



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:05 PM UTC

PDB ID : 5J5V / pdb_00005j5v
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

<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
Mogul : 2022.3.0, CSD as543be (2022)
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

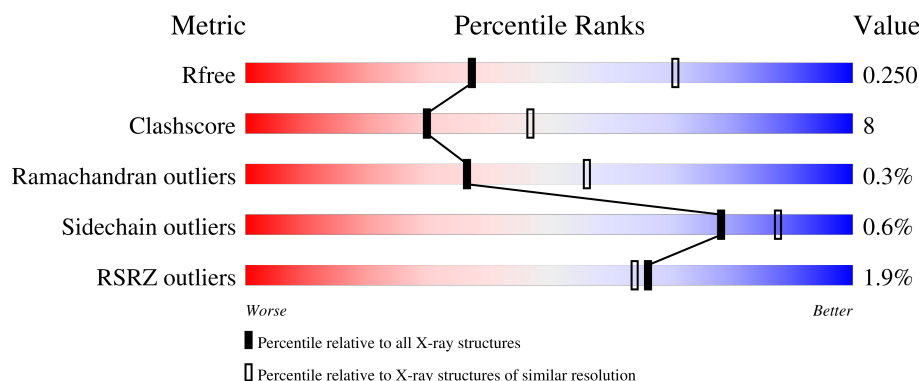
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	323	 86% 11%
1	D	323	 85% 11%
2	B	228	 2% 29% 12% 58%
2	E	228	 36% 5% 58%
3	C	138	 5% 59% 29% 11%

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Mol	Chain	Length	Quality of chain
3	F	138	4% 67% 22% 9% ••

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

- Molecule 1: Cysteine synthase A



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 48.83 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.83-2.75) 93.5 (48.83-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.06 (at 2.08Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.196 , 0.248 0.200 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 18.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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 4.03% 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: LLP

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	0.45	0/2354	0.54	0/3185
1	D	0.48	0/2354	0.55	0/3185
2	B	0.53	0/757	0.65	2/1011 (0.2%)
2	E	0.49	0/757	0.75	2/1011 (0.2%)
3	C	0.40	0/996	0.62	0/1345
3	F	0.48	0/1025	0.80	3/1383 (0.2%)
All	All	0.47	0/8243	0.62	7/11120 (0.1%)

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	111	ASP	N-CA-C	12.02	136.39	110.80
3	F	112	ILE	N-CA-C	-8.97	90.67	109.34
2	E	136	GLN	N-CA-C	-8.67	101.46	114.64
3	F	111	ASP	CB-CA-C	-7.11	96.27	110.42
2	B	136	GLN	N-CA-C	-7.03	103.95	114.64
2	E	135	LYS	N-CA-C	5.56	122.64	110.80
2	B	135	LYS	N-CA-C	5.34	122.18	110.80

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	2413	23	0
1	D	2346	0	2413	27	0
2	B	750	0	746	26	2
2	E	750	0	746	18	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	8385	141	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 (141) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:66:LYS:HD3	3:F:66:LYS:C	2.16	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: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:C:106:GLN:C	3:C:107:LEU:HD12	2.30	0.57
3:F:80:ALA:HA	3:F:116:LEU:HD13	1.87	0.56
3:F:111:ASP:OD1	3:F:111:ASP:C	2.48	0.56
2:B:172:ASN:ND2	2:B:173:GLY:O	2.38	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:36:GLU:H	3:F:36:GLU:CD	2.14	0.54
3:F:104:ILE:O	3:F:107:LEU:HD13	2.07	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:2:GLY:N	1:D:166:ASP:OD1	2.43	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:F:106:GLN:C	3:F:107:LEU:HD12	2.36	0.50
2:E:135:LYS:C	2:E:135:LYS:HD2	2.37	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:86:LYS:HZ2	3:F:88:GLU:HB3	1.77	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: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: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
3:C:116:LEU:O	3:C:120:ILE:HG13	2.15	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:HA	1:A:87:LYS:HD3	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
1:A:44:ARG:HH22	1:A:160:GLU:CD	2.24	0.46
3:C:105:ASN:OD1	3:C:121:LEU:HD11	2.16	0.46
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
1:D:44:ARG:HH22	1:D:160:GLU:CD	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:148:LYS:HE2	2:E:214:ALA:HB2	1.98	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
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
1:A:45:ILE:HB	1:A:49:MET:HE3	1.99	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
2:E:135:LYS:HZ1	2:E:136:GLN:HG2	1.83	0.43
3:F:116:LEU:O	3:F:120:ILE:HG13	2.18	0.43
1:A:92:MET:HE1	1:A:111:LEU:HD22	2.01	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:HD12	1:A:152:ILE:HA	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:97:SER:O	1:D:101:ARG:HG3	2.21	0.40
1:A:45:ILE:HD12	1:A:49:MET:HE1	2.04	0.40
1:A:69:THR:HA	1:A:120:MET:HE1	2.02	0.40
2:B:136:GLN:C	2:B:136:GLN:CD	2.89	0.40
2:B:134:GLN:HG3	2:B:201:ASN:ND2	2.37	0.40
2:B:134:GLN:HG3	2:B:201:ASN:HD22	1.86	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%)	7	14
3	F	124/138 (90%)	113 (91%)	10 (8%)	1 (1%)	16	30
All	All	1053/1378 (76%)	998 (95%)	52 (5%)	3 (0%)	36	56

