Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 04:10 AM EDT

PDB ID	:	7SBC
Title	:	Crystal structure of a GMP synthase from Acinetobacter baumannii AB5075-UW
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2021-09-24
Resolution	:	1.95 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

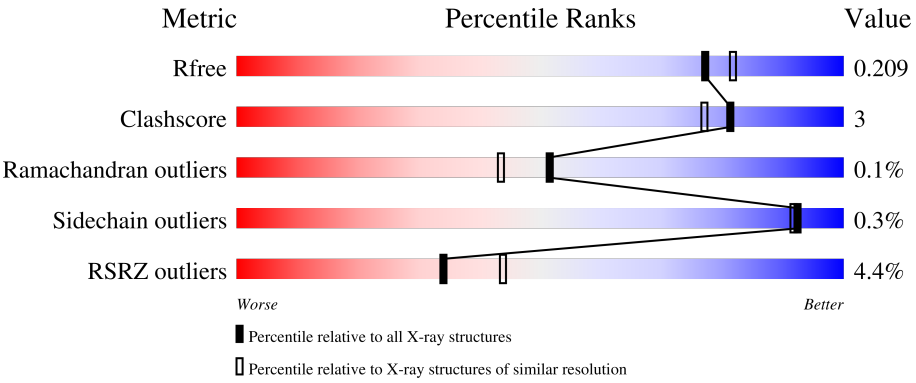
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	530	2% 89% 5% 6%
1	B	530	8% 88% 8% 5%
1	C	530	3% 90% 6% 5%
1	D	530	4% 89% 6% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17323 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 GMP synthase [glutamine-hydrolyzing].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	7	0
			3908	2484	668	740	16			
1	B	504	Total	C	N	O	S	0	6	0
			3921	2492	674	738	17			
1	C	505	Total	C	N	O	S	0	11	0
			3984	2532	683	750	19			
1	D	503	Total	C	N	O	S	0	5	0
			3919	2489	673	739	18			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP A0A0R1BBX7
A	-6	ALA	-	expression tag	UNP A0A0R1BBX7
A	-5	HIS	-	expression tag	UNP A0A0R1BBX7
A	-4	HIS	-	expression tag	UNP A0A0R1BBX7
A	-3	HIS	-	expression tag	UNP A0A0R1BBX7
A	-2	HIS	-	expression tag	UNP A0A0R1BBX7
A	-1	HIS	-	expression tag	UNP A0A0R1BBX7
A	0	HIS	-	expression tag	UNP A0A0R1BBX7
B	-7	MET	-	initiating methionine	UNP A0A0R1BBX7
B	-6	ALA	-	expression tag	UNP A0A0R1BBX7
B	-5	HIS	-	expression tag	UNP A0A0R1BBX7
B	-4	HIS	-	expression tag	UNP A0A0R1BBX7
B	-3	HIS	-	expression tag	UNP A0A0R1BBX7
B	-2	HIS	-	expression tag	UNP A0A0R1BBX7
B	-1	HIS	-	expression tag	UNP A0A0R1BBX7
B	0	HIS	-	expression tag	UNP A0A0R1BBX7
C	-7	MET	-	initiating methionine	UNP A0A0R1BBX7
C	-6	ALA	-	expression tag	UNP A0A0R1BBX7
C	-5	HIS	-	expression tag	UNP A0A0R1BBX7
C	-4	HIS	-	expression tag	UNP A0A0R1BBX7
C	-3	HIS	-	expression tag	UNP A0A0R1BBX7

