



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2016 – 12:34 PM EST

PDB ID : 5KND  
Title : Crystal structure of the Pi-bound V1 complex  
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Deposited on : 2016-06-28  
Resolution : 2.89 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](mailto: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.

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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

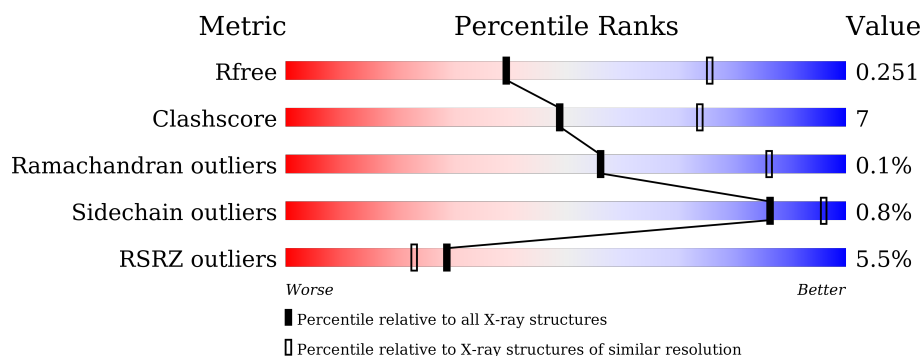
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	600	<div> <div>9%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	B	600	<div> <div>3%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	C	600	<div> <div>5%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
2	D	465	<div> <div>3%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
2	E	465	<div> <div>2%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>
2	F	465	<div> <div>2%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>

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

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 26416 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	586	Total	C	N	O	S	0	0	0
			4467	2810	750	881	26			
1	B	592	Total	C	N	O	S	0	0	0
			4549	2859	759	905	26			
1	C	586	Total	C	N	O	S	0	0	0
			4522	2841	756	899	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	452	Total	C	N	O	S	0	0	0
			3506	2227	598	667	14			
2	E	452	Total	C	N	O	S	0	0	0
			3526	2235	605	672	14			
2	F	455	Total	C	N	O	S	0	1	0
			3562	2262	607	678	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	178	Total	C	N	O	S	0	0	0
			1415	889	248	268	10			

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	102	Total	C	N	O	S	0	0	0
			762	480	128	152	2			

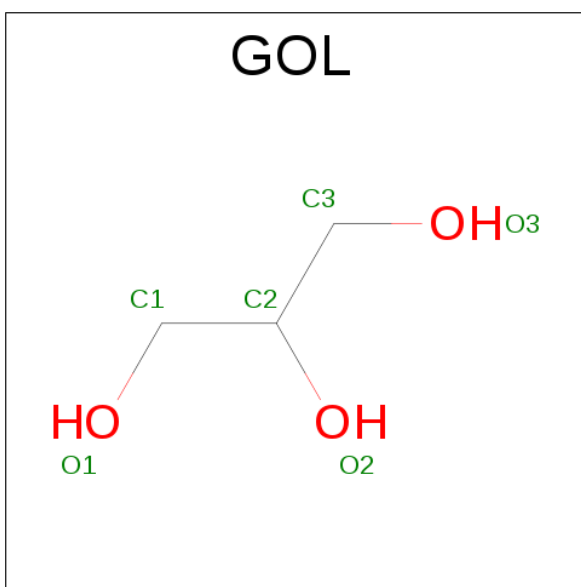
There are 12 discrepancies between the modelled and reference sequences:

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

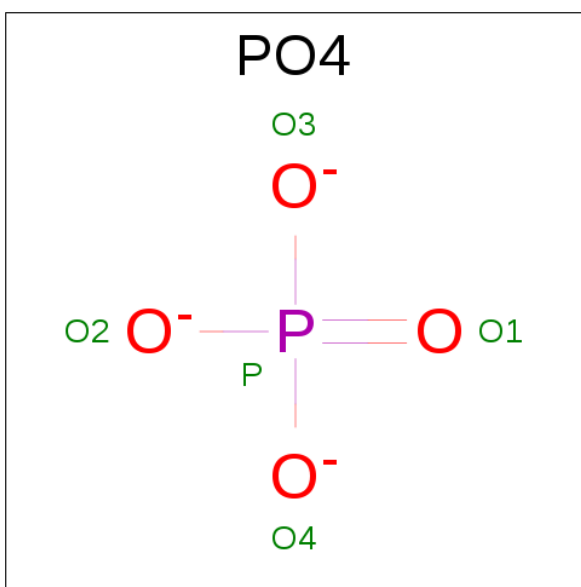
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



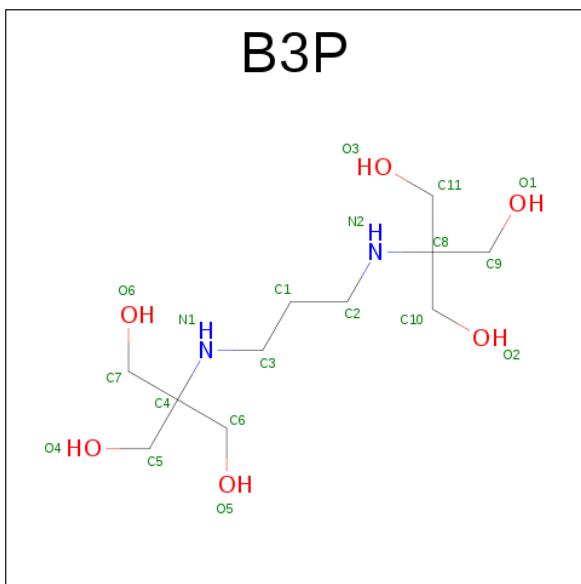
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula:  $C_{11}H_{26}N_2O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	F	1	Total	C	N	O	0	0
			19	11	2	6		

- Molecule 9 is water.

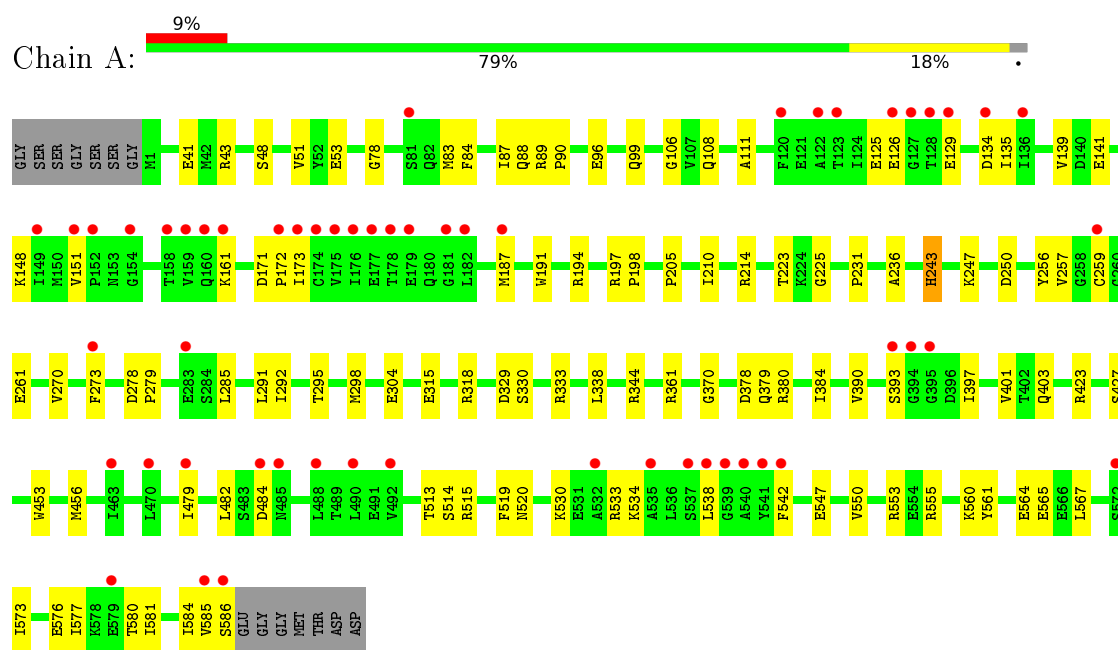
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	14	Total	O	0	0
			14	14		
9	B	14	Total	O	0	0
			14	14		
9	C	18	Total	O	0	0
			18	18		
9	D	2	Total	O	0	0
			2	2		
9	E	8	Total	O	0	0
			8	8		
9	F	5	Total	O	0	0
			5	5		
9	G	2	Total	O	0	0
			2	2		
9	H	1	Total	O	0	0
			1	1		



