



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2016 – 10:42 PM EDT

PDB ID : 5GO3
Title : Crystal structure of a di-nucleotide cyclase Vibrio mutant
Authors : Ming, Z.H.; Wang, W.; Xie, Y.C.; Chen, Y.C.; Yan, L.M.; Lou, Z.Y.
Deposited on : 2016-07-26
Resolution : 2.20 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 : unknown
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

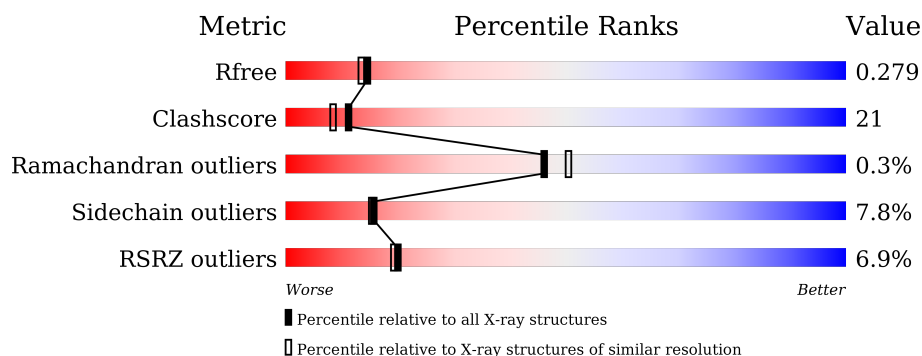
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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 $\leq 5\%$. 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	447	<div> <div>7%</div> <div> <div></div> <div>50%</div> <div>26%</div> <div>5%</div> <div>19%</div> </div> </div>
1	B	447	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>21%</div> <div>•</div> <div>19%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6104 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 Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2904	1837	503	548	16			
1	B	364	Total	C	N	O	S	0	0	0
			2922	1849	506	551	16			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q9KVG7
A	-3	PRO	-	expression tag	UNP Q9KVG7
A	-2	LEU	-	expression tag	UNP Q9KVG7
A	-1	GLY	-	expression tag	UNP Q9KVG7
A	0	SER	-	expression tag	UNP Q9KVG7
A	131	ASN	ASP	engineered mutation	UNP Q9KVG7
A	133	ASN	ASP	engineered mutation	UNP Q9KVG7
A	437	HIS	-	expression tag	UNP Q9KVG7
A	438	HIS	-	expression tag	UNP Q9KVG7
A	439	HIS	-	expression tag	UNP Q9KVG7
A	440	HIS	-	expression tag	UNP Q9KVG7
A	441	HIS	-	expression tag	UNP Q9KVG7
A	442	HIS	-	expression tag	UNP Q9KVG7
B	-4	GLY	-	expression tag	UNP Q9KVG7
B	-3	PRO	-	expression tag	UNP Q9KVG7
B	-2	LEU	-	expression tag	UNP Q9KVG7
B	-1	GLY	-	expression tag	UNP Q9KVG7
B	0	SER	-	expression tag	UNP Q9KVG7
B	131	ASN	ASP	engineered mutation	UNP Q9KVG7
B	133	ASN	ASP	engineered mutation	UNP Q9KVG7
B	437	HIS	-	expression tag	UNP Q9KVG7
B	438	HIS	-	expression tag	UNP Q9KVG7
B	439	HIS	-	expression tag	UNP Q9KVG7
B	440	HIS	-	expression tag	UNP Q9KVG7
B	441	HIS	-	expression tag	UNP Q9KVG7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	442	HIS	-	expression tag	UNP Q9KVG7

