Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:10 AM GMT

PDB ID	:	3HG9
Title	:	CRYSTAL STRUCTURE OF putative pilM protein from Pseudomonas aeruginosa 2192
Authors	:	Malashkevich, V.N.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-05-13
Resolution	:	2.40 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:

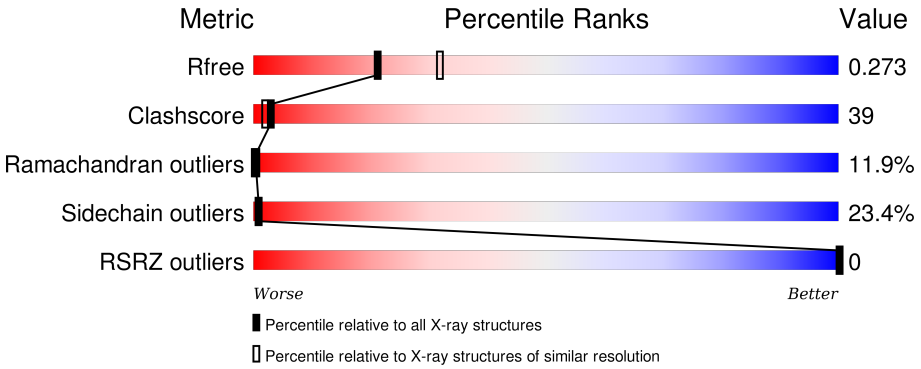
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	131	43% 30% 16% • 9%
1	B	131	42% 27% 20% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1936 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 PilM.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	119	Total 871	C 553	N 159	O 159	0	0	0
1	B	120	Total 880	C 558	N 160	O 162	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q6X3P5
A	2	SER	-	expression tag	UNP Q6X3P5
A	3	LEU	-	expression tag	UNP Q6X3P5
A	124	GLU	-	expression tag	UNP Q6X3P5
A	125	GLY	-	expression tag	UNP Q6X3P5
A	126	HIS	-	expression tag	UNP Q6X3P5
A	127	HIS	-	expression tag	UNP Q6X3P5
A	128	HIS	-	expression tag	UNP Q6X3P5
A	129	HIS	-	expression tag	UNP Q6X3P5
A	130	HIS	-	expression tag	UNP Q6X3P5
A	131	HIS	-	expression tag	UNP Q6X3P5
B	1	MET	-	expression tag	UNP Q6X3P5
B	2	SER	-	expression tag	UNP Q6X3P5
B	3	LEU	-	expression tag	UNP Q6X3P5
B	124	GLU	-	expression tag	UNP Q6X3P5
B	125	GLY	-	expression tag	UNP Q6X3P5
B	126	HIS	-	expression tag	UNP Q6X3P5
B	127	HIS	-	expression tag	UNP Q6X3P5
B	128	HIS	-	expression tag	UNP Q6X3P5
B	129	HIS	-	expression tag	UNP Q6X3P5
B	130	HIS	-	expression tag	UNP Q6X3P5
B	131	HIS	-	expression tag	UNP Q6X3P5

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ni 2 2	0	0

- Molecule 3 is water.

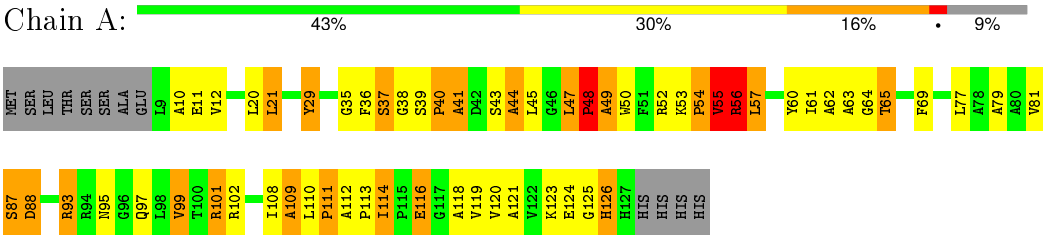
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	80	Total O 80 80	0	0
3	B	103	Total O 103 103	0	0

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.