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 [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	246/257 (96%)	245 (100%)	1 (0%)	84	91
1	D	246/257 (96%)	245 (100%)	1 (0%)	84	91
2	B	79/172 (46%)	79 (100%)	0	100	100
2	E	79/172 (46%)	78 (99%)	1 (1%)	61	76
3	C	113/127 (89%)	113 (100%)	0	100	100
3	F	117/127 (92%)	115 (98%)	2 (2%)	53	71
All	All	880/1112 (79%)	875 (99%)	5 (1%)	78	88

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

Mol	Chain	Res	Type
1	A	272	ILE
1	D	228	GLN
2	E	136	GLN
3	F	112	ILE
3	F	114	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	292	ASN
1	A	294	ASN
2	B	198	ASN

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Mol	Chain	Res	Type
2	B	205	GLN
3	C	99	GLN
3	C	105	ASN
1	D	285	GLN
2	E	136	GLN
2	E	184	ASN

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	LLP	D	42	1	23,24,25	2.30	5 (21%)	25,32,34	1.62	4 (16%)
1	LLP	A	42	1	23,24,25	2.18	6 (26%)	25,32,34	1.59	6 (24%)

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	LLP	D	42	1	-	5/16/17/19	0/1/1/1
1	LLP	A	42	1	-	3/16/17/19	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	42	LLP	C4'-NZ	6.84	1.50	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	LLP	C4'-NZ	6.47	1.48	1.27
1	D	42	LLP	C4-C4'	5.19	1.57	1.46
1	A	42	LLP	C4-C4'	5.05	1.57	1.46
1	D	42	LLP	O3-C3	3.73	1.45	1.36
1	A	42	LLP	O3-C3	3.49	1.44	1.36
1	D	42	LLP	P-OP3	-2.57	1.45	1.54
1	A	42	LLP	P-OP3	-2.35	1.46	1.54
1	D	42	LLP	C2-N1	-2.29	1.29	1.33
1	A	42	LLP	P-OP2	-2.13	1.46	1.54
1	A	42	LLP	C2-N1	-2.06	1.30	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	42	LLP	OP4-C5'-C5	4.43	117.65	109.36
1	D	42	LLP	CE-NZ-C4'	-3.88	106.30	118.72
1	A	42	LLP	CE-NZ-C4'	-3.59	107.23	118.72
1	A	42	LLP	C5-C4-C4'	-2.84	117.09	121.47
1	A	42	LLP	OP3-P-OP4	2.47	113.11	106.67
1	D	42	LLP	C5-C4-C4'	-2.47	117.67	121.47
1	D	42	LLP	OP2-P-OP4	2.36	112.83	106.67
1	A	42	LLP	CD-CE-NZ	-2.20	105.00	110.83
1	A	42	LLP	C4-C3-C2	-2.07	118.97	120.14
1	A	42	LLP	OP4-C5'-C5	2.01	113.11	109.36

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	42	LLP	CD-CE-NZ-C4'
1	D	42	LLP	C3-C4-C4'-NZ
1	A	42	LLP	C4-C4'-NZ-CE
1	A	42	LLP	CG-CD-CE-NZ
1	D	42	LLP	CA-CB-CG-CD
1	A	42	LLP	CA-CB-CG-CD
1	D	42	LLP	CG-CD-CE-NZ
1	D	42	LLP	C5-C4-C4'-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	312/323 (96%)	-0.47	1 (0%)	90 91	19, 29, 47, 64	0
1	D	312/323 (96%)	-0.56	1 (0%)	90 91	16, 26, 42, 56	0
2	B	93/228 (40%)	-0.07	4 (4%)	40 38	23, 37, 61, 72	0
2	E	93/228 (40%)	-0.20	1 (1%)	78 77	21, 33, 55, 62	0
3	C	121/138 (87%)	0.24	7 (5%)	29 29	21, 48, 76, 91	0
3	F	124/138 (89%)	-0.12	6 (4%)	35 35	20, 36, 59, 70	0
All	All	1055/1378 (76%)	-0.31	20 (1%)	66 64	16, 30, 61, 91	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	314	ASP	5.3
2	B	132	LEU	4.3
1	D	314	ASP	4.2
3	C	124	ASN	4.1
3	C	109	PRO	3.9
2	E	132	LEU	3.6
3	F	109	PRO	3.3
3	C	111	ASP	2.7
3	F	127	ILE	2.7
2	B	172	ASN	2.6
3	C	113	ASN	2.6
3	F	111	ASP	2.5
3	C	112	ILE	2.5
3	C	115	ASP	2.4
3	F	110	SER	2.4
3	F	126	ILE	2.3
2	B	139	ALA	2.2
3	C	34	PRO	2.2
3	F	107	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	134	GLN	2.0

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. 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
1	LLP	D	42	24/25	0.94	0.09	22,26,31,34	0
1	LLP	A	42	24/25	0.96	0.09	22,30,34,35	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.