



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 04:32 PM GMT

PDB ID : 3A5C
Title : Inter-subunit interaction and quaternary rearrangement defined by the central stalk of prokaryotic V1-ATPase
Authors : Numoto, N.; Hasegawa, Y.; Takeda, K.; Miki, K.
Deposited on : 2009-08-06
Resolution : 4.51 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

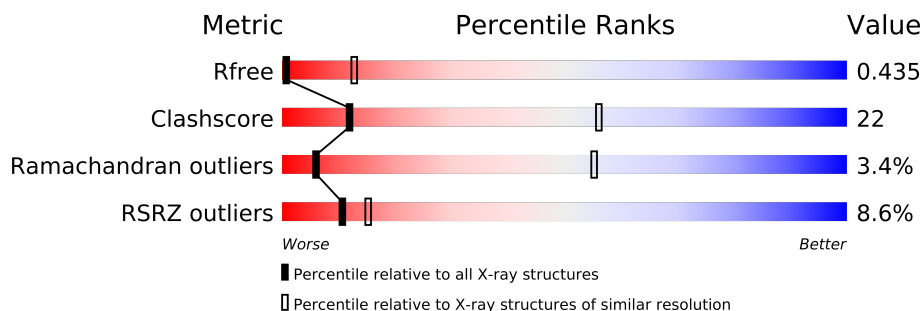
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 4.51 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}	66092	1029 (5.50-3.50)
Clashscore	79885	1300 (5.50-3.50)
Ramachandran outliers	78287	1222 (5.50-3.50)
RSRZ outliers	66119	1028 (5.50-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	578	
1	B	578	
1	C	578	
1	I	578	
1	J	578	
1	K	578	
2	D	478	
2	E	478	
2	F	478	
2	L	478	
2	M	478	
2	N	478	
3	G	223	
3	O	223	
4	H	104	
4	P	104	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32188 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ATP synthase alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	B	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	C	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	I	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	J	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	K	561	Total	C	N	O	0	0	0
			2752	1630	561	561			

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	E	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	F	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	L	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	M	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	N	450	Total	C	N	O	0	0	0
			2212	1312	450	450			

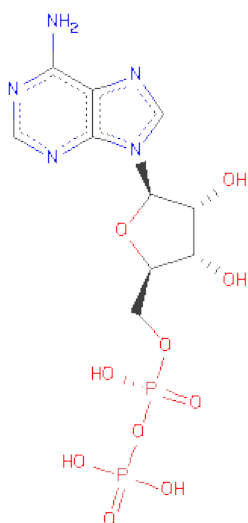
- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	129	Total	C	N	O	0	0	0
			639	381	129	129			
3	O	129	Total	C	N	O	0	0	0
			639	381	129	129			

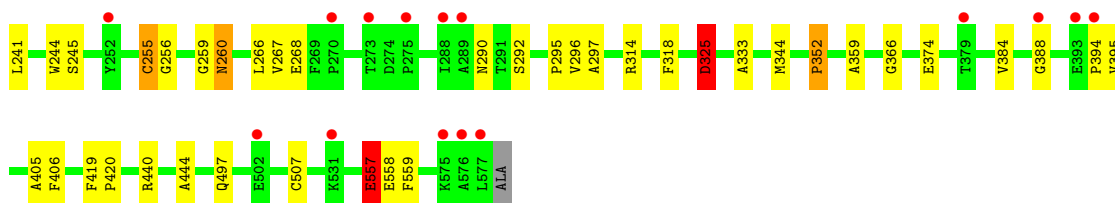
- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	104	Total	C	N	O	0	0	0
			509	301	104	104			
4	P	104	Total	C	N	O	0	0	0
			509	301	104	104			

