



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 22, 2018 – 05:06 PM EST

PDB ID : 5MRW
Title : Structure of the KdpFABC complex
Authors : Huang, C.; Pedersen, B.P.; Stokes, D.L.
Deposited on : 2016-12-27
Resolution : 2.90 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030736

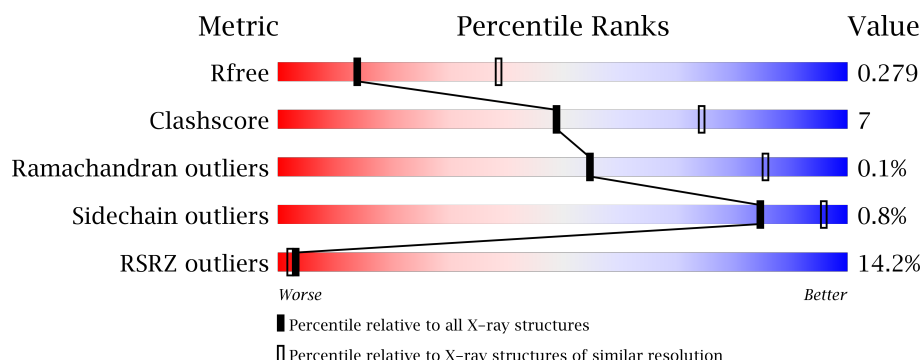
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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 $\leq 5\%$. 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	557	<div> <div>10%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
1	E	557	<div> <div>7%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
1	I	557	<div> <div>9%</div> <div>81%</div> <div>18%</div> </div>
2	B	674	<div> <div>14%</div> <div>82%</div> <div>18%</div> </div>
2	F	674	<div> <div>21%</div> <div>83%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	674	
3	C	187	
3	G	187	
3	K	187	
4	D	27	
4	H	27	
4	L	27	

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
6	PX4	A	602	-	-	-	X
6	PX4	A	603	-	-	-	X
6	PX4	E	602	-	-	-	X
6	PX4	H	101	-	-	-	X
6	PX4	I	602	-	-	-	X
6	PX4	I	603	-	-	-	X
7	BOG	A	604	-	-	-	X
7	BOG	I	604	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 32666 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 Potassium-transporting ATPase potassium-binding subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4157	2716	681	725	35			
1	E	557	Total	C	N	O	S	0	0	0
			4157	2716	681	725	35			
1	I	557	Total	C	N	O	S	0	0	0
			4157	2716	681	725	35			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	ARG	GLN	engineered mutation	UNP P03959
E	116	ARG	GLN	engineered mutation	UNP P03959
I	116	ARG	GLN	engineered mutation	UNP P03959

- Molecule 2 is a protein called Potassium-transporting ATPase ATP-binding subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	674	Total 5008	C 3187	N 864	O 932	P 1	S 24	0	0	0
2	F	674	Total 5008	C 3187	N 864	O 932	P 1	S 24	0	0	0
2	J	674	Total 5008	C 3187	N 864	O 932	P 1	S 24	0	0	0

- Molecule 3 is a protein called Potassium-transporting ATPase KdpC subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	187	Total	C	N	O	S	0	0	0
			1413	903	245	264	1			
3	G	187	Total	C	N	O	S	0	0	0
			1413	903	245	264	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	187	Total	C	N	O	S	0	0	0
			1413	903	245	264	1			

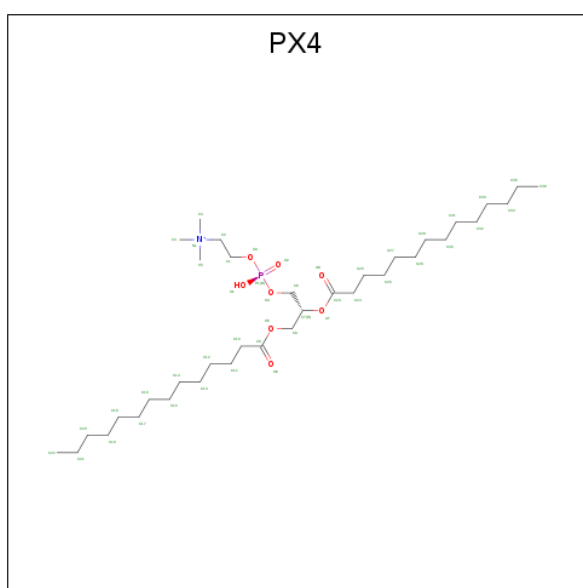
- Molecule 4 is a protein called Potassium-transporting ATPase KdpF subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	27	Total	C	N	O	S	0	0	0
			200	137	28	34	1			
4	H	27	Total	C	N	O	S	0	0	0
			200	137	28	34	1			
4	L	27	Total	C	N	O	S	0	0	0
			200	137	28	34	1			

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

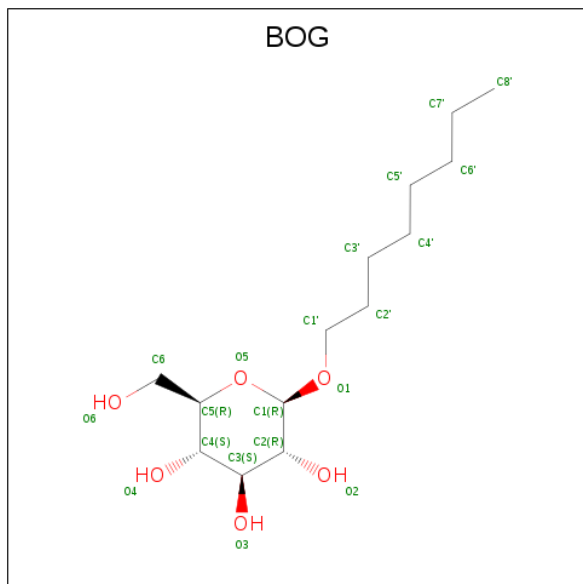
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total	K	0	0
			1	1		
5	A	1	Total	K	0	0
			1	1		
5	E	1	Total	K	0	0
			1	1		

- Molecule 6 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C₃₆H₇₃NO₈P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	0
			41	32	8	1		
6	A	1	Total	C	O	P	0	0
			41	32	8	1		
6	E	1	Total	C	O	P	0	0
			41	32	8	1		
6	H	1	Total	C	O	P	0	0
			41	32	8	1		
6	I	1	Total	C	O	P	0	0
			41	32	8	1		
6	I	1	Total	C	O	P	0	0
			41	32	8	1		

- Molecule 7 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			20	14	6		
7	B	1	Total	C	O	0	0
			20	14	6		
7	E	1	Total	C	O	0	0
			20	14	6		
7	I	1	Total	C	O	0	0
			20	14	6		

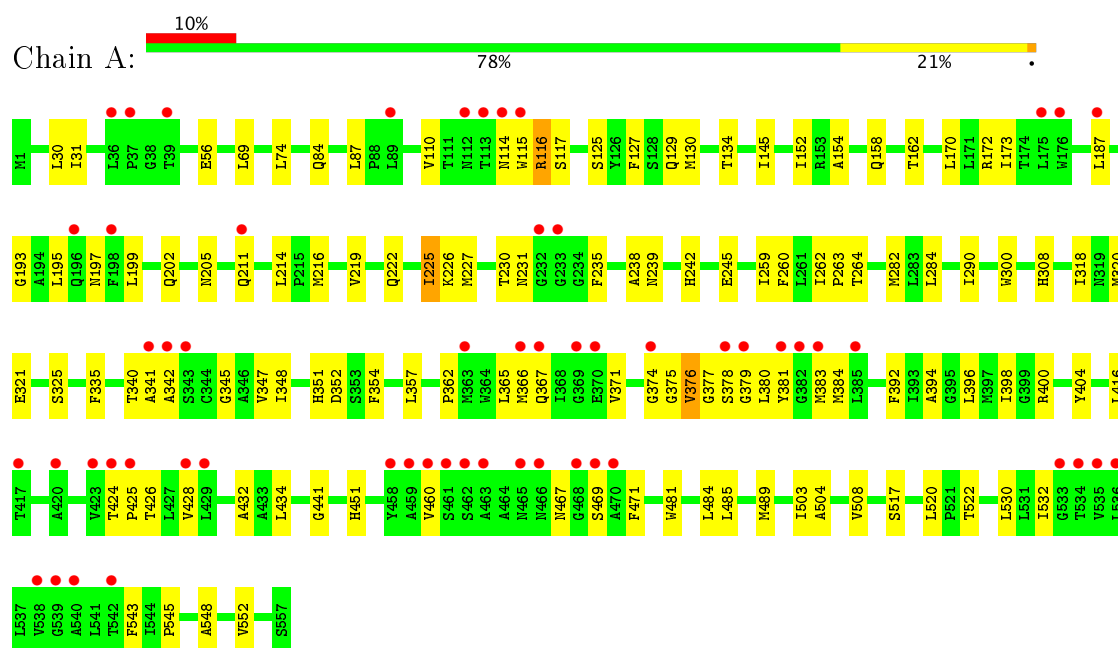
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total 1	O 1	0	0
8	F	1	Total 1	O 1	0	0
8	J	1	Total 1	O 1	0	0

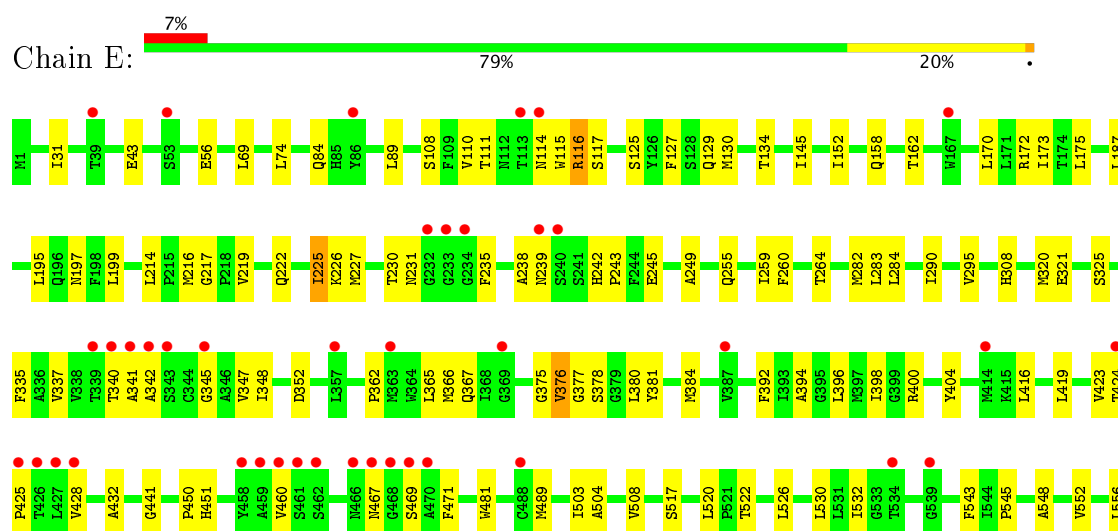
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Potassium-transporting ATPase potassium-binding subunit

