Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:26 AM GMT

PDB ID	:	2X3K
Title	:	CO-COMPLEX STRUCTURE OF ACHROMOBACTIN SYNTHETASE PROTEIN D (ACSD) WITH AMP AND SULFATE FROM PECTOBACTERIUM CHRYSANTHEMI
Authors	:	Schmelz, S.; Naismith, J.H.
Deposited on	:	2010-01-25
Resolution	:	2.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

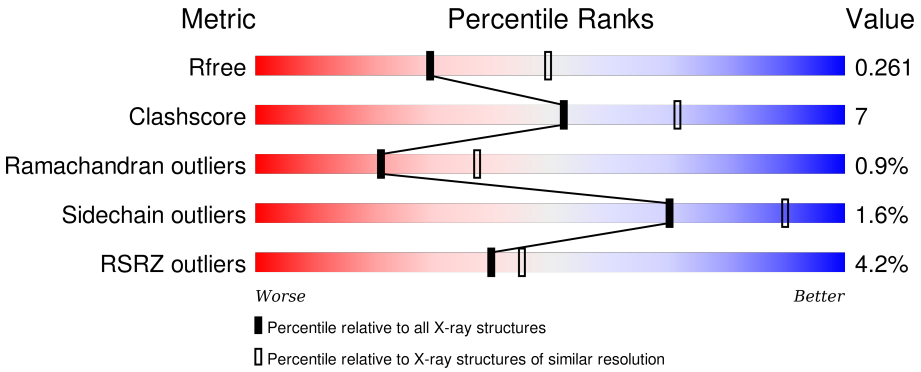
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	5% 78% 14% • 7%
1	B	620	3% 76% 15% • 8%

2 Entry composition

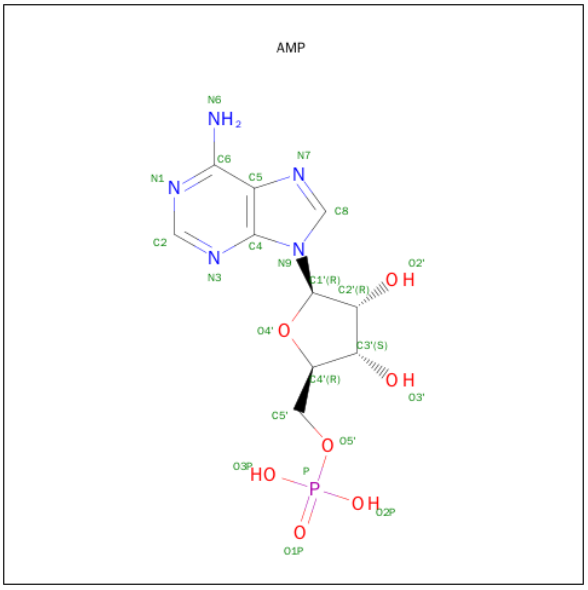
There are 4 unique types of molecules in this entry. The entry contains 9417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

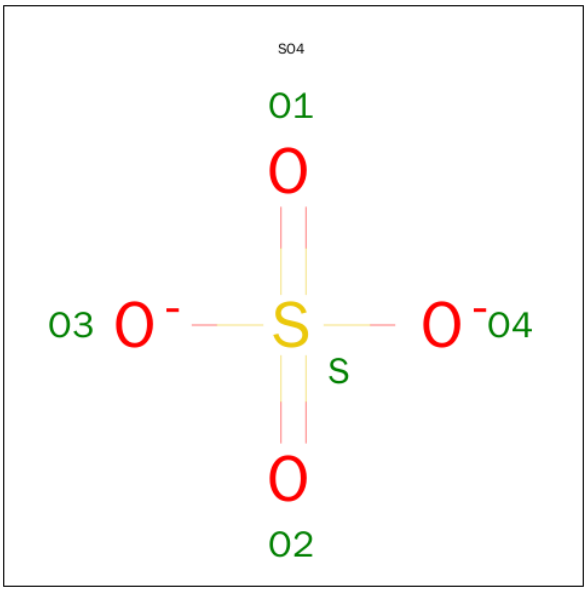
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	2	0
			4623	2940	840	823	20			
1	B	570	Total	C	N	O	S	0	0	0
			4569	2908	830	811	20			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

