 561	O 561	0	0	0
1	J	561	Total 2752	C 1630	N 561	O 561	0	0	0
1	K	561	Total 2752	C 1630	N 561	O 561	0	0	0

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	450	Total 2212	C 1312	N 450	O 450	0	0	0
2	E	450	Total 2212	C 1312	N 450	O 450	0	0	0
2	F	450	Total 2212	C 1312	N 450	O 450	0	0	0
2	L	450	Total 2212	C 1312	N 450	O 450	0	0	0
2	M	450	Total 2212	C 1312	N 450	O 450	0	0	0
2	N	450	Total 2212	C 1312	N 450	O 450	0	0	0

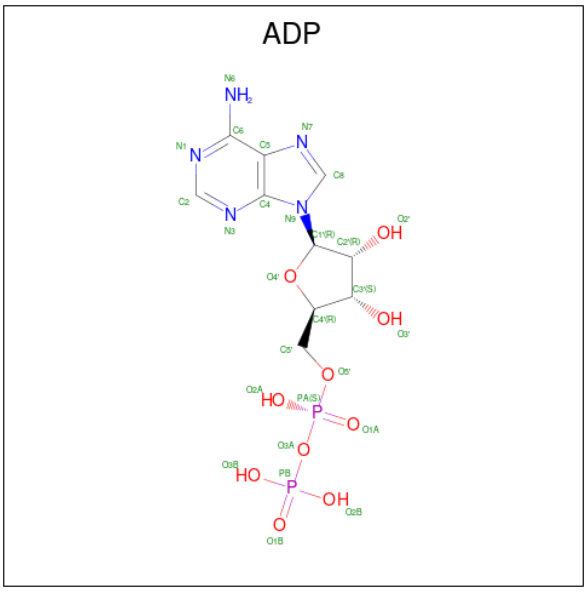
- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	129	Total	C	N	O	0	0	0
			639	381	129	129			
3	O	129	Total	C	N	O	0	0	0
			639	381	129	129			

- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	104	Total	C	N	O	0	0	0
			509	301	104	104			
4	P	104	Total	C	N	O	0	0	0
			509	301	104	104			

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



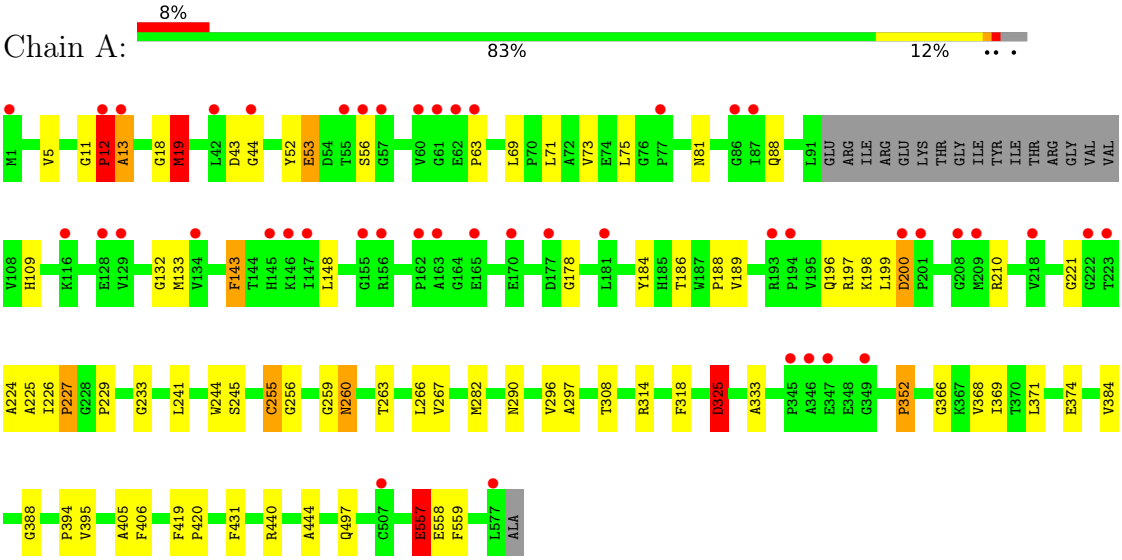
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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.

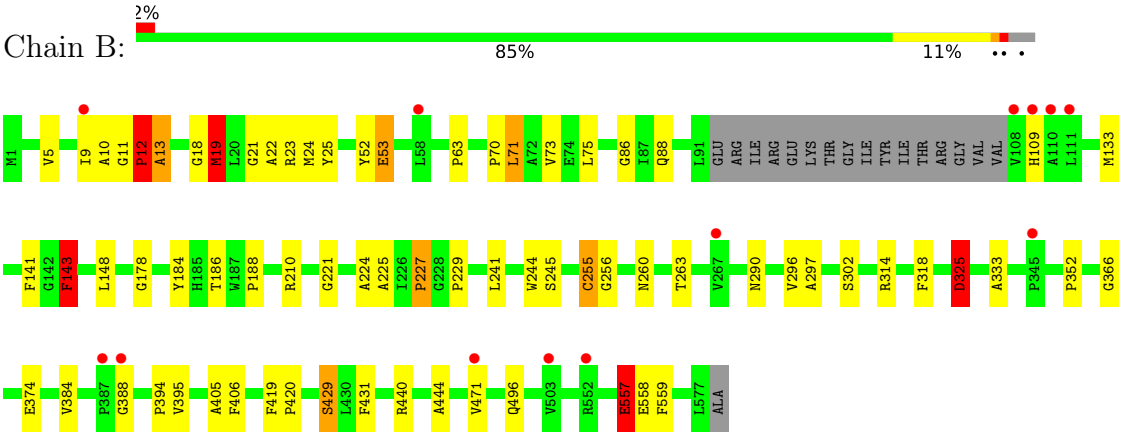
• Molecule 1: V-type ATP synthase alpha chain

Chain A:



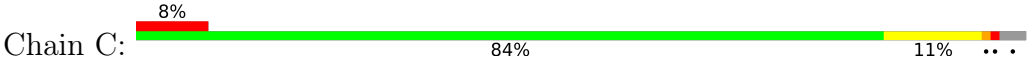
• Molecule 1: V-type ATP synthase alpha chain

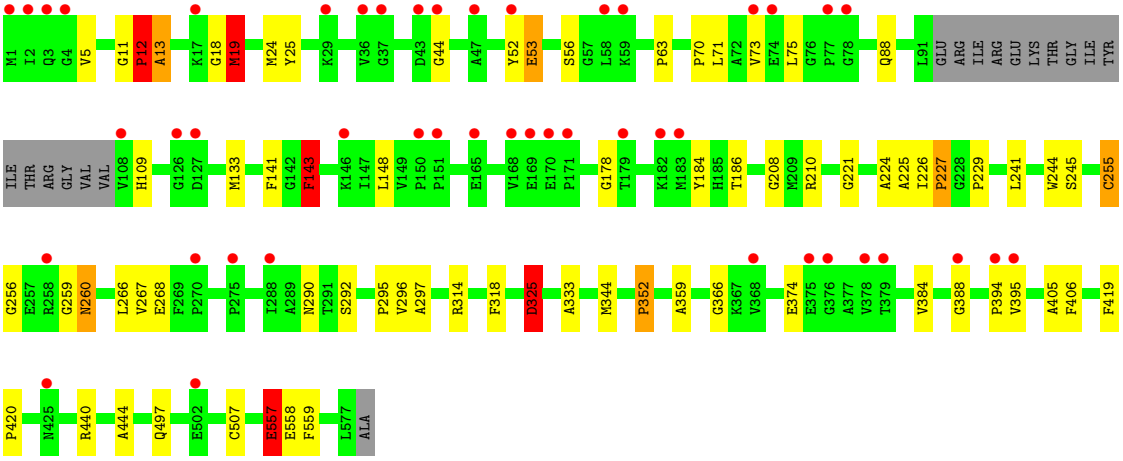
Chain B:



• Molecule 1: V-type ATP synthase alpha chain

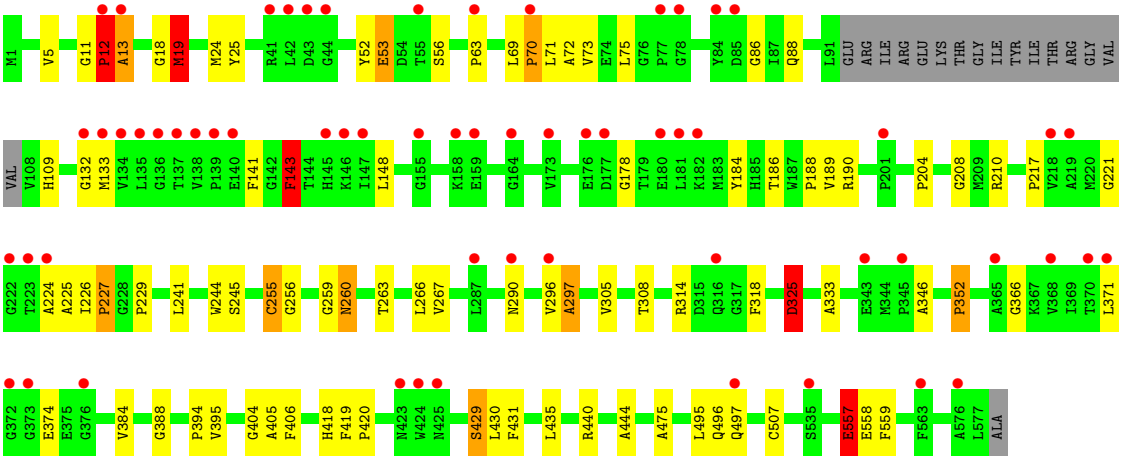
Chain C:





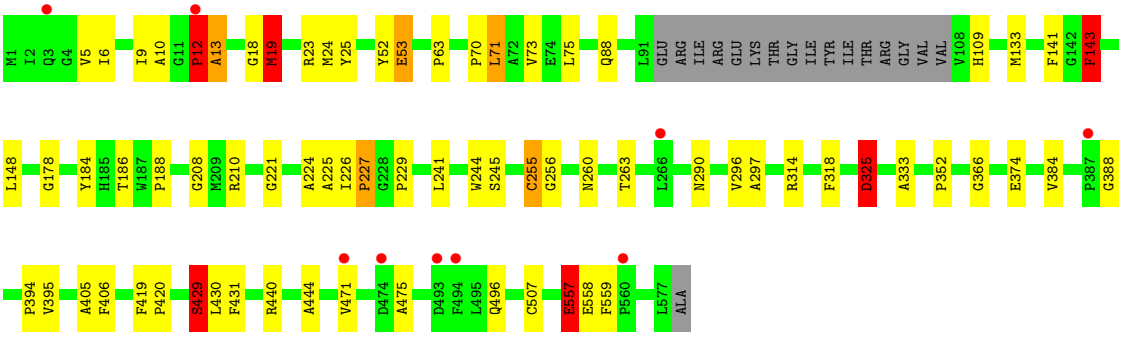
• Molecule 1: V-type ATP synthase alpha chain

Chain I:



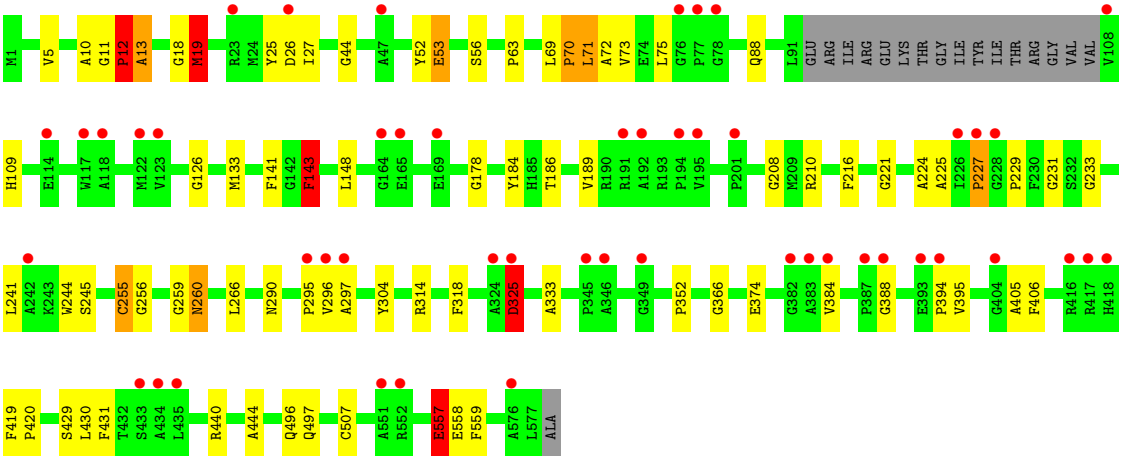
• Molecule 1: V-type ATP synthase alpha chain

Chain J:



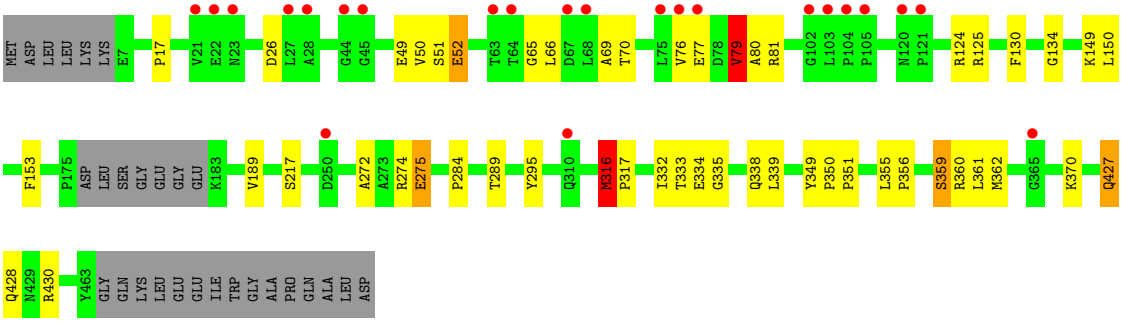
• Molecule 1: V-type ATP synthase alpha chain

Chain K:



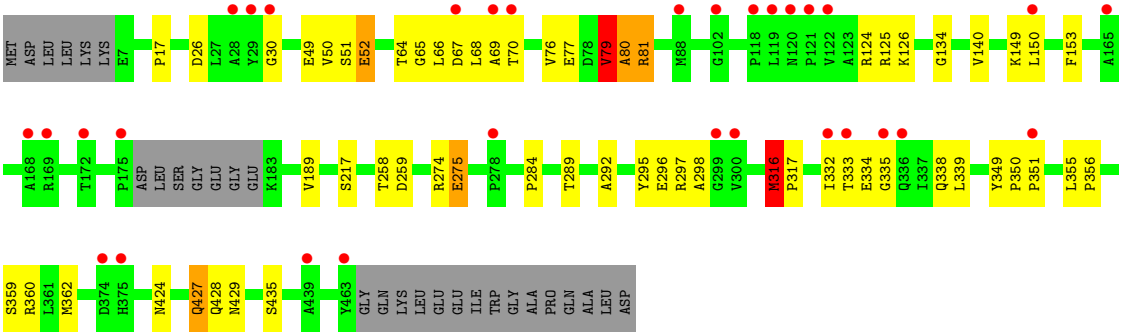
• Molecule 2: V-type ATP synthase beta chain

Chain D:



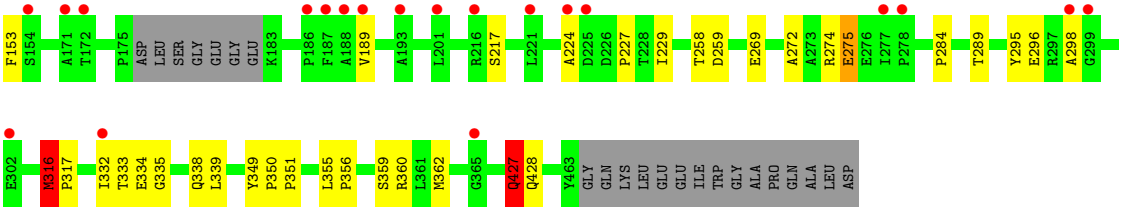
• Molecule 2: V-type ATP synthase beta chain

Chain E:



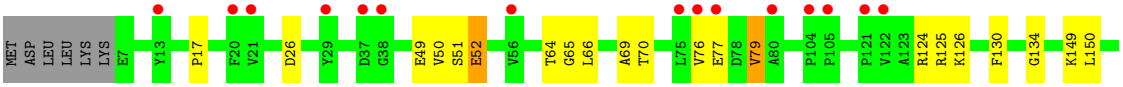
• Molecule 2: V-type ATP synthase beta chain

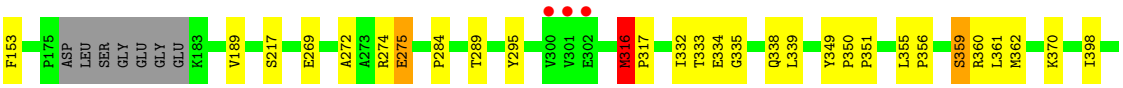
Chain F:

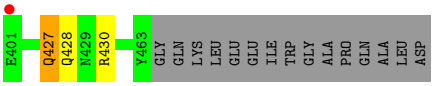


• Molecule 2: V-type ATP synthase beta chain

Chain L:

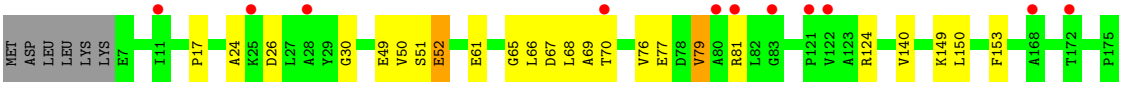


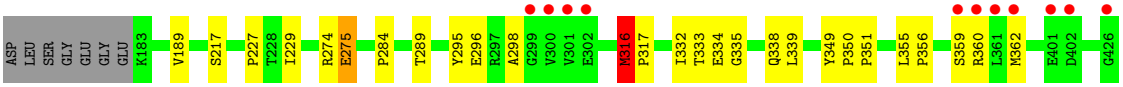




• Molecule 2: V-type ATP synthase beta chain

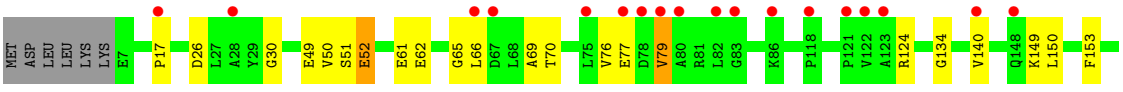
Chain M:

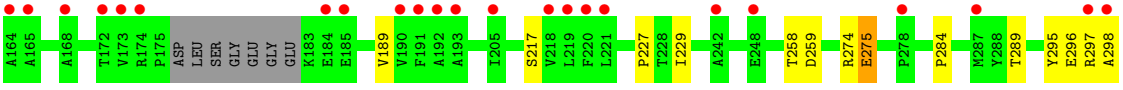


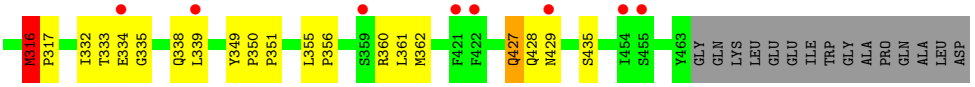


• Molecule 2: V-type ATP synthase beta chain

Chain N:

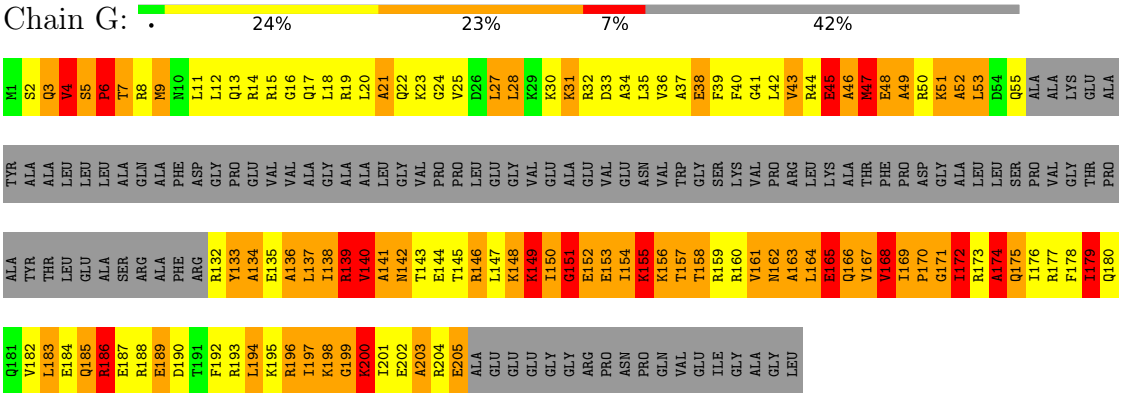






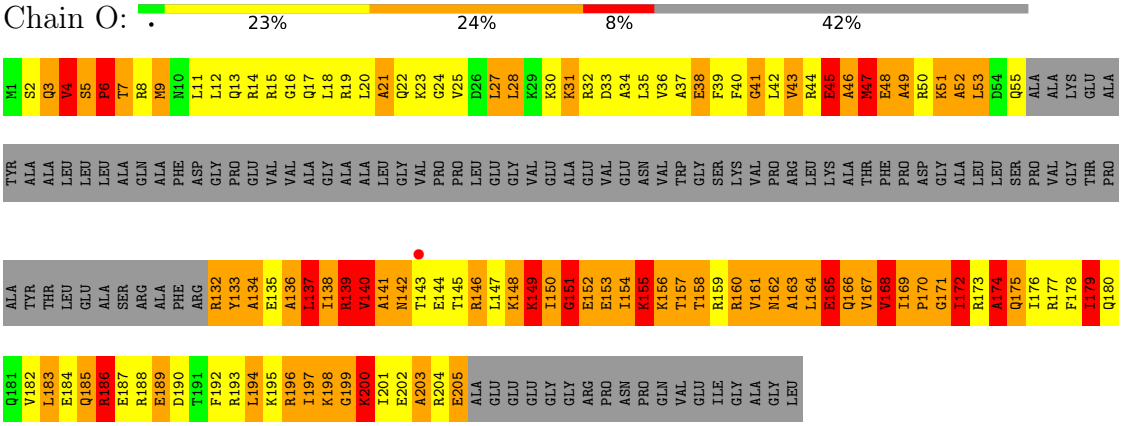
• Molecule 3: V-type ATP synthase subunit D

Chain G:



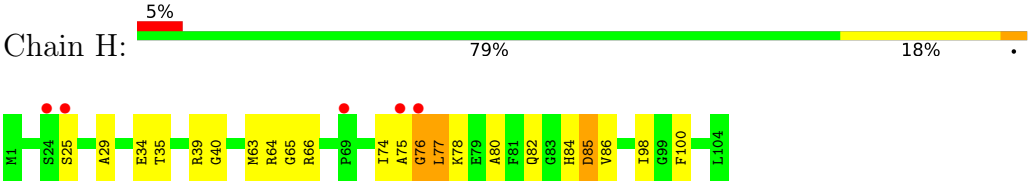
• Molecule 3: V-type ATP synthase subunit D

Chain O:



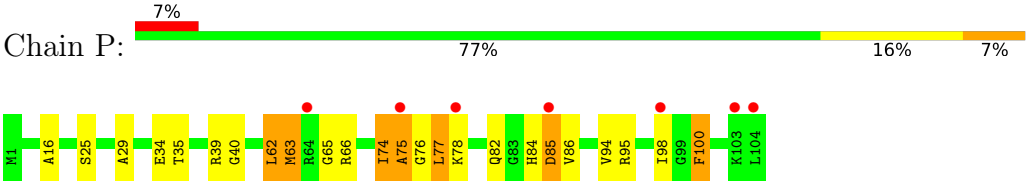
• Molecule 4: V-type ATP synthase subunit F

Chain H:



