



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 18, 2016 – 01:43 PM EDT

PDB ID : 5J5V
Title : CdiA-CT from uropathogenic Escherichia coli in complex with cognate immunity protein and CysK
Authors : Goulding, C.W.; Johnson, P.M.; Morse, R.P.
Deposited on : 2016-04-04
Resolution : 2.75 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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-20027790

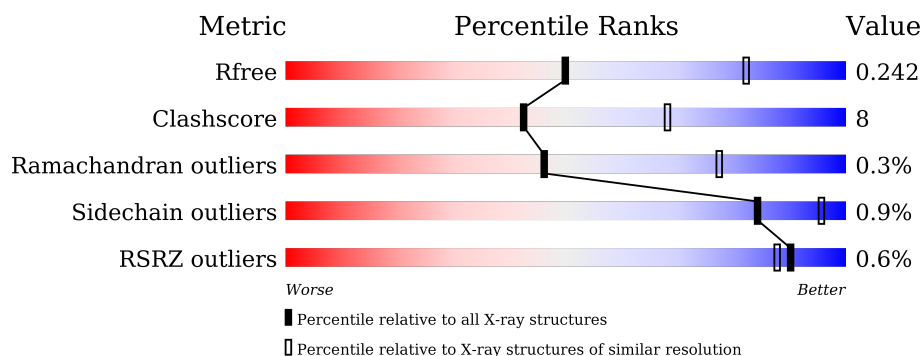
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	323	<div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	D	323	<div> <div>86%</div> <div>11%</div> <div>.</div> </div>
2	B	228	<div> <div>29%</div> <div>13%</div> <div>58%</div> </div>
2	E	228	<div> <div>36%</div> <div>6%</div> <div>58%</div> </div>
3	C	138	<div> <div>4%</div> <div>59%</div> <div>29%</div> <div>11%</div> </div>
3	F	138	<div> <div>%</div> <div>65%</div> <div>23%</div> <div>9%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8296 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 Cysteine synthase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	P	S	0	0	0
			2346	1480	404	455	1	6			
1	D	313	Total	C	N	O	P	S	0	0	0
			2346	1480	404	455	1	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	SER	engineered mutation	UNP P0ABK6
D	2	GLY	SER	engineered mutation	UNP P0ABK6

- Molecule 2 is a protein called tRNA nuclease CdiA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	96	Total	C	N	O	Se	0	0	0
			750	461	138	148	3			
2	E	96	Total	C	N	O	Se	0	0	0
			750	461	138	148	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MSE	-	initiating methionine	UNP Q0T963
E	0	MSE	-	initiating methionine	UNP Q0T963

- Molecule 3 is a protein called Immunity protein CdiI.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	123	Total	C	N	O	S	Se	0	0	0
			987	625	164	194	2	2			
3	F	126	Total	C	N	O	S	Se	0	0	0
			1016	645	169	198	2	2			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MSE	-	initiating methionine	UNP Q0T964
C	129	THR	-	expression tag	UNP Q0T964
C	130	SER	-	expression tag	UNP Q0T964
C	131	LEU	-	expression tag	UNP Q0T964
C	132	GLU	-	expression tag	UNP Q0T964
C	133	HIS	-	expression tag	UNP Q0T964
C	134	HIS	-	expression tag	UNP Q0T964
C	135	HIS	-	expression tag	UNP Q0T964
C	136	HIS	-	expression tag	UNP Q0T964
C	137	HIS	-	expression tag	UNP Q0T964
C	138	HIS	-	expression tag	UNP Q0T964
F	1	MSE	-	initiating methionine	UNP Q0T964
F	129	THR	-	expression tag	UNP Q0T964
F	130	SER	-	expression tag	UNP Q0T964
F	131	LEU	-	expression tag	UNP Q0T964
F	132	GLU	-	expression tag	UNP Q0T964
F	133	HIS	-	expression tag	UNP Q0T964
F	134	HIS	-	expression tag	UNP Q0T964
F	135	HIS	-	expression tag	UNP Q0T964
F	136	HIS	-	expression tag	UNP Q0T964
F	137	HIS	-	expression tag	UNP Q0T964
F	138	HIS	-	expression tag	UNP Q0T964