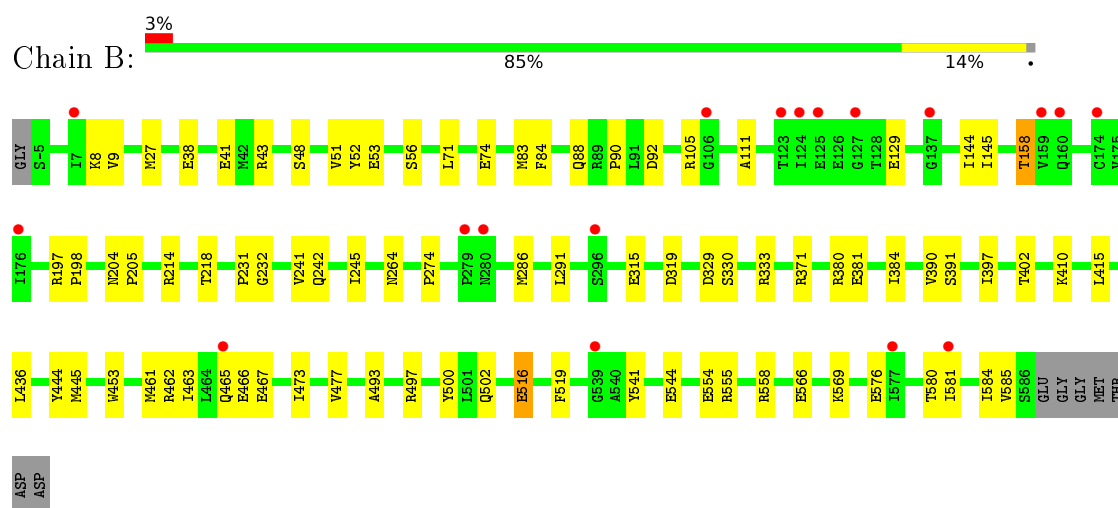
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

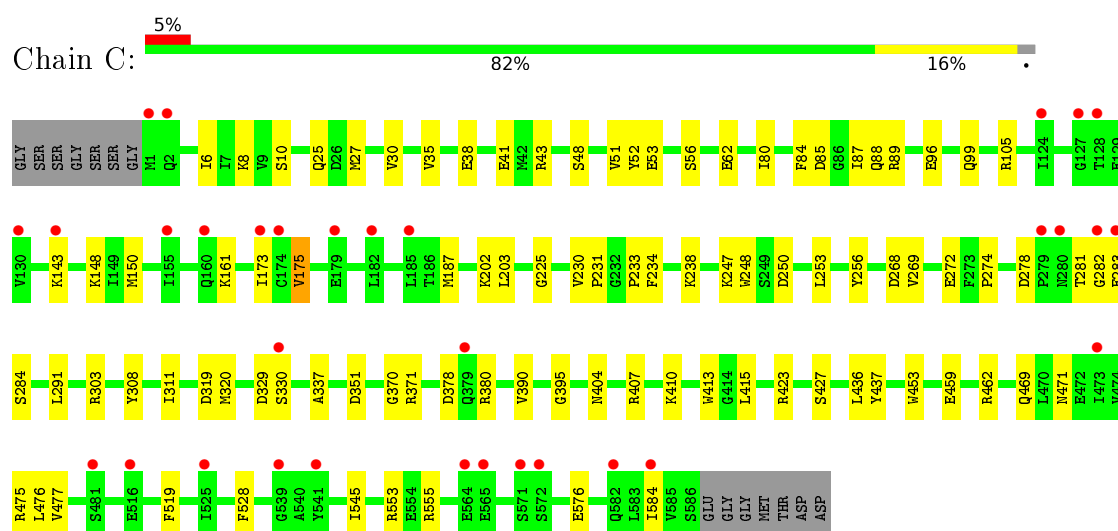
- Molecule 1: V-type sodium ATPase catalytic subunit A



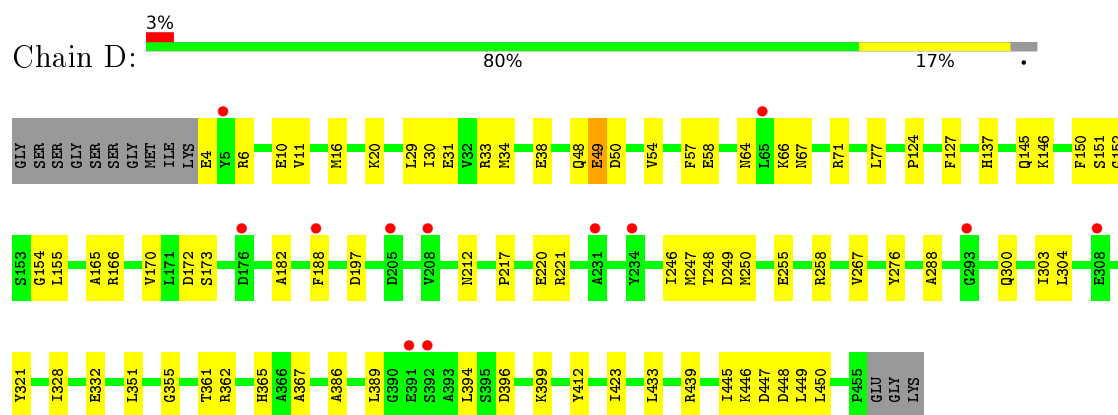
- Molecule 1: V-type sodium ATPase catalytic subunit A



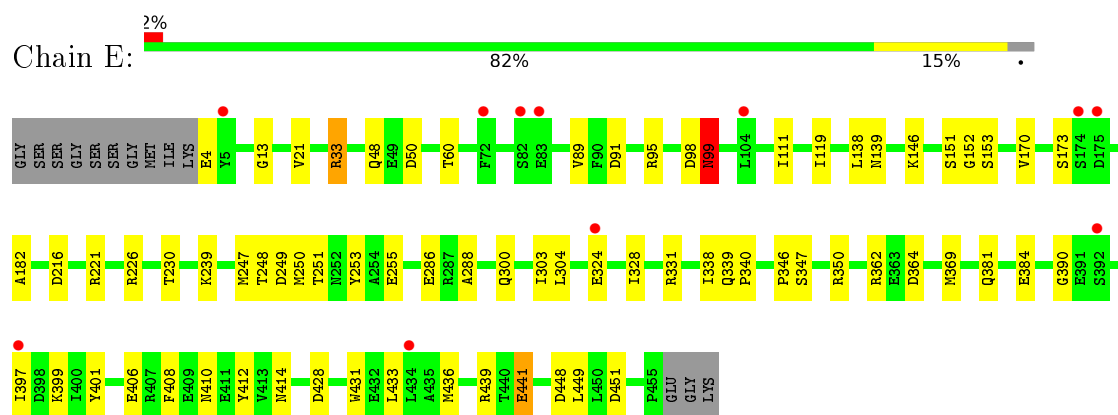
- Molecule 1: V-type sodium ATPase catalytic subunit A



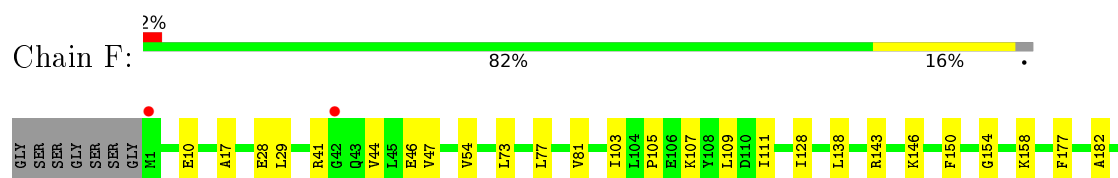
• Molecule 2: V-type sodium ATPase subunit B

