Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:00 PM GMT

PDB ID	:	3VR6
Title	:	Crystal structure of AMP-PNP bound Enterococcus hirae V1-ATPase [bV1]
Authors	:	Arai, S.; Saijo, S.; Suzuki, K.; Mizutani, K.; Kakinuma, Y.; Ishizuka-Katsura, Y.; Ohsawa, N.; Terada, T.; Shirouzu, M.; Yokoyama, S.; Iwata, S.; Yamato, I.; Murata, T.
Deposited on	:	2012-04-03
Resolution	:	2.68 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

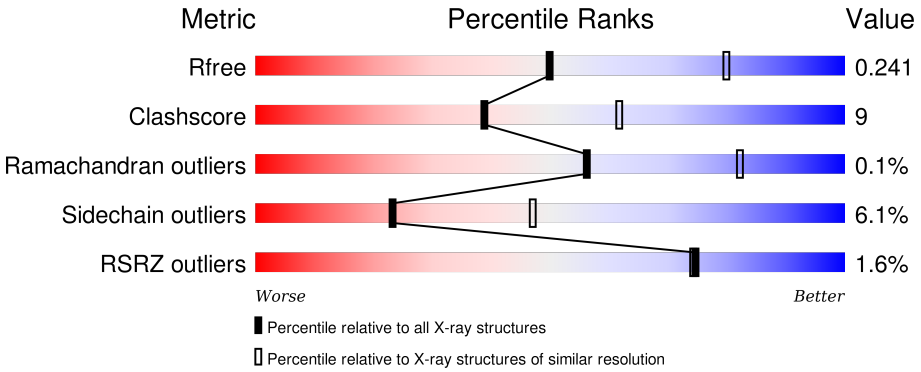
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.68 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}	91344	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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. 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	600	3% 75% 22%
1	B	600	% 81% 15%
1	C	600	% 73% 22%
2	D	465	2% 77% 18%
2	E	465	% 80% 14%

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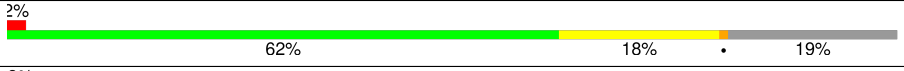
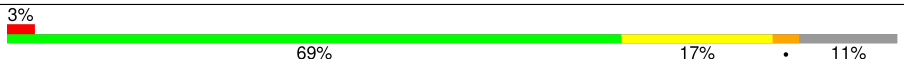
Mol	Chain	Length	Quality of chain
2	F	465	
3	G	217	
4	H	115	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27061 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called V-type sodium ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4566	2868	767	905	26			
1	B	592	Total	C	N	O	S	0	0	0
			4583	2876	770	911	26			
1	C	582	Total	C	N	O	S	0	0	0
			4536	2851	761	898	26			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP Q08636
A	-5	SER	-	EXPRESSION TAG	UNP Q08636
A	-4	SER	-	EXPRESSION TAG	UNP Q08636
A	-3	GLY	-	EXPRESSION TAG	UNP Q08636
A	-2	SER	-	EXPRESSION TAG	UNP Q08636
A	-1	SER	-	EXPRESSION TAG	UNP Q08636
A	0	GLY	-	EXPRESSION TAG	UNP Q08636
B	-6	GLY	-	EXPRESSION TAG	UNP Q08636
B	-5	SER	-	EXPRESSION TAG	UNP Q08636
B	-4	SER	-	EXPRESSION TAG	UNP Q08636
B	-3	GLY	-	EXPRESSION TAG	UNP Q08636
B	-2	SER	-	EXPRESSION TAG	UNP Q08636
B	-1	SER	-	EXPRESSION TAG	UNP Q08636
B	0	GLY	-	EXPRESSION TAG	UNP Q08636
C	-6	GLY	-	EXPRESSION TAG	UNP Q08636
C	-5	SER	-	EXPRESSION TAG	UNP Q08636
C	-4	SER	-	EXPRESSION TAG	UNP Q08636
C	-3	GLY	-	EXPRESSION TAG	UNP Q08636
C	-2	SER	-	EXPRESSION TAG	UNP Q08636
C	-1	SER	-	EXPRESSION TAG	UNP Q08636
C	0	GLY	-	EXPRESSION TAG	UNP Q08636

- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	451	Total	C	N	O	S	0	0	0
			3509	2225	601	669	14			
2	E	452	Total	C	N	O	S	0	0	0
			3549	2250	607	678	14			
2	F	455	Total	C	N	O	S	0	0	0
			3567	2261	610	681	15			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	EXPRESSION TAG	UNP Q08637
D	-5	SER	-	EXPRESSION TAG	UNP Q08637
D	-4	SER	-	EXPRESSION TAG	UNP Q08637
D	-3	GLY	-	EXPRESSION TAG	UNP Q08637
D	-2	SER	-	EXPRESSION TAG	UNP Q08637
D	-1	SER	-	EXPRESSION TAG	UNP Q08637
D	0	GLY	-	EXPRESSION TAG	UNP Q08637
E	-6	GLY	-	EXPRESSION TAG	UNP Q08637
E	-5	SER	-	EXPRESSION TAG	UNP Q08637
E	-4	SER	-	EXPRESSION TAG	UNP Q08637
E	-3	GLY	-	EXPRESSION TAG	UNP Q08637
E	-2	SER	-	EXPRESSION TAG	UNP Q08637
E	-1	SER	-	EXPRESSION TAG	UNP Q08637
E	0	GLY	-	EXPRESSION TAG	UNP Q08637
F	-6	GLY	-	EXPRESSION TAG	UNP Q08637
F	-5	SER	-	EXPRESSION TAG	UNP Q08637
F	-4	SER	-	EXPRESSION TAG	UNP Q08637
F	-3	GLY	-	EXPRESSION TAG	UNP Q08637
F	-2	SER	-	EXPRESSION TAG	UNP Q08637
F	-1	SER	-	EXPRESSION TAG	UNP Q08637
F	0	GLY	-	EXPRESSION TAG	UNP Q08637

- Molecule 3 is a protein called V-type sodium ATPase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	176	Total	C	N	O	S	0	0	0
			1412	890	250	262	10			

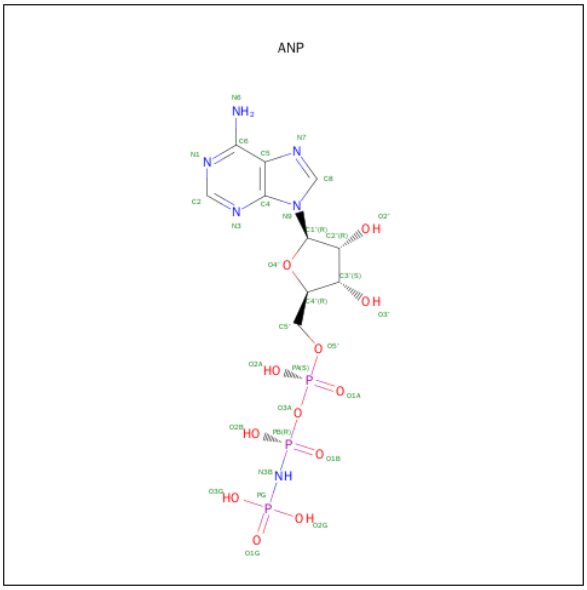
- Molecule 4 is a protein called V-type sodium ATPase subunit G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	102	Total	C	N	O	S	0	0	0
			775	494	127	152	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	104	SER	-	EXPRESSION TAG	UNP P43455
H	105	GLY	-	EXPRESSION TAG	UNP P43455
H	106	PRO	-	EXPRESSION TAG	UNP P43455
H	107	SER	-	EXPRESSION TAG	UNP P43455
H	108	SER	-	EXPRESSION TAG	UNP P43455
H	109	GLY	-	EXPRESSION TAG	UNP P43455
H	110	GLU	-	EXPRESSION TAG	UNP P43455
H	111	ASN	-	EXPRESSION TAG	UNP P43455
H	112	LEU	-	EXPRESSION TAG	UNP P43455
H	113	TYR	-	EXPRESSION TAG	UNP P43455
H	114	PHE	-	EXPRESSION TAG	UNP P43455
H	115	GLN	-	EXPRESSION TAG	UNP P43455

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

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

- Molecule 7 is water.

