



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2017 – 07:46 PM EST

PDB ID : 5TJH  
Title : hUGDH A136M Substitution  
Authors : Beattie, N.R.; Wood, Z.A.  
Deposited on : 2016-10-04  
Resolution : 2.05 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](mailto: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.

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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-20028442  
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-20028442

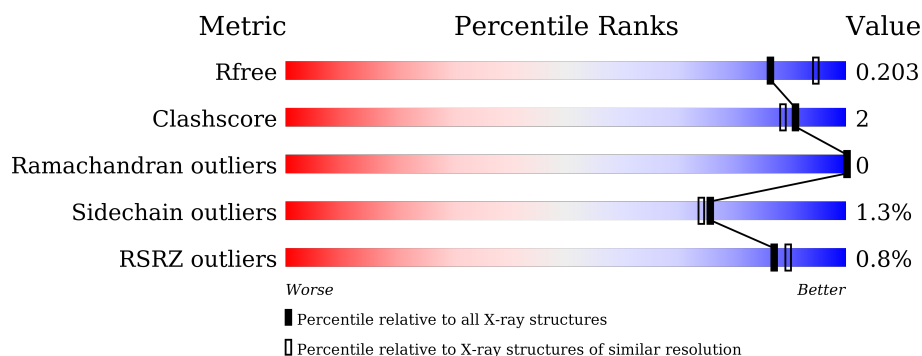
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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  $\geq 3$ , 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	494	<div> <div style="width: 87%;"></div> <div>87%</div> <div>6% • 7%</div> </div>
1	B	494	<div> <div style="width: 87%;"></div> <div>87%</div> <div>6% • 7%</div> </div>
1	C	494	<div> <div style="width: 88%;"></div> <div>88%</div> <div>5% 6%</div> </div>
1	D	494	<div> <div style="width: 86%;"></div> <div>86%</div> <div>6% • 7%</div> </div>
1	E	494	<div> <div style="width: 88%;"></div> <div>88%</div> <div>5% 7%</div> </div>
1	F	494	<div> <div style="width: 89%;"></div> <div>89%</div> <div>5% 6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	POP	A	501	-	-	-	X
2	POP	B	501	-	-	-	X
2	POP	D	501	-	-	-	X
2	POP	E	501	-	-	-	X
2	POP	F	501	-	-	-	X
4	UPG	C	501	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22615 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.

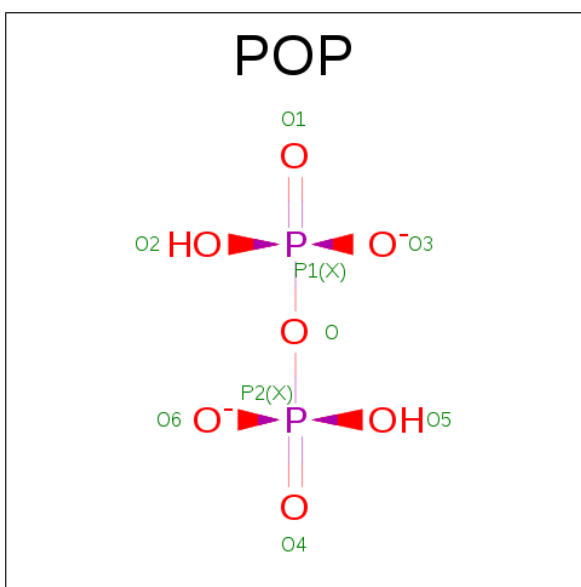
- Molecule 1 is a protein called UDP-glucose 6-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	2	0
			3615	2287	624	683	21			
1	B	460	Total	C	N	O	S	0	2	0
			3622	2292	627	682	21			
1	C	462	Total	C	N	O	S	0	4	0
			3640	2305	625	688	22			
1	D	459	Total	C	N	O	S	0	2	0
			3609	2286	622	680	21			
1	E	461	Total	C	N	O	S	0	0	0
			3615	2287	624	683	21			
1	F	463	Total	C	N	O	S	0	0	0
			3629	2294	626	688	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	MET	ALA	engineered mutation	UNP O60701
B	136	MET	ALA	engineered mutation	UNP O60701
C	136	MET	ALA	engineered mutation	UNP O60701
D	136	MET	ALA	engineered mutation	UNP O60701
E	136	MET	ALA	engineered mutation	UNP O60701
F	136	MET	ALA	engineered mutation	UNP O60701

- Molecule 2 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).