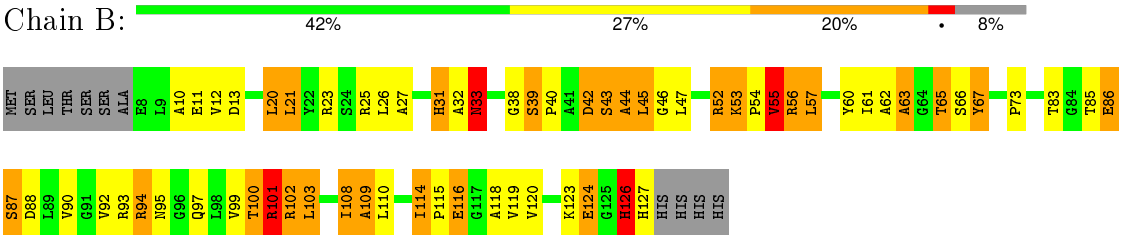
- Molecule 1: PilM

Chain A:



- Molecule 1: PilM

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α, β, γ	64.52Å 64.52Å 143.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.40 44.04 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.7 (50.00-2.40) 93.9 (44.04-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.235 , 0.267 0.249 , 0.273	Depositor DCC
R_{free} test set	616 reflections (5.23%)	DCC
Wilson B-factor (Å^2)	58.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 99.5	EDS
Estimated twinning fraction	0.503 for H, K, L 0.497 for -H-K, K, -L 0.210 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.503 for H, K, L 0.497 for -H-K, K, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.39$	Xtriage
Outliers	0 of 12417 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	1936	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.28% 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: NI

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	1.11	0/891	1.20	6/1217 (0.5%)
1	B	1.07	0/900	1.13	4/1229 (0.3%)
All	All	1.09	0/1791	1.17	10/2446 (0.4%)

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	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	120	VAL	CB-CA-C	-6.94	98.21	111.40
1	A	126	HIS	N-CA-C	6.22	127.78	111.00
1	A	56	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	39	SER	N-CA-C	-5.94	94.97	111.00
1	B	20	LEU	CA-CB-CG	-5.81	101.93	115.30
1	B	21	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	A	21	LEU	CA-CB-CG	-5.19	103.36	115.30
1	B	120	VAL	CB-CA-C	-5.07	101.77	111.40
1	A	47	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	GLU	Peptide
1	B	55	VAL	Peptide
1	B	94	ARG	Peptide

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	871	0	880	74	0
1	B	880	0	886	76	1
2	A	2	0	0	0	0
3	A	80	0	0	7	2
3	B	103	0	0	6	3
All	All	1936	0	1766	138	3

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 39.