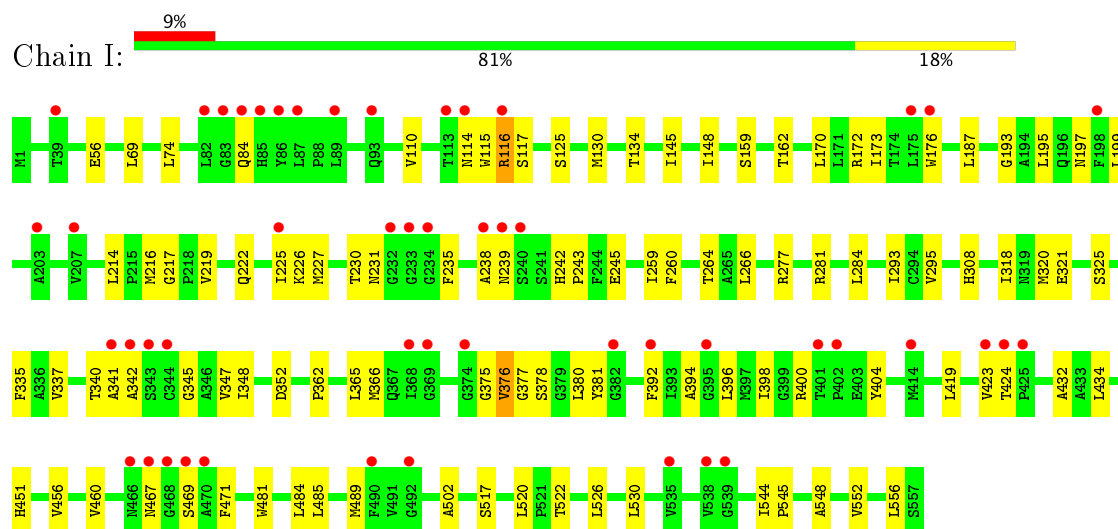


- Molecule 1: Potassium-transporting ATPase potassium-binding subunit

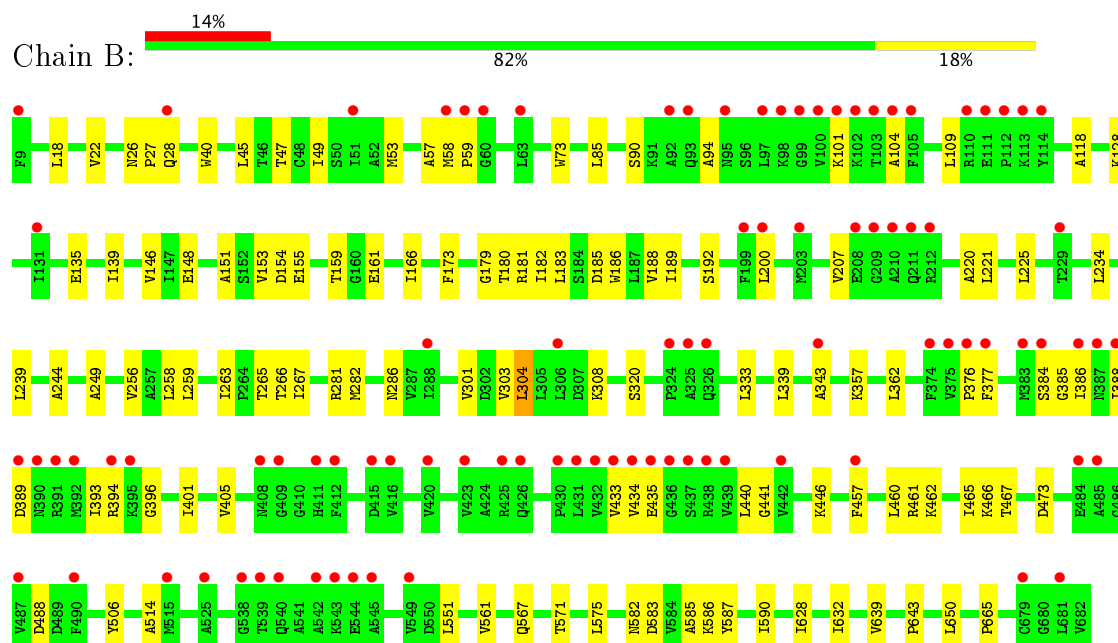


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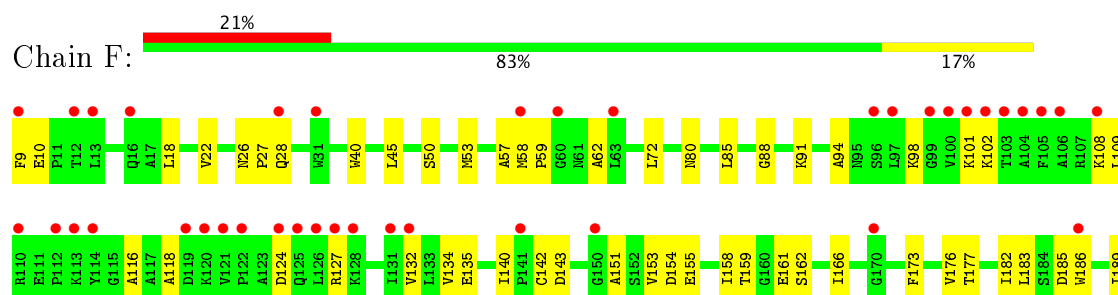
- Molecule 1: Potassium-transporting ATPase potassium-binding subunit

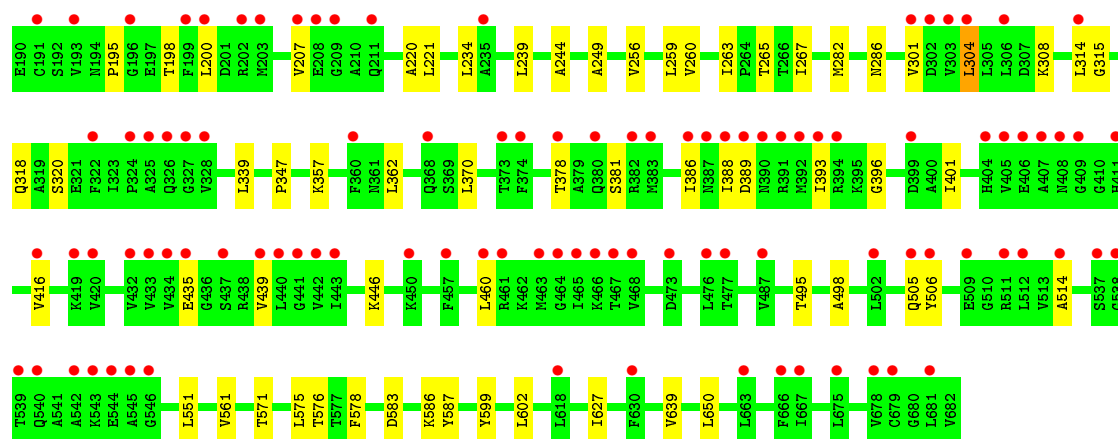


- Molecule 2: Potassium-transporting ATPase ATP-binding subunit

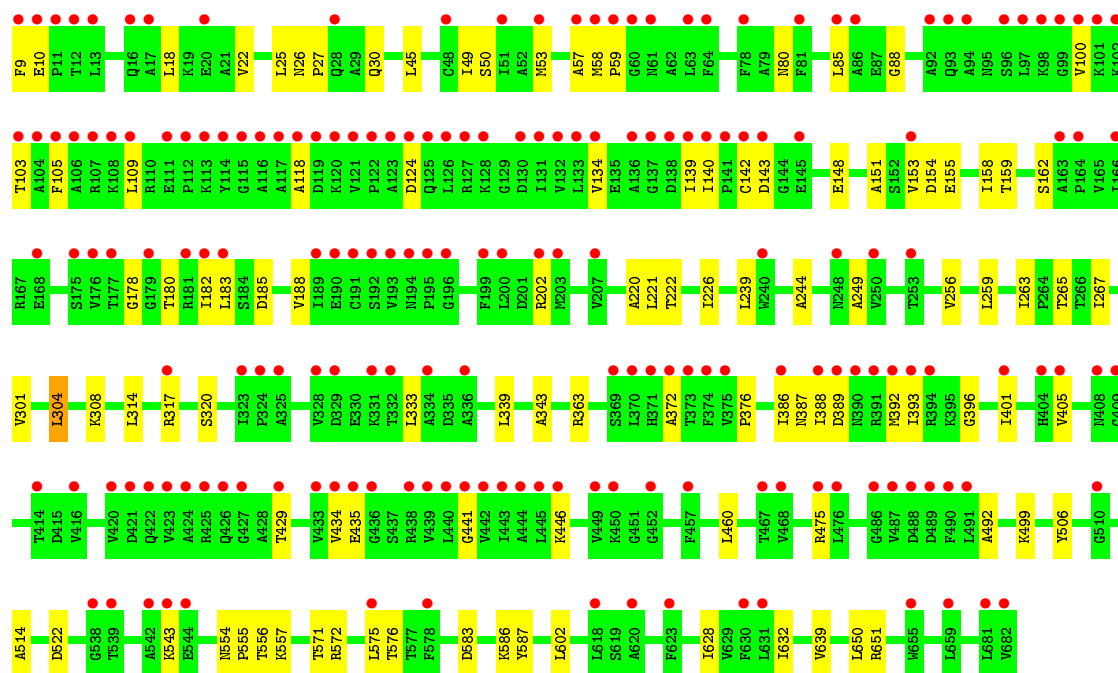
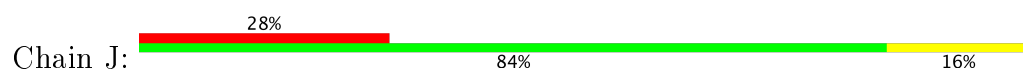


- Molecule 2: Potassium-transporting ATPase ATP-binding subunit

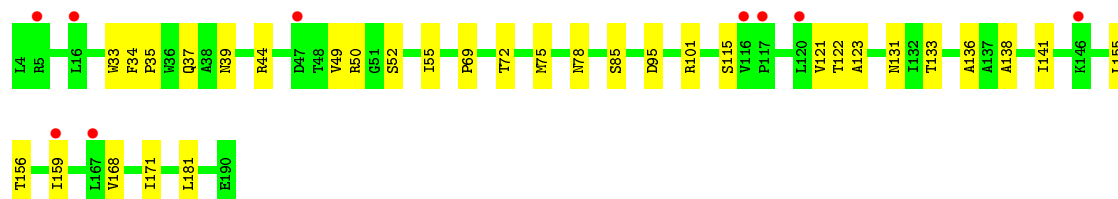
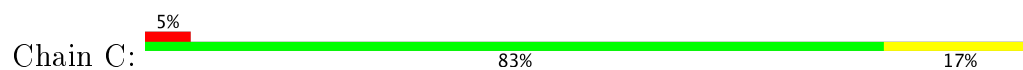




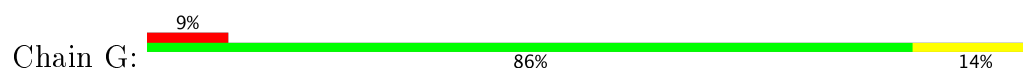
• Molecule 2: Potassium-transporting ATPase ATP-binding subunit

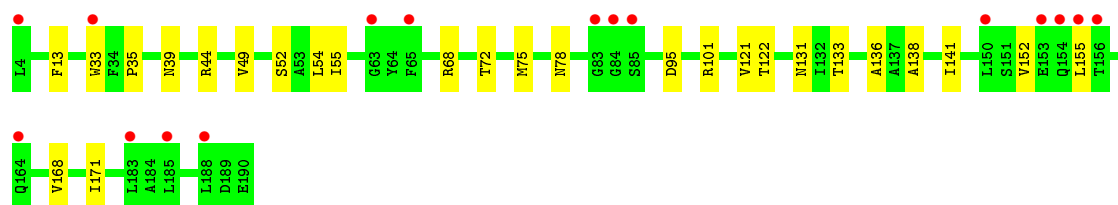


• Molecule 3: Potassium-transporting ATPase KdpC subunit

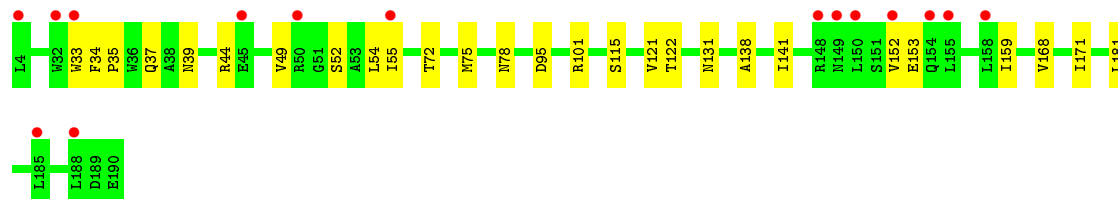
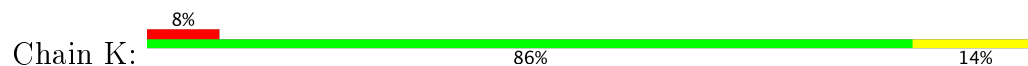


• Molecule 3: Potassium-transporting ATPase KdpC subunit

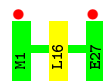




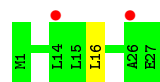
- Molecule 3: Potassium-transporting ATPase KdpC subunit



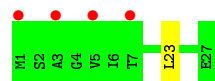
- Molecule 4: Potassium-transporting ATPase KdpF subunit



- Molecule 4: Potassium-transporting ATPase KdpF subunit



- Molecule 4: Potassium-transporting ATPase KdpF subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	124.72Å 166.29Å 196.30Å 90.00° 107.41° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 49.88 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.90) 99.4 (49.88-2.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.243 , 0.275 0.248 , 0.279	Depositor DCC
R_{free} test set	8370 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	94.7	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 92.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32666	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, BOG, PX4, SEP

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	0.25	0/4249	0.39	0/5784
1	E	0.27	1/4249 (0.0%)	0.39	0/5784
1	I	0.26	1/4249 (0.0%)	0.39	0/5784
2	B	0.24	0/5072	0.40	0/6889
2	F	0.24	0/5072	0.40	0/6889
2	J	0.24	0/5072	0.40	0/6889
3	C	0.24	0/1444	0.40	0/1977
3	G	0.24	0/1444	0.39	0/1977
3	K	0.24	0/1444	0.38	0/1977
4	D	0.23	0/202	0.37	0/275
4	H	0.23	0/202	0.36	0/275
4	L	0.23	0/202	0.37	0/275
All	All	0.25	2/32901 (0.0%)	0.39	0/44775

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	217	GLY	C-N	7.48	1.48	1.34
1	I	217	GLY	C-N	5.58	1.44	1.34

There are no bond angle outliers.

