



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:35 am BST

PDB ID : 6V4K
Title : Structure of TrkH-TrkA in complex with ADP
Authors : Zhou, M.; Zhang, H.
Deposited on : 2019-11-27
Resolution : 3.53 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 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 : 2.11
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) : 2.11

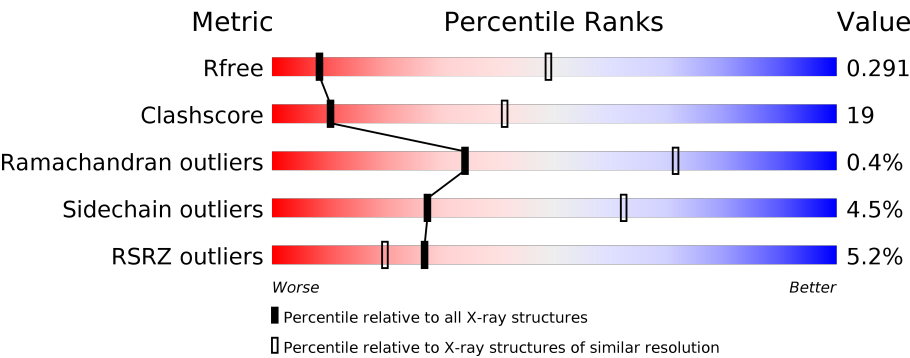
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.53 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	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	485	<div><div>%</div><div><div></div><div>61%</div><div>30%</div><div>• 5%</div></div></div>
1	B	485	<div><div>%</div><div><div></div><div>64%</div><div>28%</div><div>• 5%</div></div></div>
1	C	485	<div><div>2%</div><div><div></div><div>67%</div><div>27%</div><div>• 5%</div></div></div>
1	D	485	<div><div>2%</div><div><div></div><div>65%</div><div>28%</div><div>• 5%</div></div></div>
2	E	458	<div><div>4%</div><div><div></div><div>66%</div><div>30%</div><div>• •</div></div></div>
2	F	458	<div><div>11%</div><div><div></div><div>66%</div><div>32%</div><div>• •</div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	458	<div> <div>7%</div> <div>63%</div> <div>33%</div> <div>..</div> </div>
2	H	458	<div> <div>12%</div> <div>59%</div> <div>36%</div> <div>...</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28234 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.

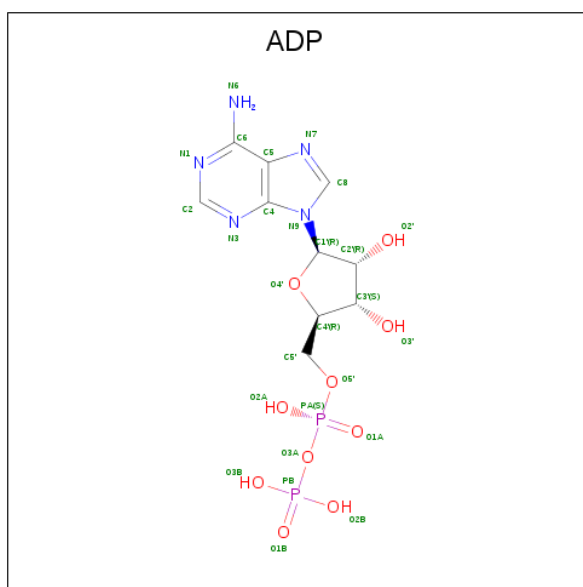
- Molecule 1 is a protein called Trk system potassium uptake protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3539	2370	559	593	17			
1	B	459	Total	C	N	O	S	0	0	0
			3549	2377	559	596	17			
1	C	459	Total	C	N	O	S	0	0	0
			3549	2377	559	596	17			
1	D	459	Total	C	N	O	S	0	0	0
			3549	2377	559	596	17			

- Molecule 2 is a protein called Potassium transporter peripheral membrane component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	455	Total	C	N	O	S	0	0	0
			3490	2190	614	674	12			
2	F	455	Total	C	N	O	S	0	0	0
			3496	2193	617	674	12			
2	G	455	Total	C	N	O	S	0	0	0
			3464	2172	611	669	12			
2	H	455	Total	C	N	O	S	0	0	0
			3490	2190	614	674	12			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

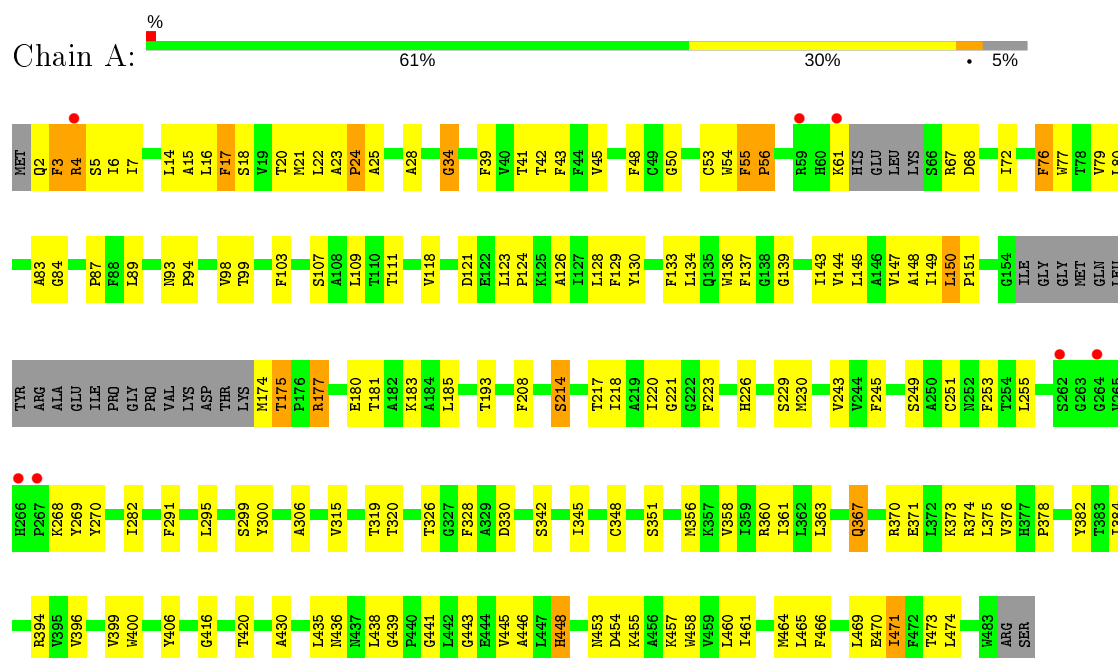


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	H	1	Total 27	C 10	N 5	O 10	P 2	0	0

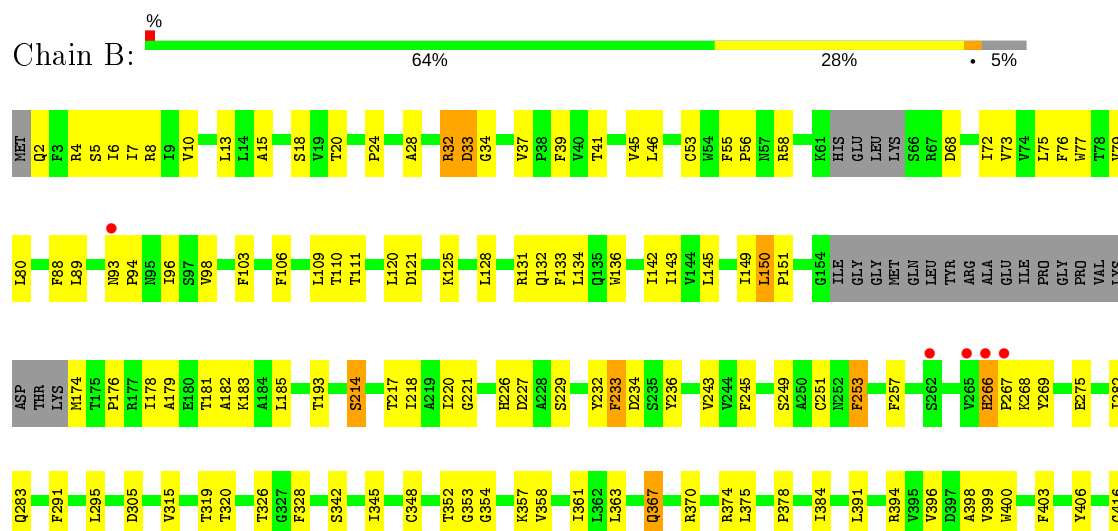
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Trk system potassium uptake protein