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

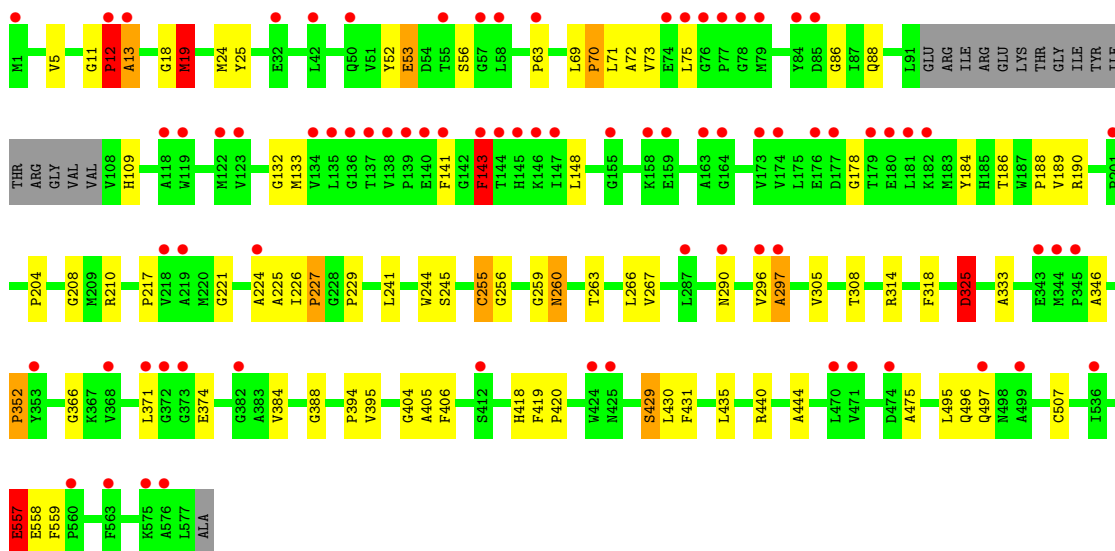


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		



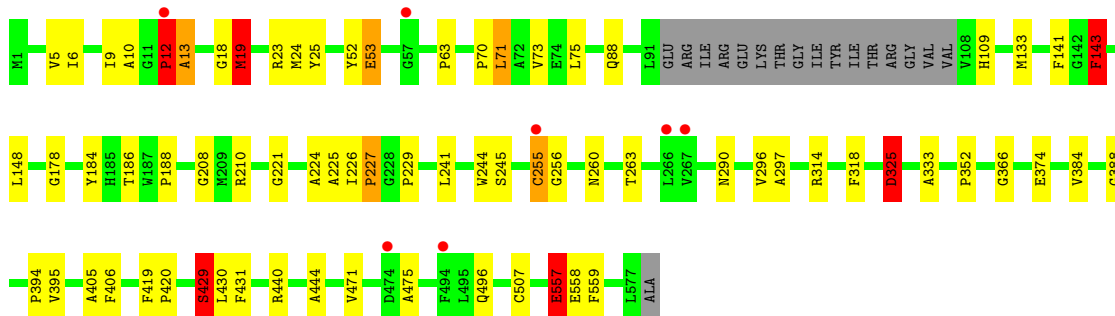
• Molecule 1: V-type ATP synthase alpha chain

Chain I:



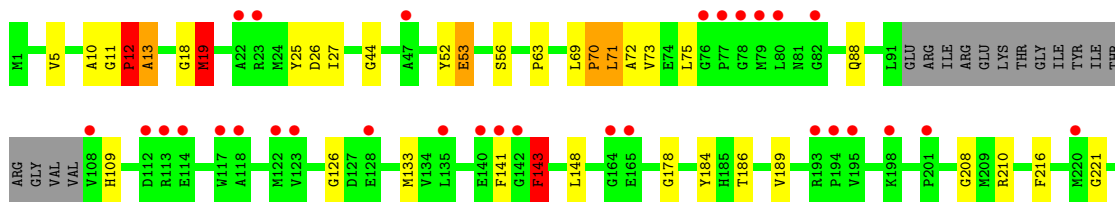
• Molecule 1: V-type ATP synthase alpha chain

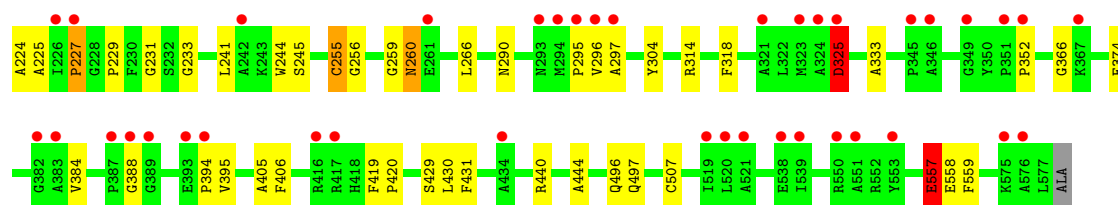
Chain J:



• Molecule 1: V-type ATP synthase alpha chain

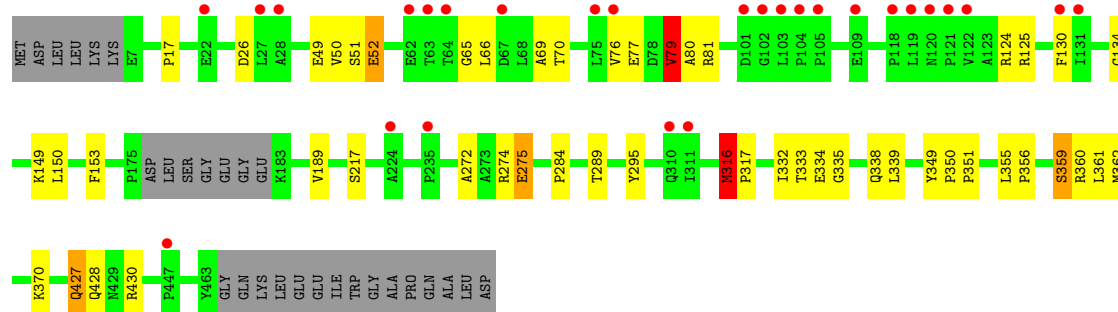
Chain K:





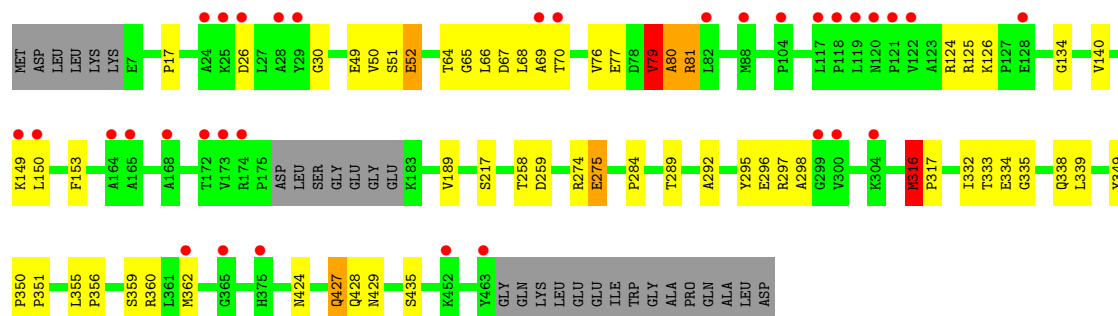
• Molecule 2: V-type ATP synthase beta chain

Chain D:



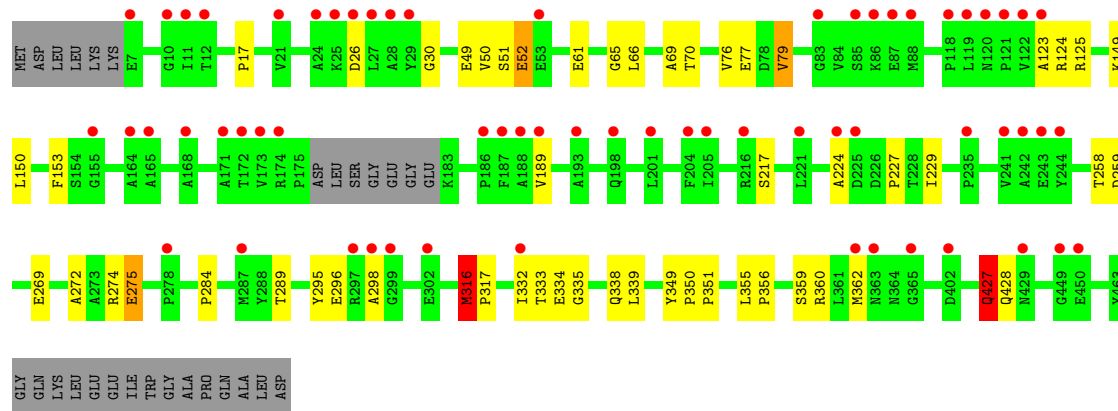
• Molecule 2: V-type ATP synthase beta chain

Chain E:



• Molecule 2: V-type ATP synthase beta chain

Chain F:



• Molecule 2: V-type ATP synthase beta chain

Government	Percentage
Current government	95%
Previous government	5%



ALA TYR THR LEU GLU ALA SER ARG ALA PHE ARG R132 Y132 Y133 A134 A134 Y135 R196 R197 R198 R199 R200 I201 A141 N142 N143 T143 E144 T145 R146 R147 K148 K149 I150 G151 E152 E153 A154 K155 K156 T157 T158 R159 R160 V161 N162 A163 L164 E165 Q166 V167 V168 I169 P170 G171 I172 R173 A174 Q175 I176 R177 F178 I179 Q180

Q181 V182 E183 E184 S185 R186 E187 R188 E189 D190 T191 F192 R193 L194 L195 R196 R197 R198 R199 R200 I201 A141 N142 N143 T143 E144 T145 R146 R147 K148 K149 I150 G151 E152 E153 A154 K155 K156 T157 T158 R159 R160 V161 N162 A163 L164 E165 Q166 V167 V168 I169 P170 G171 I172 R173 A174 Q175 I176 R177 F178 I179 Q180

• Molecule 3: V-type ATP synthase subunit D

Chain O:

M1 S2 Q3 V4 S5 P6 T7 R8 M9 N10 L11 L12 Q13 R14 R15 G16 A17 L18 R19 L20 A21 Q22 K23 Q24 V25 D26 L27 L28 K29 K30 K31 R32 D33 A34 L35 V36 A37 E38 F39 F40 G41 L42 L43 R44 E45 A46 M47 E48 A49 K51 A52 L53 D54 Q55 A56 L57 L58 L59 L60 L61 L62 L63 L64 L65 L66 L67 L68 L69 L70 L71 L72 L73 L74 L75 L76 L77 L78 L79 L80

TYR ALA ALA LEU LEU LEU ALA ALA GLN ALA ALA PHE ASP GLY PRO GLU VAL VAL GLY ALA ALA ALA LEU LEU LEU LEU LYS ALA THR PHE PRO ASP GLY ALA LEU SER PRO VAL THR PRO

ALA TYR THR LEU GLU ALA SER ARG ALA PHE ARG R132 Y132 Y133 A134 A134 Y135 R196 R197 R198 R199 R200 I201 A141 N142 N143 T143 E144 T145 R146 R147 K148 K149 I150 G151 E152 E153 A154 K155 K156 T157 T158 R159 R160 V161 N162 A163 L164 E165 Q166 V167 V168 I169 P170 G171 I172 R173 A174 Q175 I176 R177 F178 I179 Q180

Q181 V182 E183 E184 S185 R186 E187 R188 E189 D190 T191 F192 R193 L194 L195 R196 R197 R198 R199 R200 I201 A141 N142 N143 T143 E144 T145 R146 R147 K148 K149 I150 G151 E152 E153 A154 K155 K156 T157 T158 R159 R160 V161 N162 A163 L164 E165 Q166 V167 V168 I169 P170 G171 I172 R173 A174 Q175 I176 R177 F178 I179 Q180

• Molecule 4: V-type ATP synthase subunit F

Chain H:

H1 S24 S25 A29 E34 T35 R39 G40 M63 R64 G65 R66 I74 A75 G76 L77 K78 E79 A80 F81 Q82 Q83 H84 D85 V86 T97 T98 G99 F100 L104

• Molecule 4: V-type ATP synthase subunit F

Chain P:

H1 A16 S25 A29 E34 T35 R39 G40 L62 M63 G65 R66 P69 I74 A75 G76 L77 K78 Q82 Q83 H84 D85 V86 V94 R95 I98 G99 F100 K103 L104