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	4157	0	4286	78	0
1	E	4157	0	4286	78	0
1	I	4157	0	4286	70	0
2	B	5008	0	5195	71	0
2	F	5008	0	5195	72	0
2	J	5008	0	5195	66	0
3	C	1413	0	1428	24	0
3	G	1413	0	1428	22	0
3	K	1413	0	1428	21	0
4	D	200	0	221	1	0
4	H	200	0	221	1	0
4	L	200	0	221	1	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
5	I	1	0	0	0	0
6	A	82	0	118	1	0
6	E	41	0	59	1	0
6	H	41	0	59	0	0
6	I	82	0	118	3	0
7	A	20	0	28	0	0
7	B	20	0	28	0	0
7	E	20	0	28	1	0
7	I	20	0	28	1	0
8	B	1	0	0	0	0
8	F	1	0	0	0	0
8	J	1	0	0	0	0
All	All	32666	0	33856	453	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 (453) 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)
1:A:545:PRO:HB2	2:B:239:LEU:HD21	1.65	0.79
1:I:545:PRO:HB2	2:J:239:LEU:HD21	1.65	0.76
1:E:545:PRO:HB2	2:F:239:LEU:HD21	1.69	0.72
1:E:340:THR:HG21	1:E:362:PRO:HB3	1.72	0.72
1:A:116:ARG:NH1	1:A:345:GLY:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:461:ARG:NH1	2:B:488:ASP:OD1	2.26	0.69
1:A:264:THR:HG23	1:A:284:LEU:HD11	1.75	0.69
2:B:303:VAL:HG22	2:B:466:LYS:HB2	1.75	0.69
1:A:340:THR:HG21	1:A:362:PRO:HB3	1.76	0.68
1:I:264:THR:HG23	1:I:284:LEU:HD11	1.76	0.68
1:I:116:ARG:NH1	1:I:345:GLY:O	2.26	0.67
1:A:214:LEU:HD11	3:C:55:ILE:HD11	1.77	0.67
1:I:398:ILE:HD11	2:J:650:LEU:HB2	1.76	0.66
2:B:385:GLY:HA3	2:B:394:ARG:HD3	1.78	0.66
1:A:195:LEU:HD21	1:A:216:MET:HA	1.78	0.65
2:J:158:ILE:HG13	2:J:159:THR:HG23	1.79	0.65
1:I:130:MET:O	1:I:134:THR:OG1	2.14	0.65
2:B:393:ILE:HG12	2:B:435:GLU:HG2	1.78	0.64
1:E:264:THR:HG23	1:E:284:LEU:HD11	1.79	0.64
2:J:45:LEU:HD11	2:J:256:VAL:HG21	1.80	0.64
1:I:214:LEU:HD11	3:K:55:ILE:HD11	1.79	0.64
2:B:396:GLY:H	2:B:401:ILE:HD11	1.61	0.64
1:E:195:LEU:HD21	1:E:216:MET:HA	1.80	0.64
3:K:35:PRO:O	3:K:39:ASN:ND2	2.31	0.64
2:J:304:LEU:HD21	2:J:460:LEU:HD21	1.80	0.63
3:C:168:VAL:HB	3:C:171:ILE:HG12	1.80	0.63
1:E:214:LEU:HD11	3:G:55:ILE:HD11	1.79	0.63
1:A:130:MET:O	1:A:134:THR:OG1	2.17	0.63
1:A:398:ILE:HD11	2:B:650:LEU:HB2	1.80	0.63
1:E:69:LEU:HD22	1:E:170:LEU:HD13	1.80	0.63
2:J:100:VAL:HG13	2:J:139:ILE:HD12	1.81	0.63
1:E:226:LYS:HA	1:E:231:ASN:HB2	1.81	0.63
1:I:230:THR:HG21	1:I:375:GLY:HA3	1.81	0.63
1:E:398:ILE:HD11	2:F:650:LEU:HB2	1.81	0.63
1:E:341:ALA:HB2	1:E:365:LEU:HD13	1.81	0.62
1:A:366:MET:SD	1:A:467:ASN:ND2	2.67	0.62
1:I:195:LEU:HD21	1:I:216:MET:HA	1.81	0.61
2:B:47:THR:HG21	2:B:73:TRP:HE1	1.63	0.61
1:A:400:ARG:NH2	1:A:517:SER:OG	2.33	0.61
3:G:168:VAL:HB	3:G:171:ILE:HG12	1.81	0.61
1:A:321:GLU:OE2	3:C:85:SER:OG	2.18	0.61
1:E:130:MET:O	1:E:134:THR:OG1	2.18	0.61
1:I:340:THR:HG21	1:I:362:PRO:HB3	1.83	0.61
2:F:45:LEU:HD11	2:F:256:VAL:HG21	1.82	0.61
1:A:226:LYS:HA	1:A:231:ASN:HB2	1.82	0.60
3:C:35:PRO:O	3:C:39:ASN:ND2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:304:LEU:HD21	2:F:460:LEU:HD21	1.83	0.60
2:J:396:GLY:H	2:J:401:ILE:HD11	1.66	0.60
2:B:154:ASP:HB2	2:B:183:LEU:HD11	1.82	0.60
1:I:376:VAL:O	1:I:378:SER:N	2.32	0.60
1:A:376:VAL:O	1:A:378:SER:N	2.33	0.60
1:A:239:ASN:HD21	1:A:347:VAL:H	1.50	0.60
2:F:339:LEU:HB3	2:F:386:ILE:HG21	1.84	0.60
1:I:392:PHE:HZ	2:J:220:ALA:HB1	1.65	0.60
1:I:526:LEU:HD22	2:J:651:ARG:HE	1.67	0.59
2:F:18:LEU:HD11	2:F:88:GLY:HA3	1.84	0.59
1:A:230:THR:HG21	1:A:375:GLY:HA3	1.84	0.59
3:G:35:PRO:O	3:G:39:ASN:ND2	2.33	0.59
3:K:168:VAL:HB	3:K:171:ILE:HG12	1.84	0.59
1:A:227:MET:HE1	1:A:259:ILE:HD11	1.85	0.59
2:B:304:LEU:HD21	2:B:460:LEU:HD21	1.84	0.58
1:I:308:HIS:ND1	3:K:95:ASP:OD2	2.33	0.58
2:B:101:LYS:HD3	2:B:200:LEU:HD12	1.85	0.58
1:I:400:ARG:NH2	1:I:517:SER:OG	2.37	0.58
1:A:341:ALA:HB2	1:A:365:LEU:HD13	1.85	0.58
1:I:239:ASN:HD21	1:I:347:VAL:H	1.50	0.58
1:E:239:ASN:HD21	1:E:347:VAL:H	1.51	0.58
2:F:571:THR:HG22	2:F:639:VAL:HG23	1.86	0.58
1:I:226:LYS:HA	1:I:231:ASN:HB2	1.85	0.57
1:I:239:ASN:HD21	1:I:347:VAL:N	2.02	0.57
1:I:366:MET:SD	1:I:467:ASN:ND2	2.68	0.57
1:A:239:ASN:HD21	1:A:347:VAL:N	2.02	0.57
2:F:315:GLY:O	2:F:318:GLN:NE2	2.36	0.57
1:E:227:MET:HE1	1:E:259:ILE:HD11	1.87	0.57
2:B:18:LEU:HD13	2:B:85:LEU:HA	1.86	0.57
2:J:267:ILE:HD12	2:J:576:THR:HG22	1.85	0.57
2:F:101:LYS:HD2	2:F:200:LEU:HD12	1.86	0.57
2:F:396:GLY:H	2:F:401:ILE:HD11	1.70	0.57
1:E:398:ILE:HD12	1:E:520:LEU:HD11	1.86	0.56
1:E:392:PHE:HZ	2:F:220:ALA:HB1	1.70	0.56
2:B:435:GLU:HG3	2:B:440:LEU:HD11	1.87	0.56
1:E:239:ASN:HD21	1:E:347:VAL:N	2.02	0.56
1:A:290:ILE:HD11	1:A:532:ILE:HG23	1.86	0.56
1:E:404:TYR:HD1	1:E:522:THR:HG21	1.71	0.56
2:J:25:LEU:O	2:J:30:GLN:NE2	2.35	0.56
1:I:197:ASN:HD22	3:K:39:ASN:HA	1.70	0.56
3:G:72:THR:OG1	3:G:75:MET:O	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:TYR:HD1	1:A:522:THR:HG21	1.70	0.56
2:B:45:LEU:HD11	2:B:256:VAL:HG21	1.88	0.56
1:E:396:LEU:HD21	2:F:221:LEU:HB3	1.88	0.55
1:I:352:ASP:OD1	1:I:451:HIS:NE2	2.31	0.55
2:J:22:VAL:HG13	2:J:80:ASN:HB2	1.89	0.55
1:A:398:ILE:HD12	1:A:520:LEU:HD11	1.88	0.55
1:A:308:HIS:ND1	3:C:95:ASP:OD2	2.39	0.55
1:E:230:THR:HG21	1:E:375:GLY:HA3	1.88	0.55
3:G:138:ALA:HA	3:G:141:ILE:HG13	1.89	0.55
2:J:554:ASN:HB3	2:J:557:LYS:HG3	1.87	0.55
1:E:295:VAL:HA	1:E:337:VAL:HG21	1.88	0.55
3:G:141:ILE:HG23	3:G:155:LEU:HD23	1.88	0.55
2:J:109:LEU:HD23	2:J:118:ALA:HB2	1.87	0.55
1:A:396:LEU:HD21	2:B:221:LEU:HB3	1.88	0.55
1:E:400:ARG:NH2	1:E:517:SER:OG	2.39	0.55
1:I:260:PHE:HE1	1:I:342:ALA:HB2	1.72	0.55
2:J:339:LEU:HB3	2:J:386:ILE:HG21	1.89	0.55
3:C:72:THR:OG1	3:C:75:MET:O	2.23	0.55
2:F:162:SEP:HB3	2:F:357:LYS:HE2	1.88	0.55
1:A:260:PHE:HE1	1:A:342:ALA:HB2	1.71	0.55
1:E:416:LEU:HB2	1:E:503:ILE:HD11	1.89	0.55
1:A:197:ASN:HB2	1:A:199:LEU:HD13	1.89	0.54
1:I:69:LEU:HD22	1:I:170:LEU:HD13	1.88	0.54
2:J:162:SEP:O1P	2:J:363:ARG:NH2	2.40	0.54
2:F:135:GLU:HA	2:F:186:TRP:HA	1.89	0.54
2:B:571:THR:HG22	2:B:639:VAL:HG23	1.89	0.54
1:E:366:MET:SD	1:E:467:ASN:ND2	2.68	0.54
1:A:548:ALA:HA	1:A:552:VAL:HB	1.90	0.54
1:E:116:ARG:NH1	1:E:345:GLY:O	2.40	0.54
1:I:341:ALA:HB2	1:I:365:LEU:HD13	1.89	0.54
3:K:138:ALA:HA	3:K:141:ILE:HG13	1.89	0.54
1:E:325:SER:HB2	3:G:131:ASN:HB2	1.89	0.54
3:G:101:ARG:HB2	3:G:121:VAL:HG23	1.90	0.54
2:B:179:GLY:HA3	2:B:200:LEU:HD11	1.90	0.54
1:I:396:LEU:HD21	2:J:221:LEU:HB3	1.90	0.54
1:A:416:LEU:HB2	1:A:503:ILE:HD11	1.90	0.53
1:E:376:VAL:O	1:E:378:SER:N	2.33	0.53
3:K:101:ARG:HB2	3:K:121:VAL:HG23	1.89	0.53
2:F:495:THR:HG23	2:F:498:ALA:H	1.74	0.53
1:I:325:SER:HB2	3:K:131:ASN:HB2	1.90	0.53
2:B:339:LEU:HB3	2:B:386:ILE:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:ILE:HD11	1:E:532:ILE:HG23	1.90	0.53
1:E:260:PHE:HE1	1:E:342:ALA:HB2	1.73	0.53
1:E:548:ALA:HA	1:E:552:VAL:HB	1.90	0.53
1:I:394:ALA:HB2	1:I:530:LEU:HD21	1.90	0.53
3:C:115:SER:HB3	1:E:158:GLN:HG3	1.89	0.53
1:I:227:MET:HE1	1:I:259:ILE:HD11	1.91	0.53
1:A:352:ASP:HB2	1:A:471:PHE:O	2.09	0.53
2:B:153:VAL:HG12	2:B:182:ILE:HG13	1.91	0.53
1:I:398:ILE:HD12	1:I:520:LEU:HD11	1.89	0.53
1:A:352:ASP:OD1	1:A:451:HIS:NE2	2.27	0.53
2:B:433:VAL:HG13	2:B:440:LEU:HB2	1.90	0.53
2:F:18:LEU:HD13	2:F:85:LEU:HA	1.90	0.52
1:A:321:GLU:HA	3:C:122:THR:HB	1.91	0.52
1:A:432:ALA:HB2	1:A:460:VAL:HG21	1.91	0.52
1:I:392:PHE:CZ	2:J:220:ALA:HB1	2.43	0.52
2:J:154:ASP:HB2	2:J:183:LEU:HD11	1.90	0.52
