



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2016 – 04:37 PM EDT

PDB ID : 4NH0
Title : Cytoplasmic domain of the Thermomonospora curvata Type VII Secretion ATPase EccC
Authors : Rosenberg, O.S.; Cox, J.S.; Stroud, R.M.; Strauli, N.; Dovala, D.
Deposited on : 2013-11-03
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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

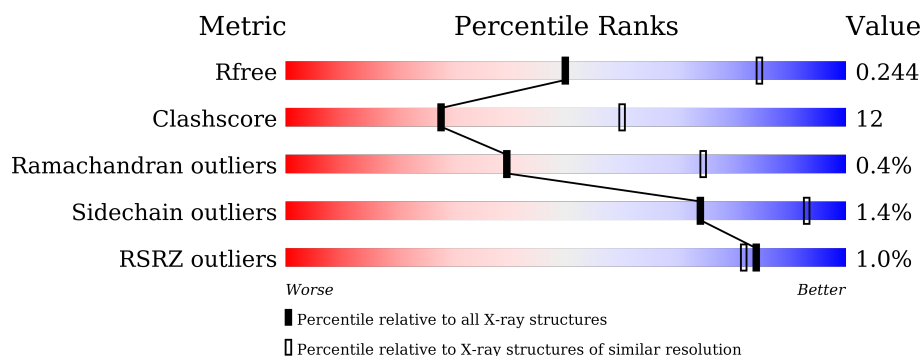
1 Overall quality at a glance

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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	1147	<div> <div></div> <div>60%14%25%</div> </div>
1	B	1147	<div> <div>%</div> <div>56%17%25%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13435 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 Cell divisionFtsK/SpoIIIE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	861	Total	C	N	O	S	0	0	0
			6663	4212	1181	1249	21			
1	B	859	Total	C	N	O	S	0	0	0
			6626	4186	1175	1244	21			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	MET	-	EXPRESSION TAG	UNP D1A4G7
A	170	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	171	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	172	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	173	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	174	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	175	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	176	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	177	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	178	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	179	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	180	SER	-	EXPRESSION TAG	UNP D1A4G7
A	181	GLU	-	EXPRESSION TAG	UNP D1A4G7
A	182	PHE	-	EXPRESSION TAG	UNP D1A4G7
A	183	SER	-	EXPRESSION TAG	UNP D1A4G7
A	184	ILE	-	EXPRESSION TAG	UNP D1A4G7
A	185	ASP	-	EXPRESSION TAG	UNP D1A4G7
A	186	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	187	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	188	SER	-	EXPRESSION TAG	UNP D1A4G7
A	189	LEU	-	EXPRESSION TAG	UNP D1A4G7
A	190	GLU	-	EXPRESSION TAG	UNP D1A4G7
A	191	VAL	-	EXPRESSION TAG	UNP D1A4G7
A	192	LEU	-	EXPRESSION TAG	UNP D1A4G7
A	193	PHE	-	EXPRESSION TAG	UNP D1A4G7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	194	GLN	-	EXPRESSION TAG	UNP D1A4G7
A	195	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	196	PRO	-	EXPRESSION TAG	UNP D1A4G7
A	197	SER	-	EXPRESSION TAG	UNP D1A4G7
A	198	SER	-	EXPRESSION TAG	UNP D1A4G7
A	199	PRO	-	EXPRESSION TAG	UNP D1A4G7
B	169	MET	-	EXPRESSION TAG	UNP D1A4G7
B	170	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	171	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	172	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	173	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	174	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	175	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	176	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	177	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	178	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	179	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	180	SER	-	EXPRESSION TAG	UNP D1A4G7
B	181	GLU	-	EXPRESSION TAG	UNP D1A4G7
B	182	PHE	-	EXPRESSION TAG	UNP D1A4G7
B	183	SER	-	EXPRESSION TAG	UNP D1A4G7
B	184	ILE	-	EXPRESSION TAG	UNP D1A4G7
B	185	ASP	-	EXPRESSION TAG	UNP D1A4G7
B	186	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	187	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	188	SER	-	EXPRESSION TAG	UNP D1A4G7
B	189	LEU	-	EXPRESSION TAG	UNP D1A4G7
B	190	GLU	-	EXPRESSION TAG	UNP D1A4G7
B	191	VAL	-	EXPRESSION TAG	UNP D1A4G7
B	192	LEU	-	EXPRESSION TAG	UNP D1A4G7
B	193	PHE	-	EXPRESSION TAG	UNP D1A4G7
B	194	GLN	-	EXPRESSION TAG	UNP D1A4G7
B	195	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	196	PRO	-	EXPRESSION TAG	UNP D1A4G7
B	197	SER	-	EXPRESSION TAG	UNP D1A4G7
B	198	SER	-	EXPRESSION TAG	UNP D1A4G7
B	199	PRO	-	EXPRESSION TAG	UNP D1A4G7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

