



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:06 PM UTC

PDB ID : 5KND / pdb_00005knd
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

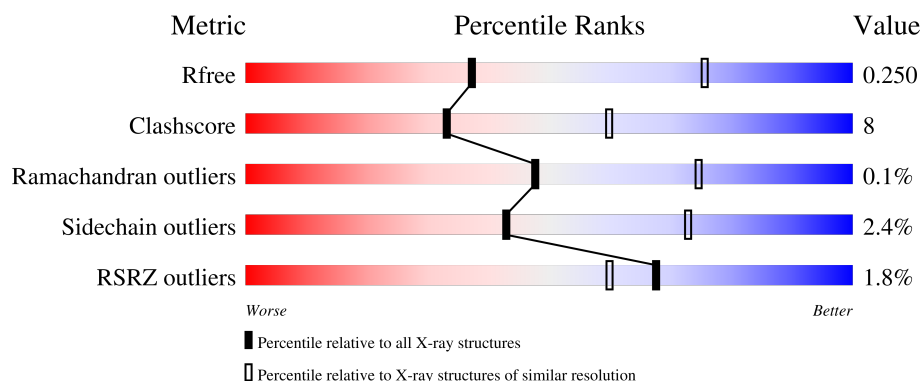
1 Overall quality at a glance

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}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 2% 76% 21% ..
1	B	600	 83% 15% .
1	C	600	 % 80% 16% ..
2	D	465	 2% 79% 18% ..

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Mol	Chain	Length	Quality of chain
2	E	465	% 80% 15% • •
2	F	465	2% 82% 16% •
3	G	217	3% 53% 27% • 18%
4	H	115	9% 52% 31% • • 11%

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			

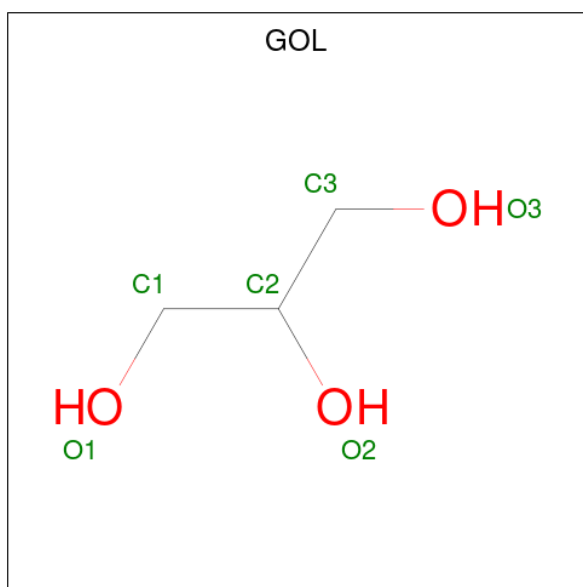
There are 12 discrepancies between the modelled and reference sequences:

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 (CCD ID: MG) (formula: Mg).

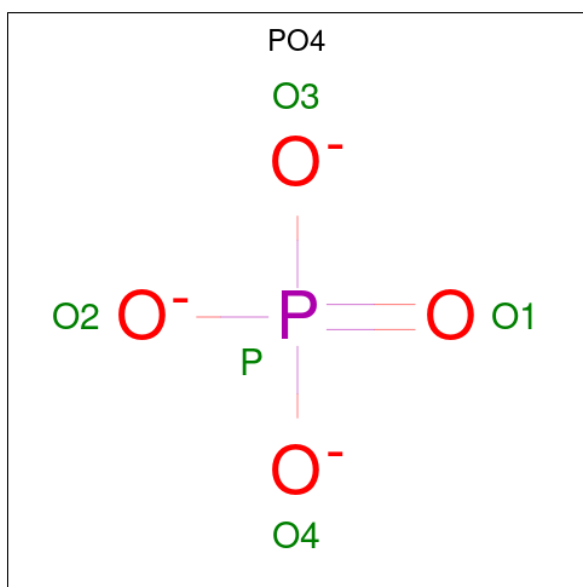
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



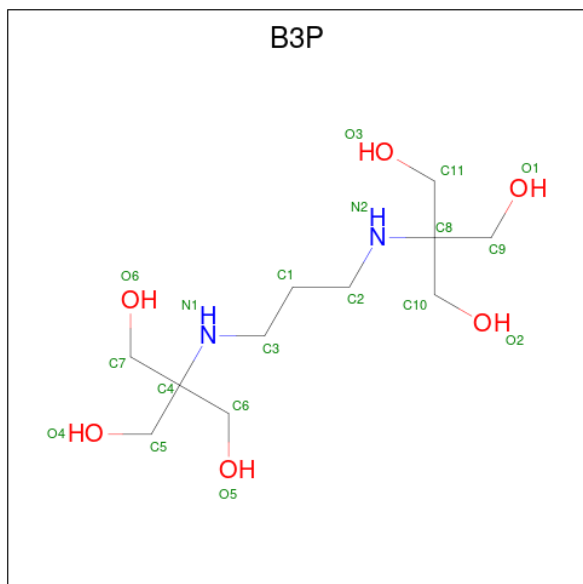
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: 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		