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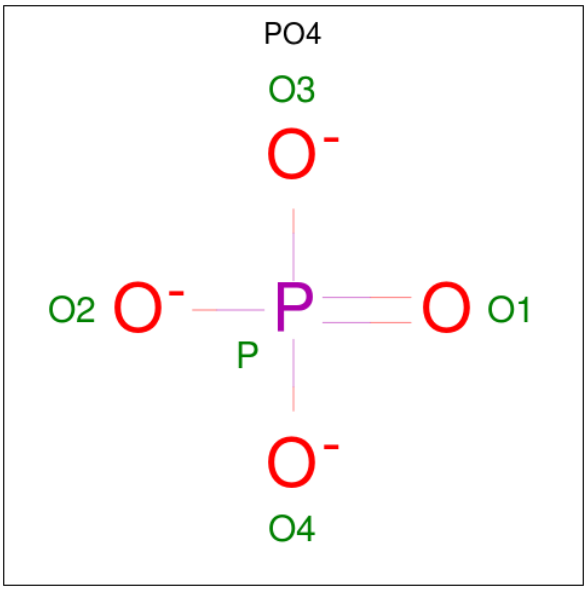
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP A0A0R1BBX7
C	-1	HIS	-	expression tag	UNP A0A0R1BBX7
C	0	HIS	-	expression tag	UNP A0A0R1BBX7
D	-7	MET	-	initiating methionine	UNP A0A0R1BBX7
D	-6	ALA	-	expression tag	UNP A0A0R1BBX7
D	-5	HIS	-	expression tag	UNP A0A0R1BBX7
D	-4	HIS	-	expression tag	UNP A0A0R1BBX7
D	-3	HIS	-	expression tag	UNP A0A0R1BBX7
D	-2	HIS	-	expression tag	UNP A0A0R1BBX7
D	-1	HIS	-	expression tag	UNP A0A0R1BBX7
D	0	HIS	-	expression tag	UNP A0A0R1BBX7

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Cl 3 3	0	0
3	B	3	Total Cl 3 3	0	0
3	C	3	Total Cl 3 3	0	0
3	D	3	Total Cl 3 3	0	0

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

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

- Molecule 5 is water.

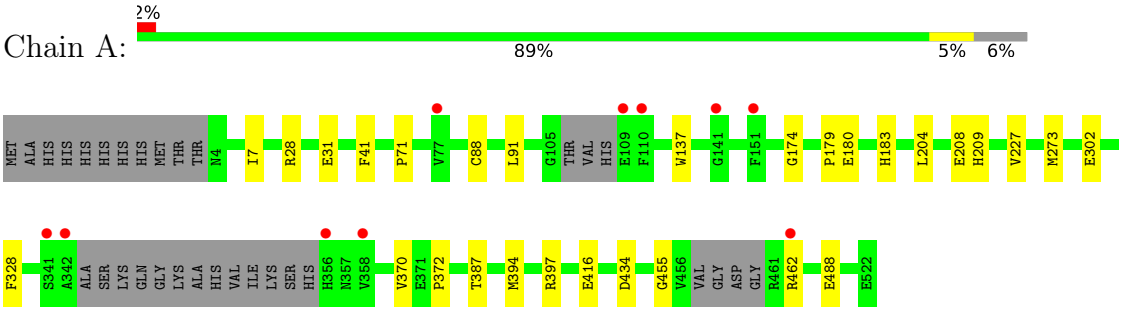
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	422	Total O 422 422	0	0
5	B	384	Total O 384 384	0	0
5	C	390	Total O 390 390	0	0
5	D	361	Total O 361 361	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

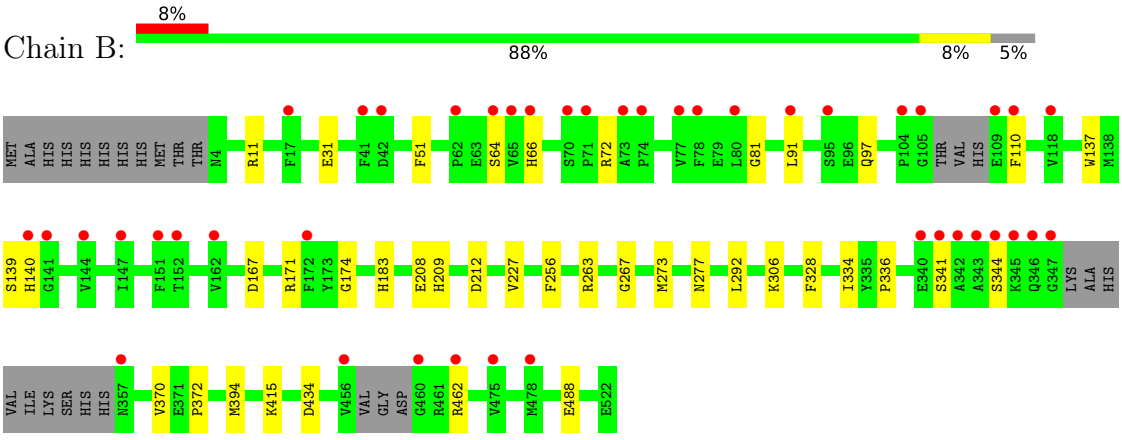
• Molecule 1: GMP synthase [glutamine-hydrolyzing]

Chain A:



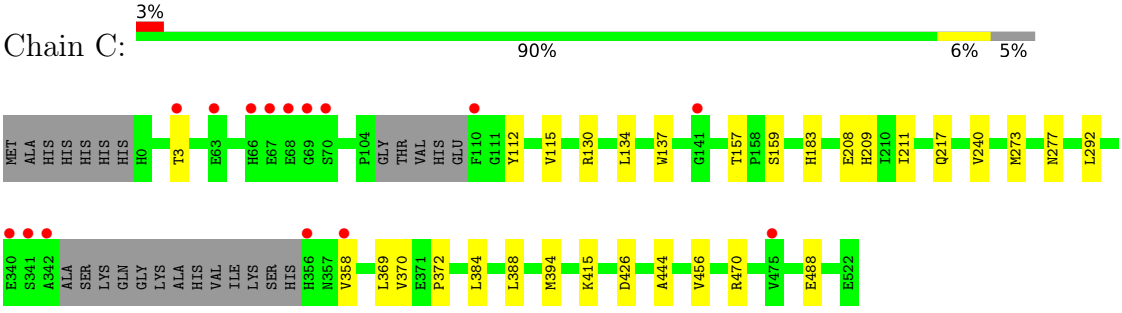
• Molecule 1: GMP synthase [glutamine-hydrolyzing]

Chain B:



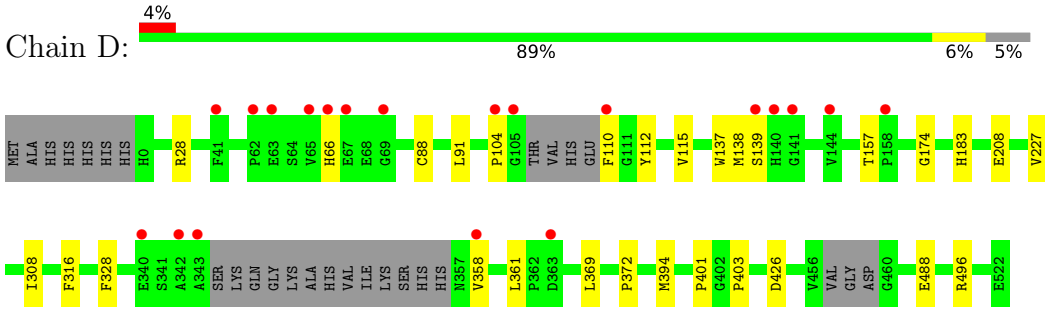
• Molecule 1: GMP synthase [glutamine-hydrolyzing]

Chain C:



• Molecule 1: GMP synthase [glutamine-hydrolyzing]

Chain D:


4%
89%
6%
5%
MET ALA HIS HIS HIS HIS HIS HO R28 F41 P62 E63 S64 V65 H66 E67 E68 G69 C88 L91 P104 G105 THR VAL HIS GLU F110 G111 Y112 V115 W137 M138 S139 H140 G141 V144 T157 P158 G174 H183 E208 V227 V240 M273
I308 F316 F328 E340 S341 A342 A343 SER LYS GLN GLY LYS ALA HIS VAL ILE LYS SER HIS HIS N357 V358 L361 P362 D363 L369 P372 M394 P401 G402 P403 D426 V456 VAL GLY ASP G460 E488 R496 E522

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	81.00Å 83.18Å 104.35Å 98.91° 109.83° 106.84°	Depositor
Resolution (Å)	48.82 – 1.95 48.83 – 1.95	Depositor EDS
% Data completeness (in resolution range)	91.9 (48.82-1.95) 91.9 (48.83-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 1.95Å)	Xtriage
Refinement program	PHENIX dev-4274	Depositor
R, R_{free}	0.177 , 0.208 0.177 , 0.209	Depositor DCC
R_{free} test set	1935 reflections (1.23%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17323	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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, 0.333 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: CL, PO4, MG

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	0.31	0/4005	0.54	0/5425
1	B	0.30	0/4015	0.53	0/5438
1	C	0.30	0/4094	0.53	0/5543
1	D	0.29	0/4007	0.53	0/5429
All	All	0.30	0/16121	0.53	0/21835

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	3908	0	3851	21	0
1	B	3921	0	3859	29	0
1	C	3984	0	3959	21	0
1	D	3919	0	3861	19	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	422	0	0	4	0
5	B	384	0	0	5	0
5	C	390	0	0	1	0
5	D	361	0	0	1	0
All	All	17323	0	15530	82	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 3.