All (138) 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:55:VAL:HG13	3:B:146:HOH:O	1.42	1.16
1:B:101:ARG:O	1:B:101:ARG:HG2	1.49	1.11
1:A:114:ILE:CD1	1:A:118:ALA:HB3	1.80	1.10
1:B:114:ILE:HD11	1:B:118:ALA:HB3	1.10	1.09
1:A:37:SER:HA	1:A:61:ILE:O	1.53	1.06
1:A:114:ILE:HD11	1:A:118:ALA:HB3	1.39	1.03
1:B:94:ARG:NH2	3:B:225:HOH:O	1.90	1.03
1:B:114:ILE:CD1	1:B:118:ALA:HB3	1.92	0.98
1:B:114:ILE:HD11	1:B:118:ALA:CB	1.94	0.98
1:B:56:ARG:CD	1:B:56:ARG:H	1.79	0.94
1:A:123:LYS:NZ	3:A:134:HOH:O	2.00	0.94
1:B:85:THR:O	1:B:86:GLU:HB2	1.67	0.92
1:A:36:PHE:CZ	1:A:38:GLY:HA3	2.10	0.86
1:A:53:LYS:HD3	1:A:57:LEU:HB3	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:TYR:HD2	1:A:45:LEU:HD23	1.41	0.83
1:B:101:ARG:O	1:B:101:ARG:CG	2.27	0.82
1:A:56:ARG:HD3	3:A:164:HOH:O	1.79	0.82
1:A:55:VAL:O	1:A:56:ARG:HG2	1.78	0.82
1:B:114:ILE:CD1	1:B:118:ALA:CB	2.56	0.80
1:B:86:GLU:O	1:B:87:SER:HB2	1.83	0.79
1:A:114:ILE:CD1	1:A:118:ALA:CB	2.62	0.77
1:B:63:ALA:HB3	1:B:65:THR:HG23	1.64	0.77
1:B:56:ARG:H	1:B:56:ARG:HD2	1.50	0.76
1:B:93:ARG:NH1	1:B:95:ASN:OD1	2.15	0.76
1:A:29:TYR:CD2	1:A:45:LEU:HD23	2.21	0.75
1:A:55:VAL:O	1:A:56:ARG:NH1	2.20	0.74
1:A:55:VAL:O	1:A:56:ARG:CG	2.36	0.74
1:A:37:SER:CA	1:A:61:ILE:O	2.33	0.73
1:A:62:ALA:C	1:A:64:GLY:H	1.89	0.73
1:A:60:TYR:CE2	1:A:62:ALA:HB2	2.24	0.73
1:B:61:ILE:HG12	1:B:66:SER:HB3	1.70	0.72
1:A:87:SER:HA	1:B:88:ASP:O	1.89	0.72
1:A:111:PRO:HB3	1:B:60:TYR:CE2	2.25	0.71
1:A:119:VAL:HG23	1:B:73:PRO:HB3	1.71	0.71
1:B:102:ARG:CZ	1:B:102:ARG:HB2	2.19	0.71
1:B:92:VAL:O	1:B:99:VAL:HG12	1.90	0.71
1:B:11:GLU:C	1:B:13:ASP:H	1.94	0.71
1:B:11:GLU:HA	1:B:13:ASP:OD2	1.91	0.71
1:A:82:ASP:HA	1:B:90:VAL:HG21	1.73	0.71
1:A:99:VAL:HG12	1:A:99:VAL:O	1.90	0.71
1:A:64:GLY:O	1:A:65:THR:OG1	2.09	0.70
1:A:93:ARG:HG2	1:A:116:GLU:HA	1.74	0.70
1:A:114:ILE:HD12	1:A:118:ALA:HB3	1.73	0.69
1:B:86:GLU:O	1:B:87:SER:CB	2.39	0.68
1:B:42:ASP:HB3	1:B:47:LEU:HD12	1.76	0.68
1:A:125:GLY:O	3:A:209:HOH:O	2.11	0.68
1:B:56:ARG:NE	1:B:56:ARG:H	1.94	0.66
1:B:67:TYR:N	1:B:67:TYR:CD2	2.62	0.66
1:B:53:LYS:HD3	1:B:57:LEU:HB3	1.77	0.66
1:B:99:VAL:O	1:B:99:VAL:HG13	1.95	0.65
1:B:25:ARG:HG3	1:B:47:LEU:HD23	1.78	0.65
1:A:54:PRO:O	1:A:55:VAL:C	2.36	0.64
1:A:48:PRO:O	1:A:49:ALA:CB	2.45	0.64
1:A:112:ALA:HB3	1:A:113:PRO:HD3	1.79	0.64
1:B:55:VAL:CG1	3:B:146:HOH:O	2.18	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:GLU:C	1:B:13:ASP:N	2.52	0.63
1:A:77:LEU:O	1:A:81:VAL:HG23	1.99	0.62
1:A:62:ALA:O	1:A:64:GLY:N	2.30	0.62
1:A:29:TYR:CE2	1:A:40:PRO:HB3	2.34	0.62
1:A:114:ILE:HD12	1:A:118:ALA:CB	2.29	0.62
1:A:93:ARG:CG	1:A:116:GLU:HA	2.29	0.62
1:B:38:GLY:HA2	1:B:40:PRO:HD3	1.81	0.62
1:B:85:THR:O	1:B:86:GLU:CB	2.46	0.61
1:B:42:ASP:OD2	1:B:53:LYS:NZ	2.34	0.61
1:A:99:VAL:CG1	1:A:99:VAL:O	2.49	0.61
1:A:55:VAL:HA	3:A:139:HOH:O	2.01	0.60
1:A:64:GLY:O	3:A:158:HOH:O	2.16	0.60
1:B:86:GLU:HA	1:B:126:HIS:HB3	1.82	0.60
1:A:101:ARG:O	3:A:143:HOH:O	2.17	0.60
1:A:48:PRO:O	1:A:49:ALA:HB3	2.03	0.59
1:A:86:GLU:O	1:A:87:SER:CB	2.52	0.58