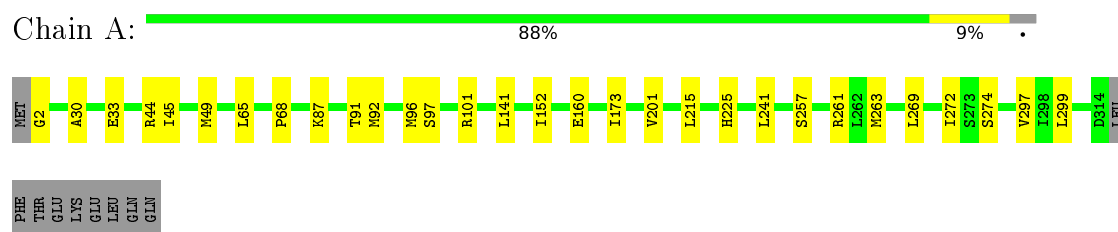
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	37	Total O 37 37	0	0
4	B	6	Total O 6 6	0	0
4	C	7	Total O 7 7	0	0
4	D	31	Total O 31 31	0	0
4	E	8	Total O 8 8	0	0
4	F	12	Total O 12 12	0	0

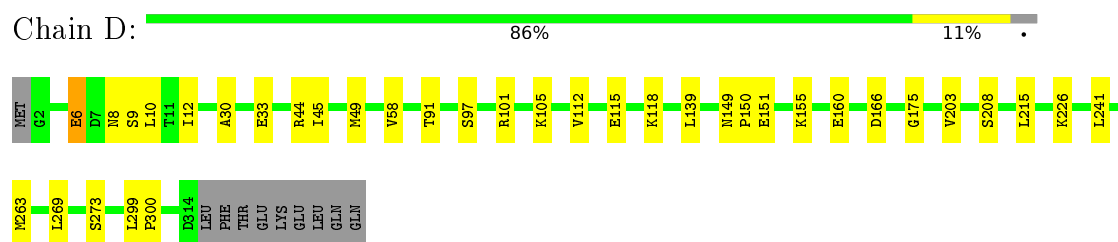
3 Residue-property plots [i](#)

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.