1:E:352:ASP:HB2	1:E:471:PHE:O	2.10	0.52
1:E:321:GLU:HA	3:G:122:THR:HB	1.90	0.52
1:I:335:PHE:HB3	1:I:348:ILE:HG21	1.91	0.52
1:E:197:ASN:HD22	3:G:39:ASN:HA	1.75	0.52
1:E:432:ALA:HB2	1:E:460:VAL:HG21	1.90	0.52
1:A:238:ALA:O	1:A:242:HIS:HB2	2.09	0.52
3:C:138:ALA:HA	3:C:141:ILE:HG13	1.91	0.52
1:I:243:PRO:HB2	3:K:54:LEU:HB3	1.91	0.52
1:A:69:LEU:HD22	1:A:170:LEU:HD13	1.92	0.52
3:C:75:MET:HG3	3:C:78:ASN:HB2	1.92	0.52
1:I:295:VAL:HA	1:I:337:VAL:HG21	1.90	0.52
2:J:103:THR:HG21	2:J:139:ILE:HD11	1.91	0.52
3:K:72:THR:OG1	3:K:75:MET:O	2.26	0.52
1:E:352:ASP:OD1	1:E:451:HIS:NE2	2.28	0.51
1:I:544:ILE:HG22	1:I:545:PRO:HD3	1.92	0.51
2:B:90:SER:HB2	2:B:207:VAL:HG13	1.91	0.51
1:E:378:SER:HA	1:E:381:TYR:CZ	2.44	0.51
1:A:187:LEU:HD13	3:C:33:TRP:HZ3	1.76	0.51
2:F:153:VAL:HG12	2:F:182:ILE:HG13	1.91	0.51
2:F:53:MET:HA	2:F:57:ALA:HB3	1.92	0.51
1:I:548:ALA:HA	1:I:552:VAL:HB	1.91	0.51
2:J:393:ILE:HG12	2:J:435:GLU:HG2	1.93	0.51
2:F:109:LEU:HD22	2:F:116:ALA:HB3	1.92	0.51
1:A:197:ASN:HD22	3:C:39:ASN:HA	1.75	0.51
2:B:159:THR:HG23	2:B:161:GLU:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:THR:HG21	1:E:489:MET:HB3	1.91	0.51
2:J:49:ILE:O	2:J:53:MET:N	2.34	0.51
1:A:378:SER:HA	1:A:381:TYR:CE2	2.46	0.51
2:B:135:GLU:HA	2:B:186:TRP:HA	1.92	0.51
1:I:321:GLU:HA	3:K:122:THR:HB	1.93	0.51
1:I:432:ALA:HB2	1:I:460:VAL:HG21	1.93	0.51
1:I:84:GLN:OE1	1:I:125:SER:N	2.44	0.51
1:E:43:GLU:OE1	1:E:172:ARG:NH1	2.44	0.50
3:C:44:ARG:HG2	3:C:49:VAL:HA	1.93	0.50
1:E:335:PHE:HB3	1:E:348:ILE:HG21	1.92	0.50
1:I:197:ASN:HB2	1:I:199:LEU:HD13	1.93	0.50
2:F:154:ASP:HB2	2:F:183:LEU:HD11	1.93	0.50
1:I:238:ALA:O	1:I:242:HIS:HB2	2.11	0.50
2:J:571:THR:HG22	2:J:639:VAL:HG23	1.92	0.50
2:B:49:ILE:O	2:B:53:MET:N	2.34	0.50
2:B:466:LYS:HD3	3:K:153:GLU:OE2	2.12	0.50
2:B:18:LEU:O	2:B:22:VAL:HG23	2.12	0.50
1:E:238:ALA:O	1:E:242:HIS:HB2	2.11	0.50
2:J:301:VAL:HG21	2:J:514:ALA:HB2	1.93	0.50
2:F:109:LEU:HD23	2:F:118:ALA:HB2	1.94	0.49
1:E:378:SER:HA	1:E:381:TYR:CE2	2.47	0.49
2:B:281:ARG:NH2	2:B:567:GLN:OE1	2.45	0.49
1:I:114:ASN:ND2	1:I:231:ASN:HB3	2.28	0.49
2:B:583:ASP:HA	2:B:586:LYS:HD3	1.95	0.49
1:E:394:ALA:HB2	1:E:530:LEU:HD21	1.95	0.49
3:K:44:ARG:HG2	3:K:49:VAL:HA	1.95	0.49
1:I:148:ILE:HD13	1:I:381:TYR:HB3	1.95	0.49
2:B:109:LEU:HD23	2:B:118:ALA:HB2	1.94	0.49
1:E:197:ASN:HB2	1:E:199:LEU:HD13	1.93	0.49
6:I:603:PX4:H55	6:I:603:PX4:H16	1.95	0.49
2:B:53:MET:HG3	2:B:59:PRO:HG2	1.95	0.48
3:G:44:ARG:HG2	3:G:49:VAL:HA	1.94	0.48
1:I:378:SER:HA	1:I:381:TYR:CZ	2.47	0.48
2:F:134:VAL:HG11	2:F:140:ILE:HD13	1.95	0.48
2:F:159:THR:HG23	2:F:161:GLU:H	1.79	0.48
1:A:114:ASN:ND2	1:A:231:ASN:HB3	2.28	0.48
2:B:396:GLY:N	2:B:401:ILE:HD11	2.28	0.48
1:I:352:ASP:HB2	1:I:471:PHE:O	2.13	0.48
2:J:103:THR:HB	2:J:105:PHE:CE2	2.48	0.48
3:C:101:ARG:HB2	3:C:121:VAL:HG23	1.96	0.48
2:B:286:ASN:HB3	2:B:551:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ALA:HB2	2:B:139:ILE:HD11	1.95	0.48
2:J:405:VAL:HG22	2:J:434:VAL:HG11	1.96	0.48
2:F:98:LYS:HG2	2:F:102:LYS:NZ	2.29	0.48
1:I:404:TYR:HD1	1:I:522:THR:HG21	1.79	0.47
2:F:9:PHE:CD2	2:F:10:GLU:HG3	2.49	0.47
2:J:53:MET:HA	2:J:57:ALA:HB3	1.95	0.47
2:B:357:LYS:HA	2:B:362:LEU:H	1.80	0.47
1:E:219:VAL:HG11	1:E:245:GLU:HG2	1.96	0.47
2:F:98:LYS:HG2	2:F:102:LYS:HZ1	1.78	0.47
2:F:158:ILE:HG21	2:F:177:THR:HG21	1.95	0.47
1:I:502:ALA:HB1	7:I:604:BOG:H2'2	1.96	0.47
1:A:394:ALA:HB2	1:A:530:LEU:HD21	1.96	0.47
1:A:145:ILE:HB	1:A:173:ILE:HD13	1.96	0.47
2:B:282:MET:HE3	2:B:561:VAL:HG22	1.95	0.47
2:J:244:ALA:HB2	2:J:249:ALA:HB2	1.97	0.47
3:K:75:MET:HG3	3:K:78:ASN:HB2	1.96	0.47
1:E:416:LEU:HD11	7:E:603:BOG:H4'2	1.97	0.47
2:J:9:PHE:CD2	2:J:10:GLU:HG3	2.50	0.47
1:E:74:LEU:HB3	1:E:110:VAL:HG21	1.96	0.47
2:F:26:ASN:N	2:F:27:PRO:HD2	2.30	0.47
2:J:343:ALA:HB1	2:J:376:PRO:HA	1.97	0.47
1:A:378:SER:HA	1:A:381:TYR:CZ	2.50	0.47
1:A:434:LEU:HD23	1:A:484:LEU:HD13	1.97	0.47
1:A:335:PHE:HB3	1:A:348:ILE:HG21	1.96	0.47
2:F:108:LYS:HA	2:F:132:VAL:HA	1.96	0.47
2:J:153:VAL:HG12	2:J:182:ILE:HG13	1.97	0.47
2:B:308:LYS:NZ	2:B:473:ASP:OD2	2.40	0.47
2:B:53:MET:HA	2:B:57:ALA:HB3	1.97	0.47
3:G:52:SER:OG	3:G:55:ILE:HG13	2.14	0.47
1:A:345:GLY:HA2	1:A:469:SER:OG	2.15	0.47
2:F:378:THR:HG1	2:F:381:SER:HG	1.55	0.47
1:I:56:GLU:HB3	1:I:162:THR:HB	1.97	0.46
2:J:221:LEU:HD21	2:J:572:ARG:HD3	1.96	0.46
2:J:267:ILE:HG22	2:J:575:LEU:HB3	1.98	0.46
1:A:158:GLN:HG3	3:K:115:SER:HB3	1.96	0.46
2:B:244:ALA:HB2	2:B:249:ALA:HB2	1.98	0.46
2:B:343:ALA:HB1	2:B:376:PRO:HA	1.96	0.46
2:B:146:VAL:HG22	2:B:189:ILE:HG22	1.97	0.46
1:E:392:PHE:CZ	2:F:220:ALA:HB1	2.48	0.46
2:F:357:LYS:HA	2:F:362:LEU:H	1.81	0.46
1:E:345:GLY:HA2	1:E:469:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:462:LYS:HB2	2:B:643:PRO:HB2	1.97	0.46
2:F:320:SER:HB2	2:F:446:LYS:HG2	1.97	0.46
1:E:114:ASN:ND2	1:E:231:ASN:HB3	2.31	0.46
1:I:345:GLY:HA2	1:I:469:SER:OG	2.15	0.46
2:J:155:GLU:HG2	2:J:180:THR:HG21	1.97	0.46
2:J:26:ASN:N	2:J:27:PRO:HD2	2.30	0.46
1:E:556:LEU:HD12	2:F:602:LEU:HD23	1.98	0.46
2:J:222:THR:O	2:J:226:ILE:HG12	2.16	0.46
1:E:56:GLU:HB3	1:E:162:THR:HB	1.97	0.46
2:F:416:VAL:HG11	2:F:439:VAL:HG11	1.98	0.46
2:B:26:ASN:N	2:B:27:PRO:HD2	2.31	0.45
1:I:187:LEU:HD13	3:K:33:TRP:HZ3	1.81	0.45
2:B:139:ILE:HG22	2:B:181:ARG:HB2	1.99	0.45
2:J:18:LEU:HD11	2:J:88:GLY:HA3	1.98	0.45
3:K:52:SER:OG	3:K:55:ILE:HG13	2.16	0.45
1:A:374:GLY:HA3	1:A:379:GLY:HA3	1.98	0.45
1:A:129:GLN:O	1:A:134:THR:HG23	2.17	0.45
1:E:419:LEU:O	1:E:423:VAL:HG23	2.17	0.45
1:E:450:PRO:HG3	2:F:599:TYR:CE1	2.52	0.45
2:F:53:MET:HG3	2:F:59:PRO:HG2	1.99	0.45
2:J:50:SER:HA	2:J:53:MET:HB3	1.98	0.45
2:B:173:PHE:CE2	2:B:343:ALA:HA	2.51	0.45
1:I:219:VAL:HG11	1:I:245:GLU:HG2	1.98	0.45
1:I:219:VAL:HG22	1:I:235:PHE:CG	2.52	0.45
2:B:263:ILE:O	2:B:265:THR:N	2.49	0.45
1:I:378:SER:HA	1:I:381:TYR:CE2	2.51	0.45
1:I:419:LEU:O	1:I:423:VAL:HG23	2.17	0.45
2:J:124:ASP:N	2:J:124:ASP:OD1	2.50	0.45
2:J:628:ILE:O	2:J:632:ILE:HG13	2.17	0.45
1:A:325:SER:OG	3:C:131:ASN:HB2	2.17	0.45
2:F:318:GLN:HE22	2:F:347:PRO:HB2	1.81	0.45
1:A:56:GLU:HB3	1:A:162:THR:HB	1.99	0.45
2:J:388:ILE:HG23	2:J:389:ASP:H	1.80	0.45
1:I:193:GLY:HA2	3:K:37:GLN:HB3	1.98	0.44
2:J:317:ARG:HH11	2:J:429:THR:HG23	1.82	0.44
2:J:320:SER:HB2	2:J:446:LYS:HG2	1.98	0.44
2:B:155:GLU:O	2:B:159:THR:HG22	2.17	0.44
2:B:148:GLU:HB2	2:B:188:VAL:HB	1.99	0.44
1:E:89:LEU:HB2	1:E:127:PHE:HB2	1.99	0.44
1:E:243:PRO:HB2	3:G:54:LEU:HB3	1.99	0.44
2:F:22:VAL:HG13	2:F:80:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:393:ILE:HG12	2:F:435:GLU:HG2	1.98	0.44
3:C:141:ILE:HG23	3:C:155:LEU:HD23	2.00	0.44
2:F:301:VAL:HG21	2:F:514:ALA:HB2	2.00	0.44
2:J:18:LEU:HD13	2:J:85:LEU:HA	1.99	0.44
2:J:583:ASP:HA	2:J:586:LYS:HD3	1.99	0.44
1:A:74:LEU:HB3	1:A:110:VAL:HG21	1.98	0.44
2:F:124:ASP:OD1	2:F:124:ASP:N	2.49	0.44
2:J:134:VAL:HG11	2:J:140:ILE:HD13	2.00	0.44
1:A:318:ILE:HG22	1:A:320:MET:HG2	2.00	0.44
2:B:320:SER:HB2	2:B:446:LYS:HG2	1.98	0.44
2:B:388:ILE:HG23	2:B:389:ASP:H	1.83	0.44
2:B:234:LEU:HD21	4:D:16:LEU:HD11	1.99	0.44
1:E:129:GLN:O	1:E:134:THR:HG23	2.17	0.44
2:F:263:ILE:O	2:F:265:THR:N	2.50	0.44