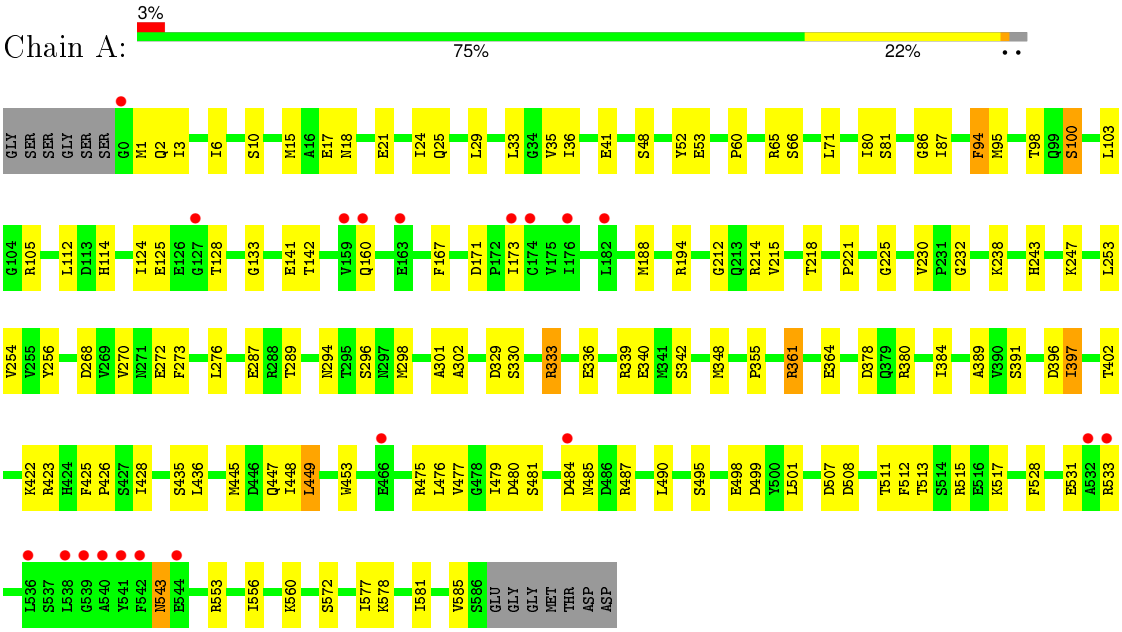
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	78	Total O 78 78	0	0
7	B	115	Total O 115 115	0	0
7	C	91	Total O 91 91	0	0
7	D	46	Total O 46 46	0	0
7	E	83	Total O 83 83	0	0
7	F	71	Total O 71 71	0	0
7	G	11	Total O 11 11	0	0
7	H	5	Total O 5 5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

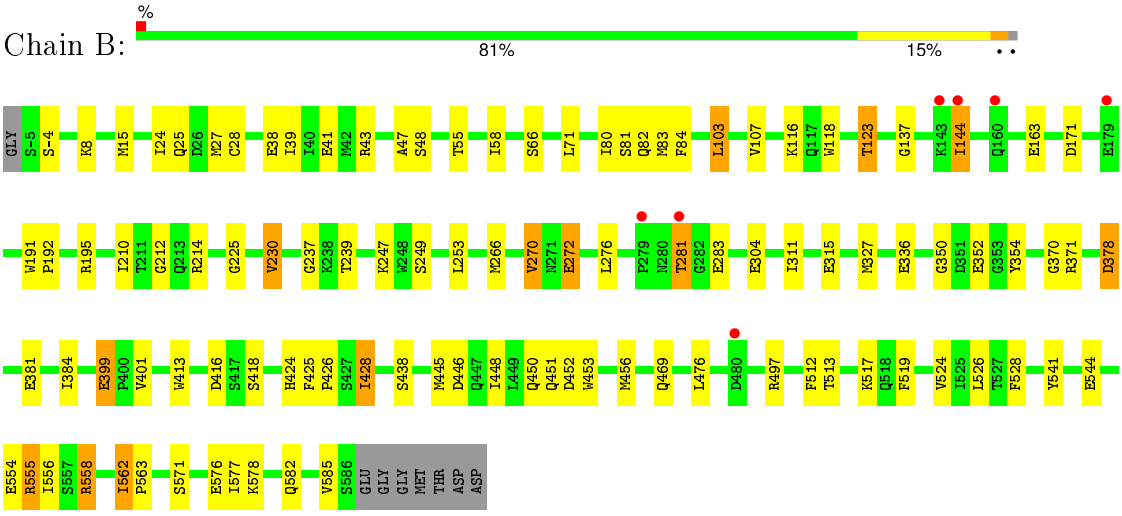
- Molecule 1: V-type sodium ATPase catalytic subunit A

Chain A:

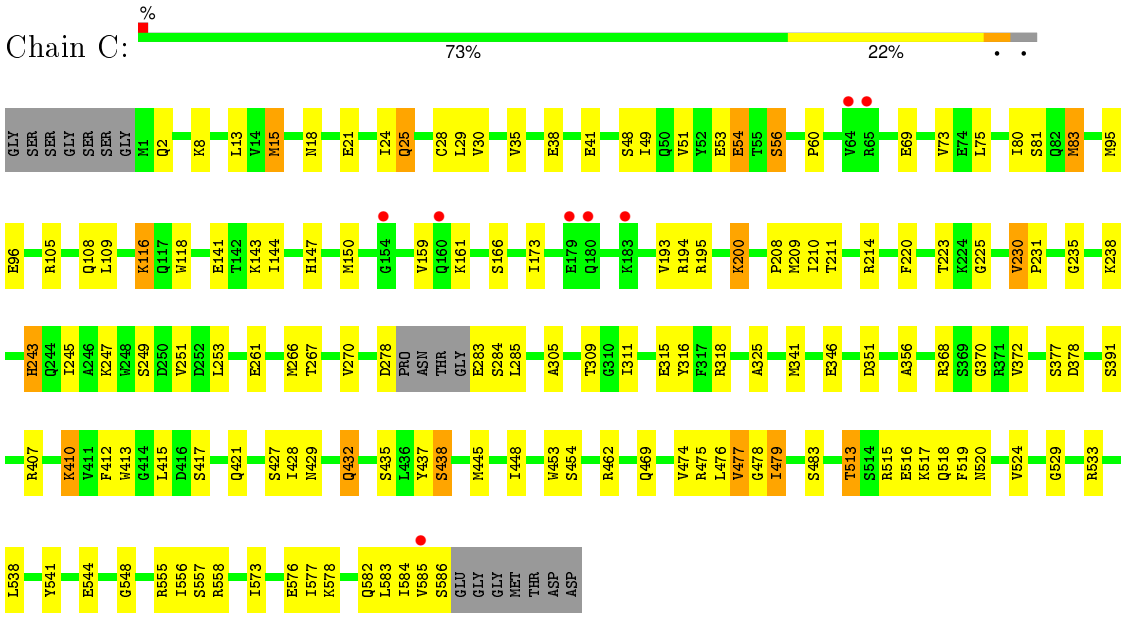


- Molecule 1: V-type sodium ATPase catalytic subunit A

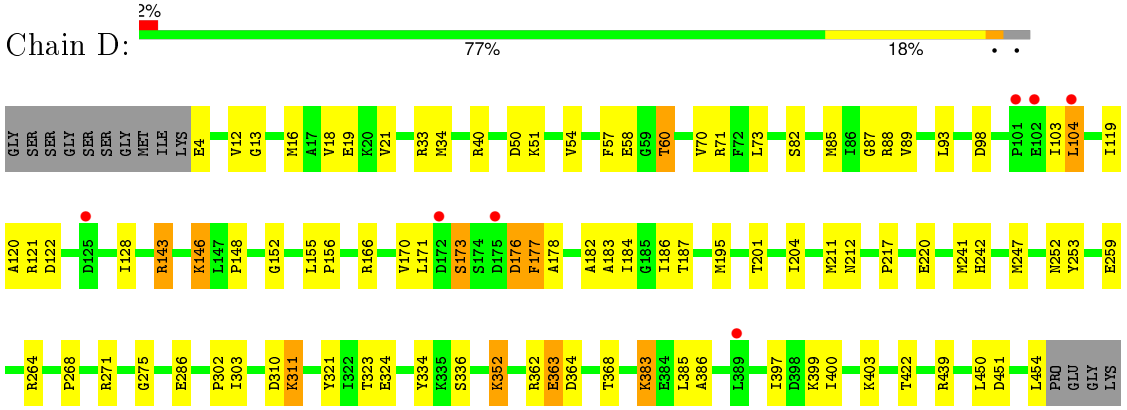
Chain B:



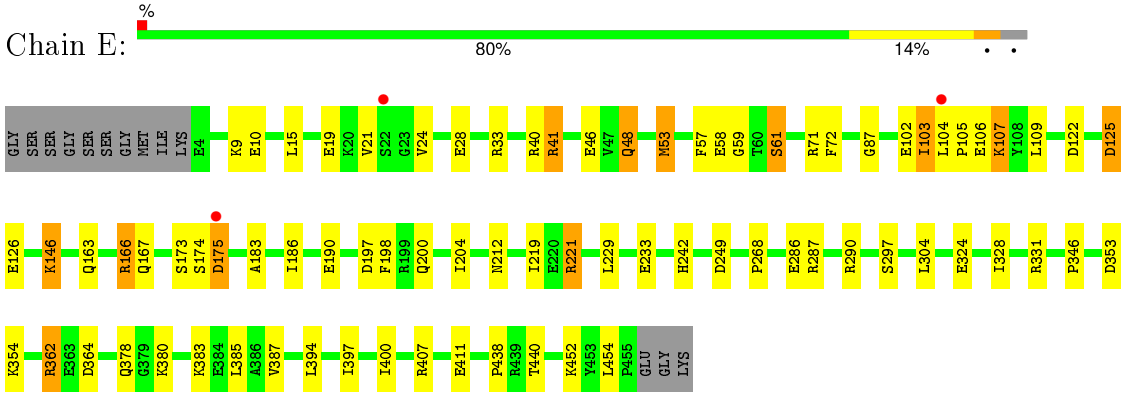
- Molecule 1: V-type sodium ATPase catalytic subunit A