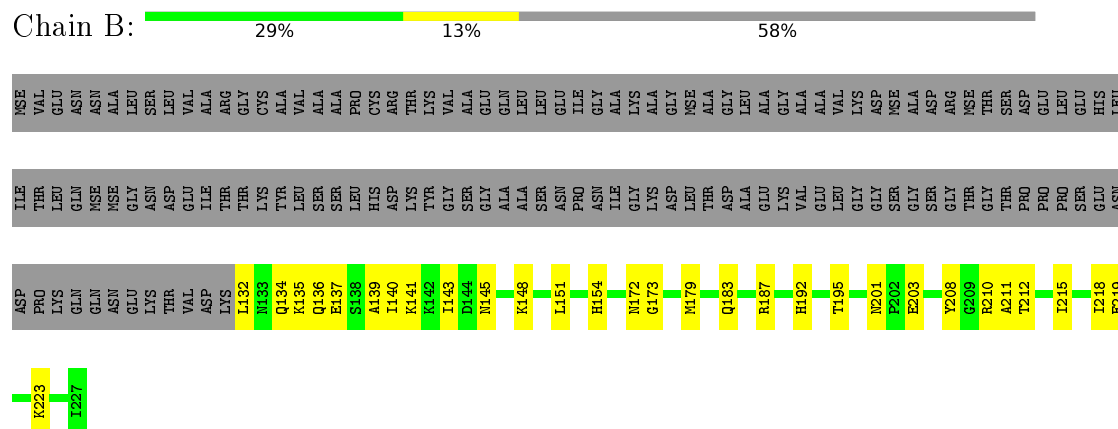
• Molecule 1: Cysteine synthase A



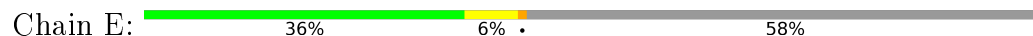
• Molecule 1: Cysteine synthase A



• Molecule 2: tRNA nuclease CdiA



• Molecule 2: tRNA nuclease CdiA



MSE	VAL	THR	LEU	ASN	ASN	ALA	LEU	SER	LEU	VAL	ALA	ARG	GLY	CYS	ALA	VAL	ALA	ALA	PRO	CYS	ARG	THR	LYS	LYS	VAL	ALA	GLU	GLN	LEU	LEU	ASN	ILE	GLY	ALA	ASP	LEU	THR	ASP	GLY	ALA	LEU	GLY	ALA	VAL	VAL	LYS	ASP	MSE	ALA	ARG	MSE	THR	SER	ASP	PRO	GLU	LEU	GLU	HIS	LEU	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASP	PRO	LYS	GLN	GLN	ASN	GLU	LYS	THR	VAL	ASP	LYS	L132	K135	Q136	E137	I140	I147	K148	L151	P169	M179	R187	T195	A214	I218	E219	K223	I227
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

● Molecule 3: Immunity protein CdiI



MSE	I2	T3	R5	M10	I11	M12	K15	Q19	E24	I31	D32	N33	P34	L35	E36	K37	L38	O44	C52	I53	D54	P57	P58	T65	A80	S83	L90	K91	D92	O93	K94	F97	T98	O99	I100	R101	Q102	L103	I104	N105	Q106	L107	E108	P109	S110
-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------

D111	I112	M113	D114	L115	D116	R117	K118	D119	I120	L121	K122	I123	N124	GLN	ILE	ILE	VAL	THR	SER	LEU	GLU	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 3: Immunity protein CdiI



MSE	I2	R5	M13	T14	K15	Q19	I31	L35	E36	K37	L38	R59	E62	K66	Y73	A80	S83	K86	G87	E88	T96	I100	R101	I104	N105	Q106	L107	E108	P109	S110	D111	M113	D114	D115	L116	R117	K118	D119	I120	L121	K122	I123	N124
-----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

Q125	I126	I127	VAL	THR	SER	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	81.25Å 195.54Å 175.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.83 – 2.75 48.82 – 2.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.83-2.75) 76.8 (48.82-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.08Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.196 , 0.248 0.194 , 0.242	Depositor DCC
R_{free} test set	847 reflections (2.47%)	DCC
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 20.4	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	8296	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: IT1

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	0/2354	0.59	0/3185
1	D	0.50	1/2354 (0.0%)	0.60	0/3185
2	B	0.46	0/757	0.60	0/1011
2	E	0.48	0/757	0.68	0/1011
3	C	0.45	1/996 (0.1%)	0.62	0/1345
3	F	0.50	0/1025	0.77	4/1383 (0.3%)
All	All	0.48	2/8243 (0.0%)	0.63	4/11120 (0.0%)

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
2	B	0	1
2	E	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	208	SER	C-N	5.51	1.44	1.34
3	C	44	CYS	CB-SG	-5.43	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	111	ASP	N-CA-C	9.40	136.39	111.00
3	F	112	ILE	N-CA-C	-7.53	90.67	111.00
3	F	111	ASP	CB-CA-C	-7.07	96.27	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	107	LEU	CA-CB-CG	5.43	127.80	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	148	LYS	Peptide
2	E	148	LYS	Peptide

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	2346	0	2412	20	0
1	D	2346	0	2412	28	0
2	B	750	0	746	25	2
2	E	750	0	746	17	0
3	C	987	0	1013	34	0
3	F	1016	0	1054	28	0
4	A	37	0	0	0	0
4	B	6	0	0	0	0
4	C	7	0	0	2	0
4	D	31	0	0	2	0
4	E	8	0	0	0	0
4	F	12	0	0	0	0
All	All	8296	0	8383	137	2

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 8.