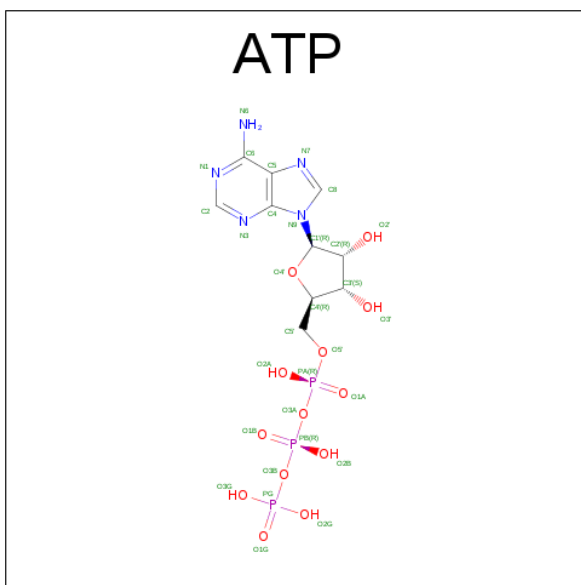


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	B	4	Total O 4 4	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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cell divisionFtsK/SpoIIIE



- Molecule 1: Cell divisionFtsK/SpoIIIE



W1176	Y1001	L850	ARG	S655	L589	GLU	ASN	GLU	MET
R1177	E1002	L851	ALA	R656	R601	GLU	GLU	ASP	HIS
K1180	D1006	R852	GLU	V657	R660	VAL	ALA	THR	HIS
M1183	K1009	T853	ASN	V658	S662	LEU	MET	GLY	HIS
L1187	Y1013	P854	LYS	G660	Y665	S414	LEU	PRO	HIS
P1188	R1020	F859	SER	V661	Y671	A415	GLU	GLY	HIS
P1189	G1021	D863	SER	Y665	E572	M416	LEU	ILE	HIS
L1192	F1029	L743	ALA	B666	B575	L419	LYS	ASP	HIS
R1200	L1030	L744	GLU	L667	B576	L422	THR	PRO	GLY
S1201	L1033	D745	LYS	P668	E577	Y429	ARG	GLY	SER
P1227	P1034	V746	SER	Y675	G578	D432	ARG	PHE	PHE
R1236	R1035	V747	ALA	R685	A579	P433	VAL	GLY	SER
D1237	I1036	P756	GLU	Y690	G579	A434	TYR	ALA	ILE
I1238	D1037	E757	GLU	V691	P580	V435	VAL	ARG	GLY
L1242	G1038	P758	GLU	S692	L581	Q442	LYS	ALA	GLY
I1243	T1040	T883	GLU	P694	P585	R445	ARG	CYS	SER
I1244	T1044	R884	GLU	V695	F594	L446	ALA	ALA	LEU
M1248	T1048	R891	GLU	D696	S595	P449	LYS	GLY	VAL
G1275	T1051	E905	PRO	E697	R601	D453	ARG	LEU	PHE
G1294	T1052	Q906	GLN	L772	L607	R457	THR	VAL	GLN
F1298	V1053	E910	THR	S782	R613	D462	SER	GLY	PRO
I1308	K1054	S783	ARG	A783	L614	I463	VAL	GLY	SER
Q1309	E1058	R797	GLU	G796	A625	K464	GLN	GLY	PRO
T1310	A1059	R798	GLY	R797	S626	Q468	ARG	LYS	ASP
S1315	W1060	H799	ILE	ILE	Q627	M471	PRO	ALA	LEU
	A1065	L804	VAL	VAL	R628	S483	GLN	TYR	VAL
	P1066	V805	ARG	ARG	L629	E487	ALA	ASP	ILE
	L1071	D806	GLN	GLN	B630	G475	ILE	GLN	SER
	P1072	R807	VAL	VAL	B631	L476	ALA	ILE	LEU
	D1095	P808	LEU	LEU	G632	T491	GLU	GLY	LEU
	E1096	F809	PRO	PRO	K633	E503	ALA	GLY	PRO
	D1117	D810	TYR	TYR	L634	L524	GLY	ASP	GLY
	C1120	Q811	LEU	LEU	G636	L534	ALA	VAL	ASP
	G1121	R812	THR	THR	L637	V541	PRO	ARG	ASP
	K1122	R813	ASP	ASP	D638	D542	PHE	LEU	PRO
	D1148	D819	ILE	ILE	T639	R644	ARG	LEU	LYS
	S1152	G822	ARG	ARG	L640	L647	THR	THR	ALA
	L1153	G823	PRO	PRO	L641	D642	SER	GLY	TYR
	A1166	A824	GLN	GLN	S642	F650	ALA	VAL	GLY
	L1175	G828	PRO	PRO	R643	M653	ASP	ALA	MET
		L939	GLU	GLU	R644	B654	GLU	GLU	VAL
		E904	GLN	GLN	L647		PRO	THR	ARG
		L995	PRO	PRO			ALA	ALA	
		R996	GLN	GLN			ASP	THR	
		L997	PRO	PRO			GLU	GLY	
			GLN	GLN			THR	VAL	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	251.82Å 116.32Å 174.11Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	48.93 – 2.90 48.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.93-2.90) 86.2 (48.93-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.226 , 0.246 0.225 , 0.244	Depositor DCC
R_{free} test set	1330 reflections (1.42%)	DCC
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13435	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, 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	0.25	0/6813	0.41	1/9264 (0.0%)
1	B	0.27	0/6774	0.47	2/9215 (0.0%)
All	All	0.26	0/13587	0.44	3/18479 (0.0%)

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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	807	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	B	579	ALA	C-N-CD	6.66	142.39	128.40
1	A	563	GLY	N-CA-C	-5.68	98.91	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	807	ARG	Peptide

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	6663	0	6636	118	0
1	B	6626	0	6588	196	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	62	0	24	1	0
4	B	62	0	24	4	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
All	All	13435	0	13272	314	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 12.