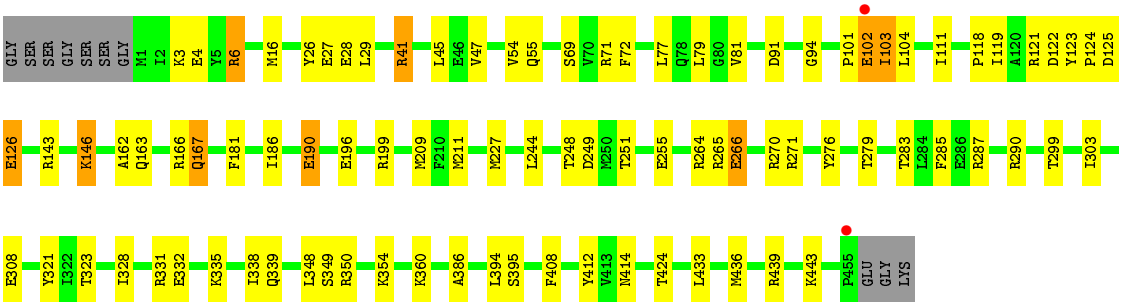
- Molecule 2: V-type sodium ATPase subunit B



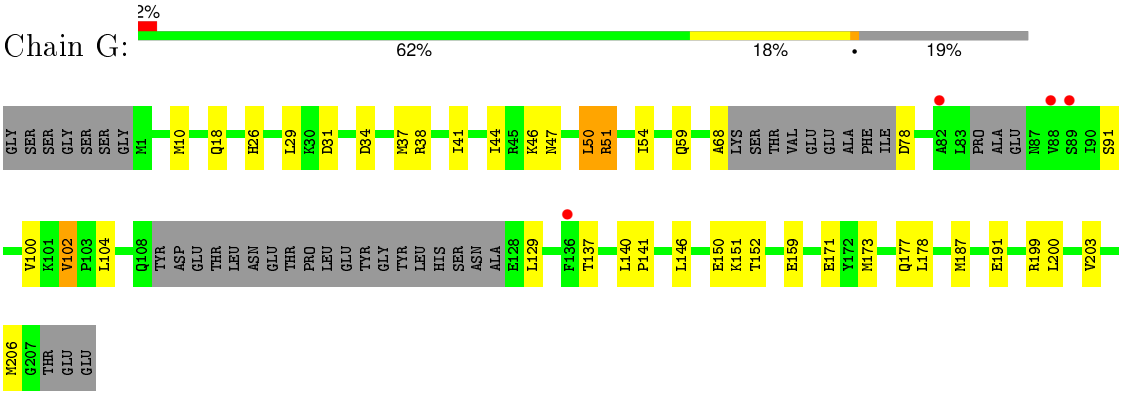
- Molecule 2: V-type sodium ATPase subunit B



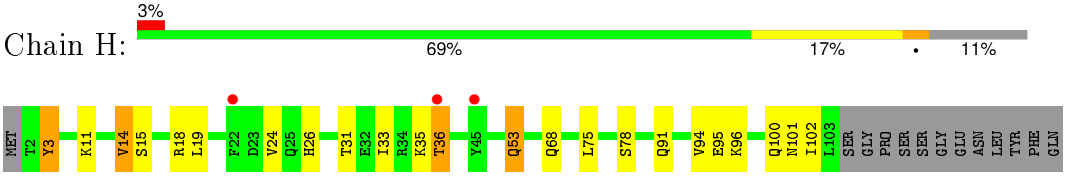
- Molecule 2: V-type sodium ATPase subunit B



- Molecule 3: V-type sodium ATPase subunit D



- Molecule 4: V-type sodium ATPase subunit G



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	126.15Å 127.42Å 225.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.58 – 2.68 48.58 – 2.68	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.58-2.68) 95.0 (48.58-2.68)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.182 , 0.246 0.180 , 0.241	Depositor DCC
R_{free} test set	4864 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	44.1	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.4	EDS
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 97194 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	27061	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ANP

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	0.51	0/4642	0.62	0/6280
1	B	0.57	1/4659 (0.0%)	0.65	0/6304
1	C	0.55	1/4610 (0.0%)	0.63	0/6234
2	D	0.51	0/3570	0.63	0/4830
2	E	0.55	0/3612	0.66	0/4884
2	F	0.56	0/3630	0.65	0/4908
3	G	0.44	0/1420	0.57	0/1899
4	H	0.42	0/787	0.59	0/1068
All	All	0.54	2/26930 (0.0%)	0.63	0/36407

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	28	CYS	CB-SG	-6.57	1.71	1.82
1	B	272	GLU	CG-CD	5.22	1.59	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4566	0	4531	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4583	0	4534	72	0
1	C	4536	0	4503	95	0
2	D	3509	0	3510	64	0
2	E	3549	0	3570	61	0
2	F	3567	0	3586	64	0
3	G	1412	0	1478	29	0
4	H	775	0	772	20	0
5	B	31	0	13	3	0
5	C	31	0	13	2	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	78	0	0	8	0
7	B	115	0	0	13	0
7	C	91	0	0	14	0
7	D	46	0	0	7	0
7	E	83	0	0	4	0
7	F	71	0	0	3	0
7	G	11	0	0	2	0
7	H	5	0	0	0	0
All	All	27061	0	26510	479	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 9.