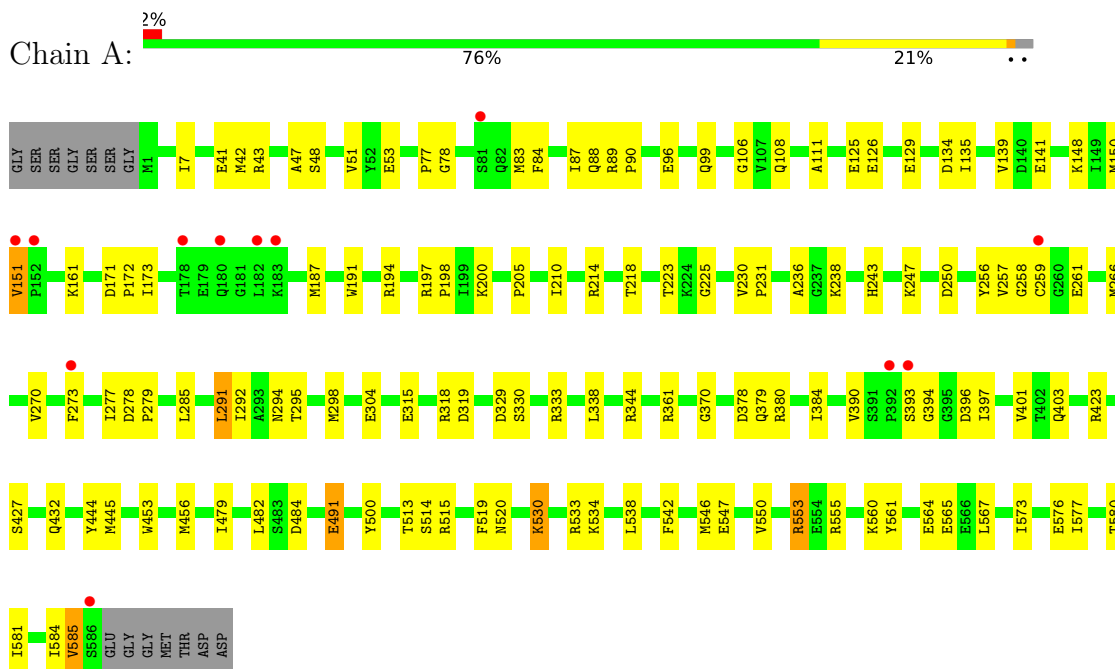
- Molecule 9 is water.

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 [i](#)

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

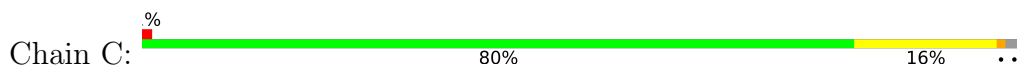
- Molecule 1: V-type sodium ATPase catalytic subunit A