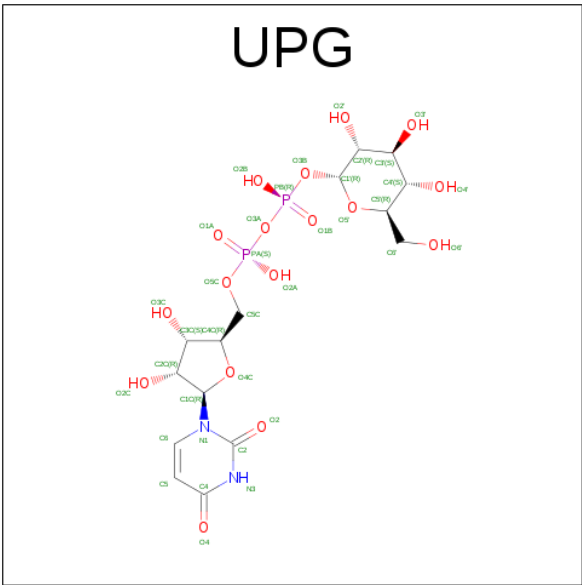


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 9 7 2	0	0
2	B	1	Total O P 9 7 2	0	0
2	D	1	Total O P 9 7 2	0	0
2	E	1	Total O P 9 7 2	0	0
2	F	1	Total O P 9 7 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0

- Molecule 4 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: C<sub>15</sub>H<sub>24</sub>N<sub>2</sub>O<sub>17</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

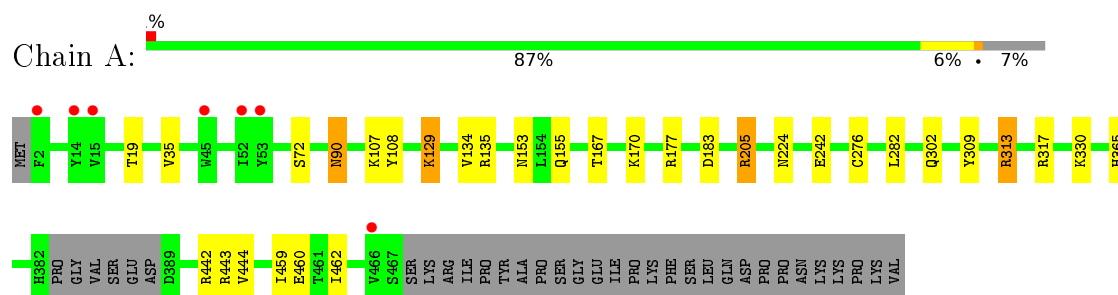
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	96	Total	O	0	0
			96	96		
5	B	133	Total	O	0	0
			133	133		
5	C	219	Total	O	0	0
			219	219		
5	D	129	Total	O	0	0
			129	129		
5	E	82	Total	O	0	0
			82	82		
5	F	143	Total	O	0	0
			143	143		

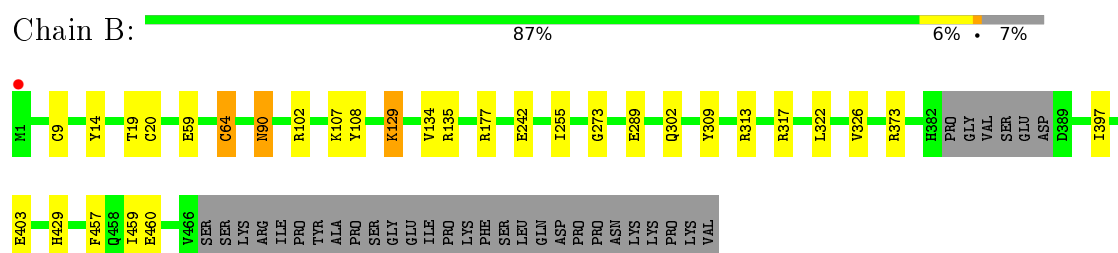
### 3 Residue-property plots [i](#)

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.

