



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:55 AM GMT

PDB ID : 3Q8V
Title : Crystal structure of Staphylococcus aureus nucleoside diphosphate kinase complexed with UDP
Authors : Srivastava, S.K.; Rajasree, K.; Gopal, B.
Deposited on : 2011-01-07
Resolution : 2.50 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

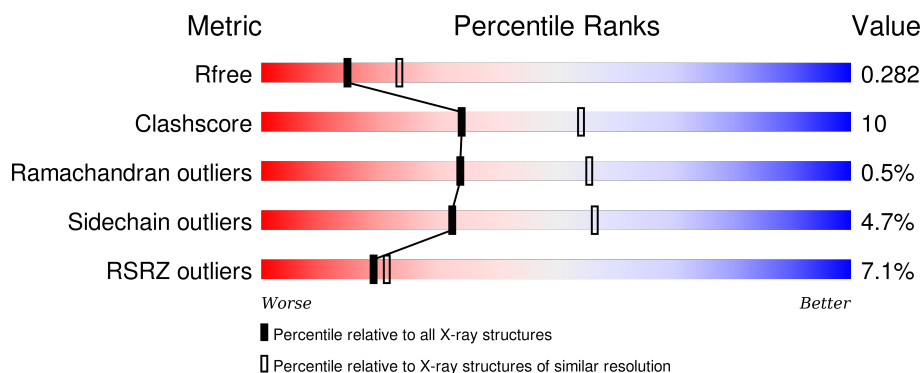
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	157	<div> <div>3%</div> <div>76% 15% • 5%</div> </div>
1	B	157	<div> <div>%</div> <div>72% 20% • 5%</div> </div>
1	C	157	<div> <div>3%</div> <div>73% 18% • • 5%</div> </div>
1	D	157	<div> <div>3%</div> <div>77% 16% • 5%</div> </div>
1	E	157	<div> <div>6%</div> <div>73% 17% • 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	157	<div><div></div><div>3%</div><div>81%</div><div>12%</div><div>• 5%</div></div>
1	G	157	<div><div></div><div>14%</div><div>80%</div><div>13%</div><div>• 5%</div></div>
1	H	157	<div><div></div><div>22%</div><div>76%</div><div>17%</div><div>• 5%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9448 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1151	724	201	221	5			
1	B	149	Total	C	N	O	S	0	0	0
			1154	728	202	219	5			
1	C	149	Total	C	N	O	S	0	0	0
			1153	727	201	220	5			
1	D	149	Total	C	N	O	S	0	0	0
			1161	731	202	223	5			
1	E	149	Total	C	N	O	S	0	0	0
			1142	718	202	217	5			
1	F	149	Total	C	N	O	S	0	0	0
			1149	725	201	218	5			
1	G	149	Total	C	N	O	S	0	0	0
			1116	700	199	212	5			
1	H	149	Total	C	N	O	S	0	0	0
			1133	710	200	218	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	LEU	-	EXPRESSION TAG	UNP Q5HJV4
A	151	GLU	-	EXPRESSION TAG	UNP Q5HJV4
A	152	HIS	-	EXPRESSION TAG	UNP Q5HJV4
A	153	HIS	-	EXPRESSION TAG	UNP Q5HJV4
A	154	HIS	-	EXPRESSION TAG	UNP Q5HJV4
A	155	HIS	-	EXPRESSION TAG	UNP Q5HJV4
A	156	HIS	-	EXPRESSION TAG	UNP Q5HJV4
A	157	HIS	-	EXPRESSION TAG	UNP Q5HJV4
B	150	LEU	-	EXPRESSION TAG	UNP Q5HJV4
B	151	GLU	-	EXPRESSION TAG	UNP Q5HJV4
B	152	HIS	-	EXPRESSION TAG	UNP Q5HJV4
B	153	HIS	-	EXPRESSION TAG	UNP Q5HJV4
B	154	HIS	-	EXPRESSION TAG	UNP Q5HJV4