All (479) 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:F:102:GLU:CB	2:F:103:ILE:HA	1.54	1.28
2:F:102:GLU:HB3	2:F:103:ILE:CA	1.66	1.25
2:E:221:ARG:HG3	2:E:221:ARG:HH11	0.98	1.15
1:A:98:THR:HG22	1:A:100:SER:HB3	1.32	1.06
2:E:41:ARG:HG3	2:E:41:ARG:HH11	1.14	1.04
1:A:98:THR:CG2	1:A:100:SER:HB3	1.88	1.04
1:A:160:GLN:HB3	7:A:711:HOH:O	1.61	1.01
1:A:333:ARG:HG2	1:A:333:ARG:HH11	1.25	0.99
1:A:1:MET:HB3	1:A:65:ARG:HH21	1.29	0.95
2:F:79:LEU:HD13	2:F:227:MET:HE3	1.47	0.95
1:A:94:PHE:O	1:A:98:THR:HB	1.67	0.93
4:H:100:GLN:CB	4:H:101:ASN:HA	1.98	0.92
2:F:181:PHE:HD2	2:F:211:MET:HE3	1.35	0.90
2:F:3:LYS:HG3	7:F:531:HOH:O	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:362:ARG:HD2	2:D:364:ASP:OD1	1.71	0.90
3:G:51:ARG:NH2	4:H:75:LEU:O	2.05	0.89
2:E:221:ARG:NH1	2:E:221:ARG:HG3	1.76	0.88
1:A:95:MET:CE	2:D:120:ALA:HB2	2.03	0.88
1:C:267:THR:HG22	2:F:118:PRO:O	1.71	0.88
2:D:146:LYS:NZ	2:D:286:GLU:OE1	2.07	0.88
1:B:237:GLY:HA2	7:B:701:HOH:O	1.73	0.87
1:A:25:GLN:HG3	2:E:61:SER:HB2	1.60	0.83
4:H:91:GLN:HE22	4:H:101:ASN:ND2	1.78	0.82
2:F:181:PHE:CD2	2:F:211:MET:HE3	2.14	0.81
1:B:304:GLU:OE2	7:B:779:HOH:O	1.99	0.80
1:B:27:MET:CE	1:B:38:GLU:HB2	2.12	0.80
1:C:150:MET:SD	7:C:746:HOH:O	2.38	0.80
2:D:146:LYS:HE3	2:D:324:GLU:OE2	1.82	0.79
1:A:95:MET:HE1	2:D:120:ALA:HB2	1.65	0.78
2:D:93:LEU:HG	2:D:220:GLU:HG2	1.68	0.76
1:C:267:THR:HG21	2:F:121:ARG:HB2	1.68	0.76
2:D:50:ASP:HA	7:D:534:HOH:O	1.86	0.76
1:C:25:GLN:HG2	7:D:539:HOH:O	1.86	0.76
1:C:41:GLU:HB2	1:C:48:SER:HB2	1.68	0.76
3:G:51:ARG:NH1	3:G:150:GLU:OE1	2.19	0.75
2:D:34:MET:HE3	2:D:40:ARG:NE	2.02	0.75
1:A:41:GLU:HB2	1:A:48:SER:HB2	1.67	0.75
1:A:160:GLN:CB	7:A:711:HOH:O	2.26	0.74
1:C:200:LYS:HD2	7:C:740:HOH:O	1.86	0.74
2:E:41:ARG:HG3	2:E:41:ARG:NH1	1.93	0.74
1:A:95:MET:HE3	2:D:120:ALA:HB2	1.69	0.74
5:B:601:ANP:O2A	7:B:701:HOH:O	2.05	0.73
1:C:116:LYS:HE2	1:C:118:TRP:CZ2	2.24	0.72
1:A:215:VAL:HG23	1:A:501:LEU:HD22	1.72	0.72
1:B:28:CYS:HB3	1:B:66:SER:HA	1.71	0.72
2:F:186:ILE:HD12	2:F:190:GLU:HG2	1.70	0.72
4:H:11:LYS:HA	4:H:26:HIS:CE1	2.26	0.71
1:A:333:ARG:HH11	1:A:333:ARG:CG	2.02	0.71
2:F:79:LEU:HD13	2:F:227:MET:CE	2.19	0.71
1:B:554:GLU:O	1:B:558:ARG:HG3	1.91	0.71
2:D:439:ARG:NH1	2:D:451:ASP:OD1	2.20	0.71
2:F:102:GLU:HB3	2:F:103:ILE:HA	0.76	0.71
1:C:283:GLU:HG3	7:C:765:HOH:O	1.91	0.70
3:G:151:LYS:HE2	4:H:68:GLN:O	1.89	0.70
2:E:362:ARG:HD2	2:E:364:ASP:OD1	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:181:PHE:HB3	2:F:209:MET:HG3	1.73	0.70
1:B:451:GLN:HG2	1:B:519:PHE:CE1	2.27	0.70
2:F:338:ILE:HG23	2:F:414:ASN:HB2	1.73	0.70
2:D:166:ARG:HD2	2:D:201:THR:HG21	1.73	0.70
1:B:27:MET:HE2	1:B:38:GLU:HB2	1.73	0.70
2:D:34:MET:CE	2:D:40:ARG:NE	2.55	0.69
1:A:477:VAL:HG23	1:A:481:SER:HB3	1.74	0.69
1:C:267:THR:CG2	2:F:118:PRO:O	2.40	0.69
3:G:173:MET:O	3:G:177:GLN:HG3	1.93	0.69
1:A:2:GLN:HG3	1:A:21:GLU:HB2	1.74	0.68
2:D:18:VAL:HG11	2:D:70:VAL:HG11	1.75	0.68
4:H:100:GLN:CB	4:H:101:ASN:CA	2.72	0.68
1:A:142:THR:HB	1:A:287:GLU:OE1	1.93	0.68
1:A:333:ARG:NH2	2:D:321:TYR:O	2.25	0.68
1:C:578:LYS:O	1:C:582:GLN:HB2	1.94	0.68
1:B:237:GLY:C	7:B:701:HOH:O	2.33	0.68
1:A:133:GLY:O	1:A:380:ARG:NH2	2.26	0.67
1:A:577:ILE:O	1:A:581:ILE:HG12	1.94	0.67
2:E:362:ARG:NH1	2:E:364:ASP:OD2	2.28	0.67
4:H:15:SER:O	4:H:18:ARG:HB2	1.94	0.67
1:A:2:GLN:HB3	1:A:66:SER:HB3	1.77	0.66
1:A:378:ASP:HB2	1:A:380:ARG:NH1	2.09	0.66
2:E:229:LEU:HD13	2:E:287:ARG:HG3	1.77	0.66
2:D:183:ALA:HB1	2:D:186:ILE:HG12	1.77	0.66
1:C:478:GLY:C	1:C:479:ILE:HG13	2.17	0.66
1:A:80:ILE:O	1:A:81:SER:HB2	1.95	0.65
1:B:451:GLN:HG2	1:B:519:PHE:CZ	2.32	0.65
1:A:426:PRO:HB2	1:A:428:ILE:CD1	2.26	0.65
2:E:41:ARG:CG	2:E:41:ARG:HH11	2.00	0.65
1:A:340:GLU:HG3	2:D:275:GLY:O	1.97	0.65
1:B:578:LYS:O	1:B:582:GLN:HG3	1.96	0.65
1:A:342:SER:HB2	1:A:355:PRO:HG3	1.78	0.64
1:B:171:ASP:OD2	7:B:726:HOH:O	2.14	0.64
2:F:102:GLU:CB	2:F:103:ILE:CA	2.41	0.64
1:B:116:LYS:HD3	1:B:118:TRP:CE2	2.33	0.64
2:F:126:GLU:OE2	2:F:143:ARG:NH1	2.31	0.64
1:C:60:PRO:HD3	2:F:47:VAL:HG13	1.80	0.64
2:D:87:GLY:HA2	2:D:204:ILE:O	1.98	0.63
1:B:452:ASP:O	1:B:456:MET:HG3	1.98	0.63
1:A:98:THR:HG22	1:A:100:SER:CB	2.20	0.63
2:E:146:LYS:HE3	2:E:324:GLU:OE2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ILE:HD12	1:A:402:THR:HG21	1.81	0.63
1:B:237:GLY:CA	7:B:701:HOH:O	2.38	0.63
2:E:122:ASP:HB3	2:E:290:ARG:HB2	1.80	0.63
2:F:163:GLN:O	2:F:167:GLN:HG3	1.98	0.63
2:F:339:GLN:OE1	7:F:554:HOH:O	2.15	0.63
2:E:186:ILE:HB	2:E:190:GLU:OE1	1.99	0.63
2:F:94:GLY:HA3	2:F:227:MET:CE	2.29	0.63
1:C:41:GLU:OE2	2:D:12:VAL:HG13	1.99	0.63
1:A:543:ASN:N	1:A:543:ASN:OD1	2.31	0.63
1:B:123:THR:HB	1:B:137:GLY:HA2	1.81	0.63
2:D:146:LYS:HE3	2:D:324:GLU:CD	2.18	0.63
2:F:29:LEU:HD13	2:F:77:LEU:HD13	1.81	0.63
1:C:410:LYS:HG3	1:C:437:TYR:OH	1.98	0.62
4:H:33:ILE:O	4:H:36:THR:HG22	1.98	0.62
2:E:212:ASN:OD1	2:E:221:ARG:HG2	1.99	0.62
3:G:199:ARG:O	3:G:203:VAL:HG23	2.00	0.61
1:A:487:ARG:HD2	7:A:728:HOH:O	1.99	0.61
1:C:477:VAL:HG21	3:G:29:LEU:HD21	1.83	0.61
2:D:82:SER:O	2:D:85:MET:HG2	2.00	0.61
1:A:1:MET:HB3	1:A:65:ARG:NH2	2.09	0.61
1:C:235:GLY:H	5:C:601:ANP:HNB1	1.48	0.61
2:F:6:ARG:HG3	2:F:69:SER:HB3	1.82	0.61
1:A:141:GLU:HG2	1:A:142:THR:HG23	1.82	0.61
1:A:581:ILE:O	1:A:585:VAL:HG23	2.01	0.61
2:F:28:GLU:OE2	2:F:72:PHE:HB3	2.01	0.61
1:B:27:MET:HE2	1:B:38:GLU:CB	2.30	0.60
2:F:103:ILE:H	2:F:103:ILE:HD13	1.66	0.60
1:B:453:TRP:CZ3	1:B:519:PHE:HA	2.36	0.60
2:E:163:GLN:HE21	2:E:167:GLN:HE22	1.49	0.60
1:C:80:ILE:O	1:C:81:SER:HB2	2.01	0.60
2:E:40:ARG:HD3	2:E:58:GLU:HB2	1.83	0.60
1:C:193:VAL:O	1:C:368:ARG:NH2	2.28	0.60
2:D:176:ASP:O	7:D:508:HOH:O	2.15	0.59
2:E:362:ARG:HB3	2:E:364:ASP:OD1	2.03	0.59
1:A:426:PRO:HB2	1:A:428:ILE:HD13	1.84	0.59
2:E:221:ARG:CG	2:E:221:ARG:HH11	1.92	0.59
2:E:397:ILE:HA	2:E:400:ILE:HD12	1.85	0.59
1:A:336:GLU:OE1	1:A:339:ARG:NH1	2.35	0.59
1:C:513:THR:HG23	1:C:517:LYS:HD2	1.84	0.58
1:A:194:ARG:NH2	1:A:364:GLU:OE1	2.36	0.58
2:D:352:LYS:HE2	7:D:506:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:GLN:CG	1:A:21:GLU:HB2	2.33	0.58
1:A:268:ASP:O	1:A:272:GLU:HG3	2.04	0.58
1:C:278:ASP:HB3	7:C:750:HOH:O	2.02	0.58
1:B:27:MET:HE1	1:B:38:GLU:HB2	1.86	0.58
3:G:102:VAL:HG21	3:G:152:THR:HG23	1.85	0.58
2:E:125:ASP:O	2:E:126:GLU:HB2	2.02	0.58
2:D:16:MET:HB3	2:D:54:VAL:HG23	1.86	0.57
3:G:102:VAL:CG2	3:G:152:THR:HG23	2.35	0.57
2:D:148:PRO:HA	2:D:302:PRO:HD2	1.87	0.57
1:C:558:ARG:HH11	1:C:558:ARG:HG2	1.68	0.57
2:D:40:ARG:HD3	2:D:58:GLU:HB2	1.85	0.57
1:C:24:ILE:O	1:C:25:GLN:HB2	2.04	0.57
1:A:296:SER:OG	2:D:286:GLU:OE2	2.22	0.57
1:B:247:LYS:NZ	1:B:272:GLU:OE1	2.37	0.57
1:C:410:LYS:HG3	1:C:437:TYR:CZ	2.39	0.57
1:C:211:THR:HG22	1:C:245:ILE:HG12	1.87	0.57
1:C:141:GLU:OE2	1:C:147:HIS:ND1	2.29	0.56
2:F:146:LYS:HD3	2:F:285:PHE:O	2.05	0.56
1:B:453:TRP:HZ3	1:B:519:PHE:HA	1.70	0.56
2:E:9:LYS:HB2	2:E:19:GLU:HG2	1.86	0.56
4:H:91:GLN:NE2	4:H:101:ASN:ND2	2.52	0.56
3:G:151:LYS:CE	4:H:68:GLN:O	2.53	0.56
2:E:40:ARG:NH1	2:E:59:GLY:O	2.39	0.56
2:E:221:ARG:NH1	2:E:221:ARG:CG	2.60	0.56
1:C:150:MET:HE1	7:C:746:HOH:O	2.06	0.56
1:B:24:ILE:O	1:B:25:GLN:HB2	2.06	0.56
2:F:181:PHE:HD2	2:F:211:MET:CE	2.13	0.56
1:C:261:GLU:OE1	7:C:741:HOH:O	2.18	0.56
1:C:305:ALA:O	1:C:309:THR:HG23	2.06	0.55