2:J:499:LYS:NZ	2:J:522:ASP:OD1	2.48	0.44
2:J:53:MET:HG3	2:J:59:PRO:HG2	2.00	0.44
1:A:205:ASN:OD1	1:A:211:GLN:NE2	2.51	0.44
2:F:176:VAL:HG11	2:F:189:ILE:HG21	1.99	0.44
1:I:197:ASN:ND2	3:K:39:ASN:HA	2.33	0.44
2:F:583:ASP:HA	2:F:586:LYS:HD3	1.99	0.44
3:K:141:ILE:HG21	3:K:152:VAL:HG13	2.00	0.44
1:A:219:VAL:HG11	1:A:245:GLU:HG2	1.99	0.44
1:A:351:HIS:HA	1:A:354:PHE:CD1	2.53	0.44
2:B:151:ALA:HB2	2:B:185:ASP:HB2	2.00	0.44
3:C:133:THR:HG23	3:C:136:ALA:H	1.83	0.44
3:C:159:ILE:HG12	3:C:181:LEU:HD21	2.00	0.44
2:F:282:MET:HE3	2:F:561:VAL:HG22	1.99	0.44
3:G:75:MET:HG3	3:G:78:ASN:HB2	1.99	0.44
2:J:148:GLU:HB2	2:J:188:VAL:HB	2.00	0.44
2:J:18:LEU:O	2:J:22:VAL:HG23	2.18	0.44
2:J:333:LEU:HD11	2:J:441:GLY:HA3	2.00	0.44
1:A:371:VAL:HG13	1:A:383:MET:HB2	2.00	0.43
2:B:377:PHE:HB2	2:B:384:SER:HB3	2.00	0.43
2:F:388:ILE:HG23	2:F:389:ASP:H	1.82	0.43
2:F:58:MET:N	2:F:59:PRO:HD2	2.33	0.43
2:J:314:LEU:O	2:J:555:PRO:HG2	2.18	0.43
2:B:457:PHE:CE1	2:B:467:THR:HG21	2.53	0.43
1:E:249:ALA:HB1	3:G:171:ILE:HG22	2.00	0.43
1:I:222:GLN:HA	1:I:225:ILE:HD12	1.99	0.43
1:A:115:TRP:HE1	1:A:117:SER:HB3	1.82	0.43
1:A:84:GLN:OE1	1:A:125:SER:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ILE:HD13	1:E:152:ILE:HG21	1.99	0.43
1:I:434:LEU:HD23	1:I:484:LEU:HD13	1.99	0.43
1:I:544:ILE:HA	1:I:544:ILE:HD12	1.86	0.43
2:J:308:LYS:HG3	2:J:314:LEU:HD23	2.00	0.43
2:J:372:ALA:HB2	2:J:388:ILE:HA	2.00	0.43
1:A:154:ALA:HA	1:A:508:VAL:HG22	2.00	0.43
2:F:244:ALA:HB2	2:F:249:ALA:HB2	2.01	0.43
1:A:441:GLY:HA2	1:A:481:TRP:HE1	1.83	0.43
2:B:128:LYS:HG3	2:B:192:SER:HA	2.01	0.43
1:A:392:PHE:CZ	2:B:220:ALA:HB1	2.54	0.43
2:F:91:LYS:HD2	2:F:94:ALA:HB3	1.99	0.43
2:J:314:LEU:O	2:J:556:THR:OG1	2.37	0.43
2:J:475:ARG:HG2	2:J:492:ALA:HB3	2.00	0.43
1:A:441:GLY:HA2	1:A:481:TRP:NE1	2.33	0.43
3:C:52:SER:OG	3:C:55:ILE:HG13	2.18	0.43
2:F:127:ARG:NH1	2:F:195:PRO:HG2	2.34	0.43
2:F:18:LEU:O	2:F:22:VAL:HG23	2.17	0.43
2:J:58:MET:N	2:J:59:PRO:HD2	2.33	0.43
2:B:155:GLU:HG2	2:B:180:THR:HG21	2.01	0.43
1:I:556:LEU:HD12	2:J:602:LEU:HD23	2.01	0.43
2:B:301:VAL:HG21	2:B:514:ALA:HB2	2.00	0.43
1:E:222:GLN:HA	1:E:225:ILE:HD12	2.00	0.43
1:E:441:GLY:HA2	1:E:481:TRP:NE1	2.34	0.43
1:E:84:GLN:OE1	1:E:125:SER:N	2.52	0.43
1:I:115:TRP:HE1	1:I:117:SER:HB3	1.84	0.43
1:A:260:PHE:CE1	1:A:342:ALA:HB2	2.52	0.43
1:A:380:LEU:O	1:A:384:MET:HG2	2.18	0.43
2:F:578:PHE:HE2	2:F:627:ILE:HD11	1.83	0.43
2:J:263:ILE:O	2:J:265:THR:N	2.51	0.43
2:B:258:LEU:HB2	2:B:590:ILE:HG21	2.00	0.42
1:E:425:PRO:HA	1:E:428:VAL:HG22	2.00	0.42
1:I:293:ILE:HG22	6:I:603:PX4:H48	2.01	0.42
1:I:485:LEU:O	1:I:489:MET:HG3	2.19	0.42
2:J:202:ARG:HH22	2:J:543:LYS:HD3	1.84	0.42
2:B:333:LEU:HD11	2:B:441:GLY:HA3	2.01	0.42
1:E:115:TRP:HE1	1:E:117:SER:HB3	1.83	0.42
3:G:133:THR:HG23	3:G:136:ALA:H	1.84	0.42
3:G:141:ILE:HG21	3:G:152:VAL:HG13	2.00	0.42
1:E:197:ASN:ND2	3:G:39:ASN:HA	2.33	0.42
1:E:260:PHE:CE1	1:E:342:ALA:HB2	2.54	0.42
1:I:145:ILE:HB	1:I:173:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:159:ILE:HG12	3:K:181:LEU:HD21	2.01	0.42
2:B:58:MET:N	2:B:59:PRO:HD2	2.33	0.42
1:I:74:LEU:HB3	1:I:110:VAL:HG21	2.00	0.42
2:F:155:GLU:O	2:F:159:THR:HG22	2.18	0.42
3:C:156:THR:HG21	2:F:505:GLN:HG2	2.00	0.42
1:I:266:LEU:HB3	1:I:380:LEU:HD22	2.01	0.42
2:F:101:LYS:NZ	2:F:198:THR:HG21	2.35	0.42
1:I:456:VAL:HG13	1:I:481:TRP:HH2	1.84	0.42
1:A:426:THR:HG21	6:A:602:PX4:H48	2.00	0.42
2:B:28:GLN:HG2	2:B:40:TRP:CH2	2.54	0.42
1:E:219:VAL:HG22	1:E:235:PHE:CG	2.54	0.42
2:J:142:CYS:SG	2:J:143:ASP:N	2.92	0.42
1:A:31:ILE:HD13	1:A:152:ILE:HG21	2.01	0.42
1:A:300:TRP:HZ3	1:A:357:LEU:HD12	1.84	0.42
2:B:225:LEU:HD21	2:B:267:ILE:HD11	2.02	0.42
2:B:460:LEU:HG	2:B:465:ILE:HB	2.01	0.42
2:J:226:ILE:HG21	4:L:23:LEU:HB2	2.02	0.42
2:B:166:ILE:HG13	2:B:173:PHE:HD2	1.84	0.42
2:B:94:ALA:HB2	2:B:207:VAL:HG11	2.02	0.42
1:E:504:ALA:O	1:E:508:VAL:HG23	2.19	0.42
2:J:143:ASP:OD1	2:J:178:GLY:N	2.35	0.42
1:E:108:SER:HB3	1:E:115:TRP:H	1.85	0.41
1:A:367:GLN:HB3	1:A:543:PHE:CE2	2.54	0.41
1:E:255:GLN:O	1:E:259:ILE:HG13	2.20	0.41
1:I:318:ILE:HG22	1:I:320:MET:HG2	2.01	0.41
2:J:387:ASN:CG	2:J:392:MET:HG2	2.40	0.41
1:A:222:GLN:HA	1:A:225:ILE:HD12	2.03	0.41
1:A:197:ASN:ND2	3:C:39:ASN:HA	2.34	0.41
1:E:145:ILE:HB	1:E:173:ILE:HD13	2.03	0.41
2:F:142:CYS:SG	2:F:143:ASP:N	2.93	0.41
2:F:308:LYS:HG3	2:F:314:LEU:HD23	2.01	0.41
2:J:26:ASN:N	2:J:27:PRO:CD	2.84	0.41
2:F:151:ALA:HB2	2:F:185:ASP:HB2	2.02	0.41
1:E:175:LEU:HD11	3:G:13:PHE:HE2	1.85	0.41
1:I:260:PHE:CE1	1:I:342:ALA:HB2	2.52	0.41
6:I:602:PX4:H62	6:I:602:PX4:H69	1.92	0.41
2:J:151:ALA:HB2	2:J:185:ASP:HB2	2.02	0.41
2:F:28:GLN:HG2	2:F:40:TRP:CH2	2.56	0.41
1:A:219:VAL:HG22	1:A:235:PHE:CG	2.56	0.41
1:A:504:ALA:O	1:A:508:VAL:HG23	2.20	0.41
2:B:628:ILE:O	2:B:632:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:LEU:HD13	3:G:33:TRP:HZ3	1.86	0.41
2:F:26:ASN:N	2:F:27:PRO:CD	2.83	0.41
1:I:214:LEU:HA	1:I:214:LEU:HD23	1.93	0.41
2:B:582:ASN:HA	2:B:665:PRO:HG3	2.01	0.41
2:F:267:ILE:HD12	2:F:576:THR:HG22	2.03	0.41
2:F:94:ALA:HB2	2:F:207:VAL:HG11	2.03	0.41
1:E:308:HIS:ND1	3:G:95:ASP:OD2	2.53	0.41
1:A:202:GLN:HB3	1:A:214:LEU:HB2	2.03	0.41
2:B:405:VAL:HG22	2:B:434:VAL:HG11	2.03	0.41
1:E:367:GLN:HB3	1:E:543:PHE:CZ	2.56	0.41
1:E:441:GLY:HA2	1:E:481:TRP:HE1	1.84	0.41
1:I:172:ARG:HG2	1:I:176:TRP:CZ3	2.55	0.41
1:A:425:PRO:HA	1:A:428:VAL:HG22	2.03	0.41
1:A:87:LEU:HD13	1:A:127:PHE:CE2	2.55	0.41
6:E:602:PX4:H54	6:E:602:PX4:H49	1.81	0.41
2:F:370:LEU:HB3	2:F:388:ILE:HG13	2.03	0.41
2:F:50:SER:HA	2:F:53:MET:HB3	2.03	0.41
1:I:277:ARG:HB3	1:I:281:ARG:NH1	2.35	0.41
2:B:585:ALA:HB3	2:B:665:PRO:HB2	2.02	0.41
3:C:69:PRO:HG2	3:C:123:ALA:HA	2.02	0.41
2:F:234:LEU:HD21	4:H:16:LEU:HD11	2.02	0.41
1:E:526:LEU:HD21	2:F:650:LEU:HD23	2.02	0.41
1:A:485:LEU:O	1:A:489:MET:HG3	2.21	0.41
2:B:267:ILE:HG22	2:B:575:LEU:HB3	2.03	0.41
2:B:26:ASN:N	2:B:27:PRO:CD	2.84	0.41
1:E:380:LEU:O	1:E:384:MET:HG2	2.21	0.41
2:F:72:LEU:HD22	2:F:260:VAL:HG11	2.03	0.41
3:C:50:ARG:HA	3:C:50:ARG:HD3	1.89	0.40
2:F:53:MET:SD	2:F:62:ALA:HA	2.61	0.40
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.95	0.40
1:A:193:GLY:HA2	3:C:37:GLN:HB3	2.04	0.40
1:E:283:LEU:HA	1:E:283:LEU:HD12	1.92	0.40
1:A:30:LEU:HD22	1:A:172:ARG:HD2	2.03	0.40
1:E:320:MET:O	3:G:68:ARG:NH2	2.53	0.40
2:F:166:ILE:HG13	2:F:173:PHE:HD2	1.86	0.40
2:F:286:ASN:HB3	2:F:551:LEU:HB2	2.04	0.40
2:F:575:LEU:HD23	2:F:575:LEU:HA	1.93	0.40
1:A:262:ILE:N	1:A:263:PRO:HD2	2.37	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	555/557 (100%)	529 (95%)	24 (4%)	2 (0%)	38	72
1	E	555/557 (100%)	531 (96%)	22 (4%)	2 (0%)	38	72
1	I	555/557 (100%)	529 (95%)	24 (4%)	2 (0%)	38	72
2	B	671/674 (100%)	648 (97%)	23 (3%)	0	100	100
2	F	671/674 (100%)	647 (96%)	24 (4%)	0	100	100
2	J	671/674 (100%)	647 (96%)	24 (4%)	0	100	100
3	C	185/187 (99%)	174 (94%)	11 (6%)	0	100	100
3	G	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
3	K	185/187 (99%)	174 (94%)	11 (6%)	0	100	100
4	D	25/27 (93%)	25 (100%)	0	0	100	100
4	H	25/27 (93%)	25 (100%)	0	0	100	100
4	L	25/27 (93%)	25 (100%)	0	0	100	100
All	All	4308/4335 (99%)	4129 (96%)	173 (4%)	6 (0%)	55	85

