



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:13 PM UTC

PDB ID : 4G6V / pdb_00004g6v
Title : CdiA-CT/CdiI toxin and immunity complex from Burkholderia pseudomallei
Authors : Morse, R.P.; Nikolakakis, K.; Willet, J.; Gerrick, E.; Low, D.A.; Hayes, C.S.;
Goulding, C.W.
Deposited on : 2012-07-19
Resolution : 2.64 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

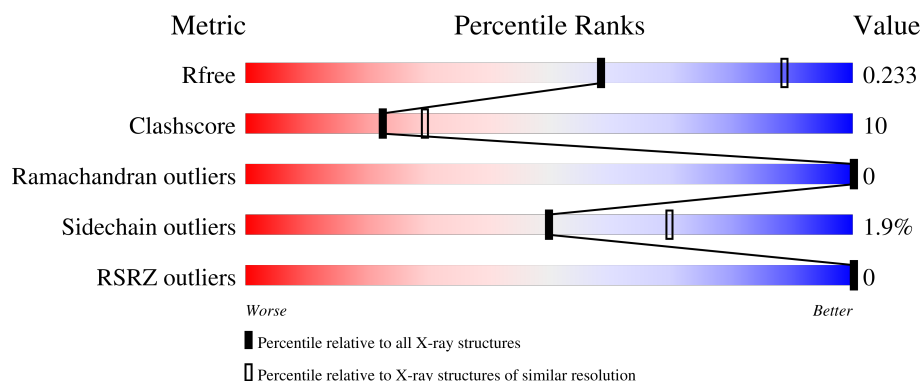
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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 $\leq 5\%$. 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	176	
1	C	176	
1	E	176	
1	G	176	
2	B	111	

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Mol	Chain	Length	Quality of chain
2	D	111	 77% 14% • 7%
2	F	111	 73% 16% • 9%
2	H	111	 71% 20% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6969 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 Adhesin/hemolysin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	0	0	0
			949	590	164	195			
1	C	132	Total	C	N	O	0	0	0
			949	590	164	195			
1	E	132	Total	C	N	O	0	0	0
			949	590	164	195			
1	G	132	Total	C	N	O	0	0	0
			949	590	164	195			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	MET	-	expression tag	UNP I2KQ03
C	122	MET	-	expression tag	UNP I2KQ03
E	122	MET	-	expression tag	UNP I2KQ03
G	122	MET	-	expression tag	UNP I2KQ03

- Molecule 2 is a protein called CdiI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	103	Total	C	N	O	S	0	0	0
			785	501	132	151	1			
2	D	103	Total	C	N	O	S	0	0	0
			785	501	132	151	1			
2	F	101	Total	C	N	O	S	0	0	0
			781	499	131	150	1			
2	H	101	Total	C	N	O	S	0	0	0
			781	499	131	150	1			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	102	THR	-	expression tag	UNP H9T8H3
B	103	SER	-	expression tag	UNP H9T8H3
B	104	LEU	-	expression tag	UNP H9T8H3
B	105	GLU	-	expression tag	UNP H9T8H3
B	106	HIS	-	expression tag	UNP H9T8H3
B	107	HIS	-	expression tag	UNP H9T8H3
B	108	HIS	-	expression tag	UNP H9T8H3
B	109	HIS	-	expression tag	UNP H9T8H3
B	110	HIS	-	expression tag	UNP H9T8H3
B	111	HIS	-	expression tag	UNP H9T8H3
D	102	THR	-	expression tag	UNP H9T8H3
D	103	SER	-	expression tag	UNP H9T8H3
D	104	LEU	-	expression tag	UNP H9T8H3
D	105	GLU	-	expression tag	UNP H9T8H3
D	106	HIS	-	expression tag	UNP H9T8H3
D	107	HIS	-	expression tag	UNP H9T8H3
D	108	HIS	-	expression tag	UNP H9T8H3
D	109	HIS	-	expression tag	UNP H9T8H3
D	110	HIS	-	expression tag	UNP H9T8H3
D	111	HIS	-	expression tag	UNP H9T8H3
F	102	THR	-	expression tag	UNP H9T8H3
F	103	SER	-	expression tag	UNP H9T8H3
F	104	LEU	-	expression tag	UNP H9T8H3
F	105	GLU	-	expression tag	UNP H9T8H3
F	106	HIS	-	expression tag	UNP H9T8H3
F	107	HIS	-	expression tag	UNP H9T8H3
F	108	HIS	-	expression tag	UNP H9T8H3
F	109	HIS	-	expression tag	UNP H9T8H3
F	110	HIS	-	expression tag	UNP H9T8H3
F	111	HIS	-	expression tag	UNP H9T8H3
H	102	THR	-	expression tag	UNP H9T8H3
H	103	SER	-	expression tag	UNP H9T8H3
H	104	LEU	-	expression tag	UNP H9T8H3
H	105	GLU	-	expression tag	UNP H9T8H3
H	106	HIS	-	expression tag	UNP H9T8H3
H	107	HIS	-	expression tag	UNP H9T8H3
H	108	HIS	-	expression tag	UNP H9T8H3
H	109	HIS	-	expression tag	UNP H9T8H3
H	110	HIS	-	expression tag	UNP H9T8H3
H	111	HIS	-	expression tag	UNP H9T8H3