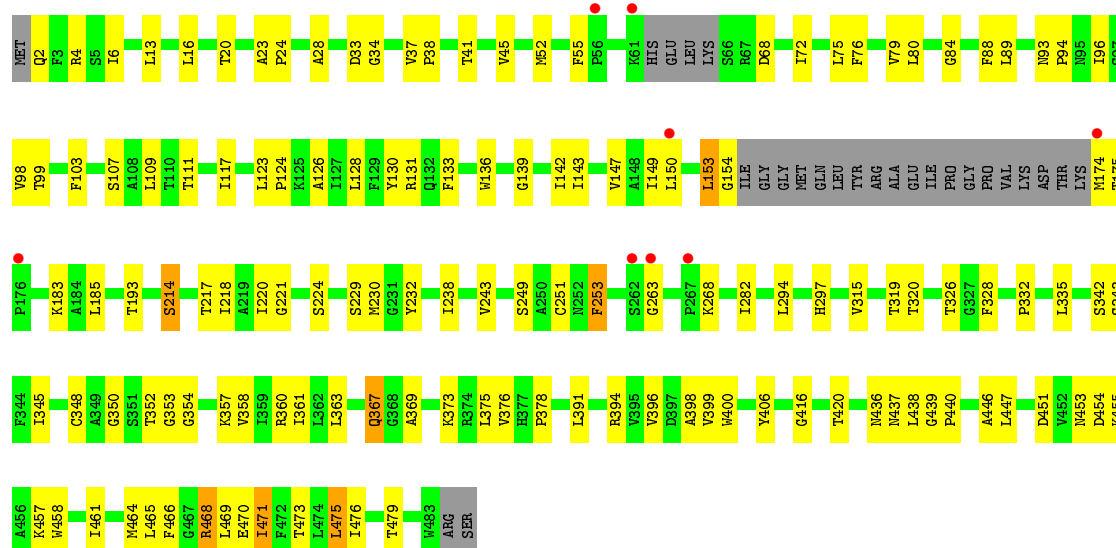


- Molecule 1: Trk system potassium uptake protein

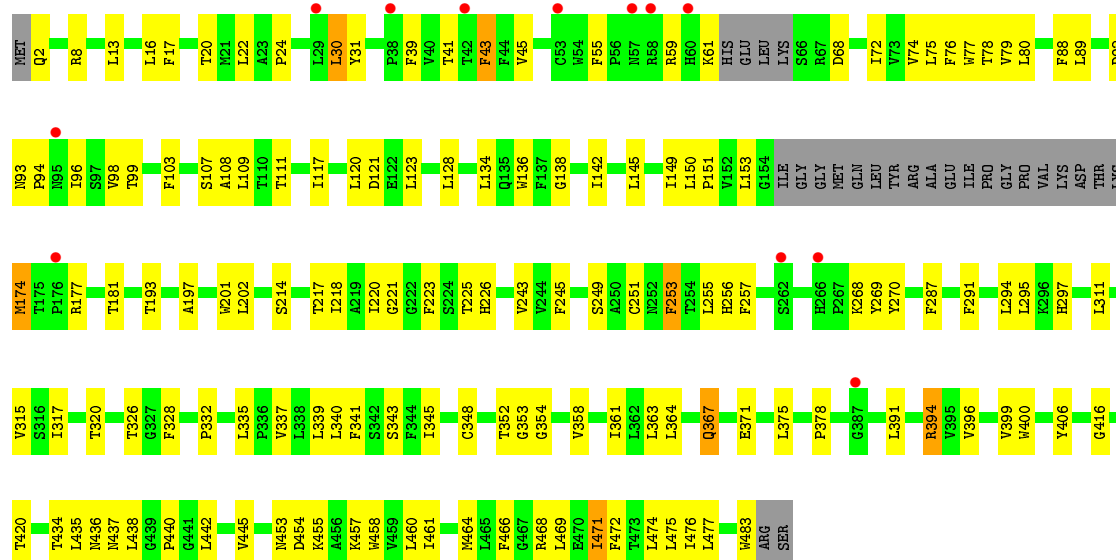




- Molecule 1: Trk system potassium uptake protein

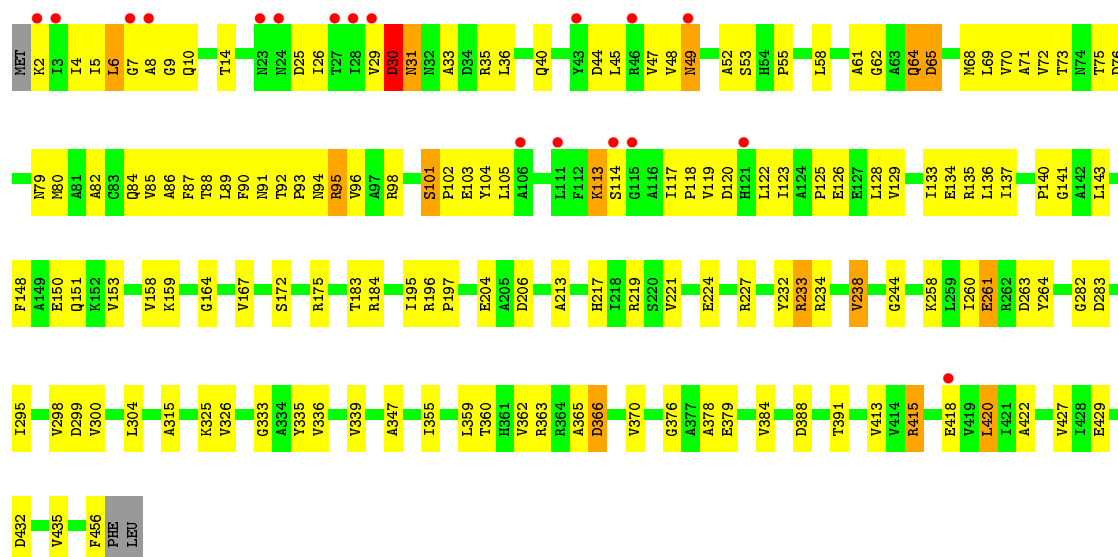


- Molecule 1: Trk system potassium uptake protein

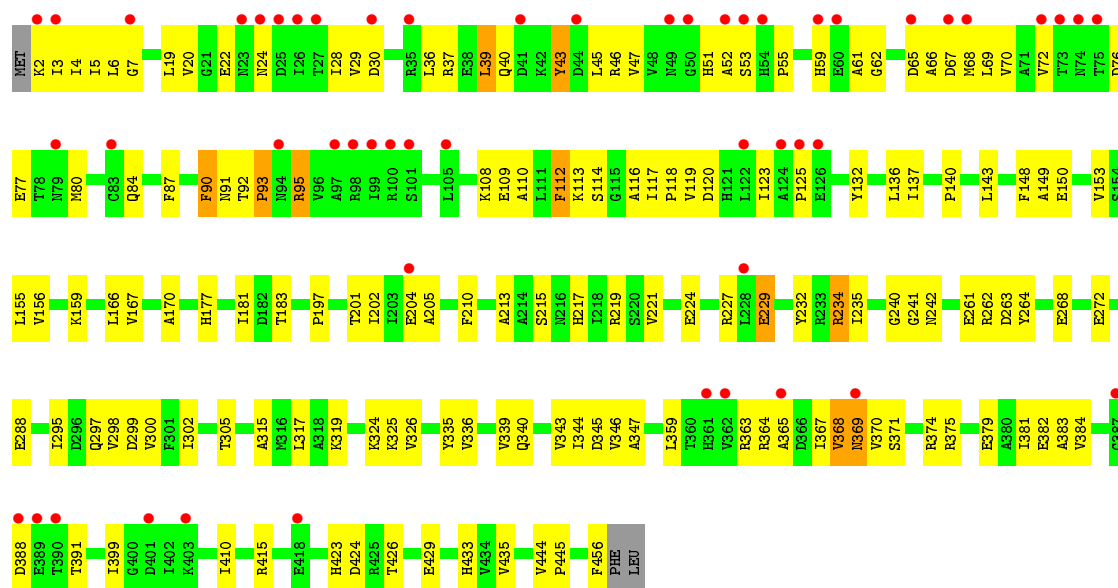


- Molecule 2: Potassium transporter peripheral membrane component

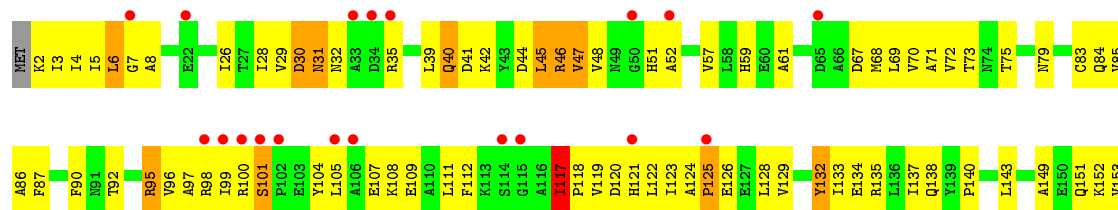


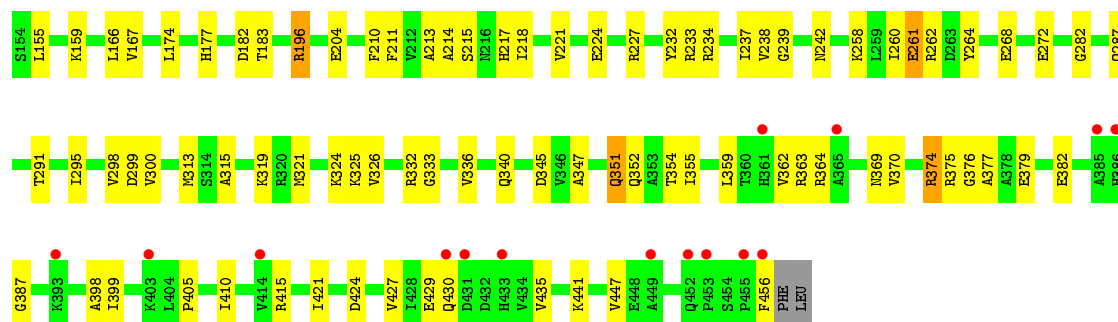


• Molecule 2: Potassium transporter peripheral membrane component

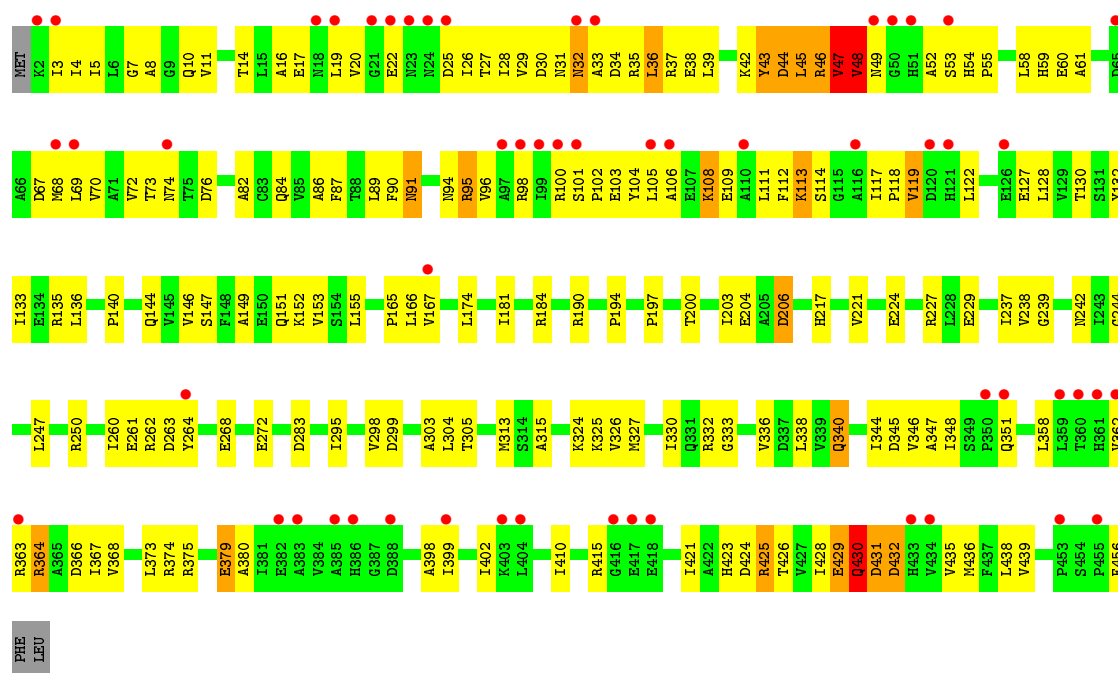


• Molecule 2: Potassium transporter peripheral membrane component





• Molecule 2: Potassium transporter peripheral membrane component



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	262.10Å 188.50Å 187.91Å 90.00° 133.16° 90.00°	Depositor
Resolution (Å)	49.82 – 3.53 49.82 – 3.53	Depositor EDS
% Data completeness (in resolution range)	84.3 (49.82-3.53) 84.3 (49.82-3.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.250 , 0.291 0.250 , 0.291	Depositor DCC
R_{free} test set	3403 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.001 for h+2*k,-h-l 0.011 for k+l,h+l,-l 0.005 for -k+l,-h-l,-l 0.007 for -h+k-l,-l,-k 0.000 for -h-k-l,l,k 0.001 for h-k+l,l,-h-l 0.000 for -k-l,-h-l,k 0.001 for h+k+l,-l,-h-l 0.002 for k-l,h+l,-k 0.007 for h,-k,-h-l 0.017 for -h-2*k,-k,l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	28234	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.29	0/3639	0.56	1/4961 (0.0%)
1	B	0.27	0/3650	0.50	1/4976 (0.0%)
1	C	0.27	0/3650	0.51	1/4976 (0.0%)
1	D	0.27	0/3650	0.50	1/4976 (0.0%)
2	E	0.31	0/3540	0.61	2/4805 (0.0%)
2	F	0.29	0/3546	0.56	0/4812
2	G	0.30	0/3513	0.65	4/4770 (0.1%)
2	H	0.32	0/3540	0.62	2/4805 (0.0%)
All	All	0.29	0/28728	0.57	12/39081 (0.0%)

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	1
1	B	0	4
1	C	0	1
2	E	0	2
2	F	0	2
2	G	0	2
2	H	0	6
All	All	0	18

