Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:15 PM GMT

PDB ID	:	4X6L
Title	:	Crystal structure of S. aureus TarM in complex with UDP
Authors	:	Worrall, L.J.; Sobhanifar, S.; Gruninger, R.J.; Strynadka, N.C.
Deposited on	:	2014-12-08
Resolution	:	3.19 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

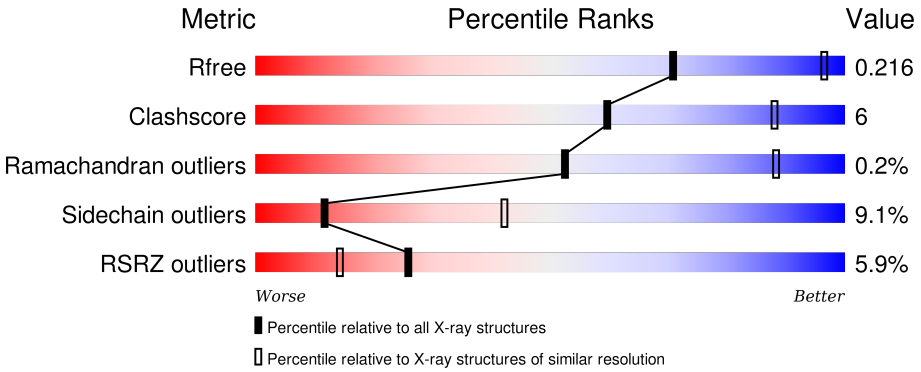
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 <=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	493	% 80% 19% ·
1	B	493	80% 17% ·
1	C	493	79% 19% ·
1	D	493	23% 79% 19% ·

2 Entry composition

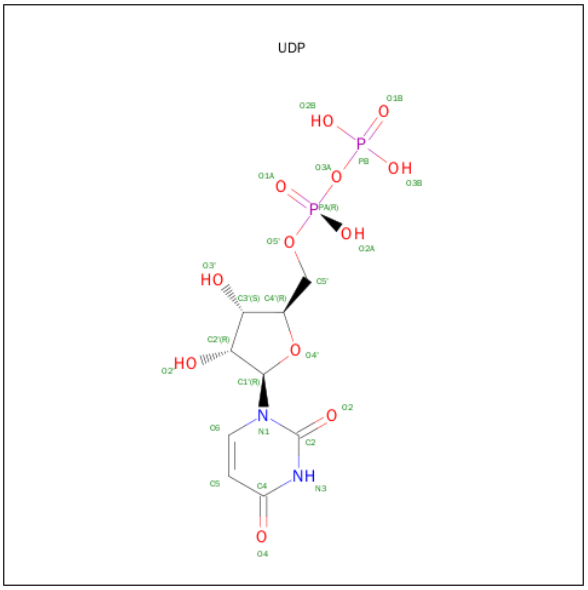
There are 2 unique types of molecules in this entry. The entry contains 16207 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TarM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			4033	2581	681	752	19			
1	B	493	Total	C	N	O	S	0	0	0
			4033	2581	681	752	19			
1	C	493	Total	C	N	O	S	0	0	0
			4033	2581	681	752	19			
1	D	493	Total	C	N	O	S	0	0	0
			4033	2581	681	752	19			

- 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		

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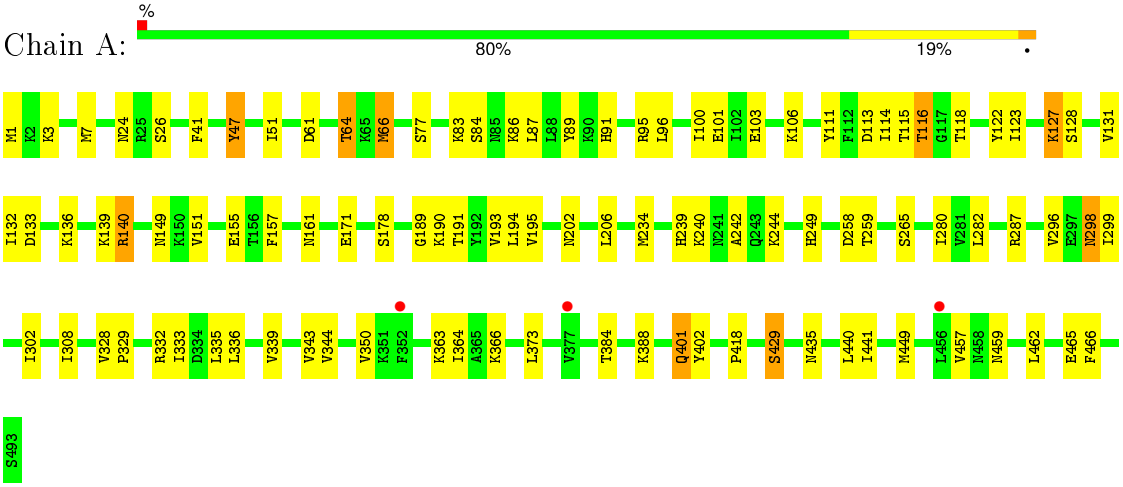
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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.