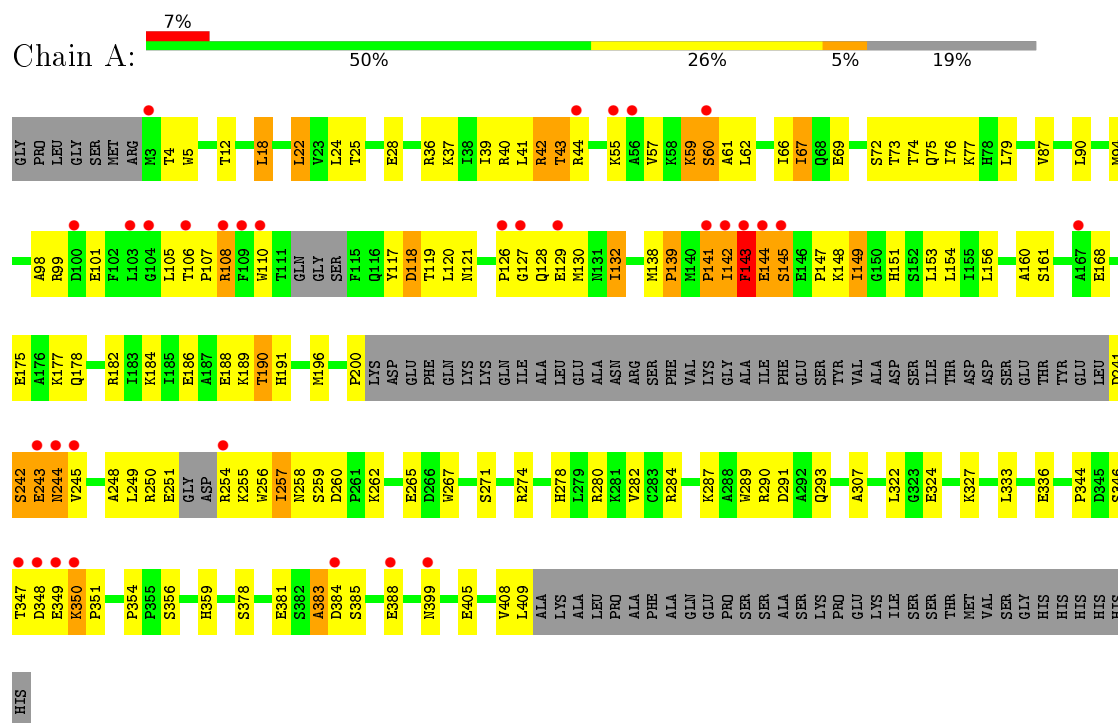
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	126	Total 126	O 126	0	0
2	B	152	Total 152	O 152	0	0

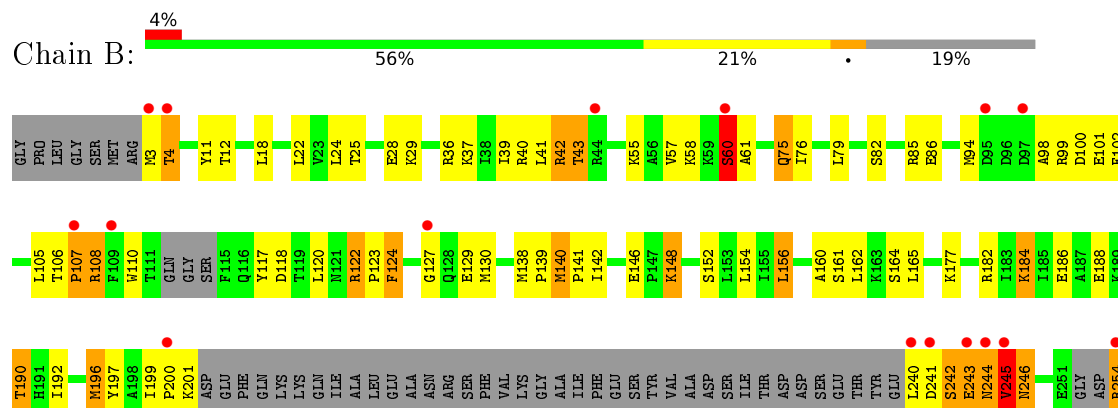
3 Residue-property plots [i](#)

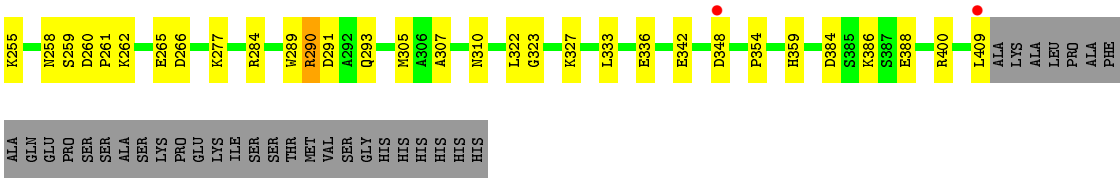
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Cyclic GMP-AMP synthase



• Molecule 1: Cyclic GMP-AMP synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.75Å 46.27Å 121.79Å 90.00° 99.82° 90.00°	Depositor
Resolution (Å)	43.17 – 2.20 43.17 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.17-2.20) 95.0 (43.17-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.228 , 0.292 0.222 , 0.279	Depositor DCC
R_{free} test set	2019 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6104	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.57 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.6827e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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	0.48	1/2961 (0.0%)	0.84	16/3991 (0.4%)
1	B	0.44	0/2979	0.96	21/4014 (0.5%)
All	All	0.46	1/5940 (0.0%)	0.90	37/8005 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	PRO	N-CD	13.36	1.66	1.47