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	117	ILE	CG1-CB-CG2	-12.29	84.37	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	447	LEU	CA-CB-CG	7.54	132.64	115.30
1	C	153	LEU	CA-CB-CG	6.96	131.31	115.30
2	G	32	ASN	N-CA-C	6.84	129.48	111.00
2	H	44	ASP	N-CA-C	6.35	128.14	111.00
2	G	42	LYS	N-CA-C	6.33	128.10	111.00
1	A	24	PRO	CA-N-CD	-6.21	102.81	111.50
2	H	45	LEU	N-CA-C	5.87	126.85	111.00
1	D	30	LEU	CA-CB-CG	5.68	128.37	115.30
2	E	6	LEU	CA-CB-CG	5.62	128.22	115.30
2	E	30	ASP	CB-CG-OD2	-5.50	113.35	118.30
2	G	6	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	GLY	Peptide
1	B	32	ARG	Peptide
1	B	33	ASP	Peptide
1	B	34	GLY	Peptide
1	B	447	LEU	Peptide
1	C	263	GLY	Peptide
2	E	101	SER	Peptide
2	E	238	VAL	Peptide
2	F	114	SER	Peptide
2	F	205	ALA	Peptide
2	G	101	SER	Peptide
2	G	61	ALA	Peptide
2	H	340	GLN	Peptide
2	H	429	GLU	Peptide
2	H	430	GLN	Peptide
2	H	431	ASP	Peptide
2	H	432	ASP	Peptide
2	H	47	VAL	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3539	0	3609	128	0
1	B	3549	0	3618	118	0
1	C	3549	0	3618	94	0
1	D	3549	0	3618	100	0
2	E	3490	0	3517	143	0
2	F	3496	0	3529	146	0
2	G	3464	0	3477	156	0
2	H	3490	0	3519	226	0
3	E	27	0	12	2	0
3	F	27	0	12	7	0
3	G	27	0	12	2	0
3	H	27	0	11	5	0
All	All	28234	0	28552	1061	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1061) 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)
2:G:30:ASP:HB3	2:G:35:ARG:CB	1.26	1.56
2:F:36:LEU:HD21	2:F:47:VAL:CG2	1.12	1.54
2:H:30:ASP:CB	2:H:35:ARG:CB	1.85	1.53
2:H:30:ASP:HB2	2:H:35:ARG:CB	0.99	1.46
2:F:36:LEU:CD2	2:F:47:VAL:HG21	0.92	1.39
1:B:178:ILE:HG21	2:F:43:TYR:CD2	1.56	1.38
2:H:29:VAL:HA	2:H:47:VAL:CG2	1.58	1.34
2:G:39:LEU:CB	2:G:47:VAL:HG11	1.64	1.26
2:H:29:VAL:CA	2:H:47:VAL:HG22	1.56	1.25
2:G:30:ASP:CB	2:G:35:ARG:CB	2.14	1.25
1:B:178:ILE:CG2	2:F:43:TYR:CD2	2.17	1.24
2:H:261:GLU:OE2	3:H:501:ADP:O3'	1.54	1.22
2:G:26:ILE:O	2:G:45:LEU:CB	1.78	1.15
1:B:178:ILE:CG2	2:F:43:TYR:HD2	1.53	1.12
2:H:47:VAL:HG13	2:H:48:VAL:N	1.66	1.10
2:G:40:GLN:HA	2:G:40:GLN:HE21	1.17	1.10
2:F:36:LEU:CD2	2:F:47:VAL:CG2	1.87	1.09
1:B:178:ILE:HG13	2:F:43:TYR:O	1.51	1.09
2:F:36:LEU:HD23	2:F:47:VAL:HG21	1.26	1.09
2:H:28:ILE:HD13	2:H:43:TYR:HE2	1.11	1.07
2:F:261:GLU:OE2	3:F:501:ADP:O2'	1.70	1.05
2:H:100:ARG:CZ	2:H:127:GLU:OE2	2.05	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:LEU:HD11	2:H:47:VAL:CG1	1.87	1.03
2:H:47:VAL:CG1	2:H:48:VAL:N	2.21	1.02
2:G:26:ILE:O	2:G:45:LEU:HB2	1.56	1.02
1:B:178:ILE:HG21	2:F:43:TYR:CE2	1.95	1.01
2:F:36:LEU:HD22	2:F:47:VAL:HG21	1.42	1.01
2:H:146:VAL:HG22	2:H:374:ARG:HH22	1.21	1.00
1:B:178:ILE:CG2	2:F:43:TYR:CE2	2.44	0.99
2:H:100:ARG:NH2	2:H:127:GLU:OE2	1.95	0.99
2:H:30:ASP:HB2	2:H:35:ARG:CA	1.93	0.99
2:H:36:LEU:CD1	2:H:47:VAL:HG11	1.90	0.99
2:H:36:LEU:HD11	2:H:48:VAL:O	1.62	0.99
2:F:36:LEU:HD21	2:F:47:VAL:HG23	1.45	0.98
2:H:112:PHE:HA	2:H:117:ILE:HG12	1.43	0.97
2:H:36:LEU:CD1	2:H:47:VAL:CG1	2.42	0.97
2:H:28:ILE:HD13	2:H:43:TYR:CE2	1.99	0.96
2:H:36:LEU:HD12	2:H:47:VAL:HG11	1.45	0.96
1:B:178:ILE:CG1	2:F:43:TYR:O	2.13	0.96
2:H:47:VAL:HG22	2:H:48:VAL:HG12	1.49	0.93
2:E:36:LEU:HD21	2:E:47:VAL:HG11	1.50	0.93
2:H:100:ARG:NH1	2:H:127:GLU:OE2	2.01	0.93
2:H:340:GLN:HE21	2:H:375:ARG:HD2	1.33	0.93
1:C:320:THR:HG21	1:C:354:GLY:H	1.34	0.92
2:G:31:ASN:O	2:G:35:ARG:CB	2.19	0.91
2:H:30:ASP:CA	2:H:35:ARG:CB	2.49	0.90
2:H:36:LEU:HD21	2:H:48:VAL:O	1.70	0.90
2:H:133:ILE:HD11	2:H:348:ILE:HD13	1.53	0.90
2:G:26:ILE:O	2:G:45:LEU:HB3	1.69	0.90
1:B:178:ILE:HG23	2:F:43:TYR:HD2	1.36	0.89
2:G:111:LEU:HB3	2:G:118:PRO:HD2	1.54	0.89
2:G:95:ARG:NE	2:G:119:VAL:O	2.07	0.88
2:H:46:ARG:O	2:H:47:VAL:HB	1.72	0.88
2:H:7:GLY:C	2:H:31:ASN:OD1	2.11	0.87
2:H:8:ALA:N	2:H:31:ASN:OD1	2.10	0.85
2:H:84:GLN:HA	2:H:119:VAL:HG21	1.56	0.85
1:C:142:ILE:HG12	1:C:468:ARG:HH11	1.42	0.85
2:E:6:LEU:HG	2:E:71:ALA:HA	1.58	0.84
2:G:39:LEU:CB	2:G:47:VAL:CG1	2.53	0.84
2:H:39:LEU:HD21	2:H:47:VAL:HB	1.60	0.84
1:B:447:LEU:HD22	1:B:448:HIS:HA	1.60	0.83
1:C:320:THR:HG21	1:C:354:GLY:N	1.93	0.83
2:H:36:LEU:HD11	2:H:47:VAL:HG13	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:ARG:NH2	1:C:470:GLU:OE2	2.12	0.83
2:H:47:VAL:CG1	2:H:48:VAL:H	1.88	0.82
1:A:438:LEU:HB3	1:A:439:GLY:HA2	1.61	0.82
2:G:261:GLU:OE2	3:G:501:ADP:O3'	1.97	0.82
1:A:315:VAL:O	1:A:319:THR:OG1	1.97	0.82
2:H:39:LEU:CD2	2:H:47:VAL:HG11	2.09	0.82
1:D:437:ASN:OD1	1:D:468:ARG:NH1	2.12	0.82
2:H:146:VAL:HG22	2:H:374:ARG:NH2	1.93	0.81
1:C:345:ILE:HG22	1:C:361:ILE:HG13	1.63	0.81
2:H:29:VAL:HA	2:H:47:VAL:HG22	0.82	0.81
2:H:340:GLN:HE22	2:H:347:ALA:H	1.27	0.81
2:H:3:ILE:HA	2:H:68:MET:HB3	1.60	0.81
1:B:178:ILE:HG23	2:F:43:TYR:CD2	2.09	0.80
1:C:438:LEU:HB3	1:C:439:GLY:HA2	1.64	0.80
1:B:315:VAL:O	1:B:319:THR:OG1	2.00	0.79
2:H:47:VAL:HG13	2:H:48:VAL:H	1.46	0.79
1:A:249:SER:O	1:A:351:SER:OG	2.01	0.79
1:A:55:PHE:HD2	1:A:56:PRO:HD2	1.45	0.79
1:A:345:ILE:HG22	1:A:361:ILE:HG13	1.65	0.79
1:B:438:LEU:HB3	1:B:439:GLY:HA2	1.63	0.78
2:H:146:VAL:HG13	2:H:374:ARG:HH12	1.48	0.78
2:E:261:GLU:OE2	3:E:501:ADP:O2'	2.02	0.78
1:B:345:ILE:HG22	1:B:361:ILE:HG13	1.66	0.78
2:H:95:ARG:HG3	2:H:119:VAL:O	1.82	0.78
2:H:36:LEU:CD1	2:H:48:VAL:O	2.31	0.77
2:F:30:ASP:HB2	2:F:36:LEU:HD21	1.65	0.77
2:G:26:ILE:HG12	2:G:45:LEU:HD21	1.65	0.77
1:A:136:TRP:HE1	1:A:193:THR:HG21	1.49	0.77
1:B:136:TRP:HE1	1:B:193:THR:HG21	1.49	0.76
1:D:177:ARG:NH1	2:E:44:ASP:OD1	2.18	0.76
1:A:378:PRO:O	1:C:394:ARG:NH2	2.18	0.76
2:E:33:ALA:HA	2:E:36:LEU:HB2	1.65	0.75
2:F:6:LEU:HA	2:F:29:VAL:HB	1.69	0.75
2:G:40:GLN:HA	2:G:40:GLN:NE2	1.97	0.75
2:G:4:ILE:HD11	2:G:69:LEU:HD13	1.67	0.75
2:H:340:GLN:HG2	2:H:375:ARG:HD2	1.69	0.75
1:B:214:SER:HA	1:B:217:THR:HG22	1.69	0.75
1:D:174:MET:N	2:E:49:ASN:OD1	2.20	0.74
1:A:360:ARG:NH2	1:A:470:GLU:OE2	2.18	0.74
1:C:136:TRP:HE1	1:C:193:THR:HG21	1.52	0.74
1:A:28:ALA:HB2	1:A:126:ALA:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ARG:HH21	1:A:374:ARG:HH12	1.36	0.74
1:C:214:SER:HA	1:C:217:THR:HG22	1.70	0.74
2:G:39:LEU:CB	2:G:47:VAL:HG21	2.17	0.74
2:H:29:VAL:CA	2:H:47:VAL:CG2	2.32	0.74
1:A:220:ILE:HD11	1:A:249:SER:HB3	1.69	0.73
2:H:47:VAL:HG22	2:H:48:VAL:CG1	2.18	0.73
1:D:320:THR:HG21	1:D:354:GLY:N	2.03	0.73
2:F:39:LEU:HD12	2:F:45:LEU:HB2	1.70	0.73
2:G:143:LEU:HD11	2:G:159:LYS:HB2	1.69	0.73
2:E:91:ASN:OD1	2:E:92:THR:N	2.22	0.72
2:E:87:PHE:HB3	2:E:119:VAL:HG11	1.71	0.72
2:H:36:LEU:CD2	2:H:48:VAL:O	2.36	0.72
1:A:214:SER:HA	1:A:217:THR:HG22	1.70	0.72
2:F:4:ILE:HD12	2:F:61:ALA:HB1	1.72	0.72
2:E:55:PRO:HD2	2:H:103:GLU:OE1	1.90	0.71
1:B:445:VAL:N	1:B:446:ALA:HA	2.04	0.71
2:E:36:LEU:CD2	2:E:47:VAL:HG11	2.20	0.71
2:F:66:ALA:HB3	2:F:92:THR:HG23	1.72	0.71
1:A:34:GLY:HA3	1:A:124:PRO:HB3	1.72	0.71
2:F:36:LEU:HD21	2:F:47:VAL:HG22	1.59	0.71
2:F:150:GLU:OE2	2:F:364:ARG:HB2	1.90	0.71
2:G:8:ALA:HA	2:G:30:ASP:OD1	1.90	0.71
2:H:7:GLY:HA3	2:H:31:ASN:N	2.05	0.71
2:E:84:GLN:HG3	2:E:117:ILE:O	1.90	0.71
2:F:30:ASP:HB2	2:F:36:LEU:CD2	1.76	0.71
1:D:406:TYR:OH	1:D:436:ASN:OD1	2.08	0.70
1:D:317:ILE:HG23	1:D:438:LEU:HD21	1.72	0.70
1:C:143:ILE:HG21	1:C:253:PHE:HD2	1.56	0.70
2:G:92:THR:O	2:G:95:ARG:NH1	2.21	0.70
1:C:353:GLY:O	1:C:357:LYS:NZ	2.23	0.70
1:D:320:THR:HG21	1:D:354:GLY:H	1.56	0.70
2:H:190:ARG:HD3	2:H:203:ILE:HD12	1.74	0.70
1:D:136:TRP:HE1	1:D:193:THR:HG21	1.56	0.70
2:E:8:ALA:O	2:E:35:ARG:NH1	2.23	0.70
1:D:24:PRO:HB2	1:D:39:PHE:CE2	2.27	0.70
2:H:340:GLN:NE2	2:H:347:ALA:H	1.89	0.70
1:A:55:PHE:CD2	1:A:56:PRO:HD2	2.26	0.69
2:F:149:ALA:N	2:F:382:GLU:OE2	2.24	0.69
1:A:177:ARG:HH22	2:H:25:ASP:HB3	1.57	0.69
2:F:95:ARG:NH2	2:F:120:ASP:OD2	2.24	0.69
2:G:46:ARG:HG2	2:G:46:ARG:O	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:60:GLU:OE1	2:H:60:GLU:N	2.25	0.69
2:G:315:ALA:HB1	2:G:326:VAL:HG13	1.72	0.69
2:E:117:ILE:HG21	2:H:118:PRO:HB3	1.73	0.69
1:D:435:LEU:HD11	1:D:471:ILE:HD11	1.74	0.69
1:B:406:TYR:OH	1:B:436:ASN:OD1	2.09	0.69
2:H:87:PHE:HB3	2:H:119:VAL:HG11	1.73	0.69
1:A:370:ARG:HH11	1:A:384:ILE:HG13	1.58	0.68
2:H:153:VAL:HG21	2:H:435:VAL:HG21	1.75	0.68
2:H:20:VAL:HG23	2:H:26:ILE:HG21	1.75	0.68
1:B:394:ARG:NH2	1:D:378:PRO:O	2.25	0.68
1:D:121:ASP:OD1	1:D:226:HIS:ND1	2.26	0.68
2:H:340:GLN:NE2	2:H:375:ARG:HD2	2.07	0.68
2:H:147:SER:HB2	2:H:151:GLN:HA	1.76	0.68
2:H:340:GLN:HE21	2:H:375:ARG:CD	2.04	0.68
2:H:39:LEU:HD21	2:H:47:VAL:CB	2.23	0.68
2:H:76:ASP:OD2	2:H:101:SER:OG	2.07	0.68
2:E:6:LEU:HD22	2:E:29:VAL:HG21	1.77	0.67
2:F:137:ILE:HG23	2:F:300:VAL:HG21	1.77	0.67
2:F:84:GLN:NE2	2:F:116:ALA:O	2.26	0.67
1:A:406:TYR:OH	1:A:436:ASN:OD1	2.11	0.67
2:F:369:ASN:HA	2:F:383:ALA:HA	1.75	0.67
1:B:143:ILE:HG21	1:B:253:PHE:HD2	1.58	0.67
2:G:232:TYR:HD1	2:G:299:ASP:HB3	1.59	0.67
2:H:374:ARG:HG2	2:H:374:ARG:HH11	1.58	0.67
2:G:40:GLN:CA	2:G:40:GLN:HE21	2.00	0.67
2:H:87:PHE:CB	2:H:119:VAL:HG11	2.25	0.67
1:D:24:PRO:HB2	1:D:39:PHE:HE2	1.59	0.66
2:E:55:PRO:HA	2:E:58:LEU:HB2	1.76	0.66
2:H:167:VAL:HG23	2:H:204:GLU:HB3	1.78	0.66
1:A:469:LEU:HB3	1:A:473:THR:HB	1.77	0.66
1:D:420:THR:O	1:D:453:ASN:ND2	2.29	0.66
2:G:117:ILE:HG22	2:G:118:PRO:HD3	1.77	0.66
1:C:13:LEU:HD21	1:C:76:PHE:HD1	1.60	0.66
1:D:343:SER:OG	1:D:436:ASN:ND2	2.27	0.66
2:H:22:GLU:OE2	2:H:364:ARG:NH2	2.28	0.66
1:D:343:SER:HB2	1:D:438:LEU:HD22	1.78	0.66
2:H:36:LEU:HD12	2:H:39:LEU:HD23	1.78	0.66
2:H:98:ARG:HH22	2:H:100:ARG:HD2	1.61	0.66
1:A:469:LEU:HD12	1:A:474:LEU:HB2	1.78	0.65
2:E:159:LYS:HE3	2:E:206:ASP:HB3	1.78	0.65
2:F:148:PHE:HB2	2:F:153:VAL:HG13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:105:LEU:HD21	2:G:128:LEU:HD22	1.78	0.65
1:D:434:THR:HG21	1:D:460:LEU:HD22	1.78	0.65
2:G:129:VAL:HG21	2:G:354:THR:HG22	1.78	0.65
2:E:7:GLY:O	2:E:35:ARG:NH2	2.30	0.65
2:G:155:LEU:HD22	2:G:374:ARG:HH22	1.62	0.65
2:F:346:VAL:HA	2:F:375:ARG:HH12	1.61	0.65
2:F:143:LEU:HD11	2:F:159:LYS:HD2	1.77	0.65
2:E:53:SER:HB3	2:E:82:ALA:HB2	1.78	0.65
2:H:421:ILE:HD13	2:H:423:HIS:HB2	1.79	0.65
1:B:367:GLN:HG3	1:B:400:TRP:CH2	2.32	0.65
2:E:84:GLN:O	2:E:88:THR:HG22	1.97	0.65
2:F:136:LEU:O	2:F:325:LYS:NZ	2.30	0.65
2:H:73:THR:O	2:H:98:ARG:NH1	2.27	0.65
2:G:30:ASP:CG	2:G:35:ARG:CB	2.66	0.64
1:A:430:ALA:HB2	1:A:445:VAL:HG11	1.79	0.64
1:B:178:ILE:CD1	2:F:43:TYR:O	2.46	0.64
2:H:43:TYR:HE1	2:H:46:ARG:H	1.43	0.64
2:H:47:VAL:HG12	2:H:48:VAL:H	1.63	0.64
1:D:466:PHE:HE1	1:D:474:LEU:HD22	1.63	0.64
2:F:232:TYR:HD2	2:F:300:VAL:HG23	1.63	0.64
2:G:377:ALA:O	2:G:441:LYS:N	2.31	0.64
2:H:340:GLN:HE22	2:H:347:ALA:N	1.96	0.64
1:C:420:THR:O	1:C:453:ASN:ND2	2.30	0.63
2:G:30:ASP:OD1	2:G:35:ARG:CB	2.46	0.63
1:B:13:LEU:HD21	1:B:76:PHE:HD1	1.63	0.63
1:C:34:GLY:HA2	1:C:124:PRO:HB3	1.81	0.63
1:A:420:THR:O	1:A:453:ASN:ND2	2.31	0.63
2:G:355:ILE:O	2:G:359:LEU:HB2	1.98	0.63
1:A:93:ASN:HB3	1:A:94:PRO:HD3	1.81	0.63
2:E:153:VAL:HG21	2:E:435:VAL:HG21	1.81	0.63
2:F:242:ASN:OD1	3:F:501:ADP:O1A	2.17	0.63
2:G:340:GLN:HB3	2:G:375:ARG:HG2	1.81	0.63
2:H:268:GLU:O	2:H:272:GLU:HG3	1.99	0.63
2:G:2:LYS:O	2:G:67:ASP:N	2.22	0.63
2:G:319:LYS:HB2	2:G:326:VAL:HG21	1.81	0.63
2:H:10:GLN:HG3	2:H:74:ASN:HD21	1.62	0.63
2:E:9:GLY:O	2:E:35:ARG:NH2	2.32	0.62
2:E:62:GLY:HA3	2:E:90:PHE:CG	2.34	0.62
1:C:139:GLY:HA2	1:C:142:ILE:HD12	1.81	0.62
1:C:326:THR:HG23	1:C:328:PHE:H	1.62	0.62
1:C:406:TYR:OH	1:C:436:ASN:OD1	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:30:ASP:HB3	2:G:35:ARG:CA	2.22	0.62
2:G:7:GLY:O	2:G:30:ASP:OD2	2.17	0.62
1:A:20:THR:HB	1:A:133:PHE:CE2	2.34	0.62
2:F:261:GLU:OE1	2:F:263:ASP:N	2.27	0.62
2:E:300:VAL:HG22	2:E:325:LYS:HB3	1.81	0.62
2:G:234:ARG:HH11	2:G:234:ARG:HB2	1.64	0.62
2:H:47:VAL:HG13	2:H:48:VAL:CA	2.28	0.62
2:H:98:ARG:NH2	2:H:100:ARG:HD2	2.15	0.62
1:A:16:LEU:O	1:A:20:THR:HG23	2.00	0.62
2:E:26:ILE:HD13	2:E:45:LEU:HD12	1.82	0.62
2:F:2:LYS:NZ	2:F:65:ASP:OD2	2.29	0.62
1:B:121:ASP:OD1	1:B:226:HIS:HA	2.00	0.61
2:G:149:ALA:N	2:G:382:GLU:OE2	2.23	0.61
2:H:415:ARG:HH22	2:H:428:ILE:HG22	1.64	0.61
2:F:166:LEU:HB3	2:F:202:ILE:HD11	1.80	0.61
2:H:410:ILE:HG12	2:H:436:MET:HG3	1.81	0.61
1:A:2:GLN:HE22	1:A:61:LYS:HA	1.65	0.61
1:A:67:ARG:HH21	1:C:376:VAL:HG21	1.65	0.61
2:H:33:ALA:HB1	2:H:37:ARG:HD3	1.82	0.61
2:H:431:ASP:N	2:H:431:ASP:OD1	2.32	0.61
2:H:28:ILE:CD1	2:H:43:TYR:HE2	2.01	0.61
1:D:466:PHE:CE1	1:D:474:LEU:HD22	2.35	0.61
1:B:367:GLN:HG3	1:B:400:TRP:HH2	1.64	0.61
1:D:153:LEU:HD11	1:D:472:PHE:HD2	1.66	0.61
1:C:93:ASN:HB3	1:C:94:PRO:HD3	1.81	0.61
2:E:333:GLY:HA2	2:E:336:VAL:HG12	1.81	0.61
2:F:315:ALA:HB1	2:F:326:VAL:HG13	1.82	0.61
2:F:234:ARG:HG3	2:F:298:VAL:HA	1.83	0.60
1:C:88:PHE:HB3	1:C:96:ILE:HD11	1.83	0.60
2:E:315:ALA:HB1	2:E:326:VAL:HG13	1.83	0.60
1:B:233:PHE:N	1:B:234:ASP:HA	2.16	0.60
2:E:336:VAL:HG23	2:E:347:ALA:HB3	1.82	0.60
2:F:112:PHE:HB2	2:F:117:ILE:HD11	1.82	0.60
1:D:218:ILE:HD11	1:D:245:PHE:HD2	1.67	0.60
2:E:261:GLU:O	2:E:282:GLY:N	2.34	0.60
2:E:6:LEU:O	2:E:8:ALA:N	2.29	0.60
1:C:142:ILE:HG12	1:C:468:ARG:NH1	2.12	0.60
1:A:326:THR:HG23	1:A:328:PHE:H	1.64	0.60
2:F:22:GLU:OE1	2:F:22:GLU:N	2.33	0.60
2:F:423:HIS:O	2:F:426:THR:OG1	2.19	0.60
2:H:39:LEU:CD2	2:H:47:VAL:CG1	2.79	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:THR:HA	1:D:438:LEU:HD13	1.84	0.60
1:D:13:LEU:HD21	1:D:76:PHE:HD1	1.67	0.60
2:G:415:ARG:CZ	2:G:429:GLU:OE2	2.50	0.59
2:E:91:ASN:OD1	2:E:93:PRO:HD3	2.01	0.59
2:E:85:VAL:O	2:E:89:LEU:HB2	2.02	0.59
2:E:58:LEU:HD13	2:E:86:ALA:HA	1.83	0.59
2:F:30:ASP:OD1	2:F:36:LEU:HB2	1.99	0.59
1:A:83:ALA:O	1:A:87:PRO:HD2	2.02	0.59
1:B:6:ILE:HG23	1:B:72:ILE:HD13	1.83	0.59
2:F:55:PRO:HB3	2:F:90:PHE:HE2	1.67	0.59
2:G:152:LYS:O	2:G:215:SER:N	2.31	0.59
1:B:460:LEU:O	1:B:464:MET:HG2	2.02	0.59
2:F:325:LYS:HA	2:F:345:ASP:OD2	2.03	0.59
2:G:333:GLY:HA2	2:G:336:VAL:HG12	1.83	0.59
1:B:378:PRO:O	1:D:394:ARG:NH2	2.35	0.59
1:C:469:LEU:HB3	1:C:473:THR:HB	1.85	0.59
2:E:184:ARG:NH2	2:E:422:ALA:O	2.36	0.59
2:E:73:THR:HG22	2:E:75:THR:H	1.68	0.59
2:H:428:ILE:HB	2:H:430:GLN:HG3	1.85	0.59
2:F:137:ILE:HG21	2:F:235:ILE:HD11	1.84	0.58
2:H:262:ARG:NH1	3:H:501:ADP:C2	2.70	0.58
1:D:345:ILE:HG22	1:D:361:ILE:HG13	1.85	0.58
2:G:117:ILE:HG22	2:G:118:PRO:CD	2.32	0.58
1:B:326:THR:HG23	1:B:328:PHE:H	1.67	0.58
2:E:72:VAL:HA	2:E:98:ARG:HB3	1.86	0.58
2:F:39:LEU:HD12	2:F:45:LEU:CB	2.32	0.58
1:B:142:ILE:HG21	1:B:352:THR:HA	1.86	0.58
1:D:16:LEU:O	1:D:20:THR:HG23	2.03	0.58
2:E:143:LEU:HD11	2:E:159:LYS:HD2	1.84	0.58
2:F:268:GLU:O	2:F:272:GLU:HG3	2.02	0.58
2:F:67:ASP:O	2:F:93:PRO:HD2	2.02	0.58
2:H:10:GLN:NE2	2:H:74:ASN:OD1	2.34	0.58
2:H:424:ASP:O	2:H:426:THR:HG23	2.04	0.58
1:B:178:ILE:CG2	2:F:43:TYR:HE2	2.11	0.58
1:C:143:ILE:HG21	1:C:253:PHE:CD2	2.38	0.58
1:C:80:LEU:HB3	1:C:109:LEU:HD11	1.85	0.58
2:E:388:ASP:H	2:E:391:THR:HG22	1.69	0.58
2:H:39:LEU:HD23	2:H:47:VAL:HG11	1.86	0.58
2:E:415:ARG:NH2	2:E:427:VAL:O	2.37	0.57
2:F:183:THR:HA	2:F:213:ALA:HB2	1.86	0.57
1:B:476:ILE:HD11	1:D:375:LEU:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:242:ASN:N	3:F:501:ADP:O1A	2.34	0.57
2:H:102:PRO:O	2:H:106:ALA:N	2.37	0.57
1:A:319:THR:O	1:A:320:THR:HG22	2.04	0.57
2:H:399:ILE:HD12	2:H:426:THR:HG21	1.85	0.57
1:C:375:LEU:HG	1:C:376:VAL:HG12	1.86	0.57
2:E:58:LEU:O	2:E:62:GLY:N	2.26	0.57
1:D:340:LEU:HD22	1:D:442:LEU:HD22	1.87	0.57
2:H:29:VAL:CB	2:H:47:VAL:HG22	2.32	0.57
1:A:76:PHE:HE1	1:A:80:LEU:HD22	1.70	0.57
2:E:359:LEU:O	2:E:362:VAL:HG12	2.04	0.57
2:H:43:TYR:CG	2:H:44:ASP:N	2.72	0.57
1:A:76:PHE:CE1	1:A:80:LEU:HD22	2.38	0.57
2:G:268:GLU:O	2:G:272:GLU:HG3	2.04	0.57
2:G:340:GLN:O	2:G:375:ARG:HG2	2.04	0.57
1:A:28:ALA:CB	1:A:126:ALA:HB2	2.35	0.57
1:A:282:ILE:HD13	1:A:345:ILE:HD12	1.87	0.57
1:B:143:ILE:HG21	1:B:253:PHE:CD2	2.39	0.57
1:C:153:LEU:HD12	1:C:154:GLY:N	2.20	0.57
1:C:461:ILE:HA	1:C:464:MET:SD	2.45	0.57
1:A:460:LEU:O	1:A:464:MET:HG2	2.05	0.56
2:E:84:GLN:HE22	2:H:118:PRO:HG3	1.70	0.56
1:A:435:LEU:HD11	1:A:471:ILE:HD11	1.86	0.56
1:B:266:HIS:ND1	1:B:267:PRO:HD2	2.20	0.56
1:C:16:LEU:O	1:C:20:THR:HG23	2.05	0.56
2:E:101:SER:OG	2:E:104:TYR:HD2	1.88	0.56
2:H:111:LEU:O	2:H:114:SER:OG	2.23	0.56