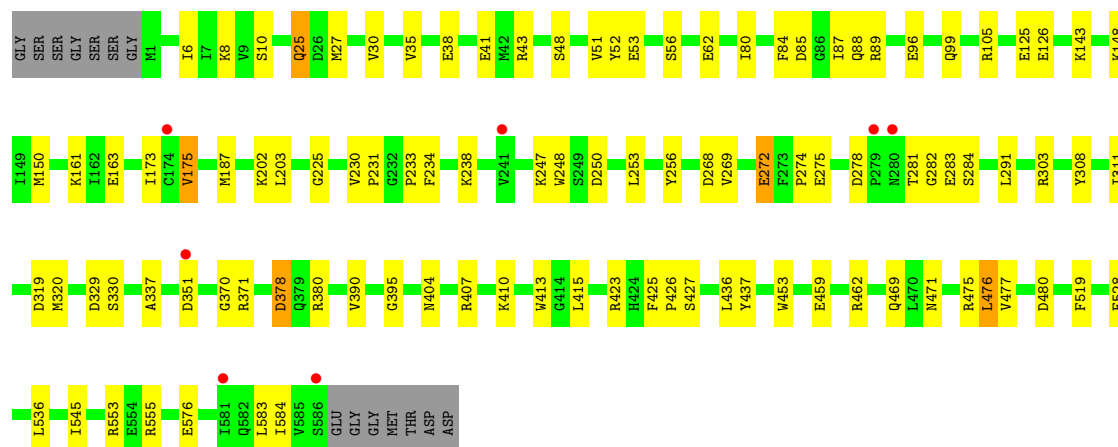


- Molecule 1: V-type sodium ATPase catalytic subunit A

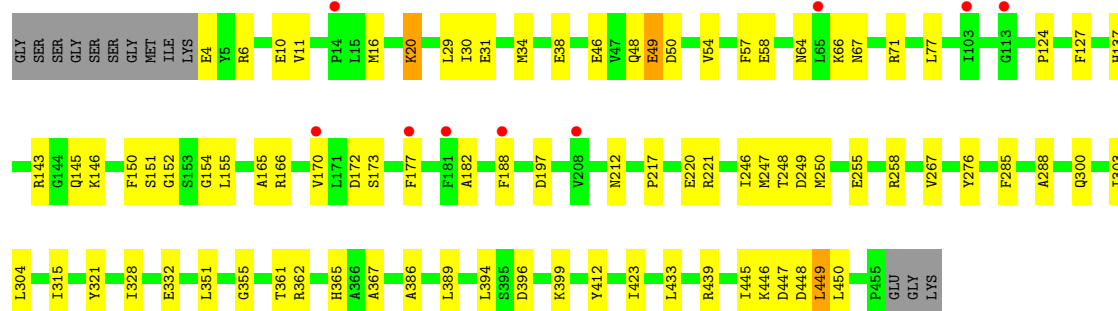
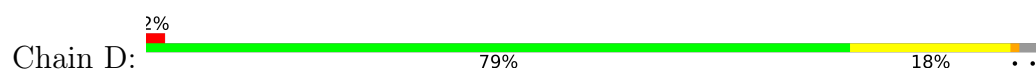


- Molecule 1: V-type sodium ATPase catalytic subunit A

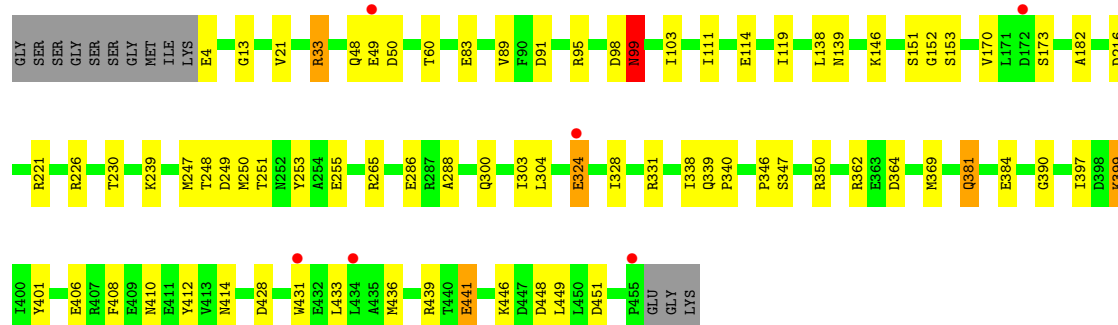
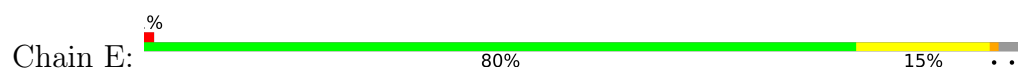




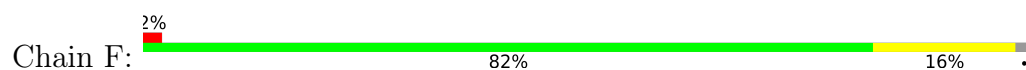
• Molecule 2: V-type sodium ATPase subunit B

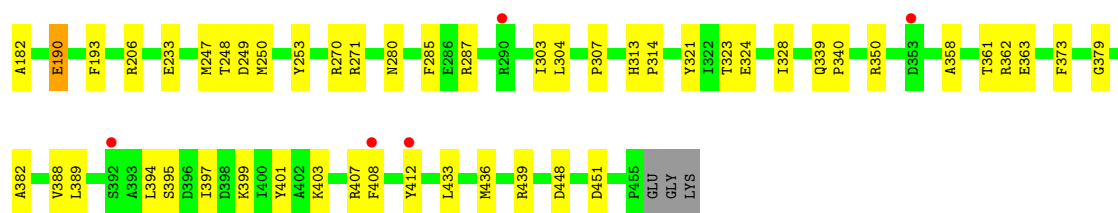


• Molecule 2: V-type sodium ATPase subunit B

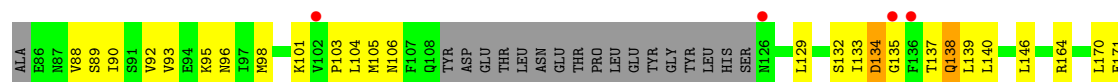
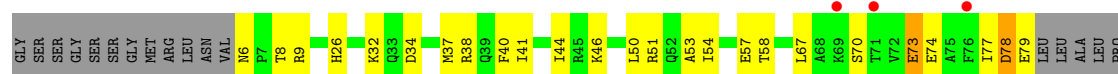


