W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2017 – 03:50 am GMT

|		
PDB ID	:	5KOY
Title	:	Mouse pgp 34 linker deleted bound with ATP
Authors	:	Xia, D.; Esser, L.; Zhou, F.
Deposited on	:	2016-07-01
Resolution	:	3.85 Å(reported)

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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 3.85 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	Percentile Ranks	Value
Rfree		0.301
Clashscore		1
Ramachandran outliers		0.4%
Sidechain outliers		2.7%
RSRZ outliers		12.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
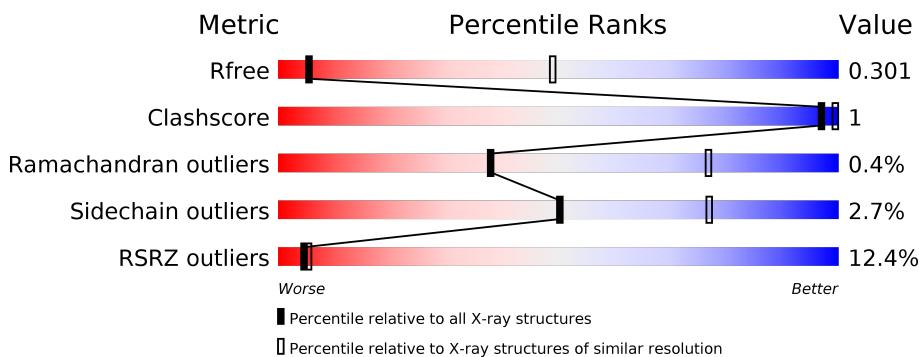
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1009 (4.16-3.56)
Clashscore	112137	1029 (4.12-3.60)
Ramachandran outliers	110173	1017 (4.14-3.58)
Sidechain outliers	110143	1010 (4.14-3.58)
RSRZ outliers	101464	1023 (4.16-3.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1248	11% 90% 5% 5%
1	B	1248	12% 88% 6% 5%
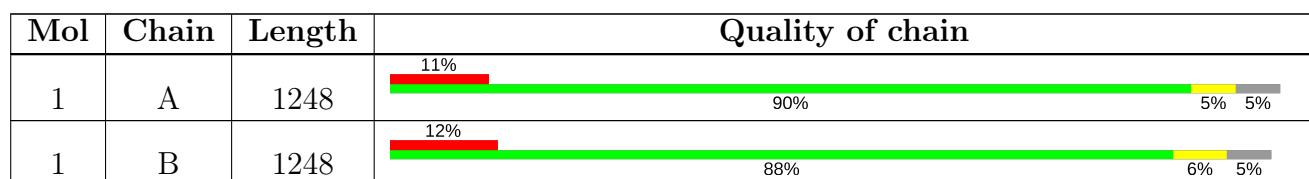
2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 37055 atoms, of which 18673 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 Multidrug resistance protein 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1182	Total	C	H	N	O	S	0	0	0
			18488	5890	9326	1554	1680	38			
1	B	1181	Total	C	H	N	O	S	0	0	0
			18481	5888	9323	1553	1679	38			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	GLN	GLU	engineered mutation	UNP P21447
A	?	-	MET	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	LYS	deletion	UNP P21447
A	?	-	ASP	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	GLY	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	LEU	deletion	UNP P21447
A	?	-	ILE	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	THR	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	LYS	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	ILE	deletion	UNP P21447
A	?	-	CYS	deletion	UNP P21447
A	?	-	GLY	deletion	UNP P21447
A	?	-	PRO	deletion	UNP P21447
A	?	-	HIS	deletion	UNP P21447