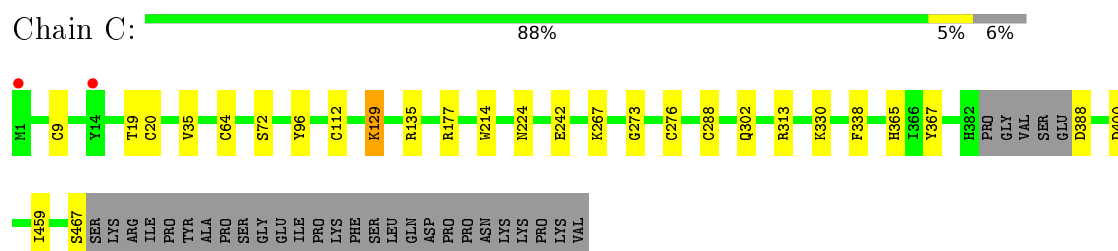
- Molecule 1: UDP-glucose 6-dehydrogenase



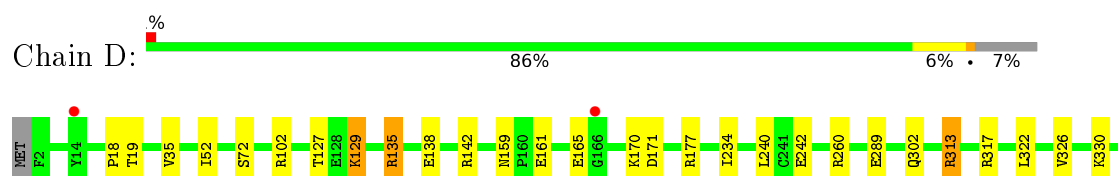
- Molecule 1: UDP-glucose 6-dehydrogenase

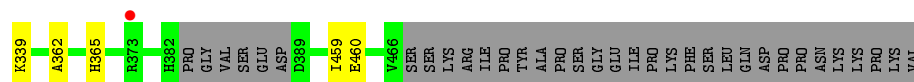


- Molecule 1: UDP-glucose 6-dehydrogenase

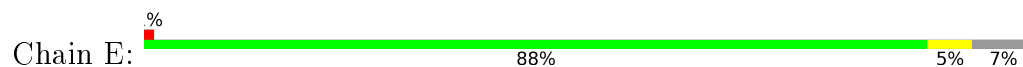


- Molecule 1: UDP-glucose 6-dehydrogenase

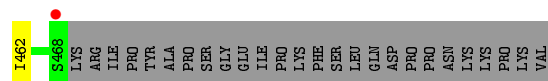
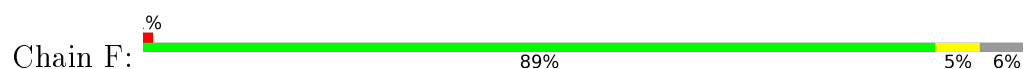




- Molecule 1: UDP-glucose 6-dehydrogenase



- Molecule 1: UDP-glucose 6-dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.35Å 104.59Å 107.71Å 64.82° 68.35° 73.72°	Depositor
Resolution (Å)	37.17 – 2.05 93.63 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.0 (37.17-2.05) 86.2 (93.63-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.171 , 0.203 0.170 , 0.203	Depositor DCC
$R_{free}$ test set	10305 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	22615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UPG, POP, CL