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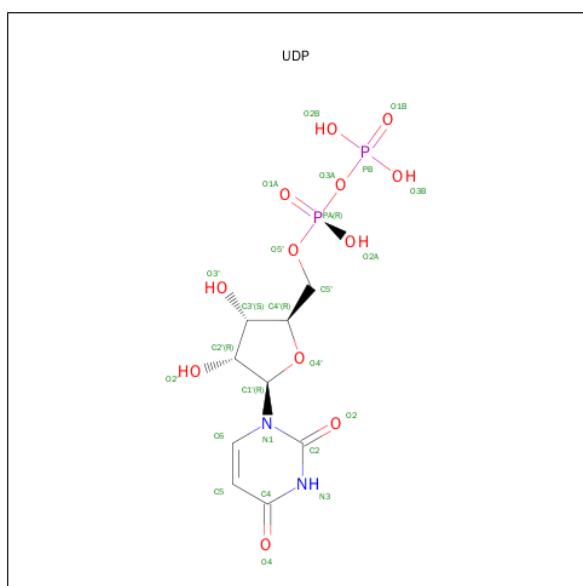
Chain	Residue	Modelled	Actual	Comment	Reference
B	155	HIS	-	EXPRESSION TAG	UNP Q5HJV4
B	156	HIS	-	EXPRESSION TAG	UNP Q5HJV4
B	157	HIS	-	EXPRESSION TAG	UNP Q5HJV4
C	150	LEU	-	EXPRESSION TAG	UNP Q5HJV4
C	151	GLU	-	EXPRESSION TAG	UNP Q5HJV4
C	152	HIS	-	EXPRESSION TAG	UNP Q5HJV4
C	153	HIS	-	EXPRESSION TAG	UNP Q5HJV4
C	154	HIS	-	EXPRESSION TAG	UNP Q5HJV4
C	155	HIS	-	EXPRESSION TAG	UNP Q5HJV4
C	156	HIS	-	EXPRESSION TAG	UNP Q5HJV4
C	157	HIS	-	EXPRESSION TAG	UNP Q5HJV4
D	150	LEU	-	EXPRESSION TAG	UNP Q5HJV4
D	151	GLU	-	EXPRESSION TAG	UNP Q5HJV4
D	152	HIS	-	EXPRESSION TAG	UNP Q5HJV4
D	153	HIS	-	EXPRESSION TAG	UNP Q5HJV4
D	154	HIS	-	EXPRESSION TAG	UNP Q5HJV4
D	155	HIS	-	EXPRESSION TAG	UNP Q5HJV4
D	156	HIS	-	EXPRESSION TAG	UNP Q5HJV4
D	157	HIS	-	EXPRESSION TAG	UNP Q5HJV4
E	150	LEU	-	EXPRESSION TAG	UNP Q5HJV4
E	151	GLU	-	EXPRESSION TAG	UNP Q5HJV4
E	152	HIS	-	EXPRESSION TAG	UNP Q5HJV4
E	153	HIS	-	EXPRESSION TAG	UNP Q5HJV4
E	154	HIS	-	EXPRESSION TAG	UNP Q5HJV4
E	155	HIS	-	EXPRESSION TAG	UNP Q5HJV4
E	156	HIS	-	EXPRESSION TAG	UNP Q5HJV4
E	157	HIS	-	EXPRESSION TAG	UNP Q5HJV4
F	150	LEU	-	EXPRESSION TAG	UNP Q5HJV4
F	151	GLU	-	EXPRESSION TAG	UNP Q5HJV4
F	152	HIS	-	EXPRESSION TAG	UNP Q5HJV4
F	153	HIS	-	EXPRESSION TAG	UNP Q5HJV4
F	154	HIS	-	EXPRESSION TAG	UNP Q5HJV4
F	155	HIS	-	EXPRESSION TAG	UNP Q5HJV4
F	156	HIS	-	EXPRESSION TAG	UNP Q5HJV4
F	157	HIS	-	EXPRESSION TAG	UNP Q5HJV4
G	150	LEU	-	EXPRESSION TAG	UNP Q5HJV4
G	151	GLU	-	EXPRESSION TAG	UNP Q5HJV4
G	152	HIS	-	EXPRESSION TAG	UNP Q5HJV4
G	153	HIS	-	EXPRESSION TAG	UNP Q5HJV4
G	154	HIS	-	EXPRESSION TAG	UNP Q5HJV4
G	155	HIS	-	EXPRESSION TAG	UNP Q5HJV4
G	156	HIS	-	EXPRESSION TAG	UNP Q5HJV4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	157	HIS	-	EXPRESSION TAG	UNP Q5HFV4
H	150	LEU	-	EXPRESSION TAG	UNP Q5HFV4
H	151	GLU	-	EXPRESSION TAG	UNP Q5HFV4
H	152	HIS	-	EXPRESSION TAG	UNP Q5HFV4
H	153	HIS	-	EXPRESSION TAG	UNP Q5HFV4
H	154	HIS	-	EXPRESSION TAG	UNP Q5HFV4
H	155	HIS	-	EXPRESSION TAG	UNP Q5HFV4
H	156	HIS	-	EXPRESSION TAG	UNP Q5HFV4
H	157	HIS	-	EXPRESSION TAG	UNP Q5HFV4

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0

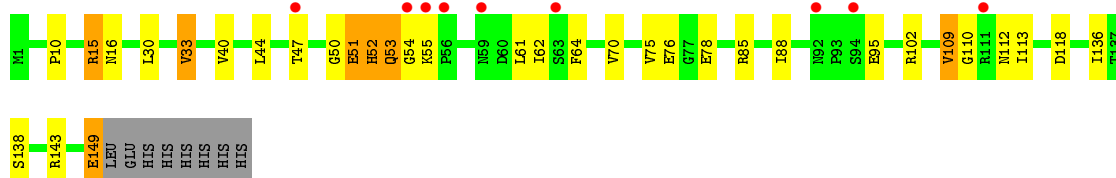
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total 30	O 30	0	0
4	B	42	Total 42	O 42	0	0
4	C	44	Total 44	O 44	0	0
4	D	28	Total 28	O 28	0	0
4	E	31	Total 31	O 31	0	0
4	F	16	Total 16	O 16	0	0
4	G	7	Total 7	O 7	0	0
4	H	13	Total 13	O 13	0	0