All (137) 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)
2:E:187:ARG:HH12	3:F:116:LEU:HD11	1.27	1.00
2:B:145:ASN:HD21	2:B:210:ARG:HH11	1.26	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:GLU:OE2	1:D:155:LYS:NZ	2.13	0.81
2:B:187:ARG:HH12	3:C:116:LEU:HD11	1.46	0.80
3:F:101:ARG:NH2	3:F:123:ILE:O	2.15	0.78
1:A:92:MET:SD	1:A:96:MET:SD	2.82	0.77
2:E:187:ARG:NH1	3:F:116:LEU:HD11	1.99	0.77
1:D:226:LYS:HE3	2:E:179:MSE:HE1	1.65	0.77
2:E:169:PRO:HG2	3:F:13:MSE:SE	2.35	0.76
3:C:105:ASN:HD21	3:C:121:LEU:HD21	1.51	0.74
2:B:141:LYS:HZ3	2:B:203:GLU:HG2	1.53	0.74
1:D:226:LYS:CE	2:E:179:MSE:HE1	2.19	0.73
3:F:59:ARG:NH1	3:F:62:GLU:OE1	2.22	0.72
2:E:140:ILE:HG13	2:E:195:THR:HG21	1.72	0.71
3:C:110:SER:HB2	3:C:114:ASP:OD1	1.92	0.69
3:F:108:GLU:HB3	3:F:109:PRO:HD3	1.74	0.69
3:C:52:CYS:SG	4:C:206:HOH:O	2.51	0.69
3:F:13:MSE:HE2	3:F:15:LYS:HE2	1.74	0.68
2:E:135:LYS:O	2:E:136:GLN:OE1	2.13	0.67
3:F:66:LYS:C	3:F:66:LYS:HD3	2.16	0.66
3:C:91:LYS:HG3	3:C:92:ASP:OD1	1.97	0.65
3:C:101:ARG:HD2	3:C:121:LEU:HD23	1.79	0.65
2:B:145:ASN:OD1	2:B:210:ARG:NH1	2.29	0.65
1:D:6:GLU:HG2	1:D:10:LEU:CD1	2.26	0.65
2:E:151:LEU:HD21	2:E:218:ILE:HD11	1.79	0.63
2:B:219:GLU:O	2:B:223:LYS:HG3	2.00	0.61
2:E:136:GLN:O	2:E:140:ILE:HG12	2.01	0.60
2:B:141:LYS:NZ	2:B:203:GLU:HG2	2.16	0.60
2:B:151:LEU:HD21	2:B:218:ILE:HD11	1.84	0.60
2:B:187:ARG:NH1	3:C:116:LEU:HD11	2.16	0.59
2:E:135:LYS:NZ	2:E:136:GLN:HG2	2.17	0.59
1:A:30:ALA:HB1	1:A:299:LEU:HD22	1.84	0.59
1:D:115:GLU:OE1	1:D:118:LYS:NZ	2.36	0.59
1:D:6:GLU:HG2	1:D:10:LEU:HD12	1.85	0.58
2:B:145:ASN:ND2	2:B:210:ARG:HH11	1.97	0.58
1:D:44:ARG:NH2	1:D:160:GLU:OE2	2.36	0.58
3:F:80:ALA:HA	3:F:116:LEU:HD13	1.87	0.56
2:B:172:ASN:ND2	2:B:173:GLY:O	2.38	0.56
1:A:45:ILE:HB	1:A:49:MET:HE3	1.88	0.56
2:E:147:ILE:HG12	3:F:73:TYR:HD1	1.71	0.55
1:A:45:ILE:O	1:A:49:MET:HB2	2.07	0.55
2:B:187:ARG:HH22	3:C:116:LEU:HD11	1.70	0.54
3:F:104:ILE:O	3:F:107:LEU:HD13	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:ILE:HD12	2:B:195:THR:HG21	1.89	0.54