• Molecule 4: V-type ATP synthase subunit F

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	381.58Å 381.58Å 147.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.92 – 4.51 49.81 – 4.51	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.92-4.51) 96.8 (49.81-4.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 4.45Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.429 , 0.437 0.409 , 0.418	Depositor DCC
R_{free} test set	3589 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	145.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.01 , -10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.28$, $< L^2 > = 0.13$	Xtriage
Estimated twinning fraction	0.217 for -h,-k,l	Xtriage
F_o,F_c correlation	0.69	EDS
Total number of atoms	32188	wwPDB-VP
Average B, all atoms (Å^2)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ADP

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	0.59	3/2750 (0.1%)	1.20	9/3815 (0.2%)
1	B	0.59	3/2750 (0.1%)	1.21	12/3815 (0.3%)
1	C	0.59	3/2750 (0.1%)	1.20	10/3815 (0.3%)
1	I	0.59	3/2750 (0.1%)	1.38	13/3815 (0.3%)
1	J	0.59	3/2750 (0.1%)	1.21	11/3815 (0.3%)
1	K	0.60	3/2750 (0.1%)	1.34	13/3815 (0.3%)
2	D	0.80	7/2210 (0.3%)	1.03	13/3068 (0.4%)
2	E	0.85	7/2210 (0.3%)	1.04	10/3068 (0.3%)
2	F	0.73	3/2210 (0.1%)	0.99	7/3068 (0.2%)
2	L	0.74	3/2210 (0.1%)	1.01	9/3068 (0.3%)
2	M	0.75	3/2210 (0.1%)	1.00	8/3068 (0.3%)
2	N	0.73	3/2210 (0.1%)	0.99	7/3068 (0.2%)
3	G	4.09	122/637 (19.2%)	2.62	48/885 (5.4%)
3	O	4.09	126/637 (19.8%)	2.63	50/885 (5.6%)
4	H	1.48	6/508 (1.2%)	1.43	9/703 (1.3%)
4	P	1.78	10/508 (2.0%)	2.16	15/703 (2.1%)
All	All	1.08	308/32050 (1.0%)	1.27	244/44474 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	5
1	C	0	5
1	I	0	6
1	J	0	6
1	K	0	6
2	D	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	4
2	F	0	3
2	L	0	4
2	M	0	3
2	N	0	3
4	H	0	3
4	P	0	2
All	All	0	60

All (308) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	47	MET	CA-CB	-25.00	0.98	1.53
3	G	47	MET	CA-CB	-24.93	0.99	1.53
3	O	27	LEU	CA-CB	14.81	1.87	1.53
3	G	27	LEU	CA-CB	14.78	1.87	1.53
4	P	75	ALA	N-CA	13.48	1.73	1.46
3	O	7	THR	CA-CB	12.79	1.86	1.53
3	G	7	THR	CA-CB	12.64	1.86	1.53
3	O	31	LYS	N-CA	12.38	1.71	1.46
3	G	31	LYS	N-CA	12.15	1.70	1.46
3	G	196	ARG	CA-C	12.11	1.84	1.52
3	G	138	ILE	CA-CB	-12.09	1.27	1.54
3	O	138	ILE	CA-CB	-12.06	1.27	1.54
3	O	196	ARG	CA-C	12.06	1.84	1.52
4	P	76	GLY	CA-C	11.97	1.71	1.51
3	O	205	GLU	CA-CB	11.22	1.78	1.53
3	O	52	ALA	CA-CB	11.20	1.75	1.52
3	G	52	ALA	CA-CB	11.16	1.75	1.52
3	G	168	VAL	CA-CB	-11.09	1.31	1.54
3	G	16	GLY	CA-C	11.05	1.69	1.51
3	O	16	GLY	CA-C	11.05	1.69	1.51
4	P	75	ALA	CA-C	11.02	1.81	1.52
3	O	168	VAL	CA-CB	-11.01	1.31	1.54
3	G	205	GLU	CA-CB	10.98	1.78	1.53
3	G	167	VAL	CA-C	10.92	1.81	1.52
3	O	167	VAL	CA-C	10.87	1.81	1.52
2	E	81	ARG	N-CA	10.68	1.67	1.46
4	H	34	GLU	C-O	10.58	1.43	1.23
3	O	171	GLY	CA-C	10.58	1.68	1.51
4	P	34	GLU	C-O	10.56	1.43	1.23
3	G	171	GLY	CA-C	10.52	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	16	GLY	C-O	10.30	1.40	1.23
3	G	189	GLU	CA-CB	10.27	1.76	1.53
3	O	189	GLU	CA-CB	10.16	1.76	1.53
3	G	16	GLY	C-O	9.98	1.39	1.23
2	E	80	ALA	CA-C	9.83	1.78	1.52
3	O	4	VAL	CA-C	9.79	1.78	1.52
4	P	76	GLY	N-CA	9.77	1.60	1.46
3	G	4	VAL	CA-C	9.76	1.78	1.52
2	E	80	ALA	N-CA	9.63	1.65	1.46
2	E	81	ARG	CA-C	9.58	1.77	1.52
3	O	19	ARG	N-CA	9.50	1.65	1.46
3	G	19	ARG	N-CA	9.48	1.65	1.46
3	O	50	ARG	C-O	9.25	1.41	1.23
3	G	32	ARG	C-O	9.14	1.40	1.23
3	O	32	ARG	C-O	9.14	1.40	1.23
3	G	164	LEU	C-O	9.13	1.40	1.23
3	O	164	LEU	C-O	9.08	1.40	1.23
3	G	50	ARG	C-O	9.07	1.40	1.23
3	G	184	GLU	CA-CB	9.05	1.73	1.53
3	O	184	GLU	CA-CB	9.05	1.73	1.53
3	O	163	ALA	C-O	8.95	1.40	1.23
3	G	184	GLU	N-CA	8.95	1.64	1.46
3	G	6	PRO	C-O	8.93	1.41	1.23
3	O	184	GLU	N-CA	8.92	1.64	1.46
3	G	163	ALA	C-O	8.87	1.40	1.23
3	O	169	ILE	C-O	8.76	1.40	1.23
3	G	169	ILE	C-O	8.71	1.40	1.23
3	O	6	PRO	C-O	8.69	1.40	1.23
3	O	142	ASN	CA-CB	8.65	1.75	1.53
3	G	142	ASN	CA-CB	8.62	1.75	1.53
3	G	183	LEU	C-O	8.62	1.39	1.23
3	G	194	LEU	CA-C	8.56	1.75	1.52
3	O	183	LEU	C-O	8.54	1.39	1.23
3	O	194	LEU	CA-C	8.47	1.75	1.52
3	G	163	ALA	CA-C	8.46	1.75	1.52
3	O	38	GLU	N-CA	8.39	1.63	1.46
3	O	163	ALA	CA-C	8.36	1.74	1.52
3	G	38	GLU	N-CA	8.33	1.63	1.46
3	G	182	VAL	N-CA	8.28	1.62	1.46
3	O	182	VAL	N-CA	8.26	1.62	1.46
2	D	81	ARG	N-CA	8.25	1.62	1.46
4	P	40	GLY	C-O	8.24	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	40	GLY	C-O	8.09	1.36	1.23
3	O	155	LYS	N-CA	8.04	1.62	1.46
3	O	34	ALA	CA-CB	-8.03	1.35	1.52
3	G	34	ALA	CA-CB	-8.01	1.35	1.52
3	G	155	LYS	N-CA	8.00	1.62	1.46
3	G	195	LYS	N-CA	7.95	1.62	1.46
3	O	185	GLN	C-O	7.89	1.38	1.23
3	O	205	GLU	CA-C	7.89	1.73	1.52
3	O	195	LYS	N-CA	7.88	1.62	1.46
3	O	170	PRO	CA-C	7.88	1.68	1.52
3	G	185	GLN	C-O	7.83	1.38	1.23
3	G	205	GLU	CA-C	7.82	1.73	1.52
3	G	24	GLY	CA-C	7.72	1.64	1.51
3	G	170	PRO	CA-C	7.71	1.68	1.52
3	O	198	LYS	C-O	7.70	1.38	1.23
3	G	198	LYS	C-O	7.67	1.38	1.23
3	G	46	ALA	C-O	7.62	1.37	1.23
3	G	192	PHE	C-O	7.60	1.37	1.23
3	O	24	GLY	CA-C	7.57	1.64	1.51
2	D	80	ALA	CA-C	7.57	1.72	1.52
3	O	192	PHE	C-O	7.56	1.37	1.23
3	O	46	ALA	C-O	7.54	1.37	1.23
3	O	51	LYS	C-O	7.48	1.37	1.23
3	G	134	ALA	CA-CB	7.44	1.68	1.52
3	O	4	VAL	CA-CB	7.43	1.70	1.54
3	G	4	VAL	CA-CB	7.41	1.70	1.54
3	G	33	ASP	N-CA	7.39	1.61	1.46
3	O	33	ASP	N-CA	7.39	1.61	1.46
3	O	134	ALA	N-CA	7.37	1.61	1.46
3	O	134	ALA	CA-CB	7.36	1.67	1.52
3	G	51	LYS	C-O	7.33	1.37	1.23
3	G	134	ALA	N-CA	7.31	1.60	1.46
3	O	146	ARG	CA-CB	7.30	1.70	1.53
3	G	6	PRO	CA-CB	7.28	1.68	1.53
3	G	167	VAL	CA-CB	7.28	1.70	1.54
3	G	22	GLN	C-O	7.27	1.37	1.23
3	G	146	ARG	CA-CB	7.26	1.70	1.53
3	O	53	LEU	N-CA	7.24	1.60	1.46
3	O	22	GLN	C-O	7.22	1.37	1.23
3	O	20	LEU	CA-C	7.20	1.71	1.52
3	G	20	LEU	CA-C	7.20	1.71	1.52
3	O	167	VAL	CA-CB	7.14	1.69	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	6	PRO	CA-CB	7.14	1.67	1.53
3	O	172	ILE	N-CA	7.14	1.60	1.46
3	G	193	ARG	N-CA	7.13	1.60	1.46
3	O	193	ARG	N-CA	7.11	1.60	1.46
3	G	172	ILE	N-CA	7.09	1.60	1.46
3	G	53	LEU	N-CA	7.08	1.60	1.46
3	O	27	LEU	N-CA	7.08	1.60	1.46
3	G	188	ARG	N-CA	7.06	1.60	1.46
3	G	154	ILE	C-O	7.04	1.36	1.23
2	D	81	ARG	CA-C	7.03	1.71	1.52
3	G	27	LEU	N-CA	7.02	1.60	1.46
3	O	52	ALA	N-CA	7.02	1.60	1.46
3	O	188	ARG	N-CA	7.01	1.60	1.46
3	G	199	GLY	N-CA	6.96	1.56	1.46
3	G	179	ILE	C-O	6.95	1.36	1.23
3	G	4	VAL	C-O	6.95	1.36	1.23
3	O	11	LEU	CA-CB	6.94	1.69	1.53
3	G	52	ALA	N-CA	6.93	1.60	1.46
3	G	156	LYS	CA-C	6.92	1.71	1.52
3	G	32	ARG	CA-C	6.91	1.71	1.52
3	G	11	LEU	CA-CB	6.91	1.69	1.53
3	O	179	ILE	C-O	6.88	1.36	1.23
3	O	156	LYS	CA-C	6.88	1.70	1.52
3	O	32	ARG	CA-C	6.87	1.70	1.52
3	O	4	VAL	C-O	6.84	1.36	1.23
3	O	154	ILE	C-O	6.80	1.36	1.23
3	O	199	GLY	N-CA	6.71	1.56	1.46
4	P	75	ALA	C-N	6.69	1.45	1.33
3	O	169	ILE	N-CA	6.62	1.59	1.46
2	D	80	ALA	N-CA	6.61	1.59	1.46
3	G	204	ARG	N-CA	6.60	1.59	1.46
3	O	175	GLN	CA-CB	-6.60	1.39	1.53
3	G	5	SER	CA-CB	6.58	1.62	1.52
3	G	17	GLN	CA-CB	-6.57	1.39	1.53
3	O	204	ARG	N-CA	6.56	1.59	1.46
3	G	169	ILE	N-CA	6.54	1.59	1.46
3	O	32	ARG	C-N	6.53	1.49	1.34
3	G	189	GLU	CA-C	6.49	1.69	1.52
3	G	32	ARG	C-N	6.48	1.49	1.34
3	G	175	GLN	CA-CB	-6.47	1.39	1.53
3	O	17	GLN	CA-CB	-6.47	1.39	1.53
3	G	148	LYS	CA-CB	6.46	1.68	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	148	LYS	CA-CB	6.43	1.68	1.53
3	G	14	ARG	N-CA	6.42	1.59	1.46
3	O	189	GLU	CA-C	6.41	1.69	1.52
3	O	9	MET	CA-C	-6.39	1.36	1.52
3	O	5	SER	CA-CB	6.38	1.62	1.52
3	O	31	LYS	C-O	6.35	1.35	1.23
3	O	196	ARG	CA-CB	6.34	1.68	1.53
3	G	28	LEU	CA-C	6.33	1.69	1.52
3	G	14	ARG	C-O	6.32	1.35	1.23
3	G	196	ARG	CA-CB	6.31	1.67	1.53
3	O	14	ARG	C-O	6.29	1.35	1.23
3	G	9	MET	CA-C	-6.28	1.36	1.52
4	H	40	GLY	C-N	6.22	1.44	1.33
3	O	14	ARG	N-CA	6.20	1.58	1.46
3	O	28	LEU	CA-C	6.19	1.69	1.52
3	O	192	PHE	CA-C	6.19	1.69	1.52
3	G	31	LYS	C-O	6.18	1.35	1.23
3	O	24	GLY	C-O	6.17	1.33	1.23
3	G	192	PHE	CA-C	6.16	1.69	1.52
4	P	40	GLY	C-N	6.14	1.44	1.33
3	O	45	GLU	C-O	6.11	1.34	1.23
1	J	13	ALA	CA-CB	-6.09	1.39	1.52
1	B	13	ALA	CA-CB	-6.08	1.39	1.52
3	G	164	LEU	N-CA	6.08	1.58	1.46
1	K	13	ALA	CA-CB	-6.07	1.39	1.52
1	C	13	ALA	CA-CB	-6.05	1.39	1.52
3	O	164	LEU	N-CA	6.03	1.58	1.46
3	O	201	ILE	CA-CB	-6.03	1.41	1.54
1	A	13	ALA	CA-CB	-6.02	1.39	1.52
3	O	203	ALA	N-CA	-6.01	1.34	1.46
3	G	205	GLU	C-O	6.01	1.34	1.23
3	G	201	ILE	CA-CB	-6.00	1.41	1.54
1	I	13	ALA	CA-CB	-6.00	1.39	1.52
3	G	45	GLU	C-O	6.00	1.34	1.23
3	O	194	LEU	C-O	6.00	1.34	1.23
3	G	194	LEU	C-O	5.98	1.34	1.23
3	O	205	GLU	C-O	5.98	1.34	1.23
3	G	7	THR	CA-C	5.96	1.68	1.52
3	G	166	GLN	CA-CB	-5.95	1.40	1.53
3	O	7	THR	CA-C	5.95	1.68	1.52
3	O	166	GLN	CA-CB	-5.91	1.41	1.53
3	G	24	GLY	C-O	5.86	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	203	ALA	N-CA	-5.80	1.34	1.46
3	G	21	ALA	C-O	5.80	1.34	1.23
3	O	14	ARG	CA-CB	5.79	1.66	1.53
3	G	37	ALA	CA-CB	-5.79	1.40	1.52
3	O	141	ALA	CA-CB	5.75	1.64	1.52
3	G	23	LYS	N-CA	5.72	1.57	1.46
3	O	23	LYS	N-CA	5.72	1.57	1.46
3	G	52	ALA	C-O	5.70	1.34	1.23
3	G	170	PRO	N-CA	5.70	1.56	1.47
3	O	21	ALA	C-O	5.69	1.34	1.23
3	O	52	ALA	C-O	5.69	1.34	1.23
3	G	49	ALA	N-CA	5.66	1.57	1.46
2	L	275	GLU	CA-CB	-5.65	1.41	1.53
3	O	37	ALA	CA-CB	-5.64	1.40	1.52
2	N	275	GLU	CA-CB	-5.64	1.41	1.53
4	H	25	SER	CA-CB	5.62	1.61	1.52
3	G	49	ALA	CA-CB	-5.62	1.40	1.52
3	O	170	PRO	N-CA	5.61	1.56	1.47
3	G	141	ALA	CA-CB	5.60	1.64	1.52
3	O	47	MET	C-O	5.59	1.33	1.23
3	G	47	MET	C-O	5.59	1.33	1.23
2	M	275	GLU	CA-CB	-5.59	1.41	1.53
3	G	14	ARG	CA-CB	5.58	1.66	1.53
3	G	158	THR	CA-CB	-5.58	1.38	1.53
2	F	275	GLU	CA-CB	-5.57	1.41	1.53
2	E	275	GLU	CA-CB	-5.56	1.41	1.53
3	G	15	ARG	CA-CB	5.56	1.66	1.53
3	G	25	VAL	N-CA	5.55	1.57	1.46
3	O	25	VAL	N-CA	5.54	1.57	1.46
3	O	158	THR	CA-CB	-5.54	1.39	1.53
3	O	171	GLY	C-O	5.53	1.32	1.23
3	G	148	LYS	N-CA	5.52	1.57	1.46
3	O	49	ALA	N-CA	5.52	1.57	1.46
3	O	148	LYS	N-CA	5.51	1.57	1.46
3	O	15	ARG	CA-CB	5.51	1.66	1.53
2	L	289	THR	C-N	5.51	1.46	1.34
4	P	25	SER	CA-CB	5.48	1.61	1.52
3	G	171	GLY	C-O	5.48	1.32	1.23
2	D	275	GLU	CA-CB	-5.47	1.42	1.53
3	O	187	GLU	CA-C	5.47	1.67	1.52
3	G	36	VAL	CA-C	5.46	1.67	1.52
3	O	49	ALA	CA-CB	-5.46	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	7	THR	C-O	5.44	1.33	1.23
3	G	187	GLU	CA-C	5.43	1.67	1.52
3	G	163	ALA	C-N	5.43	1.46	1.34
3	O	163	ALA	C-N	5.43	1.46	1.34
2	L	316	MET	C-N	-5.42	1.24	1.34
2	E	316	MET	C-N	-5.42	1.24	1.34
3	O	7	THR	C-O	5.42	1.33	1.23
3	O	36	VAL	CA-C	5.39	1.67	1.52
1	J	19	MET	CA-CB	-5.38	1.42	1.53
2	N	316	MET	C-N	-5.38	1.24	1.34
1	K	19	MET	CA-CB	-5.36	1.42	1.53
2	M	289	THR	C-N	5.36	1.46	1.34
1	I	19	MET	CA-CB	-5.35	1.42	1.53
3	O	28	LEU	C-O	5.35	1.33	1.23
1	C	19	MET	CA-CB	-5.34	1.42	1.53
1	I	352	PRO	CA-CB	-5.33	1.42	1.53
2	M	316	MET	C-N	-5.33	1.24	1.34
1	J	352	PRO	CA-CB	-5.32	1.43	1.53
2	N	289	THR	C-N	5.32	1.46	1.34
2	E	289	THR	C-N	5.31	1.46	1.34
2	F	289	THR	C-N	5.31	1.46	1.34
1	A	19	MET	CA-CB	-5.30	1.42	1.53
1	B	19	MET	CA-CB	-5.30	1.42	1.53
2	D	289	THR	C-N	5.30	1.46	1.34
3	G	15	ARG	C-O	5.29	1.33	1.23
4	H	75	ALA	N-CA	5.29	1.56	1.46
2	F	316	MET	C-N	-5.26	1.24	1.34
3	O	7	THR	N-CA	5.26	1.56	1.46
1	B	352	PRO	CA-CB	-5.25	1.43	1.53
3	G	28	LEU	C-O	5.25	1.33	1.23
1	K	352	PRO	CA-CB	-5.25	1.43	1.53
4	P	29	ALA	CA-CB	-5.24	1.41	1.52
1	A	352	PRO	CA-CB	-5.23	1.43	1.53
3	G	7	THR	N-CA	5.22	1.56	1.46
3	O	196	ARG	C-O	5.21	1.33	1.23
3	G	153	GLU	N-CA	5.21	1.56	1.46
3	O	138	ILE	CA-C	-5.20	1.39	1.52
3	O	49	ALA	CA-C	-5.19	1.39	1.52
3	G	162	ASN	C-O	5.19	1.33	1.23
4	H	29	ALA	CA-CB	-5.19	1.41	1.52
3	G	200	LYS	CA-C	5.17	1.66	1.52
3	O	153	GLU	N-CA	5.17	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	143	THR	N-CA	5.17	1.56	1.46
3	G	201	ILE	C-O	5.17	1.33	1.23
3	G	49	ALA	CA-C	-5.16	1.39	1.52
3	G	196	ARG	C-O	5.16	1.33	1.23
3	G	36	VAL	C-O	5.15	1.33	1.23
3	G	37	ALA	C-O	5.15	1.33	1.23
3	O	201	ILE	C-O	5.13	1.33	1.23
3	O	15	ARG	C-O	5.13	1.33	1.23
2	D	316	MET	C-N	-5.13	1.24	1.34
3	O	143	THR	N-CA	5.12	1.56	1.46
3	G	165	GLU	C-O	5.12	1.33	1.23
3	G	139	ARG	CA-CB	5.12	1.65	1.53
3	O	36	VAL	CA-CB	5.12	1.65	1.54
3	O	162	ASN	C-O	5.12	1.33	1.23
3	G	22	GLN	C-N	5.11	1.45	1.34
3	O	165	GLU	C-O	5.10	1.33	1.23
3	O	200	LYS	CA-C	5.08	1.66	1.52
3	O	165	GLU	N-CA	5.08	1.56	1.46
3	G	138	ILE	CA-C	-5.06	1.39	1.52
1	C	352	PRO	CA-CB	-5.05	1.43	1.53
3	O	160	ARG	C-O	5.04	1.32	1.23
3	O	22	GLN	C-N	5.04	1.45	1.34
3	O	132	ARG	C-O	5.04	1.32	1.23
3	O	37	ALA	C-O	5.03	1.32	1.23
3	O	36	VAL	C-O	5.03	1.32	1.23
3	O	41	GLY	C-O	5.00	1.31	1.23