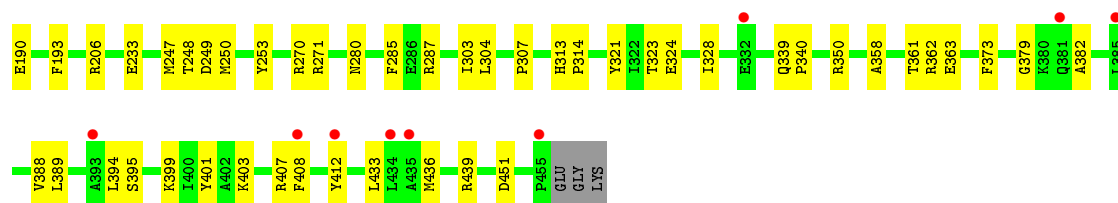


• Molecule 2: V-type sodium ATPase subunit B

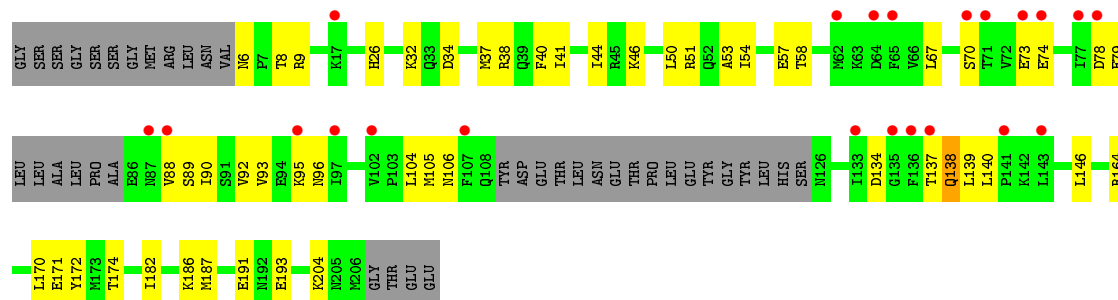


• Molecule 2: V-type sodium ATPase subunit B

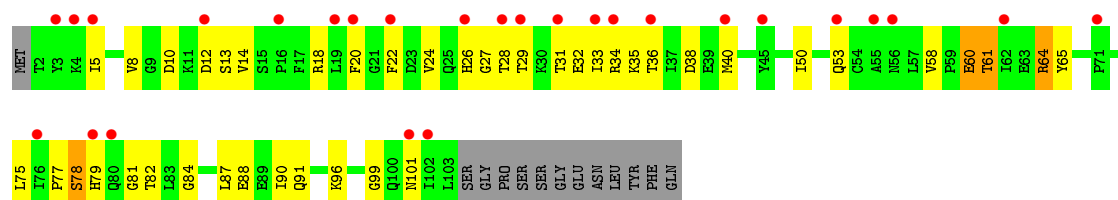




• Molecule 3: V-type sodium ATPase subunit D



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.22Å 128.35Å 228.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 2.89 49.04 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.04-2.89) 99.3 (49.04-2.89)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.206 , 0.251 0.207 , 0.251	Depositor DCC
$R_{free}$ test set	4213 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.5	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	26416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, B3P, MG

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	0.24	0/4543	0.43	0/6162
1	B	0.23	0/4625	0.40	0/6266
1	C	0.23	0/4598	0.40	0/6230
2	D	0.24	0/3569	0.45	0/4835
2	E	0.24	0/3589	0.44	1/4857 (0.0%)
2	F	0.22	0/3625	0.41	0/4903
3	G	0.27	0/1424	0.50	0/1908
4	H	0.37	0/774	0.61	0/1052
All	All	0.24	0/26747	0.43	1/36213 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	399	LYS	CA-CB-CG	5.15	124.72	113.40

There are no chirality outliers.

There are no planarity outliers.

### 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	4467	0	4331	68	0
1	B	4549	0	4449	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4522	0	4425	58	0
2	D	3506	0	3471	58	0
2	E	3526	0	3524	47	0
2	F	3562	0	3554	50	0
3	G	1415	0	1450	34	0
4	H	762	0	718	38	0
5	C	1	0	0	0	0
6	C	6	0	8	1	0
6	F	6	0	8	0	0
6	G	6	0	8	0	0
7	C	5	0	0	1	0
8	F	19	0	26	0	0
9	A	14	0	0	2	0
9	B	14	0	0	0	0
9	C	18	0	0	1	0
9	D	2	0	0	0	0
9	E	8	0	0	0	0
9	F	5	0	0	0	0
9	G	2	0	0	0	0
9	H	1	0	0	0	0
All	All	26416	0	25972	378	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 7.