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ALA	N-CA-CB	-16.81	86.56	110.10
1	A	141	PRO	N-CA-C	15.45	152.26	112.10
1	B	107	PRO	CB-CA-C	-13.04	79.39	112.00
1	B	60	SER	CB-CA-C	-12.65	86.06	110.10
1	B	3	MET	N-CA-CB	-12.64	87.85	110.60
1	B	3	MET	N-CA-C	-12.49	77.28	111.00
1	B	108	ARG	N-CA-CB	-12.20	88.64	110.60
1	A	61	ALA	N-CA-CB	-11.70	93.72	110.10
1	B	245	VAL	N-CA-CB	-11.34	86.55	111.50
1	B	244	ASN	CB-CA-C	10.28	130.96	110.40
1	B	245	VAL	N-CA-C	9.83	137.53	111.00
1	A	60	SER	CB-CA-C	-9.62	91.83	110.10
1	B	245	VAL	CB-CA-C	-9.61	93.14	111.40
1	B	4	THR	N-CA-C	-9.45	85.50	111.00
1	A	60	SER	N-CA-C	-9.41	85.60	111.00
1	A	346	SER	CB-CA-C	-9.37	92.29	110.10
1	A	142	ILE	CB-CA-C	-9.13	93.33	111.60
1	A	144	GLU	CB-CA-C	8.95	128.30	110.40
1	B	3	MET	CB-CA-C	-8.76	92.88	110.40
1	B	243	GLU	CB-CA-C	-8.52	93.37	110.40
1	A	145	SER	N-CA-CB	-8.07	98.39	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	SER	CB-CA-C	7.96	125.22	110.10
1	B	400	ARG	N-CA-C	7.82	132.11	111.00
1	A	142	ILE	N-CA-C	-7.79	89.96	111.00
1	A	107	PRO	CA-N-CD	-7.46	101.05	111.50
1	A	383	ALA	CB-CA-C	-7.40	99.00	110.10
1	A	243	GLU	CB-CA-C	-6.98	96.44	110.40
1	A	59	LYS	CB-CA-C	-6.89	96.62	110.40
1	B	246	ASN	CB-CA-C	6.62	123.64	110.40
1	B	244	ASN	N-CA-C	-6.34	93.87	111.00
1	B	246	ASN	N-CA-C	-6.24	94.15	111.00
1	B	124	PHE	CB-CA-C	-5.91	98.58	110.40
1	B	290	ARG	NE-CZ-NH1	-5.77	117.41	120.30
1	A	143	PHE	N-CA-CB	-5.67	100.39	110.60
1	A	128	GLN	N-CA-C	-5.43	96.33	111.00
1	B	400	ARG	N-CA-CB	-5.41	100.86	110.60
1	A	141	PRO	CB-CA-C	-5.08	99.30	112.00

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	2904	0	2899	137	0
1	B	2922	0	2926	105	1
2	A	126	0	0	6	0
2	B	152	0	0	8	0
All	All	6104	0	5825	241	1

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 21.