2:H:4:ILE:HD12	2:H:61:ALA:HB2	1.87	0.56
2:E:376:GLY:HA2	2:E:378:ALA:H	1.70	0.56
2:E:4:ILE:HG23	2:E:69:LEU:HA	1.87	0.56
2:G:26:ILE:CG1	2:G:45:LEU:HD21	1.98	0.56
2:H:3:ILE:HD12	2:H:26:ILE:HG13	1.86	0.56
2:H:327:MET:HA	2:H:346:VAL:O	2.05	0.56
2:H:36:LEU:HD12	2:H:47:VAL:CG1	2.18	0.56
1:B:7:ILE:HG22	1:B:53:CYS:HB3	1.88	0.56
2:E:102:PRO:O	2:E:105:LEU:N	2.38	0.56
2:F:69:LEU:HB3	2:F:95:ARG:HA	1.87	0.56
2:E:224:GLU:OE1	2:E:227:ARG:NH2	2.38	0.56
2:H:11:VAL:O	2:H:14:THR:OG1	2.23	0.56
1:D:138:GLY:O	1:D:142:ILE:HG13	2.06	0.56
1:B:374:ARG:HH21	1:D:394:ARG:HD2	1.71	0.56
2:E:58:LEU:HB3	2:E:90:PHE:HE1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:234:ARG:NH1	2:G:234:ARG:HB2	2.20	0.56
2:H:140:PRO:HG2	2:H:229:GLU:HB3	1.87	0.56
1:B:370:ARG:HH11	1:B:384:ILE:HG13	1.70	0.56
1:B:24:PRO:HB2	1:B:39:PHE:CE2	2.41	0.56
2:E:129:VAL:O	2:E:133:ILE:HG13	2.06	0.56
2:E:30:ASP:OD2	2:E:36:LEU:HG	2.05	0.56
2:F:62:GLY:HA3	2:F:66:ALA:HB2	1.88	0.56
2:H:27:THR:HG22	2:H:46:ARG:HG2	1.87	0.56
2:H:151:GLN:HG2	2:H:151:GLN:O	2.06	0.56
1:A:177:ARG:NH2	2:H:25:ASP:HB3	2.20	0.56
2:G:3:ILE:HG12	2:G:68:MET:HG2	1.87	0.56
2:H:100:ARG:HH12	2:H:127:GLU:CG	2.19	0.56
1:A:20:THR:HB	1:A:133:PHE:HE2	1.71	0.56
1:B:179:ALA:O	1:B:182:ALA:N	2.39	0.56
2:G:100:ARG:HG3	2:G:100:ARG:O	2.06	0.56
1:D:214:SER:HA	1:D:217:THR:HG22	1.88	0.55
1:A:453:ASN:OD1	1:A:454:ASP:N	2.40	0.55
2:E:233:ARG:HH11	2:E:233:ARG:HG2	1.71	0.55
2:E:125:PRO:HD2	2:E:128:LEU:HD21	1.87	0.55
2:G:72:VAL:HG12	2:G:98:ARG:HB3	1.88	0.55
2:H:379:GLU:OE2	2:H:380:ALA:N	2.39	0.55
1:D:149:ILE:HD12	1:D:149:ILE:O	2.05	0.55
2:F:345:ASP:O	2:F:375:ARG:NH2	2.39	0.55
2:F:240:GLY:HA3	2:F:261:GLU:HG2	1.88	0.55
2:F:415:ARG:CZ	2:F:429:GLU:OE2	2.54	0.55
2:G:6:LEU:HD23	2:G:52:ALA:HB1	1.88	0.55
2:H:16:ALA:HB1	2:H:28:ILE:HG12	1.88	0.55
1:C:375:LEU:HG	1:C:376:VAL:N	2.21	0.55
2:H:315:ALA:HB1	2:H:326:VAL:HG13	1.87	0.55
1:C:220:ILE:HD11	1:C:249:SER:HB3	1.89	0.55
1:C:367:GLN:HG3	1:C:400:TRP:CH2	2.42	0.55
1:C:174:MET:HB2	2:G:48:VAL:HG23	1.89	0.55
2:H:27:THR:CG2	2:H:46:ARG:HG2	2.37	0.55
1:D:68:ASP:O	1:D:72:ILE:HG12	2.07	0.55
2:E:134:GLU:O	2:E:137:ILE:HG22	2.06	0.55
2:F:299:ASP:OD2	2:F:324:LYS:HE2	2.06	0.55
2:F:399:ILE:HG23	2:F:410:ILE:HD12	1.88	0.55
2:G:132:TYR:HD2	2:G:135:ARG:HH21	1.55	0.55
1:B:80:LEU:HB3	1:B:109:LEU:HD11	1.89	0.55
2:E:315:ALA:HB1	2:E:326:VAL:CG1	2.36	0.55
2:G:100:ARG:HD3	2:G:126:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:THR:HG23	1:D:328:PHE:H	1.72	0.54
1:A:14:LEU:HD11	1:A:50:GLY:CA	2.37	0.54
2:G:399:ILE:HG23	2:G:410:ILE:HD12	1.90	0.54
2:G:336:VAL:HG23	2:G:347:ALA:HB3	1.89	0.54
2:H:132:TYR:HE1	2:H:348:ILE:HG22	1.71	0.54
1:B:420:THR:O	1:B:453:ASN:ND2	2.40	0.54
1:D:335:LEU:O	1:D:339:LEU:HG	2.07	0.54
2:G:112:PHE:CE1	2:G:118:PRO:HG3	2.43	0.54
2:G:87:PHE:CB	2:G:119:VAL:HG21	2.37	0.54
1:B:18:SER:HB3	1:B:46:LEU:HB2	1.90	0.54
1:C:136:TRP:NE1	1:C:193:THR:HG21	2.22	0.54
2:G:69:LEU:O	2:G:96:VAL:N	2.41	0.54
1:A:15:ALA:O	1:A:18:SER:OG	2.21	0.54
2:E:355:ILE:O	2:E:359:LEU:HB3	2.08	0.54
2:H:340:GLN:NE2	2:H:347:ALA:N	2.55	0.54
1:C:153:LEU:HD12	1:C:154:GLY:H	1.73	0.54
1:D:469:LEU:HD23	1:D:474:LEU:HB2	1.89	0.54
2:H:166:LEU:HD22	2:H:174:LEU:HD21	1.90	0.54
1:A:177:ARG:HH12	2:H:25:ASP:CG	2.12	0.54
1:B:128:LEU:O	1:B:132:GLN:HG2	2.08	0.54
1:B:453:ASN:OD1	1:B:454:ASP:N	2.41	0.54
2:E:58:LEU:HD12	2:E:85:VAL:HG12	1.89	0.54
1:A:28:ALA:HB2	1:A:126:ALA:CB	2.37	0.53
1:B:15:ALA:O	1:B:18:SER:OG	2.20	0.53
1:C:476:ILE:O	1:C:479:THR:OG1	2.22	0.53
1:D:123:LEU:HB3	1:D:128:LEU:HD23	1.91	0.53
2:G:100:ARG:NH1	2:G:126:GLU:OE2	2.41	0.53
2:H:100:ARG:HH12	2:H:127:GLU:HG3	1.73	0.53
2:H:184:ARG:NH2	2:H:421:ILE:O	2.42	0.53
2:H:425:ARG:H	2:H:425:ARG:HD2	1.73	0.53
1:D:253:PHE:CE1	1:D:256:HIS:HD2	2.26	0.53
2:G:111:LEU:O	2:G:118:PRO:HG2	2.09	0.53
2:F:415:ARG:HD3	2:F:429:GLU:OE2	2.08	0.53
2:G:262:ARG:NH1	3:G:501:ADP:N7	2.57	0.53
1:D:8:ARG:NH1	1:D:59:ARG:O	2.42	0.53
2:F:2:LYS:N	2:F:24:ASN:HD21	2.06	0.53
1:C:34:GLY:CA	1:C:124:PRO:HB3	2.39	0.53
1:A:17:PHE:O	1:A:21:MET:HG3	2.09	0.53
1:B:120:LEU:HD12	1:B:227:ASP:HA	1.91	0.53
2:H:43:TYR:CD1	2:H:44:ASP:N	2.77	0.53
1:D:150:LEU:N	1:D:151:PRO:HD3	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:PHE:CZ	1:A:4:ARG:HD3	2.44	0.52
1:D:103:PHE:CD2	1:D:457:LYS:HG2	2.44	0.52
2:E:6:LEU:HA	2:E:29:VAL:HG23	1.91	0.52
2:H:181:ILE:HG23	2:H:217:HIS:HB3	1.90	0.52
2:F:87:PHE:CD2	2:F:118:PRO:HG3	2.44	0.52
1:A:363:LEU:HD12	1:A:399:VAL:HG21	1.91	0.52
1:B:178:ILE:HG22	2:F:43:TYR:HE2	1.73	0.52
2:H:283:ASP:OD1	3:H:501:ADP:N6	2.42	0.52
1:B:283:GLN:HE22	1:B:319:THR:HG23	1.74	0.52
1:A:394:ARG:NH2	1:C:378:PRO:O	2.31	0.52
1:C:68:ASP:O	1:C:72:ILE:HG12	2.08	0.52
2:F:2:LYS:HD2	2:F:65:ASP:O	2.09	0.52
1:A:24:PRO:HB2	1:A:39:PHE:HE2	1.74	0.52
1:B:8:ARG:NH1	1:B:58:ARG:O	2.42	0.52
1:A:68:ASP:O	1:A:72:ILE:HG12	2.10	0.52
1:B:111:THR:HG22	1:B:221:GLY:HA2	1.90	0.52
1:C:243:VAL:HG13	1:C:315:VAL:HG21	1.91	0.52
1:C:345:ILE:CG2	1:C:361:ILE:HG13	2.38	0.52
2:G:232:TYR:CD1	2:G:299:ASP:HB3	2.42	0.52
2:H:299:ASP:OD2	2:H:324:LYS:HE2	2.10	0.52
2:E:8:ALA:C	2:E:35:ARG:HH22	2.13	0.52
2:F:335:TYR:O	2:F:339:VAL:HG22	2.10	0.52
2:G:355:ILE:HG23	2:G:359:LEU:HD22	1.92	0.52
1:B:218:ILE:HD11	1:B:245:PHE:HD2	1.74	0.52
2:F:22:GLU:HB3	2:F:367:ILE:HG12	1.91	0.52
2:F:315:ALA:HB1	2:F:326:VAL:CG1	2.39	0.52
1:D:453:ASN:OD1	1:D:454:ASP:N	2.42	0.52
1:D:93:ASN:HB3	1:D:94:PRO:HD3	1.91	0.52
2:E:72:VAL:HG13	2:E:98:ARG:HD2	1.92	0.52
2:F:336:VAL:O	2:F:340:GLN:HB2	2.09	0.52
2:H:84:GLN:CA	2:H:119:VAL:HG21	2.35	0.52
2:F:4:ILE:CD1	2:F:61:ALA:HB1	2.38	0.51
2:G:107:GLU:HB3	2:G:109:GLU:HG2	1.92	0.51
2:H:29:VAL:HA	2:H:47:VAL:HG21	1.78	0.51
1:A:23:ALA:HB3	1:A:24:PRO:HD2	1.91	0.51
1:C:297:HIS:ND1	1:C:332:PRO:HG3	2.25	0.51
2:G:351:GLN:OE1	2:G:352:GLN:N	2.44	0.51
2:E:217:HIS:O	2:E:221:VAL:HG13	2.11	0.51
2:H:105:LEU:O	2:H:108:LYS:HD2	2.09	0.51
2:H:5:ILE:HG12	2:H:28:ILE:HG23	1.92	0.51
1:A:177:ARG:HH22	2:H:25:ASP:CB	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:HG21	1:A:253:PHE:CD2	2.46	0.51
1:C:348:CYS:HA	1:C:358:VAL:HG12	1.91	0.51
2:H:112:PHE:CA	2:H:117:ILE:HG12	2.28	0.51
2:H:144:GLN:OE1	2:H:375:ARG:NH1	2.40	0.51
1:C:438:LEU:HG	1:C:440:PRO:HD2	1.92	0.51
2:G:111:LEU:HD12	2:G:117:ILE:HB	1.92	0.51
1:A:147:VAL:HG11	1:A:185:LEU:HD11	1.93	0.51
1:A:136:TRP:NE1	1:A:193:THR:HG21	2.21	0.51
1:A:24:PRO:HB2	1:A:39:PHE:CE2	2.45	0.51
1:B:33:ASP:OD2	1:B:125:LYS:HB2	2.11	0.51
1:C:37:VAL:N	1:C:38:PRO:HD2	2.26	0.51
1:C:367:GLN:HG3	1:C:400:TRP:HH2	1.76	0.51
2:E:36:LEU:HD21	2:E:47:VAL:CG1	2.31	0.51
2:E:61:ALA:O	2:E:64:GLN:O	2.29	0.51
2:H:426:THR:O	2:H:428:ILE:HG13	2.10	0.51
1:B:218:ILE:O	1:B:249:SER:OG	2.21	0.51
1:D:220:ILE:HD11	1:D:249:SER:HB3	1.93	0.51
2:G:217:HIS:O	2:G:221:VAL:HG13	2.11	0.51
1:D:30:LEU:O	1:D:31:TYR:HD1	1.93	0.51
2:F:217:HIS:O	2:F:221:VAL:HG13	2.11	0.51
2:F:336:VAL:HG23	2:F:347:ALA:HB3	1.91	0.51
2:G:107:GLU:HB3	2:G:109:GLU:CG	2.41	0.51
2:H:46:ARG:HG3	2:H:47:VAL:H	1.76	0.51
2:H:67:ASP:O	2:H:94:ASN:HB2	2.10	0.51
1:A:443:GLY:O	1:A:446:ALA:HB2	2.11	0.50
1:C:13:LEU:HD21	1:C:76:PHE:CD1	2.45	0.50
2:H:224:GLU:OE1	2:H:227:ARG:NH2	2.44	0.50
1:A:2:GLN:NE2	1:A:61:LYS:HA	2.26	0.50
1:D:353:GLY:O	1:D:468:ARG:NH2	2.29	0.50
2:G:375:ARG:HH11	2:G:376:GLY:H	1.59	0.50
2:H:146:VAL:CG1	2:H:374:ARG:HH12	2.22	0.50
1:A:25:ALA:HB2	1:A:39:PHE:HB3	1.94	0.50
2:F:117:ILE:O	2:F:117:ILE:HG13	2.11	0.50
2:H:108:LYS:HD3	2:H:109:GLU:N	2.26	0.50
1:A:143:ILE:HD12	1:A:144:VAL:N	2.26	0.50
1:B:348:CYS:HA	1:B:358:VAL:HG12	1.94	0.50
1:B:416:GLY:O	1:B:420:THR:HG23	2.12	0.50
1:C:315:VAL:O	1:C:319:THR:OG1	2.20	0.50
2:E:148:PHE:HB2	2:E:153:VAL:HG23	1.94	0.50
2:E:415:ARG:HH12	2:E:429:GLU:HG3	1.76	0.50
2:H:20:VAL:HA	2:H:26:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:70:VAL:HG12	2:H:72:VAL:HG23	1.92	0.50
1:B:103:PHE:CD2	1:B:457:LYS:HG2	2.46	0.50
2:E:365:ALA:HB3	2:E:370:VAL:HG11	1.94	0.50
1:B:178:ILE:HG22	2:F:43:TYR:CE2	2.40	0.50
2:G:39:LEU:CA	2:G:47:VAL:HG11	2.37	0.50
2:H:104:TYR:O	2:H:108:LYS:HB3	2.11	0.50
1:A:367:GLN:HG3	1:A:400:TRP:CH2	2.46	0.50
1:B:20:THR:HB	1:B:133:PHE:CE2	2.46	0.50
1:B:20:THR:HB	1:B:133:PHE:HE2	1.75	0.50
1:C:453:ASN:OD1	1:C:454:ASP:N	2.44	0.50
2:G:140:PRO:HA	2:G:232:TYR:HE2	1.77	0.50
2:H:425:ARG:H	2:H:425:ARG:CD	2.24	0.50
2:H:43:TYR:C	2:H:43:TYR:CD1	2.85	0.50
1:A:103:PHE:CD2	1:A:457:LYS:HG2	2.47	0.50
1:A:80:LEU:HB3	1:A:109:LEU:HD11	1.93	0.50
1:C:99:THR:HG23	1:C:458:TRP:CE2	2.47	0.50
2:F:5:ILE:HA	2:F:70:VAL:HB	1.94	0.50
2:E:335:TYR:CE1	2:G:313:MET:HB3	2.46	0.50
2:E:93:PRO:HA	2:E:95:ARG:NH2	2.27	0.50
1:A:375:LEU:HB2	1:C:476:ILE:HD11	1.93	0.50
2:E:140:PRO:HA	2:E:232:TYR:CE2	2.47	0.50
1:A:144:VAL:O	1:A:148:ALA:HB3	2.12	0.49
1:A:243:VAL:HG13	1:A:315:VAL:HG21	1.94	0.49
2:E:40:GLN:HA	2:E:45:LEU:HD23	1.94	0.49
2:F:224:GLU:OE1	2:F:227:ARG:NH2	2.44	0.49
2:E:234:ARG:HD3	2:E:258:LYS:NZ	2.27	0.49
2:E:65:ASP:OD2	2:E:92:THR:HA	2.11	0.49
2:F:234:ARG:HD3	2:F:297:GLN:O	2.12	0.49
1:A:218:ILE:HD11	1:A:245:PHE:HD2	1.76	0.49
2:G:234:ARG:HD3	2:G:258:LYS:NZ	2.27	0.49
2:H:315:ALA:HB1	2:H:326:VAL:CG1	2.42	0.49
2:H:95:ARG:H	2:H:95:ARG:CD	2.25	0.49
1:A:77:TRP:CD1	1:A:469:LEU:HD21	2.46	0.49
2:E:126:GLU:O	2:E:129:VAL:HG12	2.12	0.49
2:F:181:ILE:HG23	2:F:217:HIS:HB3	1.94	0.49
1:B:145:LEU:O	1:B:149:ILE:HG12	2.12	0.49
1:B:447:LEU:HD13	1:B:448:HIS:CG	2.48	0.49
2:E:96:VAL:HG22	2:E:122:LEU:HB3	1.94	0.49
2:E:55:PRO:HD2	2:H:103:GLU:CD	2.31	0.49
2:F:365:ALA:HB1	2:F:370:VAL:HG21	1.95	0.49
2:G:30:ASP:CB	2:G:35:ARG:CA	2.88	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PHE:HB2	1:A:208:PHE:CZ	2.47	0.49
1:B:68:ASP:O	1:B:72:ILE:HG12	2.13	0.49
1:D:13:LEU:HD21	1:D:76:PHE:CD1	2.48	0.49
1:D:77:TRP:CD1	1:D:469:LEU:HD11	2.48	0.49
2:E:167:VAL:HG23	2:E:204:GLU:HB3	1.94	0.49
2:E:283:ASP:OD1	3:E:501:ADP:N6	2.30	0.49
2:E:6:LEU:HA	2:E:29:VAL:CG2	2.43	0.49
2:F:415:ARG:NH1	2:F:429:GLU:OE2	2.46	0.49
2:G:340:GLN:HB3	2:G:375:ARG:CG	2.43	0.49
2:H:91:ASN:ND2	2:H:91:ASN:O	2.44	0.49
1:C:28:ALA:HB2	1:C:126:ALA:HB2	1.95	0.49
2:E:65:ASP:OD2	2:E:93:PRO:HD2	2.13	0.49
2:F:84:GLN:CD	2:G:117:ILE:HG13	2.33	0.49
1:A:255:LEU:HD21	1:A:270:TYR:HA	1.94	0.49
1:A:348:CYS:HA	1:A:358:VAL:HG12	1.95	0.49
1:C:416:GLY:O	1:C:420:THR:HG23	2.13	0.49
1:C:75:LEU:O	1:C:79:VAL:HB	2.13	0.49
1:D:460:LEU:O	1:D:464:MET:HG2	2.12	0.49
1:D:471:ILE:O	1:D:475:LEU:HD12	2.13	0.49
2:E:183:THR:HA	2:E:213:ALA:HB2	1.94	0.49
2:H:194:PRO:HG3	2:H:439:VAL:HG11	1.95	0.49
2:F:369:ASN:ND2	2:F:369:ASN:O	2.44	0.48
2:H:155:LEU:HD22	2:H:374:ARG:HH21	1.77	0.48
2:G:155:LEU:HD21	2:G:210:PHE:HD2	1.78	0.48
2:H:108:LYS:O	2:H:112:PHE:HB2	2.13	0.48
2:H:117:ILE:O	2:H:117:ILE:HD12	2.14	0.48
2:E:87:PHE:CB	2:E:119:VAL:HG11	2.43	0.48
1:A:371:GLU:HG2	1:C:398:ALA:HA	1.95	0.48
2:E:30:ASP:CG	2:E:36:LEU:HG	2.33	0.48
2:F:45:LEU:HD12	2:F:46:ARG:H	1.78	0.48
2:G:137:ILE:HD13	2:G:300:VAL:HG21	1.94	0.48
2:G:83:CYS:SG	2:G:95:ARG:HG3	2.54	0.48
2:H:217:HIS:O	2:H:221:VAL:HG13	2.14	0.48
2:H:261:GLU:OE2	3:H:501:ADP:H1'	2.13	0.48
1:B:438:LEU:HG	1:B:440:PRO:HD2	1.95	0.48
2:F:261:GLU:OE1	2:F:262:ARG:N	2.46	0.48
1:A:99:THR:HG23	1:A:458:TRP:CE2	2.48	0.48
2:E:118:PRO:O	2:E:119:VAL:HG12	2.13	0.48
2:E:365:ALA:HB1	2:E:370:VAL:HG21	1.96	0.48
2:F:112:PHE:CD2	2:F:119:VAL:HG11	2.49	0.48
2:H:7:GLY:CA	2:H:31:ASN:OD1	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:TRP:CD1	1:B:469:LEU:HD11	2.49	0.48
2:F:155:LEU:HD21	2:F:210:PHE:HD2	1.79	0.48
2:G:51:HIS:O	2:G:57:VAL:HG21	2.13	0.48
2:H:39:LEU:CD2	2:H:47:VAL:CB	2.91	0.48
2:E:102:PRO:O	2:E:105:LEU:HB2	2.14	0.48
2:F:359:LEU:HD12	2:F:363:ARG:HB3	1.95	0.48
2:G:84:GLN:NE2	2:G:85:VAL:HG23	2.28	0.48
2:H:27:THR:HA	2:H:46:ARG:HB3	1.96	0.48
1:C:89:LEU:HD21	1:C:98:VAL:HA	1.95	0.48
1:D:396:VAL:HG12	1:D:400:TRP:CH2	2.49	0.48
1:D:41:THR:O	1:D:45:VAL:HG23	2.14	0.48
2:E:232:TYR:CD1	2:E:299:ASP:HB3	2.48	0.48
2:E:415:ARG:HG3	2:E:432:ASP:OD2	2.13	0.48
2:G:375:ARG:HG3	2:G:376:GLY:N	2.29	0.48
1:C:396:VAL:HG12	1:C:400:TRP:CH2	2.49	0.48
2:E:10:GLN:CD	2:E:10:GLN:H	2.14	0.48
2:F:288:GLU:OE1	2:H:42:LYS:HE3	2.14	0.48
1:A:291:PHE:CZ	1:A:295:LEU:HD11	2.49	0.47
1:A:370:ARG:HE	1:A:374:ARG:NH1	2.11	0.47
1:C:2:GLN:OE1	1:C:2:GLN:HA	2.14	0.47
1:D:291:PHE:CZ	1:D:295:LEU:HD11	2.49	0.47
2:G:291:THR:HA	2:G:295:ILE:HG22	1.96	0.47
2:H:165:PRO:HD3	2:H:229:GLU:HG2	1.96	0.47
1:A:42:THR:HG21	1:A:87:PRO:HG3	1.96	0.47
1:B:464:MET:HG2	1:B:464:MET:H	1.55	0.47
2:E:70:VAL:HG12	2:E:72:VAL:HG23	1.96	0.47
2:F:108:LYS:HB2	2:F:112:PHE:CE1	2.49	0.47
2:H:237:ILE:HG22	2:H:239:GLY:H	1.79	0.47
1:A:174:MET:SD	1:A:175:THR:N	2.87	0.47
1:A:4:ARG:HD2	1:A:4:ARG:HA	1.57	0.47
1:A:55:PHE:HB2	1:A:56:PRO:HD3	1.96	0.47
1:B:178:ILE:HD12	2:F:43:TYR:O	2.13	0.47
1:B:41:THR:O	1:B:45:VAL:HG23	2.14	0.47
2:E:113:LYS:HD2	2:E:114:SER:H	1.79	0.47
2:G:5:ILE:HA	2:G:70:VAL:O	2.14	0.47
2:H:374:ARG:NH1	2:H:374:ARG:HG2	2.26	0.47
2:E:68:MET:HA	2:E:94:ASN:HB2	1.96	0.47
2:H:43:TYR:OH	2:H:46:ARG:N	2.48	0.47
1:B:89:LEU:HD21	1:B:98:VAL:HA	1.96	0.47
1:D:457:LYS:O	1:D:461:ILE:HG13	2.15	0.47
1:D:177:ARG:HH21	2:E:25:ASP:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3:ILE:HG12	2:F:68:MET:HB2	1.96	0.47
2:G:233:ARG:HG3	2:G:233:ARG:HH11	1.80	0.47
2:H:155:LEU:HD22	2:H:374:ARG:NH2	2.28	0.47
1:A:123:LEU:HB3	1:A:128:LEU:HD23	1.96	0.47
1:B:220:ILE:HD11	1:B:249:SER:HB3	1.97	0.47
2:E:36:LEU:HD23	2:E:36:LEU:HA	1.41	0.47
2:G:299:ASP:OD2	2:G:324:LYS:HE2	2.14	0.47
2:H:128:LEU:HD12	2:H:128:LEU:HA	1.77	0.47
2:H:14:THR:O	2:H:17:GLU:HG2	2.14	0.47
1:A:18:SER:HB2	1:A:43:PHE:CD2	2.50	0.47
1:A:4:ARG:NE	1:A:7:ILE:HD11	2.29	0.47
1:B:291:PHE:CZ	1:B:295:LEU:HD11	2.50	0.47
1:D:225:THR:HG23	1:D:226:HIS:CE1	2.49	0.47
2:H:333:GLY:HA2	2:H:336:VAL:HG12	1.96	0.47
2:H:348:ILE:HG13	2:H:348:ILE:O	2.15	0.47
1:A:2:GLN:OE1	1:A:61:LYS:HA	2.14	0.47
1:B:2:GLN:HG3	1:B:5:SER:HB3	1.97	0.47
2:G:153:VAL:HG21	2:G:435:VAL:HG21	1.97	0.47
2:G:5:ILE:HG22	2:G:70:VAL:HB	1.96	0.47
2:H:58:LEU:HB2	2:H:90:PHE:HE2	1.79	0.47
1:B:283:GLN:NE2	1:B:319:THR:HG23	2.30	0.47
1:B:93:ASN:HB3	1:B:94:PRO:HD3	1.97	0.47
1:C:103:PHE:CD2	1:C:457:LYS:HG2	2.50	0.47
2:H:415:ARG:NH2	2:H:428:ILE:HG22	2.30	0.47
1:A:373:LYS:HG2	1:A:382:TYR:CZ	2.50	0.47
1:C:268:LYS:HA	1:C:268:LYS:HD3	1.79	0.47
2:G:182:ASP:HB3	2:G:421:ILE:HD13	1.96	0.47
2:E:5:ILE:HG22	2:E:70:VAL:HB	1.97	0.47
2:E:73:THR:HB	2:E:79:ASN:HB2	1.97	0.47
2:G:362:VAL:HG12	2:G:363:ARG:HG2	1.97	0.47
2:H:118:PRO:C	2:H:119:VAL:HG22	2.35	0.47
2:H:136:LEU:O	2:H:325:LYS:NZ	2.41	0.47
1:B:183:LYS:HD3	1:B:183:LYS:HA	1.73	0.46
2:F:319:LYS:HB2	2:F:326:VAL:HG21	1.96	0.46
2:F:335:TYR:CE1	2:H:313:MET:HB3	2.50	0.46
2:H:108:LYS:HB2	2:H:112:PHE:CD1	2.50	0.46
1:A:465:LEU:HA	1:A:465:LEU:HD23	1.82	0.46
1:C:457:LYS:O	1:C:461:ILE:HG13	2.16	0.46
1:B:236:TYR:OH	1:B:305:ASP:OD1	2.21	0.46
2:F:343:VAL:O	2:F:344:ILE:HD13	2.15	0.46
2:G:120:ASP:OD1	2:G:122:LEU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:HG	1:A:43:PHE:CD2	2.51	0.46
1:A:396:VAL:HG12	1:A:400:TRP:CH2	2.50	0.46
2:G:295:ILE:O	2:G:298:VAL:HG12	2.16	0.46
1:A:174:MET:C	1:A:174:MET:SD	2.94	0.46
1:B:457:LYS:O	1:B:461:ILE:HG13	2.15	0.46
1:C:111:THR:OG1	1:C:142:ILE:HD11	2.16	0.46
1:C:6:ILE:HG23	1:C:72:ILE:HD13	1.98	0.46
2:G:73:THR:OG1	2:G:75:THR:O	2.33	0.46
2:H:101:SER:OG	2:H:104:TYR:HD2	1.97	0.46
1:B:88:PHE:HB3	1:B:96:ILE:HD11	1.97	0.46
1:C:41:THR:O	1:C:45:VAL:HG23	2.15	0.46
1:D:117:ILE:HG13	1:D:120:LEU:HD21	1.97	0.46
2:E:172:SER:HB3	2:E:175:ARG:HH21	1.81	0.46
1:A:145:LEU:O	1:A:149:ILE:N	2.47	0.46
1:B:149:ILE:O	1:B:149:ILE:HG13	2.16	0.46
2:H:261:GLU:OE1	2:H:263:ASP:N	2.30	0.46
2:H:32:ASN:HB3	2:H:33:ALA:H	1.54	0.46
1:A:7:ILE:HG22	1:A:53:CYS:O	2.16	0.46
1:B:128:LEU:HA	1:B:131:ARG:HD3	1.98	0.46
2:E:164:GLY:O	2:E:167:VAL:HG12	2.16	0.46
2:G:261:GLU:OE1	2:G:262:ARG:N	2.49	0.46
2:G:39:LEU:CB	2:G:47:VAL:CG2	2.91	0.46
2:H:340:GLN:CG	2:H:375:ARG:HD2	2.44	0.46
1:A:300:TYR:HD2	1:A:306:ALA:HA	1.81	0.46
2:F:5:ILE:HG12	2:F:28:ILE:HG22	1.97	0.46
2:H:47:VAL:HG12	2:H:48:VAL:N	2.18	0.46