- Molecule 3 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Br 2	0	0
3	C	2	Total 2	Br 2	0	0
3	E	1	Total 1	Br 1	0	0
3	F	1	Total 1	Br 1	0	0
3	G	1	Total 1	Br 1	0	0
3	H	1	Total 1	Br 1	0	0

- Molecule 4 is water.

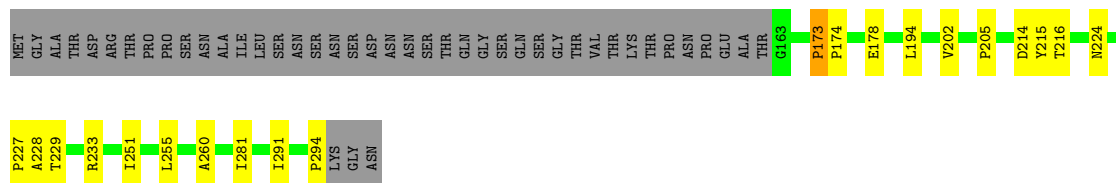
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total 6	O 6	0	0
4	B	4	Total 4	O 4	0	0
4	C	5	Total 5	O 5	0	0
4	D	3	Total 3	O 3	0	0
4	E	5	Total 5	O 5	0	0
4	F	3	Total 3	O 3	0	0
4	G	5	Total 5	O 5	0	0
4	H	2	Total 2	O 2	0	0

3 Residue-property plots

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.

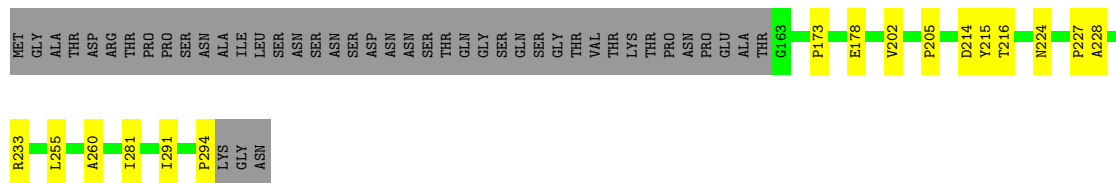
• Molecule 1: Adhesin/hemolysin

Chain A: 