All (241) 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:385:SER:HB3	1:A:388:GLU:OE1	1.22	1.29
1:A:245:VAL:HG12	1:A:259:SER:N	1.53	1.21
1:B:290:ARG:NH1	1:B:291:ASP:OD1	1.73	1.20
1:A:385:SER:CB	1:A:388:GLU:OE1	2.02	1.08
1:B:24:LEU:HD11	1:B:130:MET:HE1	1.38	1.04
1:A:245:VAL:HB	1:A:258:ASN:OD1	1.58	1.03
1:B:142:ILE:HD12	1:B:142:ILE:H	1.26	0.99
1:A:245:VAL:O	1:A:258:ASN:HA	1.61	0.99
1:A:350:LYS:NZ	1:A:350:LYS:HA	1.80	0.97
1:A:245:VAL:HG11	1:A:258:ASN:ND2	1.78	0.96
1:A:200:PRO:HD3	1:A:243:GLU:O	1.66	0.95
1:B:101:GLU:HG3	1:B:148:LYS:HE2	1.49	0.94
1:A:350:LYS:HD3	1:A:351:PRO:HD2	1.52	0.92
1:A:245:VAL:O	1:A:259:SER:N	2.03	0.91
1:A:241:ASP:O	1:A:245:VAL:CG2	2.19	0.89
1:B:105:LEU:HD21	1:B:138:MET:CE	2.01	0.89
1:A:24:LEU:HD11	1:A:130:MET:HE1	1.53	0.89
1:A:245:VAL:HG12	1:A:258:ASN:C	1.92	0.89
1:B:199:ILE:HG22	1:B:244:ASN:O	1.73	0.87
1:B:108:ARG:HH21	1:B:108:ARG:HG3	1.38	0.87
1:B:200:PRO:HD3	1:B:243:GLU:O	1.74	0.87
1:B:245:VAL:CG1	1:B:258:ASN:HA	2.05	0.86
1:A:74:THR:O	1:A:77:LYS:HE3	1.76	0.86
1:B:79:LEU:HD11	1:B:160:ALA:HB2	1.56	0.86
1:B:254:ARG:HG2	1:B:254:ARG:HH11	1.42	0.85
1:A:117:TYR:O	1:A:118:ASP:HB2	1.75	0.85
1:B:24:LEU:HD11	1:B:130:MET:CE	2.07	0.84
1:B:120:LEU:HD21	1:B:130:MET:HE2	1.57	0.84
1:B:245:VAL:HG11	1:B:258:ASN:OD1	1.80	0.81
1:B:242:SER:O	1:B:258:ASN:OD1	1.98	0.81
1:A:245:VAL:HG13	1:A:260:ASP:N	1.96	0.80
1:B:28:GLU:OE2	1:B:122:ARG:NH1	2.16	0.79
1:B:245:VAL:HG23	1:B:260:ASP:HB2	1.64	0.79
1:B:307:ALA:HB1	1:B:336:GLU:HG2	1.66	0.78
1:A:350:LYS:CE	1:A:350:LYS:HA	2.07	0.77
1:B:105:LEU:HD21	1:B:138:MET:HE3	1.65	0.77
1:A:350:LYS:HD3	1:A:351:PRO:CD	2.14	0.77
1:B:245:VAL:HG22	1:B:259:SER:N	1.98	0.77
1:A:79:LEU:HD11	1:A:160:ALA:HB2	1.66	0.76
1:B:58:LYS:NZ	1:B:100:ASP:OD1	2.16	0.76
1:A:118:ASP:O	1:A:284:ARG:NH1	2.18	0.76
1:B:245:VAL:HG11	1:B:258:ASN:HA	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ARG:HD2	2:B:547:HOH:O	1.86	0.75
1:B:36:ARG:HD3	1:B:40:ARG:CZ	2.16	0.75
1:A:290:ARG:NH1	1:A:291:ASP:OD1	2.21	0.73
1:B:142:ILE:CD1	1:B:142:ILE:H	2.01	0.73
1:B:245:VAL:HG13	1:B:258:ASN:HA	1.69	0.73
1:B:245:VAL:O	1:B:245:VAL:HG13	1.82	0.73
1:A:120:LEU:HD22	1:A:132:ILE:HD11	1.71	0.72
1:A:200:PRO:HG3	1:A:243:GLU:HB2	1.71	0.72
1:A:399:ASN:ND2	2:A:501:HOH:O	2.17	0.72
1:A:105:LEU:HD21	1:A:138:MET:HE2	1.71	0.72
1:A:347:THR:O	1:A:348:ASP:OD1	2.07	0.71
1:B:24:LEU:CD1	1:B:130:MET:HE1	2.18	0.71
1:A:245:VAL:O	1:A:258:ASN:CA	2.38	0.71
1:A:245:VAL:HB	1:A:258:ASN:CG	2.12	0.69
1:A:42:ARG:NH1	2:A:503:HOH:O	2.25	0.69
1:B:240:LEU:HB2	1:B:244:ASN:HD22	1.55	0.69
1:A:43:THR:HG22	1:A:161:SER:HB3	1.73	0.69
1:A:354:PRO:O	1:A:359:HIS:HE1	1.76	0.68
1:B:142:ILE:HD12	1:B:142:ILE:N	2.06	0.68
1:B:254:ARG:NH1	1:B:254:ARG:HG2	2.05	0.68
1:A:245:VAL:CG1	1:A:258:ASN:ND2	2.55	0.68
1:A:249:LEU:HD11	1:A:257:ILE:HG13	1.76	0.68
1:A:245:VAL:HG12	1:A:259:SER:CA	2.23	0.68
1:B:201:LYS:HD2	2:B:589:HOH:O	1.93	0.67
1:A:105:LEU:HD22	1:A:149:ILE:HD12	1.75	0.67
1:A:43:THR:HG22	1:A:161:SER:CB	2.25	0.67
1:B:245:VAL:HG22	1:B:259:SER:C	2.15	0.67
1:A:24:LEU:HD21	1:A:130:MET:HE3	1.76	0.66
1:A:129:GLU:OE1	1:A:191:HIS:CD2	2.49	0.66
1:A:57:VAL:O	1:A:60:SER:O	2.15	0.65
1:A:241:ASP:O	1:A:245:VAL:HG21	1.96	0.65
1:B:307:ALA:CB	1:B:336:GLU:HG2	2.27	0.65
1:B:94:MET:HE1	1:B:98:ALA:O	1.97	0.64
1:A:101:GLU:HG3	1:A:148:LYS:CE	2.28	0.64
1:A:5:TRP:NE1	1:A:383:ALA:O	2.25	0.64
1:B:245:VAL:HG21	1:B:258:ASN:OD1	1.98	0.64
1:A:350:LYS:HZ2	1:A:350:LYS:HA	1.61	0.64
1:A:36:ARG:HD3	1:A:40:ARG:CZ	2.28	0.62