• Molecule 2: V-type sodium ATPase subunit B

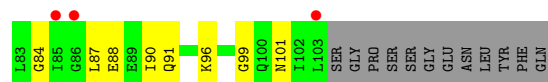
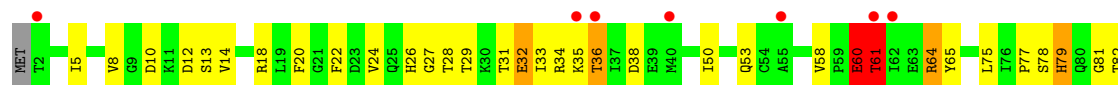




● Molecule 3: V-type sodium ATPase subunit D



● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.206 , 0.251 0.210 , 0.250	Depositor DCC
R_{free} test set	4215 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	63.5	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GOL, 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	0.30	0/4543	0.76	0/6162
1	B	0.29	0/4625	0.72	2/6266 (0.0%)
1	C	0.29	0/4598	0.73	1/6230 (0.0%)
2	D	0.30	0/3569	0.77	3/4835 (0.1%)
2	E	0.32	0/3589	0.75	2/4857 (0.0%)
2	F	0.29	0/3625	0.72	0/4903
3	G	0.37	0/1424	0.87	6/1908 (0.3%)
4	H	0.51	0/774	0.96	1/1052 (0.1%)
All	All	0.31	0/26747	0.76	15/36213 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	61	THR	N-CA-C	8.58	120.41	111.14
3	G	73	GLU	N-CA-C	6.86	119.34	111.11
3	G	78	ASP	N-CA-C	-6.43	104.70	112.54
2	E	49	GLU	CB-CA-C	-6.35	109.26	116.63
1	C	480	ASP	N-CA-C	6.31	118.16	111.28
3	G	134	ASP	N-CA-C	-6.01	105.21	112.54
2	D	177	PHE	N-CA-C	5.73	118.54	110.23
2	D	315	ILE	CA-C-N	-5.65	113.85	119.56
2	D	315	ILE	C-N-CA	-5.65	113.85	119.56
3	G	181	THR	N-CA-C	-5.43	105.44	111.36
3	G	78	ASP	CA-C-N	5.32	131.28	121.70
3	G	78	ASP	C-N-CA	5.32	131.28	121.70
2	E	399	LYS	CA-CB-CG	5.31	124.72	114.10
1	B	197	ARG	CA-C-N	5.10	125.01	119.76
1	B	197	ARG	C-N-CA	5.10	125.01	119.76