All (244) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	325	ASP	O-C-N	-39.90	58.86	122.70
1	J	325	ASP	O-C-N	-39.89	58.87	122.70
1	C	325	ASP	O-C-N	-39.89	58.87	122.70
1	A	325	ASP	O-C-N	-39.88	58.89	122.70
1	K	325	ASP	O-C-N	-39.85	58.94	122.70
1	B	325	ASP	O-C-N	-39.85	58.95	122.70
1	K	70	PRO	C-N-CA	-27.45	53.06	121.70
4	P	76	GLY	N-CA-C	26.75	179.98	113.10
1	I	429	SER	O-C-N	25.71	163.84	122.70
1	I	429	SER	CA-C-N	-25.54	61.02	117.20
1	I	429	SER	C-N-CA	-21.28	68.49	121.70
1	K	70	PRO	CA-C-N	-19.68	73.90	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	74	ILE	O-C-N	-18.90	92.46	122.70
1	C	325	ASP	C-N-CA	-18.30	75.94	121.70
1	A	325	ASP	C-N-CA	-18.27	76.03	121.70
1	K	325	ASP	C-N-CA	-18.24	76.09	121.70
1	B	325	ASP	C-N-CA	-18.22	76.15	121.70
1	J	325	ASP	C-N-CA	-18.21	76.16	121.70
1	I	325	ASP	C-N-CA	-18.17	76.27	121.70
2	D	316	MET	O-C-N	-15.68	91.31	121.10
2	L	316	MET	O-C-N	-15.62	91.42	121.10
2	E	316	MET	O-C-N	-15.62	91.42	121.10
2	F	316	MET	O-C-N	-15.60	91.47	121.10
2	N	316	MET	O-C-N	-15.55	91.55	121.10
2	M	316	MET	O-C-N	-15.55	91.56	121.10
1	I	325	ASP	CA-C-N	15.11	150.44	117.20
1	B	325	ASP	CA-C-N	15.10	150.42	117.20
1	J	325	ASP	CA-C-N	15.07	150.36	117.20
1	A	325	ASP	CA-C-N	15.01	150.22	117.20
1	K	325	ASP	CA-C-N	15.00	150.20	117.20
1	C	325	ASP	CA-C-N	14.99	150.17	117.20
4	P	76	GLY	CA-C-N	14.65	149.44	117.20
1	K	70	PRO	O-C-N	13.39	144.13	122.70
4	H	77	LEU	C-N-CA	-13.22	88.66	121.70
4	P	74	ILE	CA-C-N	12.92	145.62	117.20
4	P	75	ALA	N-CA-C	12.21	143.98	111.00
4	P	77	LEU	C-N-CA	-11.86	92.06	121.70
4	P	76	GLY	CA-C-O	-11.47	99.96	120.60
3	O	47	MET	N-CA-C	10.66	139.78	111.00
3	G	47	MET	N-CA-C	10.63	139.70	111.00
3	O	139	ARG	N-CA-C	-10.47	82.73	111.00
3	G	139	ARG	N-CA-C	-10.45	82.78	111.00
4	P	76	GLY	C-N-CA	10.11	146.97	121.70
3	O	6	PRO	C-N-CA	-9.82	97.15	121.70
3	G	6	PRO	C-N-CA	-9.73	97.38	121.70
3	G	6	PRO	N-CA-CB	9.70	114.94	103.30
2	D	316	MET	CA-C-N	9.48	143.66	117.10
2	F	316	MET	CA-C-N	9.45	143.57	117.10
2	L	316	MET	CA-C-N	9.45	143.57	117.10
2	N	316	MET	CA-C-N	9.46	143.57	117.10
2	M	316	MET	CA-C-N	9.45	143.55	117.10
3	O	6	PRO	N-CA-CB	9.45	114.64	103.30
2	E	79	VAL	O-C-N	-9.44	107.59	122.70
2	E	316	MET	CA-C-N	9.44	143.53	117.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	9	MET	C-N-CA	-9.37	98.27	121.70
3	G	9	MET	C-N-CA	-9.36	98.31	121.70
1	J	429	SER	O-C-N	-9.29	107.84	122.70
3	O	49	ALA	C-N-CA	-9.14	98.84	121.70
4	P	75	ALA	C-N-CA	9.12	141.44	122.30
3	G	49	ALA	C-N-CA	-9.11	98.92	121.70
4	P	77	LEU	CA-C-N	8.73	136.40	117.20
1	I	63	PRO	N-CA-CB	8.72	113.76	103.30
1	C	63	PRO	N-CA-CB	8.68	113.71	103.30
1	K	63	PRO	N-CA-CB	8.64	113.67	103.30
1	B	63	PRO	N-CA-CB	8.60	113.62	103.30
3	G	47	MET	C-N-CA	-8.57	100.27	121.70
3	O	47	MET	C-N-CA	-8.57	100.28	121.70
1	A	63	PRO	N-CA-CB	8.55	113.56	103.30
1	J	63	PRO	N-CA-CB	8.55	113.56	103.30
3	G	187	GLU	N-CA-C	8.43	133.77	111.00
3	O	187	GLU	N-CA-C	8.36	133.58	111.00
3	G	31	LYS	CA-C-N	-8.29	98.97	117.20
3	O	31	LYS	CA-C-N	-8.27	99.00	117.20
1	B	429	SER	O-C-N	8.27	135.93	122.70
4	H	74	ILE	O-C-N	-8.23	109.53	122.70
2	E	81	ARG	N-CA-C	8.18	133.09	111.00
4	P	76	GLY	O-C-N	-8.06	109.81	122.70
4	H	76	GLY	C-N-CA	8.02	141.74	121.70
3	O	186	ARG	C-N-CA	-7.85	102.08	121.70
3	O	203	ALA	N-CA-C	-7.81	89.91	111.00
3	G	203	ALA	N-CA-C	-7.79	89.96	111.00
4	H	75	ALA	N-CA-C	7.75	131.93	111.00
3	G	186	ARG	C-N-CA	-7.65	102.56	121.70
3	G	167	VAL	O-C-N	-7.49	110.72	122.70
3	O	167	VAL	O-C-N	-7.47	110.74	122.70
4	H	77	LEU	CA-C-N	7.45	133.59	117.20
4	P	63	MET	N-CA-C	7.37	130.90	111.00
3	G	31	LYS	O-C-N	7.32	134.40	122.70
3	O	31	LYS	O-C-N	7.30	134.37	122.70
3	G	167	VAL	C-N-CA	-7.27	103.53	121.70
3	O	167	VAL	C-N-CA	-7.27	103.53	121.70
2	L	289	THR	O-C-N	-7.24	111.11	122.70
3	G	7	THR	C-N-CA	-7.20	103.71	121.70
2	D	289	THR	O-C-N	-7.18	111.21	122.70
2	E	289	THR	O-C-N	-7.18	111.22	122.70
2	M	289	THR	O-C-N	-7.15	111.27	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	289	THR	O-C-N	-7.14	111.27	122.70
3	O	7	THR	C-N-CA	-7.14	103.85	121.70
2	E	80	ALA	N-CA-C	7.10	130.17	111.00
3	O	170	PRO	N-CA-CB	7.10	111.82	103.30
3	O	30	LYS	C-N-CA	7.09	139.44	121.70
2	F	289	THR	O-C-N	-7.09	111.35	122.70
3	O	133	TYR	N-CA-C	-7.09	91.85	111.00
3	G	153	GLU	N-CA-C	7.09	130.14	111.00
3	G	30	LYS	C-N-CA	7.09	139.41	121.70
3	G	133	TYR	N-CA-C	-7.06	91.95	111.00
3	O	157	THR	N-CA-C	-7.01	92.07	111.00
3	O	153	GLU	N-CA-C	7.01	129.91	111.00
3	G	157	THR	N-CA-C	-6.99	92.12	111.00
3	G	170	PRO	N-CA-CB	6.99	111.69	103.30
3	G	202	GLU	CA-C-N	-6.97	101.87	117.20
3	O	182	VAL	O-C-N	6.97	133.85	122.70
4	P	77	LEU	O-C-N	-6.93	111.61	122.70
3	O	156	LYS	N-CA-C	6.90	129.63	111.00
3	O	202	GLU	CA-C-N	-6.90	102.03	117.20
3	G	151	GLY	N-CA-C	-6.89	95.88	113.10
3	G	156	LYS	N-CA-C	6.88	129.58	111.00
3	O	151	GLY	N-CA-C	-6.83	96.02	113.10
3	G	182	VAL	O-C-N	6.79	133.56	122.70
1	C	12	PRO	N-CA-CB	6.75	111.39	103.30
3	G	167	VAL	CA-C-N	6.73	132.01	117.20
3	G	12	LEU	N-CA-C	-6.70	92.92	111.00
3	O	167	VAL	CA-C-N	6.69	131.91	117.20
1	K	12	PRO	N-CA-CB	6.67	111.30	103.30
3	O	12	LEU	N-CA-C	-6.66	93.02	111.00
1	A	12	PRO	N-CA-CB	6.60	111.22	103.30
1	J	12	PRO	N-CA-CB	6.59	111.21	103.30
1	B	12	PRO	N-CA-CB	6.59	111.21	103.30
1	I	12	PRO	N-CA-CB	6.55	111.16	103.30
3	G	49	ALA	CA-C-N	-6.51	102.87	117.20
3	O	49	ALA	CA-C-N	-6.51	102.88	117.20
4	H	76	GLY	CA-C-N	6.50	131.49	117.20
3	G	154	ILE	N-CA-C	-6.47	93.52	111.00
2	D	289	THR	CA-C-N	6.47	131.44	117.20
2	E	289	THR	CA-C-N	6.47	131.43	117.20
3	G	156	LYS	C-N-CA	-6.46	105.54	121.70
3	O	156	LYS	C-N-CA	-6.45	105.58	121.70
3	O	154	ILE	N-CA-C	-6.44	93.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	143	PHE	N-CA-C	6.44	128.38	111.00
3	G	196	ARG	CB-CA-C	6.43	123.27	110.40
2	L	289	THR	CA-C-N	6.42	131.33	117.20
2	N	289	THR	CA-C-N	6.42	131.32	117.20
3	O	196	ARG	N-CA-CB	-6.40	99.08	110.60
1	C	143	PHE	N-CA-C	6.39	128.25	111.00
3	G	196	ARG	N-CA-CB	-6.39	99.10	110.60
1	J	143	PHE	N-CA-C	6.38	128.24	111.00
1	C	229	PRO	N-CA-CB	6.38	110.96	103.30
3	O	196	ARG	CB-CA-C	6.38	123.17	110.40
1	K	143	PHE	N-CA-C	6.38	128.21	111.00
1	B	143	PHE	N-CA-C	6.37	128.20	111.00
2	M	289	THR	CA-C-N	6.37	131.21	117.20
2	D	81	ARG	N-CA-C	6.35	128.15	111.00
2	F	289	THR	CA-C-N	6.34	131.14	117.20
1	B	429	SER	CA-C-N	-6.32	103.31	117.20
1	I	229	PRO	N-CA-CB	6.31	110.87	103.30
1	A	143	PHE	N-CA-C	6.29	127.97	111.00
1	B	229	PRO	N-CA-CB	6.28	110.84	103.30
3	G	199	GLY	N-CA-C	-6.27	97.42	113.10
1	J	229	PRO	N-CA-CB	6.26	110.82	103.30
3	O	199	GLY	N-CA-C	-6.25	97.47	113.10
1	K	229	PRO	N-CA-CB	6.23	110.77	103.30
2	L	360	ARG	N-CA-C	-6.16	94.36	111.00
3	O	21	ALA	O-C-N	6.14	132.53	122.70
1	A	229	PRO	N-CA-CB	6.09	110.61	103.30
3	G	21	ALA	O-C-N	6.06	132.40	122.70
2	D	17	PRO	N-CA-CB	6.00	110.50	103.30
2	F	17	PRO	N-CA-CB	5.99	110.49	103.30
2	E	17	PRO	N-CA-CB	5.99	110.49	103.30
3	G	194	LEU	N-CA-C	5.97	127.12	111.00
3	O	149	LYS	N-CA-C	-5.93	94.98	111.00
3	O	194	LEU	N-CA-C	5.93	127.02	111.00
2	L	284	PRO	N-CA-CB	5.92	110.40	103.30
2	N	351	PRO	N-CA-CB	5.92	110.40	103.30
2	L	17	PRO	N-CA-CB	5.91	110.39	103.30
2	D	284	PRO	N-CA-CB	5.90	110.38	103.30
2	N	284	PRO	N-CA-CB	5.90	110.38	103.30
2	N	17	PRO	N-CA-CB	5.89	110.37	103.30
2	M	351	PRO	N-CA-CB	5.89	110.36	103.30
3	G	149	LYS	N-CA-C	-5.87	95.15	111.00
2	E	284	PRO	N-CA-CB	5.87	110.34	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	17	PRO	N-CA-CB	5.86	110.33	103.30
3	G	188	ARG	N-CA-CB	5.85	121.13	110.60
2	D	351	PRO	N-CA-CB	5.84	110.31	103.30
2	D	79	VAL	CA-C-N	-5.83	104.37	117.20
2	M	284	PRO	N-CA-CB	5.82	110.29	103.30
3	O	21	ALA	CB-CA-C	-5.79	101.42	110.10
1	J	557	GLU	O-C-N	-5.78	113.45	122.70
2	F	284	PRO	N-CA-CB	5.77	110.23	103.30
2	L	351	PRO	N-CA-CB	5.77	110.22	103.30
3	O	136	ALA	N-CA-C	-5.76	95.45	111.00
1	C	557	GLU	O-C-N	-5.76	113.49	122.70
3	O	188	ARG	N-CA-CB	5.74	120.93	110.60
2	F	351	PRO	N-CA-CB	5.73	110.18	103.30
1	B	557	GLU	O-C-N	-5.73	113.54	122.70
1	A	557	GLU	O-C-N	-5.72	113.54	122.70
2	E	351	PRO	N-CA-CB	5.72	110.17	103.30
3	G	21	ALA	CB-CA-C	-5.72	101.52	110.10
1	I	557	GLU	O-C-N	-5.71	113.56	122.70
1	C	70	PRO	N-CA-C	-5.71	97.26	112.10
1	K	557	GLU	O-C-N	-5.69	113.60	122.70
3	G	47	MET	N-CA-CB	-5.69	100.36	110.60
3	O	47	MET	N-CA-CB	-5.67	100.40	110.60
3	G	142	ASN	N-CA-C	-5.66	95.71	111.00
3	G	136	ALA	N-CA-C	-5.64	95.77	111.00
1	B	429	SER	C-N-CA	-5.64	107.60	121.70
1	C	244	TRP	N-CA-C	5.63	126.21	111.00
1	K	244	TRP	N-CA-C	5.63	126.19	111.00
1	J	244	TRP	N-CA-C	5.62	126.17	111.00
1	I	244	TRP	N-CA-C	5.61	126.15	111.00
1	A	244	TRP	N-CA-C	5.61	126.13	111.00
1	B	244	TRP	N-CA-C	5.60	126.12	111.00
3	O	142	ASN	N-CA-C	-5.58	95.94	111.00
2	D	79	VAL	O-C-N	-5.57	113.79	122.70
3	G	47	MET	CA-C-O	5.45	131.55	120.10
1	J	429	SER	CA-C-N	5.44	129.17	117.20
4	H	76	GLY	CA-C-O	-5.43	110.83	120.60
3	G	174	ALA	C-N-CA	-5.42	108.14	121.70
2	L	359	SER	N-CA-C	-5.41	96.40	111.00
4	P	35	THR	CB-CA-C	-5.40	97.01	111.60
4	H	74	ILE	CA-C-N	5.40	129.08	117.20
4	H	35	THR	CB-CA-C	-5.40	97.03	111.60
2	D	360	ARG	N-CA-C	-5.38	96.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	155	LYS	C-N-CA	-5.37	108.27	121.70
3	O	174	ALA	C-N-CA	-5.37	108.27	121.70
3	O	140	VAL	N-CA-C	5.37	125.49	111.00
3	O	47	MET	CA-C-O	5.36	131.36	120.10
3	G	155	LYS	C-N-CA	-5.34	108.36	121.70
3	G	140	VAL	N-CA-C	5.33	125.38	111.00
1	I	70	PRO	N-CA-C	-5.28	98.37	112.10
3	O	171	GLY	N-CA-C	-5.22	100.04	113.10
3	G	31	LYS	CB-CA-C	-5.20	100.00	110.40
1	K	430	LEU	N-CA-C	-5.19	97.00	111.00
3	O	31	LYS	CB-CA-C	-5.18	100.03	110.40
2	D	80	ALA	N-CA-C	5.16	124.92	111.00
3	G	171	GLY	N-CA-C	-5.14	100.25	113.10
3	O	137	LEU	O-C-N	-5.13	114.48	122.70
3	O	156	LYS	CA-C-N	5.09	128.40	117.20
3	G	156	LYS	CA-C-N	5.09	128.39	117.20
2	M	81	ARG	N-CA-C	5.07	124.69	111.00
3	O	21	ALA	CA-C-N	-5.06	106.06	117.20
2	D	359	SER	N-CA-C	-5.05	97.35	111.00
3	G	21	ALA	CA-C-N	-5.04	106.11	117.20
3	O	47	MET	CB-CA-C	-5.03	100.35	110.40
4	P	62	LEU	C-N-CA	-5.02	109.16	121.70

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLY	Peptide
1	A	210	ARG	Mainchain
1	A	297	ALA	Mainchain
1	A	325	ASP	Mainchain
1	A	557	GLU	Mainchain
1	A	69	LEU	Peptide
1	B	178	GLY	Peptide
1	B	210	ARG	Mainchain
1	B	297	ALA	Mainchain
1	B	325	ASP	Mainchain
1	B	557	GLU	Mainchain
1	C	178	GLY	Peptide
1	C	210	ARG	Mainchain
1	C	297	ALA	Mainchain
1	C	325	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	C	557	GLU	Mainchain
2	D	316	MET	Mainchain
2	D	427	GLN	Peptide
2	D	79	VAL	Mainchain,Peptide
2	E	316	MET	Mainchain
2	E	427	GLN	Peptide
2	E	79	VAL	Mainchain,Peptide
2	F	316	MET	Mainchain
2	F	427	GLN	Peptide
2	F	79	VAL	Mainchain
4	H	39	ARG	Peptide
4	H	76	GLY	Peptide
4	H	82	GLN	Peptide
1	I	178	GLY	Peptide
1	I	210	ARG	Mainchain
1	I	297	ALA	Mainchain
1	I	325	ASP	Mainchain
1	I	557	GLU	Mainchain
1	I	69	LEU	Peptide
1	J	178	GLY	Peptide
1	J	210	ARG	Mainchain
1	J	297	ALA	Mainchain
1	J	325	ASP	Mainchain
1	J	429	SER	Mainchain
1	J	557	GLU	Mainchain
1	K	178	GLY	Peptide
1	K	210	ARG	Mainchain
1	K	297	ALA	Mainchain
1	K	325	ASP	Mainchain
1	K	557	GLU	Mainchain
1	K	70	PRO	Mainchain
2	L	316	MET	Mainchain
2	L	427	GLN	Peptide
2	L	79	VAL	Mainchain,Peptide
2	M	316	MET	Mainchain
2	M	427	GLN	Peptide
2	M	79	VAL	Mainchain
2	N	316	MET	Mainchain
2	N	427	GLN	Peptide
2	N	79	VAL	Mainchain
4	P	39	ARG	Peptide
4	P	82	GLN	Peptide

5.2 Too-close contacts (i)

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	2752	0	1302	92	0
1	B	2752	0	1303	65	0
1	C	2752	0	1303	100	0
1	I	2752	0	1300	122	0
1	J	2752	0	1303	61	2
1	K	2752	0	1302	94	0
2	D	2212	0	1009	66	0
2	E	2212	0	1008	80	0
2	F	2212	0	1009	94	0
2	L	2212	0	1009	80	0
2	M	2212	0	1009	59	2
2	N	2212	0	1009	76	0
3	G	639	0	299	131	0
3	O	639	0	299	136	0
4	H	509	0	255	12	0
4	P	509	0	255	23	0
5	A	27	0	12	2	0
5	C	27	0	12	1	0
5	I	27	0	12	0	0
5	K	27	0	12	5	0
All	All	32188	0	15022	1021	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 22.