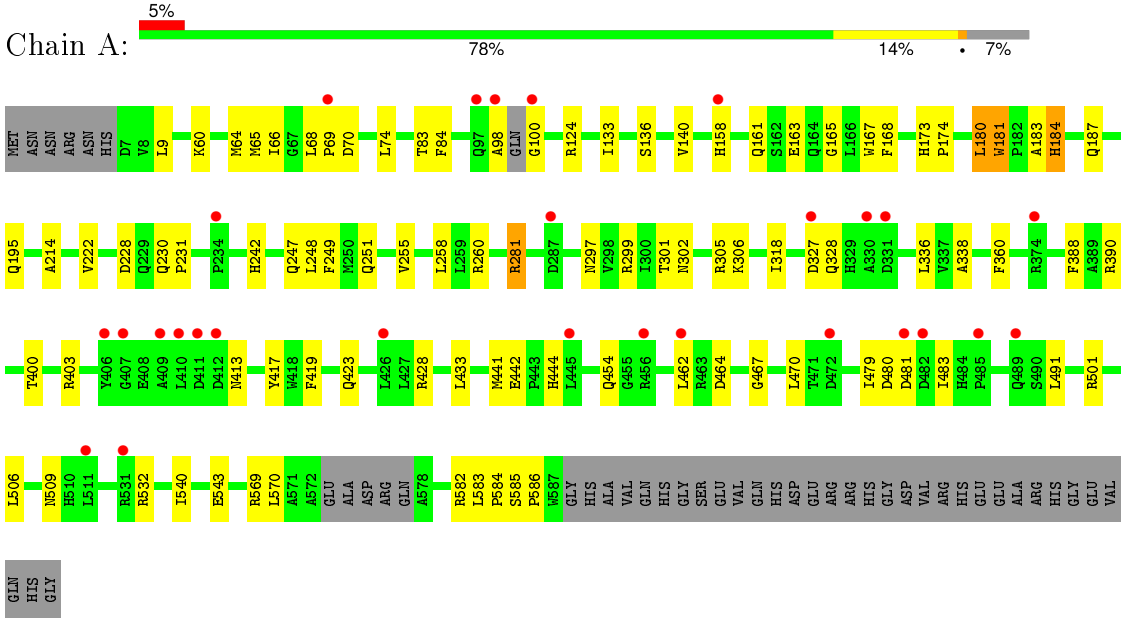
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	87	Total O 87 87	0	0
4	B	82	Total O 82 82	0	0

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.

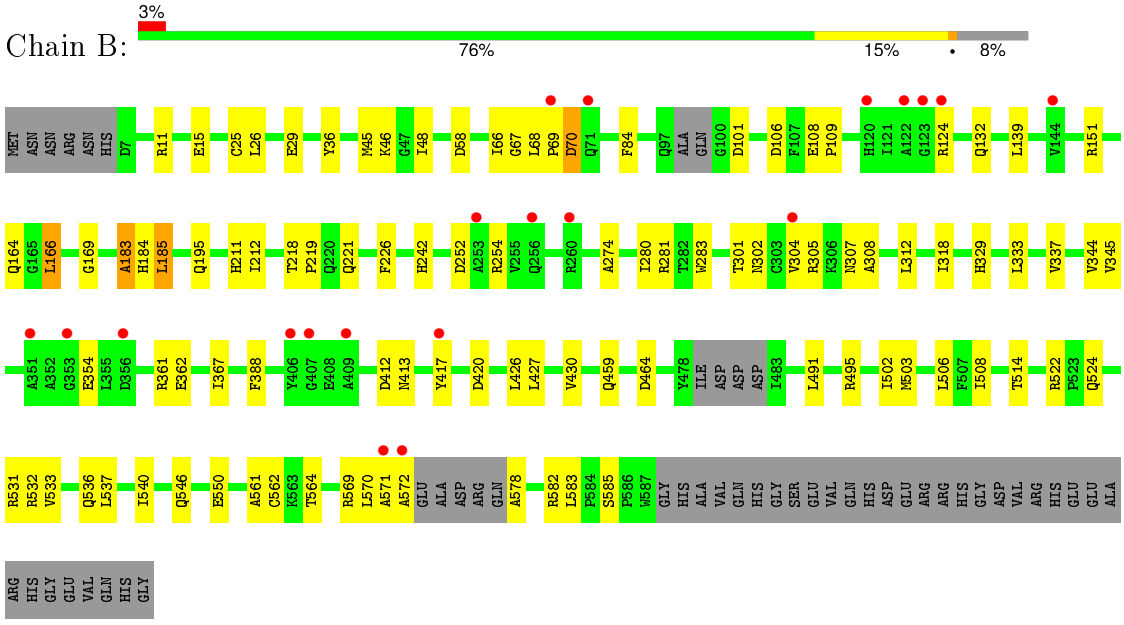
- Molecule 1: ACSD

Chain A:



- Molecule 1: ACSD

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.70Å 70.00Å 96.00Å 95.00° 101.90° 94.70°	Depositor
Resolution (Å)	39.66 – 2.50 36.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.6 (39.66-2.50) 93.5 (36.96-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.205 , 0.261 0.207 , 0.261	Depositor DCC
R_{free} test set	2469 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 48647 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9417	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, SO4

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	0.73	4/4748 (0.1%)	0.76	1/6452 (0.0%)
1	B	0.71	1/4688 (0.0%)	0.78	1/6368 (0.0%)
All	All	0.72	5/9436 (0.1%)	0.77	2/12820 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	PHE	CE2-CZ	5.31	1.47	1.37
1	B	25	CYS	CB-SG	-5.18	1.73	1.81
1	A	454	GLN	CD-OE1	5.16	1.35	1.24
1	A	195	GLN	CD-OE1	5.11	1.35	1.24
1	A	168	PHE	CG-CD1	5.01	1.46	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	166	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	281	ARG	NE-CZ-NH1	5.18	122.89	120.30

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	4623	0	4537	56	0
1	B	4569	0	4495	67	0
2	A	23	0	12	0	0
2	B	23	0	12	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	87	0	0	3	0
4	B	82	0	0	5	0
All	All	9417	0	9056	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (122) 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:184:HIS:CG	1:B:185:LEU:H	1.56	1.21
1:B:413:ASN:O	1:B:417:TYR:HD1	1.37	1.03
1:B:184:HIS:CD2	1:B:185:LEU:H	1.80	0.99
1:B:184:HIS:CG	1:B:185:LEU:N	2.29	0.94
1:B:301:THR:O	1:B:301:THR:HG22	1.73	0.88
1:B:124:ARG:HH11	1:B:572:ALA:HB2	1.38	0.87
1:B:413:ASN:O	1:B:417:TYR:CD1	2.29	0.83
1:A:467:GLY:O	1:A:501:ARG:NH1	2.17	0.78
1:B:184:HIS:CD2	1:B:185:LEU:N	2.50	0.78
1:B:420:ASP:OD1	1:B:532:ARG:HD3	1.84	0.77
1:A:180:LEU:HD22	1:A:299:ARG:HB3	1.66	0.76
1:B:218:THR:OG1	1:B:221:GLN:HG3	1.89	0.71
1:B:361:ARG:HD2	4:B:2049:HOH:O	1.89	0.71
1:B:108:GLU:HB2	1:B:109:PRO:CD	2.21	0.70
1:A:163:GLU:OE1	4:A:2017:HOH:O	2.12	0.68
1:A:183:ALA:O	1:A:184:HIS:HB3	1.95	0.66
1:A:480:ASP:O	1:A:483:ILE:HG12	1.95	0.66
1:B:68:LEU:O	1:B:70:ASP:OD1	2.13	0.65
1:B:546:GLN:O	4:B:2074:HOH:O	2.14	0.65
1:B:183:ALA:O	1:B:184:HIS:ND1	2.30	0.64
1:A:9:LEU:HD11	1:B:58:ASP:HA	1.80	0.63
1:B:502:ILE:HG23	1:B:506:LEU:HD12	1.80	0.63