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	4467	0	4331	86	0
1	B	4549	0	4449	54	0
1	C	4522	0	4425	59	0
2	D	3506	0	3471	59	0
2	E	3526	0	3524	49	0
2	F	3562	0	3554	50	0
3	G	1415	0	1450	41	0
4	H	762	0	718	37	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	410	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 (410) 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:N	2:E:99:ASN:HD22	1.71	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	2:E:99:ASN:H	1.19	0.84
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:H	3:G:138:GLN:NE2	1.78	0.79
1:A:295:THR:H	1:A:298:MET:HE3	1.49	0.78
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	3:G:138:GLN:HE21	1.46	0.62
1:A:546:MET:HE3	1:A:553:ARG:HH11	1.64	0.62
1:A:150:MET:HE1	1:A:319:ASP:HB3	1.81	0.61
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
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:250:MET:HE3	2:D:285:PHE:HE1	1.67	0.59
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:58:GLU:OE1	2:D:58:GLU:N	2.34	0.59
2:D:447:ASP:HA	2:D:450:LEU:HB3	1.83	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
1:B:445:MET:HE1	1:B:515:ARG:CZ	2.33	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
1:A:77:PRO:HG2	1:A:187:MET:HE2	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
1:A:491:GLU:HG2	1:A:546:MET:HE1	1.87	0.56
2:D:172:ASP:CG	2:D:173:SER:H	2.13	0.56
1:B:273:PHE:HB2	1:B:286:MET:HE2	1.86	0.56
1:A:150:MET:HE3	1:A:380:ARG:HH12	1.70	0.56
4:H:29:THR:N	4:H:32:GLU:OE2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:G:203:VAL:HA	3:G:206:MET:HE3	1.86	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:B:461:MET:SD	1:B:465:GLN:NE2	2.79	0.55
1:C:238:LYS:NZ	7:C:603:PO4:O2	2.31	0.55
1:C:96:GLU:O	1:C:99:GLN:NE2	2.33	0.55
4:H:12:ASP:C	4:H:79:HIS:HE1	2.15	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
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:A:546:MET:HE3	1:A:553:ARG:NH1	2.22	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
1:A:514:SER:OG	1:A:564:GLU:OE2	2.17	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
1:A:423:ARG:HG2	1:A:423:ARG:HH11	1.74	0.53
2:D:389:LEU:HD22	3:G:32:LYS:HD2	1.91	0.53
2:E:364:ASP:OD2	2:E:431:TRP:NE1	2.24	0.53
1:B:264:ASN:ND2	2:E:324:GLU:OE2	2.42	0.53
1:B:516:GLU:CD	1:B:516:GLU:H	2.17	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:84:PHE:HB3	1:A:88:GLN:HA	1.91	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:83:MET:HE2	1:A:291:LEU:HD22	1.92	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:A:261:GLU:HB2	1:A:266:MET:HE2	1.93	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
2:E:247:MET:HB3	2:E:250:MET:HE3	1.92	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:HB2	1:A:530:LYS:NZ	2.26	0.50
1:C:351:ASP:OD2	2:D:258:ARG:NH2	2.45	0.50
1:A:42:MET:HE2	1:A:47:ALA:HB2	1.93	0.50
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:396:ASP:OD1	2:D:399:LYS:NZ	2.39	0.50
2:D:29:LEU:HD11	2:D:77:LEU:HD23	1.93	0.49
1:A:456:MET:HE1	1:A:519:PHE:CD1	2.47	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:29:LEU:HD21	2:F:41:ARG:HH21	1.77	0.49
2:F:270:ARG:NH2	2:F:314:PRO:HD3	2.27	0.49
1:A:139:VAL:HG21	1:A:187:MET:HE1	1.95	0.49
1:B:92:ASP:HB3	2:E:119:ILE:HD13	1.94	0.49
1:C:407:ARG:NH2	2:D:255:GLU:OE2	2.46	0.49
2:D:165:ALA:HB2	2:D:246:ILE:HD12	1.94	0.49
2:F:307:PRO:HG2	2:F:313:HIS:CE1	2.47	0.49
4:H:33:ILE:HB	4:H:58:VAL:HG11	1.95	0.49
4:H:91:GLN:HE22	4:H:101:ASN:ND2	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:G:78:ASP:C	3:G:79:GLU:HG2	2.38	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:56:SER:O	1:B:105:ARG:NH2	2.44	0.48
1:B:231:PRO:HB3	1:B:390:VAL:HB	1.94	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:E:99:ASN:N	2:E:99:ASN:ND2	2.44	0.48
2:D:446:LYS:HG3	2:D:449:LEU:HB2	1.95	0.48
1:B:38:GLU:OE1	1:B:52:TYR:OH	2.24	0.47
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
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
1:B:43:ARG:HG2	2:F:10:GLU:HB2	1.97	0.47
2:D:30:ILE:HD13	2:D:54:VAL:HG11	1.97	0.47
2:F:248:THR:HB	2:F:303:ILE:HD12	1.96	0.47
3:G:37:MET:HA	3:G:40:PHE:HB3	1.96	0.47
3:G:103:PRO:HB2	3:G:105:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:G:98:MET:HE3	3:G:98:MET:HB2	1.78	0.47
4:H:60:GLU:O	4:H:64:ARG:HG2	2.14	0.47
1:A:295:THR:N	1:A:298:MET:HE3	2.25	0.46
2:F:28:GLU:H	2:F:44:VAL:HB	1.80	0.46
2:F:107:LYS:HE2	2:F:109:LEU:HD21	1.96	0.46
1:A:218:THR:OG1	1:A:500:TYR:OH	2.28	0.46
2:D:217:PRO:HB2	2:D:220:GLU:HG3	1.96	0.46
2:E:397:ILE:HD11	2:E:441:GLU:CD	2.40	0.46
1:A:445:MET:HE1	1:A:515:ARG:CZ	2.45	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:8:VAL:O	4:H:50:ILE:HA	2.15	0.46
4:H:91:GLN:HE22	4:H:101:ASN:HD22	1.64	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: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
2:D:412:TYR:HB2	2:D:433:LEU:HD11	1.99	0.45
1:A:87:ILE:HG13	1:A:89:ARG:HG3	1.99	0.45
1:A:236:ALA:O	1:A:427:SER:OG	2.34	0.45
1:C:150:MET:HE1	1:C:319:ASP:HB3	1.98	0.45
2:D:34:MET:HE2	2:D:38:GLU:HB3	1.98	0.45
4:H:27:GLY:CA	4:H:32:GLU:HG3	2.46	0.45
1:B:218:THR:OG1	1:B:500:TYR:OH	2.24	0.45
1:C:453:TRP:HZ3	1:C:519:PHE:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:545:ILE:HA	1:C:584:ILE:HD13	1.98	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:83:MET:HG3	1:B:291:LEU:HD23	1.98	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: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
1:A:250:ASP:OD1	1:A:250:ASP:N	2.44	0.44
2:E:139:ASN:HD21	2:E:347:SER:CB	2.31	0.44
3:G:135:GLY:C	3:G:138:GLN:NE2	2.75	0.44
4:H:32:GLU:O	4:H:36:THR:OG1	2.35	0.44
1:B:150:MET:HE1	1:B:319:ASP:HB2	2.00	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:A:294:ASN:HA	1:A:298:MET:HE3	1.99	0.44
1:A:444:TYR:HD2	1:A:445:MET:HE2	1.83	0.44
1:B:229:ALA:C	1:B:231:PRO:HD3	2.43	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:439:ARG:NH2	2:E:451:ASP:OD1	2.34	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:A:445:MET:HE1	1:A:515:ARG:NE	2.33	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:231:PRO:HA	1:A:390:VAL:O	2.17	0.43
1:A:257:VAL:HA	1:A:292:ILE:HB	1.99	0.43
1:A:555:ARG:NH1	1:A:576:GLU:OE2	2.52	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:B:445:MET:HE1	1:B:515:ARG:NE	2.34	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:A:394:GLY:C	1:A:396:ASP:H	2.27	0.43
1:C:308:TYR:HA	1:C:311:ILE:HG22	2.01	0.43
1:C:425:PHE:HA	1:C:426:PRO:C	2.44	0.43
1:A:218:THR:HG1	1:A:500:TYR:HH	1.62	0.43
1:A:278:ASP:HA	1:A:279:PRO:HD3	1.88	0.43
1:A:338:LEU:HA	1:A:338:LEU:HD23	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:A:456:MET:HE1	1:A:519:PHE:CE1	2.55	0.42
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:HE	1:A:553:ARG:HB2	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:26:HIS:CD2	3:G:171:GLU:HB2	2.54	0.42
3:G:137:THR:N	3:G:138:GLN:HE21	2.17	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:96:GLU:O	1:A:99:GLN:NE2	2.49	0.42
1:A:210:ILE:HG12	1:A:515:ARG:NH2	2.35	0.42
1:A:258:GLY:HA3	1:A:266:MET:HE1	2.02	0.42
2:F:408:PHE:O	2:F:412:TYR:HB3	2.20	0.42
1:B:194:ARG:HH22	1:B:304:GLU:CD	2.26	0.41
1:C:87:ILE:HD11	1:C:89:ARG:CZ	2.51	0.41
1:C:329:ASP:HA	1:C:330:SER:HA	1.66	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
2:E:369:MET:HE2	2:E:369:MET:HB3	1.96	0.41
3:G:9:ARG:HH22	3:G:193:GLU:CD	2.28	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: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)
1:C:234:PHE:HB3	2:F:321:TYR:CD1	2.56	0.41
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
3:G:129:LEU:O	3:G:132:SER:OG	2.35	0.41
1:B:8:LYS:HG2	1:B:9:VAL:N	2.36	0.41
1:B:232:GLY:HA3	1:B:415:LEU:HB2	2.02	0.41
1:C:250:ASP:OD1	1:C:250:ASP:N	2.46	0.41
2:D:146:LYS:HE2	2:D:146:LYS:HB2	1.91	0.41
3:G:44:ILE:HD11	4:H:90:ILE:HG23	2.01	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
3:G:77:ILE:C	3:G:79:GLU:N	2.79	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:29:LEU:HD23	2:F:73:LEU:HD22	2.02	0.40
2:F:361:THR:OG1	2:F:362:ARG:N	2.53	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:B:425:PHE:HA	1:B:426:PRO:C	2.46	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:HD12	2:D:423:ILE:HA	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: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:8:LYS:HA	2:F:47:VAL:O	2.21	0.40
1:C:43:ARG:HG2	2:D:10:GLU:HB3	2.04	0.40
1:C:231:PRO:HA	1:C:390: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%)	43	70
2	E	450/465 (97%)	438 (97%)	11 (2%)	1 (0%)	43	70
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%)	12	35
All	All	3384/3527 (96%)	3282 (97%)	99 (3%)	3 (0%)	48	74

