Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2016 – 11:51 AM EST

PDB ID	:	5KNB
Title	:	Crystal structure of the 2 ADP-bound V1 complex
Authors	:	Suzuki, K.; Mizutani, K.; Maruyama, S.; Shimono, K.; Imai, F.L.; Muneyuki, E.; Kakinuma, Y.; Ishizuka-Katsura, Y.; Shirouzu, M.; Yokoyama, S.; Yamato, I.; Murata, T.
Deposited on	:	2016-06-28
Resolution	:	3.25 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 ⓘ symbol.

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

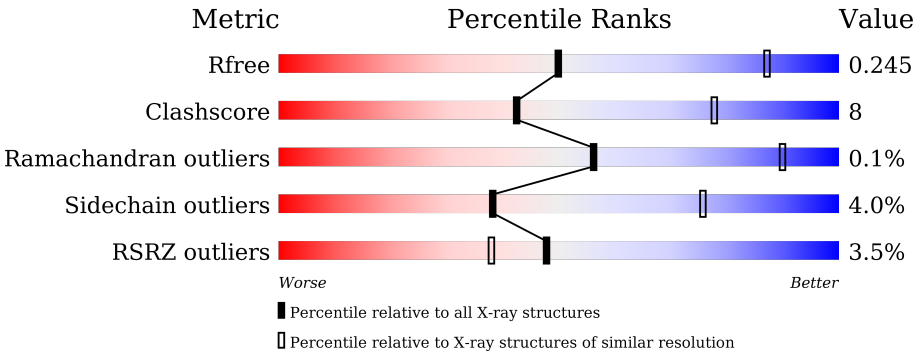
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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	5% 77% 20%
1	B	600	% 87% 12%
1	C	600	4% 73% 23%
2	D	465	% 74% 23%
2	E	465	78% 19%
2	F	465	% 74% 23%

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Mol	Chain	Length	Quality of chain
3	G	217	10% 45% 24% 6% 24%
4	H	115	26% 52% 27% 17%

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
7	GOL	E	501	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26077 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
			4431	2779	747	880	25			
1	B	592	Total	C	N	O	S	0	0	0
			4557	2858	763	910	26			
1	C	586	Total	C	N	O	S	0	0	0
			4428	2782	746	874	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	453	Total	C	N	O	S	0	0	0
			3475	2201	589	671	14			
2	E	454	Total	C	N	O	S	0	1	0
			3552	2253	609	676	14			
2	F	455	Total	C	N	O	S	0	0	0
			3541	2243	606	677	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	164	Total	C	N	O	S	0	0	0
			1308	822	233	244	9			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	GLY	-	expression tag	UNP P43435
G	-5	SER	-	expression tag	UNP P43435

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	SER	-	expression tag	UNP P43435
G	-3	GLY	-	expression tag	UNP P43435
G	-2	SER	-	expression tag	UNP P43435
G	-1	SER	-	expression tag	UNP P43435
G	0	GLY	-	expression tag	UNP P43435

- Molecule 4 is a protein called V-type sodium ATPase subunit NtpG (F).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	95	Total	C	N	O	S	0	0	0
			684	436	112	135	1			

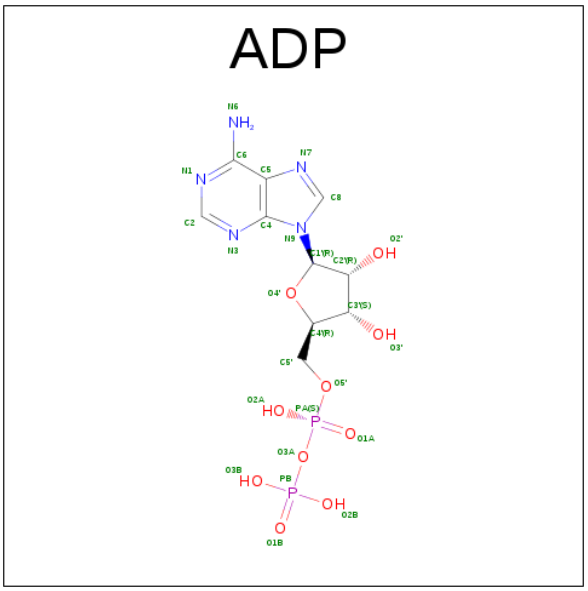
There are 12 discrepancies between the modelled and reference sequences:

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

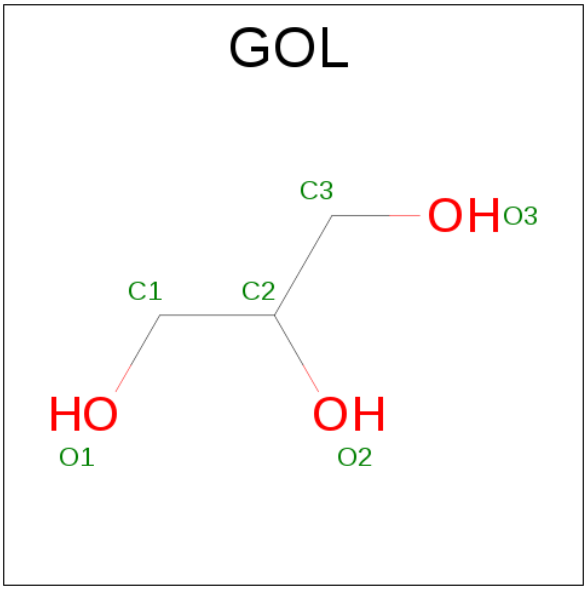
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	O		0	0
			6	3	3			
7	E	1	Total	C	O		0	0
			6	3	3			

- Molecule 8 is water.

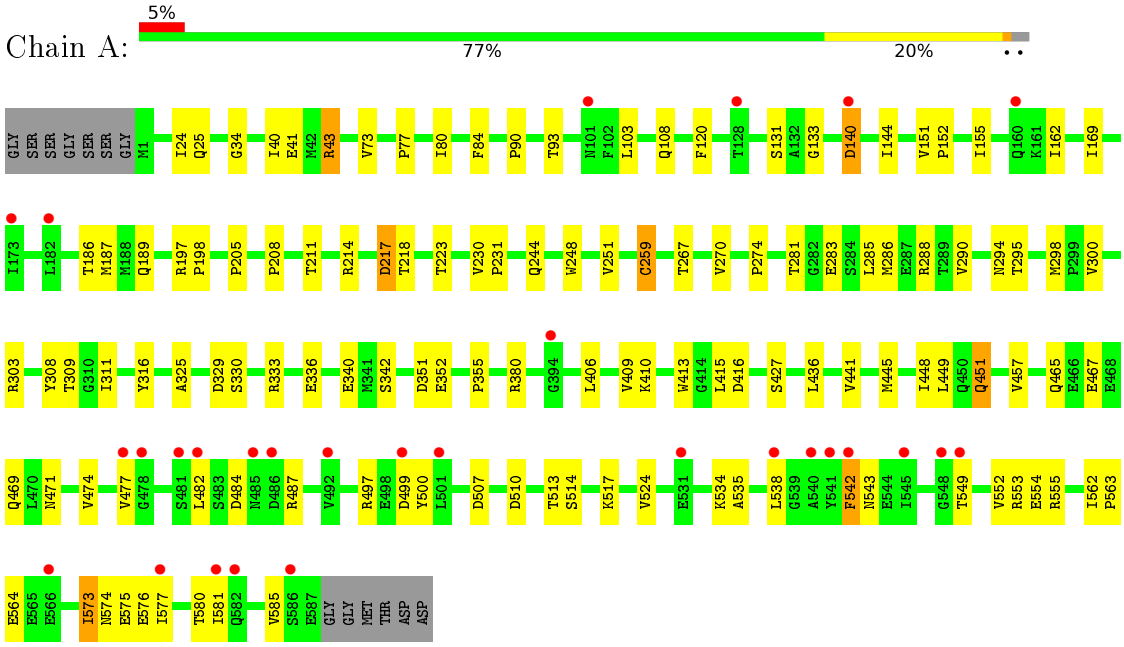
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	7	Total O 7 7	0	0
8	B	10	Total O 10 10	0	0
8	C	6	Total O 6 6	0	0
8	D	1	Total O 1 1	0	0
8	E	8	Total O 8 8	0	0
8	F	1	Total O 1 1	0	0

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.