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	GLY
1	I	377	GLY
1	E	377	GLY
1	A	376	VAL
1	E	376	VAL
1	I	376	VAL

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	439/439 (100%)	435 (99%)	4 (1%)	82	95
1	E	439/439 (100%)	435 (99%)	4 (1%)	82	95
1	I	439/439 (100%)	436 (99%)	3 (1%)	87	97
2	B	523/523 (100%)	518 (99%)	5 (1%)	80	95
2	F	523/523 (100%)	519 (99%)	4 (1%)	85	96
2	J	523/523 (100%)	519 (99%)	4 (1%)	85	96
3	C	149/149 (100%)	148 (99%)	1 (1%)	87	97
3	G	149/149 (100%)	149 (100%)	0	100	100
3	K	149/149 (100%)	148 (99%)	1 (1%)	87	97
4	D	21/21 (100%)	21 (100%)	0	100	100
4	H	21/21 (100%)	21 (100%)	0	100	100
4	L	21/21 (100%)	21 (100%)	0	100	100
All	All	3396/3396 (100%)	3370 (99%)	26 (1%)	85	96

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ARG
1	A	225	ILE
1	A	282	MET
1	A	424	THR
2	B	259	LEU
2	B	266	THR
2	B	304	LEU
2	B	506	TYR
2	B	587	TYR
3	C	34	PHE
1	E	116	ARG
1	E	225	ILE
1	E	282	MET
1	E	424	THR
2	F	259	LEU
2	F	304	LEU
2	F	506	TYR
2	F	587	TYR

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Mol	Chain	Res	Type
1	I	116	ARG
1	I	159	SER
1	I	424	THR
2	J	259	LEU
2	J	304	LEU
2	J	506	TYR
2	J	587	TYR
3	K	34	PHE

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	112	ASN
1	A	114	ASN
1	A	211	GLN
1	A	239	ASN
1	E	114	ASN
1	E	239	ASN
2	F	624	ASN
2	J	624	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
2	SEP	B	162	2	9,9,10	1.53	2 (22%)	9,12,14	1.78	2 (22%)
2	SEP	F	162	2	9,9,10	1.53	2 (22%)	9,12,14	1.63	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SEP	J	162	2	9,9,10	1.55	2 (22%)	9,12,14	1.75	2 (22%)

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
2	SEP	B	162	2	-	0/5/8/10	0/0/0/0
2	SEP	F	162	2	-	0/5/8/10	0/0/0/0
2	SEP	J	162	2	-	0/5/8/10	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	162	SEP	CA-C	2.01	1.52	1.50
2	F	162	SEP	CA-C	2.02	1.52	1.50
2	J	162	SEP	CA-C	2.15	1.53	1.50
2	F	162	SEP	P-O1P	3.13	1.61	1.50
2	B	162	SEP	P-O1P	3.13	1.61	1.50
2	J	162	SEP	P-O1P	3.15	1.61	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	162	SEP	P-OG-CB	-3.36	109.03	118.30
2	J	162	SEP	P-OG-CB	-3.26	109.30	118.30
2	F	162	SEP	P-OG-CB	-3.18	109.54	118.30
2	F	162	SEP	OG-CB-CA	2.88	111.01	108.17
2	J	162	SEP	OG-CB-CA	3.30	111.42	108.17
2	B	162	SEP	OG-CB-CA	3.34	111.46	108.17

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
2	F	162	SEP	1	0
2	J	162	SEP	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	PX4	A	602	-	40,40,45	1.25	4 (10%)	42,45,53	1.19	2 (4%)
6	PX4	A	603	-	40,40,45	1.25	5 (12%)	42,45,53	1.14	2 (4%)
7	BOG	A	604	-	20,20,20	1.23	1 (5%)	25,25,25	0.81	0
7	BOG	B	701	-	20,20,20	1.23	1 (5%)	25,25,25	0.82	0
6	PX4	E	602	-	40,40,45	1.24	5 (12%)	42,45,53	1.15	2 (4%)
7	BOG	E	603	-	20,20,20	1.24	1 (5%)	25,25,25	0.83	0
6	PX4	H	101	-	40,40,45	1.25	4 (10%)	42,45,53	1.15	2 (4%)
6	PX4	I	602	-	40,40,45	1.25	5 (12%)	42,45,53	1.10	2 (4%)
6	PX4	I	603	-	40,40,45	1.24	4 (10%)	42,45,53	1.19	2 (4%)
7	BOG	I	604	-	20,20,20	1.23	1 (5%)	25,25,25	0.86	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	PX4	A	602	-	-	0/44/44/49	0/0/0/0
6	PX4	A	603	-	-	0/44/44/49	0/0/0/0
7	BOG	A	604	-	-	0/11/31/31	0/1/1/1
7	BOG	B	701	-	-	0/11/31/31	0/1/1/1
6	PX4	E	602	-	-	0/44/44/49	0/0/0/0
7	BOG	E	603	-	-	0/11/31/31	0/1/1/1
6	PX4	H	101	-	-	0/44/44/49	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PX4	I	602	-	-	0/44/44/49	0/0/0/0
6	PX4	I	603	-	-	0/44/44/49	0/0/0/0
7	BOG	I	604	-	-	0/11/31/31	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	101	PX4	O7-C7	-2.50	1.40	1.46
6	E	602	PX4	O7-C7	-2.48	1.40	1.46
6	A	603	PX4	O7-C7	-2.47	1.40	1.46
6	I	602	PX4	O7-C7	-2.44	1.40	1.46
6	A	602	PX4	O7-C7	-2.38	1.40	1.46
6	I	603	PX4	O7-C7	-2.25	1.40	1.46
6	E	602	PX4	P1-O4	2.00	1.67	1.59
6	A	603	PX4	P1-O4	2.02	1.67	1.59
6	I	602	PX4	P1-O4	2.03	1.67	1.59
6	A	602	PX4	P1-O3	2.17	1.67	1.59
6	I	602	PX4	P1-O3	2.21	1.67	1.59
6	I	603	PX4	P1-O3	2.21	1.67	1.59
6	H	101	PX4	P1-O3	2.22	1.67	1.59
6	A	603	PX4	P1-O3	2.22	1.67	1.59
6	E	602	PX4	P1-O3	2.23	1.67	1.59
6	E	602	PX4	O7-C23	2.94	1.42	1.34
6	H	101	PX4	O7-C23	2.97	1.42	1.34
6	A	603	PX4	O7-C23	2.98	1.42	1.34
6	I	602	PX4	O7-C23	2.98	1.42	1.34
6	A	602	PX4	O7-C23	3.02	1.43	1.34
6	I	603	PX4	O7-C23	3.07	1.43	1.34
6	I	603	PX4	O5-C9	3.17	1.42	1.33
6	E	602	PX4	O5-C9	3.19	1.42	1.33
6	I	602	PX4	O5-C9	3.20	1.42	1.33
6	A	603	PX4	O5-C9	3.24	1.42	1.33
6	A	602	PX4	O5-C9	3.27	1.42	1.33
6	H	101	PX4	O5-C9	3.27	1.43	1.33
7	B	701	BOG	O5-C1	3.60	1.50	1.41
7	E	603	BOG	O5-C1	3.62	1.50	1.41
7	A	604	BOG	O5-C1	3.63	1.50	1.41
7	I	604	BOG	O5-C1	3.66	1.50	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	602	PX4	O5-C9-C10	2.71	119.77	111.90
6	H	101	PX4	O5-C9-C10	2.76	119.94	111.90
6	E	602	PX4	O5-C9-C10	2.81	120.07	111.90
6	I	603	PX4	O5-C9-C10	2.81	120.08	111.90
6	A	603	PX4	O5-C9-C10	2.85	120.18	111.90
6	A	602	PX4	O5-C9-C10	2.93	120.41	111.90
6	I	602	PX4	O7-C23-C24	3.78	119.41	111.55
6	E	602	PX4	O7-C23-C24	3.93	119.71	111.55
6	A	603	PX4	O7-C23-C24	3.93	119.72	111.55
6	H	101	PX4	O7-C23-C24	4.02	119.90	111.55
6	A	602	PX4	O7-C23-C24	4.18	120.24	111.55
6	I	603	PX4	O7-C23-C24	4.64	121.19	111.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	PX4	1	0
6	E	602	PX4	1	0
7	E	603	BOG	1	0
6	I	602	PX4	1	0
6	I	603	PX4	2	0
7	I	604	BOG	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, 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	557/557 (100%)	0.52	57 (10%) 7 5	84, 115, 153, 208	0
1	E	557/557 (100%)	0.41	40 (7%) 16 11	83, 116, 151, 232	0
1	I	557/557 (100%)	0.51	50 (8%) 10 7	92, 121, 160, 225	0
2	B	673/674 (99%)	0.71	93 (13%) 3 2	107, 152, 241, 371	0
2	F	673/674 (99%)	0.98	140 (20%) 1 1	108, 162, 253, 364	0
2	J	673/674 (99%)	1.37	186 (27%) 1 0	117, 184, 310, 484	0
3	C	187/187 (100%)	0.37	9 (4%) 31 27	102, 128, 169, 226	0
3	G	187/187 (100%)	0.39	16 (8%) 11 8	109, 134, 184, 250	0
3	K	187/187 (100%)	0.35	15 (8%) 13 10	103, 134, 191, 267	0
4	D	27/27 (100%)	0.17	2 (7%) 15 11	122, 149, 186, 203	0
4	H	27/27 (100%)	-0.05	2 (7%) 15 11	118, 143, 187, 212	0
4	L	27/27 (100%)	0.39	4 (14%) 3 2	132, 158, 231, 255	0
All	All	4332/4335 (99%)	0.71	614 (14%) 3 2	83, 138, 246, 484	0