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%)	452 (96%)	18 (4%)	29	61
1	B	489/511 (96%)	482 (99%)	7 (1%)	59	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	487/511 (95%)	476 (98%)	11 (2%)	44	74
2	D	361/387 (93%)	356 (99%)	5 (1%)	59	83
2	E	371/387 (96%)	360 (97%)	11 (3%)	36	67
2	F	371/387 (96%)	367 (99%)	4 (1%)	65	86
3	G	152/198 (77%)	147 (97%)	5 (3%)	33	65
4	H	77/99 (78%)	71 (92%)	6 (8%)	11	32
All	All	2778/2991 (93%)	2711 (98%)	67 (2%)	43	73

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	129	GLU
1	A	151	VAL
1	A	200	LYS
1	A	230	VAL
1	A	238	LYS
1	A	259	CYS
1	A	270	VAL
1	A	277	ILE
1	A	291	LEU
1	A	378	ASP
1	A	379	GLN
1	A	401	VAL
1	A	432	GLN
1	A	491	GLU
1	A	530	LYS
1	A	553	ARG
1	A	585	VAL
1	B	25	GLN
1	B	27	MET
1	B	158	THR
1	B	230	VAL
1	B	253	LEU
1	B	379	GLN
1	B	516	GLU
1	C	25	GLN
1	C	125	GLU
1	C	126	GLU
1	C	163	GLU