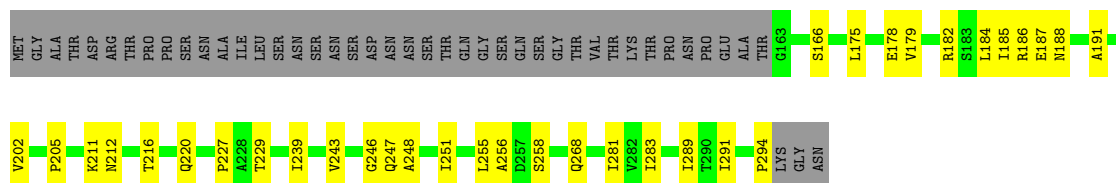
• Molecule 1: Adhesin/hemolysin

Chain C: 



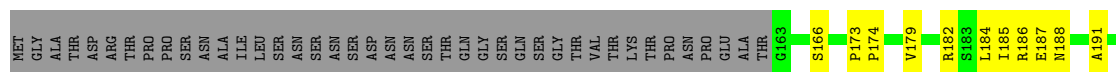
• Molecule 1: Adhesin/hemolysin

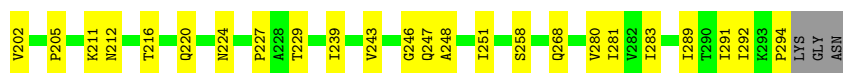
Chain E: 



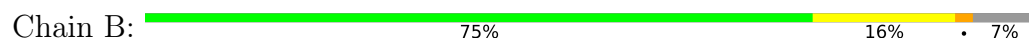
• Molecule 1: Adhesin/hemolysin

Chain G: 

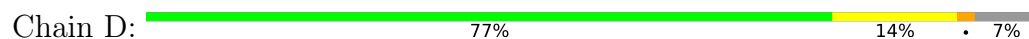




- Molecule 2: CdiI



- Molecule 2: CdiI



- Molecule 2: CdiI



- Molecule 2: CdiI



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	151.96Å 173.65Å 174.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.40 – 2.64 43.40 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.40-2.64) 95.4 (43.40-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.68 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.204 , 0.245 0.194 , 0.233	Depositor DCC
R_{free} test set	1721 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	1.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 10.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.406 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6969	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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

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	0.62	0/963	1.02	3/1322 (0.2%)
1	C	0.62	0/963	1.01	3/1322 (0.2%)
1	E	0.69	2/963 (0.2%)	0.98	1/1322 (0.1%)
1	G	0.68	2/963 (0.2%)	0.99	1/1322 (0.1%)
2	B	0.63	0/797	0.87	0/1077
2	D	0.59	0/797	0.87	0/1077
2	F	0.57	0/793	0.87	0/1070
2	H	0.57	0/793	0.88	0/1070
All	All	0.63	4/7032 (0.1%)	0.94	8/9582 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	268	GLN	CD-NE2	-6.91	1.18	1.33
1	G	268	GLN	CD-NE2	-6.15	1.20	1.33
1	G	268	GLN	CD-OE1	-6.04	1.12	1.23
1	E	268	GLN	CD-OE1	-5.68	1.12	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	294	PRO	N-CA-CB	6.56	110.22	103.00
1	E	294	PRO	N-CA-CB	6.53	110.18	103.00
1	C	294	PRO	N-CA-CB	5.75	109.32	103.00
1	A	173	PRO	CA-C-N	5.67	125.79	119.32
1	A	173	PRO	C-N-CA	5.67	125.79	119.32
1	A	294	PRO	N-CA-CB	5.58	109.14	103.00
1	C	173	PRO	CA-C-N	5.28	125.33	119.32
1	C	173	PRO	C-N-CA	5.28	125.33	119.32

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	949	0	936	32	0
1	C	949	0	936	28	0
1	E	949	0	936	22	0
1	G	949	0	936	22	0
2	B	785	0	769	18	0
2	D	785	0	769	15	0
2	F	781	0	775	20	0
2	H	781	0	775	22	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	6	0	0	1	0
4	B	4	0	0	0	0
4	C	5	0	0	0	0
4	D	3	0	0	0	0
4	E	5	0	0	0	0
4	F	3	0	0	0	0
4	G	5	0	0	0	0
4	H	2	0	0	0	0
All	All	6969	0	6832	144	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 10.

