Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 02:19 AM EDT

PDB ID	:	4HQJ
Title	:	Crystal structure of Na+,K+-ATPase in the Na+-bound state
Authors	:	Nyblom, M.; Reinhard, L.; Gourdon, P.; Nissen, P.
Deposited on	:	2012-10-25
Resolution	:	4.30 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 (i) 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 (i)) were used in the production of this report:

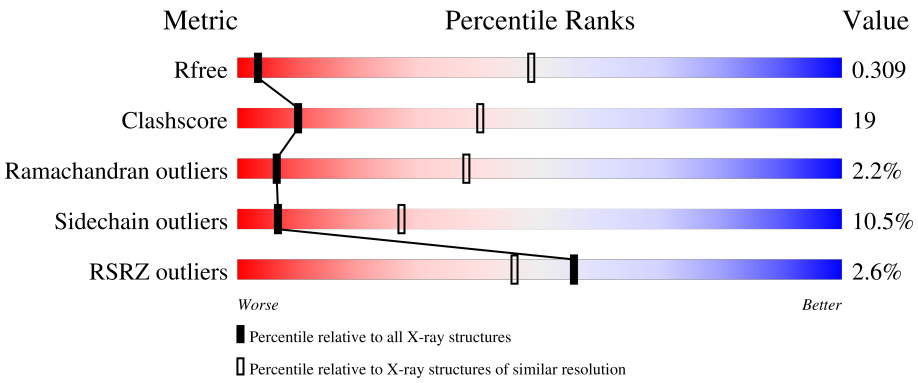
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 4.30 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	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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	1021	% 58% 34% • •
1	C	1021	2% 58% 34% • •
2	B	303	6% 45% 40% 8% • 6%
2	D	303	5% 43% 41% 10% • 6%
3	E	65	29% 11% 5% 55%

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Mol	Chain	Length	Quality of chain
3	G	65	26% 11% 5% 58%

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	ALF	A	1102	-	-	X	-
5	ALF	C	1102	-	-	X	-
8	CLR	D	400	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 20571 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 Sodium/potassium-transporting ATPase subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	985	7629	4864	1284	1435	46	0	0	0
1	C	987	7647	4875	1287	1439	46	0	0	0

- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	285	2322	1498	380	431	13	0	0	0
2	D	285	2322	1498	380	431	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	151	SER	PHE	SEE REMARK 999	UNP P05027
D	151	SER	PHE	SEE REMARK 999	UNP P05027

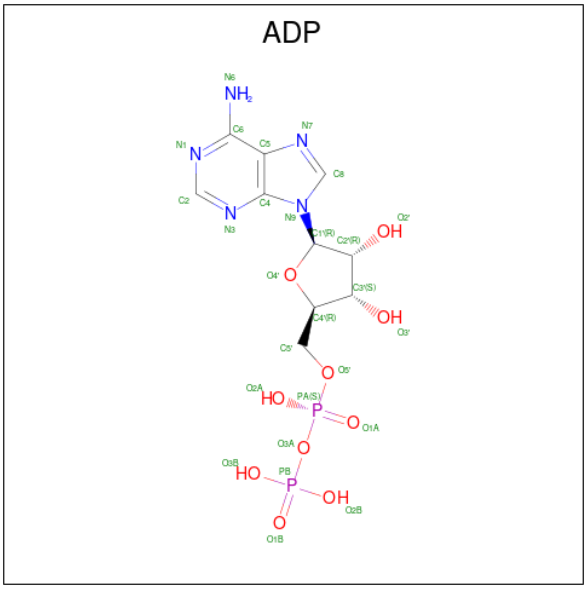
- Molecule 3 is a protein called Na+/K+ ATPase gamma subunit transcript variant a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	G	27	208	141	31	36	0	0	0
3	E	29	231	159	33	39	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

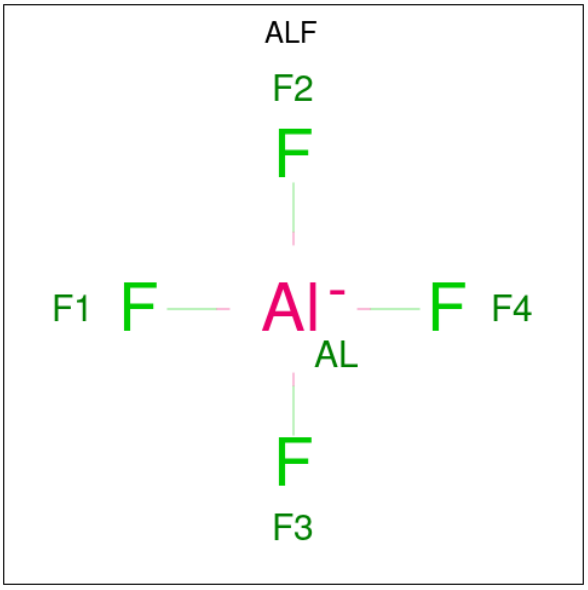
Chain	Residue	Modelled	Actual	Comment	Reference
G	45	LEU	ILE	CONFLICT	UNP Q58K79
E	45	LEU	ILE	CONFLICT	UNP Q58K79

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
5	A	1	5	1	4	0	0
5	C	1	5	1	4	0	0

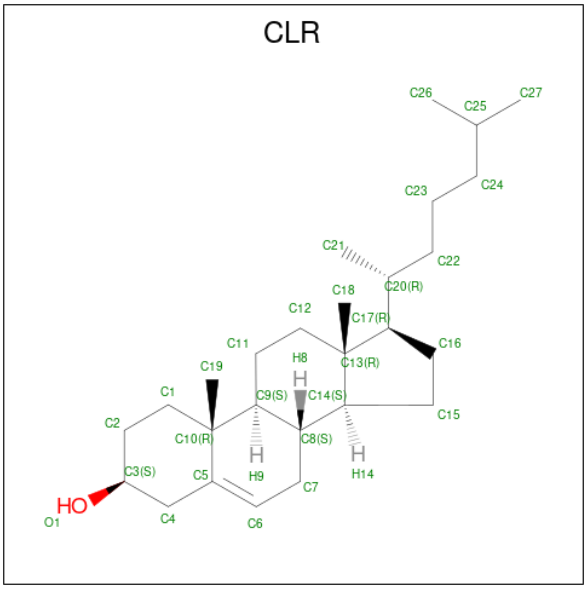
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	1	1	1	0	0
6	C	1	1	1	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
7	A	3	3	3	0	0
7	C	3	3	3	0	0

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	28	27	1	0	0

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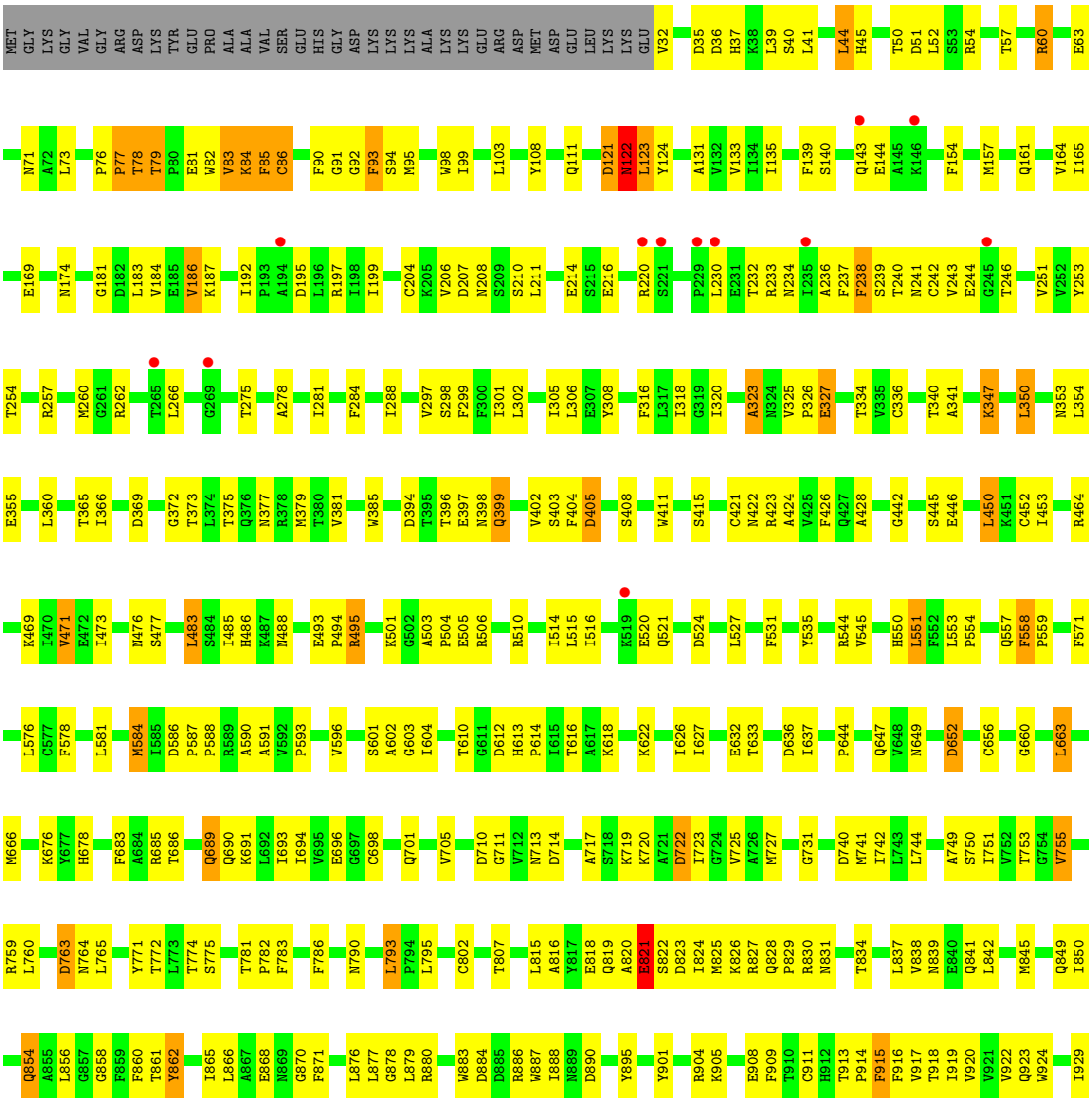
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	28	27	1	0	0
			Total	C	O		
8	C	1	28	27	1	0	0
			Total	C	O		
8	C	1	28	27	1	0	0
			Total	C	O		
8	D	1	28	27	1	0	0

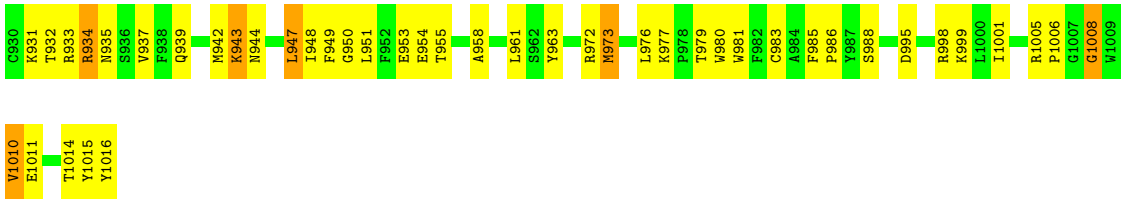
3 Residue-property plots (i)

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: Sodium/potassium-transporting ATPase subunit alpha-1

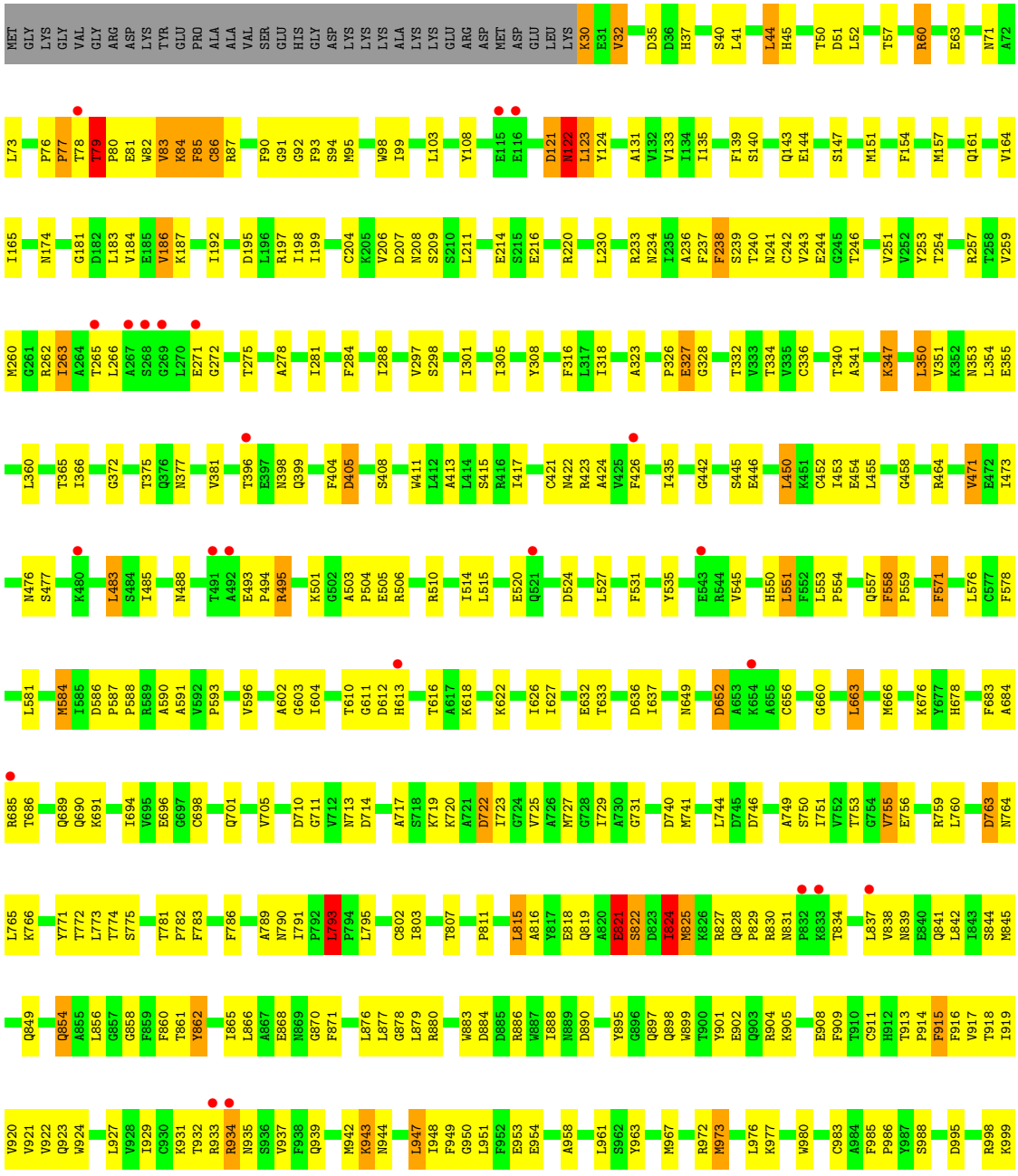
Chain A:

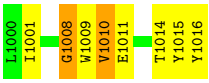




• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

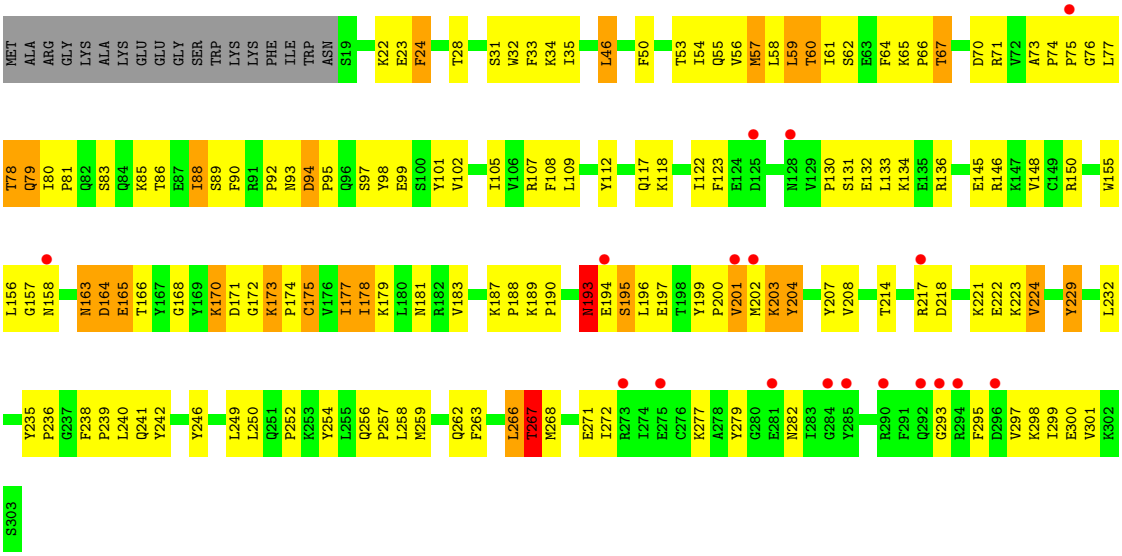
Chain C:





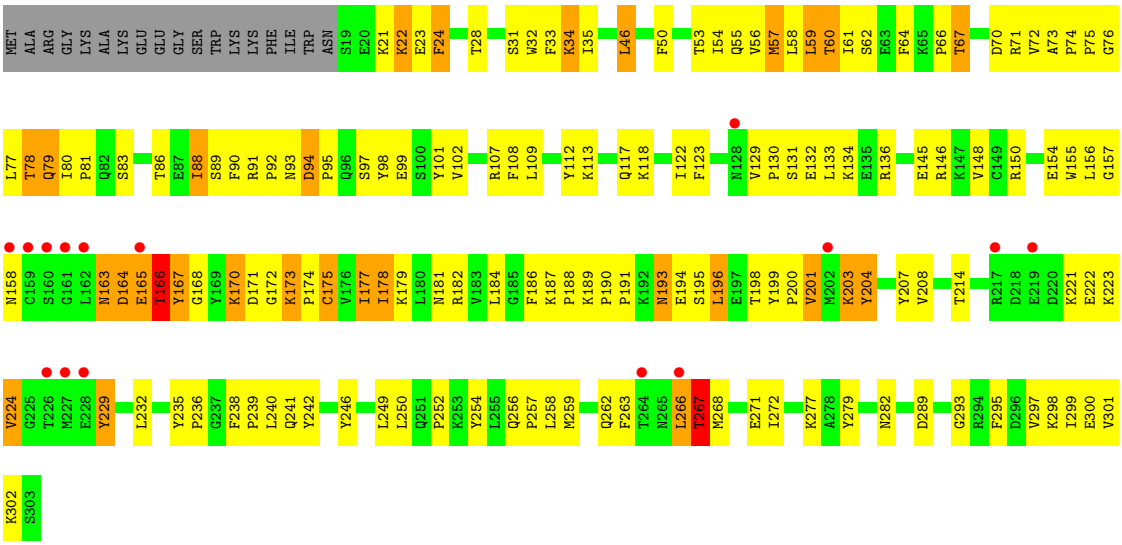
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain B:



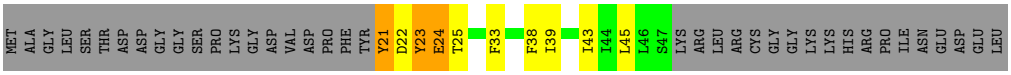
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain D:



• Molecule 3: Na+/K+ ATPase gamma subunit transcript variant a

Chain G:



• Molecule 3: Na+/K+ ATPase gamma subunit transcript variant a

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	109.07Å 219.58Å 261.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 4.30 49.99 – 4.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (12.00-4.30) 100.0 (49.99-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.261 , 0.288 0.283 , 0.309	Depositor DCC
R_{free} test set	2188 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	156.5	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 121.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	20571	wwPDB-VP
Average B, all atoms (Å^2)	211.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ALF, MG, ADP, CLR, NA

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	0.36	0/7779	0.56	0/10562
1	C	0.34	0/7797	0.54	2/10585 (0.0%)
2	B	0.35	0/2381	0.58	0/3210
2	D	0.35	0/2381	0.59	0/3210
3	E	0.32	0/236	0.52	0/320
3	G	0.32	0/211	0.57	0/286
All	All	0.35	0/20785	0.56	2/28173 (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	C	0	1
2	B	0	3
2	D	0	3
All	All	0	8