1:C:582:GLN:O	1:C:585:VAL:HG22	2.06	0.55
1:B:83:MET:CE	1:B:266:MET:HB3	2.36	0.55
1:C:161:LYS:HE3	7:C:767:HOH:O	2.06	0.55
1:C:108:GLN:NE2	7:C:714:HOH:O	2.39	0.55
2:F:386:ALA:HB2	2:F:394:LEU:HD22	1.87	0.55
2:F:94:GLY:HA3	2:F:227:MET:HE1	1.88	0.55
1:C:208:PRO:HA	1:C:223:THR:HA	1.88	0.55
4:H:91:GLN:HA	4:H:91:GLN:OE1	2.07	0.55
1:B:225:GLY:O	1:B:370:GLY:HA2	2.07	0.55
1:A:247:LYS:HD3	1:A:276:LEU:HD22	1.88	0.55
2:D:352:LYS:CE	7:D:506:HOH:O	2.54	0.54
3:G:37:MET:O	3:G:41:ILE:HG13	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:45:LEU:HD13	2:F:264:ARG:HD2	1.89	0.54
2:F:433:LEU:O	2:F:436:MET:HB2	2.07	0.54
2:E:378:GLN:OE1	7:E:522:HOH:O	2.18	0.54
1:B:27:MET:CE	1:B:71:LEU:HB2	2.38	0.54
2:E:438:PRO:HB2	2:E:440:THR:HG22	1.89	0.54
1:A:112:LEU:O	1:A:114:HIS:HD2	1.91	0.54
2:E:87:GLY:HA2	2:E:204:ILE:O	2.08	0.54
1:A:531:GLU:HG3	1:A:578:LYS:HG2	1.88	0.54
1:C:407:ARG:NH1	7:C:713:HOH:O	2.40	0.54
2:D:156:PRO:HG3	2:D:334:TYR:CE1	2.43	0.54
2:E:229:LEU:O	2:E:233:GLU:HG3	2.09	0.54
2:E:397:ILE:H	2:E:397:ILE:HD12	1.72	0.54
1:A:378:ASP:CB	1:A:380:ARG:NH1	2.71	0.53
3:G:68:ALA:HB1	3:G:129:LEU:HG	1.90	0.53
1:A:333:ARG:NH1	1:A:333:ARG:HG2	2.05	0.53
2:E:103:ILE:O	2:E:105:PRO:HD3	2.09	0.53
2:F:26:TYR:O	2:F:27:GLU:HB2	2.08	0.53
4:H:91:GLN:HE22	4:H:101:ASN:HD22	1.56	0.53
4:H:11:LYS:HA	4:H:26:HIS:HE1	1.71	0.53
2:D:13:GLY:O	2:D:60:THR:HG21	2.09	0.53
5:C:601:ANP:HNB1	2:F:350:ARG:HH12	1.57	0.53
1:C:13:LEU:HD13	1:C:341:MET:HE1	1.91	0.53
2:D:363:GLU:HG2	7:D:529:HOH:O	2.07	0.53
1:C:558:ARG:HG2	1:C:558:ARG:NH1	2.23	0.53
2:F:45:LEU:HD11	2:F:55:GLN:HB3	1.89	0.53
2:E:57:PHE:HA	2:E:219:ILE:HD12	1.91	0.53
2:F:126:GLU:OE1	2:F:290:ARG:NE	2.43	0.52
1:B:8:LYS:HE3	2:E:48:GLN:NE2	2.24	0.52
1:C:51:VAL:HG12	1:C:53:GLU:H	1.73	0.52
1:A:225:GLY:HA2	1:A:384:ILE:O	2.09	0.52
1:B:27:MET:CE	1:B:38:GLU:CB	2.87	0.52
1:B:272:GLU:O	1:B:276:LEU:HD13	2.09	0.52
3:G:51:ARG:NH1	3:G:150:GLU:CD	2.63	0.52
4:H:14:VAL:CG1	4:H:24:VAL:HG13	2.40	0.52
1:C:247:LYS:HA	1:C:285:LEU:HD21	1.92	0.52
2:F:186:ILE:CD1	2:F:190:GLU:HG2	2.40	0.52
1:A:528:PHE:HA	1:A:577:ILE:HG21	1.92	0.52
1:B:27:MET:SD	1:B:71:LEU:HD13	2.50	0.52
1:B:27:MET:HE2	1:B:38:GLU:CA	2.39	0.52
1:C:210:ILE:O	1:C:249:SER:HA	2.09	0.52
1:A:477:VAL:CG2	1:A:481:SER:HB3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:279:THR:O	2:F:283:THR:HG23	2.10	0.52
1:A:24:ILE:O	1:A:25:GLN:HB2	2.10	0.51
1:C:407:ARG:HD2	2:D:252:ASN:OD1	2.10	0.51
2:E:28:GLU:OE2	2:E:72:PHE:HB3	2.09	0.51
1:C:150:MET:CE	7:C:746:HOH:O	2.58	0.51
2:F:29:LEU:HD11	2:F:41:ARG:HG2	1.92	0.51
1:A:232:GLY:HA3	1:A:238:LYS:HD3	1.92	0.51
1:C:8:LYS:HB3	1:C:15:MET:HG3	1.91	0.51
1:A:447:GLN:HB3	7:A:776:HOH:O	2.11	0.51
1:A:105:ARG:NH1	7:A:758:HOH:O	2.43	0.51
1:C:143:LYS:HE3	1:C:283:GLU:HA	1.93	0.50
2:D:146:LYS:CE	2:D:324:GLU:OE2	2.55	0.50
1:B:446:ASP:O	1:B:450:GLN:N	2.42	0.50
2:D:271:ARG:NH2	2:D:310:ASP:OD2	2.44	0.50
1:A:294:ASN:HA	1:A:298:MET:HE3	1.93	0.50
3:G:78:ASP:HA	7:G:302:HOH:O	2.12	0.50
1:B:416:ASP:OD1	1:B:418:SER:HB3	2.12	0.50
1:B:107:VAL:HA	7:B:788:HOH:O	2.10	0.50
1:C:225:GLY:O	1:C:370:GLY:HA2	2.12	0.50
1:B:230:VAL:HG22	1:B:413:TRP:HE3	1.75	0.50
2:F:249:ASP:C	2:F:249:ASP:OD1	2.50	0.50
1:A:214:ARG:NH1	1:A:513:THR:OG1	2.45	0.50
2:F:102:GLU:HB2	2:F:103:ILE:HA	1.76	0.50
1:C:513:THR:HG22	1:C:517:LYS:HB3	1.94	0.50
1:C:453:TRP:CZ3	1:C:519:PHE:HA	2.47	0.50
1:C:318:ARG:HD2	1:C:372:VAL:HG21	1.92	0.50
1:B:163:GLU:HG2	7:B:773:HOH:O	2.11	0.50
2:D:57:PHE:HB3	2:D:217:PRO:HG3	1.95	0.49
1:C:243:HIS:HE1	7:C:791:HOH:O	1.93	0.49
1:C:548:GLY:HA3	1:C:584:ILE:HD11	1.94	0.49
1:C:445:MET:CE	1:C:515:ARG:HD2	2.43	0.49
1:B:378:ASP:OD1	1:B:378:ASP:N	2.44	0.49
2:D:182:ALA:HB3	2:D:247:MET:HG2	1.94	0.49
1:B:315:GLU:HA	1:B:384:ILE:HD11	1.93	0.49
2:E:33:ARG:HH21	2:E:71:ARG:NH2	2.10	0.49
3:G:199:ARG:HD2	7:G:308:HOH:O	2.11	0.49
2:E:200:GLN:O	2:E:200:GLN:NE2	2.45	0.49
4:H:53:GLN:NE2	4:H:78:SER:OG	2.46	0.49
1:B:8:LYS:HD2	2:E:48:GLN:HE21	1.78	0.49
3:G:140:LEU:HB2	3:G:141:PRO:HD3	1.95	0.49
1:A:1:MET:CB	1:A:65:ARG:HH21	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:MET:HE1	2:D:40:ARG:CZ	2.43	0.48
1:A:348:MET:CE	2:E:268:PRO:HG3	2.43	0.48
1:C:24:ILE:O	1:C:25:GLN:CB	2.61	0.48
2:E:183:ALA:HB1	2:E:186:ILE:CD1	2.44	0.48
3:G:34:ASP:O	3:G:38:ARG:HG3	2.14	0.48
2:E:328:ILE:HG13	2:E:346:PRO:HB2	1.95	0.48
1:C:30:VAL:HB	1:C:35:VAL:HG23	1.96	0.48
1:A:35:VAL:HB	1:A:53:GLU:HB2	1.96	0.48
2:D:19:GLU:O	2:D:21:VAL:HG13	2.13	0.48
1:A:378:ASP:OD2	1:A:380:ARG:NH1	2.47	0.48
1:A:475:ARG:NH2	3:G:31:ASP:OD2	2.46	0.48
1:A:425:PHE:HA	1:A:426:PRO:C	2.33	0.48
2:E:397:ILE:N	2:E:397:ILE:HD12	2.28	0.48
2:E:166:ARG:NH1	2:E:197:ASP:OD2	2.47	0.48
2:D:128:ILE:HD11	2:D:143:ARG:HG2	1.94	0.48
1:C:318:ARG:HD2	1:C:372:VAL:CG2	2.44	0.48
1:C:513:THR:HG23	1:C:517:LYS:CD	2.44	0.48
1:A:348:MET:HE1	2:E:268:PRO:HG3	1.96	0.48
2:E:107:LYS:HD2	2:E:109:LEU:HD21	1.94	0.48
1:B:541:TYR:N	1:B:544:GLU:OE2	2.45	0.48
3:G:46:LYS:O	3:G:50:LEU:HB2	2.13	0.48
2:F:248:THR:HB	2:F:303:ILE:HB	1.96	0.48
2:E:383:LYS:O	2:E:387:VAL:HG23	2.13	0.48
1:A:485:ASN:O	1:A:533:ARG:NH2	2.47	0.48
1:A:3:ILE:HB	1:A:65:ARG:HD2	1.96	0.48
2:F:181:PHE:CD2	2:F:211:MET:CE	2.90	0.48
1:B:225:GLY:HA2	1:B:384:ILE:O	2.14	0.48
2:D:88:ARG:NH2	2:D:98:ASP:OD1	2.47	0.48
1:C:524:VAL:CG1	1:C:556:ILE:HG12	2.44	0.48
2:F:266:GLU:OE1	2:F:276:TYR:OH	2.24	0.48
1:A:445:MET:HG2	1:A:453:TRP:CD1	2.48	0.47
1:A:52:TYR:CD2	1:A:301:ALA:HB2	2.49	0.47
4:H:31:THR:O	4:H:35:LYS:HB2	2.13	0.47
1:B:80:ILE:O	1:B:81:SER:HB2	2.14	0.47
2:E:233:GLU:HB2	7:E:518:HOH:O	2.13	0.47
1:C:193:VAL:HG11	1:C:309:THR:HG22	1.95	0.47
2:F:16:MET:HB3	2:F:54:VAL:HG22	1.96	0.47
2:F:199:ARG:HD3	7:F:540:HOH:O	2.14	0.47
3:G:54:ILE:HG21	3:G:146:LEU:HD22	1.95	0.47
1:A:498:GLU:O	1:A:560:LYS:NZ	2.42	0.47
2:F:354:LYS:O	2:F:360:LYS:CE	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LYS:HB3	1:B:15:MET:HG3	1.97	0.47
1:C:18:ASN:HA	7:C:747:HOH:O	2.14	0.47
7:C:770:HOH:O	2:D:187:THR:HB	2.14	0.47
2:D:383:LYS:O	2:D:386:ALA:HB3	2.13	0.47
1:B:239:THR:HB	5:B:601:ANP:O2A	2.15	0.47
1:A:378:ASP:HB2	1:A:380:ARG:HH12	1.77	0.47
1:C:478:GLY:O	1:C:479:ILE:HG13	2.15	0.47
1:A:238:LYS:HB3	1:A:238:LYS:HE3	1.57	0.46
1:C:311:ILE:O	1:C:315:GLU:HG3	2.15	0.46
2:F:251:THR:O	2:F:255:GLU:HG2	2.15	0.46
2:E:385:LEU:HD23	2:E:394:LEU:HD23	1.96	0.46
2:F:162:ALA:O	2:F:166:ARG:HB2	2.15	0.46
1:A:333:ARG:NH1	1:A:333:ARG:CG	2.68	0.46
3:G:44:ILE:HD12	3:G:44:ILE:HA	1.84	0.46
2:E:242:HIS:HD2	2:E:297:SER:OG	1.97	0.46
2:D:87:GLY:HA2	2:D:204:ILE:HG13	1.98	0.46
2:D:148:PRO:HD3	2:D:323:THR:HB	1.97	0.46
3:G:100:VAL:HG22	3:G:159:GLU:HG2	1.97	0.46
1:A:1:MET:HA	1:A:66:SER:O	2.16	0.46
1:C:391:SER:HB3	2:F:321:TYR:CE1	2.51	0.46
1:A:33:LEU:HD21	1:A:105:ARG:HD2	1.98	0.46
1:C:417:SER:O	1:C:421:GLN:HG3	2.16	0.46
1:B:497:ARG:NH2	7:B:787:HOH:O	2.49	0.46
2:E:9:LYS:HD3	2:E:10:GLU:HG3	1.98	0.46
2:E:48:GLN:HG2	2:E:48:GLN:O	2.15	0.46
1:B:425:PHE:HA	1:B:426:PRO:C	2.35	0.46
2:F:354:LYS:O	2:F:360:LYS:HE2	2.16	0.45
2:F:408:PHE:O	2:F:412:TYR:HB3	2.16	0.45
2:F:209:MET:HG2	2:F:211:MET:HE3	1.98	0.45
1:B:41:GLU:OE1	1:B:43:ARG:NH1	2.44	0.45
1:A:445:MET:SD	1:A:515:ARG:HD3	2.56	0.45
1:C:555:ARG:NH1	1:C:576:GLU:OE1	2.50	0.45
1:A:86:GLY:HA3	1:A:302:ALA:O	2.17	0.45
1:C:2:GLN:OE1	1:C:21:GLU:HB2	2.16	0.45