All (614) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	103	THR	11.7
2	B	539	THR	11.2
2	F	388	ILE	11.1
2	J	388	ILE	11.0
2	J	12	THR	10.8
2	J	120	LYS	10.6
2	J	60	GLY	10.5
2	J	97	LEU	10.0
2	J	106	ALA	9.7
2	J	121	VAL	9.6
2	J	389	ASP	9.4

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Mol	Chain	Res	Type	RSRZ
2	B	540	GLN	9.2
2	B	543	LYS	9.1
2	J	112	PRO	9.0
2	J	126	LEU	8.7
2	J	391	ARG	8.6
2	B	388	ILE	8.4
2	J	390	ASN	8.3
2	J	392	MET	8.2
2	J	408	ASN	8.2
2	F	465	ILE	8.1
2	J	433	VAL	7.9
2	F	105	PHE	7.7
2	J	16	GLN	7.7
2	F	390	ASN	7.6
2	J	113	LYS	7.5
2	J	100	VAL	7.5
2	F	416	VAL	7.5
2	J	488	ASP	7.4
2	B	436	GLY	7.4
2	J	58	MET	7.3
2	F	539	THR	7.2
2	J	435	GLU	7.2
2	J	119	ASP	7.2
2	J	9	PHE	7.0
2	J	59	PRO	6.9
2	B	439	VAL	6.9
2	B	538	GLY	6.9
2	F	131	ILE	6.8
2	J	436	GLY	6.8
2	J	203	MET	6.7
2	B	411	HIS	6.7
2	B	437	SER	6.6
2	J	543	LYS	6.6
2	J	122	PRO	6.6
2	F	374	PHE	6.6
2	J	141	PRO	6.5
2	F	391	ARG	6.5
2	J	131	ILE	6.5
2	J	10	GLU	6.4
2	F	325	ALA	6.4
2	J	476	LEU	6.3
2	B	99	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
2	J	164	PRO	6.3
2	F	543	LYS	6.2
2	B	58	MET	6.2
2	J	189	ILE	6.2
2	J	372	ALA	6.1
2	B	544	GLU	6.1
2	F	392	MET	6.0
2	F	433	VAL	6.0
1	E	469	SER	6.0
2	J	163	ALA	6.0
2	J	202	ARG	6.0
2	B	102	LYS	6.0
2	F	407	ALA	5.9
2	B	432	VAL	5.9
2	F	411	HIS	5.9
2	B	374	PHE	5.8
2	J	105	PHE	5.8
2	F	394	ARG	5.8
2	F	466	LYS	5.8
2	J	183	LEU	5.8
1	A	424	THR	5.8
2	F	208	GLU	5.6
1	A	176	TRP	5.5
2	F	324	PRO	5.5
2	J	393	ILE	5.5
2	J	13	LEU	5.5
2	B	114	TYR	5.4
2	J	439	VAL	5.4
2	J	145	GLU	5.4
2	F	408	ASN	5.4
2	B	100	VAL	5.4
2	J	181	ARG	5.4
2	J	371	HIS	5.4
2	J	182	ILE	5.3
2	B	390	ASN	5.3
2	F	409	GLY	5.3
2	F	439	VAL	5.3
2	B	101	LYS	5.3
2	B	110	ARG	5.3
2	B	435	GLU	5.2
2	J	123	ALA	5.2
2	J	104	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
2	F	28	GLN	5.1
1	E	424	THR	5.1
2	F	380	GLN	5.1
2	J	98	LYS	5.0
1	E	53	SER	5.0
2	J	434	VAL	5.0
2	F	211	GLN	5.0
2	F	679	CYS	4.9
1	I	424	THR	4.9
1	A	36	LEU	4.9
2	F	442	VAL	4.9
1	I	468	GLY	4.9
2	F	12	THR	4.9
2	F	114	TYR	4.8
1	I	401	THR	4.8
2	B	210	ALA	4.7
2	F	386	ILE	4.7
2	B	377	PHE	4.7
2	B	92	ALA	4.7
2	J	429	THR	4.7
1	A	89	LEU	4.7
2	B	375	VAL	4.7
2	J	207	VAL	4.6
1	I	470	ALA	4.6
2	F	538	GLY	4.6
2	F	112	PRO	4.6
2	F	419	LYS	4.6
2	F	406	GLU	4.6
2	F	387	ASN	4.6
2	B	434	VAL	4.6
2	J	153	VAL	4.6
2	F	97	LEU	4.6
2	F	373	THR	4.5
1	I	232	GLY	4.5
2	F	681	LEU	4.5
2	J	111	GLU	4.5
1	E	468	GLY	4.5
2	J	132	VAL	4.5
2	J	118	ALA	4.5
2	J	115	GLY	4.5
1	I	113	THR	4.5
2	J	127	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
2	J	125	GLN	4.5
2	B	103	THR	4.4
2	B	324	PRO	4.4
2	B	542	ALA	4.4
2	F	303	VAL	4.4
2	J	176	VAL	4.4
2	B	9	PHE	4.3
2	F	126	LEU	4.3
2	F	440	LEU	4.3
2	J	424	ALA	4.3
2	J	374	PHE	4.3
2	J	192	SER	4.3
2	F	630	PHE	4.3
2	J	404	HIS	4.3
2	J	101	LYS	4.3
2	F	326	GLN	4.3
2	F	678	VAL	4.2
2	J	325	ALA	4.2
1	I	239	ASN	4.2
2	B	211	GLN	4.2
2	J	199	PHE	4.2
2	F	104	ALA	4.1
1	I	539	GLY	4.1
2	B	97	LEU	4.1
2	F	328	VAL	4.1
1	A	369	GLY	4.1
2	B	392	MET	4.1
2	F	460	LEU	4.1
2	F	437	SER	4.1
2	F	434	VAL	4.1
2	J	416	VAL	4.1
2	B	389	ASP	4.1
2	F	101	LYS	4.1
2	J	114	TYR	4.0
2	B	391	ARG	4.0
2	F	191	CYS	4.0
2	F	202	ARG	4.0
1	A	39	THR	4.0
2	B	98	LYS	4.0
1	I	86	TYR	4.0
2	J	191	CYS	4.0
2	J	442	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
2	J	140	ILE	4.0
2	F	360	PHE	4.0
2	J	441	GLY	4.0
2	B	416	VAL	3.9
2	J	542	ALA	3.9
2	J	618	LEU	3.9
1	E	470	ALA	3.9
2	J	444	ALA	3.9
1	A	382	GLY	3.9
2	F	506	TYR	3.8
2	J	96	SER	3.8
2	J	373	THR	3.8
1	I	469	SER	3.8
2	F	666	PHE	3.8
2	B	325	ALA	3.8
2	J	440	LEU	3.8
1	I	343	SER	3.8
2	B	60	GLY	3.8
2	F	199	PHE	3.8
2	J	487	VAL	3.8
2	J	490	PHE	3.8
1	I	114	ASN	3.7
2	J	117	ALA	3.7
1	I	87	LEU	3.7
1	E	425	PRO	3.7
2	F	441	GLY	3.7
1	I	89	LEU	3.7
2	B	438	ARG	3.7
2	J	446	LYS	3.7
2	J	336	ALA	3.7
2	J	139	ILE	3.7
2	F	16	GLN	3.7
2	J	539	THR	3.7
2	J	48	CYS	3.7
2	F	63	LEU	3.7
2	J	457	PHE	3.7
2	F	304	LEU	3.7
1	A	468	GLY	3.7
2	J	240	TRP	3.7
2	B	545	ALA	3.7
2	J	94	ALA	3.7
2	J	681	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	J	130	ASP	3.6
1	E	240	SER	3.6
2	J	329	ASP	3.6
2	J	468	VAL	3.6
1	I	234	GLY	3.6
2	J	426	GLN	3.6
3	G	188	LEU	3.6
2	J	405	VAL	3.6
2	J	491	LEU	3.6
2	J	538	GLY	3.6
1	I	176	TRP	3.6
2	F	203	MET	3.6
2	F	113	LYS	3.6
2	J	53	MET	3.6
2	J	438	ARG	3.6
1	A	113	THR	3.6
2	J	370	LEU	3.6
2	J	324	PRO	3.6
2	F	675	LEU	3.6
2	J	630	PHE	3.5
1	A	469	SER	3.5
1	A	466	ASN	3.5
1	I	240	SER	3.5
2	J	425	ARG	3.5
2	F	306	LEU	3.5
3	C	116	VAL	3.5
2	F	383	MET	3.5
2	B	415	ASP	3.5
2	F	124	ASP	3.5
2	J	193	VAL	3.5
2	F	119	ASP	3.5
1	I	83	GLY	3.5
2	J	443	ILE	3.5
2	B	549	VAL	3.4
3	G	155	LEU	3.4
2	J	142	CYS	3.4
2	B	209	GLY	3.4
2	J	369	SER	3.4
1	A	428	VAL	3.4
2	J	194	ASN	3.4
1	E	233	GLY	3.4
1	A	175	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	326	GLN	3.4
3	G	154	GLN	3.4
2	F	120	LYS	3.3
2	F	509	GLU	3.3
2	J	200	LEU	3.3
1	A	37	PRO	3.3
1	A	538	VAL	3.3
2	F	9	PHE	3.3
3	K	154	GLN	3.3
2	B	386	ILE	3.3
2	B	112	PRO	3.3
2	J	108	LYS	3.3
2	F	108	LYS	3.3
3	K	188	LEU	3.3
2	F	540	GLN	3.3
2	J	409	GLY	3.3
2	J	332	THR	3.3
2	B	425	ARG	3.3
2	F	60	GLY	3.3
1	I	466	ASN	3.2
2	F	393	ILE	3.2
1	A	459	ALA	3.2
4	L	3	ALA	3.2
2	F	463	MET	3.2
1	A	367	GLN	3.2
2	B	431	LEU	3.2
2	F	389	ASP	3.2
1	A	461	SER	3.2
3	C	47	ASP	3.2
2	F	546	GLY	3.2
1	I	39	THR	3.2
2	B	105	PHE	3.2
2	B	394	ARG	3.2
2	B	95	ASN	3.2
2	F	13	LEU	3.2
1	I	203	ALA	3.2
1	E	461	SER	3.2
3	G	185	LEU	3.2
2	J	116	ALA	3.2
3	K	158	LEU	3.2
1	I	369	GLY	3.1
2	J	78	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	J	107	ARG	3.1
2	F	327	GLY	3.1
2	F	450	LYS	3.1
3	K	50	ARG	3.1
2	J	489	ASP	3.1
1	E	459	ALA	3.1
2	B	426	GLN	3.1
2	F	96	SER	3.1
2	J	510	GLY	3.1
2	B	515	MET	3.1
2	B	430	PRO	3.1
2	J	136	ALA	3.0
2	B	387	ASN	3.0
2	F	477	THR	3.0
2	B	199	PHE	3.0
2	J	445	LEU	3.0
1	E	428	VAL	3.0
1	A	379	GLY	3.0
2	J	420	VAL	3.0
2	J	86	ALA	3.0
2	F	502	LEU	3.0
2	J	133	LEU	3.0
2	J	450	LYS	3.0
1	A	423	VAL	3.0
1	E	341	ALA	3.0
1	E	342	ALA	3.0
2	B	203	MET	3.0
2	F	100	VAL	3.0
1	A	539	GLY	2.9
4	L	7	THR	2.9