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P21447
A	?	-	GLN	deletion	UNP P21447
A	?	-	ASP	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	LYS	deletion	UNP P21447
A	?	-	LEU	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	THR	deletion	UNP P21447
A	?	-	LYS	deletion	UNP P21447
A	?	-	GLU	deletion	UNP P21447
A	1197	GLN	GLU	conflict	UNP P21447
A	1277	HIS	-	expression tag	UNP P21447
A	1278	HIS	-	expression tag	UNP P21447
A	1279	HIS	-	expression tag	UNP P21447
A	1280	HIS	-	expression tag	UNP P21447
A	1281	HIS	-	expression tag	UNP P21447
A	1282	HIS	-	expression tag	UNP P21447
B	552	GLN	GLU	engineered mutation	UNP P21447
B	?	-	MET	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	LYS	deletion	UNP P21447
B	?	-	ASP	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	GLY	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	LEU	deletion	UNP P21447
B	?	-	ILE	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	THR	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	LYS	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	ILE	deletion	UNP P21447
B	?	-	CYS	deletion	UNP P21447
B	?	-	GLY	deletion	UNP P21447
B	?	-	PRO	deletion	UNP P21447
B	?	-	HIS	deletion	UNP P21447

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	deletion	UNP P21447
B	?	-	GLN	deletion	UNP P21447
B	?	-	ASP	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	LYS	deletion	UNP P21447
B	?	-	LEU	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	THR	deletion	UNP P21447
B	?	-	LYS	deletion	UNP P21447
B	?	-	GLU	deletion	UNP P21447
B	1197	GLN	GLU	conflict	UNP P21447
B	1277	HIS	-	expression tag	UNP P21447
B	1278	HIS	-	expression tag	UNP P21447
B	1279	HIS	-	expression tag	UNP P21447
B	1280	HIS	-	expression tag	UNP P21447
B	1281	HIS	-	expression tag	UNP P21447
B	1282	HIS	-	expression tag	UNP P21447