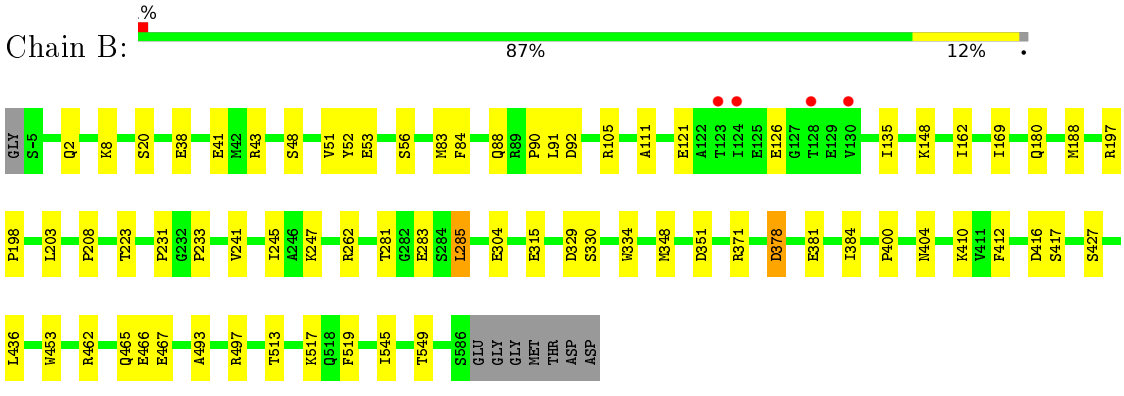
- Molecule 1: V-type sodium ATPase catalytic subunit A

Chain A:



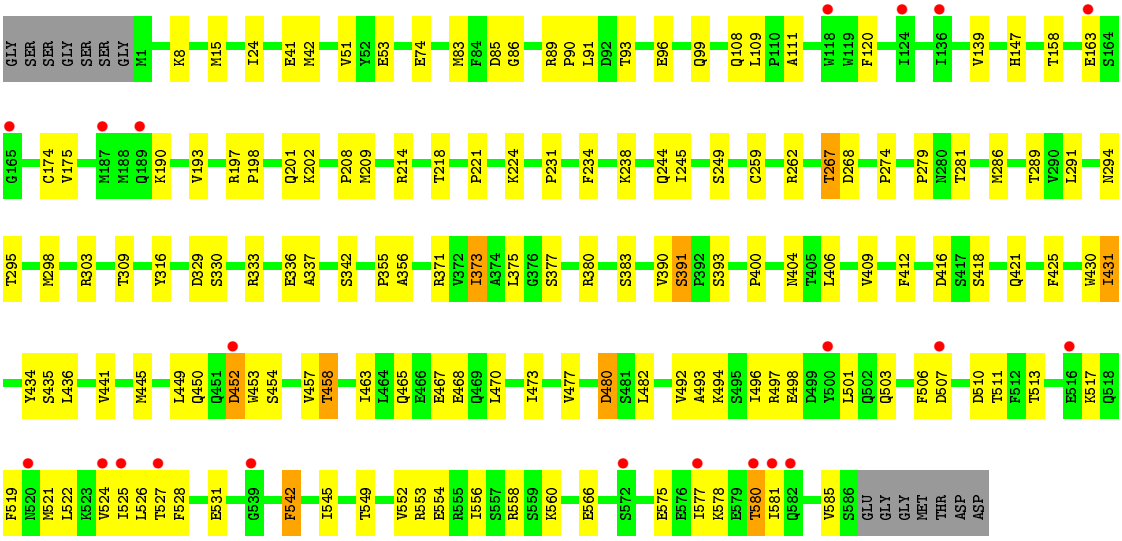
- Molecule 1: V-type sodium ATPase catalytic subunit A

Chain B:



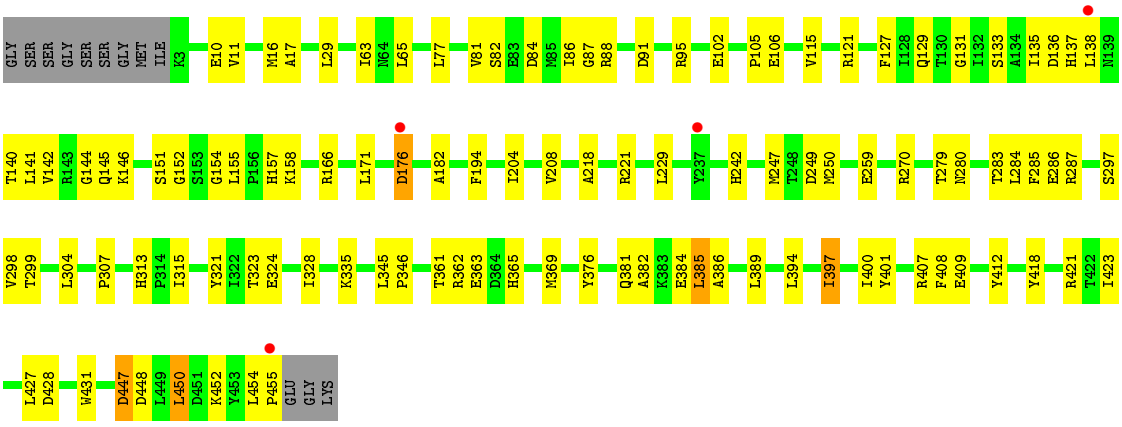
- Molecule 1: V-type sodium ATPase catalytic subunit A

Chain C:



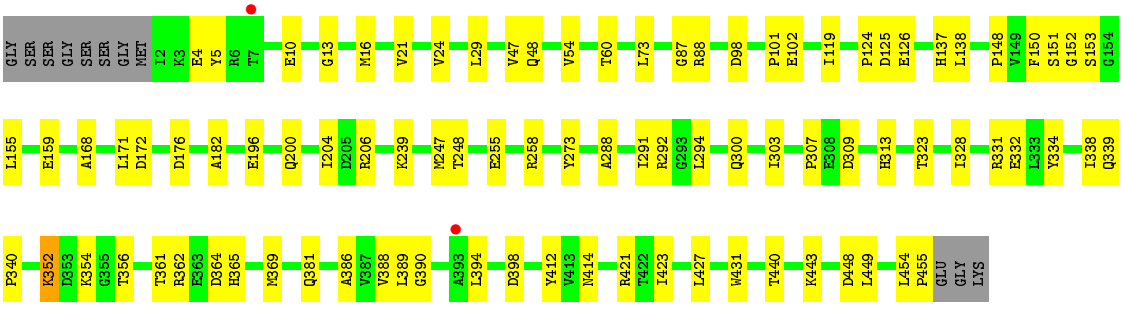
• Molecule 2: V-type sodium ATPase subunit B

Chain D:



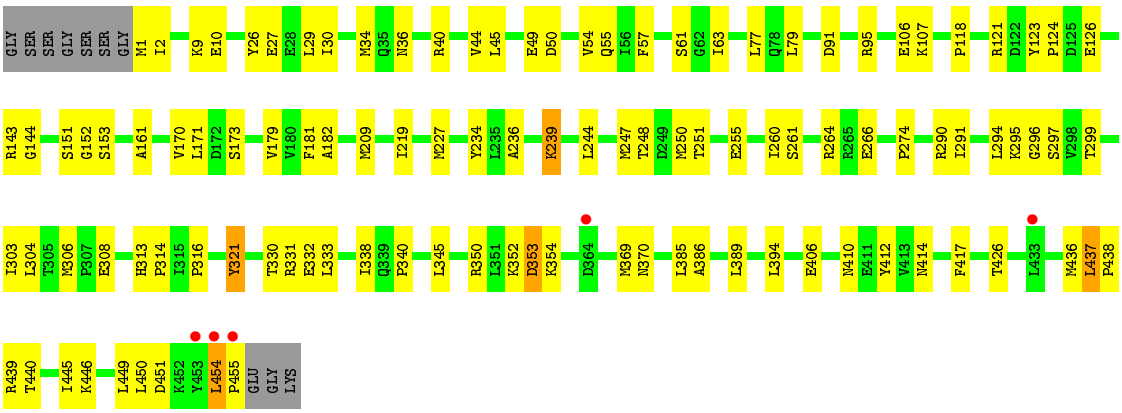
• Molecule 2: V-type sodium ATPase subunit B

Chain E:

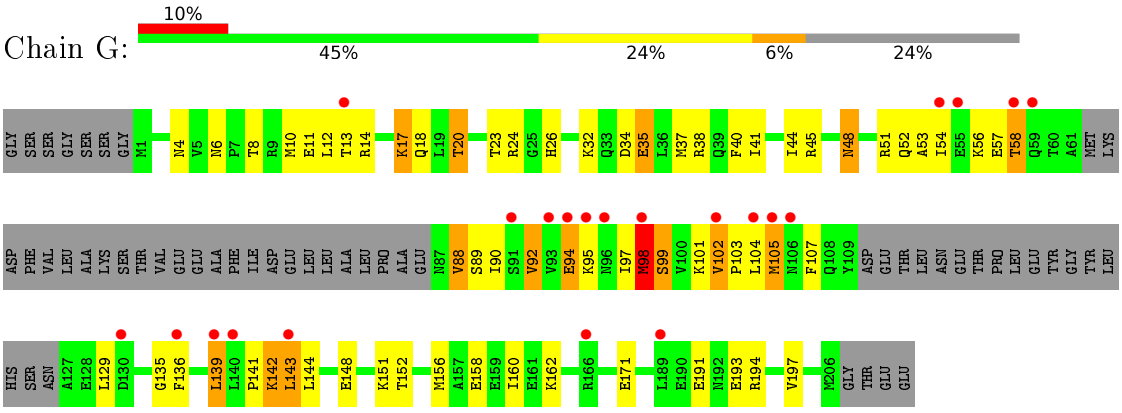


• Molecule 2: V-type sodium ATPase subunit B

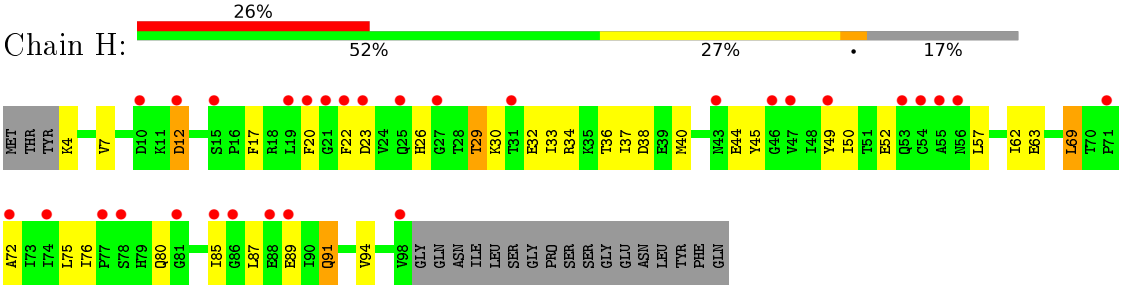
Chain F:



• Molecule 3: V-type sodium ATPase subunit D



• Molecule 4: V-type sodium ATPase subunit NtpG (F)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	127.35Å 129.62Å 237.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.55 – 3.25 46.64 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.55-3.25) 99.4 (46.64-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.209 , 0.245 0.209 , 0.245	Depositor DCC
R_{free} test set	3105 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	75.3	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 62.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
Reported twinning fraction	0.050 for k,h,-l	Depositor
Outliers	1 of 62128 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	26077	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.21	0/4507	0.40	0/6119
1	B	0.21	0/4633	0.38	0/6275
1	C	0.23	0/4503	0.41	0/6109
2	D	0.21	0/3538	0.42	0/4801
2	E	0.21	0/3615	0.39	0/4893
2	F	0.21	0/3604	0.41	0/4879
3	G	0.24	0/1316	0.49	0/1764
4	H	0.24	0/695	0.45	0/947
All	All	0.22	0/26411	0.41	0/35787

There are no bond length outliers.

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	4431	0	4235	73	0
1	B	4557	0	4458	40	0
1	C	4428	0	4264	92	0
2	D	3475	0	3388	68	0
2	E	3552	0	3548	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	3541	0	3527	70	0
3	G	1308	0	1353	44	0
4	H	684	0	635	25	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	27	0	12	0	0
6	C	27	0	12	2	0
7	B	6	0	8	0	0
7	E	6	0	8	0	0
8	A	7	0	0	3	0
8	B	10	0	0	1	0
8	C	6	0	0	2	0
8	D	1	0	0	0	0
8	E	8	0	0	0	0
8	F	1	0	0	0	0
All	All	26077	0	25448	427	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 8.