1:B:508:ILE:CD1	1:B:562:CYS:HB2	2.29	0.63
1:B:108:GLU:HB2	1:B:109:PRO:HD3	1.81	0.62
1:B:124:ARG:HB2	1:B:570:LEU:O	1.99	0.61
1:B:124:ARG:NH1	1:B:572:ALA:HB2	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:THR:CG2	1:B:301:THR:O	2.45	0.60
1:A:68:LEU:O	1:A:70:ASP:N	2.35	0.60
1:A:242:HIS:HB2	4:A:2048:HOH:O	2.02	0.59
1:B:124:ARG:HH11	1:B:572:ALA:CB	2.11	0.59
1:A:318:ILE:HD11	1:A:491:LEU:HD21	1.83	0.59
1:A:301:THR:HG22	1:A:302:ASN:H	1.68	0.58
1:B:226:PHE:CE2	1:B:345:VAL:HG12	2.38	0.58
1:A:413:ASN:O	1:A:417:TYR:HD2	1.88	0.57
1:B:11:ARG:NH1	1:B:15:GLU:OE2	2.38	0.56
1:A:441:MET:HE3	1:A:462:LEU:HD13	1.88	0.55
1:A:181:TRP:NE1	1:A:187:GLN:NE2	2.55	0.55
1:B:426:LEU:O	1:B:430:VAL:HG23	2.07	0.54
1:A:301:THR:HG22	1:A:302:ASN:N	2.23	0.54
1:A:158[A]:HIS:HB3	1:A:161:GLN:OE1	2.06	0.54
1:A:173:HIS:NE2	1:A:301:THR:HG23	2.22	0.54
1:B:412:ASP:OD1	1:B:522:ARG:HD2	2.08	0.53
1:A:165:GLY:HA2	1:A:167:TRP:CZ3	2.43	0.53
1:A:470:LEU:HD12	1:A:479:ILE:HD11	1.89	0.53
1:B:508:ILE:HD13	1:B:562:CYS:HB2	1.90	0.53
1:A:297:ASN:OD1	1:A:306:LYS:HE3	2.08	0.52
1:B:495:ARG:NE	1:B:550:GLU:OE2	2.29	0.52
1:A:260:ARG:NH2	4:A:2044:HOH:O	2.42	0.52
1:B:252:ASP:OD1	1:B:254:ARG:HB2	2.09	0.51
1:A:336:LEU:HD22	1:A:433:LEU:HD11	1.92	0.51
1:B:242:HIS:HB2	4:B:2032:HOH:O	2.10	0.51
1:B:166:LEU:HG	1:B:169:GLY:HA2	1.91	0.51
1:A:214:ALA:HB2	1:A:222:VAL:HG21	1.94	0.49
1:A:64:MET:HG2	1:A:65:MET:N	2.27	0.49
1:B:106:ASP:HB2	1:B:109:PRO:HG2	1.94	0.49
1:B:11:ARG:O	1:B:15:GLU:HG3	2.13	0.49
1:B:533:VAL:O	1:B:537:LEU:HG	2.13	0.49
1:A:133:ILE:HG12	1:A:174:PRO:O	2.12	0.49
1:B:388:PHE:CE1	1:B:514:THR:HG23	2.48	0.48
1:A:173:HIS:NE2	1:A:301:THR:CG2	2.77	0.48
1:B:307:ASN:HB3	1:B:312:LEU:HD21	1.96	0.48
1:A:444:HIS:HB2	1:A:509:ASN:OD1	2.13	0.48
1:A:158[B]:HIS:HB2	1:A:161:GLN:OE1	2.14	0.47
1:A:181:TRP:CD1	1:A:187:GLN:NE2	2.82	0.47
1:A:124:ARG:HD3	1:A:570:LEU:O	2.13	0.47
1:A:428:ARG:HG2	1:A:540:ILE:HG12	1.95	0.47
1:B:578:ALA:N	4:B:2078:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:HIS:O	1:B:333:LEU:HG	2.14	0.46
1:B:571:ALA:HB3	1:B:578:ALA:HB2	1.97	0.46
1:B:427:LEU:HD23	1:B:506:LEU:HD22	1.98	0.46
1:A:181:TRP:HE1	1:A:187:GLN:NE2	2.13	0.46
1:B:84:PHE:HA	1:B:583:LEU:HD13	1.97	0.46
1:A:470:LEU:CD1	1:A:479:ILE:HD11	2.45	0.46
1:A:388:PHE:O	1:A:390:ARG:NH1	2.49	0.46
1:A:470:LEU:HD12	1:A:479:ILE:CD1	2.45	0.46