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

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: Multidrug resistance protein 1A
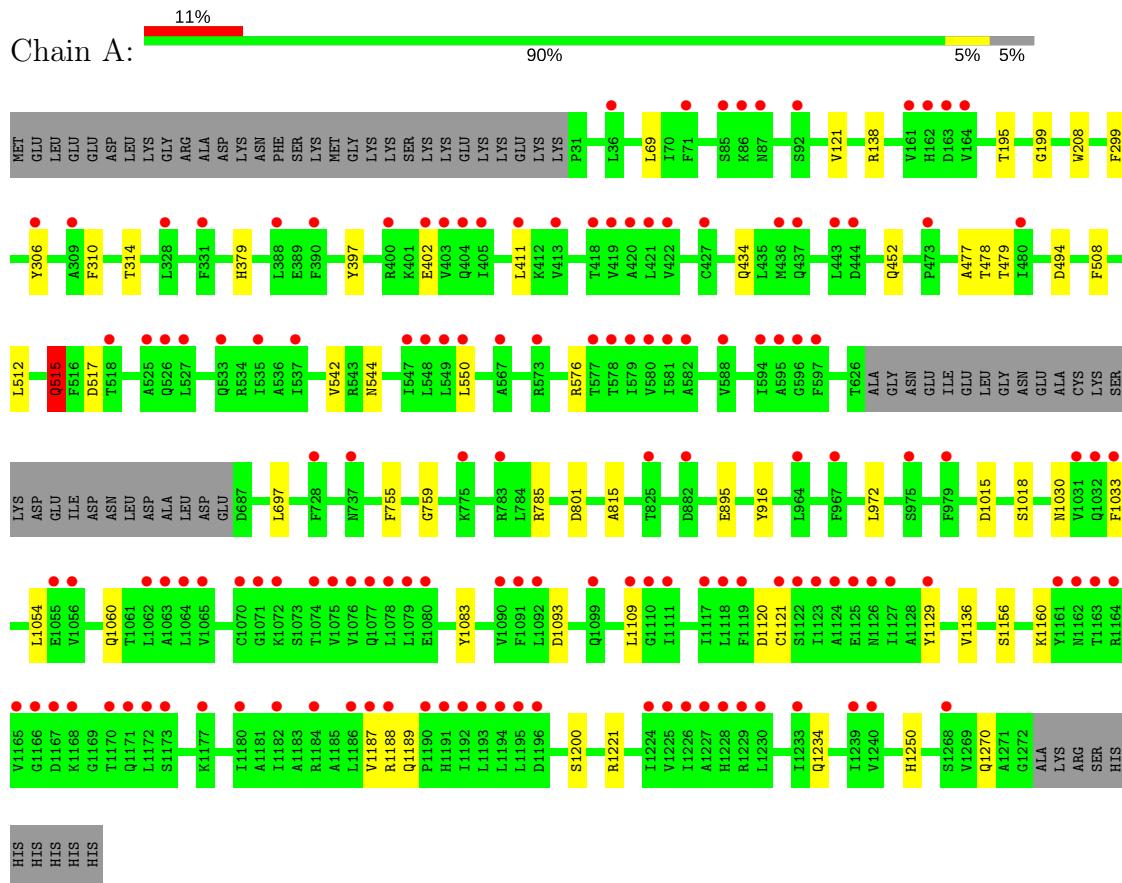
- Molecule 1: Multidrug resistance protein 1A
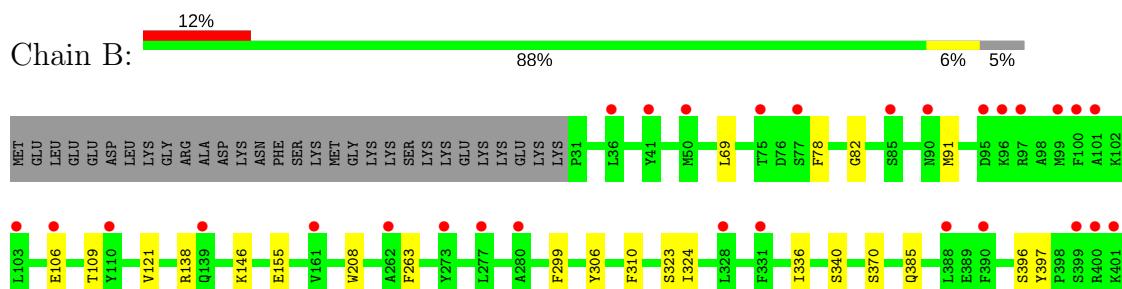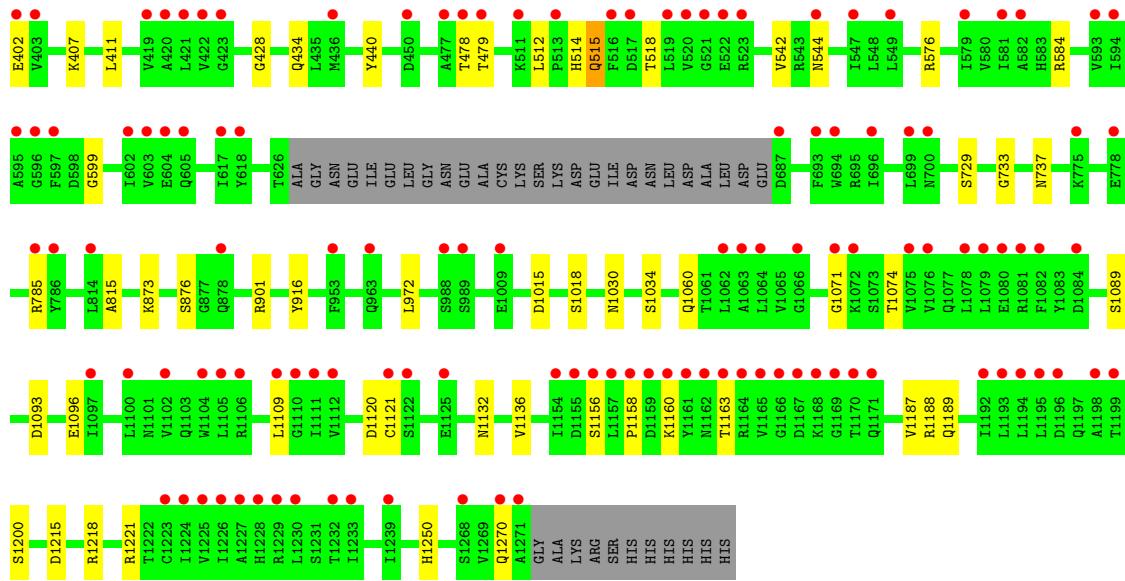
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.52Å 116.44Å 375.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.30 – 3.85 49.99 – 3.82	Depositor EDS
% Data completeness (in resolution range)	99.9 (21.30-3.85) 96.6 (49.99-3.82)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.246 , 0.289 0.256 , 0.301	Depositor DCC
R_{free} test set	3703 reflections (4.75%)	DCC
Wilson B-factor (Å^2)	137.6	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 86.3	EDS
L-test for twinning[2]	$< |L| > = 0.40, < L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	37055	wwPDB-VP
Average B, all atoms (Å^2)	197.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.34	0/9331	0.63	0/12615
1	B	0.33	0/9327	0.62	0/12610
All	All	0.34	0/18658	0.63	0/25225