1:B:240:LEU:HB2	1:B:244:ASN:ND2	2.14	0.62
1:A:69:GLU:O	1:A:72:SER:OG	2.18	0.62
1:A:141:PRO:C	1:A:142:ILE:HG13	2.20	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:SER:O	1:B:86:GLU:HG3	2.00	0.61
1:B:79:LEU:HD11	1:B:160:ALA:CB	2.29	0.60
1:B:261:PRO:O	1:B:265:GLU:HG3	2.01	0.60
1:A:94:MET:HE1	1:A:98:ALA:O	2.02	0.60
1:B:108:ARG:NH2	1:B:108:ARG:HG3	2.11	0.60
1:B:108:ARG:NH2	1:B:139:PRO:HG2	2.16	0.60
1:A:307:ALA:HB1	1:A:336:GLU:HG2	1.84	0.59
1:A:25:THR:OG1	1:A:28:GLU:HG3	2.02	0.59
1:B:39:ILE:O	1:B:43:THR:HG23	2.02	0.59
1:B:188:GLU:O	1:B:190:THR:HG23	2.03	0.59
1:A:200:PRO:HD2	1:A:244:ASN:HA	1.85	0.58
1:B:354:PRO:O	1:B:359:HIS:HE1	1.86	0.58
1:A:79:LEU:HD11	1:A:160:ALA:CB	2.33	0.58
1:A:24:LEU:HD11	1:A:130:MET:CE	2.31	0.58
1:B:55:LYS:HD3	1:B:55:LYS:C	2.24	0.57
1:A:105:LEU:HD11	1:A:138:MET:HE3	1.86	0.57
1:A:347:THR:OG1	1:A:348:ASP:N	2.36	0.57
1:B:160:ALA:O	1:B:164:SER:HB3	2.05	0.57
1:B:76:ILE:HG23	1:B:79:LEU:HD13	1.86	0.57
1:B:409:LEU:C	2:B:569:HOH:O	2.42	0.56
1:A:101:GLU:OE1	1:A:141:PRO:HG3	2.05	0.56
1:B:101:GLU:HG3	1:B:148:LYS:CE	2.30	0.56
1:A:129:GLU:HG2	1:A:189:LYS:HA	1.86	0.56
1:B:75:GLN:HG2	1:B:164:SER:HB2	1.88	0.56
1:A:241:ASP:O	1:A:245:VAL:HG22	2.05	0.55
1:A:245:VAL:CG1	1:A:259:SER:N	2.48	0.55
1:B:310:ASN:ND2	1:B:336:GLU:OE2	2.28	0.55
1:B:57:VAL:O	1:B:60:SER:O	2.25	0.55
1:A:108:ARG:HG3	1:A:139:PRO:HG3	1.89	0.55
1:A:307:ALA:CB	1:A:336:GLU:HG2	2.36	0.54
1:B:106:THR:CG2	1:B:108:ARG:CZ	2.85	0.54
1:B:28:GLU:CD	1:B:122:ARG:HH12	2.09	0.54
1:B:39:ILE:HD11	1:B:192:ILE:HD12	1.89	0.54
1:B:177:LYS:HE3	1:B:182:ARG:NH1	2.23	0.54
1:A:241:ASP:OD1	1:A:260:ASP:OD2	2.26	0.54
1:A:241:ASP:N	1:A:244:ASN:ND2	2.56	0.53
1:B:25:THR:HG23	1:B:28:GLU:OE1	2.08	0.53
1:B:106:THR:HG23	1:B:108:ARG:NE	2.24	0.53
1:B:199:ILE:HB	1:B:200:PRO:HD2	1.91	0.53
1:A:177:LYS:HE3	1:A:182:ARG:NH1	2.24	0.53
1:B:108:ARG:CG	1:B:108:ARG:HH21	2.14	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:PRO:O	1:A:142:ILE:HG13	2.09	0.52
1:B:55:LYS:HD3	1:B:55:LYS:O	2.09	0.52
1:B:105:LEU:HD21	1:B:138:MET:HE1	1.85	0.52
1:B:262:LYS:HG2	1:B:266:ASP:OD2	2.09	0.52
1:B:124:PHE:O	1:B:124:PHE:CD1	2.63	0.51
1:B:245:VAL:HG22	1:B:259:SER:H	1.72	0.51
1:B:108:ARG:NH2	1:B:108:ARG:CG	2.73	0.51
1:A:151:HIS:HB3	1:A:255:LYS:HE2	1.92	0.51
1:B:106:THR:CG2	1:B:108:ARG:NE	2.73	0.51
1:A:188:GLU:O	1:A:190:THR:HG23	2.10	0.51
1:A:271:SER:HA	1:A:274:ARG:NH1	2.26	0.51
1:A:143:PHE:HZ	1:A:256:TRP:CE2	2.29	0.50
1:A:245:VAL:CG1	1:A:259:SER:CA	2.90	0.50
1:A:245:VAL:CB	1:A:258:ASN:OD1	2.47	0.50
1:A:90:LEU:HD13	1:A:153:LEU:HB2	1.94	0.49
1:A:106:THR:HG21	1:A:108:ARG:NH2	2.27	0.49
1:A:248:ALA:HB2	1:A:256:TRP:CZ3	2.48	0.49
1:A:76:ILE:HD13	1:A:87:VAL:HG11	1.95	0.49
1:A:245:VAL:CG1	1:A:258:ASN:CG	2.81	0.49
1:A:200:PRO:CD	1:A:243:GLU:O	2.51	0.48
1:A:245:VAL:HG11	1:A:258:ASN:HD21	1.67	0.48
1:A:69:GLU:O	1:A:73:THR:HG23	2.13	0.48
1:A:12:THR:HG22	1:A:322:LEU:HD12	1.94	0.48
1:A:37:LYS:O	1:A:41:LEU:HG	2.13	0.48
1:A:129:GLU:OE1	1:A:191:HIS:NE2	2.46	0.48
1:B:110:TRP:CH2	1:B:262:LYS:HE2	2.47	0.48
1:A:129:GLU:OE2	1:A:186:GLU:HA	2.13	0.48
1:A:350:LYS:HZ3	1:A:350:LYS:HA	1.72	0.48
1:B:29:LYS:HE2	2:B:649:HOH:O	2.12	0.48
1:A:250:ARG:O	1:A:251:GLU:O	2.32	0.48
1:B:117:TYR:O	1:B:118:ASP:HB2	2.13	0.48
1:A:175:GLU:OE2	1:A:184:LYS:HE3	2.14	0.48
1:A:405:GLU:O	1:B:277:LYS:HE2	2.14	0.47
1:A:39:ILE:O	1:A:43:THR:HG23	2.14	0.47
1:A:260:ASP:OD1	1:A:262:LYS:HB3	2.15	0.47
1:B:196:MET:O	1:B:196:MET:HG3	2.15	0.47