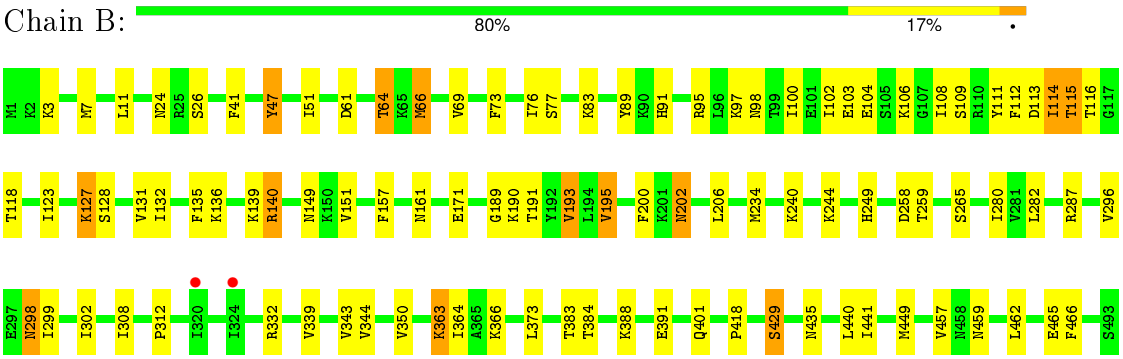
- Molecule 1: TarM

Chain A:



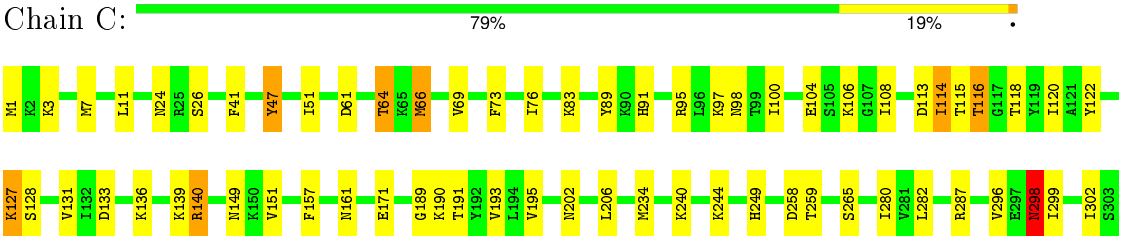
- Molecule 1: TarM

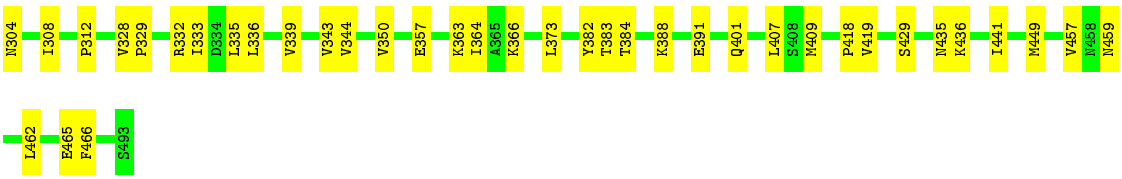
Chain B:



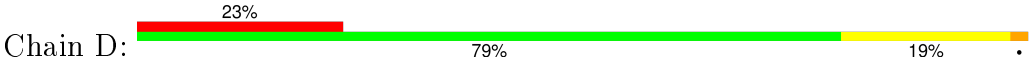
- Molecule 1: TarM

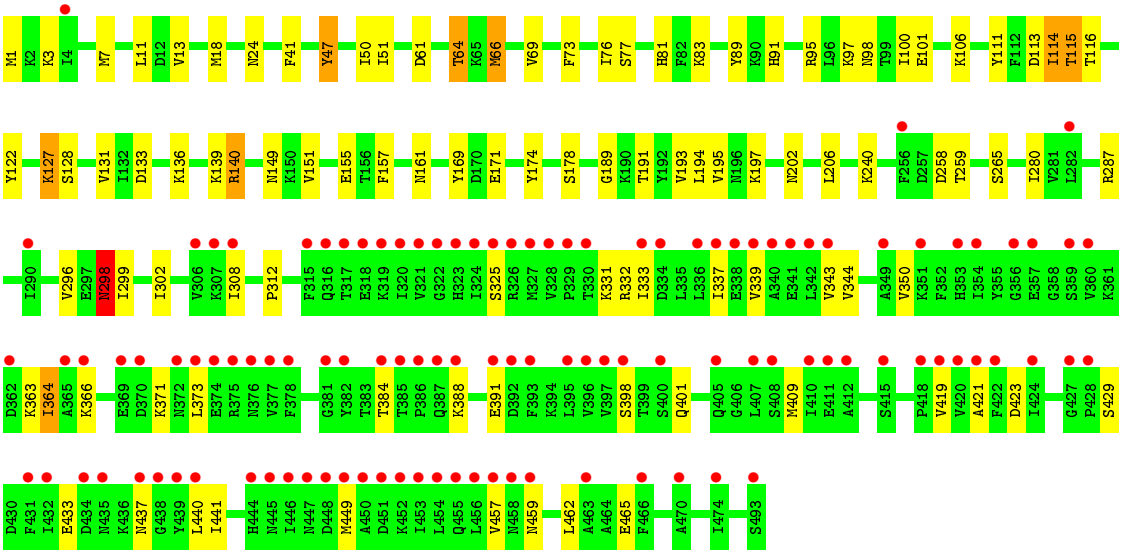
Chain C:





- Molecule 1: TarM





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	162.29Å 162.29Å 228.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	66.11 – 3.19 66.11 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (66.11-3.19) 99.9 (66.11-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 3.19Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.165 , 0.191 0.190 , 0.216	Depositor DCC
R_{free} test set	2842 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	99.2	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 73.5	EDS
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 55989 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16207	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.49	0/4110	0.71	0/5516
1	B	0.51	0/4110	0.72	0/5516
1	C	0.51	0/4110	0.73	0/5516
1	D	0.48	0/4110	0.72	0/5516
All	All	0.50	0/16440	0.72	0/22064

There are no bond length outliers.

There are no bond angle outliers.

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	4033	0	4057	41	0
1	B	4033	0	4057	49	0
1	C	4033	0	4057	50	0
1	D	4033	0	4057	46	0
2	A	25	0	11	0	0
2	B	25	0	11	1	0
2	C	25	0	11	1	0
All	All	16207	0	16261	186	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 6.