All (427) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:89:SER:HG	4:H:4:LYS:N	1.56	1.02
2:F:106:GLU:HG2	2:F:107:LYS:HG2	1.55	0.85
2:E:88:ARG:NH1	2:E:101:PRO:O	2.15	0.79
1:A:214:ARG:NH2	1:A:510:ASP:OD1	2.17	0.77
1:C:558:ARG:NH2	2:F:445:ILE:O	2.17	0.76
2:E:5:TYR:HE2	2:E:21:VAL:HA	1.52	0.73
1:A:34:GLY:O	1:A:108:GLN:NE2	2.22	0.72
2:D:218:ALA:HA	2:D:221:ARG:HD3	1.70	0.72
2:F:144:GLY:H	2:F:299:THR:HB	1.54	0.71
2:D:146:LYS:NZ	2:D:324:GLU:OE2	2.20	0.71
1:A:449:LEU:O	1:A:451:GLN:NE2	2.22	0.70
3:G:98:MET:HG2	3:G:99:SER:N	2.05	0.70
3:G:103:PRO:HD2	3:G:152:THR:HG22	1.75	0.69
3:G:103:PRO:HB3	4:H:69:LEU:HD21	1.75	0.69
1:A:281:THR:HG23	1:A:283:GLU:H	1.58	0.69
2:E:119:ILE:O	2:E:292:ARG:NH1	2.26	0.68
2:F:1:MET:N	2:F:2:ILE:HA	2.09	0.68
1:A:524:VAL:HG22	1:A:573:ILE:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:37:ILE:HA	4:H:40:MET:HB2	1.76	0.67
2:E:125:ASP:HA	2:E:354:LYS:HB3	1.76	0.67
3:G:89:SER:OG	4:H:4:LYS:N	2.27	0.67
3:G:151:LYS:HE3	4:H:72:ALA:HA	1.77	0.67
1:A:133:GLY:O	1:A:380:ARG:NH2	2.26	0.66
2:F:179:VAL:HG12	2:F:244:LEU:HB3	1.77	0.66
1:A:90:PRO:HB2	1:A:93:THR:HB	1.78	0.66
1:C:549:THR:O	1:C:553:ARG:N	2.26	0.65
1:B:51:VAL:HG12	1:B:53:GLU:H	1.63	0.63
4:H:7:VAL:HG13	4:H:49:TYR:HB2	1.79	0.63
1:C:528:PHE:HZ	1:C:549:THR:HG1	1.47	0.63
1:C:51:VAL:HG12	1:C:53:GLU:H	1.63	0.63
3:G:88:VAL:HG21	4:H:20:PHE:HD1	1.63	0.63
1:C:90:PRO:HD3	1:C:111:ALA:HA	1.81	0.63
1:C:262:ARG:NH1	8:C:701:HOH:O	2.32	0.63
1:A:230:VAL:HG12	1:A:413:TRP:HB2	1.81	0.63
2:D:447:ASP:HA	2:D:450:LEU:HD22	1.79	0.62
1:C:74:GLU:HB3	1:C:190:LYS:HE2	1.82	0.62
1:A:467:GLU:OE1	1:A:497:ARG:NH1	2.30	0.61
2:E:309:ASP:OD2	2:E:331:ARG:NH1	2.33	0.61
1:C:507:ASP:O	1:C:511:THR:OG1	2.19	0.61
1:C:198:PRO:HB2	1:C:375:LEU:HD11	1.82	0.61
1:B:467:GLU:OE2	1:B:497:ARG:NH1	2.34	0.61
1:B:462:ARG:NH1	1:B:466:GLU:OE1	2.33	0.61
2:D:129:GLN:OE1	2:D:423:ILE:N	2.33	0.61
2:E:364:ASP:OD2	2:E:431:TRP:NE1	2.21	0.61
2:F:406:GLU:O	2:F:410:ASN:ND2	2.34	0.61
1:C:147:HIS:NE2	1:C:316:TYR:OH	2.27	0.60
1:C:467:GLU:OE1	1:C:497:ARG:NH1	2.33	0.60
2:E:361:THR:HG22	2:E:362:ARG:H	1.66	0.60
2:F:153:SER:O	2:F:331:ARG:NH2	2.31	0.60
1:C:85:ASP:OD1	1:C:86:GLY:N	2.31	0.60
1:A:410:LYS:HB3	1:A:436:LEU:HB2	1.83	0.60
2:E:331:ARG:HA	2:E:334:TYR:HB3	1.84	0.60
2:E:155:LEU:HD21	2:E:331:ARG:HB3	1.83	0.60
2:D:362:ARG:HB3	2:D:427:LEU:HD13	1.85	0.59
2:F:45:LEU:HD13	2:F:264:ARG:HD2	1.84	0.59
1:C:214:ARG:NH1	1:C:510:ASP:OD1	2.34	0.59
2:F:248:THR:HB	2:F:303:ILE:HB	1.84	0.59
4:H:87:LEU:O	4:H:91:GLN:NE2	2.31	0.59
1:A:507:ASP:HB3	1:A:510:ASP:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:41:ILE:HA	3:G:44:ILE:HD12	1.83	0.59
1:A:208:PRO:HG3	1:A:441:VAL:HG22	1.84	0.59
3:G:191:GLU:OE2	3:G:194:ARG:NH1	2.36	0.59
1:A:303:ARG:HA	8:A:602:HOH:O	2.01	0.58
1:A:351:ASP:OD1	2:E:258:ARG:NH2	2.32	0.58
2:E:394:LEU:HG	2:E:398:ASP:HB3	1.86	0.58
1:B:400:PRO:O	1:B:404:ASN:ND2	2.36	0.58
1:C:238:LYS:HE3	1:C:391:SER:HB3	1.84	0.58
1:A:352:GLU:O	2:D:270:ARG:NH1	2.37	0.58
2:D:131:GLY:N	2:D:136:ASP:OD1	2.37	0.58
1:C:259:CYS:HA	1:C:294:ASN:HB3	1.85	0.58
4:H:4:LYS:HB2	4:H:45:TYR:HA	1.85	0.58
1:A:43:ARG:HD2	2:E:10:GLU:HB2	1.85	0.58
2:E:182:ALA:HB3	2:E:247:MET:HG2	1.86	0.58
2:D:182:ALA:HB3	2:D:247:MET:HG2	1.84	0.57
3:G:54:ILE:O	3:G:58:THR:OG1	2.21	0.57
3:G:136:PHE:HA	3:G:139:LEU:HD22	1.85	0.57
1:C:234:PHE:HB2	2:F:350:ARG:HH22	1.70	0.57
2:F:290:ARG:HD3	2:F:297:SER:HB3	1.87	0.57
2:D:137:HIS:ND1	2:D:412:TYR:OH	2.33	0.57
1:C:286:MET:HA	1:C:289:THR:HG22	1.85	0.57
1:A:41:GLU:OE2	1:A:43:ARG:NH1	2.35	0.56
1:C:480:ASP:OD2	1:C:480:ASP:N	2.37	0.56
1:C:90:PRO:HD2	1:C:109:LEU:HD22	1.87	0.56
1:B:233:PRO:HG3	1:B:417:SER:HB3	1.86	0.56
1:A:333:ARG:NH2	2:D:321:TYR:O	2.39	0.56
2:E:151:SER:OG	2:E:152:GLY:N	2.37	0.56
1:C:244:GLN:NE2	8:C:702:HOH:O	2.33	0.56
2:D:133:SER:OG	2:D:421:ARG:NH1	2.39	0.56
1:A:340:GLU:OE1	2:D:279:THR:OG1	2.23	0.56
1:C:494:LYS:O	1:C:498:GLU:HB3	2.07	0.56
2:F:439:ARG:NH1	2:F:451:ASP:OD1	2.37	0.55
1:B:135:ILE:HD13	1:B:148:LYS:HD3	1.88	0.55
2:D:91:ASP:OD1	2:D:95:ARG:N	2.40	0.55
2:E:153:SER:O	2:E:331:ARG:NH2	2.40	0.55
1:A:416:ASP:O	1:A:427:SER:OG	2.24	0.55
1:A:514:SER:H	1:A:517:LYS:HD2	1.70	0.55
1:C:85:ASP:OD2	1:C:89:ARG:NH2	2.39	0.55
2:D:242:HIS:HA	2:D:297:SER:HB3	1.89	0.55
2:F:182:ALA:HB3	2:F:247:MET:HG2	1.89	0.55
1:A:214:ARG:NH1	1:A:513:THR:OG1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:PRO:HG3	1:C:286:MET:HG3	1.88	0.55
3:G:105:MET:HB3	3:G:144:LEU:HD21	1.89	0.55
2:D:176:ASP:OD2	2:D:176:ASP:N	2.40	0.55
1:B:41:GLU:OE1	1:B:43:ARG:NH1	2.40	0.54
3:G:26:HIS:NE2	3:G:171:GLU:OE1	2.40	0.54
2:E:196:GLU:OE2	2:E:200:GLN:NE2	2.40	0.54
2:D:141:LEU:HD21	2:D:299:THR:HG21	1.89	0.54
2:D:328:ILE:HD12	2:D:346:PRO:HB2	1.89	0.54
1:C:201:GLN:HG2	1:C:373:ILE:HD11	1.89	0.54
1:C:375:LEU:O	1:C:380:ARG:NH2	2.41	0.54
1:B:416:ASP:O	1:B:427:SER:OG	2.24	0.54
1:B:41:GLU:HB2	1:B:48:SER:HB2	1.89	0.54
2:D:81:VAL:O	2:D:106:GLU:N	2.39	0.54
4:H:29:THR:OG1	4:H:32:GLU:HB3	2.08	0.54
2:E:5:TYR:CE2	2:E:21:VAL:HA	2.38	0.53
2:F:1:MET:H2	2:F:2:ILE:HA	1.73	0.53
2:F:290:ARG:NH1	2:F:295:LYS:O	2.42	0.53
1:A:259:CYS:HA	8:A:602:HOH:O	2.08	0.53
2:D:454:LEU:HD12	2:D:455:PRO:HD2	1.88	0.53
2:F:219:ILE:HD12	2:F:260:ILE:HD11	1.91	0.53
3:G:51:ARG:NH2	4:H:52:GLU:OE1	2.42	0.53
1:C:174:CYS:SG	1:C:175:VAL:N	2.82	0.53
1:A:535:ALA:HB3	1:A:542:PHE:HE1	1.74	0.53
1:C:8:LYS:HD3	1:C:15:MET:HG3	1.91	0.53
2:D:84:ASP:O	2:D:88:ARG:NH2	2.42	0.53
1:A:294:ASN:HB2	8:A:602:HOH:O	2.09	0.53
1:C:214:ARG:N	1:C:503:GLN:OE1	2.32	0.52
2:E:24:VAL:HG23	2:E:47:VAL:HG21	1.92	0.52
2:D:249:ASP:OD1	2:D:250:MET:N	2.42	0.52
2:F:330:THR:HG22	2:F:332:GLU:H	1.74	0.52
1:C:463:ILE:HG22	1:C:493:ALA:HB2	1.91	0.52
1:C:434:TYR:CE2	2:D:154:GLY:HA3	2.45	0.52
2:F:181:PHE:HB3	2:F:209:MET:HG2	1.92	0.52
1:C:412:PHE:HB3	1:C:434:TYR:CE1	2.44	0.52
2:E:332:GLU:OE1	2:E:332:GLU:N	2.41	0.52
2:F:151:SER:OG	2:F:152:GLY:N	2.43	0.52
3:G:105:MET:HB2	3:G:148:GLU:HG3	1.90	0.52
2:F:386:ALA:HB2	2:F:394:LEU:HD11	1.91	0.52
3:G:40:PHE:CE2	3:G:44:ILE:HD11	2.45	0.52
4:H:17:PHE:HB3	4:H:22:PHE:HD2	1.74	0.52
1:A:517:LYS:HE3	1:A:564:GLU:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:542:PHE:HA	1:C:545:ILE:HD12	1.90	0.51
2:F:406:GLU:HG2	2:F:410:ASN:HD21	1.76	0.51
1:C:549:THR:O	1:C:552:VAL:N	2.43	0.51
2:D:345:LEU:HB2	2:D:346:PRO:HD3	1.93	0.51