3:C:5:ARG:HB2	3:C:31:ILE:HG12	1.89	0.54
1:D:30:ALA:HB1	1:D:299:LEU:HD22	1.89	0.54
1:A:173:ILE:HB	1:A:297:VAL:HG22	1.88	0.53
1:A:65:LEU:HD22	1:A:141:LEU:HD21	1.91	0.52
3:F:118:LYS:HD2	3:F:122:LYS:HE3	1.90	0.52
3:C:106:GLN:C	3:C:107:LEU:HD12	2.30	0.52
1:A:2:GLY:N	1:D:166:ASP:OD1	2.43	0.52
3:F:111:ASP:OD1	3:F:111:ASP:C	2.48	0.52
3:F:5:ARG:HB2	3:F:31:ILE:HG12	1.90	0.52
1:A:274:SER:HB3	1:A:299:LEU:HG	1.92	0.51
2:B:141:LYS:HZ1	2:B:210:ARG:HH22	1.59	0.51
3:C:80:ALA:O	3:C:83:SER:HB3	2.12	0.50
3:C:120:ILE:O	3:C:123:ILE:HG12	2.11	0.50
1:D:263:MET:HG2	1:D:269:LEU:HA	1.92	0.50
3:F:36:GLU:H	3:F:36:GLU:CD	2.14	0.50
1:D:45:ILE:O	1:D:49:MET:HB2	2.12	0.49
3:F:35:LEU:HA	3:F:38:LEU:HD12	1.93	0.49
1:D:45:ILE:HB	1:D:49:MET:HE3	1.95	0.49
1:D:226:LYS:NZ	4:D:402:HOH:O	2.34	0.48
3:F:96:THR:O	3:F:100:ILE:HG13	2.12	0.48
2:B:139:ALA:O	2:B:143:ILE:HG13	2.14	0.48
3:F:111:ASP:HB3	3:F:113:ASN:H	1.79	0.48
3:F:80:ALA:O	3:F:83:SER:OG	2.20	0.47
2:B:140:ILE:HG23	2:B:192:HIS:HB3	1.95	0.47
1:D:175:GLY:HA2	1:D:203:VAL:HB	1.96	0.47
3:C:111:ASP:OD1	3:C:112:ILE:N	2.47	0.47
1:D:226:LYS:HE3	2:E:179:MSE:CE	2.40	0.47
1:A:257:SER:O	1:A:261:ARG:HG3	2.14	0.47
3:F:106:GLN:O	3:F:107:LEU:HD12	2.14	0.47
3:C:10:ASN:OD1	3:C:12:ASN:HB2	2.15	0.47
3:C:116:LEU:O	3:C:120:ILE:HG13	2.15	0.47
3:C:35:LEU:HA	3:C:38:LEU:HD12	1.95	0.47
3:C:97:PHE:HE1	3:C:101:ARG:HD3	1.80	0.47
2:E:219:GLU:O	2:E:223:LYS:HG3	2.14	0.47
2:B:135:LYS:HG3	2:B:136:GLN:H	1.80	0.47
1:D:58:VAL:HG11	1:D:139:LEU:HD13	1.98	0.46
1:A:87:LYS:HD3	1:A:87:LYS:HA	1.71	0.46
1:A:263:MET:HG2	1:A:269:LEU:HA	1.97	0.46
3:C:53:ILE:HG13	3:C:54:ASP:N	2.30	0.46
3:C:105:ASN:OD1	3:C:121:LEU:HD11	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:HIS:HA	2:B:179:MSE:HE1	1.97	0.46
3:C:36:GLU:OE1	3:C:36:GLU:N	2.44	0.45
2:E:135:LYS:HD2	2:E:135:LYS:C	2.37	0.45
2:E:148:LYS:HE2	2:E:214:ALA:HB2	1.98	0.45
3:F:106:GLN:C	3:F:107:LEU:HD12	2.36	0.45
1:D:273:SER:OG	1:D:300:PRO:HG2	2.16	0.45