1:A:370:ARG:HH21	1:A:374:ARG:NH1	2.08	0.46
1:B:232:TYR:HA	1:B:233:PHE:HA	1.73	0.46
1:D:218:ILE:O	1:D:249:SER:OG	2.30	0.46
1:D:294:LEU:HD13	1:D:335:LEU:HD12	1.98	0.46
1:D:337:VAL:O	1:D:341:PHE:HD2	1.99	0.46
2:E:125:PRO:HD2	2:E:128:LEU:CD2	2.45	0.46
2:H:415:ARG:NH1	2:H:429:GLU:H	2.14	0.46
1:B:367:GLN:HG2	1:B:384:ILE:HD11	1.97	0.45
1:B:55:PHE:CD1	1:B:56:PRO:HD3	2.51	0.45
2:F:7:GLY:HA2	2:F:72:VAL:O	2.15	0.45
2:H:149:ALA:O	2:H:152:LYS:HB2	2.16	0.45
2:H:36:LEU:HD13	2:H:36:LEU:N	2.30	0.45
1:B:181:THR:O	1:B:185:LEU:HG	2.16	0.45
1:D:145:LEU:O	1:D:149:ILE:HG13	2.16	0.45
1:D:416:GLY:O	1:D:420:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:THR:HG23	1:D:458:TRP:CE2	2.50	0.45
2:E:135:ARG:HG2	2:E:135:ARG:HH11	1.81	0.45
2:F:137:ILE:HD11	2:F:302:ILE:HD11	1.96	0.45
2:F:30:ASP:OD1	2:F:36:LEU:CB	2.54	0.45
2:H:14:THR:HG21	2:H:351:GLN:CD	2.37	0.45
1:B:363:LEU:HD12	1:B:399:VAL:HG21	1.99	0.45
1:C:111:THR:HG22	1:C:221:GLY:HA2	1.97	0.45
1:C:319:THR:O	1:C:320:THR:HG22	2.16	0.45
2:E:87:PHE:HA	2:E:90:PHE:O	2.15	0.45
2:F:415:ARG:HE	2:F:415:ARG:HB2	1.65	0.45
2:F:39:LEU:HD12	2:F:45:LEU:CD2	2.46	0.45
2:G:112:PHE:CE2	2:G:123:ILE:HG21	2.51	0.45
1:B:136:TRP:NE1	1:B:193:THR:HG21	2.26	0.45
1:B:400:TRP:HD1	1:B:403:PHE:HD2	1.64	0.45
1:D:174:MET:HA	2:E:48:VAL:HA	1.97	0.45
1:D:88:PHE:HB3	1:D:96:ILE:HD11	1.99	0.45
2:E:413:VAL:HB	2:E:420:LEU:CD1	2.47	0.45
2:F:340:GLN:CD	2:F:375:ARG:HG2	2.36	0.45
2:F:55:PRO:HB3	2:F:90:PHE:CE2	2.49	0.45
2:G:374:ARG:HG3	2:G:374:ARG:HH11	1.79	0.45
2:G:405:PRO:HG2	2:G:447:VAL:HG22	1.98	0.45
1:A:118:VAL:HB	1:A:448:HIS:CD2	2.52	0.45
1:A:79:VAL:HG12	1:A:80:LEU:HD12	1.97	0.45
1:D:445:VAL:HG12	1:D:445:VAL:O	2.17	0.45
2:F:52:ALA:HA	2:F:53:SER:HA	1.59	0.45
2:G:112:PHE:CD1	2:G:118:PRO:HG3	2.52	0.45
2:G:415:ARG:HD3	2:G:429:GLU:OE2	2.17	0.45
2:H:5:ILE:HG22	2:H:70:VAL:HB	1.98	0.45
1:C:183:LYS:HA	1:C:183:LYS:HD3	1.72	0.45
2:F:167:VAL:CG2	2:F:204:GLU:HB3	2.47	0.45
2:H:373:LEU:HD21	2:H:379:GLU:HG2	1.99	0.45
1:A:367:GLN:HG2	1:A:384:ILE:HD11	1.99	0.45
1:A:268:LYS:HD3	1:A:268:LYS:HA	1.75	0.45
1:D:111:THR:HG22	1:D:221:GLY:HA2	1.99	0.45
1:D:255:LEU:HD21	1:D:270:TYR:HA	1.98	0.45
1:D:367:GLN:HG3	1:D:400:TRP:CZ2	2.51	0.45
2:E:195:ILE:O	2:E:197:PRO:HD3	2.17	0.45
2:G:415:ARG:NH1	2:G:429:GLU:OE2	2.50	0.45
1:A:17:PHE:HZ	1:A:134:LEU:HD21	1.82	0.45
2:G:8:ALA:CA	2:G:30:ASP:OD1	2.61	0.45
2:H:67:ASP:O	2:H:94:ASN:ND2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ALA:O	1:B:32:ARG:HD2	2.17	0.45
1:C:149:ILE:HG13	1:C:149:ILE:O	2.15	0.45
1:C:363:LEU:HD12	1:C:399:VAL:HG21	1.98	0.45
2:E:87:PHE:CD2	2:E:119:VAL:HG11	2.52	0.45
2:F:384:VAL:HG22	2:F:433:HIS:HD1	1.82	0.45
1:A:80:LEU:HD23	1:A:137:PHE:CE2	2.52	0.44
2:E:31:ASN:N	2:E:31:ASN:OD1	2.49	0.44
2:E:150:GLU:OE2	2:E:363:ARG:O	2.34	0.44
2:G:121:HIS:ND1	2:G:122:LEU:HB2	2.31	0.44
2:G:155:LEU:HA	2:G:211:PHE:O	2.17	0.44
2:G:387:GLY:O	2:G:430:GLN:NE2	2.49	0.44
2:H:5:ILE:CG1	2:H:28:ILE:HG23	2.47	0.44
1:A:181:THR:O	1:A:185:LEU:HG	2.17	0.44
1:D:153:LEU:HD11	1:D:472:PHE:CD2	2.51	0.44
2:F:123:ILE:O	2:F:125:PRO:HD3	2.16	0.44
2:F:305:THR:HG23	3:F:501:ADP:C8	2.53	0.44
2:F:6:LEU:HG	2:F:29:VAL:HG21	1.99	0.44
2:H:238:VAL:HA	2:H:260:ILE:HB	2.00	0.44
1:A:89:LEU:HD21	1:A:98:VAL:HA	2.00	0.44
1:C:471:ILE:O	1:C:475:LEU:HB2	2.17	0.44
2:E:5:ILE:O	2:E:29:VAL:HG22	2.17	0.44
2:F:84:GLN:OE1	2:F:117:ILE:HG22	2.17	0.44
2:F:374:ARG:HB3	2:F:375:ARG:H	1.68	0.44
2:H:89:LEU:HB3	2:H:90:PHE:CD1	2.52	0.44
1:A:299:SER:OG	1:A:330:ASP:O	2.33	0.44
1:D:75:LEU:O	1:D:79:VAL:HB	2.17	0.44
2:F:19:LEU:HD12	2:F:20:VAL:HG13	1.98	0.44
2:G:224:GLU:OE1	2:G:227:ARG:NH2	2.51	0.44
2:G:340:GLN:C	2:G:375:ARG:HG2	2.38	0.44
2:H:59:HIS:ND1	2:H:59:HIS:O	2.45	0.44
2:G:300:VAL:HG22	2:G:325:LYS:HB3	2.00	0.44
2:H:373:LEU:HD23	2:H:373:LEU:HA	1.49	0.44
1:C:282:ILE:HD13	1:C:345:ILE:HD12	2.00	0.44
1:D:181:THR:HG22	1:D:257:PHE:CE2	2.52	0.44
2:E:335:TYR:O	2:E:339:VAL:HG22	2.17	0.44
2:E:365:ALA:O	2:E:366:ASP:OD1	2.36	0.44
2:E:6:LEU:HD13	2:E:52:ALA:HB1	2.00	0.44
2:F:317:LEU:HA	2:H:338:LEU:HD11	2.00	0.44
2:F:388:ASP:H	2:F:391:THR:CG2	2.31	0.44
2:F:43:TYR:O	2:F:43:TYR:CD2	2.70	0.44
2:G:59:HIS:HA	2:G:90:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:398:ALA:O	2:H:402:ILE:HG12	2.18	0.44
2:H:379:GLU:HB3	2:H:438:LEU:HB2	1.99	0.44
1:A:457:LYS:O	1:A:461:ILE:HG13	2.18	0.44
1:D:134:LEU:HD23	1:D:134:LEU:HA	1.84	0.44
2:E:167:VAL:CG2	2:E:204:GLU:HB3	2.48	0.44
2:G:71:ALA:O	2:G:97:ALA:HA	2.18	0.44
2:H:197:PRO:O	2:H:200:THR:HG22	2.18	0.44
2:F:335:TYR:CZ	2:H:313:MET:HB3	2.53	0.44
1:C:294:LEU:HD13	1:C:335:LEU:HD12	1.99	0.44
2:H:53:SER:OG	2:H:82:ALA:HA	2.18	0.44
2:E:295:ILE:O	2:E:298:VAL:HG12	2.18	0.44
2:E:300:VAL:HA	2:E:325:LYS:O	2.18	0.44
2:G:123:ILE:O	2:G:123:ILE:HD12	2.18	0.44
2:G:369:ASN:ND2	2:G:369:ASN:O	2.50	0.44
2:H:206:ASP:N	2:H:206:ASP:OD1	2.51	0.44
1:B:181:THR:HG22	1:B:257:PHE:HE2	1.83	0.43
1:C:23:ALA:HB3	1:C:24:PRO:HD3	1.99	0.43
1:D:117:ILE:HG13	1:D:120:LEU:CD2	2.48	0.43
2:G:101:SER:OG	2:G:104:TYR:HD2	2.01	0.43
1:A:441:GLY:O	1:A:446:ALA:HA	2.18	0.43
1:A:464:MET:H	1:A:464:MET:HG2	1.59	0.43
1:C:84:GLY:O	1:C:130:TYR:OH	2.35	0.43
2:E:76:ASP:O	2:E:80:MET:HG3	2.17	0.43
2:G:125:PRO:O	2:G:129:VAL:HG22	2.18	0.43
1:B:121:ASP:OD2	1:B:232:TYR:OH	2.24	0.43
1:B:134:LEU:HA	1:B:134:LEU:HD23	1.89	0.43
1:B:353:GLY:O	1:B:357:LYS:NZ	2.47	0.43
2:E:151:GLN:OE1	2:E:219:ARG:NH2	2.51	0.43
2:F:39:LEU:HD13	2:F:39:LEU:O	2.18	0.43
2:G:108:LYS:HB3	2:G:112:PHE:HB2	2.00	0.43
2:G:86:ALA:HB1	2:G:92:THR:HG21	2.01	0.43
2:H:130:THR:HG23	2:H:247:LEU:HD13	2.00	0.43
2:H:86:ALA:O	2:H:91:ASN:N	2.51	0.43
1:D:89:LEU:HD21	1:D:98:VAL:HA	2.01	0.43
2:G:134:GLU:HA	2:G:137:ILE:HG22	2.00	0.43
2:H:29:VAL:HG11	2:H:48:VAL:HG21	1.99	0.43
1:B:243:VAL:HG13	1:B:315:VAL:HG21	2.00	0.43
2:E:103:GLU:OE1	2:H:55:PRO:HD2	2.17	0.43
2:G:87:PHE:HB3	2:G:119:VAL:HG21	1.99	0.43
2:G:374:ARG:NH1	2:G:374:ARG:HG3	2.34	0.43
2:E:261:GLU:OE1	2:E:263:ASP:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2:LYS:HD3	2:E:64:GLN:HE22	1.84	0.43
2:F:232:TYR:CD1	2:F:232:TYR:N	2.87	0.43
2:H:250:ARG:HB2	2:H:250:ARG:HE	1.71	0.43
1:B:445:VAL:O	1:B:449:PHE:HA	2.18	0.43
1:C:218:ILE:O	1:C:249:SER:OG	2.24	0.43
1:C:438:LEU:HB3	1:C:439:GLY:CA	2.42	0.43
1:D:297:HIS:ND1	1:D:332:PRO:HG3	2.34	0.43
1:B:178:ILE:HG21	2:F:43:TYR:O	2.18	0.43
2:G:28:ILE:HG23	2:G:45:LEU:HD13	2.00	0.43
2:H:430:GLN:O	2:H:430:GLN:OE1	2.37	0.43
1:B:37:VAL:O	1:B:41:THR:OG1	2.24	0.43
1:C:117:ILE:HD11	1:C:131:ARG:NE	2.34	0.43
1:C:369:ALA:O	1:C:373:LYS:HG3	2.18	0.43
2:E:238:VAL:HG12	2:E:260:ILE:HB	2.00	0.43
2:E:58:LEU:HD23	2:E:58:LEU:HA	1.81	0.43
2:F:76:ASP:O	2:F:80:MET:HG3	2.19	0.43
2:G:375:ARG:HD2	2:G:376:GLY:H	1.83	0.43
2:H:295:ILE:O	2:H:298:VAL:HG12	2.19	0.43
2:H:58:LEU:HB2	2:H:90:PHE:CE2	2.54	0.43
1:A:6:ILE:HG23	1:A:72:ILE:HD12	2.00	0.43
1:D:61:LYS:HB2	1:D:61:LYS:HE3	1.89	0.43
2:E:6:LEU:HD22	2:E:29:VAL:CG2	2.48	0.43
2:F:167:VAL:HG23	2:F:204:GLU:HB3	2.01	0.43
2:H:113:LYS:HE2	2:H:113:LYS:HB2	1.86	0.43
2:H:16:ALA:CB	2:H:28:ILE:HG12	2.48	0.43
2:H:379:GLU:CB	2:H:438:LEU:HB2	2.49	0.43
1:A:6:ILE:HG12	1:A:72:ILE:HD11	2.01	0.43
1:B:430:ALA:HB1	1:B:460:LEU:HD21	2.01	0.43
1:C:253:PHE:N	1:C:350:GLY:O	2.34	0.43
1:D:348:CYS:HA	1:D:358:VAL:HG12	2.00	0.43
1:D:371:GLU:O	1:D:375:LEU:HD13	2.19	0.43
2:F:215:SER:O	2:F:219:ARG:HG3	2.18	0.43
2:F:371:SER:HA	2:F:381:ILE:HA	2.00	0.43
2:G:5:ILE:O	2:G:29:VAL:HG22	2.19	0.43
2:G:73:THR:OG1	2:G:79:ASN:HB2	2.19	0.43
2:H:340:GLN:HG3	2:H:344:ILE:O	2.18	0.43
2:H:367:ILE:HG22	2:H:368:VAL:N	2.34	0.43
2:H:76:ASP:N	2:H:76:ASP:OD1	2.50	0.43
2:H:90:PHE:CD1	2:H:90:PHE:N	2.87	0.43
1:B:446:ALA:HB3	1:B:447:LEU:C	2.40	0.42
2:F:170:ALA:HA	2:F:201:THR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:28:ILE:HD13	2:F:45:LEU:HD21	2.01	0.42
2:G:134:GLU:O	2:G:138:GLN:HB2	2.19	0.42
2:G:177:HIS:O	2:G:177:HIS:ND1	2.51	0.42
2:G:233:ARG:HA	2:G:233:ARG:HD2	1.88	0.42
2:G:59:HIS:O	2:G:59:HIS:ND1	2.46	0.42
1:B:150:LEU:N	1:B:151:PRO:CD	2.82	0.42
1:B:320:THR:HG21	1:B:354:GLY:N	2.34	0.42
2:E:167:VAL:HG23	2:E:204:GLU:CB	2.49	0.42
2:E:26:ILE:HD12	2:E:26:ILE:O	2.18	0.42
2:F:368:VAL:O	2:F:384:VAL:HG23	2.19	0.42
2:G:70:VAL:HA	2:G:96:VAL:HB	2.01	0.42
1:A:18:SER:O	1:A:43:PHE:HD2	2.02	0.42
2:E:120:ASP:OD2	2:E:123:ILE:HG22	2.19	0.42
2:E:122:LEU:HD13	2:E:123:ILE:N	2.35	0.42
2:F:140:PRO:HG2	2:F:229:GLU:HB3	2.02	0.42
2:F:51:HIS:CD2	2:F:52:ALA:H	2.37	0.42
1:A:41:THR:O	1:A:45:VAL:HG23	2.19	0.42
1:B:174:MET:HG3	1:B:176:PRO:HG3	2.00	0.42
1:D:92:ASP:OD1	1:D:92:ASP:N	2.51	0.42
2:G:261:GLU:O	2:G:282:GLY:N	2.48	0.42
2:G:31:ASN:N	2:G:35:ARG:CB	2.82	0.42
2:H:96:VAL:HG23	2:H:122:LEU:HG	2.02	0.42
1:A:3:PHE:CE1	1:A:4:ARG:HD3	2.53	0.42
1:B:181:THR:HG22	1:B:257:PHE:CE2	2.54	0.42
1:D:17:PHE:HZ	1:D:134:LEU:HD21	1.84	0.42
1:D:455:LYS:H	1:D:455:LYS:HG3	1.63	0.42
2:F:153:VAL:HG11	2:F:435:VAL:HG21	2.02	0.42
2:G:167:VAL:CG2	2:G:204:GLU:HB3	2.49	0.42
2:G:28:ILE:HD11	2:G:39:LEU:HA	2.02	0.42
2:H:39:LEU:HD22	2:H:47:VAL:HG21	2.00	0.42
1:A:430:ALA:HB1	1:A:460:LEU:HD21	2.00	0.42
2:E:366:ASP:HA	2:E:384:VAL:HG21	2.00	0.42
2:E:117:ILE:CG2	2:H:118:PRO:HB3	2.48	0.42
2:H:4:ILE:CD1	2:H:61:ALA:HB2	2.49	0.42
1:B:275:GLU:HG3	1:B:358:VAL:HG13	2.02	0.42
1:C:446:ALA:HA	1:C:447:LEU:HA	1.62	0.42
2:F:177:HIS:ND1	2:F:177:HIS:O	2.52	0.42
2:F:295:ILE:O	2:F:298:VAL:HG12	2.20	0.42
2:G:143:LEU:HD23	2:G:345:ASP:O	2.20	0.42
1:A:2:GLN:HG2	1:A:2:GLN:O	2.20	0.42
2:E:14:THR:HG22	2:E:355:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:39:LEU:HD22	2:F:39:LEU:HA	1.39	0.42
1:A:150:LEU:N	1:A:151:PRO:CD	2.82	0.42
1:B:178:ILE:HD12	2:F:43:TYR:HD2	1.85	0.42
1:A:20:THR:HB	1:A:133:PHE:CZ	2.55	0.42
1:A:111:THR:HG22	1:A:221:GLY:HA2	2.01	0.42
1:C:343:SER:OG	1:C:436:ASN:ND2	2.46	0.42
1:C:391:LEU:HD23	1:C:391:LEU:HA	1.85	0.42
2:E:26:ILE:HD13	2:E:45:LEU:CD1	2.50	0.42
2:G:152:LYS:O	2:G:214:ALA:HA	2.19	0.42
2:G:340:GLN:CB	2:G:375:ARG:HG2	2.50	0.42
2:H:305:THR:HG23	3:H:501:ADP:C4	2.55	0.42
1:A:121:ASP:OD1	1:A:226:HIS:ND1	2.49	0.41
1:A:374:ARG:O	1:A:374:ARG:HG2	2.19	0.41
1:B:282:ILE:HD13	1:B:345:ILE:HD12	2.02	0.41
2:E:40:GLN:HA	2:E:45:LEU:CD2	2.50	0.41
2:H:89:LEU:HB3	2:H:90:PHE:CE1	2.55	0.41
1:A:183:LYS:HD3	1:A:183:LYS:HA	1.73	0.41
1:D:317:ILE:HG21	1:D:339:LEU:HB3	2.02	0.41
2:E:14:THR:HG22	2:E:355:ILE:CD1	2.50	0.41
2:F:19:LEU:CD1	2:F:20:VAL:HG13	2.50	0.41
2:G:237:ILE:HG22	2:G:239:GLY:H	1.86	0.41
1:A:441:GLY:O	1:A:445:VAL:O	2.39	0.41
1:C:123:LEU:HB3	1:C:128:LEU:HD23	2.03	0.41
1:D:108:ALA:HB2	1:D:223:PHE:HE2	1.85	0.41
1:D:43:PHE:CD2	1:D:43:PHE:C	2.93	0.41
1:D:80:LEU:HB3	1:D:109:LEU:HD11	2.02	0.41
2:E:148:PHE:HB2	2:E:153:VAL:CG2	2.50	0.41
2:E:68:MET:HA	2:E:94:ASN:CB	2.50	0.41
2:F:36:LEU:HD22	2:F:47:VAL:CG2	2.18	0.41
2:G:117:ILE:HG21	2:G:117:ILE:HD13	1.78	0.41
2:G:363:ARG:O	2:G:364:ARG:HG2	2.20	0.41
2:H:261:GLU:OE1	2:H:262:ARG:N	2.54	0.41
1:B:75:LEU:O	1:B:79:VAL:HB	2.21	0.41
1:C:224:SER:HB3	1:C:229:SER:HA	2.02	0.41
1:D:201:TRP:CE3	1:D:202:LEU:HD12	2.55	0.41
1:D:197:ALA:N	1:D:214:SER:OG	2.52	0.41
1:D:243:VAL:HG13	1:D:315:VAL:HG21	2.01	0.41
1:D:287:PHE:CE1	1:D:311:LEU:HB2	2.55	0.41
1:B:375:LEU:CB	1:D:476:ILE:HD11	2.51	0.41
1:D:74:VAL:O	1:D:78:THR:OG1	2.30	0.41
2:E:40:GLN:NE2	2:E:45:LEU:HD23	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:47:VAL:HG12	2:E:48:VAL:N	2.35	0.41
2:G:183:THR:HA	2:G:213:ALA:HB2	2.03	0.41
2:G:336:VAL:O	2:G:375:ARG:HD3	2.21	0.41
2:H:204:GLU:OE1	2:H:204:GLU:N	2.27	0.41
2:H:36:LEU:N	2:H:36:LEU:CD1	2.84	0.41
1:A:43:PHE:C	1:A:43:PHE:CD1	2.94	0.41
1:C:20:THR:HB	1:C:133:PHE:CE2	2.55	0.41
1:A:374:ARG:HD3	1:C:394:ARG:CZ	2.50	0.41
2:G:166:LEU:HD22	2:G:174:LEU:HD21	2.01	0.41
2:G:129:VAL:CG2	2:G:354:THR:HG22	2.47	0.41
1:A:84:GLY:HA2	1:A:130:TYR:OH	2.20	0.41
1:B:106:PHE:O	1:B:110:THR:OG1	2.26	0.41
1:B:73:VAL:O	1:B:77:TRP:HD1	2.04	0.41
1:C:33:ASP:OD1	1:C:33:ASP:N	2.53	0.41
2:E:141:GLY:O	2:E:158:VAL:HA	2.20	0.41
2:E:151:GLN:HB2	2:E:360:THR:CG2	2.50	0.41
2:F:40:GLN:OE1	2:F:40:GLN:HA	2.21	0.41
2:F:59:HIS:HB2	2:F:90:PHE:CE1	2.55	0.41
2:H:330:ILE:HG22	2:H:332:ARG:H	1.86	0.41
2:H:36:LEU:HA	2:H:36:LEU:HD12	1.73	0.41
2:H:69:LEU:O	2:H:96:VAL:HG12	2.20	0.41
1:A:139:GLY:O	1:A:143:ILE:HG13	2.21	0.41
1:C:175:THR:O	2:G:46:ARG:HB2	2.20	0.41
1:B:398:ALA:HA	1:D:371:GLU:HG2	2.03	0.41
2:E:295:ILE:HD12	2:E:298:VAL:HG11	2.02	0.41
2:E:53:SER:HB3	2:E:82:ALA:CB	2.48	0.41
2:E:6:LEU:O	2:E:72:VAL:O	2.39	0.41
3:F:501:ADP:C5'	3:F:501:ADP:O3B	2.69	0.41
1:A:376:VAL:O	1:A:378:PRO:HD3	2.21	0.41
1:B:142:ILE:HB	1:B:352:THR:HG22	2.02	0.41
1:C:147:VAL:HG11	1:C:185:LEU:HD11	2.02	0.41
1:C:455:LYS:H	1:C:455:LYS:HG3	1.66	0.41
1:D:363:LEU:HD12	1:D:399:VAL:HG21	2.03	0.41
2:G:98:ARG:HA	2:G:124:ALA:O	2.21	0.41
2:G:99:ILE:HG13	2:G:99:ILE:O	2.20	0.41
1:A:177:ARG:HB2	1:A:180:GLU:HB3	2.02	0.41
1:A:55:PHE:CD2	1:A:56:PRO:CD	3.01	0.41
1:B:268:LYS:HA	1:B:268:LYS:HD3	1.79	0.41
1:C:437:ASN:OD1	1:C:468:ARG:NH2	2.53	0.41
1:D:391:LEU:HD23	1:D:391:LEU:HA	1.87	0.41
2:E:413:VAL:HB	2:E:420:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:133:ILE:O	2:G:137:ILE:HG22	2.21	0.41
2:G:238:VAL:HA	2:G:260:ILE:HB	2.02	0.41
2:G:345:ASP:N	2:G:345:ASP:OD1	2.53	0.41
2:H:364:ARG:HB2	2:H:366:ASP:OD2	2.21	0.41
2:H:399:ILE:HB	2:H:426:THR:HG21	2.03	0.41
1:A:455:LYS:H	1:A:455:LYS:HG3	1.64	0.41
1:A:50:GLY:O	1:A:54:TRP:N	2.51	0.41
1:B:438:LEU:HB3	1:B:439:GLY:CA	2.43	0.41
1:C:230:MET:HE1	1:C:238:ILE:HG22	2.02	0.41
1:C:465:LEU:HA	1:C:465:LEU:HD23	1.86	0.41
1:D:22:LEU:HG	1:D:43:PHE:HE1	1.85	0.41
2:F:241:GLY:CA	3:F:501:ADP:O1A	2.69	0.41
1:A:416:GLY:O	1:A:420:THR:HG23	2.20	0.41
2:E:136:LEU:O	2:E:325:LYS:NZ	2.53	0.41
2:F:109:GLU:HA	2:F:110:ALA:HA	1.76	0.41
2:F:95:ARG:HE	2:F:95:ARG:H	1.69	0.41
2:G:287:GLN:HB3	2:G:321:MET:CE	2.51	0.41
2:G:69:LEU:O	2:G:95:ARG:HA	2.21	0.41
2:H:96:VAL:HG23	2:H:122:LEU:HB3	2.02	0.41
1:A:14:LEU:HD11	1:A:50:GLY:HA2	2.03	0.40
1:B:396:VAL:HG12	1:B:400:TRP:CH2	2.56	0.40
1:D:142:ILE:HG21	1:D:352:THR:HG22	2.01	0.40
1:D:243:VAL:HG13	1:D:315:VAL:HG11	2.04	0.40
2:E:62:GLY:HA3	2:E:90:PHE:CD1	2.56	0.40
2:G:196:ARG:H	2:G:196:ARG:HG2	1.25	0.40
2:H:100:ARG:NH1	2:H:127:GLU:CD	2.73	0.40
2:H:19:LEU:HD11	2:H:358:LEU:HD11	2.02	0.40
2:H:238:VAL:HG22	2:H:303:ALA:HA	2.02	0.40
2:H:345:ASP:N	2:H:345:ASP:OD1	2.54	0.40
1:B:10:VAL:HG13	1:B:79:VAL:HG11	2.03	0.40
2:E:244:GLY:HA2	2:E:304:LEU:HD12	2.04	0.40
2:F:444:VAL:N	2:F:445:PRO:HD2	2.36	0.40
2:F:261:GLU:CD	3:F:501:ADP:O2'	2.51	0.40
2:H:358:LEU:O	2:H:362:VAL:N	2.54	0.40
1:B:370:ARG:HE	1:B:374:ARG:NH1	2.19	0.40
1:D:477:LEU:O	1:D:483:TRP:NE1	2.53	0.40
2:E:365:ALA:CB	2:E:370:VAL:HG21	2.51	0.40
1:B:178:ILE:HD12	2:F:43:TYR:HB2	2.02	0.40
2:G:295:ILE:HD12	2:G:298:VAL:HG11	2.02	0.40
2:H:244:GLY:HA2	2:H:304:LEU:HD12	2.03	0.40
1:B:391:LEU:HD23	1:B:391:LEU:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:LEU:HA	1:B:465:LEU:HD23	1.91	0.40
1:C:471:ILE:HG22	1:C:471:ILE:O	2.22	0.40
2:F:156:VAL:O	2:F:210:PHE:HA	2.21	0.40
2:G:332:ARG:HA	2:G:332:ARG:HD3	1.89	0.40
2:G:370:VAL:HG13	2:G:382:GLU:HB3	2.04	0.40
2:G:398:ALA:HA	2:G:427:VAL:HA	2.03	0.40
2:H:45:LEU:O	2:H:46:ARG:HD3	2.22	0.40
1:A:367:GLN:HG3	1:A:400:TRP:HH2	1.84	0.40
1:C:142:ILE:HG21	1:C:352:THR:HA	2.03	0.40
1:D:268:LYS:HD3	1:D:268:LYS:HA	1.78	0.40
2:F:77:GLU:H	2:F:77:GLU:HG2	1.69	0.40
2:F:87:PHE:HB3	2:F:118:PRO:HG3	2.04	0.40
2:G:218:ILE:HD13	2:G:218:ILE:HA	1.94	0.40
2:H:52:ALA:HA	2:H:53:SER:HA	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	453/485 (93%)	428 (94%)	21 (5%)	4 (1%)	17	58
1	B	453/485 (93%)	434 (96%)	18 (4%)	1 (0%)	47	80
1	C	453/485 (93%)	431 (95%)	21 (5%)	1 (0%)	47	80
1	D	453/485 (93%)	432 (95%)	19 (4%)	2 (0%)	34	71
2	E	453/458 (99%)	437 (96%)	16 (4%)	0	100	100
2	F	453/458 (99%)	426 (94%)	24 (5%)	3 (1%)	22	62
2	G	453/458 (99%)	429 (95%)	22 (5%)	2 (0%)	34	71
2	H	453/458 (99%)	423 (93%)	27 (6%)	3 (1%)	22	62
All	All	3624/3772 (96%)	3440 (95%)	168 (5%)	16 (0%)	34	71