2:F:385:LEU:HD11	2:F:389:LEU:HD22	1.92	0.51
3:G:90:ILE:HG21	3:G:144:LEU:HD11	1.93	0.51
2:D:376:TYR:OH	2:D:409:GLU:OE2	2.18	0.51
1:A:152:PRO:HD2	1:A:155:ILE:HD11	1.92	0.51
1:A:189:GLN:HE21	1:A:316:TYR:HE1	1.59	0.51
1:A:552:VAL:HG21	1:A:577:ILE:HD13	1.93	0.51
1:B:262:ARG:NH1	8:B:701:HOH:O	2.44	0.51
2:F:454:LEU:HD23	2:F:455:PRO:HD2	1.93	0.51
1:A:465:GLN:O	1:A:469:GLN:NE2	2.43	0.50
1:C:575:GLU:HA	1:C:578:LYS:HD2	1.93	0.50
1:A:406:LEU:HA	1:A:409:VAL:HG22	1.93	0.50
1:A:484:ASP:HA	1:A:487:ARG:HB3	1.92	0.50
1:C:24:ILE:HD13	2:D:11:VAL:HG11	1.93	0.50
2:D:155:LEU:O	2:D:157:HIS:N	2.44	0.50
3:G:136:PHE:HZ	4:H:17:PHE:HA	1.76	0.50
1:C:342:SER:HB2	1:C:355:PRO:HG3	1.93	0.50
2:E:412:TYR:O	2:E:421:ARG:NH1	2.43	0.50
1:A:482:LEU:H	1:A:482:LEU:HD22	1.77	0.50
1:C:197:ARG:HH12	1:C:316:TYR:HD1	1.60	0.50
1:A:499:ASP:OD1	1:A:500:TYR:N	2.45	0.50
3:G:48:ASN:O	3:G:52:GLN:HG2	2.12	0.50
1:C:425:PHE:HB3	6:C:602:ADP:C6	2.47	0.49
4:H:33:ILE:O	4:H:36:THR:OG1	2.26	0.49
2:D:158:LYS:HB2	2:D:194:PHE:HE1	1.77	0.49
1:C:267:THR:HG21	2:F:121:ARG:HD2	1.95	0.49
4:H:50:ILE:O	4:H:76:ILE:N	2.45	0.49
1:C:497:ARG:HA	1:C:501:LEU:HB2	1.94	0.49
2:F:450:LEU:HB3	2:F:454:LEU:HD12	1.93	0.49
3:G:141:PRO:HG2	3:G:142:LYS:NZ	2.27	0.49
1:A:471:ASN:HA	1:A:474:VAL:HG12	1.95	0.49
1:C:303:ARG:HD2	1:C:337:ALA:HB2	1.95	0.49
2:E:255:GLU:OE2	2:E:273:TYR:OH	2.25	0.49
2:F:9:LYS:HG2	2:F:10:GLU:HG3	1.95	0.49
3:G:8:THR:HB	3:G:11:GLU:HB3	1.95	0.49
1:B:203:LEU:HB2	1:B:371:ARG:HB3	1.95	0.48
1:A:285:LEU:HD11	1:A:288:ARG:HH21	1.78	0.48
1:B:378:ASP:OD1	1:B:378:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:PHE:HB2	2:F:350:ARG:NH2	2.27	0.48
2:D:408:PHE:O	2:D:412:TYR:HB3	2.13	0.48
1:B:348:MET:HE1	2:F:266:GLU:O	2.13	0.48
2:F:79:LEU:HD13	2:F:227:MET:HE3	1.96	0.48
3:G:11:GLU:O	3:G:14:ARG:HG2	2.13	0.48
1:C:453:TRP:HZ3	1:C:519:PHE:HA	1.77	0.48
2:F:126:GLU:HB2	2:F:143:ARG:HG2	1.94	0.48
4:H:34:ARG:O	4:H:38:ASP:N	2.42	0.48
4:H:49:TYR:HD1	4:H:76:ILE:HD11	1.78	0.48
1:C:90:PRO:HB2	1:C:93:THR:HB	1.96	0.48
2:E:137:HIS:HD2	2:E:365:HIS:CD2	2.31	0.48
2:F:106:GLU:OE1	2:F:234:TYR:OH	2.29	0.48
1:A:244:GLN:OE1	1:A:248:TRP:NE1	2.46	0.48
2:D:29:LEU:HD21	2:D:77:LEU:HG	1.96	0.48
2:E:338:ILE:HG23	2:E:414:ASN:HB2	1.96	0.48
2:D:428:ASP:HA	2:D:431:TRP:HD1	1.79	0.48
2:D:151:SER:OG	2:D:152:GLY:N	2.47	0.47
3:G:45:ARG:O	3:G:48:ASN:ND2	2.47	0.47
2:D:361:THR:HG22	2:D:423:ILE:HG12	1.96	0.47
2:F:450:LEU:O	2:F:454:LEU:HB2	2.15	0.47
3:G:139:LEU:HB3	3:G:143:LEU:HG	1.96	0.47
1:A:581:ILE:O	1:A:585:VAL:N	2.48	0.47
1:C:193:VAL:HG11	1:C:309:THR:HG22	1.96	0.47
2:D:307:PRO:HG2	2:D:313:HIS:CE1	2.50	0.47
1:C:452:ASP:N	1:C:452:ASP:OD2	2.44	0.47
2:D:155:LEU:O	2:D:157:HIS:ND1	2.47	0.47
1:B:281:THR:HG23	1:B:283:GLU:H	1.78	0.47
1:A:295:THR:OG1	1:A:298:MET:HG3	2.15	0.47
1:C:527:THR:O	1:C:531:GLU:HG2	2.14	0.47
4:H:49:TYR:CD1	4:H:76:ILE:HD11	2.50	0.47
1:C:108:GLN:OE1	1:C:109:LEU:N	2.48	0.47
1:A:465:GLN:HG3	1:A:469:GLN:HE22	1.80	0.47
1:C:214:ARG:HH11	1:C:513:THR:HG21	1.80	0.47
1:C:96:GLU:O	1:C:99:GLN:NE2	2.35	0.47
1:C:234:PHE:HB3	2:F:321:TYR:CD1	2.50	0.47
1:B:2:GLN:HE22	1:B:20:SER:HB2	1.80	0.47
1:C:218:THR:HG22	1:C:457:VAL:HG23	1.96	0.47
2:F:261:SER:HB2	2:F:274:PRO:HG3	1.97	0.47
2:F:40:ARG:HH12	2:F:61:SER:N	2.13	0.47
1:C:430:TRP:CD1	1:C:431:ILE:HD12	2.50	0.46
2:D:382:ALA:HA	2:D:385:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:121:ARG:NH2	2:D:286:GLU:O	2.49	0.46
2:D:386:ALA:HA	2:D:394:LEU:HD11	1.96	0.46
2:E:362:ARG:HG2	2:E:427:LEU:HD13	1.97	0.46
2:F:412:TYR:HE1	2:F:426:THR:HG23	1.80	0.46
3:G:88:VAL:HG21	4:H:20:PHE:CD1	2.48	0.46
1:C:231:PRO:HA	1:C:390:VAL:O	2.15	0.46
2:D:166:ARG:HH22	2:D:418:TYR:HA	1.81	0.46
2:F:340:PRO:HB3	2:F:417:PHE:HE1	1.79	0.46
2:F:446:LYS:HB2	2:F:449:LEU:CB	2.46	0.46
2:E:248:THR:HB	2:E:303:ILE:HB	1.98	0.46
2:E:454:LEU:HD12	2:E:455:PRO:HD2	1.97	0.46
3:G:156:MET:O	3:G:160:ILE:HG12	2.16	0.46
3:G:37:MET:O	3:G:41:ILE:HG12	2.15	0.46
1:C:329:ASP:HA	1:C:330:SER:HA	1.56	0.46
1:C:436:LEU:HD11	2:D:154:GLY:HA2	1.97	0.46
2:E:16:MET:HB3	2:E:54:VAL:HG23	1.97	0.46
1:C:400:PRO:O	1:C:404:ASN:ND2	2.47	0.46
2:D:11:VAL:HG22	2:D:16:MET:HG3	1.98	0.46
3:G:14:ARG:NH1	3:G:18:GLN:OE1	2.49	0.46
2:D:284:LEU:HA	2:D:287:ARG:HD2	1.97	0.46
1:B:38:GLU:OE1	1:B:52:TYR:OH	2.30	0.45
1:B:56:SER:O	1:B:105:ARG:NH2	2.38	0.45
1:C:42:MET:HG2	2:D:65:LEU:HD13	1.97	0.45
2:D:86:ILE:HA	2:D:208:VAL:HG22	1.98	0.45
2:F:44:VAL:HA	2:F:54:VAL:HG12	1.98	0.45
1:A:197:ARG:HA	1:A:198:PRO:HD3	1.87	0.45
1:A:445:MET:O	1:A:449:LEU:HB2	2.16	0.45
1:C:333:ARG:NH1	1:C:336:GLU:OE2	2.49	0.45
6:C:602:ADP:O3B	2:F:350:ARG:NH1	2.45	0.45
2:D:87:GLY:HA2	2:D:204:ILE:O	2.17	0.45
1:A:169:ILE:O	1:A:186:THR:HB	2.17	0.45
1:B:8:LYS:HG3	2:E:48:GLN:HB3	1.97	0.45
2:E:138:LEU:HA	2:E:369:MET:HG3	1.99	0.45
1:C:91:LEU:HD23	2:F:118:PRO:HD2	1.98	0.45
1:C:268:ASP:OD1	2:F:354:LYS:NZ	2.49	0.45
1:A:274:PRO:HG3	1:A:286:MET:HG3	1.99	0.45
1:A:80:ILE:HA	1:A:290:VAL:HG22	1.98	0.45
1:C:295:THR:OG1	1:C:298:MET:HG3	2.17	0.45
2:D:10:GLU:HB2	2:D:17:ALA:HB3	1.98	0.45
2:E:4:GLU:C	2:E:5:TYR:HD1	2.20	0.45
2:F:170:VAL:HG13	2:F:173:SER:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:306:MET:HG2	2:F:316:PRO:HB3	1.99	0.45
2:F:330:THR:HB	2:F:333:LEU:HD23	1.99	0.45
2:F:446:LYS:HB2	2:F:449:LEU:HB2	1.98	0.45
1:C:279:PRO:HA	1:C:281:THR:N	2.32	0.45
2:D:158:LYS:HB2	2:D:194:PHE:CE1	2.52	0.45
1:C:356:ALA:HB1	2:D:259:GLU:HA	1.98	0.45
1:B:197:ARG:HA	1:B:198:PRO:HD3	1.84	0.45
1:C:371:ARG:HA	1:C:383:SER:HA	1.99	0.45
2:E:29:LEU:HD23	2:E:73:LEU:HD12	1.98	0.45
2:E:150:PHE:HB2	2:E:328:ILE:HD13	1.99	0.45
2:F:250:MET:HB3	2:F:304:LEU:HB3	1.98	0.45
1:C:421:GLN:HG3	2:F:345:LEU:HB3	1.99	0.45
2:F:437:LEU:HD12	2:F:438:PRO:HD2	1.98	0.45
3:G:35:GLU:HB2	3:G:38:ARG:NH2	2.32	0.45
1:B:169:ILE:HB	1:B:188:MET:HB2	1.99	0.45
1:C:496:ILE:HG12	1:C:525:ILE:HD13	1.98	0.45
1:C:524:VAL:O	1:C:527:THR:OG1	2.34	0.45
1:B:231:PRO:HG2	1:B:412:PHE:HE1	1.81	0.44
1:B:90:PRO:HD3	1:B:111:ALA:HA	1.97	0.44
1:A:120:PHE:HE2	1:A:162:ILE:HD11	1.82	0.44
2:F:291:ILE:HD11	2:F:294:LEU:HD22	1.98	0.44
3:G:92:VAL:HG12	3:G:105:MET:HA	1.99	0.44
1:A:342:SER:HB2	1:A:355:PRO:HG3	2.00	0.44
1:B:329:ASP:HA	1:B:330:SER:HA	1.61	0.44
1:C:580:THR:HG23	1:C:581:ILE:HD12	1.98	0.44
2:F:236:ALA:O	2:F:296:GLY:HA3	2.18	0.44
3:G:40:PHE:O	3:G:44:ILE:HG13	2.17	0.44