1:A:419:PHE:CZ	1:A:423:GLN:HG2	2.51	0.45
1:B:318:ILE:HD11	1:B:491:LEU:CD2	2.46	0.45
1:A:249:PHE:O	1:A:255:VAL:HG21	2.16	0.45
1:B:211:HIS:CE1	4:B:2049:HOH:O	2.70	0.45
1:A:228:ASP:O	1:A:231:PRO:HD2	2.17	0.45
1:B:344:VAL:HG22	1:B:367:ILE:HG12	1.99	0.45
1:B:305:ARG:NH2	2:B:1588:AMP:O3P	2.50	0.44
1:B:301:THR:O	1:B:302:ASN:HB3	2.17	0.44
1:B:45:MET:HE3	1:B:48:ILE:HD12	2.00	0.44
1:A:258:LEU:HD11	1:A:360:PHE:CZ	2.53	0.44
1:B:522:ARG:HG2	1:B:524:GLN:HE22	1.83	0.43
1:B:388:PHE:CZ	1:B:514:THR:HG23	2.53	0.43
1:B:226:PHE:CE2	1:B:345:VAL:CG1	3.01	0.43
1:A:301:THR:CG2	1:A:302:ASN:H	2.30	0.43
1:B:274:ALA:HB1	1:B:283:TRP:HB3	2.00	0.43
1:A:338:ALA:HA	1:A:462:LEU:O	2.18	0.42
1:B:164:GLN:NE2	1:B:195:GLN:HA	2.34	0.42
1:B:139:LEU:HD12	1:B:139:LEU:HA	1.80	0.42
1:B:337:VAL:HG21	1:B:459:GLN:HG2	2.01	0.42
1:A:247:GLN:OE1	1:A:247:GLN:HA	2.19	0.42
1:B:503:MET:HE3	1:B:561:ALA:HB3	2.02	0.42
1:A:442:GLU:HG2	1:A:442:GLU:O	2.20	0.42
1:B:46:LYS:HD3	1:B:101:ASP:OD1	2.20	0.42
1:B:29:GLU:HG2	1:B:564:THR:HG22	2.02	0.42
1:A:84:PHE:CZ	1:A:586:PRO:HD3	2.54	0.42
1:B:536:GLN:O	1:B:540:ILE:HD12	2.20	0.41
1:B:26:LEU:HD23	1:B:26:LEU:C	2.40	0.41
1:A:301:THR:HB	1:A:305:ARG:HH21	1.85	0.41
1:B:308:ALA:HA	1:B:362:GLU:HG3	2.03	0.41
1:A:248:LEU:O	1:A:251:GLN:HB2	2.20	0.41
1:A:98:ALA:C	1:A:100:GLY:N	2.74	0.41
1:B:132:GLN:OE1	1:B:569:ARG:NH2	2.53	0.41
1:A:228:ASP:OD2	1:A:230:GLN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:SER:O	1:A:140:VAL:HG23	2.20	0.41
1:A:299:ARG:NH2	1:A:569:ARG:CZ	2.84	0.41
1:A:68:LEU:HA	1:A:68:LEU:HD23	1.84	0.41
1:B:26:LEU:HD22	1:B:66:ILE:HD13	2.02	0.41
1:A:60:LYS:HB3	1:A:60:LYS:HE2	1.90	0.41
1:A:83:THR:HG21	1:A:585:SER:O	2.21	0.41
1:A:66:ILE:HD12	1:A:74:LEU:HD22	2.03	0.41
1:B:304:VAL:HG13	1:B:304:VAL:O	2.21	0.41
1:B:36:TYR:HB3	1:B:67:GLY:O	2.21	0.40
1:A:583:LEU:HA	1:A:584:PRO:HD3	1.85	0.40
1:A:506:LEU:HA	1:A:506:LEU:HD23	1.88	0.40
1:B:301:THR:O	1:B:302:ASN:CB	2.69	0.40
1:B:212:ILE:HG21	1:B:219:PRO:HA	2.02	0.40
1:A:543:GLU:HG2	1:A:543:GLU:O	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	571/620 (92%)	538 (94%)	29 (5%)	4 (1%)	26	46
1	B	562/620 (91%)	530 (94%)	26 (5%)	6 (1%)	17	31
All	All	1133/1240 (91%)	1068 (94%)	55 (5%)	10 (1%)	21	37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	PRO
1	A	184	HIS
1	B	70	ASP
1	B	185	LEU