All (186) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ILE:HG23	1:A:114:ILE:HG22	1.31	1.10
1:C:100:ILE:HG23	1:C:114:ILE:HG22	1.46	0.95
1:D:100:ILE:HG23	1:D:114:ILE:HG22	1.55	0.87
1:D:332:ARG:HG3	1:D:401:GLN:HG2	1.63	0.80
1:B:332:ARG:HH11	1:B:401:GLN:HE22	1.31	0.76
1:C:339:VAL:HG11	1:C:449:MET:HE2	1.71	0.72
1:C:191:THR:HG21	1:C:206:LEU:HD22	1.75	0.68
1:C:113:ASP:HB3	1:C:116:THR:HG22	1.78	0.65
1:C:140:ARG:HD3	1:C:157:PHE:CD2	2.32	0.64
1:D:343:VAL:HG12	1:D:350:VAL:HG11	1.80	0.63
1:C:339:VAL:O	1:C:343:VAL:HG23	1.98	0.63
1:B:249:HIS:HA	1:B:282:LEU:HD11	1.81	0.62
1:C:335:LEU:O	1:C:339:VAL:HG23	2.00	0.61
1:A:332:ARG:HB3	1:A:335:LEU:HD12	1.82	0.60
1:D:77:SER:HB2	1:D:195:VAL:HG11	1.82	0.60
1:C:249:HIS:HA	1:C:282:LEU:HD11	1.83	0.60
1:B:100:ILE:HG23	1:B:114:ILE:HG22	1.83	0.60
1:C:339:VAL:HG21	1:C:449:MET:HE1	1.83	0.60
1:A:77:SER:HB2	1:A:195:VAL:HG11	1.85	0.59
1:D:333:ILE:HG22	1:D:364:ILE:HG12	1.84	0.58
1:C:357:GLU:HG2	1:C:382:TYR:HB2	1.84	0.58
1:A:249:HIS:HA	1:A:282:LEU:HD11	1.88	0.56
1:D:140:ARG:HD3	1:D:157:PHE:CD1	2.40	0.56
1:D:280:ILE:HG12	1:D:302:ILE:HD12	1.87	0.56
1:A:343:VAL:HG12	1:A:350:VAL:HG11	1.87	0.56
1:C:409:MET:HG2	1:C:419:VAL:HG11	1.87	0.56
1:C:122:TYR:HB3	1:C:133:ASP:HB2	1.87	0.56
1:B:280:ILE:HG12	1:B:302:ILE:HD12	1.86	0.56
1:C:343:VAL:HG12	1:C:350:VAL:HG11	1.87	0.56
1:B:191:THR:HG21	1:B:206:LEU:HD22	1.87	0.56
1:A:280:ILE:HG12	1:A:302:ILE:HD12	1.88	0.55
1:A:140:ARG:HD3	1:A:157:PHE:CD1	2.41	0.55
1:B:343:VAL:HG12	1:B:350:VAL:HG11	1.88	0.55
1:B:332:ARG:HH11	1:B:401:GLN:NE2	2.01	0.55
1:C:280:ILE:HG12	1:C:302:ILE:HD12	1.88	0.55
1:D:98:ASN:HD21	1:D:114:ILE:HG13	1.71	0.55
1:C:113:ASP:CB	1:C:116:THR:HG22	2.37	0.55
1:B:98:ASN:HD21	1:B:114:ILE:HG13	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ASP:HB3	1:D:116:THR:HG22	1.89	0.55
1:B:140:ARG:HD3	1:B:157:PHE:CD1	2.42	0.55
1:D:61:ASP:HB3	1:D:64:THR:HG22	1.90	0.54
1:A:189:GLY:O	1:A:202:ASN:HA	2.07	0.54
1:B:98:ASN:ND2	1:B:115:THR:HG22	2.22	0.54
1:B:113:ASP:HB3	1:B:116:THR:HG22	1.90	0.54
1:B:418:PRO:HB3	1:B:466:PHE:HB3	1.89	0.53
1:A:191:THR:HG21	1:A:206:LEU:HD22	1.89	0.53
1:A:333:ILE:HG23	1:A:336:LEU:HD23	1.89	0.53
1:D:100:ILE:CG2	1:D:114:ILE:HG22	2.32	0.52
1:C:61:ASP:HB3	1:C:64:THR:HG22	1.92	0.52
1:C:98:ASN:ND2	1:C:115:THR:HG22	2.25	0.52
1:D:77:SER:CB	1:D:195:VAL:HG11	2.39	0.52
1:A:61:ASP:HB3	1:A:64:THR:HG22	1.92	0.52
1:C:383:THR:O	2:C:500:UDP:H5	1.92	0.52
1:C:189:GLY:O	1:C:202:ASN:HA	2.09	0.52
1:B:123:ILE:HG12	1:B:132:ILE:HG12	1.92	0.51
1:B:287:ARG:HG3	1:B:299:ILE:HG22	1.91	0.51