HIS
HIS

- Molecule 1: Nucleoside diphosphate kinase

Chain E: 




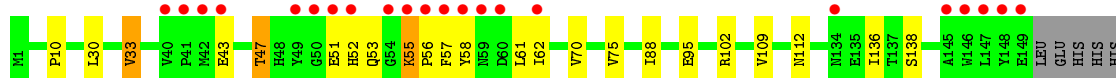
- Molecule 1: Nucleoside diphosphate kinase

Chain F: 




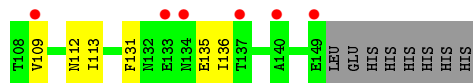
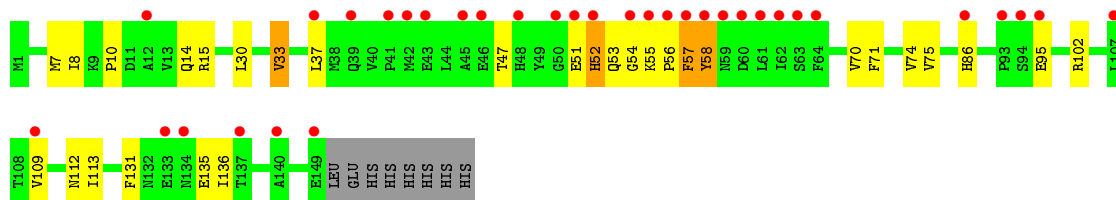
- Molecule 1: Nucleoside diphosphate kinase

Chain G: 

HIS
HIS
HIS

- Molecule 1: Nucleoside diphosphate kinase

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.66Å 72.92Å 102.14Å 90.00° 108.42° 90.00°	Depositor
Resolution (Å)	32.30 – 2.50 32.30 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (32.30-2.50) 99.5 (32.30-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	104.23 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.230 , 0.283 0.233 , 0.282	Depositor DCC
R_{free} test set	2268 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 45077 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9448	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.85	1/1174 (0.1%)	0.85	4/1589 (0.3%)
1	B	0.84	0/1177	0.86	4/1593 (0.3%)
1	C	0.83	1/1176 (0.1%)	0.77	3/1592 (0.2%)
1	D	0.76	0/1184	0.80	3/1602 (0.2%)
1	E	0.77	0/1164	0.77	1/1576 (0.1%)
1	F	0.75	1/1172 (0.1%)	0.73	1/1586 (0.1%)
1	G	0.69	1/1138 (0.1%)	0.72	0/1538
1	H	0.68	1/1154 (0.1%)	0.71	0/1560
All	All	0.77	5/9339 (0.1%)	0.78	16/12636 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	121	GLU	CG-CD	7.39	1.63	1.51
1	G	55	LYS	C-N	7.38	1.48	1.34
1	A	55	LYS	C-N	7.07	1.47	1.34
1	H	52	HIS	C-O	5.47	1.33	1.23
1	F	138	SER	C-N	-5.04	1.22	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ARG	NE-CZ-NH2	7.21	123.90	120.30
1	F	15	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	A	102	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	B	15	ARG	NE-CZ-NH1	-6.03	117.28	120.30
1	E	15	ARG	NE-CZ-NH1	-5.99	117.30	120.30
1	D	15	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	A	15	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	D	143	ARG	NE-CZ-NH2	-5.60	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	15	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	D	7	MET	CG-SD-CE	5.38	108.80	100.20
1	B	7	MET	CG-SD-CE	5.30	108.68	100.20
1	C	102	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	C	15	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	B	24	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	C	102	ARG	NE-CZ-NH2	5.04	122.82	120.30