All (378) 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:E:99:ASN:HD22	2:E:99:ASN:N	1.71	0.86
2:D:4:GLU:HG3	2:D:71:ARG:HG3	1.59	0.85
4:H:88:GLU:HA	4:H:91:GLN:HB3	1.58	0.85
2:E:99:ASN:H	2:E:99:ASN:HD22	1.19	0.84
1:A:295:THR:H	1:A:298:MET:HE3	1.44	0.82
2:D:367:ALA:HB1	2:D:445:ILE:HG22	1.62	0.81
1:B:333:ARG:HH12	1:B:391:SER:HB2	1.47	0.80
3:G:138:GLN:NE2	3:G:138:GLN:H	1.78	0.79
4:H:31:THR:OG1	4:H:34:ARG:NH1	2.18	0.77
2:E:153:SER:O	2:E:331:ARG:NH2	2.18	0.75
4:H:38:ASP:OD1	4:H:65:TYR:OH	2.04	0.75
1:B:554:GLU:O	1:B:558:ARG:NH1	2.21	0.74
1:C:404:ASN:OD1	1:C:407:ARG:NH1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:VAL:HG12	1:B:53:GLU:H	1.56	0.71
1:A:479:ILE:HD12	1:A:482:LEU:HD21	1.73	0.71
1:B:566:GLU:HB3	1:B:569:LYS:HE3	1.74	0.70
2:D:250:MET:HB2	2:D:304:LEU:HB3	1.74	0.70
2:F:270:ARG:HH21	2:F:271:ARG:HE	1.35	0.70
2:D:182:ALA:HB3	2:D:247:MET:HG2	1.73	0.69
1:C:281:THR:HG22	1:C:283:GLU:H	1.57	0.69
4:H:10:ASP:HA	4:H:26:HIS:HE1	1.58	0.68
1:A:397:ILE:O	1:A:403:GLN:NE2	2.27	0.68
2:E:182:ALA:HB3	2:E:247:MET:HG2	1.76	0.68
4:H:58:VAL:O	4:H:61:THR:OG1	2.10	0.68
1:A:333:ARG:NH2	9:A:601:HOH:O	2.27	0.68
2:E:4:GLU:OE1	2:E:33:ARG:NH2	2.27	0.67
3:G:54:ILE:HG21	3:G:146:LEU:HD22	1.77	0.67
2:E:362:ARG:NH2	2:E:428:ASP:OD1	2.26	0.67
1:A:261:GLU:OE2	1:A:330:SER:N	2.27	0.66
2:D:20:LYS:N	2:D:50:ASP:O	2.27	0.66
2:D:49:GLU:HG3	2:D:50:ASP:N	2.10	0.66
1:B:555:ARG:NH1	1:B:576:GLU:OE2	2.27	0.66
2:E:146:LYS:NZ	2:E:286:GLU:OE2	2.29	0.66
2:F:439:ARG:NH2	2:F:451:ASP:OD1	2.30	0.65
2:E:99:ASN:ND2	2:E:99:ASN:N	2.44	0.65
2:E:226:ARG:NH2	2:E:253:TYR:OH	2.30	0.64
1:A:173:ILE:HD13	1:A:187:MET:HG2	1.80	0.64
1:A:393:SER:HB2	2:D:321:TYR:OH	1.97	0.64
1:B:371:ARG:NH1	1:B:381:GLU:OE1	2.31	0.64
2:E:381:GLN:HA	2:E:384:GLU:HG2	1.81	0.63
2:F:407:ARG:NH1	2:F:436:MET:SD	2.72	0.63
4:H:77:PRO:HB3	4:H:82:THR:HG23	1.79	0.63
1:C:51:VAL:HG12	1:C:53:GLU:H	1.62	0.63
2:D:439:ARG:HG3	2:D:450:LEU:HD21	1.81	0.62
2:D:145:GLN:HG3	2:D:351:LEU:HD12	1.81	0.62
3:G:138:GLN:HE21	3:G:138:GLN:H	1.46	0.62
1:A:247:LYS:NZ	9:A:604:HOH:O	2.33	0.61
2:D:31:GLU:OE1	2:D:71:ARG:NH1	2.33	0.61
1:B:467:GLU:OE2	1:B:497:ARG:NH1	2.34	0.61
2:E:248:THR:HB	2:E:303:ILE:HB	1.83	0.61
4:H:78:SER:OG	4:H:79:HIS:N	2.34	0.61
2:D:446:LYS:HG3	2:D:449:LEU:H	1.65	0.61
3:G:90:ILE:HG23	4:H:5:ILE:HD11	1.83	0.61
3:G:134:ASP:O	3:G:138:GLN:NE2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:60:GLU:HG2	4:H:61:THR:N	2.15	0.61
1:C:555:ARG:NH1	1:C:576:GLU:OE2	2.35	0.60
2:D:288:ALA:HB2	2:D:300:GLN:HG3	1.84	0.59
4:H:22:PHE:O	4:H:24:VAL:HG23	2.02	0.59
3:G:73:GLU:N	3:G:74:GLU:HA	2.17	0.59
2:D:361:THR:HG22	2:D:362:ARG:H	1.66	0.59
2:D:447:ASP:HA	2:D:450:LEU:HB3	1.83	0.59
2:D:58:GLU:OE1	2:D:58:GLU:N	2.34	0.59
4:H:53:GLN:NE2	4:H:81:GLY:O	2.35	0.59
1:C:41:GLU:HB2	1:C:48:SER:HB2	1.85	0.59
1:B:129:GLU:OE2	1:B:158:THR:OG1	2.21	0.58
1:A:135:ILE:HG13	1:A:380:ARG:NH2	2.18	0.58
2:F:182:ALA:HB3	2:F:247:MET:HG2	1.84	0.58
2:F:358:ALA:HB2	2:F:363:GLU:HG3	1.85	0.58
2:F:253:TYR:OH	2:F:280:ASN:OD1	2.20	0.58
2:F:177:PHE:O	2:F:206:ARG:NH1	2.36	0.58
2:E:89:VAL:HB	2:E:98:ASP:HB3	1.86	0.57
4:H:31:THR:O	4:H:34:ARG:HB3	2.05	0.57
1:A:547:GLU:HA	1:A:550:VAL:HG23	1.86	0.57
1:B:84:PHE:HB3	1:B:88:GLN:HA	1.86	0.57
4:H:29:THR:N	4:H:32:GLU:OE2	2.37	0.56
1:C:471:ASN:O	1:C:475:ARG:HG2	2.06	0.56
2:F:10:GLU:HG2	2:F:17:ALA:HB3	1.88	0.56
2:E:448:ASP:OD1	2:E:449:LEU:N	2.39	0.56
3:G:170:LEU:HD12	3:G:174:THR:HB	1.87	0.56
1:C:476:LEU:HD12	1:C:477:VAL:HG13	1.87	0.56
1:A:453:TRP:HA	1:A:456:MET:HE2	1.89	0.55
1:B:461:MET:SD	1:B:465:GLN:NE2	2.79	0.55
1:C:96:GLU:O	1:C:99:GLN:NE2	2.33	0.55
1:B:315:GLU:HA	1:B:384:ILE:HD11	1.89	0.55
2:D:446:LYS:HD3	2:D:448:ASP:HB3	1.89	0.55
1:C:459:GLU:HG3	1:C:462:ARG:HH12	1.72	0.54
1:A:514:SER:OG	1:A:564:GLU:OE2	2.17	0.54
2:F:399:LYS:O	2:F:403:LYS:HG2	2.07	0.54
1:B:319:ASP:O	1:B:380:ARG:NH1	2.36	0.54
1:C:230:VAL:HG22	1:C:413:TRP:HE3	1.72	0.54
2:D:66:LYS:HG2	2:D:67:ASN:OD1	2.08	0.54
2:E:139:ASN:HD21	2:E:347:SER:HB3	1.72	0.53
4:H:34:ARG:HG2	4:H:35:LYS:N	2.23	0.53
2:F:382:ALA:HB1	2:F:394:LEU:HD21	1.90	0.53
3:G:51:ARG:NH2	4:H:75:LEU:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ARG:HG2	1:A:423:ARG:HH11	1.74	0.53
