WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:07 AM GMT

PDB ID : 2W02
Title : CO-COMPLEX STRUCTURE OF ACHROMOBACTIN SYNTHETASE
PROTEIN D (ACSD) WITH ATP FROM PECTOBACTERIUM CHRYSAN-
THEMI
Authors : Schmelz, S.; Mcmahon, S.A.; Kadi, N.; Song, L.; Oves-Costales, D.; Oke, M.;
Liu, H.; Johnson, K.A.; Carter, L.; White, M.F.; Challis, G.L.; Naismith, J.H.
Deposited on : 2008-08-08
Resolution : 2.20 Å(reported)

1   Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.
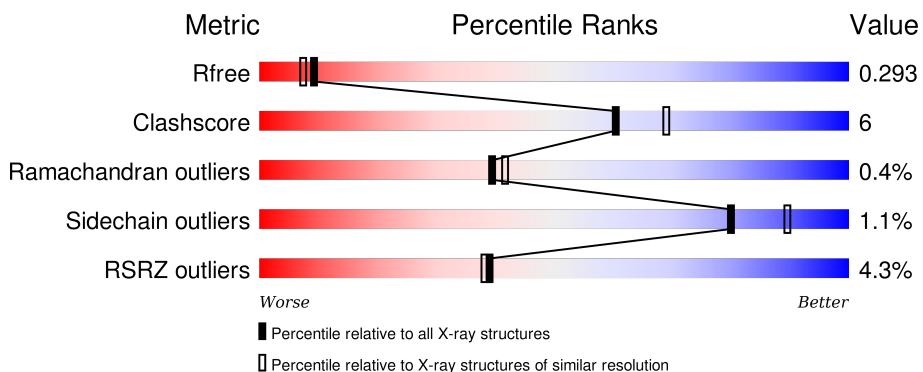
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	620	6% — 79% — 13% — 7%
1	B	620	2% — 78% — 15% — 7%
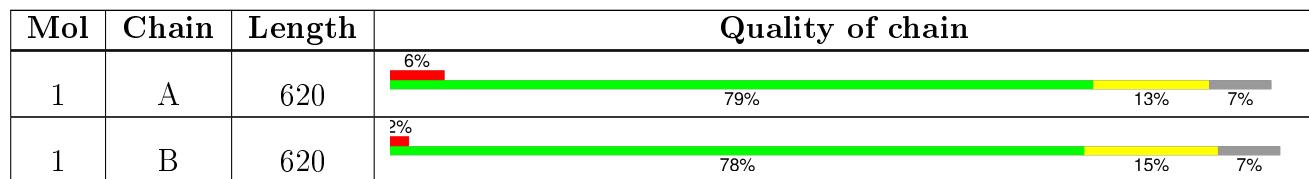
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SER	B	1590	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9600 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 ACSD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	0	0
			4609	2930	836	823	20			
1	B	579	Total	C	N	O	S	0	0	0
			4643	2949	843	831	20			