All (314) 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:629:LEU:HD21	1:B:633:LYS:CB	1.81	1.09
1:B:629:LEU:CD2	1:B:633:LYS:HB2	1.87	1.05
1:B:629:LEU:HD21	1:B:633:LYS:HB2	1.08	1.03
1:B:1122:LYS:NZ	4:B:1404:ATP:O2B	1.97	0.97
1:B:764:PRO:O	1:B:813:ARG:NH2	2.02	0.93
1:B:631:GLU:N	1:B:631:GLU:OE2	2.02	0.92
1:B:628:ARG:NH2	1:B:650:PHE:CG	2.38	0.91
1:B:636:GLY:O	1:B:640:HIS:HD2	1.52	0.91
1:A:1006:ASP:OD2	1:A:1009:LYS:N	2.04	0.89
1:A:442:GLN:O	1:A:464:LYS:NZ	2.07	0.86
1:B:905:GLU:OE2	1:B:963:ARG:NH1	2.08	0.86
1:B:644:ARG:HG3	1:B:644:ARG:HH11	1.38	0.85
1:A:442:GLN:HG3	1:A:445:ARG:HH12	1.42	0.82
1:A:543:ARG:NH1	1:A:806:ASP:OD2	2.13	0.81
1:B:471:MET:O	1:B:642:SER:OG	1.97	0.81
1:B:807:ARG:HG2	1:B:812:ARG:H	1.45	0.81
1:A:1148:ASP:OD2	1:A:1152:SER:N	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:ARG:HH21	1:B:650:PHE:CB	1.95	0.79
1:A:832:GLY:O	1:A:835:THR:OG1	1.99	0.79
1:A:1006:ASP:HB3	1:A:1009:LYS:HG3	1.65	0.79
1:B:561:HIS:CD2	1:B:562:SER:H	2.01	0.78
1:B:636:GLY:O	1:B:640:HIS:CD2	2.35	0.78
1:A:1006:ASP:CB	1:A:1009:LYS:HG3	2.14	0.78
1:B:644:ARG:HG3	1:B:644:ARG:NH1	1.98	0.78
1:B:807:ARG:NE	1:B:811:GLN:H	1.82	0.78
1:B:813:ARG:HG2	1:B:813:ARG:HH11	1.49	0.77
1:B:572:GLU:OE2	1:B:575:ARG:HG2	1.85	0.77
1:A:542:ASP:OD2	1:A:601:LYS:NZ	2.17	0.76
1:B:743:LEU:HD13	1:B:744:PHE:H	1.50	0.75
1:B:629:LEU:HD22	1:B:630:GLU:H	1.52	0.74
1:B:630:GLU:HG2	1:B:633:LYS:HG2	1.69	0.74
1:B:629:LEU:CD2	1:B:630:GLU:H	2.01	0.73
1:B:807:ARG:HE	1:B:811:GLN:H	1.35	0.73
1:A:555:ARG:NH2	1:A:585:PRO:O	2.21	0.73
1:B:629:LEU:HD23	1:B:633:LYS:HG3	1.71	0.73
1:B:575:ARG:HH11	1:B:575:ARG:HG2	1.52	0.72
1:B:837:LYS:NZ	4:B:1405:ATP:O2B	2.20	0.72
1:B:891:ARG:NH1	1:B:1096:GLU:OE2	2.24	0.71
1:B:629:LEU:CD2	1:B:633:LYS:CG	2.68	0.71
1:B:637:LEU:O	1:B:641:LEU:HG	1.90	0.71
1:B:743:LEU:HD13	1:B:744:PHE:N	2.05	0.71
1:B:629:LEU:HD11	1:B:634:LEU:HD21	1.71	0.71
1:B:691:VAL:HG23	1:B:692:SER:H	1.55	0.69
1:B:1033:LEU:O	1:B:1035:ARG:N	2.26	0.69
1:B:629:LEU:CD2	1:B:633:LYS:CB	2.58	0.68
1:B:807:ARG:HD2	1:B:807:ARG:C	2.14	0.68
1:B:807:ARG:HD2	1:B:808:PRO:N	2.08	0.68
1:B:464:LYS:NZ	1:B:468:GLN:O	2.27	0.68
1:A:1001:TYR:HD1	1:A:1002:GLU:H	1.39	0.68
1:B:807:ARG:HE	1:B:810:ASP:N	1.93	0.67
1:A:904:ARG:NE	1:A:931:ASP:OD2	2.23	0.67
1:B:692:SER:OG	1:B:693:GLY:N	2.26	0.66
1:B:1200:ARG:HH21	1:B:1236:ARG:HG2	1.60	0.66
1:B:487:GLU:OE2	1:B:692:SER:N	2.29	0.66
1:B:432:ASP:HB3	1:B:435:VAL:HG22	1.78	0.65
1:B:655:SER:OG	1:B:661:VAL:O	2.14	0.65
1:B:804:LEU:HD11	1:B:813:ARG:HB3	1.78	0.65
1:A:432:ASP:HB3	1:A:435:VAL:HG22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:SER:OG	1:A:980:GLU:OE1	2.16	0.64
1:B:975:SER:OG	1:B:980:GLU:OE1	2.15	0.64
1:B:629:LEU:CD2	1:B:633:LYS:HG3	2.28	0.64
1:A:573:LYS:O	1:A:577:GLU:N	2.30	0.63
1:B:766:LEU:H	1:B:813:ARG:HH22	1.47	0.63
1:A:658:VAL:HG23	1:A:659:LEU:HG	1.81	0.62
1:A:681:GLU:N	1:A:681:GLU:OE1	2.33	0.62
1:A:442:GLN:HG3	1:A:445:ARG:NH1	2.12	0.62
1:B:743:LEU:HA	1:B:746:VAL:HB	1.80	0.62
1:B:1177:ARG:HH11	1:B:1177:ARG:HG2	1.65	0.62
1:B:813:ARG:NH1	1:B:813:ARG:HG2	2.12	0.62
1:B:805:VAL:HA	1:B:1029:PHE:HA	1.82	0.62
1:A:543:ARG:NH2	1:A:763:LEU:O	2.33	0.61
1:A:1006:ASP:CG	1:A:1009:LYS:HG3	2.21	0.61
1:A:645:ILE:HG12	1:A:676:LEU:HD23	1.83	0.61
1:A:1189:PRO:HD2	1:A:1192:LEU:HD11	1.83	0.61
1:B:542:ASP:HA	1:B:545:TYR:HB3	1.82	0.61
1:A:920:ARG:NH1	1:A:935:ASP:OD2	2.34	0.60
1:B:1036:ILE:HG12	1:B:1052:THR:HG22	1.82	0.60
1:B:628:ARG:NH2	1:B:650:PHE:CD2	2.68	0.60
1:B:1020:ARG:CG	1:B:1030:LEU:HA	2.32	0.60