All (1021) 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)
3:O:142:ASN:CB	3:O:142:ASN:CA	1.75	1.65
3:O:189:GLU:CB	3:O:189:GLU:CA	1.76	1.64
3:G:205:GLU:CB	3:G:205:GLU:CA	1.78	1.62
3:O:52:ALA:CB	3:O:52:ALA:CA	1.76	1.59
3:G:189:GLU:CA	3:G:189:GLU:CB	1.76	1.58
1:C:352:PRO:CB	2:F:269:GLU:CA	1.80	1.58
3:O:205:GLU:CA	3:O:205:GLU:CB	1.78	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:475:ALA:HB1	4:P:100:PHE:CB	1.33	1.57
3:G:52:ALA:CB	3:G:52:ALA:CA	1.75	1.57
1:I:71:LEU:CB	1:I:188:PRO:HA	1.09	1.56
3:O:163:ALA:C	3:O:163:ALA:CA	1.74	1.55
3:G:163:ALA:C	3:G:163:ALA:CA	1.74	1.55
2:E:81:ARG:CA	2:E:81:ARG:N	1.67	1.54
3:G:7:THR:CB	3:G:7:THR:CA	1.86	1.54
3:G:142:ASN:CB	3:G:142:ASN:CA	1.75	1.54
1:K:52:TYR:HA	1:K:295:PRO:CB	1.08	1.54
3:O:31:LYS:N	3:O:31:LYS:CA	1.71	1.53
2:E:81:ARG:CA	2:E:81:ARG:C	1.77	1.53
1:I:24:MET:HA	2:L:66:LEU:CA	1.38	1.53
3:G:194:LEU:C	3:G:194:LEU:CA	1.75	1.52
1:K:52:TYR:CA	1:K:295:PRO:CB	1.85	1.51
2:N:140:VAL:CB	2:N:435:SER:CB	1.84	1.51
3:O:7:THR:CA	3:O:7:THR:CB	1.86	1.51
3:O:27:LEU:CB	3:O:27:LEU:CA	1.87	1.51
3:O:4:VAL:C	3:O:4:VAL:CA	1.78	1.51
3:O:194:LEU:C	3:O:194:LEU:CA	1.75	1.51
3:G:27:LEU:CA	3:G:27:LEU:CB	1.87	1.50
3:G:31:LYS:N	3:G:31:LYS:CA	1.70	1.50
2:E:80:ALA:C	2:E:80:ALA:CA	1.78	1.50
1:I:267:VAL:N	2:N:124:ARG:CB	1.70	1.49
3:G:4:VAL:C	3:G:4:VAL:CA	1.78	1.49
3:G:167:VAL:C	3:G:167:VAL:CA	1.81	1.49
1:C:344:MET:CB	2:F:272:ALA:HB1	1.42	1.49
3:O:167:VAL:C	3:O:167:VAL:CA	1.81	1.49
4:P:75:ALA:C	4:P:75:ALA:CA	1.81	1.49
4:P:75:ALA:CA	4:P:75:ALA:N	1.73	1.47
1:C:352:PRO:CB	2:F:269:GLU:HA	1.00	1.46
1:C:25:TYR:CB	2:F:65:GLY:HA2	1.42	1.46
3:O:196:ARG:CA	3:O:196:ARG:C	1.84	1.46
1:I:25:TYR:N	2:L:66:LEU:H	0.97	1.44
1:B:471:VAL:CB	4:H:98:ILE:CB	1.95	1.43
3:G:196:ARG:C	3:G:196:ARG:CA	1.84	1.42
1:I:24:MET:CA	2:L:66:LEU:HA	1.48	1.42
1:I:25:TYR:H	2:L:66:LEU:N	1.16	1.40
2:E:359:SER:CB	2:E:362:MET:CB	1.99	1.40
1:J:475:ALA:CB	4:P:100:PHE:CB	1.99	1.38
1:I:11:GLY:CA	2:N:50:VAL:H	1.36	1.36
1:I:266:LEU:C	2:N:124:ARG:CB	1.93	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:44:ARG:O	3:G:47:MET:CB	1.71	1.36
4:P:75:ALA:HB3	4:P:85:ASP:CB	1.53	1.35
1:C:11:GLY:HA3	2:E:50:VAL:N	1.38	1.34
3:O:44:ARG:O	3:O:47:MET:CB	1.72	1.34
1:J:9:ILE:CB	2:L:50:VAL:O	1.75	1.34
1:I:71:LEU:CB	1:I:188:PRO:CA	2.05	1.33
1:A:266:LEU:CB	2:F:124:ARG:CB	2.08	1.31
1:K:259:GLY:N	2:M:296:GLU:CA	1.83	1.31
1:B:25:TYR:O	2:E:65:GLY:HA2	1.15	1.29
1:K:69:LEU:CB	1:K:72:ALA:HB3	1.61	1.29
1:C:11:GLY:CA	2:E:50:VAL:H	1.45	1.28
1:C:344:MET:CB	2:F:272:ALA:CB	2.11	1.27
1:I:259:GLY:O	2:N:296:GLU:C	1.73	1.27
1:C:25:TYR:N	2:F:66:LEU:H	1.33	1.27
1:K:44:GLY:HA2	2:N:69:ALA:CB	1.64	1.27
2:F:427:GLN:CB	1:K:126:GLY:HA3	1.66	1.26
1:I:11:GLY:HA3	2:N:50:VAL:CA	1.63	1.26
1:I:224:ALA:CB	1:I:405:ALA:HB3	1.65	1.25
1:C:224:ALA:CB	1:C:405:ALA:HB3	1.65	1.25
4:H:84:HIS:O	4:H:86:VAL:N	1.67	1.25
1:J:224:ALA:CB	1:J:405:ALA:HB3	1.65	1.25
1:J:419:PHE:O	1:J:496:GLN:HA	1.25	1.25
1:B:224:ALA:CB	1:B:405:ALA:HB3	1.65	1.24
2:N:360:ARG:O	2:N:362:MET:N	1.70	1.24
1:C:25:TYR:H	2:F:66:LEU:N	1.30	1.24
1:I:11:GLY:HA3	2:N:50:VAL:C	1.58	1.24
1:A:224:ALA:CB	1:A:405:ALA:HB3	1.65	1.24
1:K:224:ALA:CB	1:K:405:ALA:HB3	1.66	1.23
1:B:25:TYR:O	2:E:65:GLY:CA	1.87	1.22
1:B:419:PHE:O	1:B:496:GLN:HA	1.37	1.22
1:I:11:GLY:CA	2:N:50:VAL:N	2.00	1.22
4:P:74:ILE:O	4:P:75:ALA:HA	1.35	1.21
1:C:44:GLY:HA2	2:F:69:ALA:CB	1.69	1.21
4:P:75:ALA:CB	4:P:85:ASP:CB	2.18	1.20
1:A:11:GLY:CA	2:F:50:VAL:H	1.56	1.19
2:N:61:GLU:O	2:N:227:PRO:CB	1.90	1.18
1:A:11:GLY:HA3	2:F:50:VAL:O	1.42	1.17
1:I:11:GLY:HA3	2:N:50:VAL:N	1.60	1.16
1:I:11:GLY:HA3	2:N:50:VAL:O	1.47	1.15
1:K:44:GLY:HA2	2:N:69:ALA:HB3	1.15	1.15
1:C:208:GLY:HA2	1:C:507:CYS:O	1.46	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:25:TYR:N	2:L:66:LEU:N	1.76	1.13
4:P:84:HIS:O	4:P:86:VAL:N	1.81	1.13
1:J:263:THR:CB	2:L:125:ARG:C	2.15	1.12
1:A:11:GLY:HA2	2:F:50:VAL:H	1.02	1.12
1:K:266:LEU:CB	2:M:124:ARG:CB	2.26	1.12
1:B:10:ALA:H	2:D:50:VAL:CB	1.62	1.11
1:K:69:LEU:CB	1:K:72:ALA:CB	2.27	1.11
1:A:11:GLY:HA3	2:F:50:VAL:C	1.72	1.11
1:I:24:MET:C	2:L:66:LEU:H	1.53	1.10
1:I:259:GLY:C	2:N:296:GLU:C	2.05	1.10
1:J:419:PHE:O	1:J:496:GLN:CA	1.99	1.09
1:I:266:LEU:CB	2:N:124:ARG:CB	2.30	1.09
1:J:24:MET:HA	2:M:67:ASP:O	1.52	1.09
2:L:334:GLU:O	2:L:361:LEU:N	1.86	1.08
2:D:149:LYS:O	2:D:334:GLU:N	1.87	1.07
1:A:259:GLY:N	2:F:296:GLU:HA	1.59	1.07
1:C:24:MET:HA	2:F:66:LEU:HA	1.32	1.07
1:K:10:ALA:O	2:M:50:VAL:CB	2.03	1.07
2:F:149:LYS:O	2:F:334:GLU:N	1.87	1.06
3:O:176:ILE:O	3:O:179:ILE:CB	2.03	1.06
3:G:176:ILE:O	3:G:179:ILE:CB	2.03	1.06
2:L:149:LYS:O	2:L:334:GLU:N	1.87	1.06
2:N:149:LYS:O	2:N:334:GLU:N	1.87	1.06
1:C:344:MET:CB	2:F:272:ALA:CA	2.32	1.06
2:E:149:LYS:O	2:E:334:GLU:N	1.87	1.06
1:I:24:MET:CA	2:L:66:LEU:CA	2.18	1.06
1:B:10:ALA:O	2:D:50:VAL:N	1.89	1.06
1:K:52:TYR:CB	1:K:295:PRO:CB	2.34	1.06
1:B:9:ILE:CB	2:D:50:VAL:O	2.04	1.05
2:M:149:LYS:O	2:M:334:GLU:N	1.87	1.05
1:C:208:GLY:O	1:C:507:CYS:CB	2.04	1.04
2:F:61:GLU:O	2:F:227:PRO:CB	2.06	1.03
1:K:259:GLY:O	2:M:296:GLU:C	1.96	1.03
1:K:259:GLY:O	2:M:296:GLU:O	1.74	1.03
1:A:259:GLY:N	2:F:296:GLU:CA	2.17	1.03
1:I:11:GLY:HA2	2:N:50:VAL:N	1.67	1.03
1:C:12:PRO:N	2:E:49:GLU:CB	2.22	1.02
1:C:224:ALA:HB1	1:C:405:ALA:HB3	1.41	1.02
1:A:224:ALA:HB1	1:A:405:ALA:HB3	1.41	1.01
1:C:52:TYR:CB	1:C:295:PRO:CB	2.38	1.01
1:I:224:ALA:HB1	1:I:405:ALA:HB3	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLY:CA	2:F:50:VAL:N	2.22	1.01
1:C:25:TYR:CB	2:F:65:GLY:CA	2.38	1.01
1:A:352:PRO:CB	2:D:272:ALA:HB3	1.90	1.01
1:K:44:GLY:CA	2:N:69:ALA:CB	2.38	1.01
1:A:11:GLY:HA3	2:F:50:VAL:CA	1.89	1.01
1:I:11:GLY:CA	2:N:50:VAL:O	2.07	1.01
1:K:224:ALA:HB1	1:K:405:ALA:HB3	1.42	1.00
1:K:208:GLY:O	1:K:507:CYS:O	1.79	1.00
3:O:7:THR:O	3:O:8:ARG:C	1.98	0.99
1:C:352:PRO:CB	2:F:269:GLU:CB	2.39	0.99
1:B:224:ALA:HB2	1:B:405:ALA:HB3	1.45	0.99
1:J:224:ALA:HB1	1:J:405:ALA:HB3	1.41	0.99
1:K:259:GLY:N	2:M:296:GLU:HA	1.36	0.99
1:I:24:MET:CA	2:L:66:LEU:N	2.25	0.98
1:A:11:GLY:HA3	2:F:50:VAL:N	1.78	0.98
1:B:11:GLY:HA3	2:D:49:GLU:HA	1.45	0.98
1:I:267:VAL:N	2:N:124:ARG:CA	2.22	0.98
1:C:292:SER:CB	2:E:292:ALA:HB3	1.93	0.98
1:I:25:TYR:O	2:L:65:GLY:HA2	1.62	0.98
2:N:360:ARG:C	2:N:362:MET:H	1.67	0.98
1:A:259:GLY:H	2:F:296:GLU:CA	1.75	0.97
1:B:224:ALA:HB1	1:B:405:ALA:HB3	1.42	0.97
2:D:134:GLY:HA2	2:D:430:ARG:O	1.61	0.97
3:G:199:GLY:O	3:G:203:ALA:HB2	1.63	0.97
3:G:7:THR:O	3:G:8:ARG:C	1.98	0.97
1:C:224:ALA:HB2	1:C:405:ALA:HB3	1.45	0.97
1:K:25:TYR:CB	2:N:65:GLY:HA2	1.94	0.97
1:I:224:ALA:HB2	1:I:405:ALA:HB3	1.45	0.96
3:G:199:GLY:C	3:G:203:ALA:HB2	1.86	0.96
2:L:334:GLU:CB	2:L:361:LEU:CB	2.44	0.96
2:F:149:LYS:O	2:F:333:THR:HA	1.66	0.96
1:A:224:ALA:HB2	1:A:405:ALA:HB3	1.46	0.96
2:F:427:GLN:CB	1:K:126:GLY:CA	2.43	0.96
1:I:259:GLY:O	2:N:296:GLU:O	1.82	0.96
1:J:224:ALA:HB2	1:J:405:ALA:HB3	1.45	0.96
3:O:199:GLY:O	3:O:203:ALA:HB2	1.63	0.96
2:L:150:LEU:HA	2:L:335:GLY:O	1.66	0.96
1:I:11:GLY:HA2	2:N:50:VAL:H	0.81	0.96
1:A:11:GLY:CA	2:F:50:VAL:O	2.13	0.95
1:C:259:GLY:H	2:E:296:GLU:N	1.64	0.95
1:B:11:GLY:HA3	2:D:49:GLU:CB	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:224:ALA:HB2	1:K:405:ALA:HB3	1.46	0.95
2:F:150:LEU:HA	2:F:335:GLY:O	1.66	0.95
3:G:148:LYS:O	3:G:152:GLU:CB	2.15	0.95
2:D:150:LEU:HA	2:D:335:GLY:O	1.67	0.95
2:N:150:LEU:HA	2:N:335:GLY:O	1.67	0.94
1:C:259:GLY:N	2:E:296:GLU:N	1.86	0.94
2:N:149:LYS:O	2:N:333:THR:HA	1.66	0.94
3:O:47:MET:O	3:O:49:ALA:N	2.00	0.94
2:M:150:LEU:HA	2:M:335:GLY:O	1.67	0.94
3:O:199:GLY:C	3:O:203:ALA:HB2	1.86	0.94
1:K:259:GLY:H	2:M:296:GLU:CA	1.51	0.94
2:L:149:LYS:O	2:L:333:THR:HA	1.66	0.94
2:E:150:LEU:HA	2:E:335:GLY:O	1.66	0.94
1:K:11:GLY:HA3	2:M:50:VAL:H	1.31	0.94
2:D:149:LYS:O	2:D:333:THR:HA	1.66	0.94
1:C:266:LEU:CB	2:E:124:ARG:HA	1.97	0.93
3:O:148:LYS:O	3:O:152:GLU:CB	2.15	0.93
3:G:47:MET:O	3:G:49:ALA:N	2.00	0.93
1:I:70:PRO:CB	1:I:190:ARG:CB	2.46	0.93
2:N:149:LYS:O	2:N:333:THR:CA	2.16	0.93
3:O:135:GLU:C	3:O:137:LEU:N	2.17	0.93
2:E:149:LYS:O	2:E:333:THR:HA	1.66	0.93
2:L:149:LYS:O	2:L:333:THR:CA	2.17	0.93
1:I:11:GLY:CA	2:N:50:VAL:CA	2.45	0.93
1:C:44:GLY:HA2	2:F:69:ALA:HB1	1.50	0.93
2:D:149:LYS:O	2:D:333:THR:CA	2.16	0.93
2:F:149:LYS:O	2:F:333:THR:CA	2.16	0.93
2:M:149:LYS:O	2:M:333:THR:HA	1.66	0.93
1:I:25:TYR:O	2:L:65:GLY:CA	2.17	0.93
2:E:149:LYS:O	2:E:333:THR:CA	2.17	0.92
1:B:11:GLY:HA3	2:D:49:GLU:CA	1.98	0.92
3:O:48:GLU:O	3:O:51:LYS:CB	2.18	0.92
3:G:48:GLU:O	3:G:51:LYS:CB	2.18	0.92
1:I:267:VAL:H	2:N:124:ARG:CA	1.83	0.92
2:M:149:LYS:O	2:M:333:THR:CA	2.17	0.92
1:I:260:ASN:CB	2:N:298:ALA:O	2.19	0.91
1:C:208:GLY:CA	1:C:507:CYS:O	2.19	0.91
1:B:263:THR:CB	2:D:124:ARG:C	2.39	0.90
3:G:49:ALA:O	3:G:52:ALA:HB3	1.72	0.90
1:I:25:TYR:CA	2:L:65:GLY:HA2	2.02	0.90
3:O:141:ALA:O	3:O:145:THR:CB	2.20	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:419:PHE:CB	1:I:497:GLN:O	2.20	0.89
1:J:263:THR:CB	2:L:125:ARG:CA	2.51	0.89
5:C:600:ADP:O3'	2:E:360:ARG:HA	1.73	0.88
3:O:49:ALA:O	3:O:52:ALA:HB3	1.72	0.88
1:I:25:TYR:CB	2:L:64:THR:O	2.21	0.88
3:G:141:ALA:O	3:G:145:THR:CB	2.21	0.88
3:O:51:LYS:CB	3:O:136:ALA:HB1	2.04	0.88
1:J:24:MET:CB	2:M:66:LEU:HA	2.03	0.88
2:F:295:TYR:CB	2:F:332:ILE:CB	2.52	0.87
1:K:259:GLY:C	2:M:296:GLU:C	2.33	0.87
1:C:11:GLY:HA3	2:E:50:VAL:H	0.86	0.87
2:M:295:TYR:CB	2:M:332:ILE:CB	2.52	0.87
2:N:295:TYR:CB	2:N:332:ILE:CB	2.53	0.87
1:I:419:PHE:N	1:I:496:GLN:HA	1.89	0.87
3:G:135:GLU:C	3:G:137:LEU:N	2.17	0.87
2:D:295:TYR:CB	2:D:332:ILE:CB	2.53	0.86
2:L:295:TYR:CB	2:L:332:ILE:CB	2.53	0.86
2:L:153:PHE:O	2:L:339:LEU:N	2.08	0.86
4:P:74:ILE:O	4:P:75:ALA:CA	2.19	0.86
2:L:150:LEU:CA	2:L:335:GLY:O	2.24	0.86
2:F:153:PHE:O	2:F:339:LEU:N	2.09	0.86
3:G:47:MET:O	3:G:48:GLU:C	2.09	0.86
1:I:217:PRO:O	1:I:431:PHE:CB	2.24	0.86
1:A:11:GLY:HA2	2:F:50:VAL:N	1.87	0.86
2:M:153:PHE:O	2:M:339:LEU:N	2.09	0.86
3:G:174:ALA:O	3:G:175:GLN:C	2.09	0.85
1:I:12:PRO:N	2:N:49:GLU:CB	2.38	0.85
1:J:263:THR:CB	2:L:125:ARG:N	2.40	0.85
2:E:295:TYR:CB	2:E:332:ILE:CB	2.53	0.85
2:M:150:LEU:CA	2:M:335:GLY:O	2.24	0.85
2:F:150:LEU:CA	2:F:335:GLY:O	2.24	0.85
2:N:153:PHE:O	2:N:339:LEU:N	2.09	0.85
3:O:174:ALA:O	3:O:175:GLN:C	2.09	0.85
3:O:47:MET:O	3:O:48:GLU:C	2.09	0.85
2:E:150:LEU:CA	2:E:335:GLY:O	2.24	0.85
2:D:150:LEU:CA	2:D:335:GLY:O	2.24	0.85
1:I:267:VAL:CA	2:N:124:ARG:CB	2.50	0.84
1:B:25:TYR:C	2:E:65:GLY:HA2	1.97	0.84
3:O:199:GLY:O	3:O:203:ALA:CB	2.25	0.84
2:D:153:PHE:O	2:D:339:LEU:N	2.09	0.84
2:N:150:LEU:CA	2:N:335:GLY:O	2.24	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:352:PRO:CB	2:L:269:GLU:O	2.26	0.84
1:B:419:PHE:O	1:B:496:GLN:CA	2.23	0.84
2:M:140:VAL:CB	2:M:435:SER:CB	2.56	0.83
1:I:25:TYR:CB	2:L:65:GLY:HA2	2.08	0.83
2:D:134:GLY:O	2:D:430:ARG:N	2.11	0.83
2:E:153:PHE:O	2:E:339:LEU:N	2.09	0.83
3:O:158:THR:O	3:O:161:VAL:CB	2.27	0.83
1:B:263:THR:CB	2:D:125:ARG:N	2.42	0.83
1:J:475:ALA:HB3	4:P:100:PHE:CB	2.05	0.83
1:C:344:MET:CB	2:F:272:ALA:HA	2.09	0.82
3:G:158:THR:O	3:G:161:VAL:CB	2.27	0.82
1:B:10:ALA:N	2:D:50:VAL:CB	2.41	0.82
1:C:18:GLY:O	1:C:19:MET:CB	2.28	0.82
3:G:199:GLY:O	3:G:203:ALA:CB	2.26	0.82
1:I:266:LEU:CA	2:N:124:ARG:CB	2.57	0.82
1:A:189:VAL:HA	1:A:308:THR:CB	2.10	0.82
1:I:25:TYR:C	2:L:65:GLY:HA2	1.98	0.82
4:P:75:ALA:C	4:P:75:ALA:HA	1.95	0.82
1:I:18:GLY:O	1:I:19:MET:CB	2.27	0.81
1:K:231:GLY:HA2	5:K:600:ADP:H5'1	1.61	0.81
2:E:81:ARG:N	2:E:81:ARG:HA	1.94	0.81
1:C:292:SER:CB	2:E:292:ALA:CB	2.59	0.80
3:G:167:VAL:O	3:G:168:VAL:C	2.19	0.80
1:K:18:GLY:O	1:K:19:MET:CB	2.27	0.80
1:A:259:GLY:O	2:F:296:GLU:O	1.99	0.80
2:L:134:GLY:HA2	2:L:430:ARG:O	1.81	0.80
3:O:167:VAL:O	3:O:169:ILE:N	2.14	0.80
1:J:18:GLY:O	1:J:19:MET:CB	2.28	0.80
1:K:44:GLY:HA2	2:N:69:ALA:HB2	1.62	0.80
1:J:224:ALA:HB1	1:J:405:ALA:CB	2.12	0.80
1:K:44:GLY:CA	2:N:69:ALA:HB2	2.12	0.80
1:B:18:GLY:O	1:B:19:MET:CB	2.28	0.79
3:G:167:VAL:O	3:G:169:ILE:N	2.14	0.79
2:N:134:GLY:O	2:N:429:ASN:HA	1.82	0.79
1:A:224:ALA:HB1	1:A:405:ALA:CB	2.12	0.79
1:C:224:ALA:HB1	1:C:405:ALA:CB	2.12	0.79
1:B:224:ALA:HB1	1:B:405:ALA:CB	2.12	0.79
3:G:132:ARG:N	3:G:134:ALA:HB3	1.98	0.79
1:I:267:VAL:H	2:N:124:ARG:CB	1.90	0.79
1:K:259:GLY:C	2:M:296:GLU:HA	1.81	0.79
1:I:71:LEU:CB	1:I:72:ALA:HA	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:ALA:HB1	1:I:405:ALA:CB	2.12	0.79
1:K:224:ALA:HB1	1:K:405:ALA:CB	2.13	0.79
1:C:52:TYR:HA	1:C:295:PRO:CB	2.13	0.78
1:C:352:PRO:CB	2:F:269:GLU:C	2.51	0.78
3:O:167:VAL:O	3:O:168:VAL:C	2.19	0.78
3:O:132:ARG:N	3:O:134:ALA:HB3	1.98	0.78
1:A:44:GLY:HA2	2:D:69:ALA:CB	2.13	0.78
1:A:259:GLY:O	2:F:296:GLU:C	2.21	0.78
1:A:18:GLY:O	1:A:19:MET:CB	2.28	0.78
1:A:12:PRO:N	2:F:49:GLU:CB	2.47	0.77
3:G:28:LEU:O	3:G:31:LYS:CB	2.32	0.77
1:A:81:ASN:HA	1:A:282:MET:O	1.84	0.77
3:O:28:LEU:O	3:O:31:LYS:CB	2.32	0.77
2:F:51:SER:O	2:F:52:GLU:CB	2.33	0.77
1:C:224:ALA:CB	1:C:405:ALA:CB	2.58	0.76
2:M:51:SER:O	2:M:52:GLU:CB	2.33	0.76
2:L:51:SER:O	2:L:52:GLU:CB	2.33	0.76
2:D:51:SER:O	2:D:52:GLU:CB	2.33	0.76
1:A:43:ASP:C	2:D:69:ALA:CB	2.54	0.76
1:K:11:GLY:HA3	2:M:50:VAL:N	2.00	0.76
1:K:259:GLY:C	2:M:296:GLU:CA	2.38	0.75
3:G:39:PHE:O	3:G:42:LEU:CB	2.34	0.75
2:N:51:SER:O	2:N:52:GLU:CB	2.33	0.75
1:C:52:TYR:CA	1:C:295:PRO:CB	2.65	0.75
3:O:39:PHE:O	3:O:42:LEU:CB	2.34	0.75
3:O:194:LEU:C	3:O:194:LEU:HA	2.03	0.75
1:I:224:ALA:CB	1:I:405:ALA:CB	2.58	0.75
1:I:259:GLY:O	2:N:297:ARG:N	2.18	0.75
2:E:149:LYS:CB	2:E:332:ILE:O	2.35	0.75
1:I:24:MET:CB	2:L:66:LEU:N	2.49	0.75
4:P:65:GLY:CA	4:P:66:ARG:CB	2.65	0.75
2:E:51:SER:O	2:E:52:GLU:CB	2.33	0.75
2:F:149:LYS:CB	2:F:332:ILE:O	2.35	0.75
2:L:149:LYS:CB	2:L:332:ILE:O	2.35	0.75
1:B:224:ALA:CB	1:B:405:ALA:CB	2.58	0.74
1:C:56:SER:CB	2:E:30:GLY:O	2.35	0.74
3:G:132:ARG:C	3:G:134:ALA:N	2.37	0.74
1:J:419:PHE:O	1:J:496:GLN:CB	2.35	0.74
1:K:52:TYR:C	1:K:295:PRO:CB	2.56	0.74
3:O:140:VAL:O	3:O:144:GLU:CB	2.35	0.74
1:J:263:THR:CB	2:L:125:ARG:O	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:199:GLY:C	3:G:203:ALA:CB	2.56	0.74
1:I:24:MET:CB	2:L:66:LEU:CA	2.65	0.74
3:O:199:GLY:C	3:O:203:ALA:CB	2.56	0.74