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	PHE
1	A	471	ILE
1	B	471	ILE
1	D	471	ILE
2	G	117	ILE
2	H	47	VAL
2	H	119	VAL
1	C	471	ILE
2	H	48	VAL
2	F	93	PRO
1	A	56	PRO
2	F	368	VAL
2	G	125	PRO
1	D	440	PRO
2	F	197	PRO
1	A	150	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/395 (94%)	351 (95%)	20 (5%)	22	56
1	B	373/395 (94%)	362 (97%)	11 (3%)	42	72
1	C	373/395 (94%)	358 (96%)	15 (4%)	31	65
1	D	373/395 (94%)	362 (97%)	11 (3%)	42	72
2	E	374/378 (99%)	357 (96%)	17 (4%)	27	62
2	F	375/378 (99%)	359 (96%)	16 (4%)	29	63
2	G	368/378 (97%)	348 (95%)	20 (5%)	22	56
2	H	374/378 (99%)	350 (94%)	24 (6%)	17	51
All	All	2981/3092 (96%)	2847 (96%)	134 (4%)	27	62

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	4	ARG
1	A	5	SER
1	A	17	PHE
1	A	48	PHE
1	A	76	PHE
1	A	107	SER
1	A	175	THR
1	A	177	ARG
1	A	214	SER
1	A	223	PHE
1	A	229	SER
1	A	230	MET
1	A	251	CYS
1	A	269	TYR
1	A	342	SER
1	A	356	MET
1	A	367	GLN
1	A	448	HIS
1	A	466	PHE
1	B	4	ARG
1	B	150	LEU
1	B	214	SER
1	B	229	SER
1	B	233	PHE
1	B	251	CYS
1	B	253	PHE
1	B	266	HIS
1	B	269	TYR
1	B	342	SER
1	B	367	GLN
1	C	4	ARG
1	C	52	MET
1	C	55	PHE
1	C	107	SER
1	C	150	LEU
1	C	214	SER
1	C	232	TYR
1	C	251	CYS
1	C	253	PHE
1	C	342	SER
1	C	367	GLN
1	C	451	ASP