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9162	9326	9343	17	0
1	B	9158	9323	9340	27	0
2	A	31	12	12	0	0
2	B	31	12	12	1	0
All	All	18382	18673	18707	41	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 1.

All (41) 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:B:544:ASN:OD1	1:B:576:ARG:NH2	2.24	0.70
1:B:1158:PRO:O	1:B:1163:THR:OG1	2.11	0.69
1:B:397:TYR:OH	1:B:434:GLN:NE2	2.26	0.69
1:A:138:ARG:NH2	1:B:515:GLN:OE1	2.25	0.69
1:B:440:TYR:OH	1:B:901:ARG:NH2	2.26	0.68
1:A:544:ASN:OD1	1:A:576:ARG:NH2	2.28	0.66
1:B:1215:ASP:OD1	1:B:1218:ARG:NH2	2.29	0.65
1:A:1189:GLN:OE1	1:A:1221:ARG:NH2	2.33	0.62
1:B:407:LYS:NZ	1:B:599:GLY:O	2.35	0.60
1:B:428:GLY:N	2:B:2000:ATP:O1A	2.38	0.56
1:A:397:TYR:OH	1:A:434:GLN:NE2	2.39	0.56
1:B:733:GLY:O	1:B:737:ASN:ND2	2.39	0.55
1:A:1109:LEU:O	1:A:1188:ARG:NH1	2.40	0.55
1:A:801:ASP:OD2	1:A:1083:TYR:OH	2.25	0.55
1:B:514:HIS:O	1:B:518:THR:N	2.42	0.52
1:A:515:GLN:OE1	1:B:138:ARG:NH2	2.43	0.51
1:B:1189:GLN:OE1	1:B:1221:ARG:NH2	2.44	0.51
1:B:785:ARG:NH2	1:B:815:ALA:O	2.43	0.49
1:A:1030:ASN:N	1:A:1093:ASP:OD1	2.45	0.49
1:B:155:GLU:OE2	1:B:370:SER:OG	2.29	0.49
1:B:1109:LEU:O	1:B:1188:ARG:NH1	2.45	0.48
1:A:755:PHE:O	1:A:759:GLY:N	2.43	0.48
1:A:379:HIS:ND1	1:A:452:GLN:OE1	2.45	0.48
1:B:1030:ASN:N	1:B:1093:ASP:OD1	2.46	0.47
1:B:1071:GLY:O	1:B:1074:THR:OG1	2.30	0.47
1:A:494:ASP:OD1	1:B:146:LYS:NZ	2.45	0.47
1:A:1033:PHE:O	1:A:1054:LEU:N	2.46	0.46
1:B:1015:ASP:OD2	1:B:1018:SER:N	2.49	0.45
1:A:478:THR:HG22	1:A:479:THR:H	1.82	0.45
1:B:729:SER:O	1:B:733:GLY:N	2.46	0.45
1:B:78:PHE:O	1:B:82:GLY:N	2.49	0.44
1:A:195:THR:O	1:A:199:GLY:N	2.45	0.44
1:B:106:GLU:O	1:B:109:THR:OG1	2.32	0.44
1:B:478:THR:HG22	1:B:479:THR:H	1.82	0.44
1:B:873:LYS:O	1:B:876:SER:N	2.51	0.43
1:A:477:ALA:N	1:A:895:GLU:OE2	2.52	0.43
1:A:1015:ASP:OD1	1:A:1018:SER:N	2.51	0.43
1:A:785:ARG:NH2	1:A:815:ALA:O	2.48	0.42
1:B:263:PHE:O	1:B:1132:ASN:ND2	2.53	0.42
1:B:323:SER:OG	1:B:324:ILE:N	2.53	0.42
1:B:336:ILE:O	1:B:340:SER:N	2.54	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	1178/1248 (94%)	1124 (95%)	49 (4%)	5 (0%)	38	77
1	B	1177/1248 (94%)	1122 (95%)	51 (4%)	4 (0%)	44	80
All	All	2355/2496 (94%)	2246 (95%)	100 (4%)	9 (0%)	38	77