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	1151	0	1128	20	0
1	B	1154	0	1139	26	0
1	C	1153	0	1135	32	0
1	D	1161	0	1145	24	0
1	E	1142	0	1125	27	0
1	F	1149	0	1127	18	0
1	G	1116	0	1075	13	0
1	H	1133	0	1106	34	0
2	A	25	0	11	3	0
2	B	25	0	11	1	0
2	D	25	0	11	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	30	0	0	1	0
4	B	42	0	0	5	0
4	C	44	0	0	17	0
4	D	28	0	0	8	0
4	E	31	0	0	9	0
4	F	16	0	0	6	0
4	G	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	13	0	0	20	0
All	All	9448	0	9013	184	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 (184) 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:H:33:VAL:HG12	4:H:166:HOH:O	1.14	1.26
1:C:26:GLU:HA	4:C:173:HOH:O	1.08	1.21
1:F:82:ASN:HB3	4:F:170:HOH:O	1.42	1.18
1:H:86:HIS:CE1	4:H:185:HOH:O	1.99	1.16
1:D:125:ARG:HG3	1:H:95:GLU:OE1	1.45	1.14
1:H:37:LEU:HA	4:H:169:HOH:O	0.93	1.10
1:C:61:LEU:CB	4:C:188:HOH:O	1.96	1.10
1:E:95:GLU:HG2	4:E:187:HOH:O	1.52	1.08
1:C:61:LEU:C	4:C:188:HOH:O	1.93	1.06
1:H:70:VAL:O	4:H:169:HOH:O	1.79	0.98
1:C:61:LEU:CG	4:C:188:HOH:O	2.12	0.95
1:C:61:LEU:HG	4:C:188:HOH:O	1.71	0.91
1:H:7:MET:HG3	4:H:164:HOH:O	1.69	0.91
1:F:82:ASN:CB	4:F:170:HOH:O	2.03	0.88
1:C:111:ARG:NE	4:C:203:HOH:O	1.95	0.88
1:H:86:HIS:HE1	4:H:185:HOH:O	1.44	0.86
2:A:158:UDP:O2A	4:A:182:HOH:O	1.92	0.86
1:H:70:VAL:HB	4:H:164:HOH:O	1.75	0.85
1:E:109:VAL:O	4:E:195:HOH:O	1.95	0.84
1:H:74:VAL:HB	4:H:166:HOH:O	1.77	0.83
1:C:111:ARG:NH1	4:C:203:HOH:O	2.11	0.83
1:D:121:GLU:HG2	4:D:210:HOH:O	1.77	0.82
1:D:102:ARG:HD2	1:D:112:ASN:HB2	1.60	0.82
1:A:60:ASP:HB3	4:B:185:HOH:O	1.79	0.81
1:C:102:ARG:HD2	1:C:112:ASN:HB2	1.65	0.79
1:H:131:PHE:CD2	4:H:167:HOH:O	2.36	0.77
1:D:125:ARG:CG	1:H:95:GLU:OE1	2.30	0.77
1:H:74:VAL:CB	4:H:166:HOH:O	2.33	0.76
1:G:102:ARG:HD2	1:G:112:ASN:HB2	1.67	0.76
1:D:86:HIS:ND1	4:D:180:HOH:O	2.21	0.74
1:C:61:LEU:HB3	4:C:188:HOH:O	1.75	0.73
1:D:46:GLU:OE2	4:D:211:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ARG:HD2	1:A:112:ASN:HB2	1.71	0.72
1:A:43:GLU:O	1:A:47:THR:HG22	1.90	0.72
1:H:102:ARG:HD2	1:H:112:ASN:HB2	1.71	0.72
1:D:46:GLU:HG2	4:D:211:HOH:O	1.91	0.71
1:F:102:ARG:HD2	1:F:112:ASN:HB2	1.73	0.70
1:B:102:ARG:HD2	1:B:112:ASN:HB2	1.72	0.70
1:A:15:ARG:HD2	4:B:165:HOH:O	1.92	0.70
1:E:102:ARG:HD2	1:E:112:ASN:HB2	1.72	0.70
1:H:74:VAL:CG1	4:H:166:HOH:O	2.41	0.69
1:H:55:LYS:HB2	1:H:57:PHE:CE2	2.28	0.69
1:B:55:LYS:HB3	1:B:56:PRO:HD2	1.75	0.69
1:E:149:GLU:C	4:E:184:HOH:O	2.31	0.69
4:C:197:HOH:O	1:F:15:ARG:HD2	1.93	0.68
1:H:71:PHE:HA	4:H:169:HOH:O	1.95	0.66
1:C:55:LYS:HB2	1:C:57:PHE:CE2	2.31	0.66
1:A:43:GLU:O	1:A:47:THR:CG2	2.44	0.65
1:D:53:GLN:HA	1:D:58:TYR:CD1	2.31	0.65
1:H:74:VAL:HG12	4:H:166:HOH:O	1.96	0.64
1:F:86:HIS:ND1	4:F:186:HOH:O	2.30	0.64
1:D:121:GLU:CG	4:D:210:HOH:O	2.41	0.63
1:C:62:ILE:N	4:C:188:HOH:O	2.25	0.62
1:G:52:HIS:O	1:G:58:TYR:HD1	1.84	0.61
1:H:55:LYS:HB2	1:H:57:PHE:CD2	2.36	0.61
1:H:136:ILE:HG13	4:H:167:HOH:O	2.01	0.61
1:C:121:GLU:HB2	4:C:162:HOH:O	2.02	0.59
1:G:52:HIS:O	1:G:58:TYR:CD1	2.55	0.59
1:E:64:PHE:HD2	4:E:194:HOH:O	1.85	0.59
1:B:43:GLU:OE1	4:B:174:HOH:O	2.17	0.58
1:C:52:HIS:O	1:C:54:GLY:N	2.37	0.58
1:B:88:ILE:O	1:B:102:ARG:HG3	2.03	0.57
1:E:61:LEU:O	1:E:61:LEU:HD13	2.04	0.57
1:H:71:PHE:N	4:H:164:HOH:O	2.38	0.57
1:C:111:ARG:CZ	4:C:203:HOH:O	2.33	0.57
1:A:96:ALA:O	1:B:86:HIS:NE2	2.33	0.57
1:D:88:ILE:O	1:D:102:ARG:HG3	2.07	0.55
1:C:43:GLU:O	1:C:47:THR:HG22	2.06	0.55
1:C:30:LEU:O	4:C:173:HOH:O	2.17	0.55
1:H:57:PHE:CD2	1:H:58:TYR:N	2.75	0.55
1:H:131:PHE:HD2	4:H:167:HOH:O	1.80	0.54
1:F:2:GLU:HB2	4:F:158:HOH:O	2.08	0.54
1:B:107:LEU:HD21	1:D:83:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:VAL:HG13	1:G:136:ILE:HG23	1.90	0.54
1:A:49:TYR:CE2	1:A:61:LEU:HD22	2.43	0.54
1:A:33:VAL:HG13	1:A:136:ILE:HG23	1.89	0.54
1:C:10:PRO:HD3	1:C:70:VAL:HG12	1.88	0.54
1:D:46:GLU:CG	4:D:211:HOH:O	2.52	0.54
1:E:15:ARG:HD2	4:E:181:HOH:O	2.07	0.54
2:D:158:UDP:O2B	4:D:208:HOH:O	2.19	0.53
1:B:42:MET:SD	1:B:62:ILE:CG2	2.96	0.53
1:A:88:ILE:O	1:A:102:ARG:HG3	2.09	0.53
1:B:53:GLN:HA	1:B:58:TYR:CD1	2.44	0.53
1:G:10:PRO:HD3	1:G:70:VAL:HG12	1.91	0.52
1:E:102:ARG:NH1	4:E:175:HOH:O	2.42	0.52
1:B:33:VAL:HG13	1:B:136:ILE:HG23	1.91	0.52
1:F:33:VAL:HG13	1:F:136:ILE:HG23	1.92	0.52
1:B:107:LEU:CD2	1:D:83:VAL:HG11	2.40	0.52
1:G:43:GLU:O	1:G:47:THR:HG22	2.09	0.52
1:E:50:GLY:O	1:E:52:HIS:N	2.43	0.51
1:G:53:GLN:HA	1:G:58:TYR:CD1	2.45	0.51
1:F:30:LEU:HB3	1:F:75:VAL:HG13	1.91	0.51