All (82) 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:488:GLU:HG3	1:B:488:GLU:HG3	1.40	1.01
1:C:488:GLU:HG3	1:D:488:GLU:HG3	1.69	0.76
1:A:434[B]:ASP:OD2	1:D:112:TYR:OH	2.03	0.75
1:A:88[B]:CYS:SG	5:A:976:HOH:O	2.53	0.66
1:A:416:GLU:OE2	5:A:701:HOH:O	2.14	0.65
1:B:370:VAL:HG12	1:B:372:PRO:HD3	1.80	0.62
1:D:137:TRP:HB2	1:D:183:HIS:HB2	1.82	0.62
1:C:273[B]:MET:HG2	1:C:394:MET:HE1	1.82	0.62
1:D:91:LEU:HD13	1:D:174:GLY:HA3	1.81	0.62
1:C:240:VAL:HG22	1:C:372:PRO:HG2	1.82	0.61
1:A:434[B]:ASP:OD1	1:D:183:HIS:ND1	2.33	0.61
1:B:227:VAL:HG22	1:B:328:PHE:HB2	1.86	0.58
3:A:603:CL:CL	5:A:974:HOH:O	2.54	0.58
1:C:358:VAL:HG13	1:C:369:LEU:HD13	1.87	0.56
1:C:426:ASP:OD2	5:C:701:HOH:O	2.18	0.55
1:C:137:TRP:HB2	1:C:183:HIS:HB2	1.89	0.54
1:B:434:ASP:OD1	1:C:183:HIS:ND1	2.38	0.54
1:B:11:ARG:HD2	1:B:51:PHE:O	2.09	0.53
1:A:488:GLU:CG	1:B:488:GLU:HG3	2.27	0.52
1:B:91:LEU:HD13	1:B:174:GLY:HA3	1.92	0.51
1:D:358:VAL:HG13	1:D:369:LEU:HD13	1.92	0.51
1:B:81:GLY:O	1:B:171:ARG:NH2	2.44	0.51
1:B:462:ARG:NH1	5:B:715:HOH:O	2.45	0.50
1:A:227:VAL:HG22	1:A:328:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:VAL:HG12	1:A:372:PRO:HD3	1.94	0.50
1:B:263[A]:ARG:NH1	5:B:704:HOH:O	2.28	0.49
1:C:115:VAL:HA	1:C:157:THR:HG22	1.94	0.49
1:A:91:LEU:HD13	1:A:174:GLY:HA3	1.96	0.48
1:D:88[B]:CYS:SG	1:D:139:SER:OG	2.71	0.48
5:B:753:HOH:O	1:C:130:ARG:HD2	2.14	0.48
1:A:488:GLU:HG3	1:B:488:GLU:CG	2.27	0.48
1:D:66:HIS:NE2	1:D:104:PRO:HB3	2.29	0.48
1:C:211:ILE:HD12	1:C:388:LEU:HD21	1.97	0.47
1:D:110:PHE:CE1	1:D:139:SER:HB3	2.50	0.47
1:C:3:THR:HG21	1:C:217:GLN:HG3	1.97	0.47
1:D:426:ASP:OD2	5:D:702:HOH:O	2.20	0.46
1:A:302:GLU:HG2	5:A:1063:HOH:O	2.14	0.46
1:B:334:ILE:HG13	1:B:336:PRO:HD2	1.98	0.46
1:C:273[B]:MET:HG2	1:C:394:MET:CE	2.46	0.46
1:C:370:VAL:HG12	1:C:372:PRO:HD3	1.97	0.45
1:D:316:PHE:HD2	1:D:361:LEU:HD21	1.81	0.45
1:B:212:ASP:OD2	5:B:701:HOH:O	2.21	0.45
1:B:72:ARG:HB3	1:B:97:GLN:NE2	2.32	0.45