- Molecule 2 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).
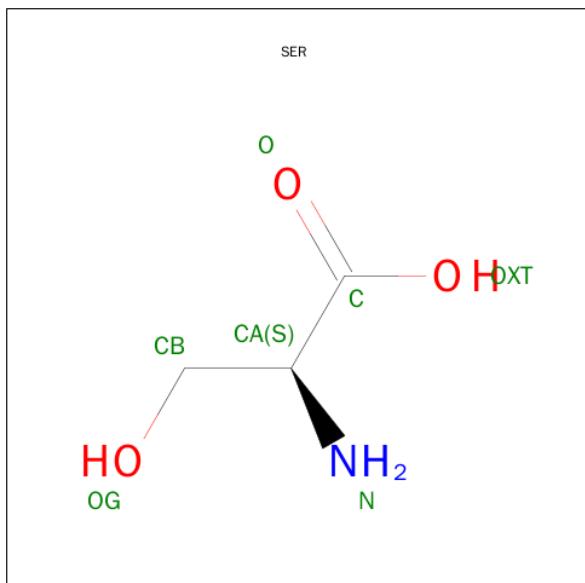
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
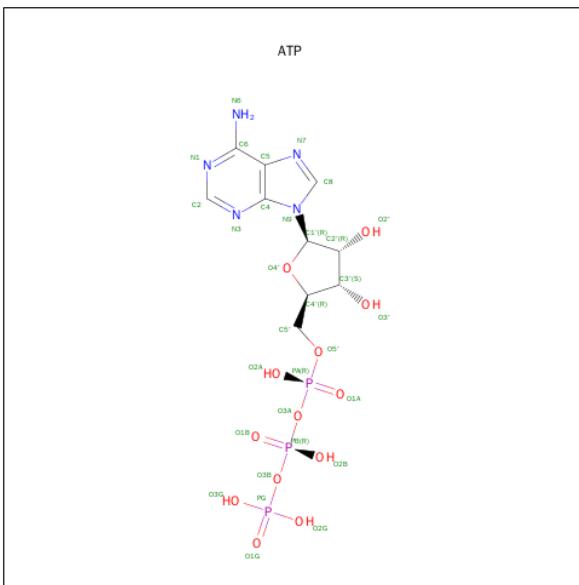
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	116	Total	O	0	0
			116	116		
5	B	161	Total	O	0	0
			161	161		

3 Residue-property plots (i)

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: ACSD
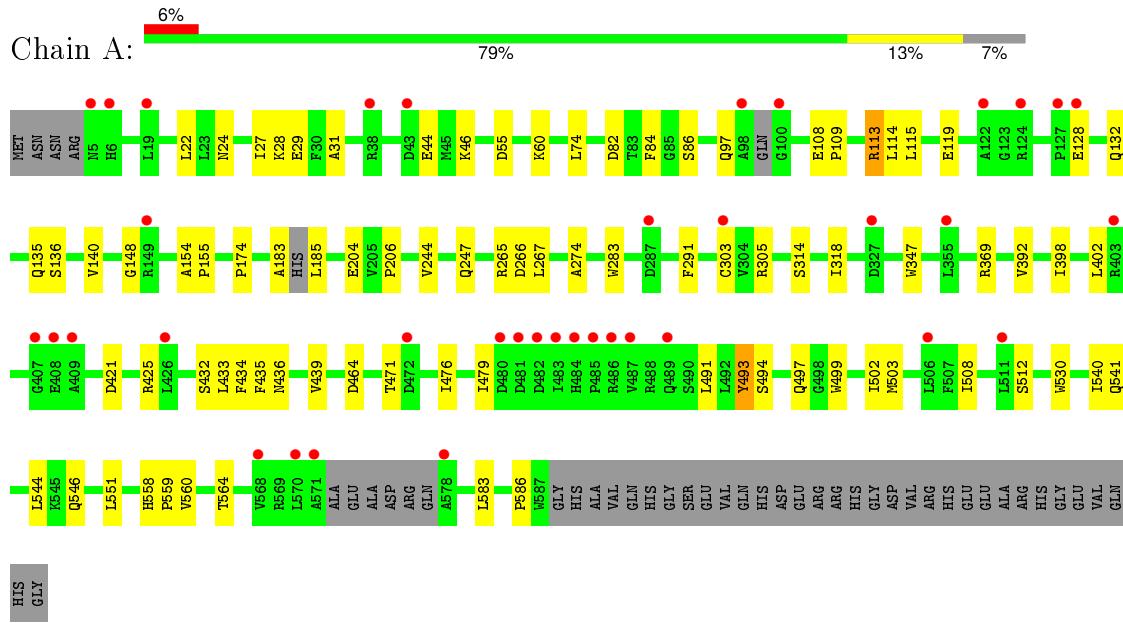
- Molecule 1: ACSD
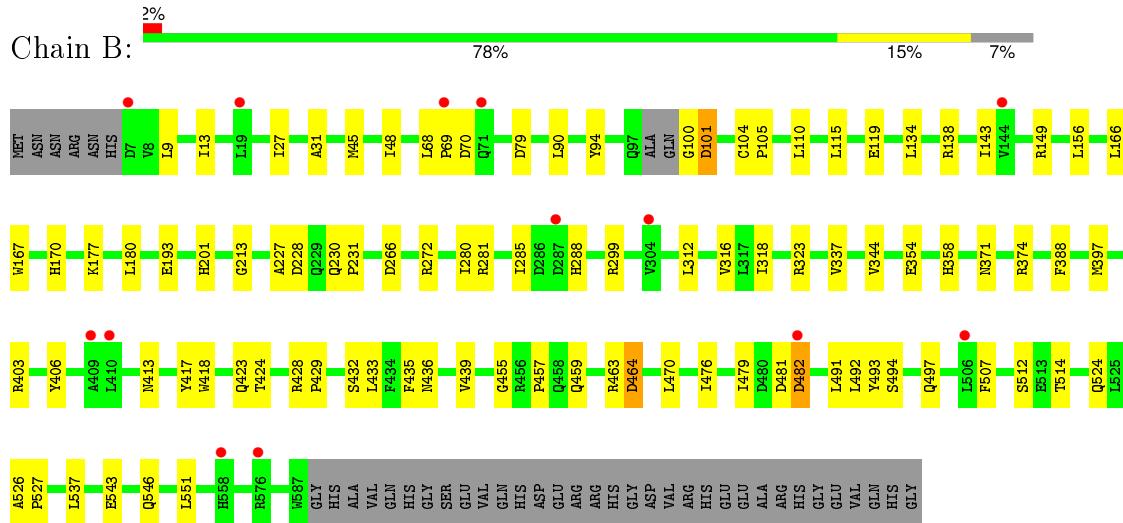
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.87Å 94.54Å 157.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.11 – 2.20 29.35 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (81.11-2.20) 100.0 (29.35-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.03 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.216 , 0.277 0.229 , 0.293	Depositor DCC
R_{free} test set	3096 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 29.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.25$	Xtriage
Outliers	1 of 61355 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9600	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.56% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, 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	0.47	0/4728	0.62	0/6423
1	B	0.47	0/4764	0.63	0/6474
All	All	0.47	0/9492	0.62	0/12897