1:A:88:ASP:OD2	1:A:88:ASP:C	2.41	0.58
1:B:52:ARG:HG2	3:B:223:HOH:O	2.04	0.58
1:A:39:SER:O	1:A:41:ALA:N	2.35	0.58
1:A:79:ALA:O	1:A:83:THR:OG1	2.18	0.57
1:B:44:ALA:O	1:B:46:GLY:N	2.36	0.57
1:A:43:SER:O	1:A:44:ALA:HB3	2.05	0.57
1:A:36:PHE:CG	1:A:37:SER:N	2.74	0.56
1:B:102:ARG:C	1:B:103:LEU:HD13	2.26	0.56
1:A:60:TYR:HE2	1:A:62:ALA:HB2	1.65	0.56
1:A:64:GLY:O	1:A:65:THR:CB	2.54	0.56
1:B:43:SER:C	1:B:44:ALA:O	2.45	0.54
1:A:38:GLY:O	1:A:60:TYR:CD1	2.60	0.53
1:A:65:THR:OG1	1:B:124:GLU:HG2	2.07	0.53
1:A:53:LYS:HD3	1:A:57:LEU:O	2.08	0.53
1:B:21:LEU:C	1:B:21:LEU:HD23	2.29	0.53
1:B:52:ARG:NH1	3:B:175:HOH:O	2.42	0.52
1:B:46:GLY:HA2	3:B:151:HOH:O	2.09	0.52
1:A:108:ILE:HG23	1:B:103:LEU:HD12	1.90	0.52
1:A:60:TYR:CD2	1:A:62:ALA:HB2	2.44	0.51
1:B:92:VAL:HB	1:B:99:VAL:CG1	2.41	0.51
1:B:95:ASN:HD21	1:B:116:GLU:HB3	1.75	0.51
1:B:55:VAL:HG12	1:B:56:ARG:HA	1.92	0.51
1:B:25:ARG:HG3	1:B:47:LEU:CD2	2.40	0.50
1:A:110:LEU:O	1:A:111:PRO:O	2.29	0.50
1:B:26:LEU:O	1:B:27:ALA:C	2.48	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PRO:HB3	1:B:60:TYR:HE2	1.75	0.50
1:B:31:HIS:O	1:B:33:ASN:N	2.41	0.49
1:B:56:ARG:N	1:B:56:ARG:CD	2.61	0.49
1:B:10:ALA:O	1:B:13:ASP:OD2	2.31	0.48
1:B:90:VAL:O	1:B:100:THR:HB	2.14	0.48
1:B:62:ALA:C	1:B:63:ALA:O	2.50	0.47
1:A:36:PHE:CD2	1:A:37:SER:N	2.80	0.47
1:A:48:PRO:HB3	1:A:50:TRP:CE2	2.50	0.47
1:B:114:ILE:HD12	1:B:115:PRO:HD2	1.95	0.47
1:A:29:TYR:CZ	1:A:40:PRO:HB3	2.49	0.47
1:B:40:PRO:HG2	1:B:45:LEU:HD11	1.96	0.47
1:A:10:ALA:HB2	3:A:152:HOH:O	2.14	0.46
1:B:93:ARG:HG3	1:B:110:LEU:HD13	1.97	0.46
1:A:121:ALA:HB1	1:B:23:ARG:HH11	1.80	0.46
1:B:102:ARG:NH1	1:B:102:ARG:HB2	2.30	0.46
1:A:43:SER:O	1:A:44:ALA:CB	2.65	0.45
1:B:99:VAL:O	1:B:99:VAL:CG1	2.65	0.45
1:A:36:PHE:HZ	1:A:38:GLY:HA3	1.71	0.45
1:A:121:ALA:HB1	1:B:23:ARG:NH1	2.32	0.45
1:A:20:LEU:HD23	1:A:20:LEU:HA	1.82	0.44
1:B:56:ARG:N	1:B:56:ARG:HD2	2.27	0.44
1:A:109:ALA:O	1:A:111:PRO:HD3	2.18	0.44
1:B:102:ARG:O	1:B:103:LEU:HD13	2.18	0.44
1:B:108:ILE:HG22	1:B:109:ALA:N	2.32	0.44
1:A:55:VAL:O	1:A:56:ARG:CB	2.66	0.43
1:B:92:VAL:HG22	1:B:119:VAL:HG22	2.00	0.42
1:A:82:ASP:CA	1:B:90:VAL:HG21	2.47	0.42
1:A:86:GLU:O	1:A:87:SER:HB2	2.20	0.42
1:B:56:ARG:HE	1:B:56:ARG:H	1.63	0.41
1:A:36:PHE:C	1:A:37:SER:OG	2.58	0.41
1:A:69:PHE:CG	1:B:114:ILE:HD13	2.54	0.41
1:A:110:LEU:O	1:A:111:PRO:C	2.57	0.41
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.80	0.41
1:B:95:ASN:ND2	1:B:116:GLU:HB3	2.35	0.41
1:B:20:LEU:HA	1:B:20:LEU:HD23	1.48	0.41
1:A:95:ASN:C	1:A:97:GLN:H	2.24	0.41
1:B:94:ARG:O	1:B:97:GLN:HB2	2.20	0.40
1:A:93:ARG:HG2	1:A:116:GLU:CA	2.49	0.40
1:B:114:ILE:HD12	1:B:118:ALA:CB	2.50	0.40
1:B:94:ARG:O	1:B:97:GLN:N	2.54	0.40
1:A:110:LEU:HD23	1:A:110:LEU:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLU:OE1	1:B:102:ARG:NH1	2.55	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:184:HOH:O	3:B:226:HOH:O[3_455]	1.95	0.25
1:B:55:VAL:O	3:B:153:HOH:O[4_455]	2.13	0.07
3:A:201:HOH:O	3:B:207:HOH:O[3_565]	2.15	0.05