All (144) 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:233:ARG:HD2	1:C:233:ARG:HH11	1.04	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:PRO:HG3	1:A:216:THR:HG23	1.35	1.07
1:C:205:PRO:HG3	1:C:216:THR:HG23	1.33	1.05
1:A:233:ARG:HH11	1:C:233:ARG:HD2	1.21	1.02
1:G:205:PRO:HG3	1:G:216:THR:HG23	1.47	0.96
1:A:233:ARG:HD2	1:C:233:ARG:NH1	1.79	0.96
1:E:205:PRO:HG3	1:E:216:THR:HG23	1.47	0.96
1:A:233:ARG:NH1	1:C:233:ARG:HD2	1.89	0.87
1:A:233:ARG:HH11	1:C:233:ARG:CD	1.90	0.84
2:F:29:GLU:HG2	2:F:30:LEU:N	1.97	0.79
1:A:233:ARG:CD	1:C:233:ARG:HH11	1.91	0.76
2:H:29:GLU:HG2	2:H:30:LEU:N	2.02	0.75
2:H:71:SER:HB3	2:H:74:LEU:HD12	1.72	0.71
2:H:9:LEU:HD11	2:H:62:PHE:HE2	1.56	0.70
2:B:29:GLU:HG2	2:B:30:LEU:N	2.07	0.70
2:D:29:GLU:HG2	2:D:30:LEU:N	2.07	0.70
2:F:9:LEU:HD11	2:F:62:PHE:HE2	1.55	0.70
2:B:29:GLU:HG2	2:B:30:LEU:H	1.58	0.69
2:D:29:GLU:HG2	2:D:30:LEU:H	1.58	0.67
2:F:29:GLU:HG2	2:F:30:LEU:H	1.58	0.67
2:F:71:SER:HB3	2:F:74:LEU:HD12	1.76	0.67
2:H:29:GLU:HG2	2:H:30:LEU:H	1.60	0.66
1:A:205:PRO:CG	1:A:216:THR:HG23	2.19	0.66
1:G:281:ILE:HG12	1:G:291:ILE:HD12	1.79	0.64
1:A:202:VAL:HB	1:A:216:THR:OG1	1.98	0.64
1:C:202:VAL:HB	1:C:216:THR:OG1	1.98	0.64
1:E:281:ILE:HG12	1:E:291:ILE:HD12	1.80	0.63
1:C:205:PRO:CG	1:C:216:THR:HG23	2.19	0.63
1:A:205:PRO:HG3	1:A:216:THR:CG2	2.22	0.59
2:H:9:LEU:HD11	2:H:62:PHE:CE2	2.37	0.59
1:E:281:ILE:HG12	1:E:291:ILE:CD1	2.33	0.59
2:F:9:LEU:HD11	2:F:62:PHE:CE2	2.36	0.59
1:G:281:ILE:HG12	1:G:291:ILE:CD1	2.34	0.58
1:A:233:ARG:CB	1:C:233:ARG:HH12	2.17	0.58
2:B:71:SER:HB3	2:B:74:LEU:HD12	1.85	0.57
1:C:205:PRO:HG3	1:C:216:THR:CG2	2.22	0.57
2:H:12:ASP:OD1	2:H:12:ASP:C	2.48	0.57
2:B:33:GLY:O	2:B:67:ASN:HB3	2.05	0.57
2:D:71:SER:HB3	2:D:74:LEU:HD12	1.86	0.56
1:C:178:GLU:CB	2:F:13:ARG:HH12	2.18	0.56
2:D:33:GLY:O	2:D:67:ASN:HB3	2.05	0.56
2:H:12:ASP:OD1	2:H:12:ASP:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ARG:HH12	1:C:233:ARG:CB	2.19	0.56
1:A:178:GLU:CB	2:H:13:ARG:HH12	2.19	0.55
2:H:12:ASP:OD1	2:H:15:ALA:N	2.30	0.55
1:G:188:ASN:O	1:G:191:ALA:HB3	2.06	0.55
2:D:29:GLU:HG2	2:D:30:LEU:HG	1.88	0.55
1:A:233:ARG:NH1	1:C:233:ARG:CD	2.60	0.55
2:B:29:GLU:HG2	2:B:30:LEU:HG	1.89	0.54
1:G:246:GLY:O	1:G:247:GLN:HB2	2.07	0.54
1:G:202:VAL:HB	1:G:216:THR:OG1	2.06	0.54
1:E:179:VAL:HG21	2:F:99:TYR:CD1	2.42	0.54
2:F:12:ASP:OD1	2:F:12:ASP:C	2.51	0.54
2:F:12:ASP:OD1	2:F:12:ASP:O	2.25	0.54
1:E:202:VAL:HB	1:E:216:THR:OG1	2.08	0.53
1:E:246:GLY:O	1:E:247:GLN:HB2	2.07	0.53
1:G:179:VAL:HG21	2:H:99:TYR:CD1	2.43	0.53
1:E:188:ASN:O	1:E:191:ALA:HB3	2.09	0.53
1:A:233:ARG:CD	1:C:233:ARG:NH1	2.61	0.52
1:A:233:ARG:HB2	1:C:233:ARG:HH12	1.75	0.52
1:A:255:LEU:HD13	1:A:260:ALA:O	2.10	0.52
2:D:9:LEU:HD23	2:D:91:ILE:HG13	1.91	0.51
1:E:229:THR:HG22	2:F:98:GLU:OE1	2.09	0.51
1:G:184:LEU:O	1:G:187:GLU:HB3	2.09	0.51
1:C:178:GLU:HB2	2:F:13:ARG:HH12	1.75	0.51
1:A:281:ILE:HG12	1:A:291:ILE:CD1	2.41	0.51
1:A:214:ASP:OD2	2:B:2:ALA:N	2.44	0.50
2:B:8:TYR:OH	2:B:97:ASN:OD1	2.28	0.50
2:B:74:LEU:O	2:B:77:ILE:HG22	2.12	0.49
1:G:247:GLN:HA	1:G:247:GLN:OE1	2.12	0.49
1:C:227:PRO:HA	2:D:98:GLU:OE1	2.13	0.49