1:H:55:LYS:HB3	1:H:56:PRO:HD2	1.92	0.51
1:H:135:GLU:C	4:H:167:HOH:O	2.50	0.51
1:E:52:HIS:HB3	1:E:55:LYS:HE3	1.91	0.51
1:G:56:PRO:HG2	1:G:57:PHE:CD2	2.47	0.50
1:A:50:GLY:O	1:A:53:GLN:HB2	2.12	0.50
1:G:61:LEU:O	1:G:62:ILE:HD12	2.12	0.50
1:E:33:VAL:HG13	1:E:136:ILE:HG23	1.94	0.50
1:B:43:GLU:O	1:B:47:THR:HG22	2.11	0.50
1:B:109:VAL:HG22	2:B:158:UDP:C2	2.47	0.49
1:C:55:LYS:CB	1:C:57:PHE:CE2	2.96	0.49
1:H:30:LEU:HB3	1:H:75:VAL:HG13	1.95	0.49
1:G:30:LEU:HB3	1:G:75:VAL:HG13	1.94	0.48
1:A:16:ASN:ND2	1:E:143:ARG:HD3	2.28	0.48
1:E:40:VAL:HG13	1:E:44:LEU:HD23	1.96	0.48
1:F:102:ARG:HD3	1:F:112:ASN:O	2.14	0.48
1:B:42:MET:SD	1:B:62:ILE:HG21	2.55	0.47
1:C:30:LEU:HB3	1:C:75:VAL:HG13	1.96	0.47
1:E:15:ARG:NH1	1:E:113:ILE:HD11	2.29	0.47
1:D:109:VAL:HG22	2:D:158:UDP:C2	2.49	0.47
1:C:15:ARG:NH1	1:C:113:ILE:HD11	2.29	0.47
1:B:10:PRO:HB3	1:B:68:ALA:HB3	1.97	0.47
1:D:33:VAL:HG13	1:D:136:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:GLU:CG	4:E:187:HOH:O	2.32	0.47
1:C:85:ARG:NE	4:C:181:HOH:O	2.42	0.46
1:E:78:GLU:OE2	4:E:183:HOH:O	2.20	0.46
1:F:82:ASN:HB2	4:F:170:HOH:O	1.89	0.46
1:F:61:LEU:HA	1:F:61:LEU:HD22	1.76	0.46
1:G:88:ILE:O	1:G:102:ARG:HG3	2.16	0.46
1:F:49:TYR:CE2	1:F:61:LEU:HD12	2.51	0.46
1:H:15:ARG:NH1	1:H:113:ILE:HD11	2.31	0.46
1:B:15:ARG:NH1	1:B:105:LEU:O	2.31	0.46
1:H:55:LYS:HB2	1:H:57:PHE:HE2	1.78	0.46
1:B:43:GLU:O	1:B:47:THR:CG2	2.64	0.46
1:D:143:ARG:HD3	1:F:16:ASN:ND2	2.31	0.46
1:H:52:HIS:C	1:H:54:GLY:H	2.20	0.46
1:F:85:ARG:NH2	4:F:162:HOH:O	2.50	0.45
1:C:57:PHE:CD1	1:C:58:TYR:N	2.85	0.45
1:E:52:HIS:C	1:E:54:GLY:H	2.20	0.45
1:B:30:LEU:HB3	1:B:75:VAL:HG13	1.99	0.45
1:H:33:VAL:HG13	1:H:136:ILE:HG23	1.98	0.45
1:B:96:ALA:O	1:D:86:HIS:NE2	2.46	0.45
1:F:88:ILE:O	1:F:102:ARG:HG3	2.16	0.45
1:D:15:ARG:NH1	1:D:105:LEU:O	2.32	0.45
1:E:61:LEU:O	1:E:62:ILE:HD12	2.17	0.44
1:C:33:VAL:HG13	1:C:136:ILE:HG23	1.98	0.44
1:B:91:THR:HG22	1:B:109:VAL:HG23	1.98	0.44
1:C:43:GLU:O	1:C:47:THR:CG2	2.65	0.44
1:A:91:THR:OG1	2:A:158:UDP:O3B	2.24	0.44
1:C:52:HIS:C	1:C:54:GLY:H	2.20	0.44
1:A:142:PRO:HB3	1:F:142:PRO:HB3	1.99	0.43
1:D:15:ARG:NH1	1:D:113:ILE:HD11	2.32	0.43
1:D:1:MET:N	1:G:95:GLU:OE2	2.49	0.43
1:E:88:ILE:O	1:E:102:ARG:HG3	2.18	0.43
1:A:30:LEU:HB3	1:A:75:VAL:CG1	2.48	0.43
1:C:27:ARG:HD3	4:C:159:HOH:O	2.18	0.43
1:C:15:ARG:NH1	1:C:105:LEU:O	2.34	0.43
1:E:110:GLY:HA2	4:E:195:HOH:O	2.17	0.43
1:A:143:ARG:HD3	1:E:16:ASN:ND2	2.33	0.43
1:A:30:LEU:HB3	1:A:75:VAL:HG13	2.00	0.43
1:H:57:PHE:CG	1:H:58:TYR:N	2.87	0.42
1:D:24:ARG:NH2	4:D:175:HOH:O	2.18	0.42
1:H:10:PRO:HD3	1:H:70:VAL:HG12	2.02	0.42
1:E:30:LEU:HB3	1:E:75:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:ILE:HD12	4:C:188:HOH:O	2.19	0.42
1:C:88:ILE:O	1:C:102:ARG:HG3	2.19	0.42
1:B:51:GLU:HG3	4:B:194:HOH:O	2.18	0.42
1:A:142:PRO:CB	1:F:142:PRO:HB3	2.50	0.42
1:A:13:VAL:HG13	1:A:18:ILE:HD11	2.01	0.42
1:E:50:GLY:C	1:E:52:HIS:H	2.23	0.42
1:E:10:PRO:HD3	1:E:70:VAL:HG12	2.02	0.42
1:A:10:PRO:HD3	1:A:70:VAL:HG12	2.01	0.41
1:B:42:MET:O	1:B:46:GLU:HG3	2.19	0.41
2:A:158:UDP:O1B	2:A:158:UDP:O3'	2.29	0.41
1:D:55:LYS:HB3	1:D:56:PRO:HD2	2.03	0.41
1:H:8:ILE:O	4:H:164:HOH:O	2.22	0.41
1:A:10:PRO:HB3	1:A:68:ALA:HB3	2.03	0.41
1:B:39:GLN:HG3	4:B:170:HOH:O	2.21	0.41
1:F:10:PRO:HB3	1:F:68:ALA:HB3	2.03	0.41
1:D:30:LEU:HB3	1:D:75:VAL:HG13	2.02	0.41
1:B:16:ASN:ND2	4:C:175:HOH:O	2.46	0.41
1:B:106:GLY:O	1:D:28:LYS:NZ	2.49	0.41
1:H:14:GLN:HG3	4:H:163:HOH:O	2.19	0.41
1:C:44:LEU:CD1	1:C:129:LEU:HG	2.50	0.41
1:C:24:ARG:HD3	1:C:101:ILE:HG12	2.01	0.41
1:E:53:GLN:HE21	1:E:53:GLN:HB2	1.67	0.41
1:B:85:ARG:HD2	1:B:118:ASP:HA	2.02	0.41
1:E:85:ARG:HD2	1:E:118:ASP:HA	2.03	0.41
1:B:42:MET:SD	1:B:62:ILE:HG23	2.61	0.40
1:H:37:LEU:HD12	4:H:169:HOH:O	2.21	0.40
1:E:52:HIS:C	1:E:54:GLY:N	2.74	0.40
1:G:53:GLN:O	1:G:53:GLN:CG	2.70	0.40
1:C:52:HIS:C	1:C:54:GLY:N	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	147/157 (94%)	140 (95%)	7 (5%)	0	100	100
1	B	147/157 (94%)	141 (96%)	6 (4%)	0	100	100
1	C	147/157 (94%)	139 (95%)	7 (5%)	1 (1%)	26	46
1	D	147/157 (94%)	142 (97%)	5 (3%)	0	100	100
1	E	147/157 (94%)	135 (92%)	11 (8%)	1 (1%)	26	46
1	F	147/157 (94%)	138 (94%)	9 (6%)	0	100	100
1	G	147/157 (94%)	134 (91%)	11 (8%)	2 (1%)	14	24
1	H	147/157 (94%)	137 (93%)	8 (5%)	2 (1%)	14	24
All	All	1176/1256 (94%)	1106 (94%)	64 (5%)	6 (0%)	34	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	51	GLU
1	G	51	GLU
1	C	53	GLN
1	H	58	TYR
1	G	55	LYS
1	H	53	GLN