1:B:810:ASP:HB3	1:B:812:ARG:NH1	2.17	0.60
1:B:644:ARG:CG	1:B:644:ARG:HH11	2.12	0.60
1:A:1006:ASP:OD2	1:A:1008:LYS:N	2.34	0.59
1:A:543:ARG:NH1	1:A:765:PRO:HA	2.18	0.59
1:B:1148:ASP:OD2	1:B:1152:SER:N	2.34	0.59
1:B:628:ARG:NH2	1:B:650:PHE:CB	2.62	0.59
1:A:568:LEU:HD13	1:A:619:GLY:HA3	1.84	0.59
1:B:1006:ASP:OD2	1:B:1009:LYS:HG3	2.02	0.59
1:B:772:LEU:HD23	1:B:850:LEU:HD12	1.83	0.59
1:B:923:ARG:NH1	1:B:933:PHE:O	2.35	0.59
1:B:807:ARG:NE	1:B:811:GLN:N	2.49	0.59
1:B:764:PRO:O	1:B:766:LEU:N	2.36	0.59
1:B:575:ARG:CG	1:B:575:ARG:HH11	2.16	0.58
1:A:508:VAL:HG23	1:A:587:LEU:HD11	1.83	0.58
1:A:525:ARG:NH1	1:A:755:GLY:O	2.37	0.58
1:B:996:ARG:HD3	1:B:1013:VAL:HG22	1.85	0.58
1:B:1037:ASP:OD1	1:B:1038:GLY:N	2.36	0.58
1:B:629:LEU:HD22	1:B:630:GLU:N	2.18	0.58
1:A:476:LEU:HB2	1:A:641:LEU:HD13	1.86	0.58
1:B:422:LEU:HD23	1:B:449:PRO:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:VAL:HG11	1:B:601:LYS:HG3	1.86	0.57
1:A:1001:TYR:CD1	1:A:1002:GLU:N	2.69	0.57
1:B:804:LEU:O	1:B:1030:LEU:N	2.37	0.57
1:A:838:SER:OG	4:A:1405:ATP:O1B	2.23	0.57
1:A:837:LYS:O	1:A:840:MET:N	2.38	0.57
1:B:572:GLU:O	1:B:575:ARG:HB3	2.05	0.57
1:B:613:ARG:NH1	1:B:614:LEU:HD21	2.20	0.57
1:B:654:GLU:H	1:B:654:GLU:CD	2.07	0.56
1:B:859:PHE:HB2	1:B:878:VAL:HG12	1.86	0.56
1:B:810:ASP:HB3	1:B:812:ARG:HH12	1.70	0.56
1:B:1117:ASP:O	1:B:1122:LYS:HE2	2.05	0.56
1:B:1120:CYS:SG	1:B:1122:LYS:HE3	2.45	0.56
1:B:475:GLY:HA3	1:B:643:TYR:CZ	2.41	0.56
1:B:1020:ARG:HD3	1:B:1030:LEU:HA	1.88	0.56
1:B:561:HIS:HD2	1:B:562:SER:H	1.53	0.56
1:B:804:LEU:HD21	1:B:813:ARG:HD3	1.88	0.56
1:B:864:PHE:H	1:B:941:ASP:HB3	1.71	0.55
1:A:1035:ARG:HH12	1:A:1044:THR:HG23	1.71	0.55
1:A:462:ASP:OD2	1:A:464:LYS:HE2	2.07	0.55
1:B:442:GLN:HA	1:B:445:ARG:NH1	2.22	0.55
1:B:1117:ASP:O	1:B:1122:LYS:CE	2.54	0.55
1:B:757:GLU:HG2	1:B:758:PRO:HD2	1.90	0.54
1:A:573:LYS:O	1:A:577:GLU:HB2	2.07	0.54
1:B:822:GLY:O	1:B:824:ALA:N	2.38	0.54
1:B:483:SER:HB2	1:B:647:LEU:HB3	1.88	0.54
1:B:1054:LYS:NZ	1:B:1058:GLU:OE2	2.38	0.54
1:B:628:ARG:HH21	1:B:650:PHE:HB3	1.71	0.54
1:A:1134:ILE:HG12	1:A:1159:THR:HG21	1.90	0.54
1:B:432:ASP:OD1	1:B:434:ALA:N	2.41	0.53
1:B:631:GLU:HA	1:B:657:VAL:HG21	1.89	0.53
1:A:1126:LEU:HD21	1:A:1245:ALA:HB2	1.90	0.53
1:A:807:ARG:HD3	1:A:1027:TYR:CE2	2.43	0.53
1:B:807:ARG:HE	1:B:809:PHE:C	2.12	0.53
1:A:1144:LEU:HD23	1:A:1209:PHE:HB2	1.90	0.53
1:A:1277:LYS:H	1:A:1277:LYS:HD2	1.73	0.53
1:B:631:GLU:OE1	1:B:653:MET:SD	2.67	0.53
1:B:561:HIS:O	1:B:562:SER:OG	2.26	0.53
1:B:593:GLU:OE2	1:B:627:GLN:CG	2.57	0.53
1:B:643:TYR:C	1:B:644:ARG:HD3	2.29	0.52
1:B:693:GLY:O	1:B:743:LEU:HD12	2.09	0.52
1:A:1126:LEU:HD12	1:A:1211:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:TYR:HD1	1:B:692:SER:HB3	1.73	0.52
1:B:561:HIS:CD2	1:B:562:SER:N	2.75	0.52
1:B:595:SER:OG	1:B:633:LYS:NZ	2.42	0.52
1:B:629:LEU:HD23	1:B:633:LYS:CG	2.36	0.52
1:B:920:ARG:NH1	1:B:935:ASP:OD2	2.43	0.52
1:B:629:LEU:HD11	1:B:634:LEU:CD2	2.40	0.52
1:A:1023:THR:HG22	1:A:1025:ASP:H	1.74	0.51
1:A:1037:ASP:OD1	1:A:1038:GLY:N	2.43	0.51
1:B:1001:TYR:CD2	1:B:1002:GLU:HG3	2.44	0.51
1:B:1071:LEU:HD12	1:B:1072:PRO:HD2	1.91	0.51
1:B:572:GLU:HA	1:B:572:GLU:OE2	2.09	0.51
1:B:593:GLU:OE2	1:B:627:GLN:HG3	2.10	0.51
1:A:1035:ARG:HA	1:A:1052:THR:HG21	1.93	0.51
1:B:1048:GLY:O	1:B:1051:THR:OG1	2.26	0.51
1:A:572:GLU:O	1:A:575:ARG:HB3	2.11	0.51
1:B:1183:MET:HB3	1:B:1238:ILE:HD12	1.93	0.51
1:A:1143:ARG:HE	1:A:1163:ILE:HD11	1.76	0.50
1:B:419:LEU:HD22	1:B:491:THR:HG23	1.93	0.50
1:A:759:HIS:NE2	1:A:811:GLN:OE1	2.42	0.50