1:E:247:GLN:HA	1:E:247:GLN:OE1	2.13	0.48
1:A:227:PRO:HA	2:B:98:GLU:OE1	2.12	0.48
1:C:255:LEU:HD13	1:C:260:ALA:O	2.13	0.48
1:C:178:GLU:HB2	2:F:13:ARG:NH1	2.28	0.48
2:H:9:LEU:HA	2:H:90:ALA:O	2.13	0.48
1:A:233:ARG:HH12	1:C:233:ARG:HB3	1.78	0.48
1:E:182:ARG:O	1:E:185:ILE:HG22	2.14	0.48
1:G:229:THR:HG22	2:H:98:GLU:OE1	2.14	0.48
1:G:182:ARG:O	1:G:185:ILE:HG22	2.13	0.48
1:G:211:LYS:HG2	1:G:212:ASN:N	2.30	0.47
2:D:74:LEU:O	2:D:77:ILE:HG22	2.15	0.47
2:B:9:LEU:HD23	2:B:91:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLU:HB2	2:H:13:ARG:HH12	1.80	0.47
1:C:214:ASP:OD2	2:D:2:ALA:N	2.48	0.46
1:G:243:VAL:HG22	1:G:248:ALA:O	2.15	0.46
2:H:92:LEU:HA	2:H:102:THR:HG21	1.97	0.46
1:A:178:GLU:HB2	2:H:13:ARG:NH1	2.29	0.46
1:E:182:ARG:O	1:E:186:ARG:HG2	2.16	0.46
2:F:9:LEU:HA	2:F:90:ALA:O	2.16	0.46
1:G:216:THR:HA	1:G:220:GLN:O	2.15	0.45
1:E:205:PRO:CG	1:E:216:THR:HG23	2.32	0.45
1:E:216:THR:HA	1:E:220:GLN:O	2.16	0.45
1:E:184:LEU:O	1:E:187:GLU:HB3	2.16	0.45
1:A:173:PRO:HA	1:A:174:PRO:HD3	1.88	0.45
1:E:243:VAL:HG22	1:E:248:ALA:O	2.16	0.45
1:C:281:ILE:HG12	1:C:291:ILE:CD1	2.46	0.45
2:B:8:TYR:N	2:B:8:TYR:CD2	2.85	0.44
1:A:229:THR:HG22	2:B:98:GLU:OE1	2.17	0.44
1:A:178:GLU:HB3	2:H:13:ARG:HH12	1.81	0.44
1:E:283:ILE:HG12	1:E:289:ILE:CD1	2.47	0.44
2:F:29:GLU:CG	2:F:30:LEU:N	2.76	0.44
1:A:215:TYR:OH	1:A:224:ASN:HB2	2.18	0.44
2:D:8:TYR:OH	2:D:97:ASN:OD1	2.29	0.44
1:E:175:LEU:HD23	1:E:175:LEU:HA	1.74	0.43
2:D:8:TYR:CD2	2:D:8:TYR:N	2.87	0.43
1:E:178:GLU:H	1:E:178:GLU:HG2	1.70	0.43
1:E:211:LYS:HG2	1:E:212:ASN:N	2.33	0.43
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.84	0.42
1:G:182:ARG:O	1:G:186:ARG:HG2	2.19	0.42
1:E:246:GLY:O	1:E:247:GLN:CB	2.67	0.42
1:A:174:PRO:HD2	4:A:404:HOH:O	2.17	0.42
1:G:283:ILE:HG12	1:G:289:ILE:CD1	2.49	0.42
1:C:178:GLU:HB3	2:F:13:ARG:HH12	1.83	0.42
2:H:29:GLU:CG	2:H:30:LEU:N	2.79	0.42
2:F:69:LYS:HA	2:F:69:LYS:HD3	1.87	0.42
1:G:173:PRO:HA	1:G:174:PRO:HD3	1.80	0.42
1:E:227:PRO:O	1:E:258:SER:HB2	2.19	0.42
2:B:49:GLU:OE1	1:C:233:ARG:NH2	2.52	0.42
1:C:228:ALA:H	2:D:98:GLU:CD	2.28	0.42
2:D:23:ILE:HD11	2:D:85:GLY:HA3	2.02	0.42
1:C:215:TYR:OH	1:C:224:ASN:HB2	2.20	0.42
1:G:227:PRO:O	1:G:258:SER:HB2	2.20	0.41
1:G:246:GLY:O	1:G:247:GLN:CB	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:35:PHE:CE2	2:H:78:VAL:HG21	2.55	0.41
1:G:224:ASN:O	2:H:2:ALA:N	2.53	0.41
2:H:27:HIS:HA	2:H:29:GLU:OE1	2.19	0.41
1:A:233:ARG:CB	1:C:233:ARG:NH1	2.82	0.41
1:G:205:PRO:CG	1:G:216:THR:HG23	2.33	0.41
2:B:61:PHE:CD2	2:B:61:PHE:C	2.98	0.41
1:G:280:VAL:HB	1:G:292:ILE:HB	2.01	0.41
2:F:35:PHE:CE2	2:F:78:VAL:HG21	2.55	0.41
1:A:228:ALA:H	2:B:98:GLU:CD	2.27	0.41
1:A:281:ILE:HG12	1:A:291:ILE:HD13	2.03	0.41
2:D:92:LEU:HD11	2:D:94:LEU:HD21	2.03	0.41
1:E:255:LEU:O	1:E:256:ALA:C	2.64	0.41
2:B:92:LEU:HD11	2:B:94:LEU:HD21	2.02	0.41
2:F:75:ILE:N	2:F:76:PRO:CD	2.83	0.40
2:H:75:ILE:N	2:H:76:PRO:CD	2.84	0.40
2:B:23:ILE:HD11	2:B:85:GLY:HA3	2.04	0.40
2:B:104:LEU:N	2:H:37:ILE:O	2.44	0.40
2:D:61:PHE:CD2	2:D:61:PHE:C	2.99	0.40
2:F:47:LEU:O	2:F:48:LYS:C	2.65	0.40
2:F:6:PHE:CE2	2:F:63:LEU:HD11	2.57	0.40