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Mol	Chain	Res	Type
1	B	464	ASP
1	B	183	ALA
1	A	464	ASP
1	A	481	ASP
1	B	69	PRO
1	B	280	ILE

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	487/522 (93%)	478 (98%)	9 (2%)	66 88
1	B	481/522 (92%)	475 (99%)	6 (1%)	78 93
All	All	968/1044 (93%)	953 (98%)	15 (2%)	70 91

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	LEU
1	A	181	TRP
1	A	281	ARG
1	A	327	ASP
1	A	328	GLN
1	A	400	THR
1	A	403	ARG
1	A	532	ARG
1	A	582	ARG
1	B	151	ARG
1	B	281	ARG
1	B	354	GLU
1	B	531	ARG
1	B	582	ARG
1	B	585	SER

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	536	GLN
1	B	164	GLN
1	B	202	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

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	$\#\|Z\| > 2$
2	AMP	A	1588	-	20,25,25	1.13	2 (10%)	22,38,38	2.55	5 (22%)
3	SO4	A	1589	-	4,4,4	0.43	0	6,6,6	0.68	0
2	AMP	B	1588	-	20,25,25	1.06	1 (5%)	22,38,38	2.50	6 (27%)
3	SO4	B	1589	-	4,4,4	0.27	0	6,6,6	0.37	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
2	AMP	A	1588	-	-	0/6/26/26	0/3/3/3
3	SO4	A	1589	-	-	0/0/0/0	0/0/0/0
2	AMP	B	1588	-	-	0/6/26/26	0/3/3/3
3	SO4	B	1589	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1588	AMP	C5-C4	2.62	1.46	1.40
2	A	1588	AMP	O4'-C1'	3.03	1.45	1.41
2	B	1588	AMP	C5-C4	3.33	1.48	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1588	AMP	N3-C2-N1	-9.45	121.66	128.89
2	B	1588	AMP	N3-C2-N1	-9.22	121.84	128.89
2	B	1588	AMP	C4-C5-N7	-3.28	106.46	109.48
2	A	1588	AMP	C2'-C1'-N9	-3.11	109.55	114.29
2	A	1588	AMP	O5'-P-O1P	-3.07	99.32	107.14
2	A	1588	AMP	C4-C5-N7	-3.00	106.72	109.48
2	B	1588	AMP	C2'-C1'-N9	-2.21	110.91	114.29
2	B	1588	AMP	O3P-P-O2P	2.33	116.25	107.38
2	A	1588	AMP	C2-N1-C6	2.51	123.25	118.77
2	B	1588	AMP	O4'-C1'-N9	2.56	113.45	108.10
2	B	1588	AMP	C2-N1-C6	2.79	123.76	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	1588	AMP	1	0

5.7 Other polymers (i)

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, 95^{th} 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%)	0.31	28 (4%)	33	38	26, 47, 66, 75	0
1	B	570/620 (91%)	0.19	20 (3%)	48	53	29, 46, 66, 80	2 (0%)
All	All	1145/1240 (92%)	0.25	48 (4%)	40	45	26, 47, 66, 80	2 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	572	ALA	4.6
1	B	123	GLY	4.6
1	A	482	ASP	4.5
1	B	124	ARG	4.3
1	A	409	ALA	4.2
1	B	304	VAL	3.9
1	A	98	ALA	3.8
1	A	410	LEU	3.8
1	A	69	PRO	3.7
1	B	69	PRO	3.7
1	B	253	ALA	3.5
1	B	406	TYR	3.5
1	A	406	TYR	3.3
1	B	260	ARG	3.3
1	B	351	ALA	3.2
1	B	571	ALA	2.9
1	B	120	HIS	2.9
1	B	122	ALA	2.9
1	A	462	LEU	2.8
1	B	417	TYR	2.8
1	A	481	ASP	2.8
1	A	485	PRO	2.7
1	B	144	VAL	2.7
1	A	331	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	234	PRO	2.5
1	B	256	GLN	2.5
1	A	407	GLY	2.5
1	B	407	GLY	2.4
1	A	411	ASP	2.4
1	A	330	ALA	2.4
1	A	426	LEU	2.4
1	A	100	GLY	2.4
1	A	531	ARG	2.4
1	A	472	ASP	2.3
1	A	445	LEU	2.3
1	A	489	GLN	2.3
1	A	511	LEU	2.2
1	A	97	GLN	2.2
1	B	353	GLY	2.2
1	A	287	ASP	2.1
1	A	158[A]	HIS	2.1
1	B	71	GLN	2.1
1	A	412	ASP	2.1
1	A	374	ARG	2.1
1	B	409	ALA	2.0
1	B	356	ASP	2.0
1	A	327	ASP	2.0
1	A	456	ARG	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, 95^{th} 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	AMP	B	1588	23/23	0.96	0.17	-0.20	48,52,57,58	0
3	SO4	A	1589	5/5	0.98	0.21	-0.28	45,46,51,51	0
2	AMP	A	1588	23/23	0.95	0.19	-0.56	41,44,51,55	0
3	SO4	B	1589	5/5	0.98	0.13	-2.25	42,43,47,48	0

6.5 Other polymers (i)

There are no such residues in this entry.