1:A:221:PRO:O	1:A:435:SER:OG	2.25	0.45
2:D:34:MET:CE	2:D:40:ARG:CD	2.95	0.45
1:C:143:LYS:HE3	1:C:283:GLU:CB	2.46	0.45
2:E:362:ARG:HH11	2:E:364:ASP:CG	2.20	0.45
1:C:477:VAL:HG22	1:C:477:VAL:O	2.15	0.45
1:B:191:TRP:CD2	1:B:192:PRO:HD2	2.51	0.45
1:A:167:PHE:HB3	1:A:171:ASP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ILE:HG21	1:B:283:GLU:OE2	2.17	0.45
2:D:34:MET:CE	2:D:40:ARG:CZ	2.95	0.45
1:C:143:LYS:HE3	1:C:283:GLU:HB3	1.99	0.45
2:D:104:LEU:HG	2:D:104:LEU:H	1.59	0.45
1:B:555:ARG:NH1	1:B:576:GLU:OE2	2.44	0.45
1:A:243:HIS:O	1:A:247:LYS:HG2	2.17	0.44
1:A:448:ILE:HG23	1:A:449:LEU:HD13	1.98	0.44
1:C:230:VAL:HG13	1:C:413:TRP:HB2	1.99	0.44
2:D:268:PRO:HD2	3:G:200:LEU:HD13	1.99	0.44
1:A:422:LYS:O	1:A:423:ARG:HB2	2.17	0.44
1:C:477:VAL:HB	3:G:29:LEU:HD11	1.98	0.44
1:C:541:TYR:HB2	1:C:544:GLU:HG3	1.98	0.44
2:E:174:SER:HB3	7:E:541:HOH:O	2.16	0.44
2:E:174:SER:HA	2:E:175:ASP:HA	1.63	0.44
1:B:513:THR:HG23	1:B:517:LYS:HD3	1.98	0.44
2:F:348:LEU:HG	2:F:349:SER:N	2.33	0.44
1:C:477:VAL:CG2	1:C:477:VAL:O	2.65	0.44
1:A:125:GLU:O	1:A:128:THR:OG1	2.28	0.44
1:B:558:ARG:HE	1:B:558:ARG:HB3	1.61	0.44
1:C:214:ARG:HG2	1:C:518:GLN:HG2	2.00	0.44
1:B:55:THR:HA	1:B:58:ILE:HD12	2.00	0.44
2:F:91:ASP:C	2:F:91:ASP:OD1	2.56	0.44
2:F:119:ILE:O	2:F:119:ILE:HG22	2.16	0.44
3:G:187:MET:O	3:G:191:GLU:HG2	2.18	0.44
1:A:479:ILE:HG23	1:A:480:ASP:OD1	2.18	0.44
1:A:17:GLU:O	1:A:18:ASN:HB2	2.17	0.44
2:E:41:ARG:CG	2:E:41:ARG:NH1	2.68	0.44
1:C:445:MET:HE2	1:C:515:ARG:HD2	1.99	0.44
1:A:212:GLY:HA3	1:A:512:PHE:CD1	2.53	0.44
1:C:38:GLU:O	1:C:49:ILE:HA	2.18	0.44
1:C:200:LYS:HB2	1:C:200:LYS:HE2	1.72	0.44
1:C:516:GLU:O	1:C:520:ASN:ND2	2.50	0.44
1:B:281:THR:OG1	1:B:283:GLU:OE1	2.33	0.43
1:A:71:LEU:HD21	1:A:87:ILE:HG22	2.00	0.43
1:A:553:ARG:HA	1:A:556:ILE:HD12	2.00	0.43
1:A:6:ILE:HG22	1:A:60:PRO:HA	2.00	0.43
1:A:507:ASP:O	1:A:511:THR:HB	2.18	0.43
3:G:51:ARG:NH1	3:G:150:GLU:OE2	2.51	0.43
1:B:212:GLY:HA3	1:B:512:PHE:CD1	2.53	0.43
1:A:528:PHE:CD2	1:A:528:PHE:C	2.91	0.43
1:A:218:THR:HG23	1:A:453:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:PRO:HG2	1:C:412:PHE:HE1	1.83	0.43
2:F:4:GLU:OE2	2:F:71:ARG:HG2	2.19	0.43
2:E:163:GLN:HE21	2:E:167:GLN:NE2	2.15	0.43
1:B:266:MET:O	1:B:270:VAL:HG22	2.17	0.43
1:A:495:SER:OG	1:A:499:ASP:OD2	2.23	0.43
1:A:230:VAL:O	1:A:389:ALA:HA	2.18	0.43
1:A:517:LYS:NZ	7:A:754:HOH:O	2.42	0.43
1:A:426:PRO:HB2	1:A:428:ILE:HD12	1.98	0.43
2:E:58:GLU:OE1	2:E:58:GLU:N	2.43	0.43
2:E:46:GLU:HB3	2:E:53:MET:HB2	2.00	0.43
2:D:183:ALA:O	2:D:212:ASN:HB3	2.19	0.43
2:D:152:GLY:N	2:D:155:LEU:HD12	2.33	0.43
1:A:396:ASP:HA	7:A:752:HOH:O	2.18	0.43
2:E:249:ASP:OD2	2:E:304:LEU:HA	2.18	0.43
4:H:3:TYR:N	4:H:3:TYR:CD1	2.87	0.43
1:A:490:LEU:HA	1:A:490:LEU:HD23	1.78	0.43
1:C:413:TRP:HB3	1:C:428:ILE:HD13	2.00	0.43
1:B:524:VAL:CG1	1:B:556:ILE:HG12	2.49	0.42
1:B:528:PHE:HA	1:B:577:ILE:HG21	2.00	0.42
1:C:238:LYS:HE2	1:C:238:LYS:HB2	1.83	0.42
2:F:331:ARG:O	2:F:335:LYS:HG2	2.19	0.42
1:C:283:GLU:OE1	1:C:283:GLU:N	2.52	0.42
1:B:82:GLN:HG2	1:B:84:PHE:CZ	2.54	0.42
5:B:601:ANP:PA	7:B:701:HOH:O	2.73	0.42
1:B:558:ARG:HD3	7:B:757:HOH:O	2.20	0.42
1:A:80:ILE:HG13	1:A:141:GLU:CD	2.40	0.42
2:E:146:LYS:NZ	2:E:286:GLU:OE2	2.53	0.42
2:E:125:ASP:OD2	2:E:354:LYS:HE3	2.19	0.42
1:B:214:ARG:NH1	1:B:513:THR:OG1	2.52	0.42
2:F:270:ARG:O	2:F:271:ARG:HB2	2.19	0.42
1:B:562:ILE:HA	1:B:563:PRO:HD3	1.83	0.42
2:F:248:THR:HA	2:F:249:ASP:HA	1.80	0.42
1:B:350:GLY:N	1:B:354:TYR:O	2.49	0.42
1:B:39:ILE:HG12	1:B:47:ALA:HB1	2.02	0.42
1:A:448:ILE:HA	1:A:448:ILE:HD12	1.90	0.42
1:C:83:MET:HE1	1:C:266:MET:HB3	2.01	0.42
2:E:407:ARG:NE	2:E:411:GLU:OE2	2.40	0.42
1:C:474:VAL:C	1:C:476:LEU:H	2.23	0.42
1:A:329:ASP:HA	1:A:330:SER:HA	1.75	0.42
1:C:150:MET:HB3	1:C:150:MET:HE2	1.84	0.42
1:B:426:PRO:HB2	1:B:428:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:529:GLY:O	1:C:533:ARG:HB2	2.20	0.42
2:F:94:GLY:CA	2:F:227:MET:HE2	2.50	0.42
4:H:14:VAL:HG13	4:H:14:VAL:O	2.19	0.42
1:A:10:SER:OG	2:D:264:ARG:HD2	2.20	0.42
1:C:415:LEU:HA	1:C:427:SER:O	2.20	0.42
2:F:125:ASP:N	2:F:125:ASP:OD1	2.51	0.42
1:C:56:SER:O	1:C:105:ARG:NH2	2.42	0.42
2:D:93:LEU:CG	2:D:220:GLU:HG2	2.46	0.41
2:E:198:PHE:HB3	2:E:204:ILE:HB	2.02	0.41
2:F:111:ILE:O	2:F:287:ARG:NH2	2.53	0.41
2:D:89:VAL:HG11	2:D:195:MET:SD	2.60	0.41
1:B:27:MET:HE2	1:B:38:GLU:HA	2.02	0.41
1:B:424:HIS:HE1	7:B:733:HOH:O	2.02	0.41
2:D:33:ARG:HH12	2:D:71:ARG:NH1	2.17	0.41
1:C:144:ILE:HG21	7:C:765:HOH:O	2.20	0.41
2:D:178:ALA:HB2	2:D:241:MET:HE2	2.01	0.41
1:C:346:GLU:HG2	3:G:206:MET:CE	2.50	0.41
2:F:244:LEU:HD12	2:F:299:THR:HB	2.01	0.41
1:B:41:GLU:HB2	1:B:48:SER:HB2	2.02	0.41
1:C:54:GLU:OE2	1:C:56:SER:HB3	2.20	0.41
7:A:770:HOH:O	2:D:121:ARG:HD3	2.20	0.41
4:H:95:GLU:HG3	4:H:96:LYS:N	2.36	0.41
1:C:251:VAL:HG11	1:C:325:ALA:HB2	2.03	0.41
2:D:148:PRO:CA	2:D:302:PRO:HD2	2.50	0.41
1:B:336:GLU:HG3	7:B:764:HOH:O	2.20	0.41
2:E:41:ARG:NE	7:E:504:HOH:O	2.35	0.41
2:D:311:LYS:H	2:D:311:LYS:HG3	1.71	0.41
2:E:21:VAL:HB	2:E:24:VAL:HG21	2.03	0.41
1:C:13:LEU:HD13	1:C:341:MET:CE	2.50	0.41
1:C:75:LEU:HD13	1:C:316:TYR:CD1	2.56	0.41
1:C:435:SER:O	1:C:438:SER:HB2	2.21	0.41
2:D:422:THR:HB	7:D:536:HOH:O	2.20	0.41
2:D:399:LYS:O	2:D:403:LYS:HG3	2.21	0.41
1:A:270:VAL:HG11	2:D:119:ILE:HG22	2.03	0.41
1:B:210:ILE:O	1:B:249:SER:HA	2.20	0.41
2:F:123:TYR:HA	2:F:124:PRO:HD3	1.84	0.41
1:A:256:TYR:C	1:A:256:TYR:CD2	2.93	0.41
1:C:356:ALA:HB1	2:D:259:GLU:HA	2.02	0.41
1:C:573:ILE:O	1:C:577:ILE:HG13	2.21	0.41
2:D:184:ILE:HG21	2:D:253:TYR:HB2	2.03	0.40
1:B:311:ILE:HD12	1:B:311:ILE:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:177:PHE:HD2	2:D:242:HIS:O	2.04	0.40
1:B:445:MET:HA	1:B:448:ILE:HG22	2.03	0.40
2:D:171:LEU:C	2:D:173:SER:H	2.23	0.40
1:B:399:GLU:OE2	1:B:401:VAL:HB	2.20	0.40
3:G:151:LYS:HA	3:G:151:LYS:HD2	1.86	0.40
1:C:513:THR:CG2	1:C:517:LYS:CD	2.99	0.40
4:H:91:GLN:O	4:H:94:VAL:HG12	2.22	0.40
3:G:41:ILE:HA	3:G:44:ILE:HG22	2.03	0.40
1:C:429:ASN:CG	1:C:432:GLN:HB2	2.42	0.40
2:F:146:LYS:HD2	2:F:323:THR:HA	2.03	0.40
1:A:254:VAL:O	1:A:289:THR:HA	2.22	0.40
3:G:26:HIS:NE2	3:G:171:GLU:HB2	2.37	0.40
1:B:103:LEU:HA	1:B:103:LEU:HD12	1.95	0.40
1:A:361:ARG:HA	1:A:361:ARG:HD3	1.47	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	585/600 (98%)	574 (98%)	11 (2%)	0	100	100
1	B	590/600 (98%)	576 (98%)	14 (2%)	0	100	100
1	C	578/600 (96%)	566 (98%)	10 (2%)	2 (0%)	46	73
2	D	449/465 (97%)	437 (97%)	12 (3%)	0	100	100
2	E	450/465 (97%)	437 (97%)	13 (3%)	0	100	100
2	F	453/465 (97%)	441 (97%)	10 (2%)	2 (0%)	39	67
3	G	168/217 (77%)	163 (97%)	5 (3%)	0	100	100
4	H	100/115 (87%)	95 (95%)	5 (5%)	0	100	100
All	All	3373/3527 (96%)	3289 (98%)	80 (2%)	4 (0%)	56	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	102	GLU
1	C	477	VAL
2	F	101	PRO
1	C	159	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	502/511 (98%)	480 (96%)	22 (4%)	35	63
1	B	503/511 (98%)	478 (95%)	25 (5%)	30	57
1	C	499/511 (98%)	457 (92%)	42 (8%)	14	28
2	D	369/387 (95%)	343 (93%)	26 (7%)	19	40
2	E	378/387 (98%)	356 (94%)	22 (6%)	25	49
2	F	379/387 (98%)	359 (95%)	20 (5%)	28	54
3	G	155/198 (78%)	144 (93%)	11 (7%)	18	39
4	H	84/99 (85%)	78 (93%)	6 (7%)	18	39
All	All	2869/2991 (96%)	2695 (94%)	174 (6%)	23	47