1:B:1177:ARG:NH1	1:B:1177:ARG:HG2	2.27	0.50
1:A:558:HIS:ND1	1:A:562:SER:OG	2.44	0.50
1:A:591:LEU:HD21	1:A:597:LEU:HD13	1.93	0.50
1:A:999:ASP:OD1	1:A:1001:TYR:N	2.44	0.50
1:B:1180:LYS:HD2	1:B:1227:PRO:HB2	1.93	0.50
1:B:1242:LEU:HD23	1:B:1244:ILE:HD11	1.94	0.50
1:B:572:GLU:HA	1:B:575:ARG:HB3	1.93	0.50
1:B:828:GLY:HA3	1:B:989:LEU:HD13	1.94	0.50
1:A:796:GLY:HA2	1:A:852:HIS:CD2	2.47	0.49
1:B:807:ARG:HD3	1:B:810:ASP:H	1.76	0.49
1:A:1193:THR:HG23	1:A:1196:GLN:H	1.77	0.49
1:B:832:GLY:O	1:B:837:LYS:NZ	2.46	0.49
1:B:782:SER:OG	1:B:783:ALA:N	2.44	0.49
1:B:872:LEU:HB3	1:B:875:LEU:HD12	1.95	0.49
1:A:638:ASP:CG	1:A:644:ARG:HH22	2.16	0.49
1:B:565:TYR:CD2	1:B:571:TYR:HA	2.47	0.48
1:B:592:ASP:HA	1:B:625:ALA:HB3	1.95	0.48
1:B:654:GLU:O	1:B:658:VAL:HG13	2.13	0.48
1:B:691:VAL:O	1:B:743:LEU:HD11	2.13	0.48
1:A:866:GLY:H	1:A:884:ARG:HH22	1.60	0.48
1:B:1035:ARG:HA	1:B:1052:THR:HG21	1.96	0.48
1:A:522:GLU:HG3	1:A:530:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:GLY:HA3	1:A:989:LEU:HD13	1.94	0.48
1:B:1020:ARG:HG3	1:B:1029:PHE:O	2.12	0.48
1:A:1191:ASP:N	1:A:1191:ASP:OD1	2.42	0.48
1:B:641:LEU:HD23	1:B:641:LEU:N	2.27	0.48
1:B:1148:ASP:OD2	1:B:1153:LEU:N	2.44	0.48
1:B:807:ARG:HE	1:B:811:GLN:N	2.07	0.48
1:B:1035:ARG:NH2	1:B:1044:THR:O	2.47	0.48
1:A:443:ARG:HA	1:A:464:LYS:HZ1	1.79	0.48
1:A:657:VAL:HG23	1:A:658:VAL:HG13	1.95	0.48
1:A:794:TRP:HA	1:A:797:ARG:HG3	1.96	0.48
1:B:690:TYR:CD1	1:B:692:SER:HB3	2.49	0.47
1:B:769:PRO:HA	1:B:1030:LEU:HD23	1.95	0.47
1:A:1151:ARG:HB3	1:A:1154:LEU:HD21	1.95	0.47
1:A:1095:ASP:HA	1:A:1308:ILE:HA	1.96	0.47
1:A:419:LEU:HD21	1:A:495:ALA:HB2	1.96	0.47
1:B:416:ASN:HB3	1:B:690:TYR:CE2	2.49	0.47
1:B:629:LEU:CD2	1:B:630:GLU:N	2.73	0.47
1:B:854:PRO:HG2	1:B:1060:TRP:CD1	2.48	0.47
1:B:545:TYR:CE1	1:B:607:LEU:HB2	2.49	0.47
1:A:1218:VAL:O	1:A:1223:ASN:ND2	2.42	0.47
1:B:807:ARG:HD2	1:B:808:PRO:CA	2.44	0.47
1:B:1248:MET:HG3	1:B:1275:GLY:HA2	1.97	0.47
1:B:631:GLU:OE1	1:B:653:MET:CG	2.62	0.47
1:B:575:ARG:NH1	1:B:575:ARG:CG	2.73	0.47
1:A:558:HIS:O	1:A:562:SER:OG	2.33	0.47
1:A:593:GLU:N	1:A:625:ALA:O	2.47	0.47
1:A:810:ASP:HB3	1:A:812:ARG:NH1	2.30	0.47
1:A:442:GLN:HA	1:A:445:ARG:NH1	2.30	0.46
1:A:1178:ASP:OD1	1:A:1178:ASP:N	2.38	0.46
1:B:675:TYR:CE1	1:B:685:ARG:HD3	2.50	0.46
1:B:807:ARG:NE	1:B:810:ASP:N	2.63	0.46
1:A:1242:LEU:HD12	1:A:1244:ILE:HD11	1.96	0.46
1:B:1187:LEU:HA	1:B:1188:PRO:HD3	1.81	0.46
1:A:1014:PRO:HG2	1:A:1020:ARG:NH1	2.31	0.46
1:B:1294:GLY:O	1:B:1310:THR:OG1	2.24	0.46
1:B:629:LEU:HD23	1:B:630:GLU:H	1.80	0.46
1:B:995:LEU:HA	1:B:1021:GLY:HA3	1.98	0.46
1:A:1277:LYS:N	1:A:1277:LYS:HD2	2.31	0.46
1:B:953:LEU:HA	1:B:956:SER:HB3	1.96	0.46
1:A:837:LYS:HB2	1:A:837:LYS:HE2	1.25	0.46
1:B:1039:ASP:OD1	1:B:1040:THR:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:675:TYR:HE1	1:B:685:ARG:HD3	1.81	0.46
1:A:416:ASN:ND2	1:A:687:LYS:NZ	2.63	0.45
1:B:628:ARG:CG	1:B:629:LEU:N	2.79	0.45
1:B:696:ASP:OD1	1:B:697:GLU:N	2.49	0.45
1:A:1183:MET:HB3	1:A:1238:ILE:HD12	1.98	0.45
1:B:1122:LYS:NZ	4:B:1404:ATP:O1G	2.49	0.45
1:B:462:ASP:OD1	1:B:464:LYS:HE3	2.17	0.45
1:B:693:GLY:C	1:B:743:LEU:HD12	2.37	0.45
1:B:1020:ARG:CD	1:B:1030:LEU:HA	2.47	0.45
1:B:476:LEU:HB2	1:B:641:LEU:HD13	1.99	0.45
1:A:837:LYS:O	1:A:839:THR:N	2.49	0.45
1:B:1200:ARG:HA	1:B:1202:TRP:CZ3	2.52	0.45
1:A:1001:TYR:O	1:A:1002:GLU:HB2	2.17	0.45
1:B:1020:ARG:HD3	1:B:1030:LEU:CA	2.47	0.45
1:B:503:GLU:HB2	1:B:756:PRO:HG2	1.98	0.45
1:A:518:PHE:HB3	1:A:521:MET:HG3	1.99	0.44
1:A:693:GLY:O	1:A:743:LEU:N	2.46	0.44