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 (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	4609	0	4524	47	0
1	B	4643	0	4556	56	0
2	B	7	0	4	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	116	0	0	0	0
5	B	161	0	0	0	0
All	All	9600	0	9108	103	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 6.

All (103) 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:503:MET:HE1	1:A:560:VAL:HA	1.63	0.78
1:B:227:ALA:HA	1:B:272:ARG:NH2	2.02	0.74
1:B:476:ILE:HD13	1:B:492:LEU:HD13	1.72	0.71
1:B:312:LEU:HD12	1:B:344:VAL:HG13	1.72	0.70
1:A:148:GLY:HA2	1:A:392:VAL:HG11	1.73	0.70
1:B:432:SER:O	1:B:436:ASN:HB2	1.92	0.69
1:B:227:ALA:HA	1:B:272:ARG:HH21	1.57	0.69
1:B:227:ALA:CA	1:B:272:ARG:NH2	2.58	0.65
1:B:476:ILE:HD12	1:B:479:ILE:HD12	1.78	0.65
1:A:303:CYS:HB3	1:A:305:ARG:HH21	1.61	0.65
1:A:494:SER:OG	1:A:497:GLN:HB2	1.96	0.65
1:B:201:HIS:HE1	1:B:266:ASP:OD1	1.78	0.65
1:A:432:SER:O	1:A:436:ASN:HB2	1.99	0.62
1:B:470:LEU:HD12	1:B:479:ILE:HD11	1.85	0.59
1:A:314:SER:HB2	1:A:491:LEU:HD21	1.82	0.59
1:B:227:ALA:C	1:B:272:ARG:HH22	2.06	0.59
1:A:185:LEU:HD13	1:A:244:VAL:HG22	1.85	0.58
1:B:100:GLY:O	1:B:101:ASP:HB2	2.05	0.57
1:A:499:TRP:O	1:A:503:MET:HG3	2.06	0.56
1:B:537:LEU:HD22	1:B:551:LEU:HD11	1.87	0.55
1:A:398:ILE:O	1:A:402:LEU:HG	2.07	0.55
1:B:476:ILE:CD1	1:B:479:ILE:HD12	2.37	0.54
1:A:148:GLY:HA2	1:A:392:VAL:CG1	2.37	0.54
1:B:213:GLY:HA3	1:B:316:VAL:HG21	1.89	0.54
1:A:74:LEU:HD12	1:A:114:LEU:HD11	1.90	0.54
1:A:476:ILE:HD12	1:A:479:ILE:HD12	1.89	0.54
1:B:435:PHE:O	1:B:546:GLN:HB2	2.07	0.54
1:B:337:VAL:HG21	1:B:459:GLN:HG2	1.89	0.53
1:B:482:ASP:OD1	1:B:482:ASP:C	2.47	0.53
1:A:435:PHE:O	1:A:546:GLN:HB2	2.10	0.52
1:B:27:ILE:HA	1:B:31:ALA:HB3	1.93	0.51
1:B:371:ASN:O	1:B:374:ARG:HG3	2.10	0.51
1:B:423:GLN:HG3	1:B:424:THR:H	1.76	0.51
1:A:29:GLU:OE1	1:A:564:THR:HB	2.11	0.51
1:A:108:GLU:HB2	1:A:109:PRO:HD3	1.92	0.51
1:B:180:LEU:HD12	1:B:299:ARG:HB2	1.93	0.51
1:A:22:LEU:HD12	1:A:174:PRO:HA	1.94	0.50
1:B:143:ILE:HD13	1:B:193:GLU:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:ILE:HD11	1:B:491:LEU:HD13	1.94	0.50
1:A:24:ASN:O	1:A:28:LYS:HG3	2.12	0.50
1:A:434:PHE:CD2	1:A:502:ILE:HD12	2.48	0.49
1:B:228:ASP:OD1	1:B:230:GLN:HB2	2.13	0.49
1:B:156:LEU:HD21	1:B:397:MET:HE3	1.92	0.49
1:B:230:GLN:CB	1:B:231:PRO:HD3	2.42	0.49
1:A:541:GLN:HG3	1:A:551:LEU:HD23	1.93	0.49
1:A:433:LEU:HB3	1:A:439:VAL:HB	1.94	0.49
1:B:455:GLY:O	1:B:457:PRO:HD3	2.13	0.49
1:B:79:ASP:HB3	1:B:90:LEU:HD11	1.94	0.48
1:B:167:TRP:O	1:B:177:LYS:HE3	2.12	0.48
1:A:185:LEU:HD11	1:A:247:GLN:OE1	2.14	0.48
1:A:204:GLU:HB3	1:A:265:ARG:HB2	1.96	0.48