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	0.38	0/3686	0.54	1/4986 (0.0%)
1	B	0.45	1/3693 (0.0%)	0.57	0/4994
1	C	0.46	2/3717 (0.1%)	0.60	0/5028
1	D	0.40	0/3680	0.56	1/4978 (0.0%)
1	E	0.38	0/3680	0.54	1/4977 (0.0%)
1	F	0.43	1/3694 (0.0%)	0.56	0/4996
All	All	0.42	4/22150 (0.0%)	0.56	3/29959 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	CYS	CB-SG	-7.33	1.69	1.82
1	C	64	CYS	CB-SG	-7.21	1.70	1.82
1	F	64	CYS	CB-SG	-6.69	1.70	1.82
1	C	112	CYS	CB-SG	-5.88	1.72	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	313	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	D	313	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	313	ARG	NE-CZ-NH1	-5.39	117.61	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	3615	0	3635	17	0
1	B	3622	0	3650	18	0
1	C	3640	0	3669	18	0
1	D	3609	0	3635	19	0
1	E	3615	0	3636	15	0
1	F	3629	0	3645	12	0
2	A	9	0	0	0	0
2	B	9	0	0	2	0
2	D	9	0	0	0	0
2	E	9	0	0	2	0
2	F	9	0	0	2	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	C	36	0	22	7	0
5	A	96	0	0	0	0
5	B	133	0	0	4	0
5	C	219	0	0	2	0
5	D	129	0	0	0	0
5	E	82	0	0	0	0
5	F	143	0	0	3	0
All	All	22615	0	21892	97	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 2.