1:B:1166:ALA:HB2	1:B:1175:LEU:HD12	1.98	0.44
1:B:667:LEU:HA	1:B:668:PRO:HD3	1.86	0.44
1:A:1111:HIS:ND1	1:A:1242:LEU:HB2	2.33	0.44
1:B:1188:PRO:HB3	1:B:1192:LEU:HD12	2.00	0.44
1:A:1202:TRP:CE2	1:A:1203:TRP:HD1	2.35	0.44
1:B:994:GLU:OE2	1:B:997:LEU:HD21	2.18	0.44
1:B:799:HIS:NE2	1:B:819:ASP:OD1	2.51	0.44
1:A:992:LYS:HD2	1:A:1004:GLU:HG2	1.99	0.43
1:B:883:THR:OG1	1:B:884:ARG:N	2.52	0.43
1:B:442:GLN:O	1:B:464:LYS:HE2	2.18	0.43
1:B:691:VAL:HG23	1:B:692:SER:N	2.30	0.43
1:B:542:ASP:HA	1:B:545:TYR:CB	2.47	0.43
1:B:654:GLU:O	1:B:657:VAL:HG12	2.18	0.43
1:A:443:ARG:HA	1:A:464:LYS:NZ	2.33	0.43
1:A:652:ALA:O	1:A:656:ARG:HG3	2.18	0.43
1:B:446:LEU:HD23	1:B:463:ILE:HG13	2.01	0.43
1:B:796:GLY:HA2	1:B:852:HIS:CD2	2.53	0.43
1:A:1230:GLU:HG2	1:A:1230:GLU:H	1.57	0.43
1:B:432:ASP:HB3	1:B:435:VAL:CG2	2.47	0.43
1:B:593:GLU:OE2	1:B:627:GLN:HG2	2.19	0.43
1:B:1189:PRO:HD2	1:B:1192:LEU:HD11	2.00	0.43
1:B:462:ASP:O	1:B:471:MET:HB2	2.19	0.43
1:B:864:PHE:HB2	1:B:942:ASN:HB3	2.01	0.43
1:A:1110:PRO:HG2	1:A:1111:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:THR:O	1:A:843:THR:HG23	2.18	0.43
1:B:834:GLN:HB3	4:B:1405:ATP:H5'1	2.01	0.43
1:B:632:GLY:O	1:B:633:LYS:C	2.57	0.43
1:B:741:GLU:HB2	1:B:742:SER:HB3	2.01	0.43
1:B:476:LEU:HB2	1:B:641:LEU:CD1	2.49	0.42
1:A:1148:ASP:OD2	1:A:1153:LEU:N	2.52	0.42
1:A:1302:ARG:O	1:A:1303:SER:OG	2.33	0.42
1:A:422:LEU:HD23	1:A:449:PRO:HB2	2.00	0.42
1:A:1035:ARG:NH2	1:A:1037:ASP:OD2	2.49	0.42
1:A:543:ARG:HH12	1:A:765:PRO:HA	1.84	0.42
1:B:1298:PHE:HB2	1:B:1308:ILE:HD13	2.02	0.42
1:B:1095:ASP:HA	1:B:1308:ILE:HA	2.01	0.42
1:B:453:ASP:OD1	1:B:457:ARG:N	2.52	0.42
1:B:580:PRO:C	1:B:581:LEU:HD12	2.40	0.42
1:A:906:GLN:O	1:A:910:GLU:HG3	2.19	0.42
1:A:1143:ARG:NE	1:A:1163:ILE:HD11	2.34	0.42
1:A:1223:ASN:HA	1:A:1224:PRO:HD3	1.85	0.42
1:A:884:ARG:H	1:A:884:ARG:HG2	1.61	0.42
1:A:1014:PRO:HB3	1:A:1017:ARG:HG3	2.01	0.42
1:A:471:MET:HA	1:A:678:PHE:CD1	2.55	0.42
1:A:1048:GLY:O	1:A:1052:THR:HG23	2.20	0.41
1:B:555:ARG:NH2	1:B:585:PRO:O	2.51	0.41
1:B:863:ASP:OD2	1:B:867:GLY:HA2	2.19	0.41
1:B:798:LEU:HD11	1:B:920:ARG:NH1	2.35	0.41
1:A:1148:ASP:CG	1:A:1152:SER:H	2.17	0.41
1:A:1179:ILE:O	1:A:1183:MET:HG2	2.20	0.41
1:A:1189:PRO:HA	1:A:1190:PRO:HD3	1.87	0.41
1:A:613:ARG:HE	1:A:614:LEU:CD1	2.33	0.41
1:B:743:LEU:O	1:B:747:VAL:N	2.43	0.41
1:A:949:ASP:N	1:A:949:ASP:OD1	2.54	0.41
1:A:1036:ILE:HG13	1:A:1052:THR:HG22	2.02	0.41
1:B:429:TYR:HE1	1:B:695:VAL:HG21	1.85	0.41
1:A:1187:LEU:HA	1:A:1188:PRO:HD3	1.81	0.41
1:B:630:GLU:OE2	1:B:633:LYS:NZ	2.33	0.41
1:A:484:GLY:N	2:A:1401:SO4:O4	2.54	0.41
1:A:954:GLU:O	1:A:958:THR:OG1	2.27	0.41
1:A:818:LEU:HG	1:A:991:THR:HG21	2.03	0.41
1:A:437:TRP:CZ2	1:A:751:LEU:HD12	2.56	0.41
1:A:571:TYR:CE1	1:A:581:LEU:HD13	2.56	0.41
1:B:1020:ARG:HG2	1:B:1030:LEU:HD12	2.03	0.41
1:B:629:LEU:HD22	1:B:630:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1146:PHE:HD2	1:A:1153:LEU:HD23	1.85	0.40
1:A:551:GLU:OE1	1:A:555:ARG:NH1	2.53	0.40
1:A:679:ALA:HB3	1:A:681:GLU:OE1	2.21	0.40
1:A:638:ASP:CG	1:A:644:ARG:NH2	2.75	0.40
1:A:864:PHE:H	1:A:941:ASP:HB3	1.86	0.40
1:B:950:TYR:HB3	1:B:953:LEU:HD13	2.03	0.40
1:A:1302:ARG:C	1:A:1304:GLY:H	2.22	0.40
1:B:1065:ALA:HA	1:B:1066:PRO:HD3	1.97	0.40
1:A:864:PHE:HB2	1:A:942:ASN:H	1.86	0.40
1:B:906:GLN:O	1:B:910:GLU:HG3	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	857/1147 (75%)	799 (93%)	56 (6%)	2 (0%)	52	84
1	B	855/1147 (74%)	793 (93%)	58 (7%)	4 (0%)	34	71
All	All	1712/2294 (75%)	1592 (93%)	114 (7%)	6 (0%)	39	74