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	124/135 (92%)	117 (94%)	7 (6%)	26	47
1	B	124/135 (92%)	118 (95%)	6 (5%)	31	55
1	C	124/135 (92%)	118 (95%)	6 (5%)	31	55
1	D	126/135 (93%)	122 (97%)	4 (3%)	46	74
1	E	122/135 (90%)	113 (93%)	9 (7%)	17	31
1	F	122/135 (90%)	117 (96%)	5 (4%)	37	63
1	G	115/135 (85%)	111 (96%)	4 (4%)	43	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	120/135 (89%)	115 (96%)	5 (4%)	36	62
All	All	977/1080 (90%)	931 (95%)	46 (5%)	32	56

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	47	THR
1	A	53	GLN
1	A	61	LEU
1	A	107	LEU
1	A	109	VAL
1	A	124	GLU
1	B	33	VAL
1	B	47	THR
1	B	51	GLU
1	B	61	LEU
1	B	109	VAL
1	B	138	SER
1	C	33	VAL
1	C	47	THR
1	C	63	SER
1	C	65	ILE
1	C	109	VAL
1	C	121	GLU
1	D	33	VAL
1	D	47	THR
1	D	61	LEU
1	D	63	SER
1	E	33	VAL
1	E	47	THR
1	E	51	GLU
1	E	52	HIS
1	E	53	GLN
1	E	76	GLU
1	E	109	VAL
1	E	138	SER
1	E	149	GLU
1	F	33	VAL
1	F	47	THR
1	F	61	LEU
1	F	63	SER