1:B:433:LEU:HB3	1:B:439:VAL:HB	1.94	0.48
1:A:82:ASP:OD2	1:A:86:SER:HB2	2.14	0.48
1:B:354:GLU:HG2	1:B:358:HIS:CE1	2.49	0.48
1:A:128:GLU:HG2	1:A:132:GLN:HE21	1.78	0.48
1:A:22:LEU:HD23	1:A:114:LEU:HD23	1.95	0.48
1:A:136:SER:O	1:A:140:VAL:HG23	2.14	0.48
1:B:428:ARG:HB2	1:B:429:PRO:HD3	1.96	0.47
1:B:227:ALA:CA	1:B:272:ARG:HH22	2.25	0.47
1:B:479:ILE:CD1	1:B:491:LEU:HD13	2.44	0.47
1:A:27:ILE:HA	1:A:31:ALA:HB3	1.97	0.47
1:A:44:GLU:HG3	1:A:46:LYS:H	1.79	0.47
1:A:206:PRO:HD2	1:A:347:TRP:CZ2	2.50	0.47
1:B:166:LEU:O	1:B:177:LYS:NZ	2.38	0.47
1:A:291:PHE:HB2	1:A:369:ARG:HB3	1.98	0.46
1:B:105:PRO:HD2	1:B:110:LEU:HD13	1.96	0.46
1:B:45:MET:HE3	1:B:48:ILE:HD12	1.98	0.46
1:A:55:ASP:HB3	1:A:60:LYS:CG	2.46	0.46
1:B:230:GLN:HB2	1:B:231:PRO:HD3	1.98	0.45
1:B:403:ARG:HE	1:B:403:ARG:HB2	1.57	0.45
1:A:115:LEU:O	1:A:119:GLU:HG3	2.17	0.45
1:B:423:GLN:HG3	1:B:424:THR:N	2.32	0.45
1:A:266:ASP:OD1	1:A:267:LEU:O	2.35	0.45
1:A:28:LYS:HE2	1:A:84:PHE:O	2.17	0.45
1:A:421:ASP:O	1:A:425:ARG:HD2	2.16	0.44
1:B:9:LEU:O	1:B:13:ILE:HG13	2.17	0.44
1:A:508:ILE:HD13	1:A:583:LEU:HD12	1.99	0.44
1:B:494:SER:OG	1:B:497:GLN:HB2	2.17	0.44
1:B:94:TYR:CE1	1:B:104:CYS:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ALA:O	1:A:185:LEU:N	2.51	0.44
1:B:318:ILE:HD11	1:B:491:LEU:HD22	2.00	0.43
1:B:406:TYR:OH	1:B:418:TRP:HD1	2.00	0.43
1:B:134:LEU:O	1:B:138:ARG:HG3	2.18	0.43
1:A:84:PHE:CZ	1:A:586:PRO:HD3	2.53	0.43
1:A:154:ALA:HB3	1:A:155:PRO:HD3	2.01	0.43
1:A:274:ALA:HB1	1:A:283:TRP:HB3	2.01	0.42
1:A:551:LEU:HD12	1:A:551:LEU:HA	1.88	0.42
1:B:149:ARG:HG3	1:B:149:ARG:HH11	1.85	0.42
1:A:97:GLN:HG3	1:A:113:ARG:HH21	1.84	0.42
1:A:540:ILE:O	1:A:544:LEU:HG	2.20	0.42
1:A:471:THR:HA	1:A:493:TYR:O	2.19	0.42
1:B:115:LEU:O	1:B:119:GLU:HG3	2.20	0.41
1:B:285:ILE:HB	1:B:288:HIS:HB3	2.02	0.41
1:B:524:GLN:O	1:B:527:PRO:HD2	2.21	0.41
1:B:388:PHE:CZ	1:B:514:THR:HG23	2.55	0.41
1:B:507:PHE:O	1:B:512:SER:HB2	2.21	0.41
1:B:413:ASN:O	1:B:417:TYR:HB2	2.21	0.41
1:B:526:ALA:HB3	1:B:527:PRO:HD3	2.02	0.40
1:B:68:LEU:O	1:B:70:ASP:N	2.54	0.40
1:A:318:ILE:HD11	1:A:491:LEU:CD2	2.51	0.40
1:A:558:HIS:ND1	1:A:559:PRO:HD2	2.36	0.40
1:A:530:TRP:CE3	1:A:530:TRP:HA	2.57	0.40
1:B:463:ARG:O	1:B:464:ASP:HB3	2.21	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	567/620 (92%)	541 (95%)	25 (4%)	1 (0%)	52 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	575/620 (93%)	556 (97%)	15 (3%)	4 (1%)	26 25
All	All	1142/1240 (92%)	1097 (96%)	40 (4%)	5 (0%)	39 42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	464	ASP
1	A	464	ASP
1	B	69	PRO
1	B	101	ASP
1	B	280	ILE