All (97) 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:F:135:ARG:NH1	1:F:138:GLU:OE1	2.18	0.77
1:F:242:GLU:OE1	1:F:313:ARG:NH1	2.16	0.75
2:F:501:POP:O2	5:F:601:HOH:O	2.06	0.72
2:B:501:POP:O2	5:B:601:HOH:O	2.08	0.70
1:A:224:ASN:ND2	1:A:276[B]:CYS:SG	2.66	0.68
1:B:373:ARG:HG2	1:B:397:ILE:HG21	1.81	0.60
4:C:501:UPG:O3'	1:D:260:ARG:NH2	2.24	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASN:OD1	1:A:155:GLN:NE2	2.36	0.59
1:B:19:THR:HG21	1:B:129:LYS:HE2	1.88	0.56
1:C:276[A]:CYS:SG	4:C:501:UPG:H6'2	2.46	0.56
1:C:338:PHE:HE1	4:C:501:UPG:H5C1	1.71	0.55
1:D:326:VAL:CG1	1:D:362:ALA:HB2	2.36	0.55
1:B:135:ARG:NH1	5:B:602:HOH:O	2.25	0.54
1:D:18:PRO:HG3	1:D:52:ILE:HD11	1.90	0.54
1:A:19:THR:HG21	1:A:129:LYS:HE2	1.90	0.53
1:E:106:LEU:HD22	1:E:136:MET:HE3	1.89	0.53
4:C:501:UPG:HO3'	1:D:260:ARG:HH22	1.53	0.53
1:E:94:LYS:NZ	1:E:98:MET:O	2.37	0.53
1:E:242:GLU:OE1	1:E:313:ARG:NH1	2.31	0.53
1:C:242:GLU:OE1	1:C:313:ARG:NH1	2.37	0.51
1:E:273:GLY:H	2:E:501:POP:P2	2.34	0.51
2:F:501:POP:O3	5:F:602:HOH:O	2.19	0.51
1:C:9:CYS:HB2	1:C:20:CYS:SG	2.52	0.50
1:E:317:ARG:NH2	1:E:460:GLU:HB3	2.26	0.50
1:B:102:ARG:HH12	1:B:289:GLU:CD	2.15	0.50
1:E:322:LEU:HD12	1:E:326:VAL:HG12	1.94	0.49
1:A:242:GLU:OE1	1:A:313:ARG:NH1	2.31	0.49
1:B:403:GLU:HG2	5:B:606:HOH:O	2.12	0.49
1:C:273:GLY:N	4:C:501:UPG:O3C	2.42	0.49
1:D:322:LEU:HD12	1:D:326:VAL:HG22	1.95	0.49
1:F:91:THR:O	1:F:279:LYS:HE2	2.13	0.48
1:A:167:THR:HB	1:A:170:LYS:HE3	1.96	0.48
1:D:170:LYS:NZ	1:D:171:ASP:OD1	2.41	0.48
1:F:224:ASN:ND2	1:F:280:ASP:HB2	2.28	0.48
1:C:224:ASN:ND2	1:C:276[B]:CYS:SG	2.86	0.48
1:B:273:GLY:N	2:B:501:POP:O3	2.41	0.47
1:A:35:VAL:HA	1:A:72:SER:O	2.14	0.47
1:B:134:VAL:O	1:B:135:ARG:HB2	2.15	0.47
1:C:302:GLN:HG3	1:D:302:GLN:HG3	1.96	0.47
1:C:267:LYS:NZ	5:C:603:HOH:O	2.39	0.47
1:D:102:ARG:HH12	1:D:289:GLU:CD	2.17	0.47
1:A:442:ARG:HB2	1:A:444:VAL:HG13	1.97	0.46
1:B:309:TYR:CZ	1:B:313:ARG:HD3	2.51	0.46
1:C:135:ARG:HD2	1:C:214:TRP:CD1	2.51	0.46
1:C:365:HIS:HD2	5:C:611:HOH:O	1.98	0.46
1:E:330:LYS:HE3	1:E:365:HIS:CG	2.51	0.46
1:D:35:VAL:HA	1:D:72:SER:O	2.15	0.46
1:C:288:CYS:SG	1:D:240[B]:LEU:HD21	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:GLU:OE1	1:D:313:ARG:NH1	2.35	0.46
1:B:255:ILE:HD11	1:E:222:ALA:HB1	1.97	0.46
1:F:19:THR:HG21	1:F:129:LYS:HE2	1.98	0.46
1:A:309:TYR:CZ	1:A:313:ARG:HD3	2.51	0.46
1:C:267:LYS:HB2	4:C:501:UPG:O4	2.16	0.46
1:B:322:LEU:HD12	1:B:326:VAL:HG12	1.98	0.46