4:H:12:ASP:OD1	4:H:12:ASP:N	2.50	0.44
1:A:40:ILE:HG22	1:A:41:GLU:HG3	1.98	0.44
1:A:329:ASP:HA	1:A:330:SER:HA	1.54	0.44
2:D:381:GLN:HA	2:D:384:GLU:HG2	1.99	0.44
2:E:307:PRO:HG2	2:E:313:HIS:CE1	2.52	0.44
4:H:30:LYS:HA	4:H:57:LEU:HB3	1.99	0.44
1:C:522:LEU:O	1:C:525:ILE:HG13	2.18	0.44
2:F:353:ASP:OD1	2:F:354:LYS:HE3	2.18	0.44
3:G:141:PRO:HG2	3:G:142:LYS:HZ3	1.83	0.44
3:G:51:ARG:NH1	4:H:75:LEU:O	2.51	0.44
1:C:492:VAL:O	1:C:496:ILE:HG13	2.17	0.44
1:C:41:GLU:HB2	2:D:11:VAL:O	2.18	0.44
2:F:251:THR:O	2:F:255:GLU:HG2	2.18	0.44
2:F:338:ILE:HG23	2:F:414:ASN:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASP:N	1:A:140:ASP:OD1	2.51	0.43
2:D:250:MET:HB2	2:D:304:LEU:HB3	1.99	0.43
2:E:13:GLY:O	2:E:60:THR:OG1	2.22	0.43
2:E:87:GLY:HA2	2:E:204:ILE:O	2.18	0.43
2:D:137:HIS:HD2	2:D:365:HIS:CD2	2.36	0.43
2:F:106:GLU:OE1	2:F:239:LYS:NZ	2.51	0.43
1:B:410:LYS:HB3	1:B:436:LEU:HB2	1.99	0.43
2:F:438:PRO:HB2	2:F:440:THR:HG22	2.01	0.43
1:C:209:MET:HG2	1:C:224:LYS:HG3	1.99	0.43
2:E:448:ASP:OD1	2:E:449:LEU:N	2.52	0.43
2:F:34:MET:HB2	2:F:36:ASN:OD1	2.18	0.43
1:C:416:ASP:OD2	1:C:418:SER:OG	2.37	0.43
2:D:229:LEU:HG	2:D:287:ARG:HD3	2.01	0.43
2:F:91:ASP:OD1	2:F:95:ARG:N	2.39	0.43
3:G:158:GLU:O	3:G:162:LYS:HG2	2.19	0.43
3:G:44:ILE:HD13	4:H:94:VAL:HG23	2.00	0.43
3:G:95:LYS:N	3:G:102:VAL:O	2.51	0.43
1:A:218:THR:HG23	1:A:457:VAL:HG22	1.99	0.43
1:C:545:ILE:HG23	1:C:581:ILE:HD11	2.00	0.43
1:A:300:VAL:HA	1:A:303:ARG:HE	1.82	0.43
1:A:465:GLN:HG3	1:A:469:GLN:NE2	2.34	0.43
2:D:146:LYS:HD3	2:D:285:PHE:O	2.18	0.43
1:A:562:ILE:HA	1:A:563:PRO:HD3	1.88	0.43
1:B:241:VAL:O	1:B:245:ILE:HG12	2.18	0.43
1:B:247:LYS:HA	1:B:285:LEU:HD11	1.99	0.43
1:B:84:PHE:HB3	1:B:88:GLN:HA	1.99	0.43
1:C:454:SER:O	1:C:458:THR:OG1	2.37	0.43
2:D:138:LEU:HD23	2:D:369:MET:HG3	2.01	0.43
2:E:440:THR:O	2:E:443:LYS:NZ	2.37	0.43
1:B:453:TRP:HZ3	1:B:519:PHE:HA	1.83	0.43
3:G:136:PHE:CZ	4:H:17:PHE:HA	2.54	0.43
1:A:574:ASN:O	1:A:577:ILE:HG22	2.19	0.42
1:A:445:MET:HA	1:A:448:ILE:HG22	2.02	0.42
2:D:144:GLY:HA2	2:D:298:VAL:O	2.19	0.42
2:D:142:VAL:HG13	2:D:145:GLN:HB2	2.01	0.42
2:E:176:ASP:N	2:E:176:ASP:OD1	2.52	0.42
2:E:88:ARG:NH2	2:E:98:ASP:OD2	2.52	0.42
2:E:356:THR:HG22	2:E:365:HIS:CE1	2.54	0.42
2:E:352:LYS:O	2:E:356:THR:HG23	2.19	0.42
2:F:57:PHE:HA	2:F:219:ILE:HB	2.01	0.42
1:C:473:ILE:O	1:C:477:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:VAL:O	1:A:288:ARG:NH1	2.52	0.42
1:B:180:GLN:N	1:B:180:GLN:OE1	2.52	0.42
1:A:103:LEU:N	2:D:115:VAL:O	2.50	0.42
2:D:397:ILE:O	2:D:400:ILE:HG22	2.19	0.42
1:C:24:ILE:HD12	2:D:63:ILE:HB	2.02	0.42
1:A:151:VAL:HA	1:A:152:PRO:HD3	1.91	0.42
1:A:73:VAL:HG11	1:A:309:THR:HG23	2.00	0.42
2:F:30:ILE:HD13	2:F:54:VAL:HG11	2.02	0.42
1:B:545:ILE:O	1:B:549:THR:OG1	2.34	0.42
2:E:159:GLU:N	2:E:159:GLU:OE1	2.48	0.42
2:E:388:VAL:HG13	2:E:389:LEU:HD13	2.01	0.42
3:G:193:GLU:O	3:G:197:VAL:HG23	2.20	0.42
1:A:554:GLU:HG2	1:A:555:ARG:HG3	2.02	0.42
2:E:386:ALA:O	2:E:390:GLY:N	2.53	0.42
2:F:123:TYR:HA	2:F:124:PRO:HD3	1.85	0.42
2:F:29:LEU:HD13	2:F:77:LEU:HD13	2.02	0.42
3:G:53:ALA:O	3:G:57:GLU:HG2	2.20	0.42
1:C:221:PRO:O	1:C:435:SER:OG	2.35	0.42
2:E:148:PRO:HD3	2:E:323:THR:HB	2.02	0.42
2:F:49:GLU:HB3	2:F:50:ASP:H	1.50	0.42
1:C:197:ARG:HA	1:C:198:PRO:HD3	1.84	0.41
2:E:288:ALA:HB2	2:E:300:GLN:HG3	2.02	0.41
1:C:506:PHE:CE1	2:F:353:ASP:HB2	2.55	0.41
1:A:24:ILE:HG22	1:A:25:GLN:HG2	2.01	0.41
1:A:534:LYS:O	1:A:538:LEU:HG	2.20	0.41
1:B:315:GLU:HA	1:B:384:ILE:HD11	2.01	0.41
1:C:208:PRO:HG3	1:C:441:VAL:HG22	2.02	0.41
1:C:449:LEU:HD23	1:C:449:LEU:HA	1.90	0.41
2:D:82:SER:HB2	2:D:105:PRO:HA	2.01	0.41
4:H:85:ILE:O	4:H:89:GLU:HG2	2.20	0.41
1:A:211:THR:OG1	1:A:217:ASP:OD2	2.36	0.41
1:B:371:ARG:NH1	1:B:381:GLU:OE1	2.53	0.41
1:B:203:LEU:N	1:B:371:ARG:O	2.44	0.41
1:C:120:PHE:HA	1:C:139:VAL:HG22	2.03	0.41
2:F:369:MET:HG3	2:F:370:ASN:N	2.34	0.41
1:A:576:GLU:O	1:A:580:THR:HG23	2.20	0.41
1:B:513:THR:HG23	1:B:517:LYS:HD3	2.03	0.41
1:B:453:TRP:CZ3	1:B:519:PHE:HA	2.55	0.41
1:B:83:MET:HG2	1:B:91:LEU:HD12	2.01	0.41
2:D:135:ILE:O	2:D:140:THR:HA	2.21	0.41
1:C:406:LEU:HA	1:C:409:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:GLY:N	2:D:299:THR:OG1	2.53	0.41
2:D:448:ASP:O	2:D:452:LYS:HB2	2.21	0.41
1:A:77:PRO:HG2	1:A:187:MET:HE2	2.02	0.41
1:A:267:THR:HA	1:A:270:VAL:HB	2.02	0.41
1:B:493:ALA:O	1:B:497:ARG:HG3	2.20	0.41
1:C:517:LYS:HE2	1:C:521:MET:CE	2.51	0.41
2:E:168:ALA:O	2:E:206[A]:ARG:NH2	2.53	0.41
2:E:291:ILE:HB	2:E:294:LEU:HD12	2.01	0.41
2:F:161:ALA:HB2	2:F:303:ILE:HD11	2.02	0.41
3:G:17:LYS:O	3:G:20:THR:HG22	2.20	0.41
3:G:94:GLU:HG3	3:G:101:LYS:HE3	2.01	0.41
1:C:506:PHE:N	1:C:506:PHE:HD2	2.19	0.41
1:C:453:TRP:CZ3	1:C:519:PHE:HA	2.56	0.41
1:A:308:TYR:HA	1:A:311:ILE:HG22	2.03	0.41
1:B:126:GLU:HG2	1:B:162:ILE:HG22	2.03	0.41
2:D:280:ASN:O	2:D:283:THR:OG1	2.39	0.41
2:D:313:HIS:CE1	2:D:315:ILE:HG12	2.56	0.41
2:E:361:THR:HG23	2:E:423:ILE:HG12	2.03	0.41
1:A:231:PRO:O	1:A:415:LEU:HB2	2.21	0.41
1:A:415:LEU:HA	1:A:427:SER:O	2.21	0.41
1:A:549:THR:OG1	1:A:553:ARG:NH1	2.54	0.41
1:C:245:ILE:O	1:C:249:SER:HB2	2.20	0.41
2:D:146:LYS:O	2:D:323:THR:HB	2.20	0.41
3:G:135:GLY:O	3:G:139:LEU:HD13	2.21	0.41
2:D:229:LEU:HD13	2:D:229:LEU:HA	1.91	0.41
2:F:26:TYR:CE2	2:F:27:GLU:HG3	2.55	0.41
1:B:208:PRO:HA	1:B:223:THR:HA	2.03	0.40
2:E:339:GLN:HA	2:E:340:PRO:HA	1.89	0.40
2:F:45:LEU:HD11	2:F:55:GLN:HB3	2.02	0.40
1:C:83:MET:HA	1:C:291:LEU:HB2	2.02	0.40
1:C:560:LYS:HE3	1:C:560:LYS:HB2	1.91	0.40
2:D:389:LEU:HD22	3:G:32:LYS:HD2	2.03	0.40
3:G:52:GLN:HG3	3:G:53:ALA:H	1.86	0.40
1:C:294:ASN:HA	1:C:298:MET:SD	2.61	0.40
1:A:205:PRO:HB2	1:A:223:THR:OG1	2.21	0.40
1:A:251:VAL:HG11	1:A:325:ALA:HB2	2.02	0.40
1:B:304:GLU:HG3	1:B:334:TRP:HE1	1.87	0.40
2:E:239:LYS:HA	2:E:239:LYS:HD3	1.86	0.40
2:F:313:HIS:CG	2:F:314:PRO:HD2	2.57	0.40
2:F:34:MET:SD	2:F:63:ILE:HG12	2.61	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%)	556 (95%)	28 (5%)	1 (0%)	52 87
1	B	590/600 (98%)	570 (97%)	20 (3%)	0	100 100
1	C	584/600 (97%)	562 (96%)	22 (4%)	0	100 100
2	D	451/465 (97%)	431 (96%)	20 (4%)	0	100 100
2	E	453/465 (97%)	442 (98%)	10 (2%)	1 (0%)	52 87
2	F	453/465 (97%)	441 (97%)	11 (2%)	1 (0%)	52 87
3	G	158/217 (73%)	146 (92%)	11 (7%)	1 (1%)	30 72
4	H	93/115 (81%)	89 (96%)	3 (3%)	1 (1%)	17 60
All	All	3367/3527 (96%)	3237 (96%)	125 (4%)	5 (0%)	56 90