5.3.2   Protein sidechains (i)

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	486/522 (93%)	482 (99%)	4 (1%)	86 93
1	B	489/522 (94%)	482 (99%)	7 (1%)	74 85
All	All	975/1044 (93%)	964 (99%)	11 (1%)	80 89

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ARG
1	A	135	GLN
1	A	493	TYR
1	A	512	SER
1	B	170	HIS
1	B	281	ARG
1	B	323	ARG
1	B	481	ASP
1	B	482	ASP
1	B	493	TYR
1	B	543	GLU

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

Mol	Chain	Res	Type
1	B	201	HIS
1	B	251	GLN
1	B	358	HIS

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 ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\#|Z| > 2$
3	ATP	A	1588	4	24,33,33	1.01	1 (4%)	31,52,52	1.97	5 (16%)
3	ATP	B	1588	4	24,33,33	1.08	1 (4%)	31,52,52	1.82	4 (12%)
2	SER	B	1590	-	3,6,6	0.03	0	1,7,7	0.29	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
3	ATP	A	1588	4	-	0/18/38/38	0/3/3/3
3	ATP	B	1588	4	-	0/18/38/38	0/3/3/3
2	SER	B	1590	-	-	0/2/6/6	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1588	ATP	C5-C4	3.21	1.47	1.40
3	B	1588	ATP	C5-C4	3.27	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1588	ATP	N3-C2-N1	-7.98	122.78	128.89
3	B	1588	ATP	N3-C2-N1	-7.07	123.48	128.89
3	A	1588	ATP	PA-O3A-PB	-4.23	120.84	132.73
3	A	1588	ATP	PB-O3B-PG	-3.02	122.55	132.67
3	B	1588	ATP	C4-C5-N7	-2.92	106.79	109.48
3	B	1588	ATP	PA-O3A-PB	-2.89	124.60	132.73
3	A	1588	ATP	C4-C5-N7	-2.44	107.23	109.48
3	A	1588	ATP	C2-N1-C6	2.18	122.67	118.77
3	B	1588	ATP	C4'-O4'-C1'	2.67	112.65	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	575/620 (92%)	0.27	37 (6%)	23	22	2, 12, 20, 31	0
1	B	579/620 (93%)	0.18	13 (2%)	65	64	2, 12, 20, 26	2 (0%)
All	All	1154/1240 (93%)	0.23	50 (4%)	39	38	2, 12, 20, 31	2 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	144	VAL	4.9
1	A	481	ASP	4.9
1	A	482	ASP	4.3
1	B	304	VAL	4.0
1	B	69	PRO	4.0
1	A	485	PRO	3.7
1	A	480	ASP	3.6
1	A	578	ALA	3.6
1	A	303	CYS	3.6
1	B	410	LEU	3.6
1	A	127	PRO	3.4
1	A	570	LEU	3.4
1	A	6	HIS	3.3
1	B	576	ARG	3.2
1	A	487	VAL	3.2
1	A	43	ASP	3.2
1	A	409	ALA	3.1
1	A	327	ASP	3.1
1	A	5	ASN	3.1
1	A	287	ASP	2.9
1	A	149	ARG	2.9
1	B	287	ASP	2.9
1	B	71	GLN	2.9
1	A	489	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	484	HIS	2.7
1	A	38	ARG	2.6
1	B	558	HIS	2.6
1	A	124	ARG	2.6
1	A	511	LEU	2.6
1	B	7	ASP	2.5
1	A	100	GLY	2.5
1	B	482	ASP	2.4
1	A	571	ALA	2.4
1	B	409	ALA	2.4
1	A	426	LEU	2.4
1	A	355	LEU	2.3
1	A	568	VAL	2.3
1	B	506	LEU	2.3
1	A	483	ILE	2.3
1	A	128	GLU	2.3
1	B	19	LEU	2.2
1	A	407	GLY	2.2
1	A	408	GLU	2.2
1	A	122	ALA	2.2
1	A	486	ARG	2.2
1	A	506	LEU	2.2
1	A	98	ALA	2.2
1	A	403	ARG	2.1
1	A	472	ASP	2.1
1	A	19	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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(Å²)	Q<0.9
2	SER	B	1590	7/7	0.89	0.15	2.06	11,12,12,13	0
3	ATP	A	1588	31/31	0.95	0.12	-1.57	14,15,17,17	0
3	ATP	B	1588	31/31	0.97	0.09	-2.52	5,8,10,10	0
4	MG	A	1589	1/1	0.83	0.10	-	22,22,22,22	0
4	MG	B	1589	1/1	0.86	0.12	-	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.