There are no symmetry-related clashes.

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	130/176 (74%)	128 (98%)	2 (2%)	0	100	100
1	C	130/176 (74%)	128 (98%)	2 (2%)	0	100	100
1	E	130/176 (74%)	126 (97%)	4 (3%)	0	100	100
1	G	130/176 (74%)	126 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	101/111 (91%)	97 (96%)	4 (4%)	0	100	100
2	D	101/111 (91%)	96 (95%)	5 (5%)	0	100	100
2	F	99/111 (89%)	95 (96%)	4 (4%)	0	100	100
2	H	99/111 (89%)	94 (95%)	5 (5%)	0	100	100
All	All	920/1148 (80%)	890 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	105/148 (71%)	104 (99%)	1 (1%)	68	80
1	C	105/148 (71%)	105 (100%)	0	100	100
1	E	105/148 (71%)	102 (97%)	3 (3%)	37	57
1	G	105/148 (71%)	102 (97%)	3 (3%)	37	57
2	B	83/96 (86%)	81 (98%)	2 (2%)	43	64
2	D	83/96 (86%)	81 (98%)	2 (2%)	43	64
2	F	84/96 (88%)	82 (98%)	2 (2%)	43	64
2	H	84/96 (88%)	83 (99%)	1 (1%)	63	78
All	All	754/976 (77%)	740 (98%)	14 (2%)	50	70