2:M:149:LYS:CB	2:M:332:ILE:O	2.35	0.74
3:G:140:VAL:O	3:G:144:GLU:CB	2.35	0.74
3:O:132:ARG:C	3:O:134:ALA:N	2.37	0.73
1:K:69:LEU:CB	1:K:72:ALA:HB2	2.19	0.73
2:N:69:ALA:O	2:N:70:THR:CB	2.36	0.73
1:B:25:TYR:N	2:E:66:LEU:H	1.86	0.73
3:G:142:ASN:O	3:G:146:ARG:CB	2.36	0.73
3:O:142:ASN:O	3:O:146:ARG:CB	2.36	0.73
1:C:11:GLY:HA2	2:E:49:GLU:HA	1.70	0.73
3:G:196:ARG:C	3:G:196:ARG:HA	2.05	0.73
1:I:52:TYR:CB	1:I:297:ALA:HB3	2.19	0.73
2:N:149:LYS:CB	2:N:332:ILE:O	2.35	0.73
4:P:75:ALA:HB2	4:P:85:ASP:CB	2.19	0.73
2:D:149:LYS:CB	2:D:332:ILE:O	2.35	0.73
3:G:45:GLU:O	3:G:46:ALA:C	2.27	0.73
1:I:56:SER:CB	2:N:30:GLY:N	2.52	0.73
3:O:45:GLU:O	3:O:46:ALA:C	2.27	0.73
2:F:69:ALA:O	2:F:70:THR:CB	2.37	0.73
2:L:69:ALA:O	2:L:70:THR:CB	2.36	0.73
1:C:44:GLY:CA	2:F:69:ALA:CB	2.61	0.73
1:C:11:GLY:CA	2:E:50:VAL:N	2.21	0.72
1:A:224:ALA:CB	1:A:405:ALA:CB	2.58	0.72
2:E:69:ALA:O	2:E:70:THR:CB	2.37	0.72
3:G:150:ILE:O	3:G:151:GLY:O	2.08	0.72
3:G:163:ALA:C	3:G:163:ALA:HA	2.04	0.72
3:O:150:ILE:O	3:O:151:GLY:O	2.07	0.72
1:I:11:GLY:CA	2:N:50:VAL:CB	2.65	0.72
1:B:86:GLY:HA2	1:B:302:SER:CB	2.19	0.72
1:C:344:MET:CA	2:F:272:ALA:HB1	2.18	0.72
1:C:267:VAL:O	2:E:125:ARG:HA	1.84	0.72
2:F:359:SER:CB	2:F:362:MET:CB	2.67	0.72
2:D:69:ALA:O	2:D:70:THR:CB	2.36	0.72
2:M:69:ALA:O	2:M:70:THR:CB	2.37	0.72
2:N:65:GLY:O	2:N:66:LEU:CB	2.38	0.71
3:O:135:GLU:O	3:O:136:ALA:C	2.28	0.71
3:G:4:VAL:C	3:G:4:VAL:HA	2.07	0.71
1:B:9:ILE:HA	2:D:50:VAL:CB	2.21	0.71
1:K:259:GLY:H	2:M:296:GLU:CB	2.02	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:196:ARG:C	3:O:196:ARG:HA	2.05	0.71
1:C:260:ASN:CB	2:E:298:ALA:HB3	2.21	0.71
3:G:135:GLU:O	3:G:136:ALA:C	2.28	0.71
4:H:77:LEU:H	4:H:80:ALA:HB3	1.55	0.71
1:B:10:ALA:C	2:D:50:VAL:H	1.94	0.71
1:I:204:PRO:CB	1:I:435:LEU:CB	2.68	0.71
2:L:359:SER:C	2:L:361:LEU:N	2.39	0.71
2:F:65:GLY:O	2:F:66:LEU:CB	2.39	0.70
1:B:11:GLY:CA	2:D:49:GLU:HA	2.20	0.70
2:E:65:GLY:O	2:E:66:LEU:CB	2.38	0.70
1:I:225:ALA:N	1:I:405:ALA:O	2.25	0.70
2:E:81:ARG:C	2:E:81:ARG:HA	2.05	0.70
1:K:44:GLY:CA	2:N:69:ALA:HB3	2.07	0.70
1:I:56:SER:CB	2:N:30:GLY:O	2.40	0.70
2:L:274:ARG:O	2:L:275:GLU:CB	2.37	0.70
2:M:65:GLY:O	2:M:66:LEU:CB	2.38	0.70
1:A:225:ALA:N	1:A:405:ALA:O	2.25	0.70
2:N:61:GLU:HA	2:N:229:ILE:CB	2.22	0.70
1:A:71:LEU:CB	1:A:188:PRO:HA	2.22	0.70
2:F:274:ARG:O	2:F:275:GLU:CB	2.37	0.70
1:A:44:GLY:N	2:D:69:ALA:CB	2.54	0.69
1:K:225:ALA:N	1:K:405:ALA:O	2.25	0.69
2:N:274:ARG:O	2:N:275:GLU:CB	2.37	0.69
2:D:65:GLY:O	2:D:66:LEU:CB	2.38	0.69
1:J:225:ALA:N	1:J:405:ALA:O	2.25	0.69
4:P:75:ALA:C	4:P:75:ALA:CB	2.60	0.69
1:A:44:GLY:HA2	2:D:69:ALA:HB1	1.74	0.69
1:C:225:ALA:N	1:C:405:ALA:O	2.25	0.69
2:F:427:GLN:O	1:K:126:GLY:N	2.25	0.69
1:I:11:GLY:HA3	2:N:50:VAL:CB	2.23	0.69
1:B:225:ALA:N	1:B:405:ALA:O	2.25	0.69
1:J:24:MET:CB	2:M:66:LEU:CA	2.69	0.69
2:E:140:VAL:CB	2:E:435:SER:CB	2.71	0.69
3:O:48:GLU:C	3:O:51:LYS:H	1.97	0.69
1:I:25:TYR:O	2:L:65:GLY:HA3	1.93	0.69
2:L:65:GLY:O	2:L:66:LEU:CB	2.39	0.69
2:M:274:ARG:O	2:M:275:GLU:CB	2.38	0.69
1:A:71:LEU:HA	1:A:188:PRO:HA	1.75	0.68
3:O:31:LYS:N	3:O:31:LYS:HA	2.02	0.68
3:O:197:ILE:O	3:O:200:LYS:CB	2.41	0.68
1:J:224:ALA:CB	1:J:405:ALA:CB	2.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:VAL:CB	1:A:18:GLY:O	2.42	0.68
3:G:197:ILE:O	3:G:200:LYS:CB	2.40	0.68
1:A:352:PRO:CB	2:D:272:ALA:CB	2.70	0.68
3:O:4:VAL:C	3:O:4:VAL:HA	2.07	0.68
1:J:5:VAL:CB	1:J:18:GLY:O	2.42	0.68
1:J:419:PHE:C	1:J:496:GLN:HA	2.13	0.68
1:I:5:VAL:CB	1:I:18:GLY:O	2.42	0.68
1:K:5:VAL:CB	1:K:18:GLY:O	2.42	0.68
1:C:259:GLY:O	2:E:296:GLU:C	2.32	0.68
1:J:10:ALA:O	2:L:49:GLU:HA	1.93	0.68
1:K:224:ALA:CB	1:K:405:ALA:CB	2.58	0.68
1:C:44:GLY:HA2	2:F:69:ALA:HB3	1.70	0.68
1:K:189:VAL:O	1:K:304:TYR:CB	2.42	0.67
1:A:11:GLY:CA	2:F:50:VAL:CA	2.68	0.67
2:E:274:ARG:O	2:E:275:GLU:CB	2.37	0.67
3:G:48:GLU:C	3:G:51:LYS:H	1.97	0.67
1:C:5:VAL:CB	1:C:18:GLY:O	2.42	0.67
1:B:5:VAL:CB	1:B:18:GLY:O	2.42	0.67
1:A:196:GLN:N	1:A:369:ILE:O	2.28	0.67
1:I:419:PHE:H	1:I:496:GLN:HA	1.59	0.67
1:B:24:MET:C	2:E:66:LEU:H	1.96	0.67
1:C:24:MET:CA	2:F:66:LEU:HA	2.18	0.67
3:G:31:LYS:N	3:G:31:LYS:HA	2.02	0.67
3:G:151:GLY:HA2	3:G:155:LYS:CB	2.25	0.67
3:G:194:LEU:C	3:G:194:LEU:HA	2.04	0.66
1:C:44:GLY:HA2	2:F:69:ALA:HB2	1.74	0.66
2:D:274:ARG:O	2:D:275:GLU:CB	2.38	0.66
3:G:3:GLN:O	3:G:5:SER:N	2.29	0.66
3:O:151:GLY:HA2	3:O:155:LYS:CB	2.26	0.66
4:P:74:ILE:C	4:P:75:ALA:CA	2.62	0.66
3:O:141:ALA:HA	3:O:144:GLU:CB	2.26	0.66
1:A:44:GLY:CA	2:D:69:ALA:HB1	2.25	0.66
1:K:27:ILE:HA	1:K:71:LEU:H	1.61	0.66
3:O:3:GLN:O	3:O:5:SER:N	2.29	0.66
1:C:419:PHE:C	1:C:497:GLN:H	1.97	0.66
2:M:61:GLU:O	2:M:227:PRO:CB	2.44	0.66
1:A:44:GLY:CA	2:D:69:ALA:CB	2.74	0.66
2:E:80:ALA:C	2:E:80:ALA:HA	2.06	0.65
3:G:141:ALA:HA	3:G:144:GLU:CB	2.26	0.65
1:C:266:LEU:C	2:E:124:ARG:CB	2.64	0.65
4:H:65:GLY:HA2	4:H:66:ARG:CB	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLY:HA2	2:D:69:ALA:HB3	1.78	0.65
2:L:334:GLU:O	2:L:361:LEU:CB	2.45	0.65
2:M:149:LYS:O	2:M:333:THR:C	2.35	0.65
1:K:56:SER:CB	2:M:30:GLY:O	2.44	0.65
2:L:334:GLU:CA	2:L:361:LEU:CB	2.75	0.65
1:I:260:ASN:N	2:N:296:GLU:HA	1.99	0.65
2:N:149:LYS:O	2:N:333:THR:C	2.35	0.65
2:E:149:LYS:O	2:E:333:THR:C	2.35	0.65
2:F:149:LYS:O	2:F:333:THR:C	2.35	0.65
4:P:65:GLY:HA2	4:P:66:ARG:CB	2.27	0.65
1:J:24:MET:CA	2:M:67:ASP:O	2.38	0.64
3:O:172:ILE:O	3:O:176:ILE:CB	2.45	0.64
1:A:43:ASP:C	2:D:69:ALA:HB2	2.18	0.64
1:C:11:GLY:HA3	2:E:49:GLU:C	2.15	0.64
2:L:149:LYS:O	2:L:333:THR:C	2.35	0.64
3:G:141:ALA:HA	3:G:145:THR:H	1.62	0.64
3:O:156:LYS:C	3:O:158:THR:N	2.44	0.64
3:O:163:ALA:C	3:O:163:ALA:HA	2.04	0.64
1:A:260:ASN:CB	2:F:298:ALA:O	2.45	0.64
3:O:156:LYS:O	3:O:157:THR:C	2.33	0.64
2:D:149:LYS:O	2:D:333:THR:C	2.35	0.64
2:E:81:ARG:N	2:E:81:ARG:CB	2.60	0.64
3:G:156:LYS:C	3:G:158:THR:N	2.44	0.64
3:G:172:ILE:O	3:G:176:ILE:CB	2.45	0.64
4:H:84:HIS:O	4:H:85:ASP:C	2.34	0.63
3:O:141:ALA:HA	3:O:145:THR:H	1.62	0.63
1:K:11:GLY:CA	2:M:49:GLU:HA	2.28	0.63
3:G:151:GLY:O	3:G:152:GLU:C	2.36	0.63
1:A:259:GLY:C	2:F:296:GLU:HA	2.10	0.63
1:C:11:GLY:CA	2:E:49:GLU:CA	2.77	0.63
3:O:151:GLY:O	3:O:152:GLU:C	2.36	0.63
1:A:81:ASN:CA	1:A:282:MET:O	2.47	0.63
3:G:18:LEU:O	3:G:21:ALA:HB3	1.99	0.63
1:K:259:GLY:C	2:M:296:GLU:O	2.35	0.63
2:N:76:VAL:O	2:N:77:GLU:CB	2.47	0.63
3:O:156:LYS:HA	3:O:159:ARG:H	1.64	0.63
1:C:25:TYR:CA	2:F:65:GLY:HA2	2.27	0.62
2:E:76:VAL:O	2:E:77:GLU:CB	2.47	0.62
2:F:76:VAL:O	2:F:77:GLU:CB	2.47	0.62
2:L:76:VAL:O	2:L:77:GLU:CB	2.47	0.62
3:O:148:LYS:O	3:O:149:LYS:O	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:156:LYS:HA	3:G:159:ARG:H	1.64	0.62
1:K:25:TYR:CB	2:N:65:GLY:CA	2.75	0.62
3:G:156:LYS:O	3:G:157:THR:C	2.33	0.62
3:O:18:LEU:O	3:O:21:ALA:HB3	1.99	0.62
2:D:334:GLU:O	2:D:361:LEU:N	2.31	0.62
1:I:208:GLY:O	1:I:507:CYS:O	2.18	0.62
2:D:134:GLY:CA	2:D:430:ARG:O	2.42	0.62
1:I:259:GLY:C	2:N:296:GLU:O	2.31	0.62
3:O:41:GLY:O	3:O:42:LEU:C	2.38	0.62
3:O:135:GLU:C	3:O:137:LEU:H	2.03	0.62
3:G:41:GLY:O	3:G:42:LEU:C	2.38	0.61
1:K:429:SER:C	1:K:431:PHE:H	2.03	0.61
2:D:76:VAL:O	2:D:77:GLU:CB	2.47	0.61
3:G:148:LYS:O	3:G:149:LYS:O	2.17	0.61
4:P:75:ALA:N	4:P:75:ALA:CB	2.56	0.61
1:A:266:LEU:CB	2:F:124:ARG:CA	2.78	0.61
1:I:25:TYR:H	2:L:65:GLY:C	1.96	0.61
1:B:25:TYR:N	2:E:66:LEU:N	2.48	0.61
2:M:76:VAL:O	2:M:77:GLU:CB	2.47	0.61
2:L:134:GLY:O	2:L:430:ARG:N	2.34	0.61
3:O:170:PRO:O	3:O:174:ALA:HB2	2.00	0.61
2:F:61:GLU:HA	2:F:229:ILE:CB	2.31	0.61
1:C:359:ALA:HB3	2:F:224:ALA:HB1	1.83	0.60
2:E:349:TYR:O	2:E:424:ASN:HA	2.01	0.60
3:G:170:PRO:O	3:G:174:ALA:HB2	2.00	0.60
3:G:135:GLU:O	3:G:137:LEU:N	2.33	0.60
3:O:158:THR:C	3:O:161:VAL:CB	2.70	0.60
1:I:12:PRO:O	1:I:13:ALA:HB3	2.01	0.60
1:C:12:PRO:O	1:C:13:ALA:HB3	2.02	0.60
3:G:158:THR:C	3:G:161:VAL:CB	2.70	0.60
1:A:12:PRO:O	1:A:13:ALA:HB3	2.02	0.60
1:C:259:GLY:O	2:E:297:ARG:N	2.35	0.60
3:G:160:ARG:O	3:G:164:LEU:CB	2.50	0.60
1:J:12:PRO:O	1:J:13:ALA:HB3	2.02	0.60
1:K:12:PRO:O	1:K:13:ALA:HB3	2.02	0.59
3:G:135:GLU:HA	3:G:138:ILE:N	2.16	0.59
3:O:150:ILE:C	3:O:151:GLY:O	2.39	0.59
1:C:266:LEU:CB	2:E:124:ARG:CA	2.78	0.59
1:J:9:ILE:CA	2:L:50:VAL:O	2.48	0.59
1:B:12:PRO:O	1:B:13:ALA:HB3	2.01	0.59
3:O:135:GLU:HA	3:O:138:ILE:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:PHE:C	1:A:497:GLN:O	2.41	0.59
1:B:9:ILE:CB	2:D:50:VAL:C	2.70	0.59
4:H:77:LEU:N	4:H:80:ALA:HB3	2.18	0.59
3:O:160:ARG:O	3:O:164:LEU:CB	2.50	0.59
2:F:427:GLN:O	1:K:126:GLY:CA	2.50	0.59
1:I:429:SER:CB	1:I:431:PHE:H	2.16	0.59
4:P:62:LEU:O	4:P:63:MET:CB	2.46	0.59
3:O:135:GLU:O	3:O:137:LEU:N	2.33	0.59
2:D:359:SER:C	2:D:361:LEU:N	2.49	0.58
1:I:25:TYR:N	2:L:65:GLY:HA2	2.18	0.58
3:G:150:ILE:C	3:G:151:GLY:O	2.39	0.58
1:A:43:ASP:O	2:D:69:ALA:HB3	2.04	0.58
1:I:189:VAL:HA	1:I:308:THR:CB	2.34	0.58
2:L:134:GLY:CA	2:L:430:ARG:O	2.51	0.58
1:A:56:SER:CB	2:F:30:GLY:N	2.67	0.58
1:C:11:GLY:CA	2:E:49:GLU:HA	2.34	0.57
2:E:80:ALA:C	2:E:80:ALA:CB	2.70	0.57
1:A:259:GLY:C	2:F:296:GLU:C	2.63	0.57
3:G:47:MET:C	3:G:49:ALA:N	2.57	0.57
3:O:186:ARG:O	3:O:190:ASP:CB	2.53	0.57
1:K:241:LEU:O	1:K:245:SER:N	2.31	0.57
2:E:134:GLY:O	2:E:429:ASN:HA	2.04	0.57
3:G:47:MET:C	3:G:49:ALA:H	2.08	0.57
1:K:260:ASN:CB	2:M:298:ALA:O	2.52	0.57
1:A:81:ASN:N	1:A:282:MET:O	2.36	0.57
1:C:266:LEU:C	2:E:124:ARG:CA	2.68	0.57
3:G:135:GLU:C	3:G:137:LEU:H	2.03	0.57
3:O:132:ARG:O	3:O:133:TYR:C	2.38	0.56
3:G:186:ARG:O	3:G:190:ASP:CB	2.53	0.56
1:J:23:ARG:O	2:M:68:LEU:HA	2.05	0.56
1:K:11:GLY:HA3	2:M:49:GLU:CA	2.35	0.56
3:O:48:GLU:O	3:O:51:LYS:N	2.38	0.56
1:A:241:LEU:O	1:A:245:SER:N	2.31	0.56
1:C:241:LEU:O	1:C:245:SER:N	2.31	0.56
3:G:189:GLU:CB	3:G:189:GLU:HA	2.18	0.56
1:I:419:PHE:HA	1:I:420:PRO:C	2.25	0.56
3:O:47:MET:C	3:O:49:ALA:H	2.09	0.56
1:C:419:PHE:HA	1:C:420:PRO:C	2.25	0.56
3:O:47:MET:C	3:O:49:ALA:N	2.57	0.56
1:C:344:MET:CB	2:F:272:ALA:C	2.73	0.56
1:K:419:PHE:CB	1:K:497:GLN:O	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:137:LEU:O	3:G:140:VAL:CB	2.54	0.56
1:I:24:MET:CB	2:L:66:LEU:HA	2.29	0.56
1:B:419:PHE:HA	1:B:420:PRO:C	2.25	0.56
1:K:419:PHE:HA	1:K:420:PRO:C	2.25	0.56
1:A:419:PHE:HA	1:A:420:PRO:C	2.25	0.56
3:G:132:ARG:N	3:G:134:ALA:CB	2.68	0.56
1:J:241:LEU:O	1:J:245:SER:N	2.32	0.56
1:C:352:PRO:CB	2:F:269:GLU:O	2.54	0.56
1:I:241:LEU:O	1:I:245:SER:N	2.31	0.56
3:O:45:GLU:C	3:O:47:MET:N	2.58	0.56
2:E:81:ARG:C	2:E:81:ARG:CB	2.67	0.55
3:O:158:THR:HA	3:O:161:VAL:CB	2.37	0.55
1:A:199:LEU:O	1:A:200:ASP:C	2.45	0.55
3:G:44:ARG:C	3:G:47:MET:CB	2.72	0.55
3:O:137:LEU:O	3:O:140:VAL:CB	2.54	0.55
3:O:142:ASN:CB	3:O:142:ASN:HA	2.16	0.55
2:D:334:GLU:CB	2:D:361:LEU:CB	2.84	0.55
1:J:419:PHE:HA	1:J:420:PRO:C	2.25	0.55
3:G:48:GLU:O	3:G:51:LYS:N	2.39	0.55
3:O:55:GLN:CB	3:O:133:TYR:CB	2.85	0.55
1:A:199:LEU:O	1:A:200:ASP:O	2.24	0.55
3:G:142:ASN:CB	3:G:142:ASN:HA	2.17	0.55
3:G:132:ARG:O	3:G:133:TYR:C	2.37	0.55
1:I:71:LEU:HA	1:I:189:VAL:H	1.72	0.55
3:O:136:ALA:O	3:O:140:VAL:CB	2.55	0.55
1:I:71:LEU:CB	1:I:72:ALA:CA	2.83	0.54
2:L:334:GLU:O	2:L:361:LEU:CA	2.54	0.54
1:C:260:ASN:N	2:E:296:GLU:HA	2.22	0.54
3:O:137:LEU:O	3:O:140:VAL:N	2.40	0.54
1:B:241:LEU:O	1:B:245:SER:N	2.31	0.54
3:G:158:THR:HA	3:G:161:VAL:CB	2.37	0.54
1:A:11:GLY:CA	2:F:50:VAL:CB	2.85	0.54
2:E:334:GLU:O	2:E:360:ARG:N	2.39	0.54
3:G:137:LEU:O	3:G:140:VAL:N	2.40	0.54
1:A:259:GLY:C	2:F:296:GLU:CA	2.69	0.54
3:G:136:ALA:O	3:G:140:VAL:CB	2.55	0.54
1:C:259:GLY:H	2:E:296:GLU:H	1.51	0.54
4:H:84:HIS:C	4:H:86:VAL:N	2.53	0.54
1:I:225:ALA:O	1:I:406:PHE:HA	2.07	0.54
1:I:404:GLY:O	1:I:430:LEU:CB	2.56	0.54
1:K:225:ALA:O	1:K:406:PHE:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:7:THR:O	3:O:9:MET:N	2.41	0.54
3:O:132:ARG:N	3:O:134:ALA:CB	2.68	0.54
1:A:225:ALA:O	1:A:406:PHE:HA	2.08	0.53
2:E:153:PHE:CB	2:E:338:GLN:HA	2.38	0.53
3:G:167:VAL:C	3:G:169:ILE:N	2.61	0.53
1:J:296:VAL:HA	1:J:333:ALA:HB1	1.90	0.53
1:B:224:ALA:CA	1:B:405:ALA:HB3	2.37	0.53
1:B:225:ALA:O	1:B:406:PHE:HA	2.07	0.53
1:C:225:ALA:O	1:C:406:PHE:HA	2.08	0.53
1:K:11:GLY:CA	2:M:50:VAL:H	2.14	0.53
1:K:224:ALA:CA	1:K:405:ALA:HB3	2.37	0.53
2:L:359:SER:C	2:L:361:LEU:H	2.07	0.53
1:A:296:VAL:HA	1:A:333:ALA:HB1	1.90	0.53
3:G:138:ILE:O	3:G:139:ARG:O	2.27	0.53
1:K:11:GLY:HA2	2:M:49:GLU:HA	1.89	0.53
1:K:429:SER:C	1:K:431:PHE:N	2.60	0.53
3:O:44:ARG:C	3:O:47:MET:CB	2.72	0.53
1:J:227:PRO:HA	1:J:384:VAL:CB	2.39	0.53
1:A:233:GLY:HA2	5:A:600:ADP:O1A	2.09	0.53
1:B:296:VAL:HA	1:B:333:ALA:HB1	1.90	0.53
2:L:153:PHE:CB	2:L:338:GLN:HA	2.39	0.53
3:O:145:THR:O	3:O:149:LYS:CB	2.57	0.53
1:A:227:PRO:HA	1:A:384:VAL:CB	2.39	0.53
1:C:25:TYR:N	2:F:66:LEU:N	2.14	0.53
2:M:153:PHE:CB	2:M:338:GLN:HA	2.39	0.53
1:I:352:PRO:CB	2:L:272:ALA:HB3	2.39	0.53
3:O:42:LEU:O	3:O:45:GLU:CB	2.57	0.53
1:B:86:GLY:O	1:B:302:SER:HA	2.09	0.53
2:D:153:PHE:CB	2:D:338:GLN:HA	2.39	0.53
3:G:166:GLN:O	3:G:169:ILE:CB	2.57	0.53
1:C:296:VAL:HA	1:C:333:ALA:HB1	1.90	0.53
1:I:227:PRO:HA	1:I:384:VAL:CB	2.39	0.53
2:N:153:PHE:CB	2:N:338:GLN:HA	2.39	0.53
3:O:138:ILE:O	3:O:139:ARG:O	2.27	0.53
2:F:153:PHE:CB	2:F:338:GLN:HA	2.39	0.53
1:B:227:PRO:HA	1:B:384:VAL:CB	2.39	0.52
1:C:419:PHE:C	1:C:497:GLN:N	2.58	0.52
3:G:145:THR:O	3:G:149:LYS:CB	2.57	0.52
1:A:224:ALA:CA	1:A:405:ALA:HB3	2.37	0.52
1:C:227:PRO:HA	1:C:384:VAL:CB	2.39	0.52
4:H:77:LEU:O	4:H:78:LYS:C	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:296:VAL:HA	1:I:333:ALA:HB1	1.91	0.52
1:C:11:GLY:C	2:E:49:GLU:CB	2.75	0.52
2:L:359:SER:CA	2:L:362:MET:H	2.22	0.52
1:A:71:LEU:CA	1:A:188:PRO:HA	2.39	0.52
1:C:420:PRO:N	1:C:497:GLN:H	2.07	0.52
1:J:225:ALA:O	1:J:406:PHE:HA	2.08	0.52
1:K:69:LEU:CA	1:K:72:ALA:HB2	2.40	0.52
3:G:138:ILE:C	3:G:139:ARG:O	2.45	0.52
3:G:165:GLU:O	3:G:166:GLN:C	2.47	0.52
3:O:166:GLN:O	3:O:169:ILE:CB	2.57	0.52
3:O:173:ARG:O	3:O:177:ARG:CB	2.58	0.52
3:G:45:GLU:C	3:G:47:MET:N	2.58	0.52
1:K:227:PRO:HA	1:K:384:VAL:CB	2.40	0.52
4:P:74:ILE:C	4:P:75:ALA:HA	2.16	0.52
1:A:44:GLY:N	2:D:69:ALA:HB1	2.22	0.52
1:A:233:GLY:HA2	5:A:600:ADP:PA	2.49	0.52
3:G:42:LEU:O	3:G:45:GLU:CB	2.57	0.52
1:I:259:GLY:O	2:N:298:ALA:N	2.42	0.52
3:O:167:VAL:C	3:O:169:ILE:N	2.61	0.52