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Mol	Chain	Res	Type
1	F	109	VAL
1	G	33	VAL
1	G	47	THR
1	G	109	VAL
1	G	138	SER
1	H	33	VAL
1	H	47	THR
1	H	51	GLU
1	H	57	PHE
1	H	109	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	134	ASN
1	B	16	ASN
1	B	53	GLN
1	C	16	ASN
1	D	16	ASN
1	E	16	ASN
1	E	53	GLN
1	E	134	ASN
1	F	16	ASN
1	G	134	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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$
2	UDP	A	158	3	18,26,26	1.28	1 (5%)	26,40,40	1.72	4 (15%)
2	UDP	B	158	3	18,26,26	1.34	3 (16%)	26,40,40	1.54	3 (11%)
2	UDP	D	158	3	18,26,26	1.20	1 (5%)	26,40,40	1.69	2 (7%)

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
2	UDP	A	158	3	-	0/12/32/32	0/2/2/2
2	UDP	B	158	3	-	0/12/32/32	0/2/2/2
2	UDP	D	158	3	-	0/12/32/32	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	158	UDP	PB-O2B	-2.39	1.46	1.54
2	B	158	UDP	PB-O3B	-2.05	1.47	1.54
2	B	158	UDP	C4-N3	2.94	1.38	1.33
2	D	158	UDP	C4-N3	3.34	1.39	1.33
2	A	158	UDP	C4-N3	3.37	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	158	UDP	PA-O3A-PB	-2.76	123.40	132.67
2	A	158	UDP	O3B-PB-O3A	2.10	114.63	105.09
2	A	158	UDP	O3A-PA-O5'	2.15	108.64	102.94
2	A	158	UDP	O4'-C1'-N1	2.20	112.72	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	158	UDP	C4'-O4'-C1'	3.57	113.64	109.72
2	B	158	UDP	C4-N3-C2	4.67	118.77	114.14
2	D	158	UDP	O3A-PA-O5'	4.71	115.42	102.94
2	D	158	UDP	C4-N3-C2	6.25	120.34	114.14
2	A	158	UDP	C4-N3-C2	6.73	120.80	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	158	UDP	3	0
2	B	158	UDP	1	0
2	D	158	UDP	2	0