1:A:41:PHE:CZ	1:A:71:PRO:HB3	2.52	0.45
1:A:208:GLU:HG3	1:A:209:HIS:N	2.31	0.45
1:B:137:TRP:HB2	1:B:183:HIS:HB2	1.99	0.45
1:D:401:PRO:HB2	1:D:403:PRO:HD2	1.98	0.45
1:B:273[B]:MET:HG2	1:B:394:MET:CE	2.46	0.44
1:B:167:ASP:O	1:B:171:ARG:N	2.51	0.44
1:D:115:VAL:HA	1:D:157:THR:HG22	2.00	0.44
1:B:273[A]:MET:SD	1:B:277:ASN:ND2	2.79	0.44
1:D:273:MET:HG2	1:D:394:MET:CE	2.48	0.43
1:B:208:GLU:HG3	1:B:209:HIS:N	2.32	0.43
1:B:341:SER:HB3	1:B:344:SER:H	1.84	0.43
1:B:306:LYS:HE3	1:B:306:LYS:HB2	1.77	0.43
1:B:31[B]:GLU:HG2	5:B:714:HOH:O	2.18	0.43
1:B:292:LEU:HD13	1:B:415:LYS:HB2	2.00	0.43
1:A:455:GLY:O	1:A:462:ARG:N	2.38	0.43
1:C:115:VAL:HG22	1:C:134:LEU:HB2	2.01	0.43
1:B:110:PHE:HE1	1:B:139:SER:HB2	1.84	0.42
1:D:227:VAL:HG22	1:D:328:PHE:HB2	2.01	0.42
1:C:211:ILE:CD1	1:C:384[B]:LEU:HG	2.49	0.42
1:D:308:ILE:HG21	1:D:403:PRO:HA	2.02	0.42
1:B:110:PHE:HB3	1:B:137:TRP:CZ2	2.55	0.41
1:C:292:LEU:HD13	1:C:415:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TRP:HB2	1:A:183:HIS:HB2	2.02	0.41
1:C:211:ILE:HD11	1:C:384[B]:LEU:HG	2.03	0.41
1:B:434:ASP:OD2	1:C:112:TYR:OH	2.28	0.41
1:B:256:PHE:CZ	1:B:267:GLY:HA2	2.55	0.41
1:B:273[B]:MET:HG2	1:B:394:MET:HE2	2.02	0.41
1:D:110:PHE:HA	1:D:138:MET:O	2.20	0.41
1:A:387:THR:HG22	1:D:208:GLU:HB3	2.03	0.41
1:C:208:GLU:HG3	1:C:209:HIS:N	2.36	0.41
1:A:28:ARG:HD2	1:A:180:GLU:HA	2.03	0.41
1:C:444:ALA:HA	1:C:470:ARG:O	2.20	0.41
1:A:28:ARG:NH1	1:A:179:PRO:O	2.54	0.40
1:A:273:MET:HG2	1:A:394:MET:CE	2.51	0.40
1:A:7:ILE:HG22	1:A:204:LEU:HB3	2.03	0.40
1:B:64:SER:HB3	1:B:66:HIS:CD2	2.56	0.40
1:D:240:VAL:HG22	1:D:372:PRO:HG2	2.03	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	498/530 (94%)	487 (98%)	11 (2%)	0	100 100
1	B	502/530 (95%)	492 (98%)	9 (2%)	1 (0%)	47 38
1	C	510/530 (96%)	499 (98%)	11 (2%)	0	100 100
1	D	500/530 (94%)	489 (98%)	11 (2%)	0	100 100
All	All	2010/2120 (95%)	1967 (98%)	42 (2%)	1 (0%)	51 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	140	HIS