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	GLN
1	A	1136	VAL
1	A	1160	LYS
1	B	515	GLN
1	B	1136	VAL
1	B	1120	ASP
1	A	411	LEU
1	A	1120	ASP
1	B	411	LEU

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	974/1031 (94%)	948 (97%)	26 (3%)	50	77
1	B	974/1031 (94%)	948 (97%)	26 (3%)	50	77
All	All	1948/2062 (94%)	1896 (97%)	52 (3%)	50	77

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	121	VAL
1	A	208	TRP
1	A	299	PHE
1	A	306	TYR
1	A	310	PHE
1	A	314	THR
1	A	402	GLU
1	A	508	PHE
1	A	512	LEU
1	A	515	GLN
1	A	517	ASP
1	A	542	VAL
1	A	550	LEU
1	A	697	LEU
1	A	916	TYR
1	A	972	LEU
1	A	1060	GLN
1	A	1121	CYS
1	A	1129	TYR
1	A	1156	SER
1	A	1187	VAL
1	A	1200	SER
1	A	1234	GLN
1	A	1250	HIS
1	A	1270	GLN
1	B	69	LEU
1	B	91	MET
1	B	121	VAL
1	B	208	TRP
1	B	299	PHE
1	B	306	TYR
1	B	310	PHE
1	B	385	GLN
1	B	396	SER
1	B	402	GLU
1	B	512	LEU
1	B	542	VAL
1	B	584	ARG
1	B	916	TYR
1	B	972	LEU
1	B	1034	SER

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Mol	Chain	Res	Type
1	B	1060	GLN
1	B	1089	SER
1	B	1096	GLU
1	B	1121	CYS
1	B	1156	SER
1	B	1160	LYS
1	B	1187	VAL
1	B	1200	SER
1	B	1250	HIS
1	B	1270	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	GLN
1	A	878	GLN
1	A	926	ASN
1	B	434	GLN
1	B	608	HIS
1	B	910	GLN
1	B	1270	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	#$|Z| > 2$
2	ATP	A	2000	-	27,33,33	0.94	1 (3%)	25,52,52	1.89	3 (12%)
2	ATP	B	2000	-	27,33,33	0.94	1 (3%)	25,52,52	1.87	4 (16%)