3	C	167	LEU	2.9
1	A	458	TYR	2.9
2	J	179	GLY	2.9
1	A	370	GLU	2.9
2	F	544	GLU	2.9
2	J	20	GLU	2.9
1	E	539	GLY	2.9
2	J	128	LYS	2.9
2	F	432	VAL	2.9
2	F	322	PHE	2.9
1	I	233	GLY	2.9
3	K	4	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	59	PRO	2.9
2	B	93	GLN	2.9
2	J	331	LYS	2.9
2	F	667	ILE	2.9
3	K	55	ILE	2.9
2	B	200	LEU	2.9
2	F	200	LEU	2.9
2	F	464	GLY	2.9
2	F	404	HIS	2.9
1	E	458	TYR	2.9
2	J	175	SER	2.9
2	J	544	GLU	2.9
2	F	235	ALA	2.9
1	A	211	GLN	2.9
2	B	208	GLU	2.9
2	B	433	VAL	2.9
1	A	470	ALA	2.9
1	I	93	GLN	2.9
3	C	5	ARG	2.9
2	F	467	THR	2.8
2	F	128	LYS	2.8
2	F	537	SER	2.8
2	F	122	PRO	2.8
1	E	234	GLY	2.8
1	E	239	ASN	2.8
1	I	207	VAL	2.8
2	B	63	LEU	2.8
4	D	27	GLU	2.8
1	A	343	SER	2.8
2	F	457	PHE	2.8
1	I	85	HIS	2.8
2	B	490	PHE	2.8
2	F	420	VAL	2.8
1	I	344	CYS	2.8
2	B	412	PHE	2.8
2	F	121	VAL	2.8
1	I	84	GLN	2.8
2	F	511	ARG	2.8
2	J	109	LEU	2.8
2	F	58	MET	2.8
1	E	232	GLY	2.8
1	I	392	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	117	PRO	2.8
2	J	253	THR	2.8
1	I	341	ALA	2.8
2	F	186	TRP	2.7
2	B	111	GLU	2.7
2	J	386	ILE	2.7
2	J	401	ILE	2.7
2	F	170	GLY	2.7
2	J	64	PHE	2.7
2	F	618	LEU	2.7
2	F	301	VAL	2.7
2	F	382	ARG	2.7
2	B	376	PRO	2.7
1	A	342	ALA	2.7
1	A	533	GLY	2.7
2	J	427	GLY	2.7
2	J	486	GLY	2.7
4	H	26	ALA	2.7
3	K	155	LEU	2.6
2	J	99	GLY	2.6
2	B	383	MET	2.6
2	J	138	ASP	2.6
2	F	209	GLY	2.6
3	K	148	ARG	2.6
1	I	423	VAL	2.6
2	F	542	ALA	2.6
3	G	150	LEU	2.6
1	E	460	VAL	2.6
2	J	11	PRO	2.6
2	B	288	ILE	2.6
2	F	127	ARG	2.6
2	F	461	ARG	2.6
2	J	414	THR	2.6
1	A	366	MET	2.6
3	G	183	LEU	2.6
2	F	302	ASP	2.6
1	A	425	PRO	2.6
2	F	505	GLN	2.6
2	B	681	LEU	2.6
1	I	425	PRO	2.6
1	I	175	LEU	2.5
3	K	185	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	378	SER	2.5
2	B	104	ALA	2.5
2	B	485	ALA	2.5
3	G	63	GLY	2.5
1	A	187	LEU	2.5
2	J	85	LEU	2.5
1	E	340	THR	2.5
1	I	414	MET	2.5
2	F	435	GLU	2.5
2	J	168	GLU	2.5
1	I	116	ARG	2.5
1	I	368	ILE	2.5
1	E	534	THR	2.5
2	F	196	GLY	2.5
1	E	39	THR	2.5
2	B	384	SER	2.5
3	C	159	ILE	2.5
1	A	232	GLY	2.5
2	F	443	ILE	2.5
3	K	149	ASN	2.5
2	B	442	VAL	2.5
2	J	449	VAL	2.5
1	E	488	CYS	2.5
2	B	51	ILE	2.5
2	B	306	LEU	2.5
2	F	476	LEU	2.5
1	A	540	ALA	2.5
2	B	395	LYS	2.5
2	J	137	GLY	2.5
2	J	631	LEU	2.5
1	A	460	VAL	2.4
2	J	248	ASN	2.4
3	G	83	GLY	2.4
3	G	156	THR	2.4
2	J	190	GLU	2.4
3	K	45	GLU	2.4
1	E	343	SER	2.4
1	A	114	ASN	2.4
1	E	363	MET	2.4
2	B	113	LYS	2.4
2	F	468	VAL	2.4
2	J	375	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
3	G	84	GLY	2.4
2	F	106	ALA	2.4
3	K	33	TRP	2.4
2	F	399	ASP	2.4
2	F	473	ASP	2.4
2	J	92	ALA	2.4
2	J	102	LYS	2.4
2	F	487	VAL	2.4
1	E	345	GLY	2.4
1	I	467	ASN	2.4
2	B	487	VAL	2.4
1	A	233	GLY	2.4
2	F	110	ARG	2.4
1	E	86	TYR	2.4
2	F	663	LEU	2.4
2	J	659	LEU	2.4
1	I	490	PHE	2.4
2	J	620	ALA	2.4
1	I	82	LEU	2.4
2	B	423	VAL	2.4
2	J	682	VAL	2.4
2	B	420	VAL	2.3
2	F	193	VAL	2.3
2	F	405	VAL	2.3
2	J	134	VAL	2.3
2	J	452	GLY	2.3
2	F	141	PRO	2.3
3	G	164	GLN	2.3
1	A	363	MET	2.3
1	E	426	THR	2.3
1	I	395	GLY	2.3
1	I	492	GLY	2.3
1	I	538	VAL	2.3
2	F	132	VAL	2.3
2	F	207	VAL	2.3
2	F	102	LYS	2.3
2	J	323	ILE	2.3
4	D	1	MET	2.3
1	A	198	PHE	2.3
1	A	465	ASN	2.3
2	J	578	PHE	2.3
2	J	394	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	J	195	PRO	2.3
2	J	421	ASP	2.3
1	A	534	THR	2.3
1	E	369	GLY	2.3
2	B	408	ASN	2.3
2	J	81	PHE	2.3
2	J	250	VAL	2.3
2	J	655	TRP	2.3
1	A	536	LEU	2.3
2	J	166	ILE	2.3
3	K	150	LEU	2.3
2	J	177	THR	2.3
1	A	462	SER	2.3
1	I	535	VAL	2.3
1	I	342	ALA	2.3
3	G	33	TRP	2.3
1	A	463	ALA	2.3
3	C	120	LEU	2.3
2	B	28	GLN	2.3
2	J	422	GLN	2.2
1	A	385	LEU	2.2
1	E	427	LEU	2.2
1	A	381	TYR	2.2
2	F	125	GLN	2.2
1	A	535	VAL	2.2
1	A	417	THR	2.2
2	F	378	THR	2.2
3	C	16	LEU	2.2
2	B	484	GLU	2.2
2	F	514	ALA	2.2
3	G	4	LEU	2.2
2	B	679	CYS	2.2
2	F	31	TRP	2.2
2	F	512	LEU	2.2
2	J	124	ASP	2.2
1	E	462	SER	2.2
2	B	212	ARG	2.2
2	F	103	THR	2.2
2	J	575	LEU	2.2
2	F	368	GLN	2.2
3	G	153	GLU	2.2
1	I	225	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	J	51	ILE	2.2
1	A	374	GLY	2.2
2	J	196	GLY	2.2
1	E	114	ASN	2.2
1	E	167	TRP	2.2
2	J	57	ALA	2.2
2	J	423	VAL	2.2
2	B	409	GLY	2.1
2	J	63	LEU	2.1
1	A	341	ALA	2.1
1	I	374	GLY	2.1
1	A	429	LEU	2.1
2	J	17	ALA	2.1
2	F	99	GLY	2.1
2	F	150	GLY	2.1
2	J	328	VAL	2.1
1	E	113	THR	2.1
2	B	131	ILE	2.1
2	J	334	ALA	2.1
1	E	466	ASN	2.1
2	F	314	LEU	2.1
1	I	238	ALA	2.1
1	E	467	ASN	2.1
4	L	1	MET	2.1
2	J	623	PHE	2.1
3	C	146	LYS	2.1
1	I	382	GLY	2.1
1	A	383	MET	2.1
2	J	475	ARG	2.1
1	A	115	TRP	2.1
1	E	339	THR	2.1
2	J	28	GLN	2.1
2	J	93	GLN	2.1
2	J	467	THR	2.1
2	B	343	ALA	2.1
2	B	525	ALA	2.1
2	J	317	ARG	2.1
1	A	112	ASN	2.1
2	J	61	ASN	2.1
3	K	32	TRP	2.1
4	H	14	LEU	2.1
2	B	457	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
3	G	65	PHE	2.1
2	J	143	ASP	2.0
1	A	542	THR	2.0
2	B	229	THR	2.0
1	I	402	PRO	2.0
3	K	152	VAL	2.0
4	L	5	VAL	2.0
1	A	196	GLN	2.0
1	E	387	VAL	2.0
1	A	420	ALA	2.0
3	G	85	SER	2.0
2	F	545	ALA	2.0
1	E	414	MET	2.0
1	I	198	PHE	2.0
1	E	357	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	SEP	F	162	10/11	0.78	0.33	-	169,175,199,205	0
2	SEP	B	162	10/11	0.94	0.19	-	153,163,177,182	0
2	SEP	J	162	10/11	0.68	0.19	-	218,226,232,235	0

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, 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	LLDF	B-factors(Å ²)	Q<0.9
6	PX4	E	602	41/46	0.31	0.74	7.26	199,227,281,284	0
6	PX4	A	602	41/46	0.58	0.47	5.59	156,188,203,205	0
6	PX4	I	602	41/46	0.47	0.67	4.73	167,183,225,228	0
6	PX4	I	603	41/46	0.74	0.44	4.41	164,204,226,228	0
7	BOG	I	604	20/20	0.89	0.41	4.17	205,221,224,227	0
6	PX4	A	603	41/46	0.66	0.45	2.37	130,169,230,232	0
7	BOG	A	604	20/20	0.85	0.32	2.11	178,191,198,198	0
6	PX4	H	101	41/46	0.69	0.42	2.01	171,197,211,214	0
7	BOG	E	603	20/20	0.79	0.23	0.69	154,184,190,194	0
5	K	A	601	1/1	0.85	0.34	-0.14	123,123,123,123	0
5	K	E	601	1/1	0.72	0.32	-0.24	124,124,124,124	0
5	K	I	601	1/1	0.76	0.36	-0.61	123,123,123,123	0
7	BOG	B	701	20/20	0.77	0.31	-	173,185,194,195	0

6.5 Other polymers ⓘ

There are no such residues in this entry.