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	29	LEU
1	A	36	ILE
1	A	94	PHE
1	A	100	SER
1	A	103	LEU
1	A	124	ILE
1	A	173	ILE
1	A	188	MET
1	A	253	LEU

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Mol	Chain	Res	Type
1	A	273	PHE
1	A	333	ARG
1	A	361	ARG
1	A	391	SER
1	A	397	ILE
1	A	436	LEU
1	A	449	LEU
1	A	476	LEU
1	A	484	ASP
1	A	508	ASP
1	A	543	ASN
1	A	572	SER
1	B	-4	SER
1	B	103	LEU
1	B	123	THR
1	B	144	ILE
1	B	195	ARG
1	B	230	VAL
1	B	253	LEU
1	B	270	VAL
1	B	281	THR
1	B	327	MET
1	B	352	GLU
1	B	371	ARG
1	B	378	ASP
1	B	381	GLU
1	B	399	GLU
1	B	428	ILE
1	B	438	SER
1	B	469	GLN
1	B	476	LEU
1	B	526	LEU
1	B	555	ARG
1	B	558	ARG
1	B	562	ILE
1	B	571	SER
1	B	585	VAL
1	C	15	MET
1	C	25	GLN
1	C	29	LEU
1	C	54	GLU
1	C	56	SER