1:B:118:ASP:O	1:B:284:ARG:NH1	2.47	0.47
1:A:118:ASP:HB2	1:A:280:ARG:NE	2.30	0.47
1:B:94:MET:HE1	1:B:102:PHE:HB2	1.95	0.47
1:A:249:LEU:CD1	1:A:257:ILE:HG13	2.42	0.46
1:A:55:LYS:C	1:A:55:LYS:HD3	2.36	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ASP:HB3	2:B:599:HOH:O	2.16	0.46
1:A:117:TYR:O	1:A:118:ASP:CB	2.53	0.46
1:A:245:VAL:CB	1:A:258:ASN:CG	2.82	0.46
1:B:289:TRP:O	1:B:293:GLN:HG2	2.16	0.46
1:A:22:LEU:HG	1:A:121:ASN:OD1	2.15	0.46
1:A:42:ARG:HH21	1:A:168:GLU:CD	2.18	0.46
1:A:76:ILE:HG23	1:A:79:LEU:HD13	1.97	0.46
1:B:43:THR:HA	1:B:161:SER:OG	2.15	0.46
1:A:120:LEU:HD21	1:A:130:MET:HE1	1.98	0.45
1:B:37:LYS:O	1:B:41:LEU:HG	2.16	0.45
1:B:42:ARG:HB3	1:B:165:LEU:HD11	1.97	0.45
1:A:178:GLN:HG3	1:A:250:ARG:O	2.15	0.45
1:B:11:TYR:CE2	1:B:323:GLY:HA2	2.52	0.45
1:A:245:VAL:HG13	1:A:260:ASP:H	1.79	0.45
1:B:36:ARG:HD3	1:B:40:ARG:NH2	2.31	0.45
1:B:260:ASP:HA	1:B:261:PRO:HD2	1.81	0.45
1:B:24:LEU:HD21	1:B:130:MET:CE	2.47	0.44
1:A:245:VAL:HG22	1:A:260:ASP:HB2	1.99	0.44
1:A:324:GLU:HG2	2:A:606:HOH:O	2.18	0.44
1:A:66:ILE:O	1:A:67:ILE:C	2.55	0.44
1:A:129:GLU:HG2	1:A:189:LYS:CA	2.48	0.44
1:A:105:LEU:HD12	1:A:139:PRO:HD2	2.00	0.44
1:B:327:LYS:HB2	1:B:327:LYS:HE3	1.85	0.44
1:B:245:VAL:HG22	1:B:259:SER:CA	2.47	0.44
1:A:324:GLU:OE1	1:A:327:LYS:NZ	2.44	0.44
1:A:79:LEU:N	1:A:79:LEU:HD12	2.32	0.44
1:B:123:PRO:HG3	1:B:130:MET:HG3	1.98	0.44
1:B:94:MET:CE	1:B:102:PHE:HB2	2.48	0.44
1:A:94:MET:CE	1:A:98:ALA:C	2.86	0.44
1:A:242:SER:C	1:A:245:VAL:HG23	2.38	0.43
1:A:408:VAL:HG12	1:A:409:LEU:N	2.33	0.43
1:A:44:ARG:O	2:A:502:HOH:O	2.21	0.43
1:B:79:LEU:N	1:B:79:LEU:HD12	2.33	0.43
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.18	0.43
1:B:197:TYR:HA	1:B:246:ASN:O	2.18	0.43
1:A:289:TRP:O	1:A:293:GLN:HG2	2.19	0.43
1:A:356:SER:HA	1:A:359:HIS:CD2	2.52	0.43
1:B:141:PRO:HG2	1:B:148:LYS:HG3	2.01	0.43
1:A:327:LYS:NZ	1:A:381:GLU:OE1	2.41	0.43
1:A:94:MET:HE2	1:A:98:ALA:C	2.39	0.42
1:B:106:THR:O	1:B:108:ARG:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:VAL:CG1	1:B:258:ASN:OD1	2.60	0.42
1:A:143:PHE:CZ	1:A:147:PRO:HG3	2.54	0.42
1:B:120:LEU:HD21	1:B:130:MET:CE	2.36	0.42
1:A:106:THR:CG2	1:A:108:ARG:NH2	2.82	0.42
1:A:256:TRP:O	1:A:257:ILE:HG12	2.20	0.42
1:A:105:LEU:HD11	1:A:138:MET:CE	2.49	0.42
1:A:242:SER:O	1:A:258:ASN:OD1	2.38	0.42
1:B:106:THR:CG2	1:B:108:ARG:NH1	2.83	0.42
1:B:322:LEU:HD23	1:B:322:LEU:HA	1.83	0.42
1:A:110:TRP:NE1	1:A:265:GLU:OE1	2.53	0.42
1:B:12:THR:HG22	1:B:322:LEU:HD12	2.02	0.42
1:A:94:MET:HE2	1:A:99:ARG:N	2.35	0.42
1:A:119:THR:HA	1:A:284:ARG:NH1	2.35	0.42
1:A:126:PRO:HA	1:A:127:GLY:HA2	1.70	0.41
1:A:245:VAL:O	1:A:258:ASN:C	2.57	0.41
1:A:59:LYS:O	1:A:59:LYS:HG2	2.19	0.41
1:B:152:SER:O	1:B:156:LEU:HD22	2.20	0.41
1:B:140:MET:O	1:B:200:PRO:O	2.37	0.41
1:A:267:TRP:CD1	1:A:344:PRO:HB3	2.55	0.41
1:B:342:GLU:HG2	2:B:647:HOH:O	2.20	0.41
1:A:76:ILE:HA	1:A:79:LEU:HD13	2.03	0.41
1:B:384:ASP:HB2	1:B:388:GLU:OE1	2.20	0.41
1:A:118:ASP:HB2	1:A:280:ARG:HE	1.84	0.41
1:A:175:GLU:OE1	1:A:177:LYS:HE2	2.20	0.41
1:A:57:VAL:C	1:A:60:SER:O	2.59	0.41
1:B:305:MET:HE1	2:B:508:HOH:O	2.21	0.41
1:A:278:HIS:O	1:A:282:VAL:HG22	2.21	0.41
1:B:188:GLU:O	1:B:190:THR:CG2	2.68	0.41
1:A:12:THR:CG2	1:A:322:LEU:HD12	2.51	0.41
1:B:184:LYS:HE2	2:B:559:HOH:O	2.20	0.41
1:A:254:ARG:HG2	2:A:613:HOH:O	2.19	0.41
1:A:287:LYS:HB3	2:A:579:HOH:O	2.19	0.40
1:B:58:LYS:HB2	1:B:99:ARG:HD2	2.02	0.40
1:A:57:VAL:HA	1:A:62:LEU:HG	2.04	0.40
1:A:18:LEU:HA	1:A:18:LEU:HD23	1.81	0.40