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	117/131 (89%)	92 (79%)	10 (8%)	15 (13%)	0	0
1	B	118/131 (90%)	95 (80%)	10 (8%)	13 (11%)	0	0
All	All	235/262 (90%)	187 (80%)	20 (8%)	28 (12%)	0	0

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	A	41	ALA
1	A	49	ALA
1	A	65	THR
1	A	87	SER
1	B	32	ALA
1	B	33	ASN
1	B	44	ALA
1	B	86	GLU
1	B	87	SER

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Mol	Chain	Res	Type
1	B	109	ALA
1	B	126	HIS
1	A	48	PRO
1	A	56	ARG
1	A	63	ALA
1	A	126	HIS
1	B	12	VAL
1	B	101	ARG
1	A	44	ALA
1	A	111	PRO
1	B	31	HIS
1	A	109	ALA
1	B	63	ALA
1	A	54	PRO
1	B	45	LEU
1	A	35	GLY
1	A	55	VAL
1	B	54	PRO

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	85/96 (88%)	68 (80%)	17 (20%)	1 1
1	B	86/96 (90%)	63 (73%)	23 (27%)	0 0
All	All	171/192 (89%)	131 (77%)	40 (23%)	1 1

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	21	LEU
1	A	29	TYR
1	A	37	SER
1	A	47	LEU

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Mol	Chain	Res	Type
1	A	48	PRO
1	A	52	ARG
1	A	55	VAL
1	A	56	ARG
1	A	57	LEU
1	A	88	ASP
1	A	93	ARG
1	A	99	VAL
1	A	101	ARG
1	A	102	ARG
1	A	114	ILE
1	A	116	GLU
1	B	33	ASN
1	B	39	SER
1	B	42	ASP
1	B	43	SER
1	B	52	ARG
1	B	53	LYS
1	B	55	VAL
1	B	56	ARG
1	B	57	LEU
1	B	65	THR
1	B	67	TYR
1	B	83	THR
1	B	100	THR
1	B	101	ARG
1	B	102	ARG
1	B	103	LEU
1	B	108	ILE
1	B	114	ILE
1	B	116	GLU
1	B	123	LYS
1	B	124	GLU
1	B	126	HIS
1	B	127	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	127	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

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	119/131 (90%)	-0.23	0	100	100	25, 44, 55, 62	0
1	B	120/131 (91%)	-0.31	0	100	100	26, 41, 56, 63	0
All	All	239/262 (91%)	-0.27	0	100	100	25, 42, 56, 63	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	NI	A	501	1/1	0.91	0.16	-	99,99,99,99	0
2	NI	A	502	1/1	0.89	0.12	-	114,114,114,114	0

6.5 Other polymers (i)

There are no such residues in this entry.