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	793	LEU	CB-CG-CD2	5.32	120.03	111.00
1	C	793	LEU	CA-CB-CG	5.26	127.41	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	78	THR	Peptide
2	B	165	GLU	Peptide
2	B	166	THR	Peptide
2	B	193	ASN	Peptide
1	C	78	THR	Peptide
2	D	165	GLU	Peptide
2	D	166	THR	Peptide
2	D	21	LYS	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	7629	0	7678	282	0
1	C	7647	0	7697	271	0
2	B	2322	0	2300	111	0
2	D	2322	0	2300	120	0
3	E	231	0	235	9	0
3	G	208	0	217	12	0
4	A	27	0	12	2	0
4	C	27	0	12	3	0
5	A	5	0	0	2	0
5	C	5	0	0	2	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	3	0	0	0	0
7	C	3	0	0	0	0
8	A	56	0	92	14	0
8	C	56	0	92	9	0
8	D	28	0	46	1	0
All	All	20571	0	20681	783	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 (783) 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:B:93:ASN:HD22	2:D:93:ASN:HB2	1.37	0.90
1:A:602:ALA:HA	1:A:826:LYS:H	1.38	0.89
1:A:830:ARG:NH2	1:A:1015:TYR:OH	2.09	0.86
1:A:495:ARG:HH22	1:A:558:PHE:HB2	1.41	0.85
1:C:830:ARG:NH2	1:C:1015:TYR:OH	2.10	0.85
2:B:157:GLY:HA2	2:B:163:ASN:HB3	1.60	0.84
2:D:92:PRO:HB3	2:D:170:LYS:HB2	1.61	0.82
2:B:136:ARG:HB3	2:B:146:ARG:HD3	1.62	0.82
2:B:92:PRO:HB3	2:B:170:LYS:HB2	1.60	0.82
2:D:157:GLY:HA2	2:D:163:ASN:HB3	1.60	0.81
1:C:495:ARG:HH22	1:C:558:PHE:HB2	1.44	0.81
1:A:372:GLY:HA2	1:A:377:ASN:HB2	1.63	0.81
2:D:136:ARG:HB3	2:D:146:ARG:HD3	1.62	0.80
1:C:493:GLU:O	1:C:495:ARG:N	2.14	0.80
1:A:493:GLU:O	1:A:495:ARG:N	2.15	0.79
1:A:826:LYS:HA	1:A:827:ARG:C	2.03	0.79
2:D:76:GLY:HA2	2:D:293:GLY:H	1.49	0.78
1:A:495:ARG:NH2	1:A:559:PRO:O	2.18	0.77
1:C:92:GLY:HA2	1:C:95:MET:H	1.49	0.77
2:B:76:GLY:HA2	2:B:293:GLY:H	1.50	0.77
2:D:112:TYR:OH	2:D:256:GLN:O	2.04	0.76
1:A:839:ASN:ND2	1:A:1016:TYR:OXT	2.18	0.76
1:C:372:GLY:HA2	1:C:377:ASN:HB2	1.65	0.76
2:D:187:LYS:O	2:D:282:ASN:ND2	2.20	0.75
1:C:365:THR:HB	1:C:705:VAL:HG12	1.69	0.75
2:D:80:ILE:HB	2:D:177:ILE:HG23	1.67	0.75
1:A:92:GLY:HA2	1:A:95:MET:H	1.50	0.75
2:B:112:TYR:OH	2:B:256:GLN:O	2.03	0.75
1:C:856:LEU:HD12	2:D:46:LEU:HD12	1.69	0.75
2:D:32:TRP:HD1	2:D:35:ILE:HD12	1.50	0.75
1:A:790:ASN:OD1	1:A:880:ARG:NH1	2.20	0.75
1:C:187:LYS:HD3	1:C:423:ARG:HH12	1.52	0.75
1:C:30:LYS:HA	1:C:262:ARG:HH12	1.51	0.75
2:B:80:ILE:HB	2:B:177:ILE:HG23	1.69	0.74
1:C:790:ASN:OD1	1:C:880:ARG:NH1	2.21	0.74
2:B:187:LYS:O	2:B:282:ASN:ND2	2.20	0.74
1:A:195:ASP:HB2	1:A:253:TYR:HB2	1.71	0.73
1:A:365:THR:HB	1:A:705:VAL:HG12	1.69	0.73
1:C:495:ARG:NH2	1:C:559:PRO:O	2.20	0.73
2:B:32:TRP:HD1	2:B:35:ILE:HD12	1.51	0.73
2:B:55:GLN:HA	2:B:58:LEU:HB2	1.71	0.73
2:B:193:ASN:HD21	2:B:196:LEU:HD13	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:HD3	1:A:423:ARG:HH12	1.52	0.72
1:C:839:ASN:ND2	1:C:1016:TYR:OXT	2.22	0.72
2:D:55:GLN:HA	2:D:58:LEU:HB2	1.71	0.71
1:C:856:LEU:HD13	2:D:50:PHE:HB2	1.71	0.71
2:D:170:LYS:O	2:D:172:GLY:N	2.24	0.71
1:C:685:ARG:NH2	4:C:1101:ADP:O3'	2.24	0.71
1:C:45:HIS:HE1	1:C:51:ASP:HA	1.56	0.70
1:C:195:ASP:HB2	1:C:253:TYR:HB2	1.73	0.70
1:A:603:GLY:HA3	1:A:828:GLN:HG2	1.73	0.70
2:B:170:LYS:O	2:B:172:GLY:N	2.24	0.70
1:C:861:THR:HG22	1:C:983:CYS:HB3	1.74	0.70
1:C:603:GLY:HA3	1:C:828:GLN:HG2	1.74	0.69
1:C:976:LEU:HD22	1:C:980:TRP:HD1	1.57	0.69
1:A:122:ASN:O	1:A:124:TYR:N	2.26	0.69
1:A:45:HIS:HE1	1:A:51:ASP:HA	1.56	0.69
2:B:200:PRO:HG2	2:B:203:LYS:HE3	1.75	0.69
1:C:919:ILE:HA	1:C:922:VAL:HG12	1.76	0.68
1:C:818:GLU:OE2	1:C:931:LYS:NZ	2.19	0.68
1:C:122:ASN:O	1:C:124:TYR:N	2.27	0.68
1:A:613:HIS:HB2	1:A:616:THR:HB	1.75	0.68
1:A:976:LEU:HD22	1:A:980:TRP:HD1	1.59	0.67
1:A:839:ASN:HB3	1:A:841:GLN:HG2	1.76	0.67
1:C:52:LEU:HD12	1:C:199:ILE:HD12	1.77	0.67
1:A:288:ILE:HG21	1:A:326:PRO:HD2	1.76	0.67
1:A:922:VAL:HA	1:A:988:SER:HB3	1.77	0.67
1:A:1008:GLY:HA3	1:A:1011:GLU:HB3	1.77	0.67
1:C:288:ILE:HG21	1:C:326:PRO:HD2	1.75	0.67
1:C:1008:GLY:HA3	1:C:1011:GLU:HB3	1.77	0.67
2:D:200:PRO:HG2	2:D:203:LYS:HE3	1.75	0.67
1:A:422:ASN:O	1:A:464:ARG:NH1	2.28	0.67
1:A:861:THR:HG22	1:A:983:CYS:HB3	1.76	0.67
1:C:244:GLU:OE1	1:C:476:ASN:ND2	2.28	0.67
1:C:793:LEU:H	1:C:793:LEU:HD23	1.60	0.67
1:A:913:THR:HG23	1:A:973:MET:HG3	1.76	0.66
1:A:818:GLU:OE2	1:A:931:LYS:NZ	2.19	0.66
1:A:551:LEU:HD12	1:A:553:LEU:HD23	1.76	0.66
1:A:919:ILE:HA	1:A:922:VAL:HG12	1.76	0.66
2:D:130:PRO:HB2	2:D:204:TYR:OH	1.96	0.66
1:C:57:THR:HB	1:C:60:ARG:HB2	1.76	0.66
1:C:913:THR:HG23	1:C:973:MET:HG3	1.77	0.66
1:C:422:ASN:O	1:C:464:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:551:LEU:HD12	1:C:553:LEU:HD23	1.77	0.66
1:C:839:ASN:HB3	1:C:841:GLN:HG2	1.78	0.66
2:B:130:PRO:HB2	2:B:204:TYR:OH	1.95	0.65
1:A:57:THR:HB	1:A:60:ARG:HB2	1.78	0.65
3:G:23:TYR:O	3:G:25:THR:N	2.29	0.65
1:C:1010:VAL:O	1:C:1014:THR:N	2.25	0.65
1:A:244:GLU:OE1	1:A:476:ASN:ND2	2.30	0.65
1:C:922:VAL:HA	1:C:988:SER:HB3	1.78	0.65
2:B:131:SER:HB2	2:B:241:GLN:HB3	1.79	0.65
1:C:422:ASN:ND2	1:C:446:GLU:O	2.30	0.65
1:C:786:PHE:HZ	1:C:793:LEU:HD22	1.62	0.64
1:C:976:LEU:HD22	1:C:980:TRP:CD1	2.31	0.64
1:A:976:LEU:HD22	1:A:980:TRP:CD1	2.32	0.64
2:B:173:LYS:HD3	2:B:263:PHE:H	1.62	0.64
1:A:656:CYS:SG	1:A:678:HIS:ND1	2.70	0.64
2:D:163:ASN:ND2	2:D:175:CYS:SG	2.71	0.64
2:B:163:ASN:ND2	2:B:175:CYS:SG	2.70	0.64
1:A:52:LEU:HD12	1:A:199:ILE:HD12	1.78	0.64
2:D:94:ASP:OD1	2:D:94:ASP:N	2.30	0.64
2:D:32:TRP:CD1	2:D:35:ILE:HD12	2.33	0.63
2:D:108:PHE:HD2	2:D:109:LEU:HD22	1.63	0.63
1:C:613:HIS:HB2	1:C:616:THR:HB	1.78	0.63
1:C:505:GLU:OE2	1:C:685:ARG:NH1	2.31	0.63
2:D:131:SER:HB2	2:D:241:GLN:HB3	1.79	0.63
2:D:173:LYS:HD3	2:D:263:PHE:H	1.62	0.63
2:D:224:VAL:HG22	2:D:267:THR:HG21	1.81	0.63
1:A:884:ASP:OD1	1:A:905:LYS:NZ	2.26	0.62
2:B:168:GLY:HA2	2:B:174:PRO:HB3	1.81	0.62
2:D:222:GLU:HG2	2:D:224:VAL:HG23	1.81	0.62
1:A:505:GLU:OE2	1:A:685:ARG:NH1	2.32	0.62
1:A:77:PRO:HB2	1:A:79:THR:HA	1.81	0.62
1:A:375:THR:HA	1:A:588:PRO:HA	1.81	0.62
1:A:827:ARG:CZ	1:A:934:ARG:HG2	2.29	0.62
3:E:23:TYR:O	3:E:25:THR:N	2.33	0.62
1:A:1010:VAL:O	1:A:1014:THR:N	2.27	0.62
1:A:931:LYS:HZ3	1:A:947:LEU:HD22	1.63	0.62
2:B:222:GLU:HG2	2:B:224:VAL:HG23	1.82	0.61
2:B:224:VAL:HG22	2:B:267:THR:HG21	1.82	0.61
1:C:98:TRP:HE1	1:C:133:VAL:HG11	1.65	0.61
1:A:880:ARG:HA	1:A:883:TRP:HB3	1.82	0.61
1:C:884:ASP:OD1	1:C:905:LYS:NZ	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:TRP:HE1	1:A:133:VAL:HG11	1.64	0.61
1:A:422:ASN:ND2	1:A:446:GLU:O	2.32	0.61
1:A:91:GLY:O	1:A:94:SER:OG	2.18	0.61
1:C:98:TRP:NE1	1:C:133:VAL:HG11	2.16	0.61
1:C:656:CYS:SG	1:C:678:HIS:ND1	2.73	0.61
1:C:868:GLU:HB2	1:C:980:TRP:HH2	1.66	0.61
2:B:32:TRP:CD1	2:B:35:ILE:HD12	2.34	0.61
1:A:856:LEU:HD12	2:B:46:LEU:HD12	1.82	0.60
1:C:663:LEU:HA	1:C:666:MET:HG2	1.81	0.60
1:C:827:ARG:CZ	1:C:934:ARG:HG2	2.31	0.60
1:A:888:ILE:O	1:A:904:ARG:NH2	2.33	0.60
2:B:108:PHE:HD2	2:B:109:LEU:HD22	1.66	0.60
1:A:663:LEU:HA	1:A:666:MET:HG2	1.83	0.60
1:C:880:ARG:HA	1:C:883:TRP:HB3	1.83	0.60
2:D:204:TYR:OH	2:D:207:TYR:HB2	2.01	0.60
1:C:931:LYS:HZ3	1:C:947:LEU:HD22	1.66	0.60
1:A:771:TYR:O	1:A:774:THR:OG1	2.20	0.60
2:B:173:LYS:HE2	2:B:262:GLN:HG3	1.84	0.60
2:D:178:ILE:HG23	2:D:259:MET:HB3	1.83	0.60
1:C:375:THR:HA	1:C:588:PRO:HA	1.82	0.60
1:A:98:TRP:NE1	1:A:133:VAL:HG11	2.16	0.60
2:B:81:PRO:HD3	2:B:177:ILE:HG23	1.84	0.59
1:A:355:GLU:CD	1:A:355:GLU:H	2.06	0.59
1:A:394:ASP:HB2	1:A:399:GLN:O	2.02	0.59
1:C:73:LEU:HD22	1:C:260:MET:HB3	1.84	0.59
1:A:204:CYS:HB2	1:A:246:THR:O	2.02	0.59
1:A:823:ASP:O	1:A:827:ARG:NH1	2.34	0.59
2:B:204:TYR:OH	2:B:207:TYR:HB2	2.02	0.59
1:A:868:GLU:HB2	1:A:980:TRP:HH2	1.68	0.59
2:D:81:PRO:HD3	2:D:177:ILE:HG23	1.85	0.59
1:C:103:LEU:HB3	1:C:318:ILE:HD11	1.85	0.59
1:C:888:ILE:O	1:C:904:ARG:NH2	2.35	0.59
1:C:204:CYS:HB2	1:C:246:THR:O	2.02	0.59
2:D:60:THR:OG1	2:D:61:ILE:N	2.31	0.59
1:A:950:GLY:O	1:A:954:GLU:HB2	2.02	0.59
1:A:601:SER:O	1:A:826:LYS:HB3	2.03	0.58
2:B:178:ILE:HG23	2:B:259:MET:HB3	1.85	0.58
2:D:75:PRO:HB3	2:D:181:ASN:HB2	1.85	0.58
1:C:207:ASP:HB2	1:C:243:VAL:HG23	1.83	0.58
1:C:488:ASN:HB3	1:C:495:ARG:O	2.04	0.58
1:A:207:ASP:HB2	1:A:243:VAL:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:759:ARG:NH2	1:C:829:PRO:HA	2.18	0.58
1:A:759:ARG:NH2	1:A:829:PRO:HA	2.18	0.58
2:B:59:LEU:N	2:B:60:THR:HA	2.17	0.58
2:D:173:LYS:HE2	2:D:262:GLN:HG3	1.85	0.58
1:C:771:TYR:O	1:C:774:THR:OG1	2.22	0.58
2:D:133:LEU:HG	2:D:240:LEU:HD23	1.86	0.58
1:A:103:LEU:HB3	1:A:318:ILE:HD11	1.86	0.58
1:A:977:LYS:HD2	1:A:980:TRP:CZ2	2.39	0.58
1:A:495:ARG:NH2	1:A:558:PHE:HB2	2.16	0.57
1:A:685:ARG:NH2	4:A:1101:ADP:O3'	2.36	0.57
1:C:366:ILE:HG13	1:C:604:ILE:HG21	1.87	0.57
1:A:488:ASN:HB3	1:A:495:ARG:O	2.04	0.57
2:B:75:PRO:HB3	2:B:181:ASN:HB2	1.85	0.57
2:B:92:PRO:HD3	2:B:170:LYS:HE2	1.86	0.57
1:C:950:GLY:O	1:C:954:GLU:HB2	2.03	0.57
1:A:696:GLU:OE1	1:A:720:LYS:HE3	2.05	0.57
2:B:60:THR:OG1	2:B:61:ILE:N	2.32	0.57
1:C:77:PRO:HB2	1:C:79:THR:HA	1.86	0.57
2:D:59:LEU:N	2:D:60:THR:HA	2.18	0.57
2:B:60:THR:O	2:B:61:ILE:HD13	2.05	0.57
2:B:188:PRO:HG2	2:B:240:LEU:HG	1.87	0.57
1:C:91:GLY:O	1:C:94:SER:OG	2.21	0.57
2:B:88:ILE:HG22	2:B:101:TYR:CE1	2.39	0.56
2:D:92:PRO:HD3	2:D:170:LYS:HE2	1.87	0.56
1:A:366:ILE:HG13	1:A:604:ILE:HG21	1.86	0.56
1:C:596:VAL:HG11	1:C:626:ILE:HD13	1.87	0.56
1:A:764:ASN:ND2	1:A:816:ALA:O	2.38	0.56
2:B:58:LEU:HA	2:B:60:THR:HB	1.86	0.56
1:C:271:GLU:N	1:C:272:GLY:HA3	2.20	0.56
2:D:95:PRO:HA	2:D:98:TYR:CZ	2.41	0.56
1:A:782:PRO:HG3	1:A:795:LEU:HD21	1.88	0.56
1:A:995:ASP:O	1:A:998:ARG:HB3	2.06	0.56
1:C:854:GLN:HB3	1:C:922:VAL:HG11	1.88	0.56
1:C:995:ASP:O	1:C:998:ARG:HB3	2.05	0.56
1:A:398:ASN:HB3	1:A:399:GLN:C	2.26	0.56
1:A:596:VAL:HG11	1:A:626:ILE:HD13	1.87	0.56
1:C:696:GLU:OE1	1:C:720:LYS:HE3	2.06	0.56
2:B:271:GLU:HA	2:B:300:GLU:HB2	1.87	0.56
1:A:262:ARG:O	1:A:266:LEU:HB2	2.05	0.55
1:A:535:TYR:HD1	1:A:545:VAL:HG11	1.71	0.55
1:A:711:GLY:N	1:A:714:ASP:OD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:186:PHE:HD1	3:E:19:PHE:CE1	2.23	0.55
1:C:263:ILE:HB	1:C:266:LEU:H	1.70	0.55
2:D:58:LEU:HA	2:D:60:THR:HB	1.87	0.55
2:B:59:LEU:HG	2:B:60:THR:O	2.07	0.55
2:B:95:PRO:HA	2:B:98:TYR:CZ	2.42	0.55
1:C:591:ALA:HB1	1:C:749:ALA:HB2	1.88	0.55
1:C:711:GLY:N	1:C:714:ASP:OD2	2.39	0.55
1:C:782:PRO:HG3	1:C:795:LEU:HD21	1.87	0.55
2:D:60:THR:O	2:D:61:ILE:HD13	2.06	0.55
2:D:88:ILE:HG22	2:D:101:TYR:CE1	2.41	0.55
2:D:109:LEU:HD11	2:D:258:LEU:HD21	1.88	0.55
2:D:193:ASN:ND2	2:D:196:LEU:HB3	2.22	0.55
1:A:495:ARG:NH1	1:A:558:PHE:O	2.40	0.55
1:A:951:LEU:HD13	8:A:1107:CLR:H261	1.88	0.55
2:B:77:LEU:HD11	2:B:178:ILE:HD11	1.89	0.55
1:A:820:ALA:HB1	1:A:823:ASP:HB2	1.89	0.55
1:C:355:GLU:H	1:C:355:GLU:CD	2.11	0.55
1:C:764:ASN:ND2	1:C:816:ALA:O	2.40	0.55
1:A:350:LEU:HD12	1:A:742:ILE:HB	1.89	0.54
1:C:350:LEU:HG	1:C:351:VAL:N	2.13	0.54
2:D:59:LEU:HG	2:D:60:THR:O	2.07	0.54
1:A:591:ALA:HB1	1:A:749:ALA:HB2	1.88	0.54
2:B:109:LEU:HD11	2:B:258:LEU:HD21	1.88	0.54
1:C:495:ARG:NH2	1:C:558:PHE:HB2	2.19	0.54
4:A:1101:ADP:H5'2	4:A:1101:ADP:O1B	2.08	0.54
2:B:133:LEU:HG	2:B:240:LEU:HD23	1.89	0.54
2:D:271:GLU:HA	2:D:300:GLU:HB2	1.88	0.54
1:A:979:THR:OG1	8:A:1108:CLR:H41	2.08	0.54
1:A:360:LEU:HD13	1:A:723:ILE:HG12	1.89	0.54
1:C:610:THR:OG1	5:C:1102:ALF:F4	2.12	0.54
1:A:402:VAL:HG23	1:A:405:ASP:H	1.72	0.54
1:A:759:ARG:HH22	1:A:829:PRO:HA	1.73	0.54
1:C:535:TYR:HD1	1:C:545:VAL:HG11	1.73	0.54
2:D:77:LEU:HD11	2:D:178:ILE:HD11	1.88	0.54
1:A:854:GLN:HB3	1:A:922:VAL:HG11	1.89	0.53
1:C:916:PHE:CE2	1:C:958:ALA:HA	2.43	0.53
1:C:495:ARG:NH1	1:C:558:PHE:O	2.41	0.53
1:C:865:ILE:HA	1:C:980:TRP:CH2	2.43	0.53
1:A:347:LYS:NZ	1:A:750:SER:O	2.35	0.53
2:B:123:PHE:HB3	2:B:150:ARG:HD3	1.91	0.53
1:A:83:VAL:O	1:A:86:CYS:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:VAL:HA	1:A:242:CYS:HA	1.91	0.53
1:C:181:GLY:H	1:C:251:VAL:HB	1.72	0.53
1:A:602:ALA:CA	1:A:826:LYS:H	2.17	0.53
1:C:347:LYS:NZ	1:C:750:SER:O	2.36	0.53
1:C:902:GLU:HB2	2:D:289:ASP:OD2	2.09	0.53