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Mol	Chain	Res	Type
1	C	466	PHE
1	C	468	ARG
1	C	475	LEU
1	D	2	GLN
1	D	43	PHE
1	D	55	PHE
1	D	107	SER
1	D	174	MET
1	D	251	CYS
1	D	253	PHE
1	D	269	TYR
1	D	364	LEU
1	D	367	GLN
1	D	394	ARG
2	E	30	ASP
2	E	31	ASN
2	E	49	ASN
2	E	64	GLN
2	E	65	ASP
2	E	95	ARG
2	E	113	LYS
2	E	196	ARG
2	E	233	ARG
2	E	261	GLU
2	E	264	TYR
2	E	366	ASP
2	E	379	GLU
2	E	415	ARG
2	E	418	GLU
2	E	420	LEU
2	E	456	PHE
2	F	37	ARG
2	F	39	LEU
2	F	43	TYR
2	F	90	PHE
2	F	91	ASN
2	F	95	ARG
2	F	112	PHE
2	F	113	LYS
2	F	132	TYR
2	F	229	GLU
2	F	234	ARG

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Mol	Chain	Res	Type
2	F	264	TYR
2	F	369	ASN
2	F	379	GLU
2	F	424	ASP
2	F	456	PHE
2	G	30	ASP
2	G	31	ASN
2	G	40	GLN
2	G	41	ASP
2	G	44	ASP
2	G	45	LEU
2	G	46	ARG
2	G	47	VAL
2	G	95	ARG
2	G	132	TYR
2	G	151	GLN
2	G	196	ARG
2	G	242	ASN
2	G	261	GLU
2	G	264	TYR
2	G	351	GLN
2	G	374	ARG
2	G	379	GLU
2	G	424	ASP
2	G	456	PHE
2	H	32	ASN
2	H	34	ASP
2	H	36	LEU
2	H	38	GLU
2	H	43	TYR
2	H	46	ARG
2	H	48	VAL
2	H	49	ASN
2	H	54	HIS
2	H	91	ASN
2	H	95	ARG
2	H	108	LYS
2	H	113	LYS
2	H	135	ARG
2	H	206	ASP
2	H	242	ASN
2	H	264	TYR

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Mol	Chain	Res	Type
2	H	363	ARG
2	H	364	ARG
2	H	379	GLU
2	H	425	ARG
2	H	430	GLN
2	H	432	ASP
2	H	456	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	74	ASN
2	G	40	GLN
2	G	84	GLN
2	H	10	GLN
2	H	74	ASN
2	H	84	GLN
2	H	340	GLN

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 carbohydrates 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
3	ADP	G	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.51	4 (13%)
3	ADP	H	501	-	24,29,29	1.13	2 (8%)	29,45,45	2.17	7 (24%)
3	ADP	E	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.37	4 (13%)
3	ADP	F	501	-	24,29,29	1.08	1 (4%)	29,45,45	2.27	8 (27%)

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
3	ADP	G	501	-	-	5/12/32/32	0/3/3/3
3	ADP	H	501	-	-	5/12/32/32	0/3/3/3
3	ADP	E	501	-	-	4/12/32/32	0/3/3/3
3	ADP	F	501	-	-	7/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	501	ADP	C2'-C1'	-3.30	1.48	1.53
3	F	501	ADP	C2'-C1'	-2.76	1.49	1.53
3	E	501	ADP	C5-C4	2.50	1.47	1.40
3	G	501	ADP	C5-C4	2.44	1.47	1.40
3	H	501	ADP	C5-C4	2.05	1.46	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	501	ADP	PA-O3A-PB	-6.94	109.03	132.83
3	H	501	ADP	PA-O3A-PB	-6.26	111.36	132.83
3	F	501	ADP	O4'-C1'-C2'	-5.50	98.89	106.93
3	H	501	ADP	O4'-C1'-C2'	-5.34	99.13	106.93
3	H	501	ADP	C3'-C2'-C1'	-4.09	94.82	100.98
3	G	501	ADP	PA-O3A-PB	-3.57	120.56	132.83
3	F	501	ADP	C4-C5-N7	-3.51	105.74	109.40
3	H	501	ADP	N3-C2-N1	-3.33	123.47	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	501	ADP	N3-C2-N1	-3.21	123.66	128.68
3	E	501	ADP	N3-C2-N1	-3.13	123.79	128.68
3	E	501	ADP	C3'-C2'-C1'	2.93	105.39	100.98
3	G	501	ADP	C4-C5-N7	-2.92	106.35	109.40
3	E	501	ADP	PA-O3A-PB	-2.84	123.09	132.83
3	F	501	ADP	N3-C2-N1	-2.79	124.31	128.68
3	G	501	ADP	O4'-C1'-C2'	-2.77	102.88	106.93
3	F	501	ADP	O3'-C3'-C4'	-2.70	103.25	111.05
3	E	501	ADP	C4-C5-N7	-2.61	106.68	109.40
3	H	501	ADP	C2-N1-C6	2.46	122.97	118.75
3	F	501	ADP	O3B-PB-O2B	2.34	116.58	107.64
3	H	501	ADP	O3'-C3'-C4'	-2.33	104.31	111.05
3	H	501	ADP	N6-C6-N1	2.31	123.37	118.57
3	F	501	ADP	O2A-PA-O1A	2.07	122.46	112.24
3	F	501	ADP	O3A-PB-O1B	-2.04	99.87	111.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

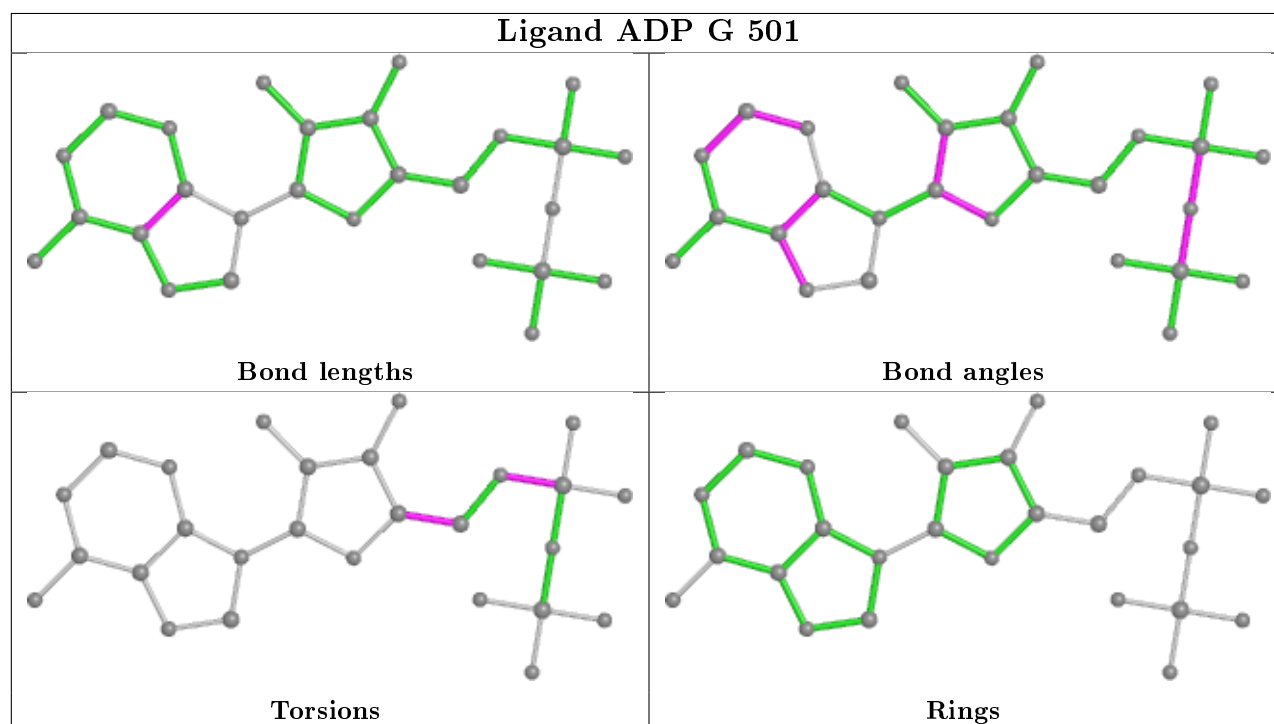
Mol	Chain	Res	Type	Atoms
3	G	501	ADP	C5'-O5'-PA-O2A
3	H	501	ADP	C5'-O5'-PA-O1A
3	H	501	ADP	C5'-O5'-PA-O3A
3	H	501	ADP	C3'-C4'-C5'-O5'
3	E	501	ADP	PA-O3A-PB-O2B
3	E	501	ADP	C5'-O5'-PA-O1A
3	F	501	ADP	C5'-O5'-PA-O1A
3	F	501	ADP	C5'-O5'-PA-O2A
3	F	501	ADP	O4'-C4'-C5'-O5'
3	F	501	ADP	C3'-C4'-C5'-O5'
3	G	501	ADP	C3'-C4'-C5'-O5'
3	H	501	ADP	O4'-C4'-C5'-O5'
3	G	501	ADP	O4'-C4'-C5'-O5'
3	F	501	ADP	PB-O3A-PA-O5'
3	G	501	ADP	C5'-O5'-PA-O3A
3	E	501	ADP	C5'-O5'-PA-O3A
3	H	501	ADP	C5'-O5'-PA-O2A
3	F	501	ADP	C4'-C5'-O5'-PA
3	F	501	ADP	C5'-O5'-PA-O3A
3	G	501	ADP	C5'-O5'-PA-O1A
3	E	501	ADP	C5'-O5'-PA-O2A

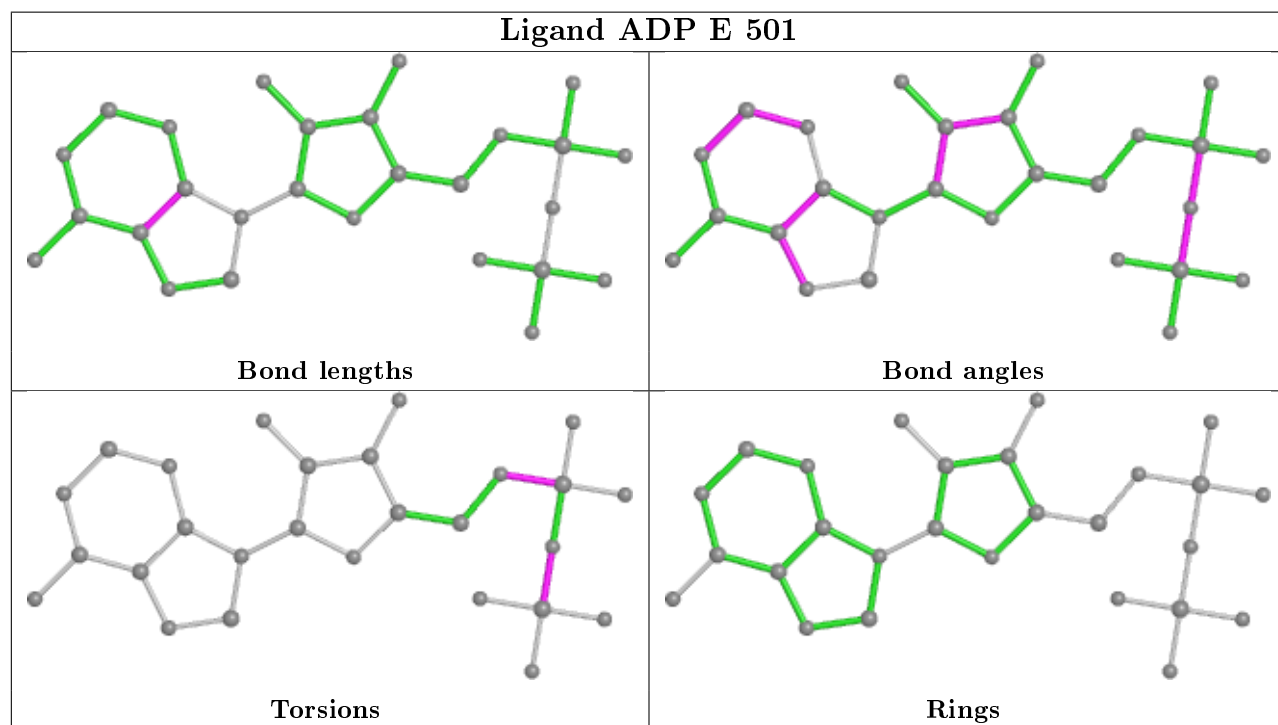
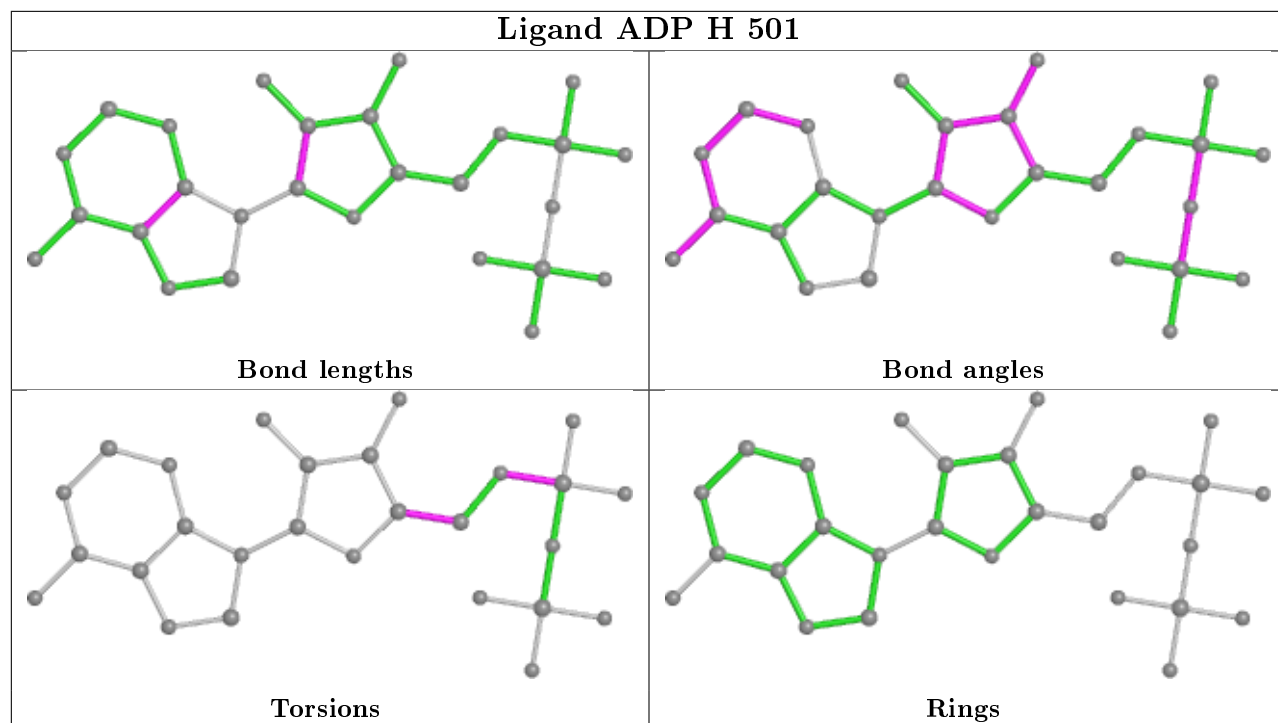
There are no ring outliers.