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	381.58Å 381.58Å 147.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.92 – 4.51 49.81 – 4.51	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.92-4.51) 96.8 (49.81-4.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 4.45Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.429 , 0.437 0.428 , 0.435	Depositor DCC
R_{free} test set	3589 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	145.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , -10.0	EDS
Estimated twinning fraction	0.217 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.13$	Xtriage
Outliers	1 of 70593 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	32188	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	3/2750 (0.1%)	1.20	9/3815 (0.2%)
1	B	0.59	3/2750 (0.1%)	1.21	12/3815 (0.3%)
1	C	0.59	3/2750 (0.1%)	1.20	10/3815 (0.3%)
1	I	0.59	3/2750 (0.1%)	1.38	13/3815 (0.3%)
1	J	0.59	3/2750 (0.1%)	1.21	11/3815 (0.3%)
1	K	0.60	3/2750 (0.1%)	1.34	13/3815 (0.3%)
2	D	0.80	7/2210 (0.3%)	1.03	13/3068 (0.4%)
2	E	0.85	7/2210 (0.3%)	1.04	10/3068 (0.3%)
2	F	0.73	3/2210 (0.1%)	0.99	7/3068 (0.2%)
2	L	0.74	3/2210 (0.1%)	1.01	9/3068 (0.3%)
2	M	0.75	3/2210 (0.1%)	1.00	8/3068 (0.3%)
2	N	0.73	3/2210 (0.1%)	0.99	7/3068 (0.2%)
3	G	4.09	122/637 (19.2%)	2.62	48/885 (5.4%)
3	O	4.09	126/637 (19.8%)	2.63	50/885 (5.6%)
4	H	1.48	6/508 (1.2%)	1.43	9/703 (1.3%)
4	P	1.78	10/508 (2.0%)	2.16	15/703 (2.1%)
All	All	1.08	308/32050 (1.0%)	1.27	244/44474 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	5
1	C	0	5
1	I	0	6
1	J	0	6
1	K	0	6
2	D	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	4
2	F	0	3
2	L	0	4
2	M	0	3
2	N	0	3
4	H	0	3
4	P	0	2
All	All	0	60

The worst 5 of 308 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	47	MET	CA-CB	-25.00	0.98	1.53
3	G	47	MET	CA-CB	-24.93	0.99	1.53
3	O	27	LEU	CA-CB	14.81	1.87	1.53
3	G	27	LEU	CA-CB	14.78	1.87	1.53
4	P	75	ALA	N-CA	13.48	1.73	1.46

The worst 5 of 244 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	325	ASP	O-C-N	-39.90	58.86	122.70
1	J	325	ASP	O-C-N	-39.89	58.87	122.70
1	C	325	ASP	O-C-N	-39.89	58.87	122.70
1	A	325	ASP	O-C-N	-39.88	58.89	122.70
1	K	325	ASP	O-C-N	-39.85	58.94	122.70

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLY	Peptide
1	A	210	ARG	Mainchain
1	A	297	ALA	Mainchain
1	A	325	ASP	Mainchain
1	A	69	LEU	Peptide

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2752	0	1302	92	0
1	B	2752	0	1303	65	0
1	C	2752	0	1303	100	0
1	I	2752	0	1300	122	0
1	J	2752	0	1303	61	2
1	K	2752	0	1302	94	0
2	D	2212	0	1009	66	0
2	E	2212	0	1008	80	0
2	F	2212	0	1009	94	0
2	L	2212	0	1009	80	0
2	M	2212	0	1009	59	2
2	N	2212	0	1009	76	0
3	G	639	0	299	131	0
3	O	639	0	299	136	0
4	H	509	0	255	12	0
4	P	509	0	255	23	0
5	A	27	0	12	2	0
5	C	27	0	12	1	0
5	I	27	0	12	0	0
5	K	27	0	12	5	0
All	All	32188	0	15022	1021	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

The worst 5 of 1021 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:O:142:ASN:CB	3:O:142:ASN:CA	1.75	1.65
3:O:189:GLU:CA	3:O:189:GLU:CB	1.76	1.64
3:G:205:GLU:CA	3:G:205:GLU:CB	1.78	1.62
3:O:52:ALA:CB	3:O:52:ALA:CA	1.76	1.59
3:G:189:GLU:CB	3:G:189:GLU:CA	1.76	1.58

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:6:ILE:CB	2:M:24:ALA:O[5_555]	2.04	0.16

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:5:VAL:CA	2:M:24:ALA:CB[5_555]	2.10	0.10

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	557/578 (96%)	491 (88%)	48 (9%)	18 (3%)	6	56
1	B	557/578 (96%)	492 (88%)	47 (8%)	18 (3%)	6	56
1	C	557/578 (96%)	492 (88%)	48 (9%)	17 (3%)	7	57
1	I	557/578 (96%)	493 (88%)	48 (9%)	16 (3%)	7	58
1	J	557/578 (96%)	492 (88%)	47 (8%)	18 (3%)	6	56
1	K	557/578 (96%)	493 (88%)	47 (8%)	17 (3%)	7	57
2	D	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	11	67
2	E	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	11	67
2	F	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	11	67
2	L	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	11	67
2	M	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	11	67
2	N	446/478 (93%)	420 (94%)	16 (4%)	10 (2%)	10	65
3	G	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	3
3	O	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	3
4	H	102/104 (98%)	89 (87%)	11 (11%)	2 (2%)	11	67
4	P	102/104 (98%)	90 (88%)	10 (10%)	2 (2%)	11	67
All	All	6472/6990 (93%)	5808 (90%)	443 (7%)	221 (3%)	6	55