1:C:330:LYS:HE3	1:C:365:HIS:CG	2.52	0.45
1:B:317:ARG:NH2	1:B:460:GLU:HB3	2.32	0.45
1:A:302:GLN:HG3	1:F:302:GLN:HG3	1.99	0.45
1:D:317:ARG:NH2	1:D:460:GLU:HB3	2.32	0.45
1:A:134:VAL:O	1:A:135:ARG:HB2	2.17	0.44
1:A:107:LYS:HE3	1:A:108:TYR:CZ	2.53	0.44
1:E:272:PHE:HB2	2:E:501:POP:O5	2.18	0.44
1:D:135:ARG:NH2	1:D:138:GLU:OE1	2.48	0.44
1:E:326:VAL:HA	1:E:329:LYS:HD2	1.98	0.44
1:C:96:TYR:N	1:C:96:TYR:CD1	2.86	0.44
1:F:330:LYS:HE3	1:F:365:HIS:CG	2.54	0.43
1:E:309:TYR:CZ	1:E:313:ARG:HD3	2.53	0.43
1:A:205:ARG:O	1:A:205:ARG:HD3	2.18	0.43
1:F:403:GLU:HG2	5:F:625:HOH:O	2.18	0.43
1:F:416:GLU:HA	1:F:444:VAL:HG11	2.01	0.43
1:D:165:GLU:O	1:D:339:LYS:NZ	2.51	0.42
1:B:107:LYS:HE3	1:B:108:TYR:CZ	2.54	0.42
1:C:19:THR:HG21	1:C:129:LYS:HE2	2.02	0.42
1:C:35:VAL:HA	1:C:72:SER:O	2.20	0.42
1:B:242:GLU:CD	1:B:313:ARG:HH12	2.22	0.42
1:C:367:TYR:CE1	1:C:400:ASP:HA	2.55	0.41
1:F:314:PHE:CD1	1:F:462:ILE:HD11	2.56	0.41
1:A:330:LYS:HE3	1:A:365:HIS:CG	2.55	0.41
1:E:153:ASN:OD1	1:E:155:GLN:NE2	2.51	0.41
1:C:338:PHE:CD1	4:C:501:UPG:H3C	2.56	0.41
1:E:106:LEU:HD22	1:E:136:MET:CE	2.50	0.41
1:A:443:ARG:HD3	1:A:462:ILE:O	2.20	0.41
1:B:102:ARG:HD3	5:B:607:HOH:O	2.21	0.41
1:B:302:GLN:HG3	1:E:302:GLN:HG3	2.02	0.41
1:D:19:THR:HG21	1:D:129:LYS:HE2	2.01	0.41
1:D:129:LYS:HE3	1:D:161:GLU:HG2	2.01	0.41
1:B:9:CYS:HB2	1:B:20:CYS:SG	2.61	0.41
1:D:127:THR:CG2	1:D:159:ASN:HB3	2.51	0.40
1:D:234:ILE:HA	1:D:234:ILE:HD12	1.95	0.40
1:D:330:LYS:HE3	1:D:365:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:HA	1:A:282:LEU:HD23	1.90	0.40
1:F:373:ARG:HG3	1:F:397:ILE:HD12	2.03	0.40
1:A:317:ARG:NH2	1:A:460:GLU:HB3	2.35	0.40
1:B:429:HIS:HB2	1:B:457:PHE:CE2	2.57	0.40
1:E:109:ILE:CD1	1:E:132:VAL:HG12	2.52	0.40
1:F:442:ARG:HB2	1:F:444:VAL:HG13	2.04	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	458/494 (93%)	449 (98%)	9 (2%)	0	100	100
1	B	458/494 (93%)	451 (98%)	7 (2%)	0	100	100
1	C	462/494 (94%)	455 (98%)	7 (2%)	0	100	100
1	D	457/494 (92%)	447 (98%)	10 (2%)	0	100	100
1	E	457/494 (92%)	450 (98%)	7 (2%)	0	100	100
1	F	459/494 (93%)	451 (98%)	8 (2%)	0	100	100
All	All	2751/2964 (93%)	2703 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	398/427 (93%)	391 (98%)	7 (2%)	66	62
1	B	398/427 (93%)	390 (98%)	8 (2%)	63	58
1	C	402/427 (94%)	397 (99%)	5 (1%)	78	76
1	D	397/427 (93%)	392 (99%)	5 (1%)	76	74
1	E	397/427 (93%)	394 (99%)	3 (1%)	86	86
1	F	399/427 (93%)	394 (99%)	5 (1%)	76	74
All	All	2391/2562 (93%)	2358 (99%)	33 (1%)	76	72