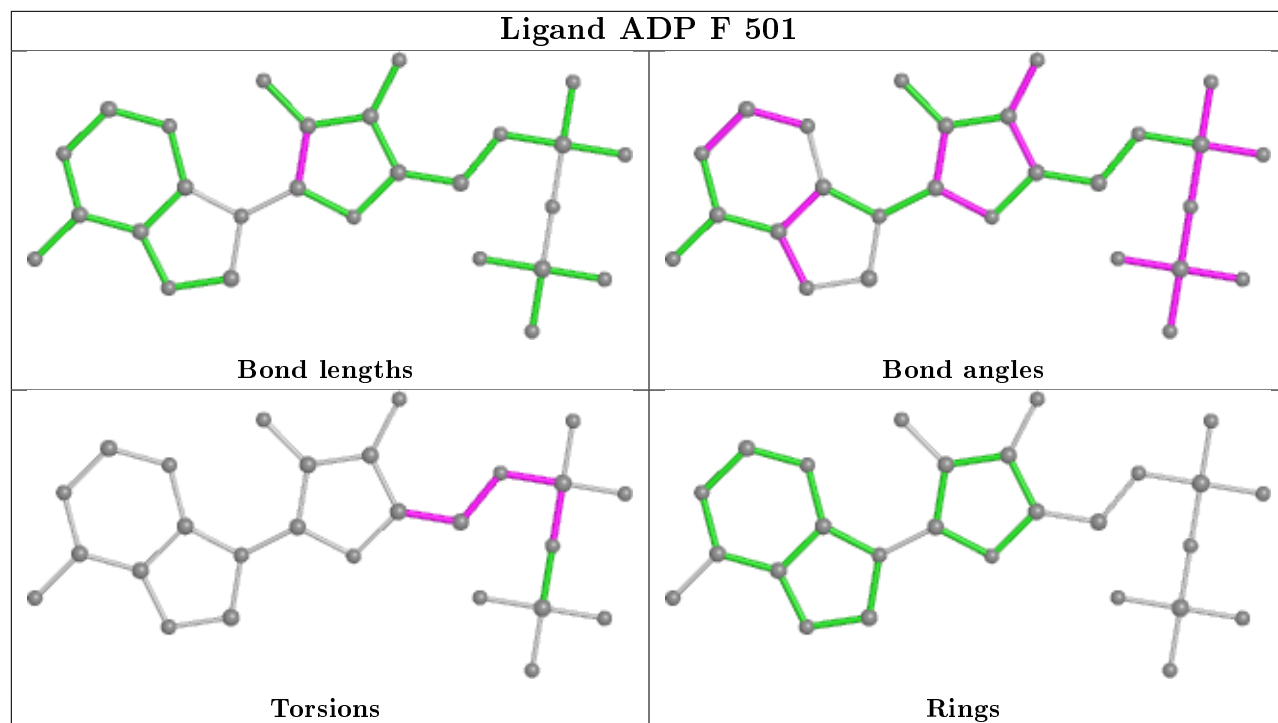
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	501	ADP	2	0
3	H	501	ADP	5	0
3	E	501	ADP	2	0
3	F	501	ADP	7	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	459/485 (94%)	-0.22	7 (1%) 73 61	13, 56, 126, 182	0
1	B	459/485 (94%)	-0.18	5 (1%) 80 69	23, 63, 139, 171	0
1	C	459/485 (94%)	-0.21	8 (1%) 70 57	12, 52, 123, 170	0
1	D	459/485 (94%)	-0.04	12 (2%) 56 42	30, 72, 127, 171	0
2	E	455/458 (99%)	0.12	18 (3%) 38 28	20, 63, 143, 180	0
2	F	455/458 (99%)	0.51	52 (11%) 5 5	32, 90, 162, 209	0
2	G	455/458 (99%)	0.40	34 (7%) 14 11	29, 92, 151, 191	0
2	H	455/458 (99%)	0.58	55 (12%) 4 4	26, 98, 172, 221	0
All	All	3656/3772 (96%)	0.12	191 (5%) 27 20	12, 73, 150, 221	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	50	GLY	13.8
2	H	25	ASP	6.7
1	B	266	HIS	6.0
2	F	30	ASP	5.8
2	F	99	ILE	5.7
2	H	33	ALA	5.5
2	G	456	PHE	5.3
2	F	100	ARG	5.0
2	F	403	LYS	4.9
2	H	23	ASN	4.8
2	F	98	ARG	4.8
2	E	115	GLY	4.7
2	G	105	LEU	4.5
2	E	114	SER	4.4
1	D	58	ARG	4.4
2	G	455	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
2	F	23	ASN	4.2
2	G	65	ASP	4.2
2	G	102	PRO	4.2
2	H	403	LYS	4.2
2	F	41	ASP	4.0
1	A	267	PRO	4.0
2	H	19	LEU	4.0
2	H	24	ASN	4.0
2	H	51	HIS	3.9
2	H	360	THR	3.8
2	F	2	LYS	3.7
2	H	361	HIS	3.7
2	H	18	ASN	3.7
2	E	27	THR	3.7
2	F	49	ASN	3.5
2	G	98	ARG	3.5
2	G	100	ARG	3.5
2	H	105	LEU	3.4
1	D	262	SER	3.4
2	F	97	ALA	3.4
2	H	106	ALA	3.4
1	D	42	THR	3.4
2	H	120	ASP	3.4
2	H	97	ALA	3.3
2	H	65	ASP	3.3
1	A	266	HIS	3.3
2	F	125	PRO	3.3
2	F	53	SER	3.3
2	F	52	ALA	3.3
1	A	262	SER	3.3
2	G	34	ASP	3.2
2	H	3	ILE	3.2
2	F	24	ASN	3.2
2	H	418	GLU	3.2
2	H	100	ARG	3.2
2	F	390	THR	3.2
2	E	29	VAL	3.1
2	F	65	ASP	3.1
2	G	361	HIS	3.1
2	G	386	HIS	3.1
2	H	383	ALA	3.0
1	B	265	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	G	33	ALA	3.0
2	E	7	GLY	3.0
2	G	106	ALA	3.0
2	H	386	HIS	3.0
2	G	403	LYS	3.0
2	F	228	LEU	3.0
2	H	22	GLU	3.0
2	G	114	SER	3.0
2	F	25	ASP	3.0
2	G	99	ILE	2.9
2	F	388	ASP	2.9
1	D	266	HIS	2.9
2	H	110	ALA	2.9
2	F	418	GLU	2.9
2	H	385	ALA	2.9
2	F	3	ILE	2.9
2	H	126	GLU	2.9
2	G	433	HIS	2.8
2	H	116	ALA	2.8
2	H	2	LYS	2.8
2	E	49	ASN	2.8
2	H	399	ILE	2.8
2	F	94	ASN	2.8
2	F	74	ASN	2.8
1	A	59	ARG	2.8
1	B	267	PRO	2.8
2	H	53	SER	2.7
2	H	433	HIS	2.7
1	D	387	GLY	2.7
2	G	430	GLN	2.7
1	A	264	GLY	2.7
2	G	431	ASP	2.7
2	H	363	ARG	2.7
2	H	404	LEU	2.6
2	F	204	GLU	2.6
2	G	101	SER	2.6
2	F	124	ALA	2.6
2	G	7	GLY	2.6
2	F	79	ASN	2.6
2	F	67	ASP	2.6
2	G	125	PRO	2.6
2	H	121	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
2	G	393	LYS	2.6
2	H	434	VAL	2.5
2	E	3	ILE	2.5
2	H	382	GLU	2.5
2	H	455	PRO	2.5
2	H	99	ILE	2.5
2	F	126	GLU	2.5
2	E	46	ARG	2.5
1	C	56	PRO	2.5
2	H	388	ASP	2.5
1	A	61	LYS	2.5
2	G	385	ALA	2.5
2	G	449	ALA	2.5
2	H	74	ASN	2.5
2	H	351	GLN	2.4
2	H	98	ARG	2.4
2	F	75	THR	2.4
2	E	121	HIS	2.4
2	H	49	ASN	2.4
2	H	101	SER	2.4
2	F	362	VAL	2.4
2	G	414	VAL	2.4
2	E	23	ASN	2.4
2	H	68	MET	2.4
2	H	69	LEU	2.4
2	H	362	VAL	2.4
1	B	93	ASN	2.4
2	F	54	HIS	2.4
2	G	452	GLN	2.4
2	E	43	TYR	2.4
2	G	115	GLY	2.4
2	E	24	ASN	2.3
2	F	73	THR	2.3
2	F	122	LEU	2.3
1	D	29	LEU	2.3
2	F	59	HIS	2.3
2	F	27	THR	2.3
2	F	369	ASN	2.3
2	H	416	GLY	2.3
2	H	359	LEU	2.3
2	E	106	ALA	2.3
2	G	22	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	21	GLY	2.2
2	H	167	VAL	2.2
2	F	72	VAL	2.2
2	F	7	GLY	2.2
1	C	150	LEU	2.2
1	C	176	PRO	2.2
1	D	53	CYS	2.2
2	F	60	GLU	2.2
1	B	262	SER	2.2
1	D	95	ASN	2.2
2	F	44	ASP	2.2
2	F	101	SER	2.2
2	G	50	GLY	2.2
1	D	57	ASN	2.2
2	H	417	GLU	2.2
2	F	401	ASP	2.2
1	C	262	SER	2.2
2	G	52	ALA	2.2
2	G	453	PRO	2.2
1	D	60	HIS	2.2
2	H	32	ASN	2.2
2	H	264	TYR	2.2
1	A	4	ARG	2.2
2	F	365	ALA	2.2
2	E	418	GLU	2.2
2	E	111	LEU	2.1
1	C	263	GLY	2.1
2	E	2	LYS	2.1
1	D	176	PRO	2.1
2	H	453	PRO	2.1
2	G	121	HIS	2.1
2	F	83	CYS	2.1
1	D	38	PRO	2.1
1	C	61	LYS	2.1
2	H	350	PRO	2.1
2	G	35	ARG	2.1
2	F	26	ILE	2.1
2	F	361	HIS	2.1
1	C	267	PRO	2.1
2	F	50	GLY	2.1
2	F	389	GLU	2.1
2	F	105	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	G	365	ALA	2.0
2	E	28	ILE	2.0
1	C	174	MET	2.0
2	E	8	ALA	2.0
2	F	387	GLY	2.0
2	F	68	MET	2.0
2	F	35	ARG	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 carbohydrates in this entry.

6.4 Ligands [i](#)

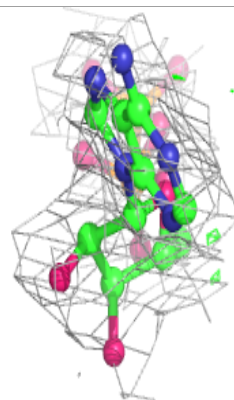
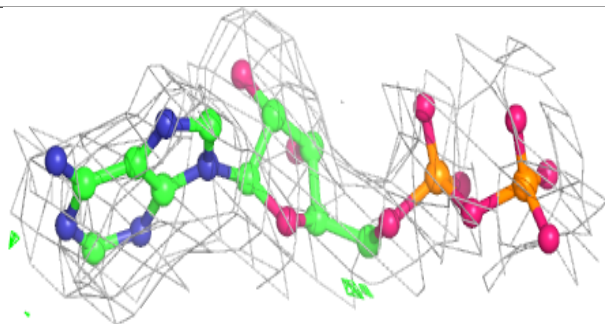
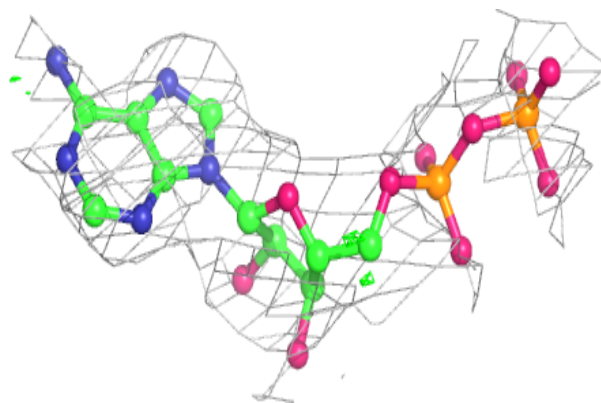
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ADP	G	501	27/27	0.74	0.29	52,88,144,145	0
3	ADP	H	501	27/27	0.79	0.29	77,107,133,135	0
3	ADP	E	501	27/27	0.83	0.25	34,52,128,131	0
3	ADP	F	501	27/27	0.85	0.20	67,89,134,136	0

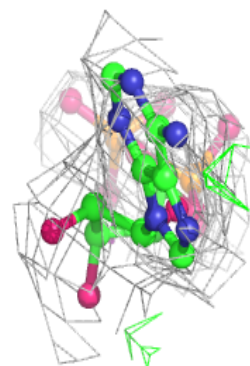
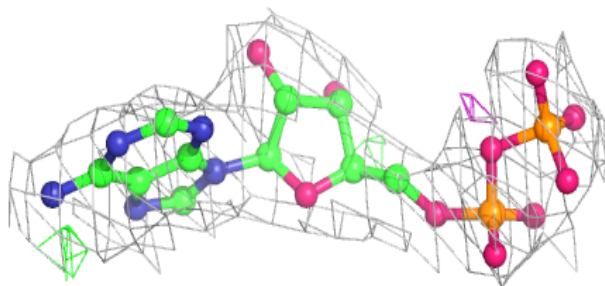
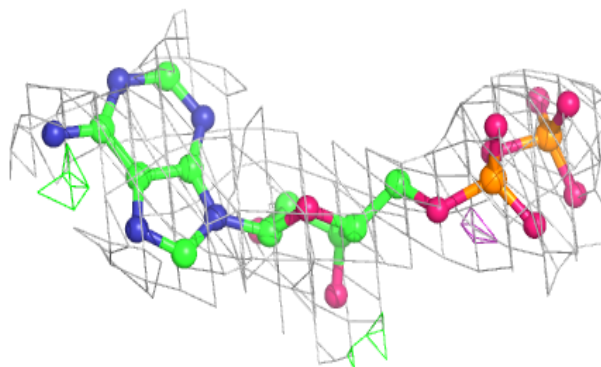
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP G 501:

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

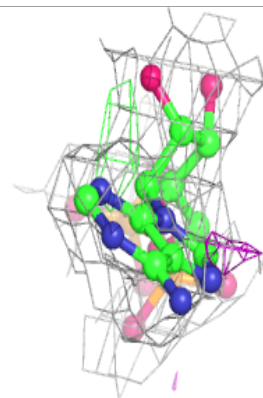
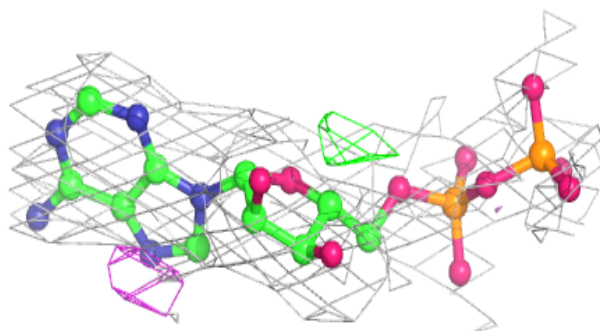
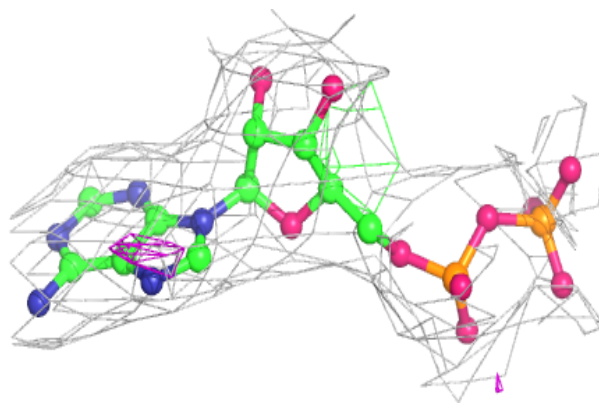
**Electron density around ADP H 501:**

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

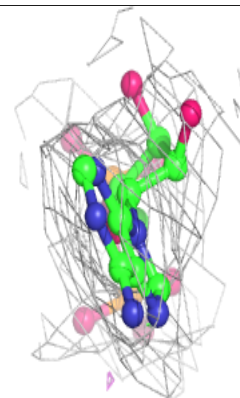
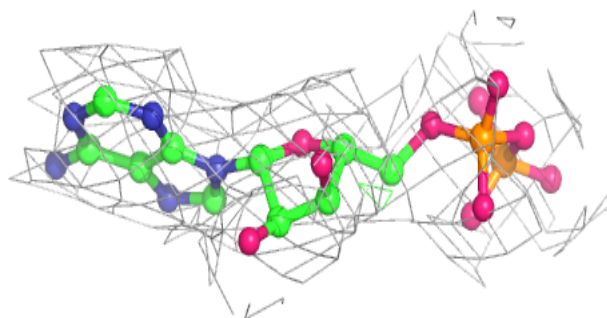
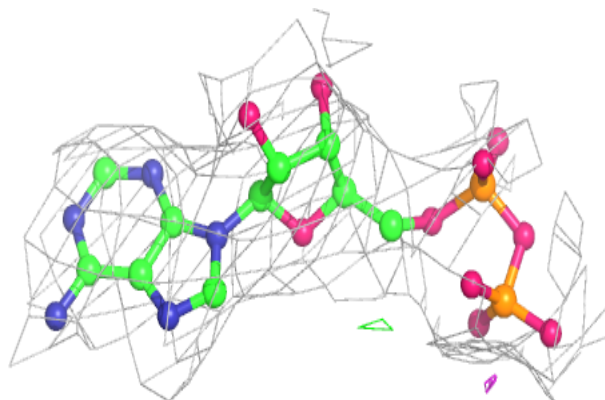


Electron density around ADP E 501:

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

**Electron density around ADP F 501:**

$2mF_o-DF_c$ (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.