5 of 221 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PRO
1	A	19	MET
1	A	53	GLU

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Mol	Chain	Res	Type
1	A	143	PHE
1	A	227	PRO

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands 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	$\# Z > 2$
5	ADP	A	600	-	29,29,29	1.15	4 (13%)	45,45,45	0.77	0
5	ADP	C	600	-	29,29,29	0.92	2 (6%)	45,45,45	0.94	3 (6%)
5	ADP	I	600	-	29,29,29	1.15	5 (17%)	45,45,45	0.76	0
5	ADP	K	600	-	29,29,29	0.92	2 (6%)	45,45,45	0.94	3 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	A	600	-	-	0/16/32/32	0/1/3/3
5	ADP	C	600	-	-	0/16/32/32	0/1/3/3
5	ADP	I	600	-	-	0/16/32/32	0/1/3/3
5	ADP	K	600	-	-	0/16/32/32	0/1/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	600	ADP	PB-O2B	-2.54	1.45	1.54
5	C	600	ADP	PB-O2B	-2.53	1.45	1.54
5	A	600	ADP	PB-O2B	-2.44	1.45	1.54
5	I	600	ADP	PB-O2B	-2.43	1.45	1.54
5	C	600	ADP	PA-O1A	-2.30	1.42	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	600	ADP	O3B-PB-O2B	2.34	116.72	107.61
5	C	600	ADP	O3B-PB-O2B	2.34	116.71	107.61
5	K	600	ADP	O4'-C1'-N9	-2.12	106.47	108.44
5	C	600	ADP	O4'-C1'-N9	-2.10	106.48	108.44
5	K	600	ADP	O4'-C4'-C3'	-2.02	101.08	105.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	561/578 (97%)	0.56	71 (12%) 4 8	103, 162, 214, 214	0
1	B	561/578 (97%)	0.22	25 (4%) 32 29	79, 130, 144, 144	0
1	C	561/578 (97%)	0.61	53 (9%) 9 14	137, 189, 210, 210	0
1	I	561/578 (97%)	0.84	78 (13%) 4 7	172, 172, 232, 232	0
1	J	561/578 (97%)	0.01	7 (1%) 75 62	50, 58, 104, 104	0
1	K	561/578 (97%)	0.75	69 (12%) 5 9	146, 177, 189, 189	0
2	D	450/478 (94%)	0.34	27 (6%) 21 22	118, 118, 188, 188	0
2	E	450/478 (94%)	0.49	33 (7%) 15 18	122, 130, 162, 162	0
2	F	450/478 (94%)	0.65	63 (14%) 3 7	109, 217, 217, 217	0
2	L	450/478 (94%)	0.28	22 (4%) 28 27	98, 98, 158, 158	0
2	M	450/478 (94%)	0.36	29 (6%) 19 21	99, 99, 148, 148	0
2	N	450/478 (94%)	0.77	69 (15%) 3 6	158, 250, 250, 250	0
3	G	129/223 (57%)	-0.39	2 (1%) 68 56	34, 34, 49, 49	0
3	O	129/223 (57%)	-0.40	0 100 100	84, 85, 85, 85	0
4	H	104/104 (100%)	0.36	6 (5%) 22 23	110, 110, 134, 134	0
4	P	104/104 (100%)	0.22	9 (8%) 10 15	94, 94, 141, 141	0
All	All	6532/6990 (93%)	0.45	563 (8%) 11 15	34, 137, 232, 250	0

The worst 5 of 563 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	145	HIS	10.5
1	K	78	GLY	10.3
2	N	192	ALA	9.5
1	K	77	PRO	9.5
1	I	180	GLU	8.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	ADP	K	600	27/27	0.46	0.24	112,112,112,112	0
5	ADP	A	600	27/27	0.27	0.00	109,109,109,109	0
5	ADP	C	600	27/27	0.28	-0.08	116,116,116,116	0
5	ADP	I	600	27/27	0.31	-0.74	110,110,110,110	0

6.5 Other polymers ⓘ

There are no such residues in this entry.