2:D:123:PHE:HB3	2:D:150:ARG:HD3	1.91	0.53
2:B:94:ASP:OD1	2:B:94:ASP:N	2.32	0.53
1:A:45:HIS:CE1	1:A:51:ASP:HA	2.42	0.53
1:A:404:PHE:HZ	1:A:411:TRP:CD2	2.27	0.53
1:A:535:TYR:OH	1:A:613:HIS:HB3	2.09	0.52
2:B:57:MET:C	2:B:59:LEU:H	2.13	0.52
2:B:196:LEU:HD12	2:B:197:GLU:H	1.74	0.52
2:D:57:MET:C	2:D:59:LEU:H	2.12	0.52
2:D:193:ASN:OD1	2:D:194:GLU:HA	2.08	0.52
2:D:188:PRO:HG2	2:D:240:LEU:HG	1.90	0.52
1:A:471:VAL:HG12	1:A:485:ILE:HB	1.92	0.52
1:C:360:LEU:HD13	1:C:723:ILE:HG12	1.92	0.52
1:C:590:ALA:O	1:C:593:PRO:HD2	2.10	0.52
1:A:78:THR:H	1:A:79:THR:HA	1.75	0.52
1:A:865:ILE:HA	1:A:980:TRP:CH2	2.45	0.52
1:C:844:SER:HB3	8:D:400:CLR:C6	2.40	0.52
1:C:953:GLU:OE2	3:E:38:PHE:HA	2.10	0.52
1:A:610:THR:OG1	5:A:1102:ALF:F4	2.16	0.52
1:C:676:LYS:HE2	1:C:701:GLN:HE22	1.75	0.52
1:A:862:TYR:CE2	1:A:866:LEU:HD12	2.45	0.52
1:A:949:PHE:CD1	3:G:45:LEU:HD13	2.44	0.52
2:B:130:PRO:HG2	2:B:235:TYR:CD1	2.45	0.52
1:C:759:ARG:HH22	1:C:829:PRO:HA	1.73	0.52
1:A:932:THR:HG21	1:A:937:VAL:HA	1.92	0.51
2:B:190:PRO:HB3	2:B:208:VAL:O	2.10	0.51
1:A:426:PHE:CZ	1:A:450:LEU:HD22	2.45	0.51
1:A:916:PHE:CE2	1:A:958:ALA:HA	2.45	0.51
1:C:45:HIS:CE1	1:C:51:ASP:HA	2.41	0.51
1:A:181:GLY:H	1:A:251:VAL:HB	1.75	0.51
1:A:590:ALA:O	1:A:593:PRO:HD2	2.11	0.51
1:C:83:VAL:O	1:C:86:CYS:HB3	2.11	0.51
1:C:424:ALA:HB2	1:C:442:GLY:HA3	1.91	0.51
1:A:886:ARG:HA	1:A:901:TYR:CD1	2.46	0.51
1:C:845:MET:O	1:C:849:GLN:HB3	2.11	0.51
1:C:916:PHE:HE2	1:C:958:ALA:HA	1.75	0.51
2:D:130:PRO:HG2	2:D:235:TYR:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ILE:HG12	1:A:240:THR:O	2.11	0.51
2:D:266:LEU:HD21	2:D:299:ILE:HD12	1.92	0.51
1:A:917:VAL:O	1:A:920:VAL:HB	2.11	0.51
1:C:238:PHE:HD1	1:C:239:SER:H	1.59	0.51
1:C:471:VAL:HG12	1:C:485:ILE:HB	1.92	0.51
1:C:862:TYR:CE2	1:C:866:LEU:HD12	2.46	0.51
1:C:924:TRP:CH2	8:C:1107:CLR:H213	2.45	0.51
1:C:977:LYS:HD2	1:C:980:TRP:CZ2	2.45	0.51
2:D:157:GLY:CA	2:D:163:ASN:HB3	2.37	0.51
1:A:514:ILE:HD12	1:A:527:LEU:HD13	1.93	0.51
1:A:949:PHE:CG	3:G:45:LEU:HD13	2.45	0.51
1:C:771:TYR:CZ	1:C:923:GLN:NE2	2.78	0.51
1:C:698:CYS:HB3	1:C:705:VAL:HG11	1.93	0.50
1:C:995:ASP:OD1	1:C:999:LYS:HE3	2.10	0.50
8:A:1108:CLR:H213	2:B:56:VAL:HG11	1.92	0.50
2:B:157:GLY:CA	2:B:163:ASN:HB3	2.37	0.50
1:C:206:VAL:HA	1:C:242:CYS:HA	1.93	0.50
1:C:220:ARG:HD3	1:C:233:ARG:O	2.12	0.50
2:D:57:MET:O	2:D:59:LEU:HD23	2.12	0.50
2:D:83:SER:HB3	2:D:86:THR:HA	1.93	0.50
1:A:916:PHE:HE2	1:A:958:ALA:HA	1.77	0.50
2:D:79:GLN:NE2	2:D:81:PRO:O	2.43	0.50
2:D:117:GLN:OE1	2:D:150:ARG:HB2	2.11	0.50
1:A:771:TYR:CZ	1:A:923:GLN:NE2	2.79	0.50
2:D:191:PRO:HG2	2:D:196:LEU:HD12	1.92	0.50
1:A:871:PHE:HB3	1:A:876:LEU:HD21	1.94	0.50
2:B:179:LYS:HD2	2:B:256:GLN:CD	2.32	0.50
1:C:949:PHE:CZ	1:C:953:GLU:HG3	2.47	0.50
2:D:190:PRO:HB3	2:D:208:VAL:O	2.10	0.50
1:C:360:LEU:HD22	1:C:741:MET:SD	2.52	0.50
1:C:426:PHE:CZ	1:C:450:LEU:HD22	2.47	0.50
2:D:165:GLU:O	2:D:166:THR:HG23	2.12	0.50
1:A:424:ALA:HB2	1:A:442:GLY:HA3	1.92	0.49
1:A:676:LYS:HE2	1:A:701:GLN:HE22	1.76	0.49
1:A:995:ASP:OD1	1:A:999:LYS:HE3	2.11	0.49
1:C:121:ASP:OD1	1:C:972:ARG:NH2	2.45	0.49
1:C:917:VAL:O	1:C:920:VAL:HB	2.12	0.49
2:B:83:SER:HB3	2:B:86:THR:HA	1.92	0.49
1:C:404:PHE:HZ	1:C:411:TRP:CD2	2.30	0.49
2:D:130:PRO:HG2	2:D:235:TYR:HD1	1.77	0.49
2:D:179:LYS:HD2	2:D:256:GLN:CD	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1108:CLR:H121	2:B:56:VAL:HG13	1.95	0.49
8:A:1108:CLR:H212	2:B:53:THR:HG22	1.94	0.49
2:B:189:LYS:N	2:B:282:ASN:HD22	2.09	0.49
1:A:238:PHE:HD1	1:A:239:SER:H	1.59	0.49
1:A:515:LEU:CD2	1:A:520:GLU:HG2	2.43	0.49
1:C:649:ASN:HB3	1:C:652:ASP:HB2	1.95	0.49
1:C:870:GLY:HA2	1:C:895:TYR:CD2	2.48	0.49
1:C:1009:TRP:CH2	2:D:34:LYS:HB2	2.47	0.49
1:A:949:PHE:CZ	1:A:953:GLU:HG3	2.48	0.49
1:C:535:TYR:OH	1:C:613:HIS:HB3	2.13	0.49
1:A:663:LEU:HD13	1:A:690:GLN:HB3	1.95	0.49
1:C:514:ILE:HD12	1:C:527:LEU:HD13	1.94	0.49
1:C:611:GLY:O	4:C:1101:ADP:H5'1	2.13	0.49
1:C:886:ARG:HA	1:C:901:TYR:CD1	2.48	0.49
2:B:57:MET:O	2:B:59:LEU:HD23	2.13	0.49
2:B:117:GLN:OE1	2:B:150:ARG:HB2	2.13	0.49
3:G:39:ILE:O	3:G:43:ILE:HG12	2.13	0.49
1:C:108:TYR:CZ	1:C:123:LEU:HD22	2.48	0.49
2:D:194:GLU:HB3	2:D:195:SER:HB2	1.95	0.49
2:B:266:LEU:HD21	2:B:299:ILE:HD12	1.94	0.49
1:C:514:ILE:HG23	1:C:578:PHE:HB3	1.95	0.48
1:C:963:TYR:HE2	1:C:976:LEU:H	1.61	0.48
3:E:23:TYR:HB3	3:E:24:GLU:H	1.41	0.48
1:A:220:ARG:HD3	1:A:233:ARG:O	2.13	0.48
1:A:397:GLU:HA	1:A:398:ASN:C	2.33	0.48
1:A:698:CYS:HB3	1:A:705:VAL:HG11	1.94	0.48
2:B:90:PHE:CE1	2:B:301:VAL:HG12	2.49	0.48
1:C:181:GLY:N	1:C:251:VAL:O	2.47	0.48
1:A:845:MET:O	1:A:849:GLN:HB3	2.12	0.48
2:B:130:PRO:HG2	2:B:235:TYR:HD1	1.77	0.48
1:C:260:MET:HA	1:C:262:ARG:O	2.13	0.48
1:C:663:LEU:HD13	1:C:690:GLN:HB3	1.96	0.48
1:A:524:ASP:HB2	1:A:527:LEU:H	1.79	0.48
2:D:95:PRO:O	2:D:99:GLU:HG2	2.14	0.48
2:D:193:ASN:CG	2:D:194:GLU:HA	2.34	0.48
2:D:229:TYR:HB2	2:D:236:PRO:HB3	1.96	0.48
1:A:181:GLY:N	1:A:251:VAL:O	2.46	0.48
1:A:210:SER:HB2	1:A:260:MET:CE	2.43	0.48
1:A:977:LYS:HB3	3:G:21:TYR:CE2	2.49	0.48
1:A:554:PRO:HB2	1:A:557:GLN:OE1	2.14	0.48
1:C:197:ARG:CZ	1:C:234:ASN:HD22	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:PHE:CG	1:C:838:VAL:HG21	2.48	0.48
1:C:786:PHE:HE2	1:C:793:LEU:HA	1.78	0.48
2:D:90:PHE:CE1	2:D:301:VAL:HG12	2.48	0.48
1:C:262:ARG:HA	1:C:263:ILE:HA	1.47	0.48
1:C:495:ARG:HD2	1:C:495:ARG:HA	1.56	0.48
1:C:725:VAL:HG11	1:C:751:ILE:HD11	1.95	0.48
2:D:94:ASP:CG	2:D:97:SER:HB2	2.34	0.48
1:A:84:LYS:HG3	1:A:85:PHE:N	2.28	0.48
2:B:155:TRP:CD2	2:B:232:LEU:HD23	2.48	0.48
1:C:802:CYS:SG	1:C:961:LEU:HD21	2.54	0.48
1:A:423:ARG:H	1:A:446:GLU:CD	2.18	0.47
2:B:246:TYR:O	2:B:250:LEU:HB3	2.14	0.47
1:A:786:PHE:HE2	1:A:793:LEU:HA	1.79	0.47
1:C:524:ASP:HB2	1:C:527:LEU:H	1.79	0.47
1:A:887:TRP:CD1	2:B:85:LYS:HA	2.49	0.47
1:A:909:PHE:HB3	1:A:972:ARG:O	2.14	0.47
2:D:277:LYS:HD2	2:D:279:TYR:OH	2.14	0.47
1:A:725:VAL:HG11	1:A:751:ILE:HD11	1.96	0.47
1:A:949:PHE:CE1	3:G:45:LEU:HD22	2.50	0.47
1:C:554:PRO:HB2	1:C:557:GLN:OE1	2.15	0.47
1:C:584:MET:SD	1:C:584:MET:N	2.88	0.47
1:C:327:GLU:CD	1:C:327:GLU:H	2.18	0.47
1:C:756:GLU:HB2	1:C:825:MET:HE1	1.97	0.47
1:C:935:ASN:HB3	1:C:939:GLN:OE1	2.15	0.47
2:D:173:LYS:HG2	2:D:174:PRO:N	2.29	0.47
2:D:246:TYR:O	2:D:250:LEU:HB3	2.15	0.47
1:A:32:VAL:HG12	1:A:262:ARG:HH12	1.78	0.47
1:A:197:ARG:CZ	1:A:234:ASN:HD22	2.27	0.47
1:A:710:ASP:O	1:A:731:GLY:HA2	2.14	0.47
1:C:932:THR:HG21	1:C:937:VAL:HA	1.95	0.47
1:A:207:ASP:O	1:A:240:THR:HB	2.15	0.47
1:C:899:TRP:CZ2	2:D:72:VAL:HG22	2.50	0.47
1:C:924:TRP:CZ2	8:C:1107:CLR:H213	2.50	0.47
1:A:514:ILE:HG23	1:A:578:PHE:HB3	1.96	0.47
2:B:22:LYS:O	2:B:24:PHE:N	2.48	0.47
2:B:94:ASP:HB3	2:D:91:ARG:NH2	2.30	0.47
1:C:821:GLU:OE2	1:C:932:THR:HA	2.14	0.47
1:A:284:PHE:CG	1:A:838:VAL:HG21	2.50	0.47
1:A:911:CYS:C	1:A:914:PRO:HD2	2.36	0.47
1:A:935:ASN:HB3	1:A:939:GLN:OE1	2.15	0.47
2:B:277:LYS:HD2	2:B:279:TYR:OH	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:963:TYR:HE2	1:A:976:LEU:H	1.63	0.46
2:B:173:LYS:HG2	2:B:174:PRO:N	2.31	0.46
1:C:207:ASP:OD2	1:C:209:SER:OG	2.14	0.46
1:C:211:LEU:HD11	1:C:230:LEU:HD22	1.96	0.46
1:A:111:GLN:OE1	1:A:122:ASN:ND2	2.48	0.46
2:B:229:TYR:HB2	2:B:236:PRO:HB3	1.98	0.46
1:C:71:ASN:ND2	1:C:71:ASN:O	2.48	0.46
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.81	0.46
1:A:495:ARG:HH12	1:A:558:PHE:CB	2.29	0.46
1:A:618:LYS:HE2	1:A:622:LYS:HE2	1.97	0.46
2:B:94:ASP:CG	2:B:97:SER:HB2	2.36	0.46
3:G:23:TYR:HD2	3:G:23:TYR:HA	1.69	0.46
1:A:161:GLN:HG2	1:A:174:ASN:HA	1.97	0.46
1:A:421:CYS:SG	1:A:501:LYS:HG2	2.56	0.46
1:C:165:ILE:HB	1:C:183:LEU:HB3	1.96	0.46
1:C:515:LEU:CD2	1:C:520:GLU:HG2	2.45	0.46
1:C:861:THR:O	1:C:865:ILE:HG12	2.15	0.46
1:A:78:THR:N	1:A:79:THR:HA	2.30	0.46
1:A:360:LEU:HD22	1:A:741:MET:SD	2.56	0.46
1:A:610:THR:OG1	5:A:1102:ALF:F2	2.23	0.46
2:B:79:GLN:HG2	2:B:295:PHE:CE1	2.51	0.46
1:C:871:PHE:HB3	1:C:876:LEU:HD21	1.97	0.46
1:C:909:PHE:HB3	1:C:972:ARG:O	2.16	0.46
1:C:911:CYS:C	1:C:914:PRO:HD2	2.36	0.46
1:A:108:TYR:CZ	1:A:123:LEU:HD22	2.51	0.46
1:A:802:CYS:SG	1:A:961:LEU:HD21	2.56	0.46
1:C:30:LYS:N	1:C:262:ARG:HH22	2.14	0.46
1:C:868:GLU:HA	2:D:67:THR:HG1	1.81	0.46
2:D:155:TRP:CD2	2:D:232:LEU:HD23	2.50	0.46
1:A:506:ARG:O	1:A:510:ARG:HG3	2.16	0.46
1:A:366:ILE:HG13	1:A:604:ILE:CG2	2.46	0.46
1:A:422:ASN:OD1	1:A:424:ALA:N	2.47	0.46
1:C:860:PHE:HZ	8:C:1108:CLR:H6	1.81	0.46
3:E:39:ILE:O	3:E:43:ILE:HG12	2.16	0.46
1:A:861:THR:O	1:A:865:ILE:HG12	2.15	0.46
2:D:207:TYR:HA	2:D:240:LEU:HD22	1.97	0.46
1:A:793:LEU:HD22	1:A:908:GLU:OE2	2.16	0.45
1:C:895:TYR:CE2	2:D:66:PRO:HA	2.50	0.45
2:D:193:ASN:HD21	2:D:196:LEU:HB3	1.81	0.45
1:A:71:ASN:O	1:A:71:ASN:ND2	2.50	0.45
1:A:211:LEU:HD11	1:A:230:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLU:HB3	1:A:216:GLU:HG2	1.98	0.45
1:A:691:LYS:HB3	1:A:717:ALA:HB2	1.98	0.45
1:A:826:LYS:HA	1:A:828:GLN:N	2.30	0.45
1:A:998:ARG:O	1:A:1001:ILE:N	2.48	0.45
1:C:154:PHE:HB3	1:C:350:LEU:HD13	1.97	0.45
1:C:405:ASP:OD2	1:C:408:SER:HB2	2.16	0.45
2:D:189:LYS:N	2:D:282:ASN:HD22	2.14	0.45
1:A:165:ILE:HB	1:A:183:LEU:HB3	1.97	0.45
1:A:210:SER:HB2	1:A:260:MET:HE1	1.99	0.45
2:B:70:ASP:OD2	2:B:71:ARG:HG2	2.15	0.45
2:B:79:GLN:NE2	2:B:81:PRO:O	2.44	0.45
2:B:148:VAL:HG21	2:B:254:TYR:HA	1.98	0.45
2:B:193:ASN:ND2	2:B:196:LEU:HD13	2.28	0.45
1:C:207:ASP:O	1:C:240:THR:HB	2.16	0.45
1:C:951:LEU:HB3	8:C:1107:CLR:H261	1.97	0.45
1:A:98:TRP:CD1	1:A:133:VAL:HG11	2.52	0.45
1:C:40:SER:O	1:C:44:LEU:N	2.45	0.45
1:C:531:PHE:HE2	1:C:581:LEU:HD21	1.81	0.45
2:D:22:LYS:O	2:D:24:PHE:N	2.50	0.45
2:D:79:GLN:HG2	2:D:295:PHE:CE1	2.51	0.45
1:A:327:GLU:H	1:A:327:GLU:CD	2.19	0.45
1:C:84:LYS:HG3	1:C:85:PHE:N	2.30	0.45
1:C:473:ILE:HB	1:C:483:LEU:HG	1.98	0.45
1:C:660:GLY:H	1:C:685:ARG:HB3	1.81	0.45
1:C:723:ILE:HD12	1:C:740:ASP:HB2	1.96	0.45
1:A:649:ASN:HB3	1:A:652:ASP:HB2	1.98	0.45
1:A:793:LEU:HD12	1:A:793:LEU:H	1.81	0.45
2:B:95:PRO:O	2:B:99:GLU:HG2	2.16	0.45
1:C:50:THR:OG1	1:C:51:ASP:N	2.47	0.45
1:C:503:ALA:HB1	1:C:505:GLU:OE2	2.17	0.45
1:A:320:ILE:O	1:A:323:ALA:HB3	2.17	0.45
1:C:506:ARG:O	1:C:510:ARG:HG3	2.15	0.45
1:C:691:LYS:HB3	1:C:717:ALA:HB2	1.99	0.45
1:C:755:VAL:O	1:C:759:ARG:HG2	2.17	0.45
1:A:790:ASN:HB2	1:A:878:GLY:HA2	1.99	0.45
1:A:986:PRO:HG3	8:A:1108:CLR:H181	1.98	0.45
2:D:92:PRO:HD3	2:D:170:LYS:CE	2.47	0.45
1:A:503:ALA:HB1	1:A:505:GLU:OE2	2.17	0.45
1:A:723:ILE:HD12	1:A:740:ASP:HB2	1.99	0.45
1:A:866:LEU:HB3	1:A:876:LEU:HD11	1.99	0.45
1:A:985:PHE:N	1:A:986:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1108:CLR:H212	8:A:1108:CLR:H183	1.98	0.45
2:B:136:ARG:HG2	2:B:146:ARG:HB3	1.99	0.45
1:C:214:GLU:HB3	1:C:216:GLU:HG2	1.99	0.45
1:C:909:PHE:CD2	1:C:972:ARG:HB3	2.52	0.45
1:A:405:ASP:OD2	1:A:408:SER:HB2	2.16	0.45
1:A:495:ARG:NH1	1:A:558:PHE:HD2	2.14	0.45
1:A:722:ASP:OD2	1:A:722:ASP:N	2.51	0.45
1:A:763:ASP:HA	1:A:933:ARG:NH2	2.31	0.45
1:A:856:LEU:HD13	2:B:50:PHE:HB2	1.99	0.45
1:A:895:TYR:CE2	2:B:66:PRO:HA	2.52	0.45
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.82	0.45
1:C:610:THR:OG1	5:C:1102:ALF:F2	2.25	0.45
2:D:59:LEU:HG	2:D:60:THR:CA	2.47	0.45
1:A:531:PHE:HE2	1:A:581:LEU:HD21	1.82	0.44
1:A:613:HIS:HA	1:A:614:PRO:HD3	1.89	0.44
1:A:909:PHE:CD2	1:A:972:ARG:HB3	2.52	0.44
1:A:981:TRP:CD1	8:A:1107:CLR:H12	2.51	0.44
2:B:207:TYR:HA	2:B:240:LEU:HD22	1.99	0.44
1:C:192:ILE:HG12	1:C:240:THR:O	2.17	0.44
1:C:618:LYS:HE2	1:C:622:LYS:HE2	1.99	0.44
1:C:868:GLU:HA	2:D:67:THR:OG1	2.17	0.44
1:C:914:PRO:HG3	1:C:976:LEU:HD21	1.99	0.44
1:A:121:ASP:OD1	1:A:972:ARG:NH2	2.51	0.44
1:A:924:TRP:CH2	8:A:1107:CLR:H17	2.52	0.44
1:C:98:TRP:CD1	1:C:133:VAL:HG11	2.52	0.44
1:A:36:ASP:HB2	1:A:39:LEU:HD12	2.00	0.44
2:B:95:PRO:HD2	2:D:302:LYS:NZ	2.33	0.44
1:C:423:ARG:H	1:C:446:GLU:CD	2.20	0.44
1:C:602:ALA:HA	1:C:825:MET:O	2.17	0.44
1:C:663:LEU:HD11	1:C:694:ILE:HD11	1.99	0.44