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90[A]	ASN
1	A	90[B]	ASN
1	A	129	LYS
1	A	177	ARG
1	A	183	ASP
1	A	205	ARG
1	A	459	ILE
1	B	14	TYR
1	B	59	GLU
1	B	64	CYS
1	B	90[A]	ASN
1	B	90[B]	ASN
1	B	129	LYS
1	B	177	ARG
1	B	459	ILE
1	C	129	LYS
1	C	177	ARG
1	C	388	ASP
1	C	459	ILE
1	C	467	SER
1	D	129	LYS
1	D	135	ARG
1	D	142	ARG
1	D	177	ARG
1	D	459	ILE
1	E	129	LYS
1	E	177	ARG
1	E	459	ILE
1	F	14	TYR
1	F	129	LYS

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Mol	Chain	Res	Type
1	F	135	ARG
1	F	177	ARG
1	F	459	ILE

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

Mol	Chain	Res	Type
1	A	118	GLN
1	A	224	ASN
1	A	365	HIS
1	B	375	GLN
1	E	449	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	POP	A	501	-	8,8,8	0.55	0	13,13,13	1.53	2 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	POP	B	501	-	8,8,8	0.55	0	13,13,13	1.44	1 (7%)
4	UPG	C	501	-	32,38,38	0.85	1 (3%)	43,58,58	1.50	6 (13%)
2	POP	D	501	-	8,8,8	0.54	0	13,13,13	1.33	1 (7%)
2	POP	E	501	-	8,8,8	0.55	0	13,13,13	1.45	1 (7%)
2	POP	F	501	-	8,8,8	0.55	0	13,13,13	1.02	1 (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	POP	A	501	-	-	0/6/6/6	0/0/0/0
2	POP	B	501	-	-	0/6/6/6	0/0/0/0
4	UPG	C	501	-	-	0/19/59/59	0/3/3/3
2	POP	D	501	-	-	0/6/6/6	0/0/0/0
2	POP	E	501	-	-	0/6/6/6	0/0/0/0
2	POP	F	501	-	-	0/6/6/6	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	UPG	C4-N3	2.65	1.37	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	POP	P2-O-P1	-4.41	119.88	132.51
2	B	501	POP	P2-O-P1	-4.27	120.26	132.51
2	D	501	POP	P2-O-P1	-4.14	120.64	132.51
2	E	501	POP	P2-O-P1	-4.04	120.93	132.51
4	C	501	UPG	C3'-C4'-C5'	-3.11	104.69	110.23
2	F	501	POP	P2-O-P1	-2.91	124.17	132.51
4	C	501	UPG	O3C-C3C-C2C	-2.37	104.19	111.86
2	A	501	POP	O-P2-O4	-2.21	100.58	107.57
4	C	501	UPG	O5'-C1'-O3B	2.21	114.28	111.36
4	C	501	UPG	O5'-C5'-C6'	2.89	113.88	106.38
4	C	501	UPG	O3A-PB-O3B	4.22	109.58	102.05
4	C	501	UPG	C4-N3-C2	4.61	119.06	114.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	POP	2	0
4	C	501	UPG	7	0
2	E	501	POP	2	0
2	F	501	POP	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	460/494 (93%)	-0.05	7 (1%)	76 81	31, 55, 99, 127	0
1	B	460/494 (93%)	-0.17	1 (0%)	95 96	26, 46, 78, 118	0
1	C	462/494 (93%)	-0.17	2 (0%)	93 94	24, 40, 65, 114	0
1	D	459/494 (92%)	-0.13	3 (0%)	89 91	25, 48, 90, 115	0
1	E	461/494 (93%)	-0.06	6 (1%)	79 83	27, 57, 93, 120	0
1	F	463/494 (93%)	-0.10	4 (0%)	85 89	30, 49, 83, 122	0
All	All	2765/2964 (93%)	-0.11	23 (0%)	87 90	24, 49, 88, 127	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	14	TYR	6.1
1	A	14	TYR	6.1
1	E	52	ILE	4.6
1	F	468	SER	4.5
1	C	1	MET	3.9
1	A	2	PHE	3.9
1	F	48	PRO	3.4
1	D	14	TYR	3.2
1	E	467	SER	3.1
1	B	1	MET	3.1
1	A	52	ILE	2.9
1	E	1	MET	2.9
1	F	49	THR	2.8
1	A	45	TRP	2.5
1	D	166	GLY	2.5
1	E	165	GLU	2.5
1	F	15	VAL	2.5
1	A	53	TYR	2.3
1	A	15	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	14	TYR	2.1
1	D	373	ARG	2.1
1	A	466	VAL	2.1
1	E	458	GLN	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	POP	B	501	9/9	0.83	0.38	21.18	68,71,84,85	9
2	POP	E	501	9/9	0.77	0.42	17.56	68,71,81,82	9
2	POP	A	501	9/9	0.78	0.38	15.44	69,75,81,83	9
2	POP	F	501	9/9	0.90	0.39	13.94	64,70,77,79	9
2	POP	D	501	9/9	0.86	0.39	11.42	42,60,70,72	9
4	UPG	C	501	36/36	0.79	0.29	8.68	25,38,62,68	36
3	CL	B	502	1/1	0.86	0.11	-0.66	78,78,78,78	0
3	CL	D	502	1/1	0.97	0.08	-	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.