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	149/157 (94%)	0.13	4 (2%) 58 62	11, 27, 52, 64	0
1	B	149/157 (94%)	-0.06	1 (0%) 89 90	10, 24, 44, 55	0
1	C	149/157 (94%)	0.10	5 (3%) 49 54	15, 30, 52, 68	0
1	D	149/157 (94%)	0.06	5 (3%) 49 54	14, 30, 60, 71	0
1	E	149/157 (94%)	0.24	9 (6%) 25 28	17, 30, 68, 85	0
1	F	149/157 (94%)	0.25	5 (3%) 49 54	19, 39, 70, 84	0
1	G	149/157 (94%)	0.93	22 (14%) 3 3	29, 46, 78, 95	0
1	H	149/157 (94%)	1.16	34 (22%) 1 1	31, 47, 80, 102	0
All	All	1192/1256 (94%)	0.35	85 (7%) 19 21	10, 35, 69, 102	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	56	PRO	7.9
1	G	148	TYR	6.1
1	H	95	GLU	5.7
1	G	54	GLY	5.6
1	G	59	ASN	5.5
1	H	54	GLY	5.3
1	G	42	MET	4.9
1	H	58	TYR	4.9
1	H	107	LEU	4.9
1	G	58	TYR	4.8
1	G	145	ALA	4.6
1	G	40	VAL	4.5
1	H	55	LYS	4.3
1	H	51	GLU	4.3
1	G	49	TYR	4.3
1	C	56	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	57	PHE	4.2
1	G	52	HIS	4.1
1	F	57	PHE	4.0
1	G	149	GLU	3.9
1	G	56	PRO	3.9
1	H	46	GLU	3.9
1	G	146	TRP	3.8
1	H	41	PRO	3.7
1	H	42	MET	3.6
1	H	48	HIS	3.6
1	E	59	ASN	3.5
1	H	45	ALA	3.4
1	E	54	GLY	3.4
1	E	55	LYS	3.4
1	D	56	PRO	3.4
1	H	94	SER	3.4
1	E	94	SER	3.3
1	G	50	GLY	3.3
1	H	60	ASP	3.3
1	G	51	GLU	3.1
1	A	53	GLN	3.1
1	C	57	PHE	3.1
1	E	56	PRO	3.1
1	G	62	ILE	3.1
1	H	43	GLU	3.1
1	C	148	TYR	3.0
1	D	54	GLY	3.0
1	H	52	HIS	3.0
1	H	137	THR	3.0
1	A	55	LYS	2.9
1	A	56	PRO	2.8
1	D	55	LYS	2.8
1	H	63	SER	2.8
1	C	54	GLY	2.8
1	H	12	ALA	2.8
1	F	42	MET	2.7
1	H	140	ALA	2.7
1	H	134	ASN	2.7
1	H	62	ILE	2.7
1	G	55	LYS	2.6
1	G	60	ASP	2.6
1	H	64	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	58	TYR	2.5
1	E	47	THR	2.5
1	A	57	PHE	2.5
1	H	149	GLU	2.5
1	H	50	GLY	2.5
1	G	134	ASN	2.4
1	G	41	PRO	2.4
1	G	147	LEU	2.4
1	B	58	TYR	2.3
1	H	59	ASN	2.3
1	H	39	GLN	2.3
1	H	37	LEU	2.3
1	E	111	ARG	2.3
1	D	57	PHE	2.3
1	H	93	PRO	2.3
1	F	59	ASN	2.2
1	H	86	HIS	2.2
1	E	63	SER	2.2
1	G	43	GLU	2.1
1	H	61	LEU	2.1
1	E	92	ASN	2.1
1	C	50	GLY	2.1
1	H	109	VAL	2.1
1	F	52	HIS	2.1
1	G	57	PHE	2.1
1	H	133	GLU	2.0
1	F	1	MET	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](#)

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
2	UDP	A	158	25/25	0.83	0.23	0.75	66,72,75,75	0
2	UDP	D	158	25/25	0.91	0.18	0.26	52,60,62,63	0
2	UDP	B	158	25/25	0.96	0.11	-1.25	25,32,35,43	0
3	MG	A	159	1/1	0.93	0.20	-	48,48,48,48	0
3	MG	B	159	1/1	0.93	0.07	-	45,45,45,45	0
3	MG	D	159	1/1	0.96	0.18	-	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.