1:A:52:TYR:O	1:A:53:GLU:CB	2.58	0.52
2:D:359:SER:C	2:D:362:MET:H	2.13	0.52
2:N:62:GLU:HA	2:N:227:PRO:CB	2.39	0.52
1:C:52:TYR:O	1:C:53:GLU:CB	2.58	0.52
1:I:52:TYR:O	1:I:53:GLU:CB	2.58	0.52
1:J:263:THR:CB	2:L:124:ARG:C	2.78	0.52
1:A:419:PHE:O	1:A:497:GLN:O	2.27	0.51
1:I:25:TYR:CB	2:L:65:GLY:CA	2.84	0.51
1:K:52:TYR:O	1:K:53:GLU:CB	2.58	0.51
1:B:71:LEU:O	1:B:188:PRO:HA	2.10	0.51
1:I:132:GLY:HA3	1:I:371:LEU:C	2.30	0.51
1:I:224:ALA:CA	1:I:405:ALA:HB3	2.37	0.51
1:I:263:THR:O	2:N:124:ARG:HA	2.10	0.51
3:O:141:ALA:CA	3:O:145:THR:H	2.22	0.51
1:K:296:VAL:HA	1:K:333:ALA:HB1	1.90	0.51
1:B:52:TYR:O	1:B:53:GLU:CB	2.59	0.51
1:C:11:GLY:CA	2:E:49:GLU:CB	2.88	0.51
3:O:165:GLU:O	3:O:166:GLN:C	2.47	0.51
3:O:171:GLY:O	3:O:174:ALA:HB3	2.11	0.51
1:B:224:ALA:HB2	1:B:405:ALA:CB	2.31	0.51
3:G:7:THR:O	3:G:9:MET:N	2.42	0.51
3:G:141:ALA:CA	3:G:145:THR:H	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:173:ARG:O	3:G:177:ARG:CB	2.58	0.51
2:M:359:SER:CB	2:M:362:MET:CB	2.88	0.51
3:O:205:GLU:CB	3:O:205:GLU:N	2.67	0.51
1:B:9:ILE:CA	2:D:50:VAL:CB	2.87	0.51
3:G:171:GLY:O	3:G:174:ALA:HB3	2.11	0.51
3:G:52:ALA:CB	3:G:52:ALA:C	2.74	0.51
1:I:346:ALA:HB2	2:L:272:ALA:CB	2.40	0.51
3:O:138:ILE:C	3:O:139:ARG:O	2.45	0.51
3:O:52:ALA:CB	3:O:52:ALA:C	2.74	0.51
1:A:132:GLY:HA3	1:A:371:LEU:O	2.11	0.50
3:G:183:LEU:O	3:G:186:ARG:CB	2.59	0.50
3:O:183:LEU:O	3:O:186:ARG:CB	2.59	0.50
1:C:73:VAL:O	1:C:186:THR:HA	2.12	0.50
3:G:194:LEU:C	3:G:194:LEU:CB	2.73	0.50
4:P:77:LEU:O	4:P:78:LYS:C	2.37	0.50
2:L:130:PHE:CB	2:L:370:LYS:O	2.60	0.50
3:O:148:LYS:O	3:O:152:GLU:CA	2.59	0.50
1:I:418:HIS:HA	1:I:496:GLN:CB	2.42	0.50
1:J:52:TYR:O	1:J:53:GLU:CB	2.58	0.50
3:O:132:ARG:C	3:O:134:ALA:H	2.13	0.50
1:A:73:VAL:O	1:A:186:THR:HA	2.12	0.50
1:J:224:ALA:CA	1:J:405:ALA:HB3	2.37	0.50
3:G:146:ARG:O	3:G:147:LEU:C	2.50	0.50
3:G:205:GLU:CB	3:G:205:GLU:N	2.66	0.50
1:J:224:ALA:HB2	1:J:405:ALA:CB	2.31	0.50
1:B:73:VAL:O	1:B:186:THR:HA	2.12	0.49
3:G:132:ARG:C	3:G:134:ALA:H	2.13	0.49
1:J:73:VAL:O	1:J:186:THR:HA	2.11	0.49
1:K:73:VAL:O	1:K:186:THR:HA	2.12	0.49
1:K:231:GLY:CA	5:K:600:ADP:H5'1	2.37	0.49
2:L:150:LEU:CB	2:L:335:GLY:O	2.60	0.49
2:N:149:LYS:O	2:N:333:THR:CB	2.59	0.49
1:J:9:ILE:HA	2:L:50:VAL:CB	2.42	0.49
2:F:149:LYS:O	2:F:333:THR:CB	2.59	0.49
3:G:146:ARG:O	3:G:149:LYS:N	2.45	0.49
3:O:43:VAL:O	3:O:44:ARG:C	2.51	0.49
1:C:11:GLY:HA3	2:E:49:GLU:CA	2.42	0.49
2:E:149:LYS:O	2:E:333:THR:CB	2.59	0.49
3:G:148:LYS:O	3:G:152:GLU:CA	2.59	0.49
2:D:149:LYS:O	2:D:333:THR:CB	2.59	0.49
2:E:150:LEU:CB	2:E:335:GLY:O	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:557:GLU:C	1:K:559:PHE:N	2.66	0.49
3:O:7:THR:O	3:O:8:ARG:O	2.30	0.49
3:O:49:ALA:O	3:O:52:ALA:CB	2.53	0.49
3:O:146:ARG:O	3:O:149:LYS:N	2.45	0.49
1:A:557:GLU:C	1:A:559:PHE:N	2.66	0.49
1:J:557:GLU:C	1:J:559:PHE:N	2.66	0.49
2:N:150:LEU:CB	2:N:335:GLY:O	2.61	0.49
3:O:142:ASN:CB	3:O:142:ASN:N	2.67	0.49
2:D:150:LEU:CB	2:D:335:GLY:O	2.60	0.49
1:I:475:ALA:HB1	2:L:398:ILE:O	2.13	0.49
1:K:216:PHE:HA	1:K:429:SER:CB	2.43	0.49
2:M:150:LEU:CB	2:M:335:GLY:O	2.61	0.49
1:B:21:GLY:O	2:E:68:LEU:CB	2.61	0.49
3:G:43:VAL:O	3:G:44:ARG:C	2.51	0.49
3:O:146:ARG:O	3:O:147:LEU:C	2.50	0.49
3:O:198:LYS:O	3:O:199:GLY:O	2.31	0.49
2:D:134:GLY:HA2	2:D:430:ARG:C	2.30	0.49
1:I:71:LEU:CB	1:I:188:PRO:CB	2.87	0.49
1:J:429:SER:C	1:J:431:PHE:H	2.17	0.49
3:O:134:ALA:O	4:P:16:ALA:HB2	2.13	0.49
1:I:24:MET:HA	2:L:66:LEU:HA	0.57	0.49
2:L:149:LYS:O	2:L:333:THR:CB	2.59	0.49
3:O:134:ALA:O	3:O:137:LEU:CB	2.61	0.49
1:A:81:ASN:HA	1:A:282:MET:C	2.33	0.48
2:M:149:LYS:O	2:M:333:THR:CB	2.60	0.48
1:B:557:GLU:C	1:B:559:PHE:N	2.66	0.48
3:G:198:LYS:O	3:G:199:GLY:O	2.31	0.48
4:H:65:GLY:CA	4:H:66:ARG:CB	2.91	0.48
1:I:73:VAL:O	1:I:186:THR:HA	2.12	0.48
1:C:208:GLY:O	1:C:507:CYS:CA	2.61	0.48
1:C:224:ALA:CA	1:C:405:ALA:HB3	2.37	0.48
1:I:557:GLU:C	1:I:559:PHE:N	2.66	0.48
3:O:198:LYS:O	3:O:199:GLY:C	2.52	0.48
1:I:440:ARG:HA	1:I:444:ALA:O	2.14	0.48
1:J:440:ARG:HA	1:J:444:ALA:O	2.14	0.48
1:J:471:VAL:CB	4:P:98:ILE:O	2.61	0.48
3:O:3:GLN:O	3:O:6:PRO:N	2.46	0.48
3:O:200:LYS:HA	3:O:203:ALA:HB3	1.96	0.48
1:C:266:LEU:O	2:E:124:ARG:CB	2.62	0.48
1:C:352:PRO:C	2:F:269:GLU:CB	2.81	0.48
3:G:134:ALA:O	3:G:137:LEU:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:259:GLY:N	2:M:296:GLU:CB	2.68	0.48
3:O:138:ILE:O	3:O:142:ASN:CB	2.62	0.48
1:C:557:GLU:C	1:C:559:PHE:N	2.66	0.48
2:F:150:LEU:CB	2:F:335:GLY:O	2.61	0.48
3:G:3:GLN:O	3:G:6:PRO:N	2.47	0.48
1:I:24:MET:CB	2:L:66:LEU:CB	2.92	0.48
3:O:48:GLU:CB	3:O:51:LYS:CB	2.92	0.48
3:G:135:GLU:HA	3:G:138:ILE:H	1.79	0.48
3:G:198:LYS:O	3:G:199:GLY:C	2.52	0.48
1:I:404:GLY:O	1:I:430:LEU:N	2.47	0.48
1:A:43:ASP:C	2:D:69:ALA:HB3	2.34	0.48
3:G:153:GLU:O	3:G:154:ILE:O	2.32	0.47
2:M:61:GLU:HA	2:M:229:ILE:CB	2.44	0.47
3:O:153:GLU:O	3:O:154:ILE:O	2.32	0.47
3:G:4:VAL:CA	3:G:5:SER:N	2.68	0.47
1:A:440:ARG:HA	1:A:444:ALA:O	2.14	0.47
3:G:167:VAL:C	3:G:169:ILE:H	2.18	0.47
1:I:25:TYR:N	2:L:65:GLY:C	2.60	0.47
1:K:233:GLY:CA	5:K:600:ADP:C8	2.97	0.47
3:O:167:VAL:C	3:O:169:ILE:H	2.17	0.47
3:G:48:GLU:CB	3:G:51:LYS:CB	2.92	0.47
2:E:150:LEU:C	2:E:335:GLY:O	2.53	0.47
3:G:138:ILE:O	3:G:142:ASN:CB	2.62	0.47
1:K:440:ARG:HA	1:K:444:ALA:O	2.14	0.47
1:B:25:TYR:CB	2:E:64:THR:O	2.63	0.47
2:F:150:LEU:C	2:F:335:GLY:O	2.53	0.47
2:M:150:LEU:C	2:M:335:GLY:O	2.53	0.47
1:I:25:TYR:N	2:L:65:GLY:CA	2.77	0.47
3:O:135:GLU:HA	3:O:138:ILE:H	1.80	0.47
1:B:429:SER:C	1:B:431:PHE:H	2.19	0.47
1:C:440:ARG:HA	1:C:444:ALA:O	2.14	0.47
1:B:440:ARG:HA	1:B:444:ALA:O	2.14	0.47
1:C:266:LEU:CB	2:E:124:ARG:CB	2.93	0.47
1:C:352:PRO:O	2:F:269:GLU:CB	2.63	0.47
2:D:150:LEU:C	2:D:335:GLY:O	2.53	0.47
3:G:200:LYS:HA	3:G:203:ALA:HB3	1.96	0.47
2:D:359:SER:CA	2:D:362:MET:H	2.27	0.46
1:I:346:ALA:HB2	2:L:272:ALA:HB2	1.97	0.46
2:L:150:LEU:C	2:L:335:GLY:O	2.52	0.46
3:O:200:LYS:CA	3:O:203:ALA:HB3	2.45	0.46
3:G:49:ALA:O	3:G:52:ALA:CB	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:132:GLY:HA3	1:I:371:LEU:O	2.16	0.46
2:L:134:GLY:C	2:L:430:ARG:O	2.54	0.46
1:A:43:ASP:O	2:D:69:ALA:CB	2.63	0.46
1:B:23:ARG:O	2:E:67:ASP:O	2.34	0.46
1:J:24:MET:CB	2:M:66:LEU:C	2.83	0.46
1:A:198:LYS:HA	1:A:368:VAL:HA	1.98	0.46
1:B:10:ALA:O	2:D:49:GLU:HA	2.16	0.46
2:F:427:GLN:O	1:K:126:GLY:HA2	2.15	0.46
1:I:419:PHE:O	1:I:495:LEU:O	2.34	0.46
2:N:150:LEU:C	2:N:335:GLY:O	2.53	0.46
3:G:7:THR:O	3:G:8:ARG:O	2.30	0.46
4:H:84:HIS:C	4:H:86:VAL:H	2.10	0.46
1:A:56:SER:CB	2:F:30:GLY:H	2.28	0.46
3:G:200:LYS:CA	3:G:203:ALA:HB3	2.45	0.46
1:A:224:ALA:HB2	1:A:405:ALA:CB	2.31	0.46
1:C:359:ALA:CB	2:F:224:ALA:HB1	2.46	0.46
1:K:419:PHE:N	1:K:496:GLN:HA	2.31	0.46
1:C:268:GLU:CB	2:E:126:LYS:CB	2.94	0.46
1:I:217:PRO:C	1:I:431:PHE:CB	2.84	0.46
1:I:419:PHE:H	1:I:496:GLN:CA	2.27	0.45
3:O:52:ALA:O	3:O:55:GLN:O	2.34	0.45
1:A:197:ARG:O	1:A:369:ILE:N	2.38	0.45
1:I:11:GLY:N	2:N:50:VAL:O	2.47	0.45
3:O:194:LEU:C	3:O:194:LEU:CB	2.73	0.45
3:G:35:LEU:O	3:G:38:GLU:CB	2.65	0.45
3:O:35:LEU:O	3:O:38:GLU:CB	2.65	0.45
3:G:52:ALA:O	3:G:55:GLN:O	2.34	0.45
1:J:71:LEU:O	1:J:188:PRO:HA	2.15	0.45
3:G:142:ASN:CB	3:G:142:ASN:N	2.67	0.45
1:K:44:GLY:N	2:N:69:ALA:HB2	2.32	0.45
1:K:296:VAL:CA	1:K:333:ALA:HB1	2.47	0.45
3:G:151:GLY:O	3:G:152:GLU:O	2.35	0.45
1:A:11:GLY:HA3	2:F:50:VAL:CB	2.42	0.45
1:J:208:GLY:O	1:J:507:CYS:CB	2.65	0.45
3:G:179:ILE:O	3:G:180:GLN:C	2.56	0.45
1:I:11:GLY:C	2:N:50:VAL:O	2.54	0.45
1:I:24:MET:CA	2:L:66:LEU:H	1.93	0.45
1:J:70:PRO:O	1:J:71:LEU:C	2.55	0.45
3:O:179:ILE:O	3:O:180:GLN:C	2.55	0.45
1:A:44:GLY:CA	2:D:69:ALA:HB3	2.44	0.45
1:C:296:VAL:CA	1:C:333:ALA:HB1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:56:SER:CB	2:N:30:GLY:CA	2.95	0.45
3:G:141:ALA:HB1	3:G:145:THR:CB	2.47	0.44
1:J:296:VAL:CA	1:J:333:ALA:HB1	2.47	0.44
1:K:26:ASP:O	1:K:71:LEU:N	2.50	0.44
3:O:4:VAL:CA	3:O:5:SER:N	2.68	0.44
1:A:263:THR:CB	2:F:123:ALA:O	2.66	0.44
2:D:153:PHE:O	2:D:338:GLN:HA	2.17	0.44
3:O:141:ALA:HB1	3:O:145:THR:CB	2.47	0.44
1:B:296:VAL:CA	1:B:333:ALA:HB1	2.47	0.44
1:C:314:ARG:HA	1:C:318:PHE:O	2.18	0.44
3:G:45:GLU:O	3:G:47:MET:N	2.50	0.44
1:K:11:GLY:HA3	2:M:49:GLU:HA	1.94	0.44
3:G:175:GLN:O	3:G:177:ARG:N	2.51	0.44
3:G:189:GLU:CB	3:G:189:GLU:N	2.69	0.44
1:J:314:ARG:HA	1:J:318:PHE:O	2.18	0.44
1:K:259:GLY:CA	2:M:296:GLU:C	2.60	0.44
1:A:314:ARG:HA	1:A:318:PHE:O	2.18	0.44
1:J:10:ALA:O	2:L:49:GLU:CA	2.65	0.44
1:J:25:TYR:O	2:M:65:GLY:HA2	2.17	0.44
3:O:151:GLY:O	3:O:152:GLU:O	2.35	0.44
3:O:175:GLN:O	3:O:177:ARG:N	2.51	0.44
1:A:296:VAL:CA	1:A:333:ALA:HB1	2.47	0.44
1:B:314:ARG:HA	1:B:318:PHE:O	2.18	0.44
1:I:86:GLY:O	1:I:305:VAL:CB	2.66	0.44
1:I:296:VAL:CA	1:I:333:ALA:HB1	2.47	0.44
1:K:233:GLY:HA2	5:K:600:ADP:C8	2.52	0.44
1:K:314:ARG:HA	1:K:318:PHE:O	2.18	0.44
2:E:153:PHE:O	2:E:338:GLN:HA	2.18	0.44
2:L:153:PHE:O	2:L:338:GLN:HA	2.18	0.44
3:O:45:GLU:O	3:O:47:MET:N	2.50	0.44
1:K:224:ALA:HB2	1:K:405:ALA:CB	2.32	0.43
2:D:349:TYR:HA	2:D:350:PRO:C	2.38	0.43
2:N:153:PHE:O	2:N:338:GLN:HA	2.18	0.43
2:N:349:TYR:HA	2:N:350:PRO:C	2.38	0.43
1:I:314:ARG:HA	1:I:318:PHE:O	2.18	0.43
2:M:153:PHE:O	2:M:338:GLN:HA	2.18	0.43
3:O:167:VAL:C	3:O:167:VAL:HA	2.16	0.43
3:O:189:GLU:CB	3:O:189:GLU:N	2.69	0.43
1:I:255:CYS:HA	1:I:290:ASN:CB	2.49	0.43
1:J:75:LEU:O	1:J:184:TYR:HA	2.19	0.43
2:M:349:TYR:HA	2:M:350:PRO:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:258:THR:HA	2:F:259:ASP:HA	1.85	0.43
1:B:241:LEU:O	1:B:245:SER:CB	2.67	0.43
2:D:334:GLU:CA	2:D:361:LEU:CB	2.97	0.43
1:A:255:CYS:HA	1:A:290:ASN:CB	2.49	0.43
1:C:292:SER:CB	2:E:292:ALA:HB1	2.45	0.43
2:F:349:TYR:HA	2:F:350:PRO:C	2.38	0.43
3:G:175:GLN:O	3:G:178:PHE:N	2.51	0.43
1:I:56:SER:CB	2:N:30:GLY:H	2.29	0.43
1:J:241:LEU:O	1:J:245:SER:CB	2.67	0.43
1:K:75:LEU:O	1:K:184:TYR:HA	2.19	0.43
3:O:135:GLU:O	3:O:139:ARG:CB	2.67	0.43
2:E:258:THR:HA	2:E:259:ASP:HA	1.85	0.43
3:G:135:GLU:O	3:G:139:ARG:CB	2.67	0.43
1:K:189:VAL:CB	1:K:304:TYR:CB	2.97	0.43
3:O:140:VAL:O	3:O:144:GLU:N	2.47	0.43
1:A:241:LEU:O	1:A:245:SER:CB	2.67	0.42
1:B:9:ILE:CB	2:D:52:GLU:N	2.82	0.42
2:F:427:GLN:C	1:K:126:GLY:HA2	2.40	0.42
3:O:189:GLU:CB	3:O:189:GLU:HA	2.18	0.42
1:B:255:CYS:HA	1:B:290:ASN:CB	2.49	0.42
1:K:255:CYS:HA	1:K:290:ASN:CB	2.49	0.42
2:F:153:PHE:O	2:F:338:GLN:HA	2.18	0.42
2:F:427:GLN:CB	1:K:126:GLY:HA2	2.43	0.42
1:K:241:LEU:O	1:K:245:SER:CB	2.67	0.42
2:M:334:GLU:O	2:M:360:ARG:N	2.49	0.42
3:O:174:ALA:O	3:O:175:GLN:O	2.37	0.42
1:B:75:LEU:O	1:B:184:TYR:HA	2.19	0.42
1:C:241:LEU:O	1:C:245:SER:CB	2.67	0.42
1:I:241:LEU:O	1:I:245:SER:CB	2.67	0.42
2:L:349:TYR:HA	2:L:350:PRO:C	2.38	0.42
1:J:255:CYS:HA	1:J:290:ASN:CB	2.49	0.42
2:D:189:VAL:O	2:D:217:SER:HA	2.20	0.42
2:E:189:VAL:O	2:E:217:SER:HA	2.20	0.42
4:H:77:LEU:H	4:H:80:ALA:CB	2.28	0.42
2:L:189:VAL:O	2:L:217:SER:HA	2.20	0.42
1:K:12:PRO:N	2:M:49:GLU:CB	2.83	0.42
1:A:11:GLY:N	2:F:50:VAL:O	2.53	0.42
1:C:75:LEU:O	1:C:184:TYR:HA	2.19	0.42
2:E:349:TYR:HA	2:E:350:PRO:C	2.39	0.42
2:N:360:ARG:C	2:N:362:MET:N	2.38	0.42
1:A:267:VAL:CB	2:F:125:ARG:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:189:VAL:O	2:F:217:SER:HA	2.20	0.42
3:G:4:VAL:C	3:G:6:PRO:N	2.71	0.42
1:A:133:MET:O	1:A:148:LEU:HA	2.20	0.42
1:A:266:LEU:CB	2:F:124:ARG:HA	2.49	0.42
1:B:25:TYR:O	2:E:65:GLY:HA3	2.02	0.42
1:I:75:LEU:O	1:I:184:TYR:HA	2.19	0.42
1:K:11:GLY:CA	2:M:49:GLU:CA	2.95	0.42
1:A:75:LEU:O	1:A:184:TYR:HA	2.19	0.41
1:A:221:GLY:O	1:A:366:GLY:HA2	2.20	0.41
1:B:227:PRO:CB	1:B:384:VAL:CB	2.98	0.41
1:J:133:MET:O	1:J:148:LEU:HA	2.20	0.41
3:O:175:GLN:O	3:O:178:PHE:N	2.51	0.41
1:B:22:ALA:HA	2:E:68:LEU:CB	2.50	0.41
1:C:133:MET:O	1:C:148:LEU:HA	2.20	0.41
2:F:334:GLU:O	2:F:360:ARG:N	2.53	0.41
2:M:189:VAL:O	2:M:217:SER:HA	2.20	0.41
3:O:48:GLU:O	3:O:51:LYS:CA	2.67	0.41
1:C:255:CYS:HA	1:C:290:ASN:CB	2.49	0.41
1:J:10:ALA:O	2:L:50:VAL:N	2.47	0.41
1:K:227:PRO:CB	1:K:384:VAL:CB	2.99	0.41
3:G:43:VAL:O	3:G:45:GLU:N	2.54	0.41
1:K:133:MET:O	1:K:148:LEU:HA	2.21	0.41
2:N:189:VAL:O	2:N:217:SER:HA	2.20	0.41
1:B:133:MET:O	1:B:148:LEU:HA	2.20	0.41
1:B:221:GLY:O	1:B:366:GLY:HA2	2.21	0.41
2:D:149:LYS:CB	2:D:333:THR:HA	2.51	0.41
1:I:133:MET:O	1:I:148:LEU:HA	2.21	0.41
2:L:334:GLU:C	2:L:361:LEU:CB	2.88	0.41
1:B:141:PHE:O	1:B:143:PHE:O	2.39	0.41
1:B:263:THR:CB	2:D:124:ARG:CA	2.97	0.41
2:F:149:LYS:CB	2:F:333:THR:HA	2.51	0.41
1:K:221:GLY:O	1:K:366:GLY:HA2	2.21	0.41
3:O:148:LYS:C	3:O:149:LYS:O	2.59	0.41
1:C:221:GLY:O	1:C:366:GLY:HA2	2.21	0.41
1:I:227:PRO:CB	1:I:384:VAL:CB	2.99	0.41
1:J:221:GLY:O	1:J:366:GLY:HA2	2.20	0.41
1:C:141:PHE:O	1:C:143:PHE:O	2.39	0.41
2:D:130:PHE:CB	2:D:370:LYS:O	2.68	0.41
2:F:427:GLN:C	1:K:126:GLY:CA	2.89	0.41
1:I:346:ALA:HB2	2:L:272:ALA:HB1	2.03	0.41
1:K:141:PHE:O	1:K:143:PHE:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:149:LYS:CB	2:N:333:THR:HA	2.51	0.41
3:O:40:PHE:O	3:O:43:VAL:CB	2.69	0.41
3:O:43:VAL:O	3:O:45:GLU:N	2.54	0.41
1:A:227:PRO:CB	1:A:384:VAL:CB	2.99	0.41
3:G:146:ARG:O	3:G:149:LYS:CB	2.69	0.41
1:C:44:GLY:CA	2:F:69:ALA:HB2	2.42	0.40
1:C:227:PRO:CB	1:C:384:VAL:CB	2.99	0.40
3:G:48:GLU:O	3:G:51:LYS:CA	2.68	0.40
3:G:174:ALA:O	3:G:175:GLN:O	2.36	0.40
1:I:221:GLY:O	1:I:366:GLY:HA2	2.21	0.40
2:N:258:THR:HA	2:N:259:ASP:HA	1.85	0.40
4:H:63:MET:CB	4:H:64:ARG:HA	2.52	0.40
1:I:226:ILE:O	1:I:384:VAL:N	2.55	0.40
2:M:149:LYS:CB	2:M:333:THR:HA	2.51	0.40
3:O:146:ARG:O	3:O:149:LYS:CB	2.69	0.40
1:A:226:ILE:O	1:A:384:VAL:N	2.55	0.40
3:G:40:PHE:O	3:G:43:VAL:CB	2.69	0.40
1:J:263:THR:CB	2:L:126:LYS:N	2.77	0.40
4:P:94:VAL:O	4:P:95:ARG:C	2.58	0.40
1:C:226:ILE:O	1:C:384:VAL:N	2.54	0.40
3:G:148:LYS:C	3:G:149:LYS:O	2.60	0.40
1:I:141:PHE:O	1:I:143:PHE:O	2.39	0.40
1:J:227:PRO:CB	1:J:384:VAL:CB	2.99	0.40
1:K:233:GLY:HA2	5:K:600:ADP:O1A	2.21	0.40
2:L:149:LYS:CB	2:L:333:THR:HA	2.51	0.40
3:O:4:VAL:C	3:O:6:PRO:N	2.71	0.40
1:B:263:THR:CB	2:D:124:ARG:HA	2.51	0.40
1:C:259:GLY:C	2:E:296:GLU:C	2.80	0.40
1:J:141:PHE:O	1:J:143:PHE:O	2.39	0.40
1:J:226:ILE:O	1:J:384:VAL:N	2.55	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:J:6:ILE:CB	2:M:24:ALA:O[5_555]	2.04	0.16
1:J:5:VAL:CA	2:M:24:ALA:CB[5_555]	2.10	0.10