1:C:710:ASP:O	1:C:731:GLY:HA2	2.18	0.44
1:C:819:GLN:HE21	1:C:943:LYS:HE3	1.83	0.44
1:C:985:PHE:N	1:C:986:PRO:HD2	2.32	0.44
1:A:192:ILE:HG21	1:A:236:ALA:HB1	1.99	0.44
8:A:1107:CLR:H193	8:A:1107:CLR:H111	1.78	0.44
1:C:422:ASN:OD1	1:C:424:ALA:N	2.49	0.44
1:C:790:ASN:HB2	1:C:878:GLY:HA2	1.99	0.44
8:C:1108:CLR:H213	8:C:1108:CLR:H231	1.74	0.44
2:D:70:ASP:OD2	2:D:71:ARG:HG2	2.17	0.44
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.52	0.44
1:A:584:MET:SD	1:A:584:MET:N	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:SER:O	1:A:301:ILE:HG12	2.17	0.44
1:C:192:ILE:HG21	1:C:236:ALA:HB1	2.00	0.44
1:C:998:ARG:O	1:C:1001:ILE:N	2.49	0.44
2:D:148:VAL:HG21	2:D:254:TYR:HA	1.99	0.44
1:A:50:THR:OG1	1:A:51:ASP:N	2.50	0.44
1:A:341:ALA:HB2	1:A:354:LEU:HD21	2.00	0.44
1:A:503:ALA:HA	1:A:504:PRO:HD2	1.86	0.44
1:A:603:GLY:HA3	1:A:828:GLN:CG	2.46	0.44
1:A:683:PHE:HB3	1:A:686:THR:HG21	2.00	0.44
1:A:786:PHE:CE2	1:A:793:LEU:HA	2.52	0.44
1:A:870:GLY:HA2	1:A:895:TYR:CD2	2.52	0.44
1:C:551:LEU:HD23	1:C:576:LEU:HA	1.99	0.44
1:C:765:LEU:HB2	1:C:837:LEU:HD11	2.00	0.44
1:C:866:LEU:HB3	1:C:876:LEU:HD11	1.99	0.44
2:D:136:ARG:HG2	2:D:146:ARG:HB3	2.00	0.44
1:A:535:TYR:HE1	1:A:545:VAL:HB	1.83	0.44
1:A:819:GLN:HE21	1:A:943:LYS:HE3	1.81	0.44
2:B:173:LYS:HB3	2:B:173:LYS:HE3	1.56	0.44
1:C:238:PHE:HD1	1:C:239:SER:N	2.16	0.44
2:D:118:LYS:H	2:D:123:PHE:HD2	1.66	0.44
2:D:271:GLU:OE1	2:D:298:LYS:HD3	2.18	0.44
1:A:37:HIS:HB2	1:A:234:ASN:HD21	1.83	0.43
2:B:89:SER:HA	2:B:300:GLU:O	2.18	0.43
3:E:22:ASP:O	3:E:24:GLU:HG2	2.18	0.43
1:A:781:THR:N	1:A:782:PRO:HD2	2.33	0.43
8:A:1107:CLR:H213	8:A:1107:CLR:H231	1.75	0.43
8:A:1108:CLR:H121	2:B:56:VAL:CG1	2.48	0.43
1:C:571:PHE:HD1	1:C:571:PHE:HA	1.66	0.43
1:C:763:ASP:HA	1:C:933:ARG:NH2	2.33	0.43
1:C:870:GLY:HA2	1:C:895:TYR:HD2	1.82	0.43
2:D:166:THR:OG1	2:D:167:TYR:N	2.51	0.43
1:A:793:LEU:H	1:A:793:LEU:CD1	2.30	0.43
1:A:821:GLU:HG3	1:A:934:ARG:HB2	2.00	0.43
2:B:118:LYS:H	2:B:123:PHE:HD2	1.65	0.43
1:C:140:SER:O	1:C:144:GLU:HB2	2.18	0.43
1:C:786:PHE:CE2	1:C:793:LEU:HA	2.53	0.43
2:D:239:PRO:HB2	2:D:241:GLN:HG2	1.99	0.43
1:C:495:ARG:NH1	1:C:558:PHE:HD2	2.16	0.43
1:C:535:TYR:HE1	1:C:545:VAL:HB	1.83	0.43
1:C:551:LEU:HD22	1:C:551:LEU:HA	1.75	0.43
2:D:74:PRO:HA	2:D:75:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:ASP:HA	1:A:933:ARG:HH22	1.83	0.43
1:A:831:ASN:HB2	1:A:834:THR:OG1	2.19	0.43
2:B:94:ASP:HB3	2:D:91:ARG:CZ	2.48	0.43
2:B:189:LYS:HA	2:B:190:PRO:HD2	1.84	0.43
3:G:23:TYR:HB3	3:G:24:GLU:H	1.44	0.43
1:C:298:SER:O	1:C:301:ILE:HG12	2.19	0.43
1:C:415:SER:OG	1:C:453:ILE:HD12	2.18	0.43
1:C:495:ARG:HH12	1:C:558:PHE:CB	2.30	0.43
1:A:239:SER:OG	1:A:260:MET:HG2	2.19	0.43
1:A:862:TYR:HD2	1:A:911:CYS:HB3	1.82	0.43
1:C:37:HIS:HB2	1:C:234:ASN:HD21	1.84	0.43
1:C:815:LEU:HD13	1:C:815:LEU:HA	1.84	0.43
1:C:961:LEU:O	1:C:967:MET:HE2	2.18	0.43
2:D:62:SER:C	2:D:64:PHE:H	2.22	0.43
1:C:454:GLU:HA	1:C:458:GLY:O	2.19	0.43
1:C:603:GLY:HA3	1:C:828:GLN:CG	2.46	0.43
1:C:858:GLY:HA3	1:C:915:PHE:CE1	2.53	0.43
1:C:862:TYR:HD2	1:C:911:CYS:HB3	1.84	0.43
1:C:944:ASN:O	1:C:948:ILE:HG13	2.18	0.43
2:D:187:LYS:HA	2:D:188:PRO:HD2	1.84	0.43
1:C:164:VAL:HG12	1:C:184:VAL:HG22	2.01	0.43
1:C:683:PHE:HB3	1:C:686:THR:HG21	2.01	0.43
1:C:741:MET:HB3	1:C:741:MET:HE2	1.67	0.43
2:D:129:VAL:HA	2:D:130:PRO:HD3	1.82	0.43
1:A:131:ALA:O	1:A:135:ILE:HG13	2.18	0.43
1:A:660:GLY:H	1:A:685:ARG:HB3	1.83	0.43
1:A:977:LYS:HB3	3:G:21:TYR:HE2	1.84	0.43
2:B:239:PRO:HB2	2:B:241:GLN:HG2	2.00	0.43
2:B:271:GLU:OE1	2:B:298:LYS:HD3	2.18	0.43
1:C:278:ALA:O	1:C:281:ILE:HB	2.19	0.43
1:C:722:ASP:OD2	1:C:722:ASP:N	2.52	0.43
1:C:821:GLU:HG3	1:C:934:ARG:HB2	2.01	0.43
8:C:1107:CLR:H182	8:C:1107:CLR:H8	1.74	0.43
1:A:402:VAL:CA	1:A:403:SER:HB3	2.49	0.43
1:A:516:ILE:HD12	1:A:521:GLN:OE1	2.19	0.43
1:A:944:ASN:O	1:A:948:ILE:HG13	2.18	0.43
2:B:92:PRO:HD3	2:B:170:LYS:CE	2.48	0.43
1:C:297:VAL:O	1:C:301:ILE:HG23	2.19	0.43
1:C:786:PHE:O	1:C:880:ARG:NH2	2.44	0.43
1:C:824:ILE:HD13	1:C:824:ILE:H	1.83	0.43
1:C:831:ASN:HB2	1:C:834:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:ILE:HD12	2:D:67:THR:HG23	2.01	0.43
1:A:495:ARG:HD2	1:A:495:ARG:HA	1.54	0.42
1:A:663:LEU:HD11	1:A:694:ILE:HD11	2.00	0.42
2:B:74:PRO:HA	2:B:75:PRO:HD3	1.89	0.42
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.54	0.42
1:C:789:ALA:O	1:C:791:ILE:N	2.46	0.42
1:C:861:THR:HG21	1:C:918:THR:HG21	2.01	0.42
1:A:122:ASN:HB2	1:A:123:LEU:H	1.48	0.42
1:A:381:VAL:HB	1:A:452:CYS:SG	2.59	0.42
1:A:504:PRO:HB2	1:A:531:PHE:HZ	1.83	0.42
1:C:781:THR:N	1:C:782:PRO:HD2	2.34	0.42
1:C:949:PHE:CE2	1:C:953:GLU:HG3	2.54	0.42
8:C:1107:CLR:H213	8:C:1107:CLR:H231	1.84	0.42
2:D:88:ILE:HG12	2:D:299:ILE:HA	2.02	0.42
2:B:59:LEU:HG	2:B:60:THR:CA	2.49	0.42
1:C:477:SER:HB3	1:C:713:ASN:HD22	1.83	0.42
2:D:53:THR:HA	2:D:56:VAL:HG12	2.00	0.42
2:B:61:ILE:HD12	2:B:67:THR:HG23	2.00	0.42
2:B:62:SER:C	2:B:64:PHE:H	2.23	0.42
1:C:131:ALA:O	1:C:135:ILE:HG13	2.20	0.42
1:C:161:GLN:HG2	1:C:174:ASN:HA	2.00	0.42
1:C:760:LEU:O	1:C:764:ASN:N	2.36	0.42
1:C:977:LYS:HG2	3:E:21:TYR:OH	2.19	0.42
1:A:404:PHE:HZ	1:A:411:TRP:CE3	2.37	0.42
1:A:495:ARG:HH12	1:A:558:PHE:HB2	1.85	0.42
1:A:755:VAL:O	1:A:759:ARG:HG2	2.20	0.42
1:A:821:GLU:OE2	1:A:932:THR:HA	2.19	0.42
2:B:133:LEU:HD12	2:B:133:LEU:H	1.84	0.42
1:C:586:ASP:HA	1:C:587:PRO:HD3	1.81	0.42
1:C:633:THR:O	1:C:637:ILE:HG12	2.20	0.42
1:C:698:CYS:CB	1:C:705:VAL:HG11	2.50	0.42
1:A:238:PHE:HD1	1:A:239:SER:N	2.17	0.42
1:A:284:PHE:CZ	1:A:288:ILE:HD11	2.54	0.42
1:A:347:LYS:HE3	1:A:753:THR:HB	2.01	0.42
1:C:435:ILE:HB	1:C:455:LEU:HD22	2.02	0.42
1:C:793:LEU:HG	1:C:908:GLU:CD	2.40	0.42
2:D:113:LYS:HB3	2:D:113:LYS:HE3	1.89	0.42
1:A:469:LYS:HG3	1:A:486:HIS:NE2	2.35	0.42
1:A:1010:VAL:HG12	1:A:1014:THR:HG23	2.01	0.42
2:B:202:MET:H	2:B:202:MET:HG2	1.41	0.42
1:C:328:GLY:O	1:C:332:THR:OG1	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:ILE:HG13	1:C:604:ILE:CG2	2.49	0.42
1:A:169:GLU:HB3	1:A:428:ALA:HB2	2.00	0.42
1:A:278:ALA:O	1:A:281:ILE:HB	2.20	0.42
1:A:326:PRO:HB3	1:A:772:THR:HG21	2.01	0.42
1:A:379:MET:SD	1:A:544:ARG:NH2	2.92	0.42
1:A:633:THR:O	1:A:637:ILE:HG12	2.20	0.42
1:A:819:GLN:NE2	1:A:943:LYS:HE3	2.35	0.42
1:A:914:PRO:HG3	1:A:976:LEU:HD21	2.01	0.42
1:C:284:PHE:CZ	1:C:288:ILE:HD11	2.55	0.42
1:C:897:GLN:HG2	2:D:184:LEU:H	1.85	0.42
2:D:99:GLU:HA	2:D:102:VAL:HB	2.00	0.42
2:D:133:LEU:HD12	2:D:133:LEU:H	1.85	0.42
1:A:140:SER:O	1:A:144:GLU:HB2	2.19	0.42
1:A:208:ASN:N	1:A:208:ASN:OD1	2.53	0.42
1:A:284:PHE:CE2	1:A:288:ILE:HD11	2.54	0.42
1:A:385:TRP:HE3	1:A:581:LEU:HG	1.85	0.42
1:A:860:PHE:HD1	2:B:54:ILE:HD12	1.85	0.42
1:C:157:MET:HB3	1:C:744:LEU:HD13	2.02	0.42
1:C:504:PRO:HB2	1:C:531:PHE:HZ	1.85	0.42
1:C:860:PHE:HD1	2:D:54:ILE:HD12	1.84	0.42
2:D:145:GLU:HG3	2:D:252:PRO:HD2	2.02	0.42
1:A:953:GLU:OE2	3:G:38:PHE:HA	2.20	0.41
1:A:977:LYS:HD3	3:G:21:TYR:CD2	2.55	0.41
2:B:78:THR:OG1	2:B:79:GLN:N	2.53	0.41
1:C:208:ASN:OD1	1:C:208:ASN:N	2.52	0.41
1:C:660:GLY:N	1:C:684:ALA:O	2.53	0.41
1:A:93:PHE:CE2	1:A:325:VAL:HG13	2.55	0.41
1:A:157:MET:HB3	1:A:744:LEU:HD13	2.01	0.41
1:A:232:THR:OG1	1:A:234:ASN:OD1	2.20	0.41
1:A:347:LYS:H	1:A:347:LYS:HG3	1.74	0.41
1:C:404:PHE:HZ	1:C:411:TRP:CE3	2.38	0.41
2:D:89:SER:HA	2:D:300:GLU:O	2.19	0.41
1:A:1005:ARG:HA	1:A:1006:PRO:HD3	1.81	0.41
1:C:803:ILE:HD13	1:C:803:ILE:HA	1.92	0.41
1:C:811:PRO:HB3	1:C:927:LEU:HD21	2.02	0.41
8:C:1108:CLR:H183	8:C:1108:CLR:H20	1.86	0.41
2:D:193:ASN:OD1	2:D:195:SER:HA	2.19	0.41
1:A:164:VAL:HG12	1:A:184:VAL:HG22	2.02	0.41
1:A:551:LEU:HA	1:A:551:LEU:HD22	1.73	0.41
1:A:586:ASP:HA	1:A:587:PRO:HD3	1.81	0.41
1:C:139:PHE:O	1:C:143:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:LYS:H	1:C:347:LYS:HG3	1.75	0.41
1:C:899:TRP:CH2	2:D:72:VAL:HG22	2.55	0.41
2:D:173:LYS:HE3	2:D:173:LYS:HB3	1.56	0.41
2:D:221:LYS:C	2:D:223:LYS:H	2.23	0.41
1:A:698:CYS:CB	1:A:705:VAL:HG11	2.51	0.41
1:A:759:ARG:O	1:A:763:ASP:N	2.53	0.41
1:A:765:LEU:HB2	1:A:837:LEU:HD11	2.02	0.41
1:A:858:GLY:HA3	1:A:915:PHE:CE1	2.55	0.41
1:C:79:THR:HG23	1:C:80:PRO:HD3	2.03	0.41
1:C:326:PRO:HB3	1:C:772:THR:HG21	2.03	0.41
1:C:963:TYR:CD1	3:E:30:GLY:HA3	2.54	0.41
2:D:186:PHE:HA	3:E:19:PHE:HE1	1.85	0.41
1:A:121:ASP:HB3	1:A:122:ASN:H	1.42	0.41
1:A:760:LEU:O	1:A:764:ASN:N	2.38	0.41
1:A:786:PHE:O	1:A:880:ARG:NH2	2.46	0.41
1:A:955:THR:HG22	3:G:33:PHE:HZ	1.84	0.41
2:B:242:TYR:HB2	2:B:257:PRO:HG3	2.03	0.41
1:C:793:LEU:H	1:C:793:LEU:CD2	2.32	0.41
1:C:921:VAL:HG13	1:C:924:TRP:CZ3	2.56	0.41
1:A:139:PHE:O	1:A:143:GLN:HG2	2.21	0.41
1:A:473:ILE:HB	1:A:483:LEU:HG	2.02	0.41
1:A:774:THR:CG2	1:A:850:ILE:HB	2.51	0.41
2:B:132:GLU:O	2:B:134:LYS:HG2	2.20	0.41
2:B:217:ARG:HB3	2:B:218:ASP:H	1.73	0.41
1:A:154:PHE:HB3	1:A:350:LEU:HD23	2.03	0.41
1:A:742:ILE:HG22	1:A:744:LEU:HD23	2.03	0.41
1:C:198:ILE:HD13	1:C:198:ILE:HA	1.84	0.41
1:C:284:PHE:CE2	1:C:288:ILE:HD11	2.56	0.41
1:C:301:ILE:O	1:C:305:ILE:HG12	2.20	0.41
2:D:58:LEU:CA	2:D:60:THR:HB	2.50	0.41
2:D:193:ASN:HD21	2:D:196:LEU:N	2.18	0.41
1:A:51:ASP:CG	1:A:54:ARG:HB2	2.41	0.41
1:A:297:VAL:O	1:A:301:ILE:HG23	2.21	0.41
1:A:741:MET:HE2	1:A:741:MET:HB3	1.71	0.41
1:A:774:THR:HG22	1:A:850:ILE:HB	2.03	0.41
8:A:1108:CLR:H213	8:A:1108:CLR:H231	1.70	0.41
2:B:75:PRO:HG3	2:B:183:VAL:HG21	2.02	0.41
2:B:99:GLU:HA	2:B:102:VAL:HB	2.02	0.41
2:B:105:ILE:HG22	2:B:165:GLU:OE2	2.21	0.41
1:C:284:PHE:HZ	1:C:773:LEU:HD21	1.85	0.41
1:C:341:ALA:HB2	1:C:354:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:VAL:HB	1:C:452:CYS:SG	2.61	0.41
4:C:1101:ADP:H5'2	4:C:1101:ADP:O1B	2.21	0.41
2:D:154:GLU:OE2	2:D:154:GLU:N	2.49	0.41
1:A:551:LEU:HD23	1:A:576:LEU:HA	2.03	0.41
1:A:644:PRO:HG2	1:A:647:GLN:HB2	2.03	0.41
8:A:1107:CLR:H8	8:A:1107:CLR:H182	1.80	0.41
1:C:766:LYS:HG3	1:C:837:LEU:O	2.20	0.41
1:C:898:GLN:HG3	2:D:182:ARG:HG2	2.03	0.41
8:C:1107:CLR:H162	8:C:1107:CLR:H221	1.77	0.41
1:A:40:SER:O	1:A:44:LEU:N	2.49	0.40
1:A:299:PHE:HA	1:A:302:LEU:HB2	2.03	0.40
1:A:301:ILE:O	1:A:305:ILE:HG12	2.21	0.40
1:A:710:ASP:N	1:A:714:ASP:OD2	2.35	0.40
2:B:58:LEU:CA	2:B:60:THR:HB	2.49	0.40
2:B:221:LYS:C	2:B:223:LYS:H	2.24	0.40
1:C:122:ASN:HB2	1:C:123:LEU:H	1.48	0.40
1:C:495:ARG:HH12	1:C:558:PHE:HB2	1.86	0.40
2:D:132:GLU:O	2:D:134:LYS:HG2	2.21	0.40
1:A:632:GLU:HB3	1:A:636:ASP:HB2	2.04	0.40
1:C:632:GLU:HB3	1:C:636:ASP:HB2	2.02	0.40
2:D:78:THR:OG1	2:D:79:GLN:N	2.55	0.40
1:A:369:ASP:O	1:A:373:THR:HB	2.21	0.40
1:A:415:SER:OG	1:A:453:ILE:HD12	2.22	0.40
1:A:477:SER:HB3	1:A:713:ASN:HD22	1.86	0.40
1:A:622:LYS:HA	1:A:627:ILE:O	2.22	0.40
2:B:65:LYS:HA	2:B:66:PRO:HD3	1.97	0.40
1:C:347:LYS:HE3	1:C:753:THR:HB	2.02	0.40
1:C:413:ALA:O	1:C:417:ILE:HG13	2.21	0.40
1:C:729:ILE:HB	1:C:746:ASP:OD2	2.20	0.40
1:A:77:PRO:HB2	1:A:78:THR:H	1.65	0.40
1:A:861:THR:HG21	1:A:918:THR:HG21	2.02	0.40
2:B:88:ILE:HG12	2:B:299:ILE:HA	2.03	0.40
2:B:117:GLN:HA	2:B:123:PHE:CE2	2.56	0.40
1:C:147:SER:O	1:C:151:MET:HG2	2.21	0.40
1:C:421:CYS:SG	1:C:501:LYS:HG2	2.61	0.40
1:C:622:LYS:HA	1:C:627:ILE:O	2.21	0.40
1:C:790:ASN:HB2	1:C:878:GLY:CA	2.52	0.40
2:D:198:THR:HG23	2:D:200:PRO:HD3	2.04	0.40
2:D:242:TYR:HB2	2:D:257:PRO:HG3	2.03	0.40
1:A:404:PHE:CZ	1:A:411:TRP:CE3	3.10	0.40
1:A:689:GLN:O	1:A:693:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:GLU:HG3	2:B:252:PRO:HD2	2.03	0.40
2:B:194:GLU:O	2:B:195:SER:HB3	2.22	0.40
1:C:660:GLY:HA3	1:C:685:ARG:O	2.22	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	983/1021 (96%)	903 (92%)	66 (7%)	14 (1%)	11 47
1	C	985/1021 (96%)	903 (92%)	64 (6%)	18 (2%)	8 42
2	B	283/303 (93%)	234 (83%)	40 (14%)	9 (3%)	4 30
2	D	283/303 (93%)	238 (84%)	33 (12%)	12 (4%)	3 25
3	E	27/65 (42%)	25 (93%)	1 (4%)	1 (4%)	3 28
3	G	25/65 (38%)	22 (88%)	1 (4%)	2 (8%)	1 14
All	All	2586/2778 (93%)	2325 (90%)	205 (8%)	56 (2%)	6 38