All (1) 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)
1:B:85:ARG:NH2	1:B:127:GLY:O[2_444]	1.90	0.30

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	354/447 (79%)	340 (96%)	12 (3%)	2 (1%)	30	29
1	B	356/447 (80%)	345 (97%)	11 (3%)	0	100	100
All	All	710/894 (79%)	685 (96%)	23 (3%)	2 (0%)	46	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ASP
1	A	67	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	320/391 (82%)	296 (92%)	24 (8%)	17	17
1	B	323/391 (83%)	297 (92%)	26 (8%)	15	15
All	All	643/782 (82%)	593 (92%)	50 (8%)	16	15

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	18	LEU
1	A	22	LEU
1	A	42	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	43	THR
1	A	75	GLN
1	A	108	ARG
1	A	132	ILE
1	A	139	PRO
1	A	143	PHE
1	A	145	SER
1	A	149	ILE
1	A	154	LEU
1	A	156	LEU
1	A	190	THR
1	A	196	MET
1	A	242	SER
1	A	244	ASN
1	A	257	ILE
1	A	333	LEU
1	A	349	GLU
1	A	350	LYS
1	A	378	SER
1	A	384	ASP
1	B	4	THR
1	B	18	LEU
1	B	22	LEU
1	B	42	ARG
1	B	43	THR
1	B	60	SER
1	B	75	GLN
1	B	107	PRO
1	B	122	ARG
1	B	129	GLU
1	B	140	MET
1	B	146	GLU
1	B	148	LYS
1	B	154	LEU
1	B	156	LEU
1	B	162	LEU
1	B	184	LYS
1	B	186	GLU
1	B	190	THR
1	B	196	MET
1	B	241	ASP
1	B	245	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	254	ARG
1	B	255	LYS
1	B	333	LEU
1	B	386	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	ASN
1	A	246	ASN
1	A	359	HIS
1	B	244	ASN
1	B	359	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](#)