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	557/578 (96%)	491 (88%)	48 (9%)	18 (3%)	4	30
1	B	557/578 (96%)	492 (88%)	47 (8%)	18 (3%)	4	30
1	C	557/578 (96%)	492 (88%)	48 (9%)	17 (3%)	4	31
1	I	557/578 (96%)	493 (88%)	48 (9%)	16 (3%)	4	32
1	J	557/578 (96%)	492 (88%)	47 (8%)	18 (3%)	4	30
1	K	557/578 (96%)	493 (88%)	47 (8%)	17 (3%)	4	31
2	D	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	7	40
2	E	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	7	40
2	F	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	7	40
2	L	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	7	40
2	M	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	7	40
2	N	446/478 (93%)	420 (94%)	16 (4%)	10 (2%)	6	38
3	G	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	1
3	O	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	1
4	H	102/104 (98%)	89 (87%)	11 (11%)	2 (2%)	7	40
4	P	102/104 (98%)	90 (88%)	10 (10%)	2 (2%)	7	40
All	All	6472/6990 (93%)	5808 (90%)	443 (7%)	221 (3%)	3	29

All (221) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PRO
1	A	19	MET
1	A	53	GLU
1	A	143	PHE
1	A	227	PRO
1	A	256	GLY

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Mol	Chain	Res	Type
1	A	260	ASN
1	A	325	ASP
1	A	394	PRO
1	A	395	VAL
1	A	558	GLU
1	B	12	PRO
1	B	19	MET
1	B	53	GLU
1	B	143	PHE
1	B	227	PRO
1	B	256	GLY
1	B	260	ASN
1	B	325	ASP
1	B	394	PRO
1	B	395	VAL
1	B	558	GLU
1	C	12	PRO
1	C	19	MET
1	C	53	GLU
1	C	143	PHE
1	C	227	PRO
1	C	256	GLY
1	C	260	ASN
1	C	325	ASP
1	C	394	PRO
1	C	395	VAL
1	C	558	GLU
2	D	52	GLU
2	D	79	VAL
2	D	316	MET
2	D	356	PRO
2	D	427	GLN
2	E	52	GLU
2	E	79	VAL
2	E	316	MET
2	E	356	PRO
2	E	427	GLN
2	F	52	GLU
2	F	316	MET
2	F	356	PRO
2	F	427	GLN
3	G	3	GLN

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Mol	Chain	Res	Type
3	G	4	VAL
3	G	43	VAL
3	G	47	MET
3	G	48	GLU
3	G	140	VAL
3	G	149	LYS
3	G	152	GLU
3	G	161	VAL
3	G	172	ILE
3	G	174	ALA
4	H	85	ASP
4	H	100	PHE
1	I	12	PRO
1	I	19	MET
1	I	53	GLU
1	I	143	PHE
1	I	227	PRO
1	I	256	GLY
1	I	260	ASN
1	I	325	ASP
1	I	394	PRO
1	I	395	VAL
1	I	558	GLU
1	J	12	PRO
1	J	19	MET
1	J	53	GLU
1	J	143	PHE
1	J	227	PRO
1	J	256	GLY
1	J	260	ASN
1	J	325	ASP
1	J	394	PRO
1	J	395	VAL
1	J	558	GLU
1	K	12	PRO
1	K	19	MET
1	K	53	GLU
1	K	71	LEU
1	K	143	PHE
1	K	227	PRO
1	K	256	GLY
1	K	260	ASN

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Mol	Chain	Res	Type
1	K	325	ASP
1	K	394	PRO
1	K	395	VAL
1	K	558	GLU
2	L	52	GLU
2	L	79	VAL
2	L	316	MET
2	L	356	PRO
2	L	427	GLN
2	M	52	GLU
2	M	316	MET
2	M	356	PRO
2	M	427	GLN
2	N	52	GLU
2	N	316	MET
2	N	356	PRO
2	N	361	LEU
2	N	427	GLN
3	O	3	GLN
3	O	4	VAL
3	O	43	VAL
3	O	47	MET
3	O	48	GLU
3	O	140	VAL
3	O	149	LYS
3	O	152	GLU
3	O	161	VAL
3	O	172	ILE
3	O	174	ALA
3	O	200	LYS
4	P	85	ASP
4	P	100	PHE
1	A	88	GLN
1	A	255	CYS
1	A	431	PHE
1	B	71	LEU
1	B	88	GLN
1	B	255	CYS
1	C	88	GLN
1	C	255	CYS
2	D	26	ASP
2	D	428	GLN

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Mol	Chain	Res	Type
2	E	26	ASP
2	E	428	GLN
2	F	26	ASP
2	F	428	GLN
3	G	2	SER
3	G	6	PRO
3	G	150	ILE
3	G	151	GLY
3	G	185	GLN
3	G	200	LYS
1	I	88	GLN
1	I	255	CYS
1	J	71	LEU
1	J	88	GLN
1	J	255	CYS
1	J	430	LEU
1	K	88	GLN
1	K	255	CYS
2	L	26	ASP
2	L	428	GLN
2	M	26	ASP
2	M	79	VAL
2	M	428	GLN
2	N	26	ASP
2	N	428	GLN
3	O	2	SER
3	O	6	PRO
3	O	13	GLN
3	O	150	ILE
3	O	151	GLY
3	O	185	GLN
1	A	109	HIS
1	B	109	HIS
1	C	109	HIS
3	G	13	GLN
3	G	139	ARG
3	G	155	LYS
3	G	162	ASN
3	G	165	GLU
1	I	109	HIS
1	J	109	HIS
1	K	109	HIS

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Mol	Chain	Res	Type
2	N	79	VAL
3	O	139	ARG
3	O	155	LYS
3	O	162	ASN
3	O	165	GLU
1	A	200	ASP
2	F	79	VAL
3	G	45	GLU
3	G	186	ARG
3	O	45	GLU
3	O	137	LEU
3	O	186	ARG
1	A	374	GLU
1	B	70	PRO
1	B	374	GLU
1	C	71	LEU
1	C	374	GLU
2	D	317	PRO
2	E	317	PRO
2	F	317	PRO
3	G	53	LEU
3	G	137	LEU
3	G	197	ILE
1	I	374	GLU
1	J	374	GLU
1	K	374	GLU
2	L	317	PRO
2	M	317	PRO
2	N	317	PRO
3	O	53	LEU
3	O	197	ILE
2	D	355	LEU
2	E	355	LEU
2	F	355	LEU
2	L	355	LEU
2	M	355	LEU
2	N	355	LEU
1	A	388	GLY
1	B	388	GLY
1	C	388	GLY
3	G	179	ILE
1	I	388	GLY

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Mol	Chain	Res	Type
1	J	388	GLY
1	K	388	GLY
3	O	179	ILE
3	G	168	VAL
3	O	168	VAL

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ADP	K	600	-	24,29,29	1.00	2 (8%)	29,45,45	1.06	4 (13%)
5	ADP	I	600	-	24,29,29	1.09	2 (8%)	29,45,45	0.89	0
5	ADP	A	600	-	24,29,29	1.09	2 (8%)	29,45,45	0.89	0
5	ADP	C	600	-	24,29,29	1.00	2 (8%)	29,45,45	1.07	4 (13%)

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
5	ADP	K	600	-	-	0/12/32/32	0/3/3/3
5	ADP	I	600	-	-	2/12/32/32	0/3/3/3
5	ADP	A	600	-	-	2/12/32/32	0/3/3/3
5	ADP	C	600	-	-	0/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	600	ADP	O4'-C1'	2.63	1.44	1.41
5	I	600	ADP	O4'-C1'	2.60	1.44	1.41
5	K	600	ADP	PB-O2B	-2.44	1.45	1.54
5	C	600	ADP	PB-O2B	-2.44	1.45	1.54
5	A	600	ADP	PB-O2B	-2.35	1.45	1.54
5	I	600	ADP	PB-O2B	-2.34	1.45	1.54
5	C	600	ADP	PA-O1A	-2.33	1.42	1.50
5	K	600	ADP	PA-O1A	-2.32	1.42	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	600	ADP	C5-C6-N6	2.41	124.01	120.35
5	K	600	ADP	O3B-PB-O2B	2.38	116.72	107.64
5	C	600	ADP	O3B-PB-O2B	2.37	116.71	107.64
5	K	600	ADP	C5-C6-N6	2.37	123.95	120.35
5	C	600	ADP	O5'-PA-O1A	2.07	117.14	109.07
5	K	600	ADP	O5'-PA-O1A	2.06	117.13	109.07
5	K	600	ADP	O4'-C4'-C3'	-2.04	101.08	105.11
5	C	600	ADP	O4'-C4'-C3'	-2.03	101.09	105.11

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	600	ADP	PA-O3A-PB-O2B
5	A	600	ADP	PA-O3A-PB-O3B
5	I	600	ADP	PA-O3A-PB-O2B
5	I	600	ADP	PA-O3A-PB-O3B

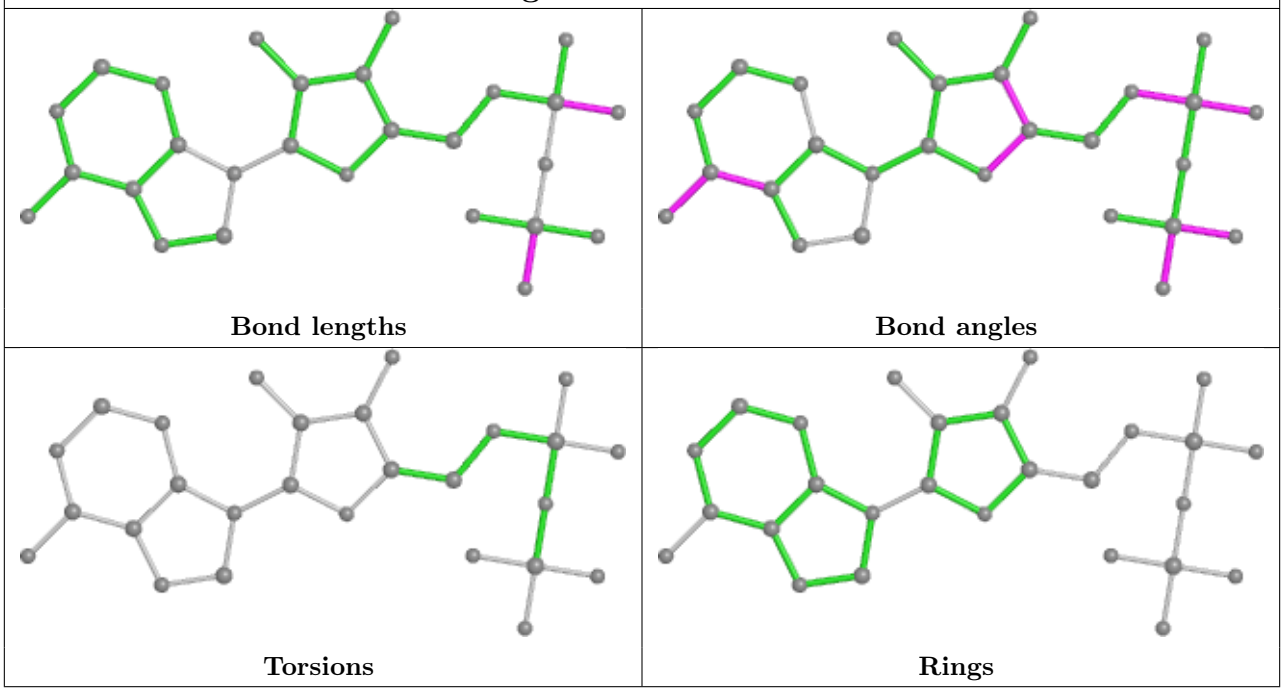
There are no ring outliers.

3 monomers are involved in 8 short contacts:

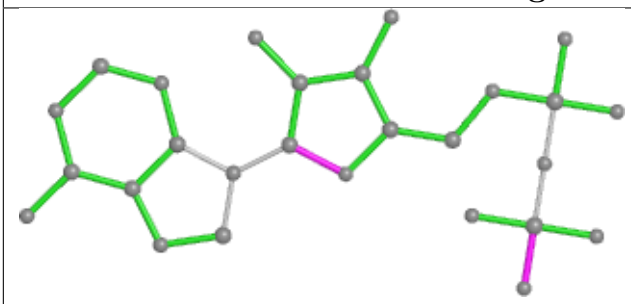
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	600	ADP	5	0
5	A	600	ADP	2	0
5	C	600	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

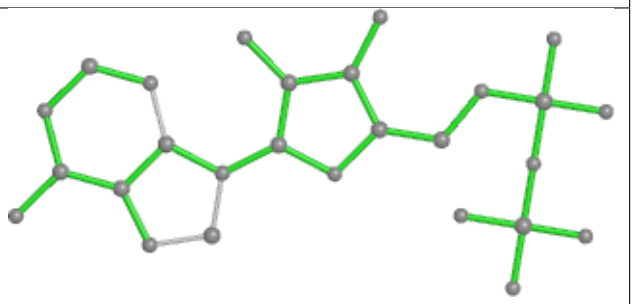
Ligand ADP K 600



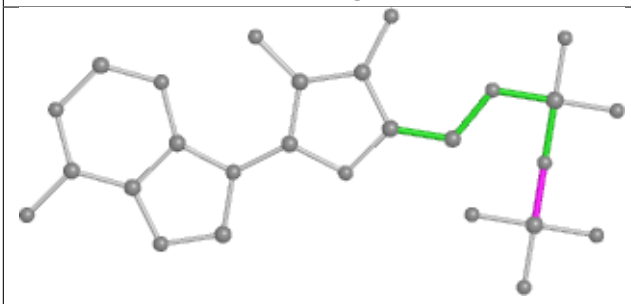
Ligand ADP I 600



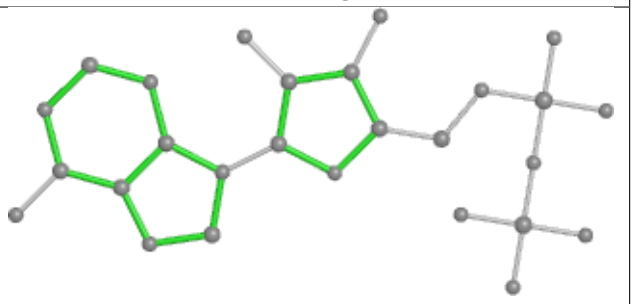
Bond lengths



Bond angles

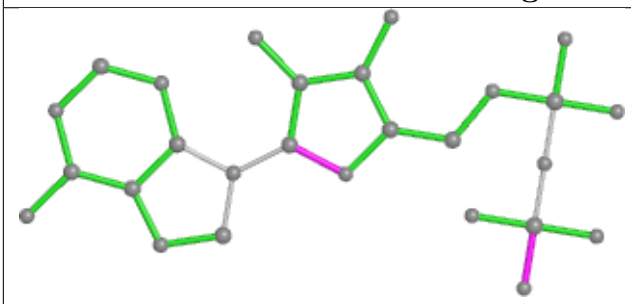


Torsions

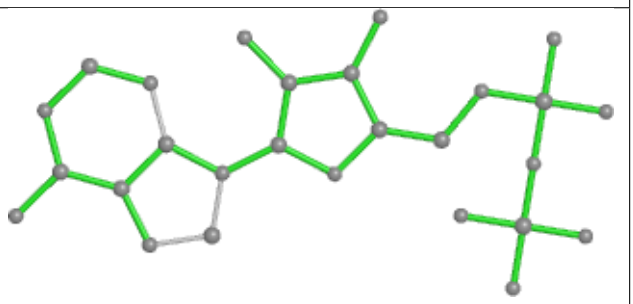


Rings

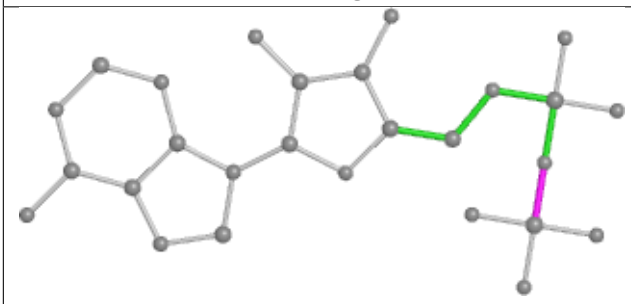
Ligand ADP A 600



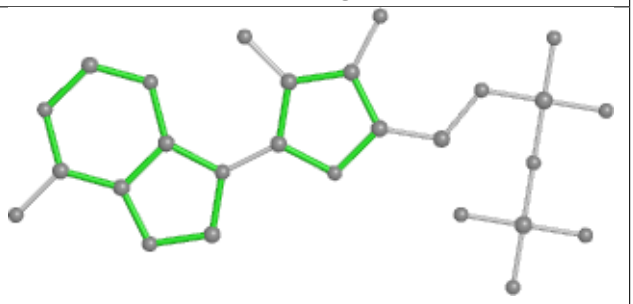
Bond lengths



Bond angles

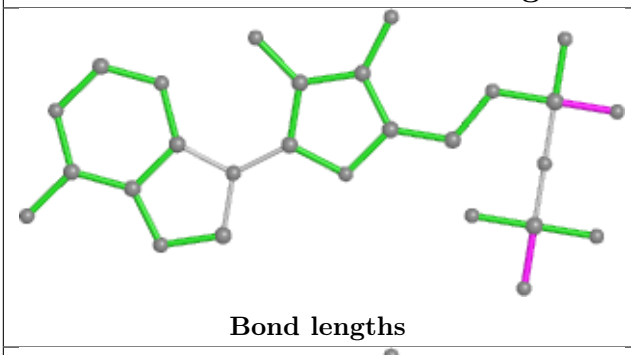


Torsions

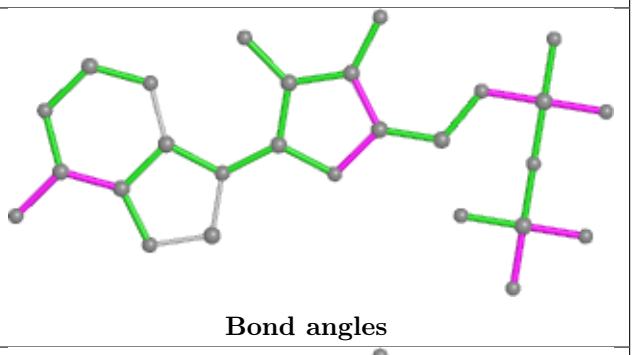


Rings

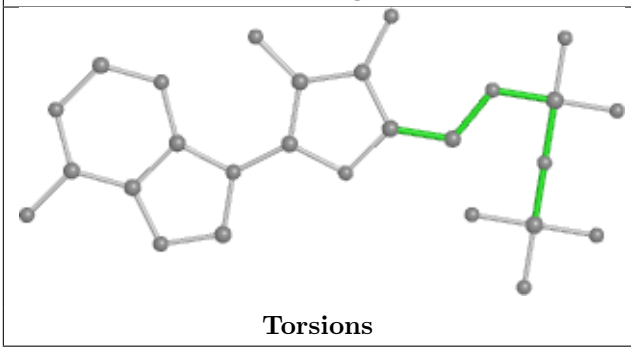
Ligand ADP C 600



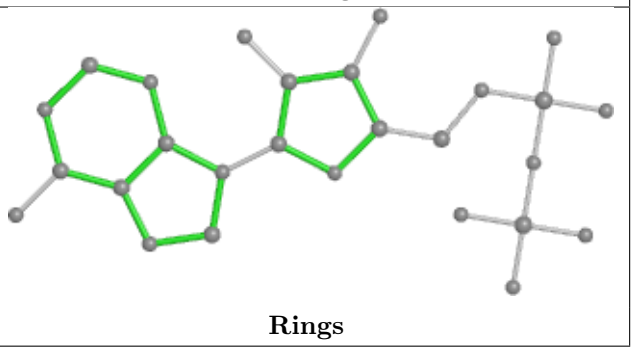
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	561/578 (97%)	0.18	45 (8%) 12 11	103, 162, 214, 214	0
1	B	561/578 (97%)	-0.18	13 (2%) 60 51	79, 130, 144, 144	0
1	C	561/578 (97%)	0.22	46 (8%) 11 10	137, 189, 210, 210	0
1	I	561/578 (97%)	0.42	61 (10%) 5 6	172, 172, 232, 232	0
1	J	561/578 (97%)	-0.35	9 (1%) 72 62	50, 58, 104, 104	0
1	K	561/578 (97%)	0.33	49 (8%) 10 9	146, 177, 189, 189	0
2	D	450/478 (94%)	-0.00	23 (5%) 28 24	118, 118, 188, 188	0
2	E	450/478 (94%)	0.15	31 (6%) 16 13	122, 130, 162, 162	0
2	F	450/478 (94%)	0.22	37 (8%) 11 10	109, 217, 217, 217	0
2	L	450/478 (94%)	-0.04	19 (4%) 36 30	98, 98, 158, 158	0
2	M	450/478 (94%)	0.02	22 (4%) 29 25	99, 99, 148, 148	0
2	N	450/478 (94%)	0.48	49 (10%) 5 6	158, 250, 250, 250	0
3	G	129/223 (57%)	-0.71	0 100 100	34, 34, 49, 49	0
3	O	129/223 (57%)	-0.61	1 (0%) 86 79	84, 85, 85, 85	0
4	H	104/104 (100%)	0.07	5 (4%) 30 26	110, 110, 134, 134	0
4	P	104/104 (100%)	-0.04	7 (6%) 17 15	94, 94, 141, 141	0
All	All	6532/6990 (93%)	0.08	417 (6%) 19 16	34, 137, 232, 250	0