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Mol	Chain	Res	Type
1	C	69	GLU
1	C	73	VAL
1	C	83	MET
1	C	95	MET
1	C	96	GLU
1	C	109	LEU
1	C	116	LYS
1	C	166	SER
1	C	173	ILE
1	C	194	ARG
1	C	195	ARG
1	C	200	LYS
1	C	209	MET
1	C	220	PHE
1	C	230	VAL
1	C	243	HIS
1	C	253	LEU
1	C	270	VAL
1	C	284	SER
1	C	351	ASP
1	C	377	SER
1	C	378	ASP
1	C	410	LYS
1	C	432	GLN
1	C	438	SER
1	C	448	ILE
1	C	454	SER
1	C	462	ARG
1	C	469	GLN
1	C	475	ARG
1	C	479	ILE
1	C	483	SER
1	C	513	THR
1	C	538	LEU
1	C	557	SER
1	C	583	LEU
1	C	586	SER
2	D	4	GLU
2	D	51	LYS
2	D	60	THR
2	D	73	LEU
2	D	103	ILE

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Mol	Chain	Res	Type
2	D	104	LEU
2	D	122	ASP
2	D	143	ARG
2	D	146	LYS
2	D	170	VAL
2	D	173	SER
2	D	176	ASP
2	D	177	PHE
2	D	211	MET
2	D	303	ILE
2	D	311	LYS
2	D	336	SER
2	D	352	LYS
2	D	363	GLU
2	D	368	THR
2	D	383	LYS
2	D	385	LEU
2	D	397	ILE
2	D	400	ILE
2	D	450	LEU
2	D	454	LEU
2	E	15	LEU
2	E	41	ARG
2	E	48	GLN
2	E	53	MET
2	E	61	SER
2	E	102	GLU
2	E	103	ILE
2	E	104	LEU
2	E	106	GLU
2	E	107	LYS
2	E	125	ASP
2	E	146	LYS
2	E	166	ARG
2	E	173	SER
2	E	175	ASP
2	E	221	ARG
2	E	331	ARG
2	E	353	ASP
2	E	362	ARG
2	E	380	LYS
2	E	452	LYS

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Mol	Chain	Res	Type
2	E	454	LEU
2	F	6	ARG
2	F	41	ARG
2	F	81	VAL
2	F	103	ILE
2	F	104	LEU
2	F	122	ASP
2	F	126	GLU
2	F	146	LYS
2	F	167	GLN
2	F	190	GLU
2	F	196	GLU
2	F	265	ARG
2	F	266	GLU
2	F	308	GLU
2	F	328	ILE
2	F	332	GLU
2	F	395	SER
2	F	424	THR
2	F	439	ARG
2	F	443	LYS
3	G	10	MET
3	G	18	GLN
3	G	47	ASN
3	G	50	LEU
3	G	51	ARG
3	G	59	GLN
3	G	91	SER
3	G	102	VAL
3	G	104	LEU
3	G	137	THR
3	G	178	LEU
4	H	3	TYR
4	H	14	VAL
4	H	19	LEU
4	H	36	THR
4	H	53	GLN
4	H	102	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	421	GLN
1	B	502	GLN
1	B	520	ASN
1	C	108	GLN
1	C	403	GLN
2	E	48	GLN
2	E	112	ASN
2	E	167	GLN
2	E	242	HIS
2	E	370	ASN
2	E	410	ASN
2	F	378	GLN
4	H	26	HIS
4	H	53	GLN
4	H	91	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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\|>2$
5	ANP	B	601	6	27,33,33	1.95	6 (22%)	30,52,52	1.49	4 (13%)
5	ANP	C	601	6	27,33,33	1.98	7 (25%)	30,52,52	2.24	7 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	B	601	6	-	0/12/38/38	0/3/3/3
5	ANP	C	601	6	-	0/12/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	ANP	C2-N3	2.12	1.35	1.32
5	C	601	ANP	C2-N3	2.20	1.36	1.32
5	C	601	ANP	PB-O3A	2.81	1.62	1.59
5	C	601	ANP	C5-C4	3.23	1.47	1.40
5	B	601	ANP	C5-C4	3.37	1.48	1.40
5	C	601	ANP	PB-N3B	3.58	1.72	1.63
5	C	601	ANP	PB-O1B	3.65	1.50	1.46
5	C	601	ANP	PG-N3B	3.67	1.73	1.63
5	B	601	ANP	PB-N3B	3.93	1.73	1.63
5	B	601	ANP	PB-O1B	3.99	1.50	1.46
5	B	601	ANP	PG-N3B	4.19	1.74	1.63
5	B	601	ANP	PG-O1G	4.30	1.51	1.46
5	C	601	ANP	PG-O1G	5.06	1.51	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	601	ANP	N3-C2-N1	-7.11	123.45	128.89
5	C	601	ANP	C2'-C1'-N9	-5.21	106.34	114.29
5	B	601	ANP	N3-C2-N1	-4.69	125.31	128.89
5	C	601	ANP	O1G-PG-N3B	-4.43	105.11	111.90
5	C	601	ANP	PA-O3A-PB	-3.40	121.25	132.67
5	C	601	ANP	C4-C5-N7	-2.84	106.86	109.48
5	B	601	ANP	O1G-PG-N3B	-2.65	107.83	111.90
5	B	601	ANP	PA-O3A-PB	-2.08	125.70	132.67
5	C	601	ANP	O2B-PB-O1B	2.64	115.51	110.00
5	B	601	ANP	O3G-PG-O2G	2.85	116.03	107.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	601	ANP	O3G-PG-O2G	3.60	118.25	107.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	601	ANP	3	0
5	C	601	ANP	2	0

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	587/600 (97%)	-0.06	20 (3%)	49	48	25, 43, 72, 91	0
1	B	592/600 (98%)	-0.14	7 (1%)	81	81	19, 34, 64, 85	0
1	C	582/600 (97%)	-0.09	8 (1%)	78	77	21, 38, 64, 90	0
2	D	451/465 (96%)	-0.13	7 (1%)	74	74	26, 43, 73, 90	0
2	E	452/465 (97%)	-0.28	3 (0%)	89	89	21, 35, 59, 77	0
2	F	455/465 (97%)	-0.35	2 (0%)	93	94	21, 35, 61, 84	0
3	G	176/217 (81%)	0.14	4 (2%)	64	62	35, 58, 121, 148	0
4	H	102/115 (88%)	0.39	3 (2%)	55	54	36, 80, 112, 126	0
All	All	3397/3527 (96%)	-0.13	54 (1%)	74	74	19, 40, 75, 148	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	82	ALA	3.9
1	A	541	TYR	3.8
2	E	175	ASP	3.4
1	A	0	GLY	3.3
2	D	125	ASP	3.2
2	D	104	LEU	3.2
1	A	160	GLN	3.2
1	A	539	GLY	3.1
1	C	160	GLN	3.0
1	C	179	GLU	2.9
2	D	175	ASP	2.9
1	A	532	ALA	2.9
1	A	173	ILE	2.9
1	B	281	THR	2.8
1	C	65	ARG	2.7
2	D	389	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	154	GLY	2.7
1	A	174	CYS	2.6
3	G	136	PHE	2.6
1	A	163	GLU	2.6
1	B	144	ILE	2.5
2	D	172	ASP	2.5
1	C	585	VAL	2.4
1	A	466	GLU	2.4
1	A	159	VAL	2.3
1	B	143	LYS	2.3
2	D	102	GLU	2.3
2	F	455	PRO	2.3
2	E	22	SER	2.3
1	A	127	GLY	2.3
3	G	89	SER	2.3
1	B	179	GLU	2.3
3	G	88	VAL	2.3
1	A	536	LEU	2.3
1	B	160	GLN	2.3
1	B	279	PRO	2.2
1	A	176	ILE	2.2
2	E	104	LEU	2.2
1	C	64	VAL	2.2
1	A	182	LEU	2.2
1	A	538	LEU	2.2
1	A	540	ALA	2.2
1	A	544	GLU	2.2
1	A	533	ARG	2.2
1	A	542	PHE	2.1
4	H	45	TYR	2.1
2	D	101	PRO	2.1
1	C	180	GLN	2.1
4	H	22	PHE	2.1
1	A	484	ASP	2.1
1	B	480	ASP	2.1
4	H	36	THR	2.0
2	F	102	GLU	2.0
1	C	183	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MG	C	602	1/1	0.98	0.19	-0.13	27,27,27,27	0
6	MG	B	602	1/1	0.96	0.20	-0.43	24,24,24,24	0
5	ANP	B	601	31/31	0.99	0.13	-1.31	12,19,23,26	0
5	ANP	C	601	31/31	0.99	0.12	-1.68	13,21,30,31	0

6.5 Other polymers (i)

There are no such residues in this entry.