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	PRO
1	A	122	ASN
1	A	123	LEU
1	A	821	GLU
2	B	171	ASP
2	B	201	VAL
3	G	24	GLU
1	C	32	VAL
1	C	77	PRO

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Mol	Chain	Res	Type
1	C	79	THR
1	C	122	ASN
1	C	123	LEU
1	C	821	GLU
2	D	166	THR
2	D	171	ASP
2	D	201	VAL
3	E	24	GLU
1	A	323	ALA
2	B	23	GLU
2	B	31	SER
2	B	158	ASN
2	B	195	SER
2	B	267	THR
1	C	323	ALA
1	C	398	ASN
1	C	822	SER
1	C	824	ILE
2	D	22	LYS
2	D	23	GLU
2	D	31	SER
2	D	158	ASN
2	D	267	THR
1	A	76	PRO
1	A	81	GLU
1	A	405	ASP
1	A	494	PRO
2	B	73	ALA
1	C	76	PRO
1	C	81	GLU
1	C	405	ASP
1	C	494	PRO
2	D	73	ALA
2	D	164	ASP
2	D	167	TYR
1	A	396	THR
1	A	824	ILE
1	A	943	LYS
2	B	164	ASP
1	C	396	THR
1	C	943	LYS
3	G	22	ASP

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Mol	Chain	Res	Type
1	C	1008	GLY
2	D	168	GLY
1	A	1008	GLY
1	A	186	VAL
1	C	186	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	836/865 (97%)	761 (91%)	75 (9%)	9 33
1	C	838/865 (97%)	758 (90%)	80 (10%)	8 30
2	B	255/269 (95%)	218 (86%)	37 (14%)	3 18
2	D	255/269 (95%)	217 (85%)	38 (15%)	3 17
3	E	23/52 (44%)	21 (91%)	2 (9%)	10 34
3	G	21/52 (40%)	19 (90%)	2 (10%)	8 30
All	All	2228/2372 (94%)	1994 (90%)	234 (10%)	7 27

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	41	LEU
1	A	44	LEU
1	A	60	ARG
1	A	63	GLU
1	A	73	LEU
1	A	79	THR
1	A	82	TRP
1	A	83	VAL
1	A	84	LYS
1	A	85	PHE
1	A	86	CYS
1	A	90	PHE

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Mol	Chain	Res	Type
1	A	93	PHE
1	A	99	ILE
1	A	121	ASP
1	A	122	ASN
1	A	186	VAL
1	A	237	PHE
1	A	238	PHE
1	A	241	ASN
1	A	254	THR
1	A	257	ARG
1	A	275	THR
1	A	306	LEU
1	A	308	TYR
1	A	316	PHE
1	A	327	GLU
1	A	334	THR
1	A	336	CYS
1	A	340	THR
1	A	347	LYS
1	A	350	LEU
1	A	353	ASN
1	A	399	GLN
1	A	445	SER
1	A	450	LEU
1	A	471	VAL
1	A	483	LEU
1	A	495	ARG
1	A	550	HIS
1	A	551	LEU
1	A	558	PHE
1	A	571	PHE
1	A	584	MET
1	A	612	ASP
1	A	652	ASP
1	A	663	LEU
1	A	689	GLN
1	A	719	LYS
1	A	722	ASP
1	A	727	MET
1	A	755	VAL
1	A	763	ASP
1	A	775	SER

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Mol	Chain	Res	Type
1	A	783	PHE
1	A	793	LEU
1	A	807	THR
1	A	815	LEU
1	A	821	GLU
1	A	822	SER
1	A	825	MET
1	A	842	LEU
1	A	854	GLN
1	A	862	TYR
1	A	877	LEU
1	A	879	LEU
1	A	890	ASP
1	A	915	PHE
1	A	929	ILE
1	A	934	ARG
1	A	942	MET
1	A	947	LEU
1	A	973	MET
1	A	1010	VAL
2	B	24	PHE
2	B	28	THR
2	B	33	PHE
2	B	34	LYS
2	B	46	LEU
2	B	57	MET
2	B	59	LEU
2	B	60	THR
2	B	67	THR
2	B	78	THR
2	B	79	GLN
2	B	88	ILE
2	B	94	ASP
2	B	107	ARG
2	B	122	ILE
2	B	156	LEU
2	B	163	ASN
2	B	164	ASP
2	B	170	LYS
2	B	173	LYS
2	B	175	CYS
2	B	177	ILE

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Mol	Chain	Res	Type
2	B	178	ILE
2	B	193	ASN
2	B	199	TYR
2	B	201	VAL
2	B	203	LYS
2	B	204	TYR
2	B	214	THR
2	B	224	VAL
2	B	229	TYR
2	B	249	LEU
2	B	266	LEU
2	B	267	THR
2	B	268	MET
2	B	272	ILE
2	B	297	VAL
3	G	21	TYR
3	G	23	TYR
1	C	30	LYS
1	C	32	VAL
1	C	35	ASP
1	C	41	LEU
1	C	44	LEU
1	C	60	ARG
1	C	63	GLU
1	C	79	THR
1	C	82	TRP
1	C	83	VAL
1	C	84	LYS
1	C	85	PHE
1	C	86	CYS
1	C	87	ARG
1	C	90	PHE
1	C	93	PHE
1	C	99	ILE
1	C	121	ASP
1	C	122	ASN
1	C	186	VAL
1	C	237	PHE
1	C	238	PHE
1	C	241	ASN
1	C	254	THR
1	C	257	ARG

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Mol	Chain	Res	Type
1	C	259	VAL
1	C	263	ILE
1	C	265	THR
1	C	275	THR
1	C	308	TYR
1	C	316	PHE
1	C	327	GLU
1	C	334	THR
1	C	336	CYS
1	C	340	THR
1	C	347	LYS
1	C	350	LEU
1	C	353	ASN
1	C	399	GLN
1	C	445	SER
1	C	450	LEU
1	C	471	VAL
1	C	483	LEU
1	C	495	ARG
1	C	550	HIS
1	C	551	LEU
1	C	558	PHE
1	C	571	PHE
1	C	584	MET
1	C	612	ASP
1	C	652	ASP
1	C	663	LEU
1	C	689	GLN
1	C	719	LYS
1	C	722	ASP
1	C	727	MET
1	C	755	VAL
1	C	763	ASP
1	C	775	SER
1	C	783	PHE
1	C	793	LEU
1	C	807	THR
1	C	815	LEU
1	C	821	GLU
1	C	822	SER
1	C	824	ILE
1	C	825	MET

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Mol	Chain	Res	Type
1	C	842	LEU
1	C	854	GLN
1	C	862	TYR
1	C	877	LEU
1	C	879	LEU
1	C	890	ASP
1	C	915	PHE
1	C	929	ILE
1	C	934	ARG
1	C	942	MET
1	C	947	LEU
1	C	973	MET
1	C	1010	VAL
2	D	24	PHE
2	D	28	THR
2	D	33	PHE
2	D	34	LYS
2	D	46	LEU
2	D	57	MET
2	D	59	LEU
2	D	60	THR
2	D	67	THR
2	D	78	THR
2	D	79	GLN
2	D	88	ILE
2	D	94	ASP
2	D	107	ARG
2	D	122	ILE
2	D	156	LEU
2	D	163	ASN
2	D	164	ASP
2	D	170	LYS
2	D	173	LYS
2	D	175	CYS
2	D	177	ILE
2	D	178	ILE
2	D	193	ASN
2	D	196	LEU
2	D	199	TYR
2	D	201	VAL
2	D	203	LYS
2	D	204	TYR

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Mol	Chain	Res	Type
2	D	214	THR
2	D	224	VAL
2	D	229	TYR
2	D	249	LEU
2	D	266	LEU
2	D	267	THR
2	D	268	MET
2	D	272	ILE
2	D	297	VAL
3	E	21	TYR
3	E	23	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	376	GLN
1	A	550	HIS
1	A	631	ASN
1	A	701	GLN
2	B	93	ASN
2	B	163	ASN
2	B	262	GLN
2	B	282	ASN
1	C	45	HIS
1	C	376	GLN
1	C	550	HIS
1	C	631	ASN
1	C	689	GLN
1	C	701	GLN
2	D	163	ASN
2	D	262	GLN
2	D	282	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 for Mogul analysis.

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	$\#\|Z\| > 2$
4	ADP	C	1101	-	24,29,29	0.98	1 (4%)	29,45,45	1.28	2 (6%)
8	CLR	C	1108	-	31,31,31	1.07	3 (9%)	48,48,48	1.57	10 (20%)
8	CLR	A	1107	-	31,31,31	1.00	2 (6%)	48,48,48	1.55	7 (14%)
8	CLR	D	400	-	31,31,31	0.86	0	48,48,48	1.14	5 (10%)
4	ADP	A	1101	-	24,29,29	1.07	1 (4%)	29,45,45	1.37	2 (6%)
5	ALF	C	1102	-	4,4,4	1.36	0	-		
5	ALF	A	1102	-	4,4,4	1.36	0	-		
8	CLR	A	1108	-	31,31,31	1.00	1 (3%)	48,48,48	1.38	6 (12%)
8	CLR	C	1107	-	31,31,31	1.10	2 (6%)	48,48,48	1.33	7 (14%)

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
4	ADP	C	1101	-	-	2/12/32/32	0/3/3/3
8	CLR	C	1108	-	-	8/10/68/68	0/4/4/4
8	CLR	A	1107	-	-	4/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLR	D	400	-	-	8/10/68/68	0/4/4/4
4	ADP	A	1101	-	-	2/12/32/32	0/3/3/3
8	CLR	A	1108	-	-	6/10/68/68	0/4/4/4
8	CLR	C	1107	-	-	6/10/68/68	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	ADP	PA-O3A	3.05	1.62	1.59
4	C	1101	ADP	PA-O3A	2.87	1.62	1.59
8	C	1108	CLR	C10-C9	-2.74	1.51	1.56
8	C	1107	CLR	C13-C17	2.63	1.59	1.55
8	A	1107	CLR	C20-C17	2.46	1.58	1.54
8	C	1108	CLR	C20-C17	2.44	1.58	1.54
8	C	1107	CLR	C10-C9	2.15	1.59	1.56
8	A	1107	CLR	C13-C17	2.13	1.58	1.55
8	A	1108	CLR	C10-C5	-2.04	1.49	1.52
8	C	1108	CLR	C4-C3	2.02	1.55	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1107	CLR	C10-C9-C8	-4.36	106.35	112.71
8	C	1108	CLR	C13-C17-C20	-4.10	113.17	119.50
8	C	1108	CLR	C11-C9-C10	-3.97	108.19	113.08
8	A	1107	CLR	C13-C14-C8	-3.82	108.99	114.41
8	A	1108	CLR	C14-C8-C9	-3.74	104.20	109.09
4	C	1101	ADP	N3-C2-N1	-3.65	123.72	128.67
8	A	1107	CLR	C8-C7-C6	-3.62	107.74	112.76
4	A	1101	ADP	N3-C2-N1	-3.61	123.78	128.67
8	C	1107	CLR	C13-C14-C8	-3.49	109.46	114.41
8	C	1108	CLR	C13-C14-C8	-3.42	109.56	114.41
8	C	1108	CLR	C10-C9-C8	-3.18	108.06	112.71
4	A	1101	ADP	C4-C5-N7	-3.11	106.05	109.34
8	A	1108	CLR	C13-C14-C8	-3.09	110.03	114.41
8	A	1107	CLR	C4-C5-C6	-2.92	116.61	120.57
8	D	400	CLR	C11-C12-C13	-2.84	107.94	112.74
8	D	400	CLR	C13-C17-C20	-2.83	115.13	119.50
8	A	1108	CLR	C3-C4-C5	-2.82	107.56	112.05
4	C	1101	ADP	C4-C5-N7	-2.72	106.47	109.34
8	C	1107	CLR	C16-C17-C20	-2.66	108.16	112.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	400	CLR	C4-C5-C6	-2.66	116.97	120.57
8	A	1107	CLR	C1-C10-C9	2.63	112.22	108.74
8	C	1108	CLR	C11-C12-C13	-2.62	108.32	112.74
8	C	1107	CLR	C4-C5-C6	-2.62	117.02	120.57
8	C	1108	CLR	C1-C2-C3	-2.51	107.16	110.48
8	C	1107	CLR	C17-C13-C14	2.50	102.97	100.10
8	C	1108	CLR	C4-C5-C6	-2.41	117.30	120.57
8	A	1108	CLR	C7-C8-C9	2.40	112.50	109.72
8	C	1107	CLR	C8-C7-C6	-2.37	109.48	112.76
8	A	1107	CLR	C19-C10-C9	-2.36	109.01	111.66
8	A	1108	CLR	C4-C5-C6	-2.29	117.47	120.57
8	A	1108	CLR	C11-C9-C10	-2.23	110.33	113.08
8	A	1107	CLR	C17-C13-C14	2.17	102.59	100.10
8	C	1107	CLR	C3-C4-C5	-2.15	108.62	112.05
8	D	400	CLR	C12-C11-C9	-2.15	109.49	113.14
8	C	1108	CLR	C8-C7-C6	-2.14	109.80	112.76
8	C	1107	CLR	C10-C5-C6	2.13	126.04	122.93
8	D	400	CLR	C1-C2-C3	-2.13	107.67	110.48
8	C	1108	CLR	C16-C17-C20	2.12	115.38	112.18
8	C	1108	CLR	C2-C1-C10	-2.04	108.45	112.78

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	ADP	O4'-C4'-C5'-O5'
4	C	1101	ADP	O4'-C4'-C5'-O5'
8	C	1107	CLR	C21-C20-C22-C23
8	D	400	CLR	C21-C20-C22-C23
4	A	1101	ADP	C3'-C4'-C5'-O5'
4	C	1101	ADP	C3'-C4'-C5'-O5'
8	A	1107	CLR	C21-C20-C22-C23
8	A	1107	CLR	C17-C20-C22-C23
8	D	400	CLR	C17-C20-C22-C23
8	A	1108	CLR	C17-C20-C22-C23
8	C	1107	CLR	C17-C20-C22-C23
8	A	1108	CLR	C20-C22-C23-C24
8	A	1108	CLR	C22-C23-C24-C25
8	D	400	CLR	C20-C22-C23-C24
8	A	1107	CLR	C20-C22-C23-C24
8	C	1107	CLR	C20-C22-C23-C24
8	C	1108	CLR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
8	A	1108	CLR	C23-C24-C25-C26
8	C	1108	CLR	C23-C24-C25-C26
8	A	1108	CLR	C23-C24-C25-C27
8	C	1108	CLR	C23-C24-C25-C27
8	C	1108	CLR	C13-C17-C20-C22
8	D	400	CLR	C22-C23-C24-C25
8	C	1107	CLR	C23-C24-C25-C26
8	C	1107	CLR	C23-C24-C25-C27
8	C	1108	CLR	C13-C17-C20-C21
8	A	1108	CLR	C21-C20-C22-C23
8	C	1108	CLR	C16-C17-C20-C21
8	A	1107	CLR	C22-C23-C24-C25
8	C	1108	CLR	C17-C20-C22-C23
8	C	1108	CLR	C16-C17-C20-C22
8	D	400	CLR	C23-C24-C25-C26
8	C	1107	CLR	C22-C23-C24-C25
8	D	400	CLR	C23-C24-C25-C27
8	D	400	CLR	C13-C17-C20-C22
8	D	400	CLR	C13-C17-C20-C21

There are no ring outliers.