All (417) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	77	PRO	10.6
1	I	372	GLY	9.8
2	N	191	PHE	9.4
2	N	122	VAL	8.9
4	H	24	SER	8.5

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Mol	Chain	Res	Type	RSRZ
2	M	121	PRO	8.4
2	N	192	ALA	8.1
2	D	67	ASP	8.0
1	C	379	THR	8.0
2	L	121	PRO	7.7
4	H	76	GLY	7.5
2	L	122	VAL	7.3
1	C	36	VAL	7.2
1	K	382	GLY	7.0
2	E	120	ASN	7.0
2	M	302	GLU	6.7
1	K	78	GLY	6.4
1	C	47	ALA	6.4
1	I	77	PRO	6.4
1	A	128	GLU	6.3
4	P	104	LEU	6.3
2	N	190	VAL	6.2
2	M	122	VAL	6.1
1	K	76	GLY	6.1
1	C	29	LYS	6.1
1	K	383	ALA	6.0
1	A	61	GLY	5.9
2	N	121	PRO	5.9
2	F	225	ASP	5.9
2	E	29	TYR	5.8
1	I	78	GLY	5.7
1	I	63	PRO	5.6
1	K	324	ALA	5.6
1	K	122	MET	5.6
1	B	109	HIS	5.6
1	K	195	VAL	5.5
1	C	37	GLY	5.4
2	E	118	PRO	5.4
1	A	146	LYS	5.4
2	D	28	ALA	5.4
2	F	86	LYS	5.4
2	N	218	VAL	5.4
2	D	102	GLY	5.4
4	P	85	ASP	5.3
2	D	68	LEU	5.3
1	I	134	VAL	5.3
2	E	119	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	147	ILE	5.2
1	K	394	PRO	5.2
2	E	172	THR	5.2
2	F	122	VAL	5.1
1	I	145	HIS	5.0
2	N	67	ASP	4.9
2	F	278	PRO	4.9
1	I	180	GLU	4.9
1	I	177	ASP	4.8
1	C	150	PRO	4.7
2	L	56	VAL	4.6
2	N	118	PRO	4.6
2	E	70	THR	4.6
1	B	110	ALA	4.5
2	F	83	GLY	4.5
2	F	121	PRO	4.5
2	E	28	ALA	4.5
2	N	123	ALA	4.5
1	A	346	ALA	4.5
1	I	576	ALA	4.5
1	C	376	GLY	4.4
1	K	194	PRO	4.4
1	C	1	MET	4.4
2	E	168	ALA	4.4
1	I	371	LEU	4.4
1	I	146	LYS	4.3
2	F	188	ALA	4.3
2	M	301	VAL	4.3
1	I	373	GLY	4.3
1	I	424	TRP	4.2
1	K	117	TRP	4.2
1	I	12	PRO	4.2
1	K	227	PRO	4.2
2	N	242	ALA	4.2
1	C	183	MET	4.2
2	M	300	VAL	4.1
2	F	221	LEU	4.1
1	A	162	PRO	4.1
1	A	77	PRO	4.0
1	A	12	PRO	4.0
1	C	77	PRO	4.0
4	P	75	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
2	E	299	GLY	4.0
2	E	69	ALA	4.0
1	I	218	VAL	4.0
2	F	189	VAL	4.0
2	N	220	PHE	4.0
1	K	345	PRO	3.9
2	L	20	PHE	3.9
1	A	194	PRO	3.9
1	B	108	VAL	3.9
2	L	21	VAL	3.9
1	I	138	VAL	3.9
1	I	155	GLY	3.9
1	I	139	PRO	3.8
2	F	187	PHE	3.8
1	A	86	GLY	3.8
2	N	359	SER	3.8
1	I	176	GLU	3.8
2	D	310	GLN	3.8
1	C	2	ILE	3.8
1	K	123	VAL	3.8
1	I	42	LEU	3.8
1	A	134	VAL	3.8
2	D	75	LEU	3.7
2	D	21	VAL	3.7
2	E	351	PRO	3.7
4	H	75	ALA	3.7
2	N	80	ALA	3.7
1	A	193	ARG	3.7
1	K	393	GLU	3.7
2	N	164	ALA	3.7
1	I	181	LEU	3.7
2	D	22	GLU	3.7
1	K	297	ALA	3.6
1	I	219	ALA	3.6
1	I	135	LEU	3.6
1	A	155	GLY	3.6
2	F	28	ALA	3.6
1	I	563	PHE	3.5
2	N	148	GLN	3.5
2	F	365	GLY	3.5
1	I	497	GLN	3.5
1	A	62	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	K	417	ARG	3.4
1	A	201	PRO	3.4
2	M	402	ASP	3.4
2	E	121	PRO	3.4
1	K	164	GLY	3.4
2	N	184	GLU	3.4
2	N	83	GLY	3.4
1	C	502	GLU	3.4
1	A	55	THR	3.4
1	K	169	GLU	3.3
4	H	25	SER	3.3
2	F	332	ILE	3.3
1	A	222	GLY	3.3
1	I	55	THR	3.3
1	K	226	ILE	3.3
1	K	165	GLU	3.3
1	K	118	ALA	3.3
1	C	368	VAL	3.2
1	C	168	VAL	3.2
2	F	224	ALA	3.2
1	C	151	PRO	3.2
2	M	168	ALA	3.2
2	F	299	GLY	3.2
1	C	182	LYS	3.2
1	A	60	VAL	3.2
2	N	429	ASN	3.2
1	K	433	SER	3.2
2	M	401	GLU	3.2
2	M	11	ILE	3.2
1	A	218	VAL	3.2
2	N	28	ALA	3.1
2	E	335	GLY	3.1
1	I	140	GLU	3.1
2	F	87	GLU	3.1
1	A	577	LEU	3.1
2	M	360	ARG	3.1
1	I	164	GLY	3.1
2	F	298	ALA	3.1
2	D	121	PRO	3.1
2	M	359	SER	3.1
2	N	82	LEU	3.1
2	N	173	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	494	PHE	3.1
2	E	333	THR	3.0
2	D	64	THR	3.0
2	F	172	THR	3.0
2	D	45	GLY	3.0
1	K	108	VAL	3.0
1	C	43	ASP	3.0
2	E	88	MET	3.0
1	C	394	PRO	3.0
3	O	143	THR	3.0
1	K	434	ALA	3.0
1	K	551	ALA	3.0
2	F	88	MET	2.9
2	E	300	VAL	2.9
1	C	388	GLY	2.9
2	D	44	GLY	2.9
1	C	108	VAL	2.9
1	I	173	VAL	2.9
2	N	185	GLU	2.9
1	K	114	GLU	2.9
1	C	58	LEU	2.9
1	A	208	GLY	2.9
1	K	325	ASP	2.9
1	I	365	ALA	2.9
2	M	81	ARG	2.9
2	M	80	ALA	2.9
1	K	295	PRO	2.8
2	E	102	GLY	2.8
1	K	576	ALA	2.8
1	C	169	GLU	2.8
1	K	47	ALA	2.8
2	N	66	LEU	2.8
1	A	1	MET	2.8
1	C	73	VAL	2.8
2	N	174	ARG	2.8
1	B	388	GLY	2.8
2	N	165	ALA	2.7
4	P	98	ILE	2.7
1	J	471	VAL	2.7
1	K	384	VAL	2.7
2	M	299	GLY	2.7
2	N	298	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	44	GLY	2.7
1	I	316	GLN	2.7
2	N	219	LEU	2.7
1	A	223	THR	2.7
2	E	165	ALA	2.7
1	B	267	VAL	2.7
1	K	201	PRO	2.7
1	B	471	VAL	2.7
1	I	84	TYR	2.7
2	N	78	ASP	2.7
2	D	104	PRO	2.7
2	D	103	LEU	2.7
2	N	421	PHE	2.7
1	I	296	VAL	2.7
1	I	132	GLY	2.6
2	M	362	MET	2.6
1	C	375	GLU	2.6
2	E	463	TYR	2.6
1	I	137	THR	2.6
1	I	224	ALA	2.6
1	A	13	ALA	2.6
2	L	105	PRO	2.6
1	K	418	HIS	2.6
2	D	77	GLU	2.6
1	A	200	ASP	2.6
1	I	158	LYS	2.6
1	A	163	ALA	2.6
1	A	347	GLU	2.6
1	I	425	ASN	2.6
2	E	375	HIS	2.6
1	C	3	GLN	2.6
2	N	205	ILE	2.6
2	F	147	GLY	2.6
2	F	193	ALA	2.6
1	B	387	PRO	2.6
1	I	13	ALA	2.6
2	M	28	ALA	2.6
2	L	37	ASP	2.6
1	I	201	PRO	2.6
1	J	266	LEU	2.6
2	F	21	VAL	2.6
1	A	57	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	41	ARG	2.6
2	D	27	LEU	2.6
2	F	277	ILE	2.6
2	L	38	GLY	2.6
1	K	296	VAL	2.5
1	K	242	ALA	2.5
2	D	23	ASN	2.5
2	L	77	GLU	2.5
2	L	302	GLU	2.5
2	E	67	ASP	2.5
1	I	85	ASP	2.5
2	F	186	PRO	2.5
2	F	201	LEU	2.5
1	B	345	PRO	2.5
1	I	368	VAL	2.5
1	K	552	ARG	2.5
1	C	270	PRO	2.5
2	M	361	LEU	2.5
2	E	175	PRO	2.5
1	I	370	THR	2.5
2	L	13	TYR	2.5
2	E	374	ASP	2.5
2	N	339	LEU	2.5
1	C	288	ILE	2.5
1	C	275	PRO	2.5
1	J	12	PRO	2.5
2	L	75	LEU	2.5
2	M	83	GLY	2.5
1	C	179	THR	2.4
2	D	76	VAL	2.4
1	B	111	LEU	2.4
2	N	193	ALA	2.4
4	P	78	LYS	2.4
1	A	63	PRO	2.4
1	C	258	ARG	2.4
1	I	159	GLU	2.4
1	K	349	GLY	2.4
1	C	74	GLU	2.4
2	F	85	SER	2.4
2	D	120	ASN	2.4
1	J	493	ASP	2.4
1	K	346	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	59	LYS	2.4
1	C	170	GLU	2.4
1	I	345	PRO	2.4
2	N	297	ARG	2.4
1	I	43	ASP	2.4
1	A	507	CYS	2.4
1	A	345	PRO	2.4
1	C	78	GLY	2.4
1	C	165	GLU	2.4
2	N	454	ILE	2.4
1	I	133	MET	2.4
1	I	44	GLY	2.4
2	M	25	LYS	2.4
1	J	387	PRO	2.4
1	K	435	LEU	2.3
1	B	503	VAL	2.3
2	F	17	PRO	2.3
1	I	222	GLY	2.3
2	N	17	PRO	2.3
2	N	168	ALA	2.3
1	K	26	ASP	2.3
1	K	192	ALA	2.3
2	E	122	VAL	2.3
2	F	10	GLY	2.3
2	E	150	LEU	2.3
1	J	474	ASP	2.3
1	A	349	GLY	2.3
1	K	23	ARG	2.3
2	N	278	PRO	2.3
2	N	79	VAL	2.3
2	E	439	ALA	2.3
1	B	58	LEU	2.3
2	M	172	THR	2.3
2	N	248	GLU	2.3
1	I	290	ASN	2.3
1	I	343	GLU	2.3
2	N	455	SER	2.2
2	E	332	ILE	2.2
1	K	228	GLY	2.2
1	A	87	ILE	2.2
1	C	171	PRO	2.2
1	I	182	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	63	THR	2.2
2	E	30	GLY	2.2
2	F	118	PRO	2.2
2	N	221	LEU	2.2
1	C	17	LYS	2.2
2	N	334	GLU	2.2
1	C	378	VAL	2.2
1	K	388	GLY	2.2
2	F	82	LEU	2.2
2	F	216	ARG	2.2
1	A	181	LEU	2.2
1	A	209	MET	2.2
1	I	376	GLY	2.2
2	E	169	ARG	2.2
2	L	80	ALA	2.2
1	A	156	ARG	2.2
2	F	171	ALA	2.2
1	A	129	VAL	2.2
1	A	44	GLY	2.2
4	P	103	LYS	2.2
2	F	123	ALA	2.2
2	D	250	ASP	2.2
1	I	423	ASN	2.2
2	N	75	LEU	2.2
2	N	86	LYS	2.2
2	D	105	PRO	2.2
2	F	154	SER	2.1
1	A	170	GLU	2.1
1	C	126	GLY	2.1
1	A	165	GLU	2.1
1	A	116	LYS	2.1
2	F	79	VAL	2.1
2	F	119	LEU	2.1
1	I	223	THR	2.1
2	L	104	PRO	2.1
1	K	191	ARG	2.1
1	A	177	ASP	2.1
1	K	404	GLY	2.1
1	B	552	ARG	2.1
1	J	3	GLN	2.1
1	B	9	ILE	2.1
1	K	416	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	M	70	THR	2.1
4	P	64	ARG	2.1
1	C	127	ASP	2.1
2	E	336	GLN	2.1
2	N	172	THR	2.1
1	I	136	GLY	2.1
1	C	425	ASN	2.1
1	I	287	LEU	2.1
1	J	560	PRO	2.1
2	N	140	VAL	2.1
2	L	29	TYR	2.1
2	N	422	PHE	2.1
1	C	395	VAL	2.1
4	H	69	PRO	2.1
1	C	146	LYS	2.0
1	I	535	SER	2.0
1	I	147	ILE	2.0
1	K	387	PRO	2.0
2	N	77	GLU	2.0
1	C	4	GLY	2.0
1	I	70	PRO	2.0
1	A	42	LEU	2.0
2	D	365	GLY	2.0
2	M	426	GLY	2.0
2	N	287	MET	2.0
1	C	52	TYR	2.0
2	L	76	VAL	2.0
1	A	56	SER	2.0
2	L	301	VAL	2.0
2	L	401	GLU	2.0
1	A	145	HIS	2.0
2	L	300	VAL	2.0
2	F	302	GLU	2.0
2	E	278	PRO	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)

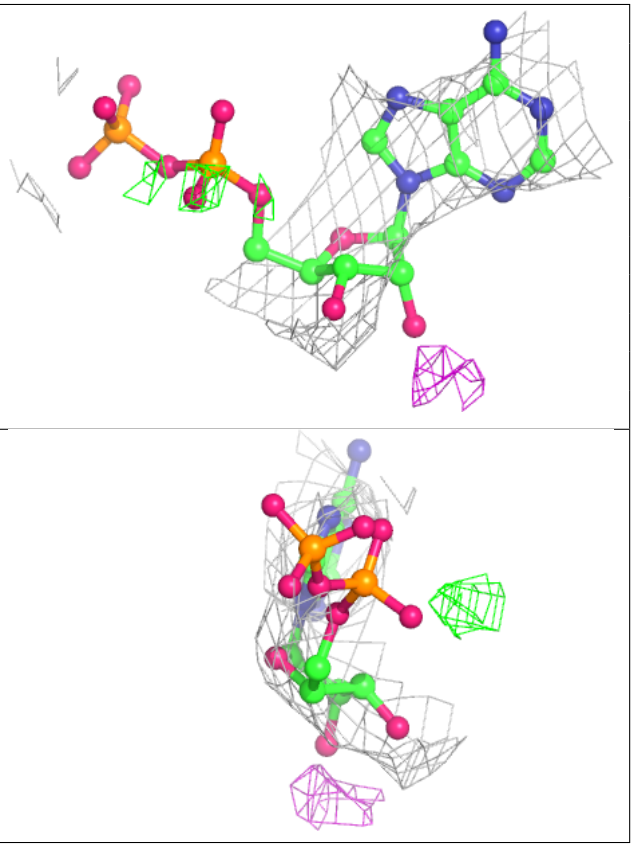
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	ADP	K	600	27/27	0.63	0.47	112,112,112,112	0
5	ADP	I	600	27/27	0.80	0.28	110,110,110,110	0
5	ADP	C	600	27/27	0.80	0.27	116,116,116,116	0
5	ADP	A	600	27/27	0.83	0.26	109,109,109,109	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.

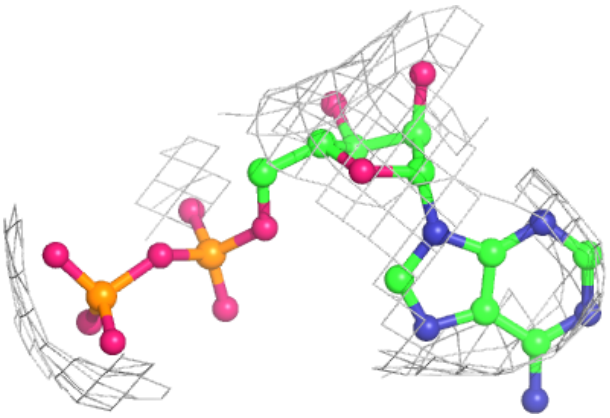
Electron density around ADP K 600:

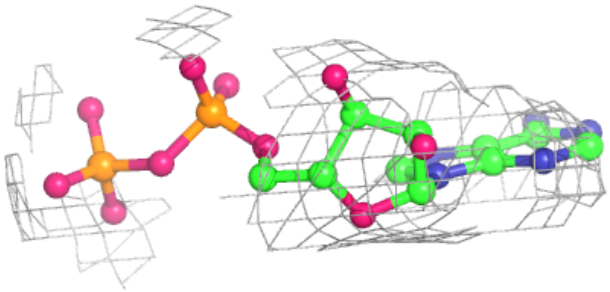
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

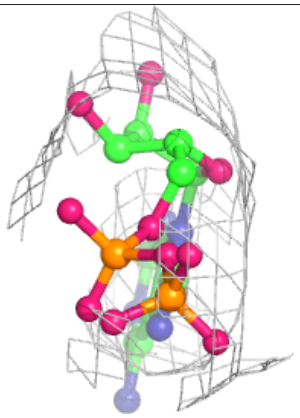


Electron density around ADP I 600:

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

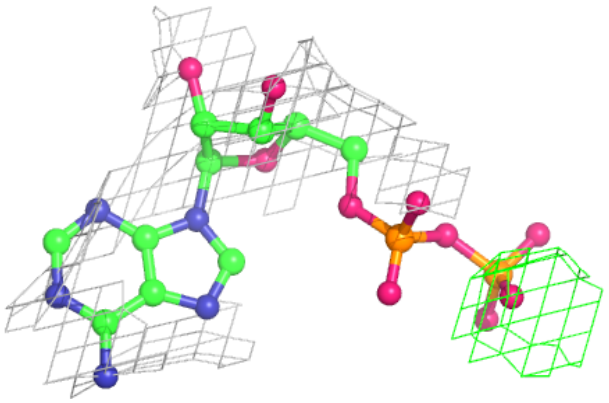


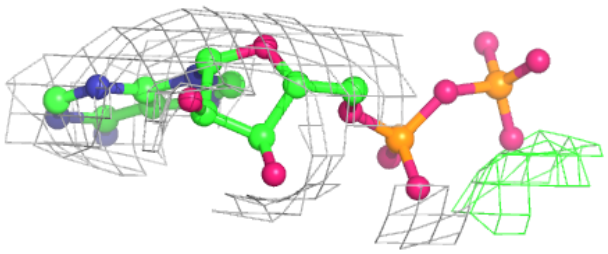


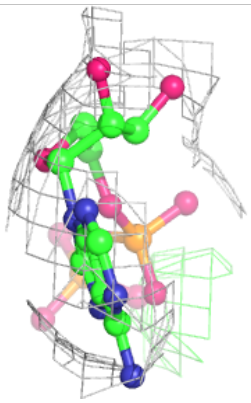


Electron density around ADP C 600:

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

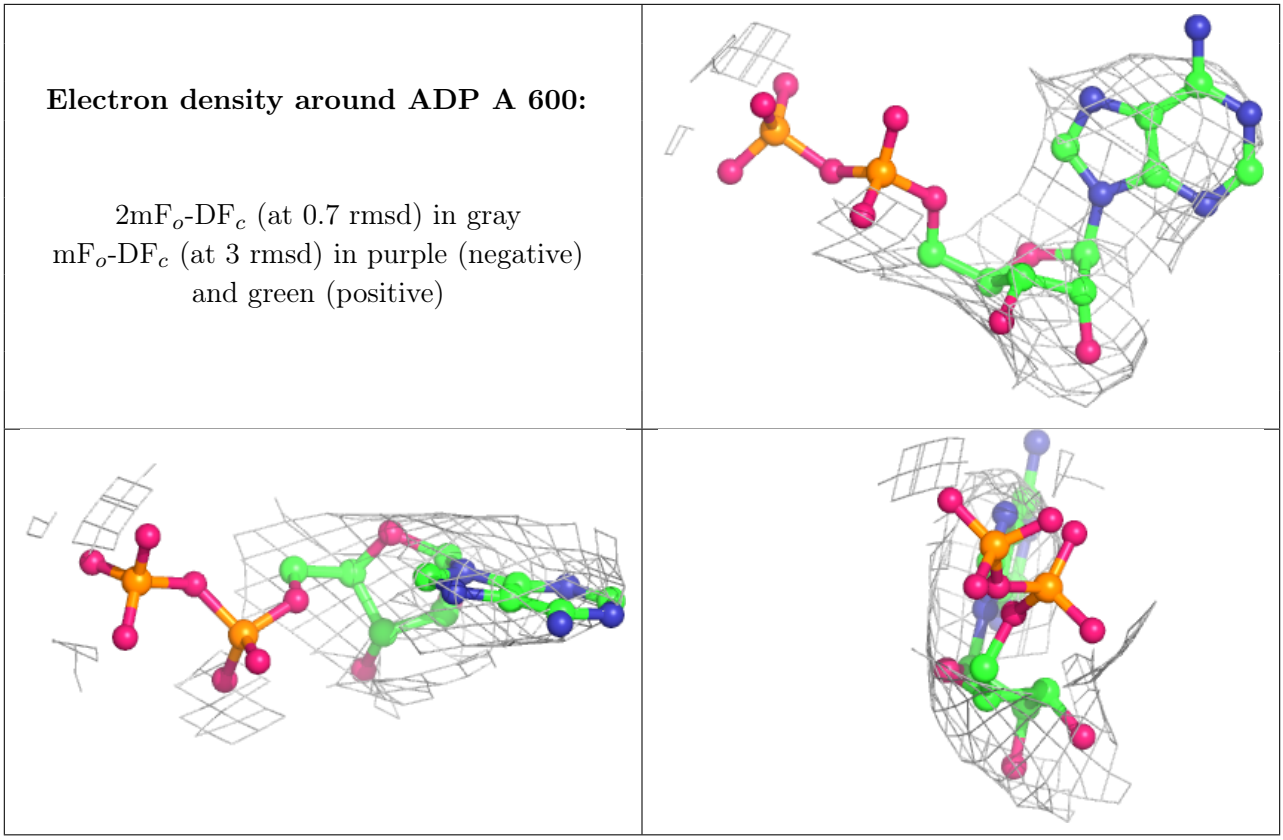






Electron density around ADP A 600:

$2mF_o$-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.