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	417/445 (94%)	416 (100%)	1 (0%)	93 93
1	B	414/445 (93%)	414 (100%)	0	100 100
1	C	428/445 (96%)	426 (100%)	2 (0%)	88 88
1	D	416/445 (94%)	414 (100%)	2 (0%)	88 88
All	All	1675/1780 (94%)	1670 (100%)	5 (0%)	92 92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	ARG
1	C	159	SER
1	C	456	VAL
1	D	28	ARG
1	D	496	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 14 are monoatomic - leaving 4 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	PO4	C	601	-	4,4,4	0.83	0	6,6,6	0.47	0
2	PO4	D	601	-	4,4,4	0.90	0	6,6,6	0.42	0
2	PO4	B	601	-	4,4,4	0.86	0	6,6,6	0.48	0
2	PO4	A	601	-	4,4,4	0.78	0	6,6,6	0.52	0

There are no bond length outliers.

There are no bond angle outliers.

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

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	499/530 (94%)	-0.11	10 (2%)	65	73	17, 30, 59, 86	0
1	B	504/530 (95%)	0.16	43 (8%)	10	17	16, 33, 76, 103	0
1	C	505/530 (95%)	-0.12	15 (2%)	50	59	16, 32, 60, 93	0
1	D	503/530 (94%)	-0.02	20 (3%)	38	48	16, 34, 68, 98	0
All	All	2011/2120 (94%)	-0.02	88 (4%)	34	44	16, 32, 67, 103	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	342	ALA	11.8
1	B	343	ALA	8.2
1	B	342	ALA	8.0
1	B	341	SER	6.8
1	C	341	SER	5.4
1	B	110	PHE	4.7
1	B	344	SER	4.4
1	D	66	HIS	4.4
1	C	68	GLU	4.3
1	B	345	LYS	4.1
1	D	139	SER	4.1
1	D	110	PHE	4.0
1	B	66	HIS	4.0
1	B	340	GLU	3.9
1	B	41	PHE	3.8
1	D	105	GLY	3.8
1	B	95	SER	3.7
1	B	347	GLY	3.6
1	D	141	GLY	3.6
1	C	356	HIS	3.6
1	D	363	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	346	GLN	3.5
1	C	69	GLY	3.4
1	B	151	PHE	3.3
1	B	460	GLY	3.3
1	C	475	VAL	3.2
1	D	358	VAL	3.2
1	B	475	VAL	3.2
1	B	74	PRO	3.2
1	C	110	PHE	3.1
1	A	141	GLY	3.1
1	A	356	HIS	3.0
1	B	105	GLY	3.0
1	D	342	ALA	3.0
1	B	104	PRO	2.9
1	A	342	ALA	2.9
1	D	65	VAL	2.9
1	A	110	PHE	2.9
1	C	340	GLU	2.8
1	C	358	VAL	2.8
1	D	340	GLU	2.8
1	D	69	GLY	2.7
1	D	62	PRO	2.7
1	B	78	PHE	2.7
1	D	63	GLU	2.6
1	D	140	HIS	2.6
1	A	151	PHE	2.6
1	D	144	VAL	2.6
1	B	62	PRO	2.5
1	B	478	MET	2.5
1	B	147	ILE	2.5
1	B	80	LEU	2.4
1	D	158	PRO	2.4
1	B	141	GLY	2.4
1	C	66	HIS	2.4
1	D	104	PRO	2.4
1	C	70	SER	2.4
1	B	17	PHE	2.3
1	B	65	VAL	2.3
1	B	144	VAL	2.3
1	A	341	SER	2.3
1	D	343	ALA	2.3
1	A	462	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	172	PHE	2.2
1	B	64	SER	2.2
1	B	140	HIS	2.2
1	B	118	VAL	2.2
1	B	456	VAL	2.2
1	B	91	LEU	2.2
1	A	109	GLU	2.2
1	B	71	PRO	2.2
1	C	141	GLY	2.2
1	B	152	THR	2.1
1	C	67	GLU	2.1
1	B	73	ALA	2.1
1	B	70	SER	2.1
1	A	77	VAL	2.1
1	B	42	ASP	2.1
1	B	77	VAL	2.1
1	B	357	ASN	2.1
1	D	41	PHE	2.1
1	C	3	THR	2.1
1	B	462	ARG	2.1
1	B	162	VAL	2.1
1	A	358	VAL	2.0
1	B	109	GLU	2.0
1	C	63	GLU	2.0
1	D	67	GLU	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	PO4	C	601	5/5	0.92	0.15	35,46,48,52	0
2	PO4	B	601	5/5	0.93	0.15	32,48,52,54	0
2	PO4	A	601	5/5	0.93	0.17	37,50,55,55	0
2	PO4	D	601	5/5	0.94	0.11	32,43,52,55	0
3	CL	A	602	1/1	0.97	0.07	32,32,32,32	0
3	CL	B	604	1/1	0.97	0.07	41,41,41,41	0
3	CL	C	604	1/1	0.97	0.05	38,38,38,38	0
4	MG	B	602	1/1	0.97	0.07	45,45,45,45	0
3	CL	C	602	1/1	0.98	0.05	34,34,34,34	0
3	CL	B	605	1/1	0.99	0.07	34,34,34,34	0
3	CL	A	604	1/1	0.99	0.07	35,35,35,35	0
3	CL	C	603	1/1	0.99	0.06	39,39,39,39	0
3	CL	B	603	1/1	0.99	0.07	32,32,32,32	0
3	CL	D	603	1/1	0.99	0.06	36,36,36,36	0
3	CL	D	604	1/1	0.99	0.05	38,38,38,38	0
3	CL	D	605	1/1	0.99	0.10	36,36,36,36	0
3	CL	A	603	1/1	0.99	0.05	32,32,32,32	0
4	MG	D	602	1/1	0.99	0.04	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.