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	98	MET
2	F	353	ASP
4	H	23	ASP
2	E	124	PRO
1	A	477	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	461/511 (90%)	448 (97%)	13 (3%)	51 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	493/511 (96%)	487 (99%)	6 (1%)	78 92
1	C	462/511 (90%)	436 (94%)	26 (6%)	26 66
2	D	356/387 (92%)	344 (97%)	12 (3%)	44 79
2	E	373/387 (96%)	367 (98%)	6 (2%)	70 89
2	F	372/387 (96%)	364 (98%)	8 (2%)	60 86
3	G	141/198 (71%)	113 (80%)	28 (20%)	1 8
4	H	66/99 (67%)	57 (86%)	9 (14%)	5 22
All	All	2724/2991 (91%)	2616 (96%)	108 (4%)	38 76

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	84	PHE
1	A	131	SER
1	A	140	ASP
1	A	144	ILE
1	A	217	ASP
1	A	259	CYS
1	A	336	GLU
1	A	451	GLN
1	A	542	PHE
1	A	543	ASN
1	A	573	ILE
1	A	575	GLU
1	B	92	ASP
1	B	121	GLU
1	B	285	LEU
1	B	351	ASP
1	B	378	ASP
1	B	465	GLN
1	C	158	THR
1	C	163	GLU
1	C	202	LYS
1	C	267	THR
1	C	373	ILE
1	C	377	SER
1	C	391	SER
1	C	393	SER
1	C	431	ILE