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	ILE
2	B	23	ILE
2	B	77	ILE
2	D	23	ILE
2	D	77	ILE
1	E	166	SER

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Mol	Chain	Res	Type
1	E	239	ILE
1	E	251	ILE
2	F	12	ASP
2	F	63	LEU
1	G	166	SER
1	G	239	ILE
1	G	251	ILE
2	H	63	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	GLN
2	B	27	HIS
1	C	203	GLN
2	D	27	HIS
1	E	224	ASN
1	G	224	ASN
1	G	268	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	132/176 (75%)	-1.42	0 100 100	27, 38, 56, 65	0
1	C	132/176 (75%)	-1.46	0 100 100	27, 39, 56, 65	0
1	E	132/176 (75%)	-1.49	0 100 100	26, 37, 54, 70	0
1	G	132/176 (75%)	-1.50	0 100 100	25, 37, 54, 71	0
2	B	103/111 (92%)	-1.47	0 100 100	24, 35, 58, 73	0
2	D	103/111 (92%)	-1.45	0 100 100	23, 35, 58, 70	0
2	F	101/111 (90%)	-1.44	0 100 100	26, 40, 57, 78	0
2	H	101/111 (90%)	-1.45	0 100 100	27, 40, 58, 79	0
All	All	936/1148 (81%)	-1.46	0 100 100	23, 38, 58, 79	0

There are no RSRZ outliers to report.

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BR	C	301	1/1	0.96	0.07	102,102,102,102	1
3	BR	F	201	1/1	0.97	0.06	61,61,61,61	1
3	BR	H	201	1/1	0.98	0.05	69,69,69,69	1
3	BR	E	301	1/1	0.99	0.02	39,39,39,39	1
3	BR	A	302	1/1	0.99	0.06	97,97,97,97	1
3	BR	C	302	1/1	0.99	0.03	39,39,39,39	1
3	BR	G	301	1/1	1.00	0.02	34,34,34,34	1
3	BR	A	301	1/1	1.00	0.01	31,31,31,31	1

6.5 Other polymers [i](#)

There are no such residues in this entry.