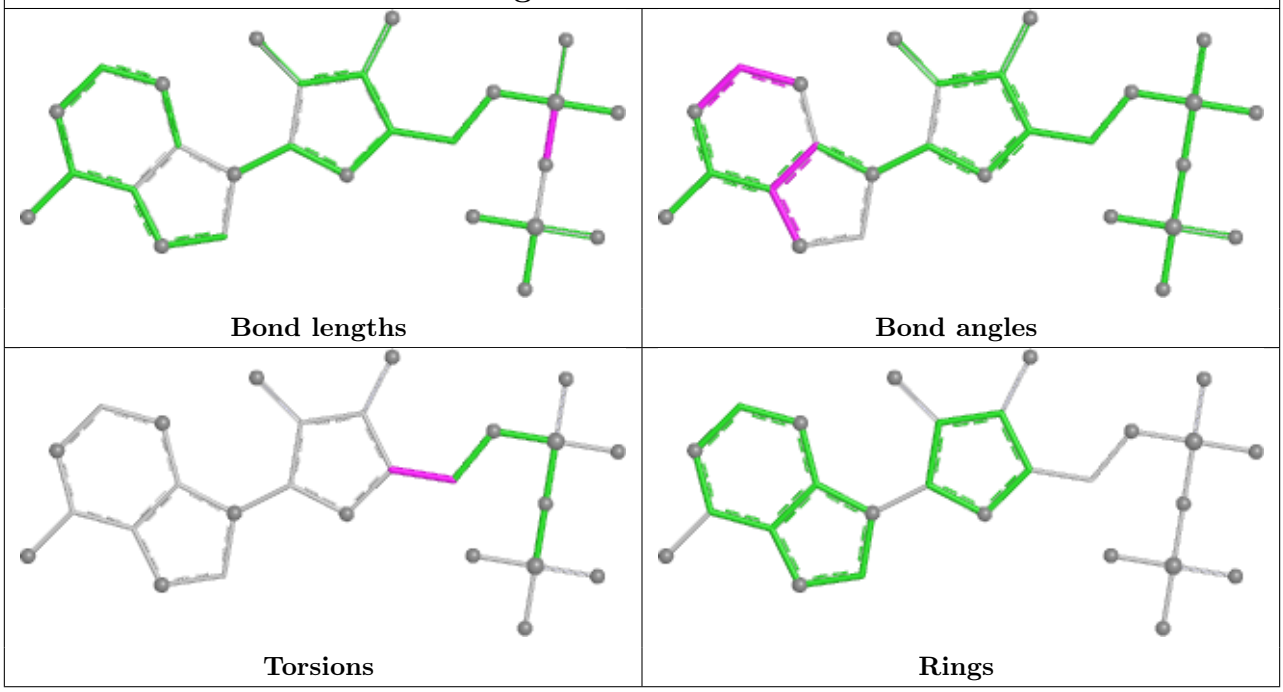
9 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1101	ADP	3	0
8	C	1108	CLR	3	0
8	A	1107	CLR	6	0
8	D	400	CLR	1	0
4	A	1101	ADP	2	0
5	C	1102	ALF	2	0
5	A	1102	ALF	2	0
8	A	1108	CLR	8	0
8	C	1107	CLR	6	0

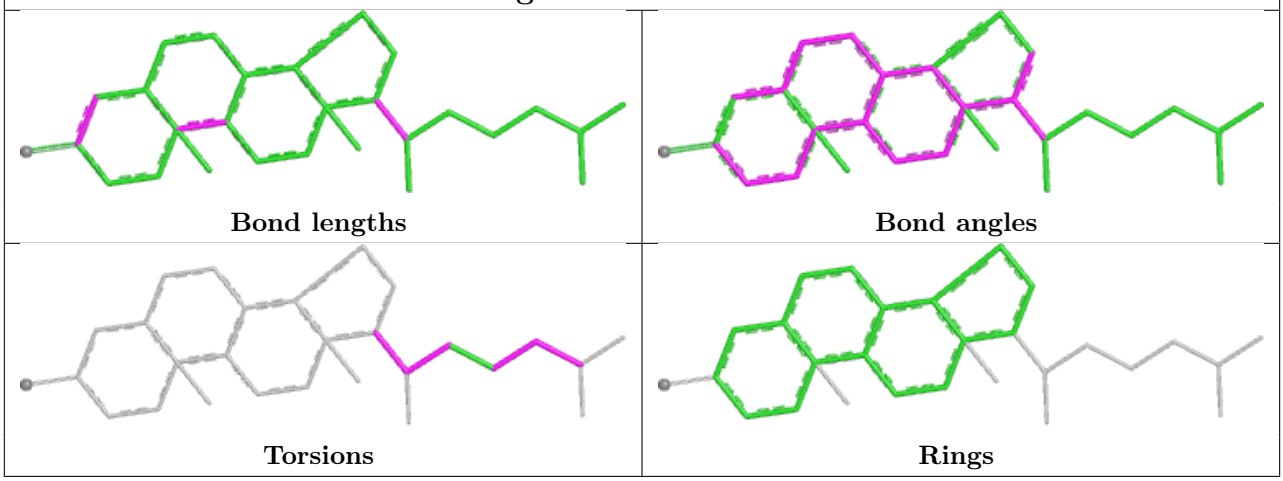
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

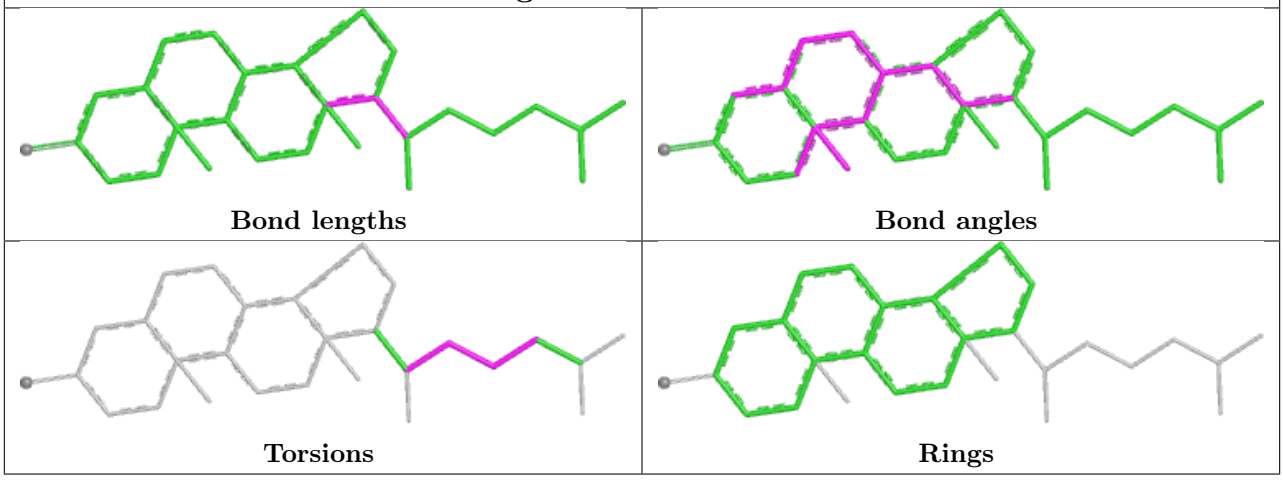
Ligand ADP C 1101



Ligand CLR C 1108



Ligand CLR A 1107



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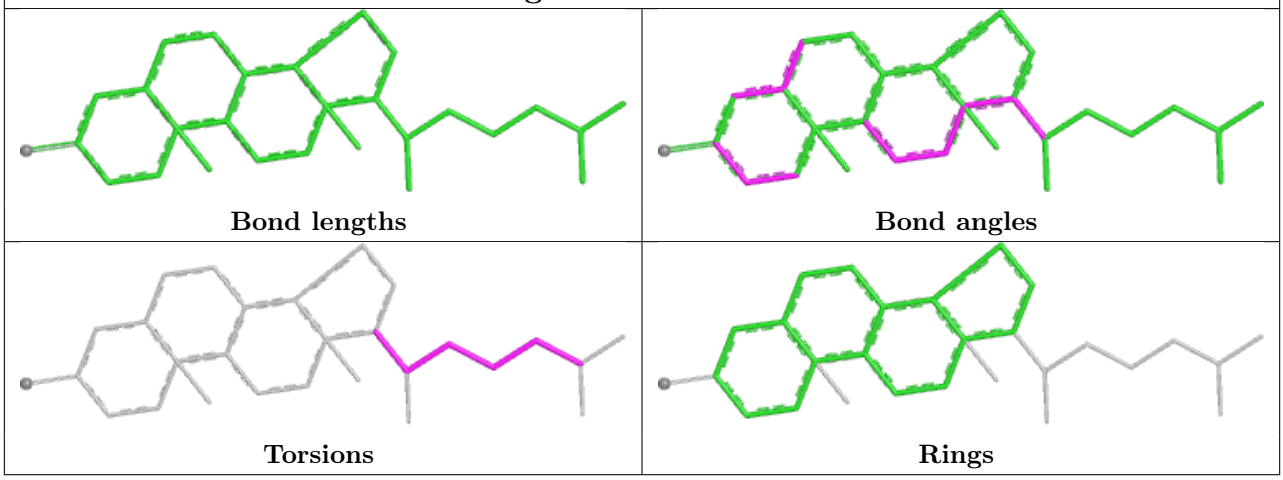

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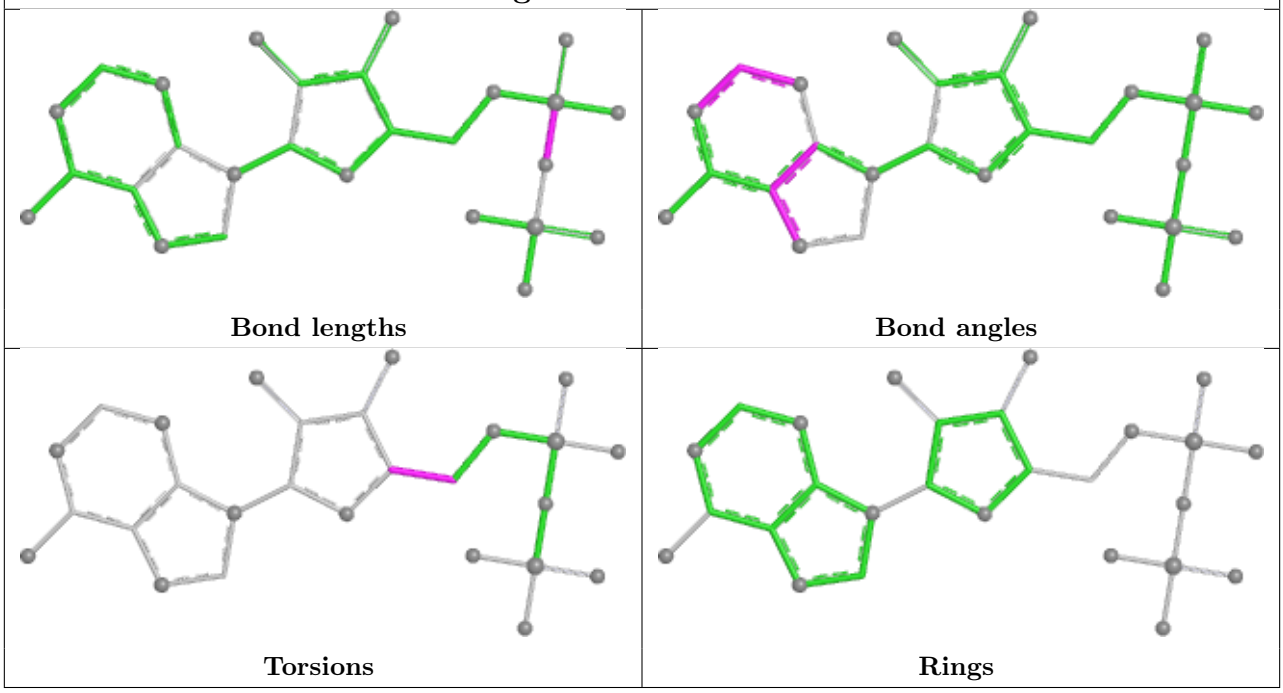

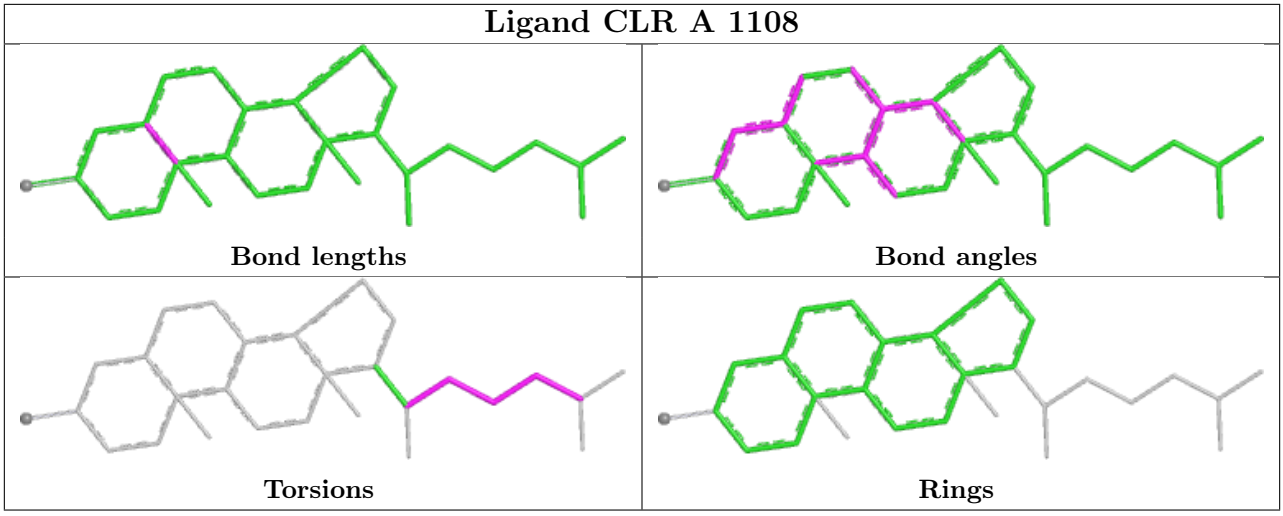

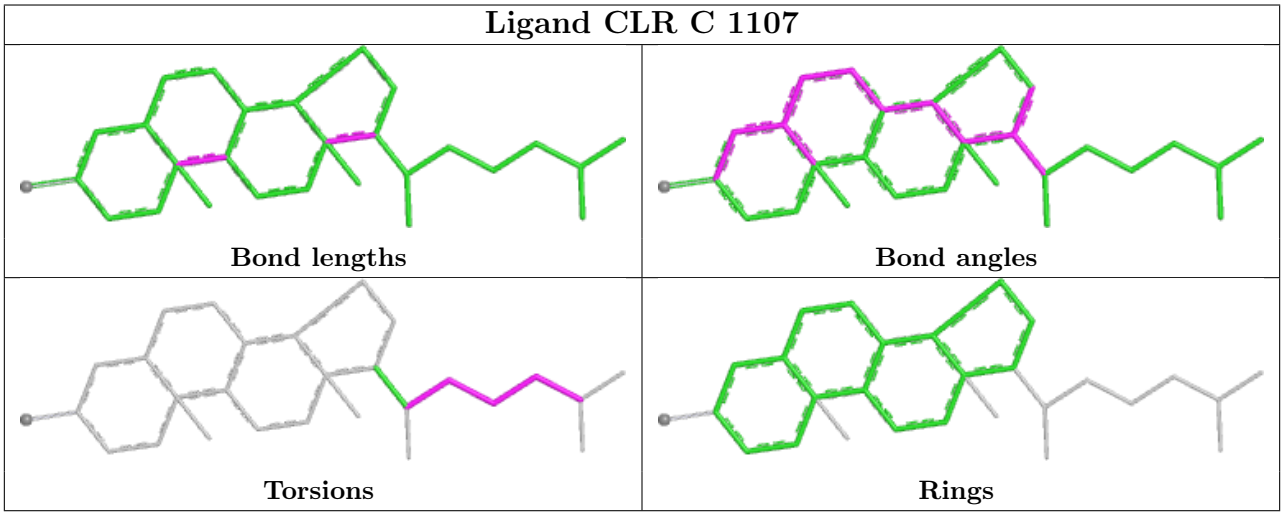

5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	985/1021 (96%)	-0.20	12 (1%)	79	70	111, 176, 234, 320	0
1	C	987/1021 (96%)	-0.10	23 (2%)	60	51	159, 209, 285, 352	0
2	B	285/303 (94%)	0.16	18 (6%)	20	16	181, 252, 296, 353	0
2	D	285/303 (94%)	-0.03	15 (5%)	26	23	165, 241, 290, 355	0
3	E	29/65 (44%)	-0.56	0	100	100	177, 210, 240, 258	0
3	G	27/65 (41%)	-0.69	0	100	100	158, 180, 238, 268	0
All	All	2598/2778 (93%)	-0.11	68 (2%)	56	46	111, 204, 280, 355	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	158	ASN	7.3
2	B	294	ARG	6.3
1	C	267	ALA	5.9
1	C	268	SER	5.9
2	B	293	GLY	5.8
2	D	161	GLY	5.7
2	D	159	CYS	5.6
2	D	227	MET	5.3
2	B	292	GLN	5.2
2	B	285	TYR	4.9
2	D	228	GLU	4.6
1	C	265	THR	4.3
1	C	491	THR	4.2
2	D	162	LEU	3.9
2	D	160	SER	3.8
2	B	158	ASN	3.6
1	C	833	LYS	3.4
1	C	269	GLY	3.3
1	A	265	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	613	HIS	3.2
2	B	296	ASP	3.2
2	B	128	ASN	3.1
1	A	235	ILE	3.1
1	C	116	GLU	3.1
2	D	202	MET	3.0
1	C	934	ARG	3.0
1	A	220	ARG	2.9
2	B	202	MET	2.9
2	D	226	THR	2.9
2	D	217	ARG	2.8
1	C	654	LYS	2.7
2	D	165	GLU	2.7
2	B	217	ARG	2.6
2	B	201	VAL	2.6
1	A	269	GLY	2.5
2	B	275	GLU	2.5
1	A	245	GLY	2.5
1	C	543	GLU	2.5
1	C	396	THR	2.5
2	B	273	ARG	2.4
1	C	271	GLU	2.4
1	C	933	ARG	2.4
2	D	266	LEU	2.4
2	B	284	GLY	2.4
1	A	146	LYS	2.4
1	C	426	PHE	2.4
2	D	264	THR	2.4
2	B	290	ARG	2.3
1	A	230	LEU	2.3
1	C	492	ALA	2.3
2	B	281	GLU	2.3
2	B	75	PRO	2.2
2	B	125	ASP	2.2
1	C	832	PRO	2.2
1	A	229	PRO	2.2
1	C	115	GLU	2.2
1	A	194	ALA	2.2
1	A	221	SER	2.1
1	C	685	ARG	2.1
1	C	480	LYS	2.1
1	C	521	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	219	GLU	2.1
1	A	519	LYS	2.1
1	A	143	GLN	2.0
1	C	837	LEU	2.0
2	B	194	GLU	2.0
2	D	128	ASN	2.0
1	C	78	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	CLR	A	1108	28/28	0.76	0.36	233,266,290,295	0
8	CLR	C	1108	28/28	0.77	0.36	294,305,319,322	0
8	CLR	D	400	28/28	0.77	0.54	288,293,294,295	0
7	NA	A	1106	1/1	0.78	0.26	154,154,154,154	0
8	CLR	A	1107	28/28	0.80	0.35	223,225,228,229	0
7	NA	C	1106	1/1	0.84	0.15	155,155,155,155	0
7	NA	A	1105	1/1	0.86	0.16	130,130,130,130	0
4	ADP	C	1101	27/27	0.87	0.36	170,220,235,237	0
8	CLR	C	1107	28/28	0.88	0.30	207,215,220,223	0
7	NA	C	1105	1/1	0.92	0.15	135,135,135,135	0
7	NA	C	1104	1/1	0.93	0.18	136,136,136,136	0
7	NA	A	1104	1/1	0.93	0.18	132,132,132,132	0
4	ADP	A	1101	27/27	0.94	0.32	107,144,156,157	0
6	MG	C	1103	1/1	0.95	0.29	232,232,232,232	0
5	ALF	A	1102	5/5	0.95	0.21	137,144,149,154	0
5	ALF	C	1102	5/5	0.95	0.22	233,236,241,242	0