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	ATP	A	2000	-	-	0/18/38/38	0/3/3/3
2	ATP	B	2000	-	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	ATP	C5-C4	2.95	1.47	1.40
2	B	2000	ATP	C5-C4	2.97	1.47	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2000	ATP	N3-C2-N1	-6.95	122.80	128.86
2	A	2000	ATP	N3-C2-N1	-6.81	122.92	128.86
2	A	2000	ATP	C4-C5-N7	-3.37	106.16	109.41
2	B	2000	ATP	C4-C5-N7	-3.12	106.40	109.41
2	A	2000	ATP	C4'-O4'-C1'	-2.71	106.89	109.77
2	B	2000	ATP	C4'-O4'-C1'	-2.43	107.18	109.77
2	B	2000	ATP	C2-N1-C6	2.02	122.31	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2000	ATP	1	0

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	1182/1248 (94%)	0.44	143 (12%)	5	5	108, 170, 249, 374	0
1	B	1181/1248 (94%)	0.60	150 (12%)	4	5	105, 175, 272, 409	0
All	All	2363/2496 (94%)	0.52	293 (12%)	4	5	105, 173, 262, 409	0

All (293) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1170	THR	15.5
1	B	1226	ILE	14.6
1	B	603	VAL	12.8
1	B	1227	ALA	11.7
1	B	1225	VAL	11.0
1	A	1172	LEU	10.1
1	B	1161	TYR	9.0
1	B	604	GLU	8.9
1	A	1171	GLN	8.6
1	B	1168	LYS	8.5
1	A	1227	ALA	8.2
1	B	1156	SER	8.0
1	B	1169	GLY	7.9
1	B	1164	ARG	7.7
1	B	1195	LEU	7.7
1	A	1126	ASN	7.6
1	B	595	ALA	7.3
1	B	1080	GLU	7.0
1	A	1226	ILE	6.9
1	B	1228	HIS	6.7
1	A	1170	THR	6.5
1	B	594	ILE	6.4
1	A	1118	LEU	6.4
1	A	1228	HIS	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	1162	ASN	6.3
1	A	1125	GLU	6.0
1	A	86	LYS	5.9
1	B	687	ASP	5.8
1	B	1224	ILE	5.8
1	A	1123	ILE	5.7
1	B	421	LEU	5.6
1	B	423	GLY	5.5
1	B	1109	LEU	5.5
1	A	1161	TYR	5.5
1	B	511	LYS	5.4
1	B	1110	GLY	5.4
1	A	1074	THR	5.4
1	B	1158	PRO	5.4
1	A	1167	ASP	5.4
1	A	1064	LEU	5.3
1	B	100	PHE	5.3
1	B	420	ALA	5.3
1	A	1065	VAL	5.2
1	B	597	PHE	5.2
1	B	1229	ARG	5.1
1	A	1071	GLY	5.1
1	A	577	THR	5.1
1	A	1225	VAL	5.1
1	B	523	ARG	5.1
1	B	963	GLN	5.1
1	A	1194	LEU	5.0
1	B	1194	LEU	5.0
1	B	596	GLY	5.0
1	B	422	VAL	5.0
1	A	1224	ILE	5.0
1	B	1271	ALA	5.0
1	B	1155	ASP	5.0
1	B	1159	ASP	4.9
1	A	1165	VAL	4.9
1	A	578	THR	4.8
1	A	550	LEU	4.8
1	A	579	ILE	4.8
1	B	1165	VAL	4.7
1	B	1154	ILE	4.7
1	B	1157	LEU	4.7
1	B	1079	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	1196	ASP	4.6