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Mol	Chain	Res	Type
1	C	445	MET
1	C	450	GLN
1	C	452	ASP
1	C	458	THR
1	C	465	GLN
1	C	468	GLU
1	C	470	LEU
1	C	480	ASP
1	C	482	LEU
1	C	526	LEU
1	C	542	PHE
1	C	554	GLU
1	C	556	ILE
1	C	566	GLU
1	C	577	ILE
1	C	580	THR
1	C	585	VAL
2	D	102	GLU
2	D	127	PHE
2	D	171	LEU
2	D	176	ASP
2	D	335	LYS
2	D	363	GLU
2	D	385	LEU
2	D	397	ILE
2	D	401	TYR
2	D	407	ARG
2	D	447	ASP
2	D	450	LEU
2	E	102	GLU
2	E	126	GLU
2	E	171	LEU
2	E	172	ASP
2	E	352	LYS
2	E	381	GLN
2	F	171	LEU
2	F	239	LYS
2	F	308	GLU
2	F	321	TYR
2	F	352	LYS
2	F	436	MET
2	F	437	LEU

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Mol	Chain	Res	Type
2	F	454	LEU
3	G	4	ASN
3	G	6	ASN
3	G	10	MET
3	G	12	LEU
3	G	13	THR
3	G	17	LYS
3	G	20	THR
3	G	23	THR
3	G	24	ARG
3	G	34	ASP
3	G	35	GLU
3	G	48	ASN
3	G	56	LYS
3	G	58	THR
3	G	88	VAL
3	G	92	VAL
3	G	94	GLU
3	G	97	ILE
3	G	98	MET
3	G	99	SER
3	G	102	VAL
3	G	104	LEU
3	G	105	MET
3	G	107	PHE
3	G	129	LEU
3	G	139	LEU
3	G	142	LYS
3	G	143	LEU
4	H	12	ASP
4	H	26	HIS
4	H	29	THR
4	H	44	GLU
4	H	62	ILE
4	H	63	GLU
4	H	69	LEU
4	H	80	GLN
4	H	91	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	GLN
2	F	410	ASN
3	G	48	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
6	ADP	B	602	5	24,29,29	1.00	1 (4%)	23,45,45	1.70	1 (4%)
7	GOL	B	603	-	5,5,5	0.35	0	5,5,5	0.24	0
6	ADP	C	602	5	24,29,29	1.08	1 (4%)	23,45,45	2.00	3 (13%)
7	GOL	E	501	-	5,5,5	0.36	0	5,5,5	0.26	0

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
6	ADP	B	602	5	-	0/12/32/32	0/3/3/3
7	GOL	B	603	-	-	0/4/4/4	0/0/0/0
6	ADP	C	602	5	-	0/12/32/32	0/3/3/3
7	GOL	E	501	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	602	ADP	C5-C4	3.16	1.47	1.40
6	C	602	ADP	C5-C4	3.52	1.48	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	602	ADP	N3-C2-N1	-7.84	122.71	128.87
6	B	602	ADP	N3-C2-N1	-6.48	123.78	128.87
6	C	602	ADP	C2'-C1'-N9	-2.40	107.05	113.47
6	C	602	ADP	C2-N1-C6	2.30	122.87	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	602	ADP	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%)	0.15	29 (4%) 33 25	40, 81, 144, 184	0
1	B	592/600 (98%)	-0.11	4 (0%) 89 84	27, 54, 91, 124	0
1	C	586/600 (97%)	0.23	21 (3%) 46 37	41, 93, 152, 185	0
2	D	453/465 (97%)	0.07	4 (0%) 85 80	63, 90, 128, 144	0
2	E	454/465 (97%)	-0.20	2 (0%) 93 91	29, 54, 93, 159	0
2	F	455/465 (97%)	-0.06	5 (1%) 82 75	41, 76, 120, 145	0
3	G	164/217 (75%)	0.69	22 (13%) 4 3	71, 119, 183, 202	0
4	H	95/115 (82%)	1.67	30 (31%) 1 1	126, 157, 190, 203	0
All	All	3386/3527 (96%)	0.10	117 (3%) 48 38	27, 79, 149, 203	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	47	VAL	9.6
4	H	55	ALA	7.2
1	A	542	PHE	5.9
1	C	520	ASN	5.3
4	H	54	CYS	5.1
3	G	94	GLU	4.7
1	A	545	ILE	4.7
4	H	46	GLY	4.7
3	G	136	PHE	4.3
4	H	49	TYR	4.1
4	H	77	PRO	4.0
1	A	101	ASN	4.0
2	D	455	PRO	4.0
4	H	43	ASN	3.9
3	G	106	ASN	3.8
4	H	78	SER	3.8

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Mol	Chain	Res	Type	RSRZ
4	H	85	ILE	3.7
4	H	53	GLN	3.6
1	C	163	GLU	3.6
1	C	577	ILE	3.6
4	H	72	ALA	3.5
1	A	541	TYR	3.5
1	C	582	GLN	3.5
1	C	136	ILE	3.5
4	H	27	GLY	3.4
1	A	540	ALA	3.4
4	H	23	ASP	3.4
3	G	96	ASN	3.4
4	H	81	GLY	3.3
2	F	455	PRO	3.3
3	G	105	MET	3.2
1	A	485	ASN	3.2
1	A	566	GLU	3.2
4	H	89	GLU	3.2
4	H	12	ASP	3.1
1	B	123	THR	3.0
1	A	160	GLN	3.0
2	D	237	TYR	2.9
1	A	586	SER	2.9
1	A	549	THR	2.9
1	A	577	ILE	2.9
1	B	128	THR	2.9
3	G	102	VAL	2.8
4	H	74	ILE	2.8
3	G	95	LYS	2.8
1	A	481	SER	2.8
4	H	31	THR	2.8
2	E	7	THR	2.7
1	A	477	VAL	2.7
1	A	140	ASP	2.7
4	H	98	VAL	2.7
3	G	59	GLN	2.7
4	H	19	LEU	2.6
1	C	187	MET	2.6
1	C	581	ILE	2.6
1	A	581	ILE	2.6
1	C	524	VAL	2.6
1	A	478	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
3	G	58	THR	2.5
1	A	492	VAL	2.5
1	C	525	ILE	2.5
1	A	486	ASP	2.5
1	A	182	LEU	2.4
4	H	56	ASN	2.4
3	G	130	ASP	2.4
3	G	91	SER	2.4
1	C	580	THR	2.4
1	B	130	VAL	2.4
1	C	516	GLU	2.4
1	A	538	LEU	2.4
3	G	140	LEU	2.4
1	C	189	GLN	2.4
4	H	71	PRO	2.4
2	D	176	ASP	2.4
1	C	118	TRP	2.3
3	G	166	ARG	2.3
4	H	22	PHE	2.3
3	G	104	LEU	2.3
1	A	394	GLY	2.3
3	G	54	ILE	2.3
2	F	364	ASP	2.3
4	H	25	GLN	2.3
3	G	55	GLU	2.3
1	A	499	ASP	2.3
4	H	88	GLU	2.2
3	G	93	VAL	2.2
3	G	98	MET	2.2
1	A	128	THR	2.2
1	A	173	ILE	2.2
1	A	582	GLN	2.2
3	G	143	LEU	2.2
2	F	454	LEU	2.2
3	G	13	THR	2.2
1	B	124	ILE	2.2
1	C	539	GLY	2.2
2	F	453	TYR	2.2
4	H	15	SER	2.2
1	C	507	ASP	2.1
4	H	10	ASP	2.1
2	E	393	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	531	GLU	2.1
1	C	124	ILE	2.1
1	A	501	LEU	2.1
1	A	482	LEU	2.1
3	G	139	LEU	2.1
4	H	21	GLY	2.1
1	A	548	GLY	2.1
1	C	165	GLY	2.1
4	H	86	GLY	2.1
2	F	433	LEU	2.1
1	C	527	THR	2.1
4	H	20	PHE	2.1
2	D	138	LEU	2.1
1	C	572	SER	2.1
1	C	452	ASP	2.0
1	C	500	TYR	2.0
3	G	189	LEU	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
7	GOL	E	501	6/6	0.88	0.29	3.23	62,63,63,64	0
5	MG	B	601	1/1	0.99	0.32	1.84	14,14,14,14	0
6	ADP	B	602	27/27	0.96	0.25	0.73	40,45,54,68	0
6	ADP	C	602	27/27	0.92	0.28	0.34	54,59,117,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	GOL	B	603	6/6	0.95	0.19	-0.35	55,58,60,61	0
5	MG	C	601	1/1	0.97	0.23	-2.41	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.