1:C:238:LYS:NZ	7:C:603:PO4:O2	2.31	0.53
2:E:364:ASP:OD2	2:E:431:TRP:NE1	2.24	0.53
2:D:389:LEU:HD22	3:G:32:LYS:HD2	1.91	0.53
1:B:264:ASN:ND2	2:E:324:GLU:OE2	2.42	0.53
1:C:10:SER:HB2	2:F:46:GLU:HG3	1.91	0.52
4:H:28:THR:H	4:H:32:GLU:HG3	1.73	0.52
1:A:453:TRP:CZ3	1:A:519:PHE:HA	2.43	0.52
3:G:182:ILE:O	3:G:186:LYS:HG3	2.08	0.52
2:D:166:ARG:NH1	2:D:197:ASP:OD2	2.43	0.52
2:F:150:PHE:HB2	2:F:328:ILE:HG12	1.92	0.52
4:H:84:GLY:O	4:H:88:GLU:HG3	2.09	0.52
1:A:106:GLY:O	1:A:108:GLN:NE2	2.43	0.52
1:A:318:ARG:HD3	1:A:384:ILE:HG13	1.92	0.52
1:A:84:PHE:HB3	1:A:88:GLN:HA	1.91	0.52
2:D:172:ASP:CG	2:D:173:SER:H	2.13	0.52
1:B:453:TRP:HZ3	1:B:519:PHE:HA	1.75	0.52
2:E:21:VAL:HG22	2:E:50:ASP:O	2.10	0.52
1:A:577:ILE:O	1:A:581:ILE:HG12	2.10	0.52
3:G:9:ARG:NH2	3:G:193:GLU:OE2	2.40	0.52
1:C:269:VAL:HG11	1:C:291:LEU:HD21	1.92	0.51
1:C:143:LYS:HB2	1:C:283:GLU:HG2	1.92	0.51
2:D:248:THR:HB	2:D:303:ILE:HB	1.93	0.51
2:F:233:GLU:OE1	2:F:287:ARG:NH1	2.39	0.51
2:F:433:LEU:O	2:F:436:MET:HG2	2.11	0.51
1:A:453:TRP:HZ3	1:A:519:PHE:HA	1.75	0.51
1:B:8:LYS:HG3	2:E:48:GLN:HB2	1.93	0.51
1:C:256:TYR:HB3	1:C:291:LEU:HD23	1.93	0.51
1:A:581:ILE:O	1:A:585:VAL:HG23	2.10	0.51
1:C:278:ASP:O	1:C:282:GLY:N	2.34	0.51
2:F:138:LEU:HB3	2:F:373:PHE:CZ	2.46	0.50
1:B:241:VAL:O	1:B:245:ILE:HG12	2.12	0.50
2:D:124:PRO:HG2	2:D:351:LEU:HD13	1.93	0.50
1:B:462:ARG:NH1	1:B:466:GLU:OE1	2.44	0.50
1:A:90:PRO:HD3	1:A:111:ALA:HA	1.93	0.50
4:H:12:ASP:C	4:H:79:HIS:HE1	2.15	0.50
2:E:251:THR:O	2:E:255:GLU:HG2	2.12	0.50
2:D:267:VAL:HG23	3:G:204:LYS:HD2	1.93	0.50
4:H:28:THR:H	4:H:32:GLU:CG	2.25	0.50
1:A:530:LYS:NZ	1:A:530:LYS:HB2	2.26	0.50
1:C:351:ASP:OD2	2:D:258:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:LYS:O	1:A:534:LYS:HG2	2.11	0.50
1:C:148:LYS:HD2	1:C:320:MET:HB3	1.93	0.50
2:D:29:LEU:HD11	2:D:77:LEU:HD23	1.93	0.49
1:B:397:ILE:HB	1:B:402:THR:HG21	1.94	0.49
2:E:170:VAL:HG23	2:E:173:SER:HB2	1.93	0.49
2:F:270:ARG:NH2	2:F:314:PRO:HD3	2.27	0.49
2:F:29:LEU:HD21	2:F:41:ARG:HH21	1.77	0.49
2:D:165:ALA:HB2	2:D:246:ILE:HD12	1.94	0.49
1:C:407:ARG:NH2	2:D:255:GLU:OE2	2.46	0.49
1:B:92:ASP:HB3	2:E:119:ILE:HD13	1.94	0.49
2:F:307:PRO:HG2	2:F:313:HIS:CE1	2.47	0.49
4:H:91:GLN:HE22	4:H:101:ASN:ND2	2.09	0.49
4:H:33:ILE:HB	4:H:58:VAL:HG11	1.95	0.49
1:B:274:PRO:HD3	1:B:286:MET:HE2	1.95	0.49
2:F:394:LEU:HD12	2:F:395:SER:H	1.77	0.49
1:C:80:ILE:HD12	1:C:253:LEU:HD11	1.94	0.49
1:B:453:TRP:CZ3	1:B:519:PHE:HA	2.47	0.49
1:C:38:GLU:OE1	1:C:52:TYR:OH	2.23	0.49
2:D:127:PHE:HB2	2:D:355:GLY:O	2.12	0.49
2:E:13:GLY:O	2:E:60:THR:OG1	2.22	0.49
4:H:10:ASP:O	4:H:14:VAL:HG22	2.13	0.49
1:B:214:ARG:NH2	1:B:502:GLN:O	2.45	0.48
2:E:216:ASP:O	2:E:221:ARG:NH1	2.46	0.48
3:G:92:VAL:HG22	3:G:105:MET:HG2	1.93	0.48
2:E:139:ASN:ND2	2:E:347:SER:HB3	2.27	0.48
2:F:388:VAL:HG13	2:F:389:LEU:HG	1.96	0.48
3:G:164:ARG:NH2	4:H:96:LYS:O	2.46	0.48
4:H:12:ASP:HB2	4:H:79:HIS:CE1	2.48	0.48
2:D:6:ARG:NH1	2:D:67:ASN:O	2.46	0.48
2:E:324:GLU:O	2:E:350:ARG:NE	2.46	0.48
1:A:135:ILE:HD13	1:A:148:LYS:HD3	1.96	0.48
2:D:445:ILE:HD13	2:D:450:LEU:HB2	1.96	0.48
1:B:231:PRO:HB3	1:B:390:VAL:HB	1.94	0.48
1:B:516:GLU:H	1:B:516:GLU:CD	2.17	0.48
1:B:56:SER:O	1:B:105:ARG:NH2	2.44	0.48
1:C:27:MET:HG3	6:C:602:GOL:H11	1.95	0.48
2:D:361:THR:HG21	2:D:365:HIS:ND1	2.29	0.48
2:D:446:LYS:HG3	2:D:449:LEU:HB2	1.95	0.48
1:B:41:GLU:HB2	1:B:48:SER:HB2	1.96	0.47
1:B:473:ILE:O	1:B:477:VAL:HG22	2.14	0.47
2:D:446:LYS:CG	2:D:449:LEU:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:ASN:OD1	2:D:67:ASN:HB2	2.14	0.47
1:A:126:GLU:OE2	1:A:161:LYS:HA	2.15	0.47
2:D:30:ILE:HD13	2:D:54:VAL:HG11	1.97	0.47
3:G:37:MET:HA	3:G:40:PHE:HB3	1.96	0.47
1:B:43:ARG:HG2	2:F:10:GLU:HB2	1.97	0.47
2:F:248:THR:HB	2:F:303:ILE:HD12	1.96	0.47
1:A:243:HIS:CE1	1:A:273:PHE:HE2	2.33	0.47
2:E:433:LEU:O	2:E:436:MET:HG2	2.14	0.47
2:F:44:VAL:HA	2:F:54:VAL:HG12	1.96	0.47
3:G:34:ASP:O	3:G:38:ARG:HG3	2.15	0.47
4:H:31:THR:O	4:H:34:ARG:CZ	2.63	0.47
1:C:436:LEU:HD21	2:D:154:GLY:HA2	1.96	0.47
2:E:401:TYR:OH	2:E:441:GLU:OE1	2.15	0.47
2:F:324:GLU:HA	2:F:350:ARG:HD2	1.97	0.47
4:H:60:GLU:O	4:H:64:ARG:HG2	2.14	0.47
2:F:107:LYS:HE2	2:F:109:LEU:HD21	1.96	0.46
2:F:28:GLU:H	2:F:44:VAL:HB	1.80	0.46