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	808	PRO
1	A	577	GLU
1	B	823	GLY
1	B	1034	PRO
1	A	580	PRO
1	B	693	GLY

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	709/953 (74%)	704 (99%)	5 (1%)	88	97
1	B	703/953 (74%)	688 (98%)	15 (2%)	61	88
All	All	1412/1906 (74%)	1392 (99%)	20 (1%)	74	93

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	573	LYS
1	A	816	TYR
1	A	837	LYS
1	A	838	SER
1	A	1023	THR
1	B	534	LEU
1	B	560	ARG
1	B	575	ARG
1	B	576	MET
1	B	577	GLU
1	B	629	LEU
1	B	630	GLU
1	B	631	GLU
1	B	638	ASP
1	B	644	ARG
1	B	658	VAL
1	B	742	SER
1	B	743	LEU
1	B	807	ARG
1	B	1020	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	416	ASN
1	B	561	HIS

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Mol	Chain	Res	Type
1	B	640	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z > 2$
2	SO4	A	1401	-	4,4,4	0.30	0	6,6,6	0.07	0
4	ATP	A	1404	3	26,33,33	0.96	1 (3%)	26,52,52	1.63	1 (3%)
4	ATP	A	1405	3	26,33,33	0.96	1 (3%)	26,52,52	1.62	1 (3%)
2	SO4	B	1401	-	4,4,4	0.29	0	6,6,6	0.08	0
4	ATP	B	1404	3	26,33,33	0.96	1 (3%)	26,52,52	1.61	1 (3%)
4	ATP	B	1405	3	26,33,33	0.97	1 (3%)	26,52,52	1.66	1 (3%)