1	B	99	MET	4.6
1	B	1081	ARG	4.6
1	A	737	ASN	4.5
1	A	1111	ILE	4.4
1	A	1124	ALA	4.4
1	A	1192	ILE	4.4
1	A	1187	VAL	4.3
1	A	1122	SER	4.3
1	B	1163	THR	4.3
1	A	1186	LEU	4.3
1	A	420	ALA	4.3
1	B	1063	ALA	4.3
1	B	1062	LEU	4.2
1	A	162	HIS	4.2
1	A	1127	ILE	4.2
1	A	1117	ILE	4.2
1	B	1193	LEU	4.2
1	A	548	LEU	4.1
1	B	103	LEU	4.1
1	A	1229	ARG	4.0
1	A	1077	GLN	3.9
1	A	580	VAL	3.8
1	B	1160	LYS	3.8
1	A	1055	GLU	3.8
1	B	1064	LEU	3.8
1	B	419	VAL	3.8
1	A	87	ASN	3.7
1	B	605	GLN	3.7
1	A	581	ILE	3.7
1	B	1232	THR	3.7
1	A	1177	LYS	3.7
1	A	533	GLN	3.7
1	A	1075	VAL	3.7
1	B	1111	ILE	3.7
1	A	1121	CYS	3.6
1	A	595	ALA	3.6
1	B	90	ASN	3.6
1	B	522	GLU	3.6
1	B	1009	GLU	3.6
1	A	419	VAL	3.6
1	B	618	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	390	PHE	3.6
1	A	1079	LEU	3.6
1	B	1106	ARG	3.5
1	B	1196	ASP	3.5
1	B	399	SER	3.5
1	A	1195	LEU	3.5
1	A	1129	TYR	3.5
1	B	402	GLU	3.5
1	A	418	THR	3.4
1	A	594	ILE	3.4
1	B	516	PHE	3.4
1	B	1233	ILE	3.4
1	A	549	LEU	3.4
1	B	617	ILE	3.4
1	A	421	LEU	3.4
1	B	97	ARG	3.4
1	A	1062	LEU	3.4
1	A	1090	VAL	3.4
1	A	1173	SER	3.4
1	A	1078	LEU	3.3
1	B	85	SER	3.3
1	B	400	ARG	3.3
1	A	525	ALA	3.3
1	B	95	ASP	3.3
1	B	388	LEU	3.3
1	B	1198	ALA	3.3
1	B	1105	LEU	3.3
1	A	1163	THR	3.3
1	B	785	ARG	3.3
1	B	1192	ILE	3.3
1	B	1230	LEU	3.3
1	A	1233	ILE	3.3
1	B	1171	GLN	3.2
1	A	404	GLN	3.2
1	B	1268	SER	3.2
1	B	1078	LEU	3.2
1	B	579	ILE	3.1
1	A	1188	ARG	3.1
1	B	273	TYR	3.1
1	A	1076	VAL	3.1
1	B	1223	CYS	3.1
1	A	1166	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	953	PHE	3.1
1	A	1070	CYS	3.1
1	A	443	LEU	3.1
1	B	814	LEU	3.1
1	A	1164	ARG	3.0
1	A	411	LEU	3.0
1	B	517	ASP	3.0
1	B	1166	GLY	3.0
1	B	602	ILE	3.0
1	A	1110	GLY	3.0
1	B	36	LEU	3.0
1	A	775	LYS	2.9
1	A	1230	LEU	2.9
1	A	526	GLN	2.9
1	A	402	GLU	2.9
1	B	694	TRP	2.9
1	A	547	ILE	2.9
1	B	521	GLY	2.9
1	A	1099	GLN	2.9
1	B	1076	VAL	2.9
1	B	328	LEU	2.9
1	A	1032	GLN	2.9
1	A	1193	LEU	2.9
1	B	582	ALA	2.9
1	A	436	MET	2.8
1	A	1056	VAL	2.8
1	B	1104	TRP	2.8
1	B	77	SER	2.8
1	A	331	PHE	2.8
1	A	783	ARG	2.8
1	A	582	ALA	2.8
1	A	1033	PHE	2.7
1	A	400	ARG	2.7
1	A	1031	VAL	2.7
1	A	527	LEU	2.7
1	A	1063	ALA	2.7
1	B	1112	VAL	2.7
1	B	280	ALA	2.7