2:D:217:PRO:HB2	2:D:220:GLU:HG3	1.96	0.46
1:B:218:THR:OG1	1:B:500:TYR:OH	2.24	0.46
1:C:378:ASP:OD2	1:C:380:ARG:NH1	2.48	0.46
2:D:11:VAL:HG22	2:D:16:MET:HG3	1.96	0.46
2:E:408:PHE:O	2:E:412:TYR:HB3	2.15	0.46
4:H:91:GLN:HE22	4:H:101:ASN:HD22	1.64	0.46
4:H:8:VAL:O	4:H:50:ILE:HA	2.15	0.46
1:A:51:VAL:HG12	1:A:53:GLU:H	1.81	0.46
2:F:249:ASP:OD1	2:F:304:LEU:HA	2.15	0.46
3:G:93:VAL:HG23	3:G:104:LEU:HB2	1.98	0.46
1:C:423:ARG:NH1	9:C:703:HOH:O	2.48	0.46
2:D:361:THR:HG22	2:D:362:ARG:N	2.29	0.46
2:F:379:GLY:HA2	2:F:401:TYR:HB3	1.97	0.46
1:A:83:MET:HG2	1:A:291:LEU:HB3	1.97	0.46
1:A:329:ASP:HA	1:A:330:SER:HA	1.61	0.46
1:C:378:ASP:HB2	1:C:380:ARG:HG3	1.97	0.46
2:D:386:ALA:HB2	2:D:394:LEU:HD11	1.96	0.46
1:A:187:MET:HE2	1:A:187:MET:HB3	1.76	0.46
1:A:41:GLU:OE2	1:A:43:ARG:NH1	2.49	0.46
1:B:144:ILE:HG23	1:B:145:ILE:HG13	1.98	0.46
1:C:202:LYS:HB3	2:D:188:PHE:CE2	2.51	0.46
1:A:78:GLY:N	1:A:141:GLU:OE2	2.43	0.46
1:C:84:PHE:HB3	1:C:88:GLN:HA	1.98	0.45
2:D:152:GLY:N	2:D:155:LEU:HD12	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:412:TYR:HB2	2:D:433:LEU:HD11	1.99	0.45
1:A:236:ALA:O	1:A:427:SER:OG	2.34	0.45
1:A:87:ILE:HG13	1:A:89:ARG:HG3	1.99	0.45
4:H:27:GLY:CA	4:H:32:GLU:HG3	2.46	0.45
1:B:38:GLU:OE1	1:B:52:TYR:OH	2.24	0.45
1:C:453:TRP:HZ3	1:C:519:PHE:HA	1.82	0.45
1:C:545:ILE:HA	1:C:584:ILE:HD13	1.98	0.45
2:D:34:MET:HE2	2:D:38:GLU:HB3	1.99	0.45
1:A:565:GLU:OE1	1:A:565:GLU:N	2.38	0.45
1:A:361:ARG:HA	1:A:361:ARG:HD3	1.76	0.45
1:B:436:LEU:HD11	2:F:154:GLY:HA2	1.99	0.45
3:G:37:MET:O	3:G:41:ILE:N	2.45	0.45
1:B:242:GLN:HE22	1:B:329:ASP:HB2	1.81	0.45
1:C:225:GLY:O	1:C:370:GLY:HA2	2.17	0.45
2:D:57:PHE:HB3	2:D:217:PRO:HG2	1.99	0.45
2:E:288:ALA:HB2	2:E:300:GLN:HG3	1.97	0.45
3:G:140:LEU:HD11	4:H:20:PHE:CE1	2.52	0.45
1:A:530:LYS:HA	1:A:533:ARG:HB2	2.00	0.44
1:C:173:ILE:HD13	1:C:187:MET:HG2	1.98	0.44
2:D:212:ASN:OD1	2:D:221:ARG:HG2	2.17	0.44
1:A:41:GLU:HB2	1:A:48:SER:HB2	2.00	0.44
1:A:573:ILE:O	1:A:577:ILE:HG13	2.16	0.44
1:B:329:ASP:HA	1:B:330:SER:HA	1.72	0.44
1:B:410:LYS:HB3	1:B:436:LEU:HB2	1.99	0.44
1:B:83:MET:HG3	1:B:291:LEU:HD23	1.98	0.44
1:A:214:ARG:NH1	1:A:513:THR:OG1	2.50	0.44
1:C:161:LYS:HB3	1:C:175:VAL:HG13	1.99	0.44
2:E:390:GLY:HA3	4:H:99:GLY:HA3	1.99	0.44
2:E:412:TYR:HB2	2:E:433:LEU:HD11	1.99	0.44
4:H:36:THR:HG22	4:H:40:MET:HE2	1.98	0.44
1:A:250:ASP:N	1:A:250:ASP:OD1	2.44	0.44
2:E:139:ASN:HD21	2:E:347:SER:CB	2.31	0.44
4:H:32:GLU:O	4:H:36:THR:OG1	2.35	0.44
2:F:146:LYS:HD2	2:F:323:THR:HA	1.99	0.44
3:G:46:LYS:O	3:G:50:LEU:HB2	2.18	0.44
1:A:125:GLU:OE2	1:A:126:GLU:HG2	2.17	0.44
1:C:247:LYS:HG3	1:C:248:TRP:CD1	2.53	0.44
2:D:48:GLN:HG2	2:D:49:GLU:HG2	1.99	0.44
2:E:362:ARG:HB3	2:E:364:ASP:OD1	2.18	0.44
3:G:6:ASN:O	3:G:8:THR:N	2.48	0.44
3:G:78:ASP:O	3:G:79:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:PRO:HB2	1:A:223:THR:OG1	2.18	0.44
1:A:344:ARG:HD2	2:D:276:TYR:HB3	1.99	0.44
3:G:95:LYS:HG2	3:G:96:ASN:N	2.32	0.44
2:E:439:ARG:NH2	2:E:451:ASP:OD1	2.34	0.44
3:G:78:ASP:C	3:G:79:GLU:HG2	2.38	0.44
1:A:134:ASP:O	1:A:151:VAL:HG12	2.18	0.43
1:B:541:TYR:HB2	1:B:544:GLU:HG2	1.99	0.43
1:C:56:SER:O	1:C:105:ARG:NH2	2.46	0.43
2:F:103:ILE:O	2:F:105:PRO:HD3	2.18	0.43
2:E:151:SER:OG	2:E:152:GLY:N	2.49	0.43
2:F:250:MET:HB2	2:F:304:LEU:HB3	2.00	0.43
1:B:580:THR:O	1:B:584:ILE:HG12	2.17	0.43
2:D:249:ASP:OD1	2:D:304:LEU:HA	2.18	0.43
2:E:248:THR:HA	2:E:249:ASP:HA	1.82	0.43
1:C:303:ARG:HD2	1:C:337:ALA:HB2	2.01	0.43
2:D:150:PHE:HB2	2:D:328:ILE:HG12	1.99	0.43
2:F:158:LYS:HD2	2:F:193:PHE:CD2	2.53	0.43
3:G:171:GLU:HG2	3:G:172:TYR:CD1	2.53	0.43
1:A:257:VAL:HA	1:A:292:ILE:HB	1.99	0.43
1:A:231:PRO:HA	1:A:390:VAL:O	2.17	0.43
1:A:555:ARG:NH1	1:A:576:GLU:OE2	2.52	0.43
1:C:150:MET:HE1	1:C:319:ASP:HB3	2.01	0.43
1:C:415:LEU:HA	1:C:427:SER:O	2.18	0.43
2:F:158:LYS:HD3	2:F:190:GLU:OE2	2.19	0.43
1:B:197:ARG:HA	1:B:198:PRO:HD3	1.78	0.43
1:C:85:ASP:OD1	1:C:89:ARG:N	2.40	0.43
3:G:88:VAL:HG11	4:H:20:PHE:HB3	2.01	0.43
1:A:256:TYR:HB3	1:A:291:LEU:HD12	1.99	0.43
1:C:308:TYR:HA	1:C:311:ILE:HG22	2.01	0.43
1:A:278:ASP:HA	1:A:279:PRO:HD3	1.88	0.43
1:A:338:LEU:HD23	1:A:338:LEU:HA	1.85	0.43
1:C:203:LEU:HB2	1:C:371:ARG:HG2	2.01	0.43
3:G:67:LEU:O	3:G:70:SER:OG	2.33	0.43