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Mol	Chain	Res	Type
1	C	175	VAL
1	C	272	GLU
1	C	275	GLU
1	C	378	ASP
1	C	476	LEU
1	C	536	LEU
1	C	583	LEU
2	D	20	LYS
2	D	46	GLU
2	D	143	ARG
2	D	170	VAL
2	D	449	LEU
2	E	33	ARG
2	E	83	GLU
2	E	99	ASN
2	E	103	ILE
2	E	114	GLU
2	E	265	ARG
2	E	324	GLU
2	E	381	GLN
2	E	399	LYS
2	E	441	GLU
2	E	446	LYS
2	F	1	MET
2	F	190	GLU
2	F	397	ILE
2	F	448	ASP
3	G	89	SER
3	G	101	LYS
3	G	106	ASN
3	G	133	ILE
3	G	138	GLN
4	H	32	GLU
4	H	36	THR
4	H	60	GLU
4	H	61	THR
4	H	64	ARG
4	H	79	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	213	GLN
1	A	244	GLN
1	A	404	ASN
1	A	424	HIS
1	A	450	GLN
1	B	201	GLN
1	B	244	GLN
1	B	424	HIS
1	B	465	GLN
1	C	117	GLN
1	C	204	ASN
1	C	244	GLN
1	C	271	ASN
1	C	403	GLN
1	C	465	GLN
2	D	48	GLN
2	D	55	GLN
2	D	139	ASN
2	D	242	HIS
2	E	99	ASN
2	E	313	HIS
2	F	129	GLN
2	F	167	GLN
2	F	313	HIS
2	F	339	GLN
3	G	26	HIS
3	G	39	GLN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
7	PO4	C	603	5	4,4,4	0.98	0	6,6,6	0.48	0
6	GOL	G	301	-	5,5,5	0.38	0	5,5,5	0.23	0
6	GOL	F	501	-	5,5,5	0.37	0	5,5,5	0.41	0
6	GOL	C	602	-	5,5,5	0.38	0	5,5,5	0.34	0
8	B3P	F	502	-	18,18,18	0.59	0	23,23,23	0.84	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	F	501	-	-	2/4/4/4	-
6	GOL	C	602	-	-	2/4/4/4	-
8	B3P	F	502	-	-	6/28/28/28	-
6	GOL	G	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	602	GOL	O1-C1-C2-C3