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	SO4	A	1401	-	-	0/0/0/0	0/0/0/0
4	ATP	A	1404	3	-	0/18/38/38	0/3/3/3
4	ATP	A	1405	3	-	0/18/38/38	0/3/3/3
2	SO4	B	1401	-	-	0/0/0/0	0/0/0/0
4	ATP	B	1404	3	-	0/18/38/38	0/3/3/3
4	ATP	B	1405	3	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1404	ATP	C5-C4	3.04	1.47	1.40
4	B	1404	ATP	C5-C4	3.06	1.47	1.40
4	A	1405	ATP	C5-C4	3.09	1.47	1.40
4	B	1405	ATP	C5-C4	3.12	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1405	ATP	N3-C2-N1	-6.58	123.70	128.87
4	A	1405	ATP	N3-C2-N1	-6.54	123.73	128.87
4	A	1404	ATP	N3-C2-N1	-6.46	123.80	128.87
4	B	1404	ATP	N3-C2-N1	-6.44	123.81	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	SO4	1	0
4	A	1405	ATP	1	0
4	B	1404	ATP	2	0
4	B	1405	ATP	2	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	861/1147 (75%)	-0.19	4 (0%) 91 90	44, 80, 113, 151	0
1	B	859/1147 (74%)	-0.10	13 (1%) 76 74	35, 84, 128, 161	0
All	All	1720/2294 (74%)	-0.15	17 (0%) 84 82	35, 82, 125, 161	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	578	GLY	3.8
1	B	580	PRO	3.5
1	B	634	LEU	3.2
1	B	565	TYR	2.5
1	B	560	ARG	2.2
1	A	580	PRO	2.2
1	B	1001	TYR	2.2
1	B	1059	ALA	2.2
1	A	565	TYR	2.2
1	B	524	LEU	2.1
1	A	414	SER	2.1
1	B	665	TYR	2.1
1	B	581	LEU	2.1
1	B	659	LEU	2.1
1	B	559	LEU	2.1
1	B	579	ALA	2.0
1	B	1021	GLY	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 [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(\AA^2)	Q<0.9
4	ATP	B	1404	31/31	0.97	0.16	0.19	34,63,78,97	0
4	ATP	A	1404	31/31	0.97	0.14	0.05	61,73,96,101	0
4	ATP	A	1405	31/31	0.97	0.14	-0.69	65,92,108,113	0
4	ATP	B	1405	31/31	0.96	0.14	-0.80	69,117,135,141	0
2	SO4	B	1401	5/5	0.92	0.11	-1.04	97,105,124,150	0
2	SO4	A	1401	5/5	0.96	0.11	-1.48	72,86,91,93	0
3	MG	A	1403	1/1	0.96	0.11	-	77,77,77,77	0
3	MG	A	1402	1/1	0.97	0.05	-	82,82,82,82	0
3	MG	B	1403	1/1	0.97	0.06	-	86,86,86,86	0
3	MG	B	1402	1/1	0.97	0.11	-	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.