1:A:534:LYS:O	1:A:538:LEU:N	2.52	0.42
1:C:528:PHE:CZ	1:C:553:ARG:HD3	2.54	0.42
1:B:554:GLU:OE1	1:B:558:ARG:NH2	2.36	0.42
2:E:250:MET:HB2	2:E:304:LEU:HB3	2.01	0.42
2:F:394:LEU:O	2:F:399:LYS:HE2	2.18	0.42
1:A:580:THR:O	1:A:584:ILE:HG12	2.20	0.42
2:D:57:PHE:HB2	2:D:58:GLU:OE1	2.19	0.42
2:E:239:LYS:HA	2:E:239:LYS:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:PRO:HA	1:C:284:SER:OG	2.20	0.42
2:E:138:LEU:HA	2:E:369:MET:HG3	2.00	0.42
1:A:553:ARG:HB2	1:A:553:ARG:HE	1.42	0.42
1:B:90:PRO:HD3	1:B:111:ALA:HA	2.02	0.42
2:E:91:ASP:OD1	2:E:95:ARG:N	2.49	0.42
2:F:395:SER:O	2:F:399:LYS:HG3	2.20	0.42
3:G:137:THR:N	3:G:138:GLN:HE21	2.17	0.42
3:G:26:HIS:CD2	3:G:171:GLU:HB2	2.54	0.42
2:E:338:ILE:HG23	2:E:414:ASN:HB2	2.02	0.42
2:F:146:LYS:HD3	2:F:285:PHE:O	2.19	0.42
2:F:248:THR:HB	2:F:303:ILE:HB	2.01	0.42
3:G:58:THR:HG23	3:G:139:LEU:HD13	2.01	0.42
1:A:315:GLU:HA	1:A:384:ILE:HD11	2.00	0.42
1:C:410:LYS:HG3	1:C:437:TYR:OH	2.19	0.42
1:A:210:ILE:HG12	1:A:515:ARG:NH2	2.35	0.42
1:A:96:GLU:O	1:A:99:GLN:NE2	2.49	0.42
1:B:444:TYR:HD1	1:B:445:MET:HE2	1.85	0.42
2:E:397:ILE:HD11	2:E:441:GLU:CD	2.40	0.42
2:F:408:PHE:O	2:F:412:TYR:HB3	2.20	0.42
1:B:27:MET:HE1	1:B:71:LEU:HB2	2.02	0.41
1:C:329:ASP:HA	1:C:330:SER:HA	1.66	0.41
1:C:87:ILE:HD11	1:C:89:ARG:CZ	2.51	0.41
2:F:128:ILE:HD11	2:F:143:ARG:HA	2.02	0.41
2:F:339:GLN:HA	2:F:340:PRO:HA	1.91	0.41
4:H:18:ARG:HD3	4:H:22:PHE:O	2.19	0.41
1:A:194:ARG:NH2	1:A:304:GLU:OE1	2.53	0.41
2:E:328:ILE:HD12	2:E:346:PRO:HB2	2.01	0.41
1:B:581:ILE:O	1:B:585:VAL:HG23	2.20	0.41
1:A:139:VAL:HG21	1:A:187:MET:HE3	2.03	0.41
2:E:362:ARG:NH1	2:E:364:ASP:OD2	2.54	0.41
2:F:313:HIS:CG	2:F:314:PRO:HD2	2.56	0.41
1:B:74:GLU:HB2	1:B:111:ALA:HB3	2.01	0.41
1:C:6:ILE:HD12	1:C:62:GLU:HB2	2.02	0.41
4:H:13:SER:N	4:H:79:HIS:HE1	2.19	0.41
1:B:231:PRO:HA	1:B:390:VAL:O	2.20	0.41
2:E:111:ILE:HA	2:E:230:THR:OG1	2.21	0.41
2:E:406:GLU:O	2:E:410:ASN:ND2	2.48	0.41
2:F:81:VAL:HG11	2:F:109:LEU:HD12	2.02	0.41
1:A:247:LYS:HB3	1:A:285:LEU:HD11	2.03	0.41
1:C:234:PHE:HB3	2:F:321:TYR:CD1	2.56	0.41
1:C:25:GLN:NE2	1:C:38:GLU:OE2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:HIS:ND1	2:D:412:TYR:OH	2.48	0.41
1:A:197:ARG:HA	1:A:198:PRO:HD3	1.85	0.41
1:A:560:LYS:HD2	1:A:561:TYR:CZ	2.56	0.41
1:C:233:PRO:HG3	1:C:395:GLY:HA3	2.03	0.41
1:C:423:ARG:HD3	1:C:423:ARG:HA	1.83	0.41
1:B:232:GLY:HA3	1:B:415:LEU:HB2	2.02	0.41
1:C:250:ASP:N	1:C:250:ASP:OD1	2.46	0.41
3:G:44:ILE:HD11	4:H:90:ILE:HG23	2.01	0.41
1:B:8:LYS:HG2	1:B:9:VAL:N	2.36	0.41
2:D:146:LYS:HE2	2:D:146:LYS:HB2	1.91	0.41
1:A:225:GLY:O	1:A:370:GLY:HA2	2.21	0.41
1:A:484:ASP:HB3	1:A:542:PHE:HB2	2.03	0.41
2:F:29:LEU:HD13	2:F:77:LEU:HD13	2.02	0.41
4:H:87:LEU:HD23	4:H:87:LEU:HA	1.92	0.41
1:B:204:ASN:HA	1:B:205:PRO:HD3	1.90	0.40
1:C:469:GLN:NE2	2:D:332:GLU:OE1	2.48	0.40
3:G:37:MET:O	3:G:41:ILE:HG12	2.21	0.40
3:G:53:ALA:O	3:G:57:GLU:HG3	2.21	0.40
2:F:361:THR:OG1	2:F:362:ARG:N	2.53	0.40
2:F:29:LEU:HD23	2:F:73:LEU:HD22	2.02	0.40
3:G:187:MET:O	3:G:191:GLU:HB2	2.21	0.40
1:A:295:THR:OG1	1:A:298:MET:HG3	2.20	0.40
1:C:268:ASP:O	1:C:272:GLU:HB2	2.21	0.40
2:D:151:SER:OG	2:D:152:GLY:N	2.54	0.40
2:D:423:ILE:HA	2:D:423:ILE:HD12	1.94	0.40
2:E:339:GLN:HA	2:E:340:PRO:HA	1.89	0.40
1:C:30:VAL:HB	1:C:35:VAL:HG23	2.03	0.40
2:D:396:ASP:OD1	2:D:399:LYS:NZ	2.39	0.40
2:F:313:HIS:CD2	2:F:314:PRO:HD2	2.56	0.40
1:A:171:ASP:HA	1:A:172:PRO:HD3	1.87	0.40
1:A:191:TRP:CZ2	1:A:198:PRO:HD3	2.56	0.40
1:A:520:ASN:OD1	1:A:567:LEU:HD21	2.22	0.40
1:B:463:ILE:HG22	1:B:493:ALA:HB2	2.03	0.40
1:C:231:PRO:HA	1:C:390:VAL:O	2.21	0.40
1:C:43:ARG:HG2	2:D:10:GLU:HB3	2.04	0.40
1:C:8:LYS:HA	2:F:47:VAL:O	2.21	0.40
2:F:111:ILE:O	2:F:287:ARG:NH2	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	584/600 (97%)	562 (96%)	22 (4%)	0	100	100
1	B	590/600 (98%)	574 (97%)	16 (3%)	0	100	100
1	C	584/600 (97%)	570 (98%)	14 (2%)	0	100	100
2	D	450/465 (97%)	434 (96%)	15 (3%)	1 (0%)	52	83
2	E	450/465 (97%)	438 (97%)	11 (2%)	1 (0%)	52	83
2	F	454/465 (98%)	444 (98%)	10 (2%)	0	100	100
3	G	172/217 (79%)	168 (98%)	4 (2%)	0	100	100
4	H	100/115 (87%)	92 (92%)	7 (7%)	1 (1%)	19	52
All	All	3384/3527 (96%)	3282 (97%)	99 (3%)	3 (0%)	56	86