There are no ligands in this entry.

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, 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	362/447 (80%)	0.46	32 (8%) 12 11	15, 31, 56, 68	0
1	B	364/447 (81%)	0.29	18 (4%) 33 33	14, 27, 47, 63	0
All	All	726/894 (81%)	0.38	50 (6%) 20 19	14, 29, 53, 68	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	ASN	9.1
1	A	245	VAL	8.2
1	A	244	ASN	7.1
1	B	3	MET	6.7
1	A	3	MET	6.0
1	A	106	THR	5.6
1	B	245	VAL	5.6
1	A	141	PRO	4.7
1	A	142	ILE	4.5
1	A	348	ASP	4.2
1	B	109	PHE	3.9
1	A	143	PHE	3.4
1	B	241	ASP	3.3
1	A	350	LYS	3.3
1	B	127	GLY	3.3
1	A	384	ASP	3.2
1	A	144	GLU	3.2
1	A	56	ALA	3.2
1	A	55	LYS	3.2
1	A	127	GLY	3.2
1	B	107	PRO	3.2
1	B	409	LEU	3.1
1	A	129	GLU	3.1
1	A	347	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	95	ASP	2.9
1	B	200	PRO	2.9
1	A	60	SER	2.8
1	B	243	GLU	2.8
1	A	44	ARG	2.8
1	B	348	ASP	2.8
1	A	109	PHE	2.7
1	A	167	ALA	2.7
1	A	349	GLU	2.7
1	A	110	TRP	2.7
1	A	254	ARG	2.5
1	A	100	ASP	2.5
1	B	97	ASP	2.4
1	A	388	GLU	2.3
1	A	104	GLY	2.3
1	B	240	LEU	2.3
1	A	243	GLU	2.2
1	A	126	PRO	2.2
1	B	254	ARG	2.2
1	A	145	SER	2.2
1	B	44	ARG	2.1
1	B	60	SER	2.1
1	B	4	THR	2.1
1	A	399	ASN	2.0
1	A	108	ARG	2.0
1	A	103	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.