1	A	1168	LYS	2.7
1	B	1270	GLN	2.6
1	B	106	GLU	2.6
1	B	1102	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1167	ASP	2.6
1	A	328	LEU	2.6
1	A	480	ILE	2.6
1	A	161	VAL	2.6
1	A	596	GLY	2.6
1	B	277	LEU	2.6
1	B	436	MET	2.6
1	A	597	PHE	2.6
1	B	331	PHE	2.6
1	A	85	SER	2.6
1	A	964	LEU	2.6
1	A	1080	GLU	2.6
1	A	537	ILE	2.5
1	B	513	PRO	2.5
1	A	1182	ILE	2.5
1	A	1162	ASN	2.5
1	B	110	TYR	2.5
1	A	473	PRO	2.5
1	B	1084	ASP	2.5
1	A	1109	LEU	2.5
1	B	878	GLN	2.5
1	B	477	ALA	2.5
1	A	825	THR	2.5
1	A	1184	ARG	2.5
1	A	975	SER	2.5
1	B	519	LEU	2.5
1	B	262	ALA	2.5
1	B	778	GLU	2.4
1	B	403	VAL	2.4
1	A	1072	LYS	2.4
1	B	1125	GLU	2.4
1	A	1191	HIS	2.4
1	A	1190	PRO	2.4
1	A	36	LEU	2.4
1	B	520	VAL	2.4
1	A	413	VAL	2.4
1	A	1240	VAL	2.4
1	B	700	ASN	2.4
1	B	161	VAL	2.4
1	B	989	SER	2.4
1	B	41	TYR	2.4
1	B	1075	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	450	ASP	2.3
1	A	1091	PHE	2.3
1	A	309	ALA	2.3
1	A	403	VAL	2.3
1	B	50	MET	2.3
1	A	1180	ILE	2.3
1	A	306	TYR	2.3
1	B	479	THR	2.3
1	A	588	VAL	2.3
1	A	535	ILE	2.3
1	A	728	PHE	2.3
1	B	581	ILE	2.3
1	B	139	GLN	2.2
1	B	786	TYR	2.2
1	A	444	ASP	2.2
1	B	696	ILE	2.2
1	A	422	VAL	2.2
1	B	547	ILE	2.2
1	B	544	ASN	2.2
1	A	967	PHE	2.2
1	A	1239	ILE	2.2
1	B	775	LYS	2.2
1	B	1121	CYS	2.2
1	B	1122	SER	2.1
1	A	573	ARG	2.1
1	A	518	THR	2.1
1	B	593	VAL	2.1
1	A	1119	PHE	2.1
1	B	1097	ILE	2.1
1	B	1066	GLY	2.1
1	A	164	VAL	2.1
1	A	1092	LEU	2.1
1	B	549	LEU	2.1
1	A	1268	SER	2.1
1	A	71	PHE	2.1
1	B	390	PHE	2.1
1	B	988	SER	2.1
1	B	1239	ILE	2.1
1	B	75	THR	2.1
1	B	693	PHE	2.1
1	A	567	ALA	2.1
1	B	1072	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1100	LEU	2.1
1	B	1199	THR	2.0
1	A	405	ILE	2.0
1	B	101	ALA	2.0
1	A	163	ASP	2.0
1	A	388	LEU	2.0
1	A	882	ASP	2.0
1	B	96	LYS	2.0
1	A	427	CYS	2.0
1	B	401	LYS	2.0
1	B	699	LEU	2.0
1	A	92	SER	2.0
1	B	478	THR	2.0
1	A	979	PHE	2.0
1	B	1082	PHE	2.0
1	B	1071	GLY	2.0
1	A	437	GLN	2.0

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	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	ATP	A	2000	31/31	0.60	0.27	-0.40	201,241,278,286	0
2	ATP	B	2000	31/31	0.83	0.26	-0.47	195,228,260,277	0

6.5 Other polymers ⓘ

There are no such residues in this entry.