3:C:5:ARG:HD2	3:C:32:ASP:OD1	2.17	0.45
3:C:80:ALA:HA	3:C:116:LEU:HD13	1.98	0.45
2:B:187:ARG:HH22	3:C:116:LEU:CD1	2.29	0.45
3:F:119:ASP:HA	3:F:122:LYS:HD2	1.98	0.45
2:B:179:MSE:O	2:B:183:GLN:HG3	2.17	0.45
1:D:91:THR:HG22	1:D:112:VAL:HB	1.98	0.45
3:F:15:LYS:HD2	3:F:19:GLN:O	2.16	0.44
2:E:137:GLU:H	2:E:137:GLU:HG3	1.48	0.44
3:F:111:ASP:OD1	3:F:112:ILE:N	2.50	0.44
3:C:3:THR:HG22	3:C:34:PRO:HG3	2.00	0.44
1:D:33:GLU:OE1	1:D:44:ARG:NH1	2.46	0.44
1:A:45:ILE:HB	1:A:49:MET:CE	2.48	0.44
1:D:9:SER:O	1:D:12:ILE:HG23	2.18	0.44
3:C:32:ASP:O	3:C:34:PRO:HD3	2.18	0.44
3:F:86:LYS:HZ2	3:F:88:GLU:HB3	1.83	0.44
2:B:187:ARG:NH2	3:C:116:LEU:HD11	2.33	0.44
3:C:15:LYS:HD2	3:C:19:GLN:O	2.18	0.43
3:C:65:THR:HA	3:C:103:LEU:HD11	2.00	0.43
2:E:147:ILE:HG12	3:F:73:TYR:CD1	2.53	0.43
3:F:86:LYS:HG3	3:F:88:GLU:H	1.83	0.43
1:A:33:GLU:OE2	1:A:44:ARG:NH1	2.41	0.43
3:F:116:LEU:O	3:F:120:ILE:HG13	2.18	0.43
1:A:97:SER:O	1:A:101:ARG:HG3	2.19	0.43
1:D:8:ASN:HB2	4:D:414:HOH:O	2.19	0.43
1:A:173:ILE:HG12	1:A:201:VAL:HB	2.01	0.42
2:B:211:ALA:O	2:B:215:ILE:HG13	2.19	0.42
2:B:208:TYR:O	2:B:212:THR:HG23	2.19	0.42
3:C:104:ILE:O	3:C:107:LEU:HD13	2.20	0.42
3:C:15:LYS:HE3	3:C:24:GLU:OE2	2.20	0.42
1:A:68:PRO:HA	1:A:91:THR:O	2.20	0.41
1:D:149:ASN:HB3	1:D:150:PRO:CD	2.50	0.41
1:D:149:ASN:HB3	1:D:150:PRO:HD3	2.02	0.41
1:A:152:ILE:HA	1:A:152:ILE:HD12	1.93	0.41
3:C:94:LYS:HE3	4:C:201:HOH:O	2.21	0.41
3:C:118:LYS:HD3	3:C:118:LYS:HA	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:VAL:CG1	1:D:139:LEU:HD13	2.50	0.41
2:B:137:GLU:H	2:B:137:GLU:HG3	1.60	0.41
1:A:44:ARG:HH22	1:A:160:GLU:CD	2.24	0.41
1:A:215:LEU:HD21	1:A:241:LEU:HD22	2.03	0.41
1:D:215:LEU:HD21	1:D:241:LEU:HD22	2.02	0.41
3:C:106:GLN:O	3:C:107:LEU:HD12	2.21	0.41
1:D:44:ARG:HH22	1:D:160:GLU:CD	2.24	0.41
1:D:97:SER:O	1:D:101:ARG:HG3	2.21	0.40
2:B:134:GLN:HG3	2:B:201:ASN:HD22	1.86	0.40
2:B:134:GLN:HG3	2:B:201:ASN:ND2	2.37	0.40
3:C:57:MSE:HB2	3:C:58:PRO:HD3	2.03	0.40
1:D:105:LYS:HD2	1:D:105:LYS:HA	1.83	0.40