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	99	ASN
4	H	60	GLU
2	D	49	GLU

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	470/511 (92%)	462 (98%)	8 (2%)	68	90
1	B	489/511 (96%)	487 (100%)	2 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	487/511 (95%)	486 (100%)	1 (0%)	95	99
2	D	361/387 (93%)	359 (99%)	2 (1%)	90	97
2	E	371/387 (96%)	368 (99%)	3 (1%)	86	96
2	F	371/387 (96%)	371 (100%)	0	100	100
3	G	152/198 (77%)	149 (98%)	3 (2%)	63	88
4	H	77/99 (78%)	74 (96%)	3 (4%)	39	74
All	All	2778/2991 (93%)	2756 (99%)	22 (1%)	86	96

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	GLU
1	A	243	HIS
1	A	259	CYS
1	A	270	VAL
1	A	378	ASP
1	A	379	GLN
1	A	401	VAL
1	A	586	SER
1	B	158	THR
1	B	516	GLU
1	C	175	VAL
2	D	33	ARG
2	D	170	VAL
2	E	33	ARG
2	E	99	ASN
2	E	441	GLU
3	G	89	SER
3	G	106	ASN
3	G	138	GLN
4	H	61	THR
4	H	64	ARG
4	H	78	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	B	465	GLN

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Mol	Chain	Res	Type
1	C	465	GLN
2	E	99	ASN
2	F	313	HIS
3	G	138	GLN
4	H	79	HIS
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 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	GOL	C	602	-	5,5,5	0.36	0	5,5,5	0.25	0
7	PO4	C	603	5	4,4,4	0.68	0	6,6,6	0.23	0
6	GOL	F	501	-	5,5,5	0.35	0	5,5,5	0.30	0
8	B3P	F	502	-	18,18,18	0.55	0	17,23,23	0.79	0
6	GOL	G	301	-	5,5,5	0.36	0	5,5,5	0.19	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	GOL	C	602	-	-	0/4/4/4	0/0/0/0
7	PO4	C	603	5	-	0/0/0/0	0/0/0/0
6	GOL	F	501	-	-	0/4/4/4	0/0/0/0
8	B3P	F	502	-	-	0/28/28/28	0/0/0/0
6	GOL	G	301	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	602	GOL	1	0
7	C	603	PO4	1	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	586/600 (97%)	0.49	55 (9%) 11 6	44, 67, 102, 115	0
1	B	592/600 (98%)	0.22	18 (3%) 54 48	33, 54, 86, 109	1 (0%)
1	C	586/600 (97%)	0.40	32 (5%) 29 23	41, 59, 89, 103	0
2	D	452/465 (97%)	0.27	12 (2%) 58 53	44, 64, 89, 120	0
2	E	452/465 (97%)	0.21	11 (2%) 62 58	32, 56, 82, 115	0
2	F	455/465 (97%)	0.15	11 (2%) 62 58	33, 55, 84, 113	0
3	G	178/217 (82%)	0.77	22 (12%) 5 3	57, 77, 133, 148	0
4	H	102/115 (88%)	1.31	27 (26%) 1 0	70, 112, 156, 171	0
All	All	3403/3527 (96%)	0.35	188 (5%) 29 23	32, 61, 102, 171	1 (0%)

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	40	MET	6.1
1	A	182	LEU	6.1
4	H	62	ILE	5.7
1	A	394	GLY	5.5
1	C	174	CYS	5.4
1	A	488	LEU	4.9
4	H	36	THR	4.9
4	H	26	HIS	4.8
1	A	178	THR	4.8
1	A	176	ILE	4.7
4	H	45	TYR	4.5
1	C	539	GLY	4.4
1	C	279	PRO	4.4
1	A	393	SER	4.4
1	C	582	GLN	4.3
3	G	71	THR	4.2

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Mol	Chain	Res	Type	RSRZ
4	H	12	ASP	4.1
1	A	160	GLN	4.0
1	A	540	ALA	4.0
3	G	135	GLY	3.9
1	A	158	THR	3.9
4	H	29	THR	3.8
3	G	136	PHE	3.8
3	G	133	ILE	3.8
1	A	586	SER	3.7
3	G	70	SER	3.6
4	H	5	ILE	3.6
3	G	77	ILE	3.6
1	A	129	GLU	3.6
1	C	182	LEU	3.6
2	F	1	MET	3.5
3	G	137	THR	3.5
1	A	159	VAL	3.5
4	H	101	ASN	3.4
4	H	55	ALA	3.4
1	C	280	ASN	3.4
1	B	123	THR	3.4
1	C	185	LEU	3.3
2	D	5	TYR	3.3
1	C	173	ILE	3.2
2	E	397	ILE	3.2
2	F	412	TYR	3.2
1	A	542	PHE	3.2
1	C	473	ILE	3.2
1	B	176	ILE	3.1
1	A	538	LEU	3.1
2	F	455	PRO	3.1
2	E	174	SER	3.1
4	H	33	ILE	3.1
4	H	79	HIS	3.1
1	C	481	SER	3.1
1	A	120	PHE	3.1
4	H	16	PRO	3.1
1	A	181	GLY	3.0
1	A	539	GLY	3.0
1	A	152	PRO	3.0
1	A	123	THR	3.0
3	G	97	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	279	PRO	2.9
3	G	107	PHE	2.9
1	A	177	GLU	2.9
1	A	579	GLU	2.9
3	G	143	LEU	2.9
1	B	539	GLY	2.9
1	A	174	CYS	2.8
1	A	151	VAL	2.8
1	B	159	VAL	2.8
4	H	76	ILE	2.8
1	C	283	GLU	2.8
3	G	102	VAL	2.8
1	B	577	ILE	2.8
1	A	122	ALA	2.8
2	F	381	GLN	2.8
1	A	572	SER	2.7
1	A	541	TYR	2.7
1	C	155	ILE	2.7
3	G	88	VAL	2.7
1	C	572	SER	2.7
1	A	532	ALA	2.7
1	A	128	THR	2.7
1	A	136	ILE	2.7
2	F	435	ALA	2.7
2	E	392	SER	2.6
3	G	64	ASP	2.6
2	E	72	PHE	2.6
1	A	149	ILE	2.6
1	C	160	GLN	2.6
1	B	127	GLY	2.6
1	A	175	VAL	2.6
1	B	160	GLN	2.5
2	D	391	GLU	2.5
1	C	130	VAL	2.5
3	G	65	PHE	2.5
2	F	42	GLY	2.5
2	E	104	LEU	2.5
1	A	535	ALA	2.5
1	B	174	CYS	2.5
4	H	53	GLN	2.5
1	A	173	ILE	2.5
1	A	187	MET	2.5

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Mol	Chain	Res	Type	RSRZ
4	H	34	ARG	2.5
1	B	581	ILE	2.5
2	F	385	LEU	2.5
1	A	283	GLU	2.5
4	H	3	TYR	2.5
4	H	19	LEU	2.5
1	A	126	GLU	2.5
1	A	273	PHE	2.5
2	F	393	ALA	2.5
2	E	5	TYR	2.5
2	E	434	LEU	2.5
1	A	127	GLY	2.4
1	C	127	GLY	2.4
3	G	78	ASP	2.4
2	F	434	LEU	2.4
1	A	479	ILE	2.4
4	H	28	THR	2.4
1	C	1	MET	2.4
2	E	83	GLU	2.4
3	G	73	GLU	2.4
4	H	56	ASN	2.4
1	B	124	ILE	2.4
2	D	392	SER	2.4
4	H	4	LYS	2.4
3	G	141	PRO	2.3
1	A	134	ASP	2.3
4	H	31	THR	2.3
1	C	571	SER	2.3
4	H	20	PHE	2.3
2	E	175	ASP	2.3
2	E	82	SER	2.3
1	C	282	GLY	2.3
1	C	541	TYR	2.3
3	G	62	MET	2.3
1	A	179	GLU	2.3
1	A	463	ILE	2.3
1	B	7	ILE	2.3
1	C	525	ILE	2.3
4	H	102	ILE	2.3
1	B	465	GLN	2.3
1	C	564	GLU	2.3
3	G	87	ASN	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	E	324	GLU	2.3
1	A	490	LEU	2.3
1	A	81	SER	2.2
3	G	74	GLU	2.2
2	F	332	GLU	2.2
1	C	2	GLN	2.2
1	A	470	LEU	2.2
1	C	330	SER	2.2
2	D	293	GLY	2.2
1	B	280	ASN	2.2
1	A	537	SER	2.2
2	D	231	ALA	2.2
2	D	208	VAL	2.2
1	B	125	GLU	2.2
3	G	17	LYS	2.2
1	A	485	ASN	2.2
2	D	205	ASP	2.2
2	F	408	PHE	2.2
1	A	154	GLY	2.2
1	A	395	GLY	2.2
1	B	137	GLY	2.2
4	H	22	PHE	2.1
4	H	71	PRO	2.1
1	C	379	GLN	2.1
1	A	484	ASP	2.1
1	C	179	GLU	2.1
1	A	492	VAL	2.1
1	C	143	LYS	2.1
2	D	234	TYR	2.1
2	D	188	PHE	2.1
2	D	176	ASP	2.1
1	C	584	ILE	2.1
1	A	585	VAL	2.1
1	A	259	CYS	2.1
4	H	80	GLN	2.1
1	C	516	GLU	2.1
1	C	565	GLU	2.1
3	G	95	LYS	2.1
1	C	124	ILE	2.0
1	C	128	THR	2.0
1	A	161	LYS	2.0
1	A	172	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	296	SER	2.0
2	D	308	GLU	2.0
1	B	106	GLY	2.0
2	D	65	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
8	B3P	F	502	19/19	0.85	0.25	1.08	69,70,72,72	0
6	GOL	C	602	6/6	0.88	0.28	0.96	75,75,75,75	0
6	GOL	F	501	6/6	0.83	0.23	0.31	80,80,80,81	0
5	MG	C	601	1/1	0.92	0.21	-1.24	46,46,46,46	0
7	PO4	C	603	5/5	0.98	0.15	-2.15	55,55,56,56	0
6	GOL	G	301	6/6	0.80	0.19	-	69,71,71,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.