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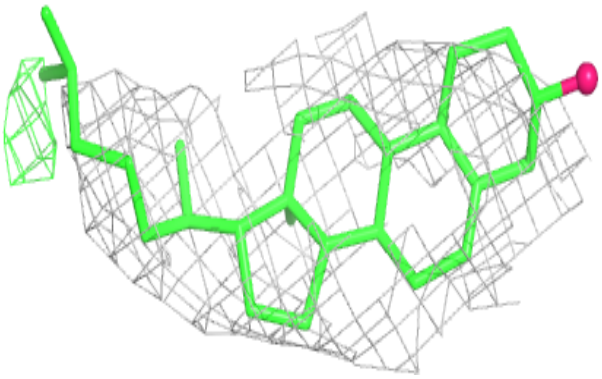
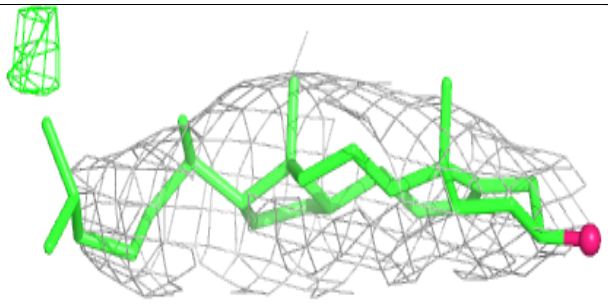
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	A	1103	1/1	0.96	0.23	133,133,133,133	0

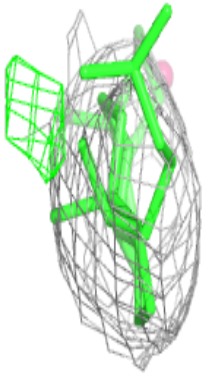
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLR A 1108:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

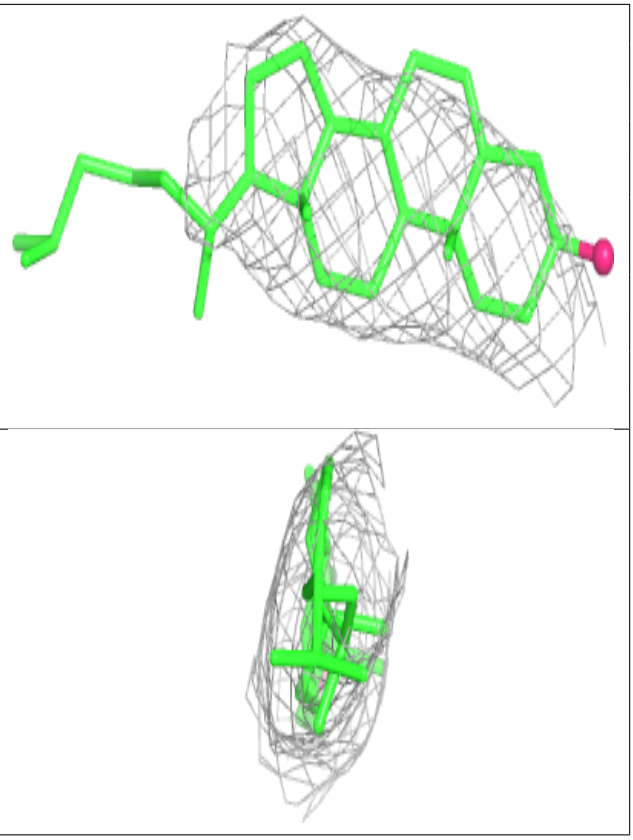






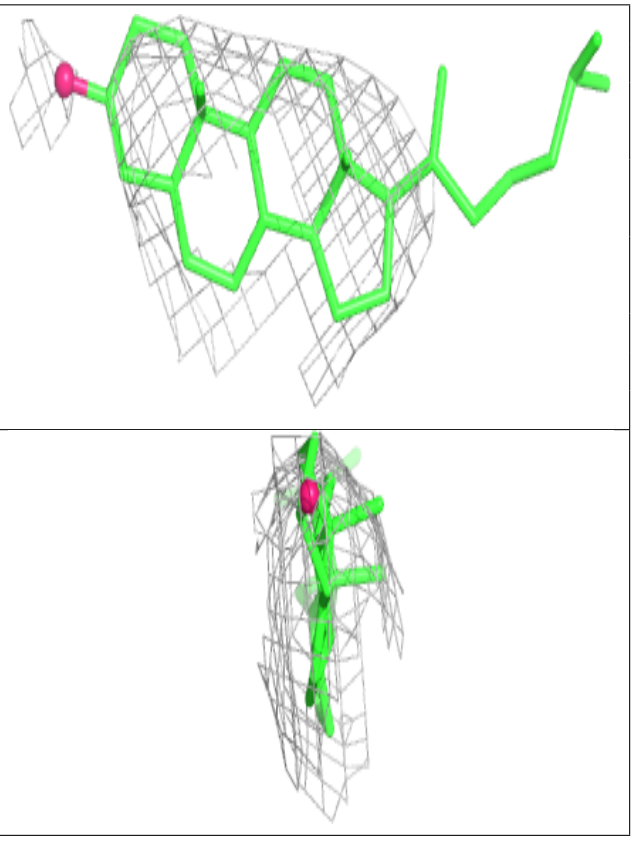
Electron density around CLR C 1108:

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



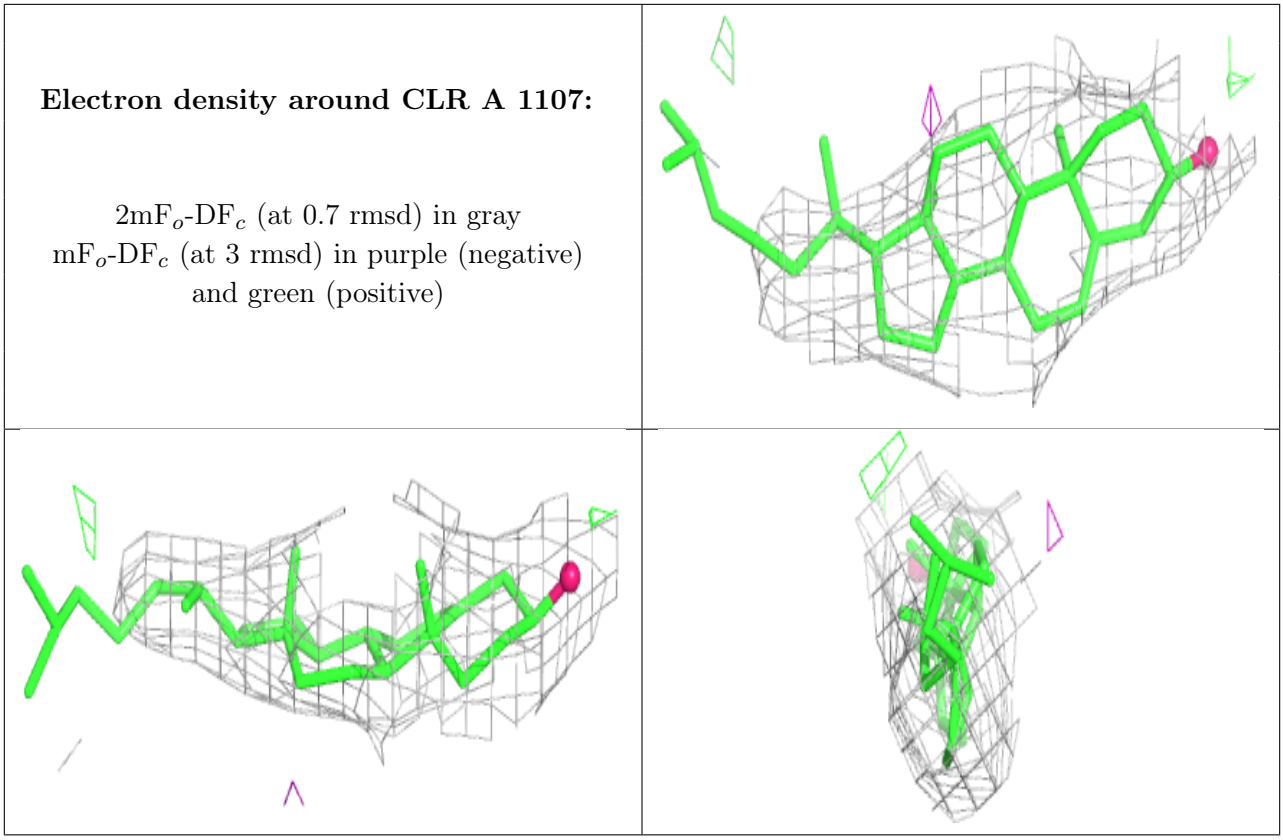
Electron density around CLR D 400:

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



Electron density around CLR A 1107:

$2mF_o$-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 1101:

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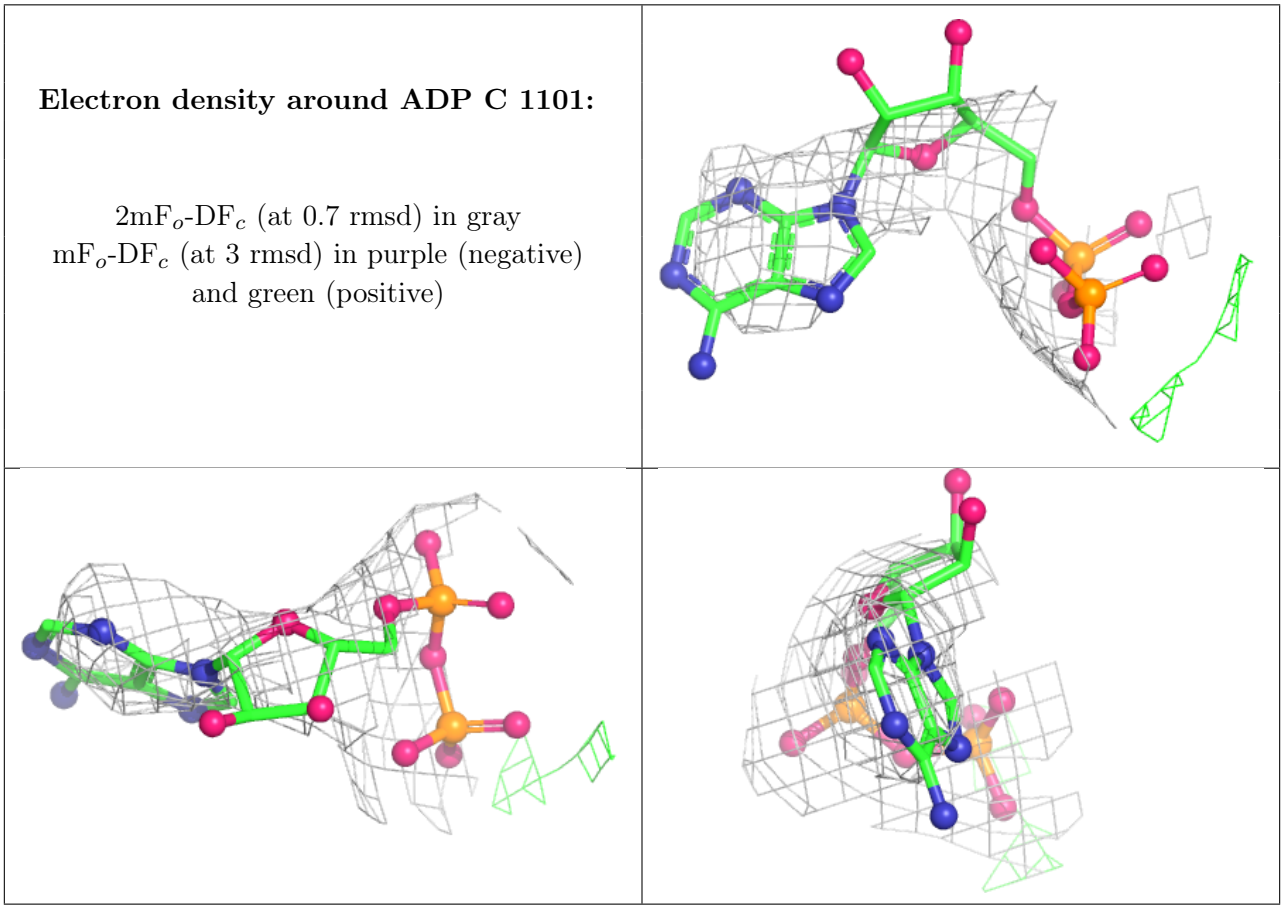
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLR C 1107:

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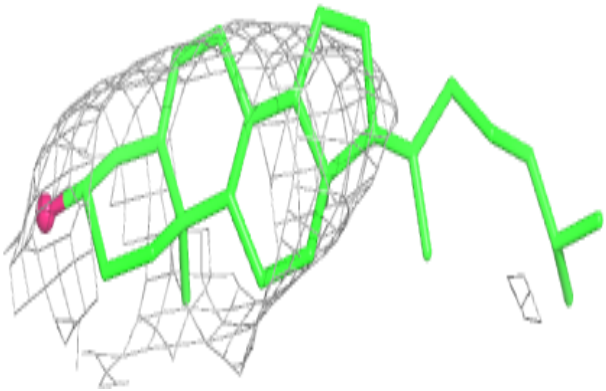
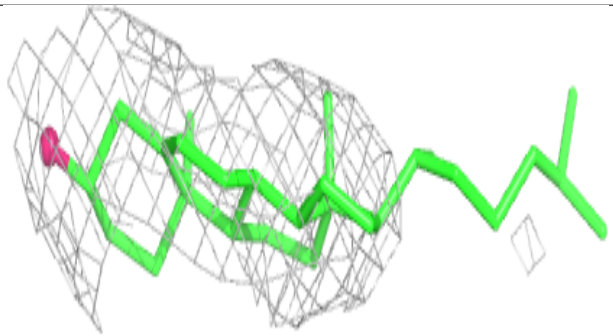
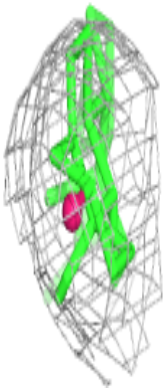
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

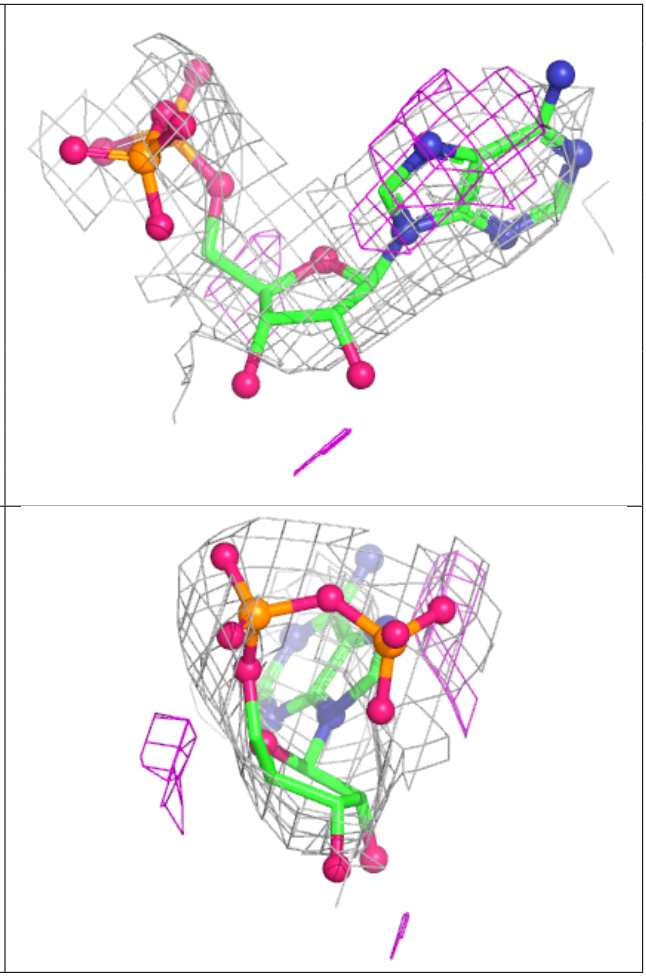






Electron density around ADP A 1101:

$2mF_o$-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.