All (2) 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)
2:B:154:HIS:CE1	2:B:154:HIS:CE1[3_654]	1.07	1.13
2:B:154:HIS:ND1	2:B:154:HIS:CE1[3_654]	1.63	0.57

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	310/323 (96%)	300 (97%)	10 (3%)	0	100	100
1	D	310/323 (96%)	300 (97%)	10 (3%)	0	100	100
2	B	94/228 (41%)	89 (95%)	5 (5%)	0	100	100
2	E	94/228 (41%)	89 (95%)	5 (5%)	0	100	100
3	C	121/138 (88%)	107 (88%)	12 (10%)	2 (2%)	11	32
3	F	124/138 (90%)	113 (91%)	10 (8%)	1 (1%)	24	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1053/1378 (76%)	998 (95%)	52 (5%)	3 (0%)	46 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	111	ASP
3	F	108	GLU
3	C	108	GLU

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	246/257 (96%)	245 (100%)	1 (0%)	93 98
1	D	246/257 (96%)	245 (100%)	1 (0%)	93 98
2	B	79/172 (46%)	78 (99%)	1 (1%)	76 93
2	E	79/172 (46%)	78 (99%)	1 (1%)	76 93
3	C	113/127 (89%)	112 (99%)	1 (1%)	84 95
3	F	117/127 (92%)	114 (97%)	3 (3%)	54 84
All	All	880/1112 (79%)	872 (99%)	8 (1%)	84 95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	ILE
2	B	132	LEU
3	C	83	SER
1	D	6	GLU
2	E	136	GLN
3	F	114	ASP
3	F	115	ASP
3	F	125	GLN

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

Mol	Chain	Res	Type
3	C	99	GLN
2	E	136	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	IT1	A	42	1	22,24,25	2.51	6 (27%)	28,32,34	1.63	6 (21%)
1	IT1	D	42	1	22,24,25	2.64	7 (31%)	28,32,34	1.42	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IT1	A	42	1	-	0/15/17/19	0/1/1/1
1	IT1	D	42	1	-	0/15/17/19	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	42	IT1	P-OP3	-2.75	1.45	1.54
1	A	42	IT1	P-OP3	-2.51	1.46	1.54
1	A	42	IT1	P-OP2	-2.27	1.46	1.54
1	D	42	IT1	C2-N1	-2.06	1.29	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	IT1	C3-C2	2.04	1.42	1.40
1	D	42	IT1	P-OP4	2.31	1.66	1.59
1	D	42	IT1	C3-C2	2.71	1.42	1.40
1	A	42	IT1	O3-C3	3.35	1.44	1.37
1	D	42	IT1	O3-C3	3.59	1.45	1.37
1	A	42	IT1	C4-C4A	6.37	1.57	1.46
1	D	42	IT1	C4-C4A	6.55	1.57	1.46
1	A	42	IT1	C4A-NZ	7.25	1.48	1.27
1	D	42	IT1	C4A-NZ	7.68	1.50	1.27

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	42	IT1	CE-NZ-C4A	-4.31	106.30	119.14
1	A	42	IT1	CE-NZ-C4A	-3.99	107.23	119.14
1	A	42	IT1	CD-CE-NZ	-3.60	105.00	110.94
1	A	42	IT1	C5-C4-C4A	-2.78	117.09	121.41
1	D	42	IT1	O-C-CA	-2.68	118.53	125.72
1	A	42	IT1	O-C-CA	-2.68	118.55	125.72
1	D	42	IT1	C5-C4-C4A	-2.41	117.67	121.41
1	D	42	IT1	OP2-P-OP4	2.09	112.83	106.72
1	D	42	IT1	C3-C4-C5	2.13	119.81	118.26
1	A	42	IT1	OP3-P-OP4	2.19	113.11	106.72
1	A	42	IT1	C3-C4-C4A	2.54	123.42	120.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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(Å²)	Q<0.9	
1	A	312/323 (96%)	-0.67	0	100	100	19, 29, 47, 64	0
1	D	312/323 (96%)	-0.71	0	100	100	16, 26, 42, 56	0
2	B	93/228 (40%)	-0.57	0	100	100	23, 37, 61, 72	0
2	E	93/228 (40%)	-0.57	0	100	100	21, 33, 55, 62	0
3	C	121/138 (87%)	-0.12	5 (4%)	41	34	21, 48, 76, 91	0
3	F	124/138 (89%)	-0.48	1 (0%)	87	83	20, 36, 59, 70	0
All	All	1055/1378 (76%)	-0.58	6 (0%)	90	88	16, 30, 61, 91	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	102	GLN	3.7
3	C	100	ILE	2.5
3	C	124	ASN	2.5
3	C	98	THR	2.4
3	F	107	LEU	2.2
3	C	90	LEU	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
1	IT1	D	42	24/25	0.94	0.16	-	22,26,31,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	IT1	A	42	24/25	0.95	0.15	-	22,30,34,35	0

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.