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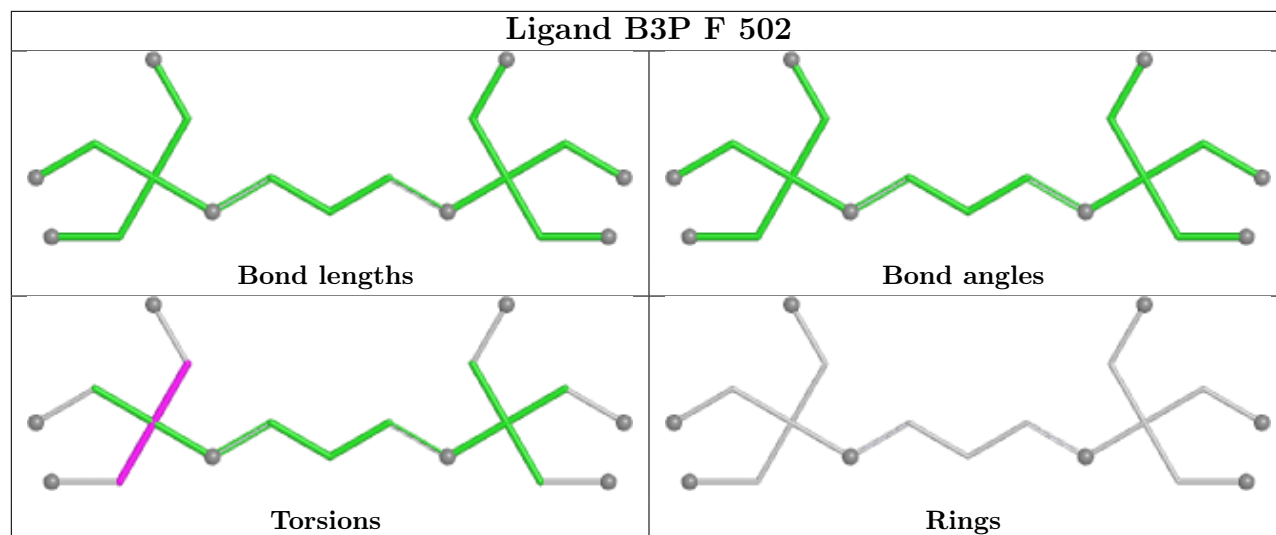
Mol	Chain	Res	Type	Atoms
6	F	501	GOL	O1-C1-C2-O2
6	G	301	GOL	O1-C1-C2-C3
8	F	502	B3P	N1-C4-C5-O4
8	F	502	B3P	C6-C4-C5-O4
8	F	502	B3P	C7-C4-C5-O4
8	F	502	B3P	N1-C4-C7-O6
8	F	502	B3P	C5-C4-C7-O6
8	F	502	B3P	C6-C4-C7-O6
6	F	501	GOL	O1-C1-C2-C3
6	G	301	GOL	O1-C1-C2-O2
6	C	602	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	603	PO4	1	0
6	C	602	GOL	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	586/600 (97%)	0.34	12 (2%) 65 57	44, 67, 102, 115	0
1	B	592/600 (98%)	0.13	2 (0%) 90 87	33, 54, 86, 109	0
1	C	586/600 (97%)	0.22	7 (1%) 76 70	41, 59, 89, 103	0
2	D	452/465 (97%)	0.28	9 (1%) 65 57	44, 64, 89, 120	0
2	E	452/465 (97%)	0.15	6 (1%) 75 68	32, 56, 82, 115	0
2	F	455/465 (97%)	0.16	7 (1%) 72 64	29, 55, 84, 113	1 (0%)
3	G	178/217 (82%)	0.55	7 (3%) 43 35	57, 77, 133, 148	0
4	H	102/115 (88%)	1.00	10 (9%) 13 11	70, 112, 156, 171	0
All	All	3403/3527 (96%)	0.26	60 (1%) 67 60	29, 61, 102, 171	1 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	62	ILE	5.2
4	H	36	THR	4.7
1	A	273	PHE	4.1
4	H	103	LEU	3.9
4	H	86	GLY	3.6
3	G	136	PHE	3.4
4	H	40	MET	3.3
1	A	392	PRO	3.1
1	C	241	VAL	2.9
2	F	42	GLY	2.9
2	E	434	LEU	2.8
1	A	178	THR	2.8
3	G	76	PHE	2.7
1	A	586	SER	2.6
2	F	7	THR	2.6
2	F	392	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	177	PHE	2.5
2	D	170	VAL	2.5
2	F	353	ASP	2.5
1	B	586	SER	2.5
4	H	35	LYS	2.4
2	D	208	VAL	2.4
1	A	152	PRO	2.4
2	F	290[A]	ARG	2.4
1	C	586	SER	2.3
2	E	324	GLU	2.3
4	H	55	ALA	2.3
1	A	180	GLN	2.3
1	B	7	ILE	2.3
2	D	103	ILE	2.3
3	G	135	GLY	2.3
3	G	71	THR	2.3
2	D	14	PRO	2.3
2	E	455	PRO	2.3
1	C	174	CYS	2.2
4	H	61	THR	2.2
1	A	151	VAL	2.2
1	A	393	SER	2.2
2	D	113	GLY	2.2
1	A	182	LEU	2.2
4	H	85	ILE	2.2
2	D	181	PHE	2.2
2	E	431	TRP	2.2
1	A	259	CYS	2.2
1	A	81	SER	2.2
1	C	581	ILE	2.1
2	E	172	ASP	2.1
2	D	65	LEU	2.1
2	D	188	PHE	2.1
1	C	351	ASP	2.1
2	F	408	PHE	2.1
2	F	412	TYR	2.1
2	E	49	GLU	2.1
1	A	183	LYS	2.0
1	C	279	PRO	2.0
3	G	126	ASN	2.0
3	G	102	VAL	2.0
1	C	280	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
4	H	2	THR	2.0
3	G	69	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

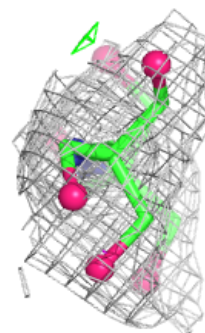
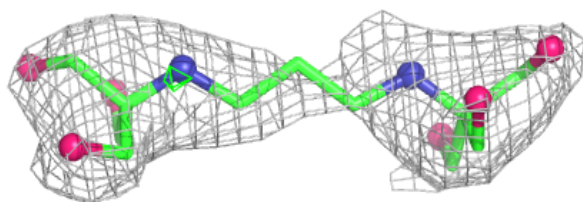
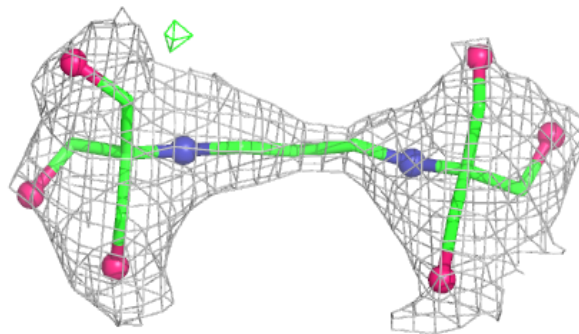
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	G	301	6/6	0.65	0.14	69,71,71,72	0
6	GOL	F	501	6/6	0.75	0.11	80,80,80,81	0
6	GOL	C	602	6/6	0.83	0.16	75,75,75,75	0
8	B3P	F	502	19/19	0.84	0.12	69,70,72,72	0
7	PO4	C	603	5/5	0.97	0.06	55,55,56,56	0
5	MG	C	601	1/1	0.99	0.04	46,46,46,46	0

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

Electron density around B3P F 502:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.