1:D:191:THR:HG21	1:D:206:LEU:HD22	1.92	0.51
1:B:61:ASP:HB3	1:B:64:THR:HG22	1.92	0.51
1:C:116:THR:HG23	1:C:118:THR:OG1	2.11	0.51
1:A:429:SER:HA	1:A:440:LEU:HD21	1.93	0.51
1:A:287:ARG:HG3	1:A:299:ILE:HG22	1.92	0.51
1:C:98:ASN:HD21	1:C:114:ILE:HG13	1.76	0.51
1:D:423:ASP:HB2	1:D:440:LEU:HG	1.93	0.50
1:A:418:PRO:HB3	1:A:466:PHE:HB3	1.93	0.50
1:D:98:ASN:ND2	1:D:115:THR:HG22	2.26	0.50
1:C:332:ARG:HB3	1:C:335:LEU:HD12	1.93	0.50
1:D:287:ARG:HG3	1:D:299:ILE:HG22	1.94	0.50
1:D:409:MET:HG2	1:D:419:VAL:HG11	1.94	0.50
1:A:122:TYR:HB3	1:A:133:ASP:HB2	1.94	0.50
1:C:73:PHE:HA	1:C:76:ILE:HD12	1.93	0.50
1:D:178:SER:HB3	1:D:194:LEU:HD11	1.93	0.49
1:C:287:ARG:HG3	1:C:299:ILE:HG22	1.94	0.49
1:D:339:VAL:HG11	1:D:449:MET:HE2	1.95	0.49
1:C:418:PRO:HB3	1:C:466:PHE:HB3	1.94	0.49
1:B:441:ILE:HG21	1:B:449:MET:HB2	1.95	0.48
1:B:116:THR:HG23	1:B:118:THR:H	1.78	0.48
1:B:73:PHE:HA	1:B:76:ILE:HD12	1.96	0.48
1:B:339:VAL:HG11	1:B:449:MET:HE2	1.95	0.48
1:C:339:VAL:HG21	1:C:449:MET:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:ILE:HG21	1:C:449:MET:HB2	1.95	0.48
1:A:101:GLU:HB2	1:A:111:TYR:CE2	2.49	0.48
1:D:73:PHE:HA	1:D:76:ILE:HD12	1.96	0.48
1:B:339:VAL:O	1:B:343:VAL:HG23	2.15	0.47
1:A:47:TYR:CZ	1:A:66:MET:HE1	2.49	0.47
1:D:122:TYR:HB3	1:D:133:ASP:HB2	1.97	0.47
1:D:433:GLU:HB2	1:D:437:ASN:HD21	1.80	0.46
1:A:328:VAL:HB	1:A:329:PRO:CD	2.46	0.46
1:A:441:ILE:HG21	1:A:449:MET:HB2	1.98	0.46
1:B:111:TYR:CE2	1:B:123:ILE:HD12	2.50	0.46
1:B:127:LYS:HG2	1:B:128:SER:H	1.80	0.46
1:B:429:SER:HA	1:B:440:LEU:HD21	1.96	0.46
1:B:189:GLY:O	1:B:202:ASN:HA	2.16	0.46
1:B:113:ASP:CB	1:B:116:THR:HG22	2.46	0.46
1:A:333:ILE:HD12	1:A:333:ILE:H	1.80	0.46
1:A:113:ASP:HB3	1:A:116:THR:HG22	1.98	0.46
1:A:123:ILE:HG12	1:A:132:ILE:HG12	1.98	0.46
1:D:127:LYS:HG2	1:D:128:SER:H	1.80	0.46
1:A:401:GLN:HB3	1:A:402:TYR:CD2	2.51	0.45
1:D:77:SER:O	1:D:81:HIS:HD2	1.99	0.45
1:D:441:ILE:HG21	1:D:449:MET:HB2	1.98	0.45
1:C:104:GLU:HB3	1:C:108:ILE:HG22	1.98	0.45
1:D:189:GLY:O	1:D:202:ASN:HA	2.16	0.45
1:A:140:ARG:HD2	1:A:161:ASN:OD1	2.16	0.45
1:C:332:ARG:HH11	1:C:401:GLN:NE2	2.15	0.45
1:B:7:MET:HG2	1:B:41:PHE:CZ	2.52	0.45
1:D:337:ILE:HG22	1:D:371:LYS:HD2	1.97	0.45
1:C:328:VAL:HB	1:C:329:PRO:CD	2.48	0.45
1:B:11:LEU:HD12	1:B:66:MET:HE2	1.99	0.44
1:B:41:PHE:HA	1:B:69:VAL:HG12	1.99	0.44
1:D:13:VAL:HG13	1:D:50:ILE:HG23	2.00	0.44
1:B:140:ARG:HD2	1:B:161:ASN:OD1	2.18	0.44
1:B:383:THR:O	2:B:500:UDP:H5	1.99	0.44
1:C:47:TYR:CZ	1:C:66:MET:HE1	2.52	0.44
1:A:7:MET:HG2	1:A:41:PHE:CZ	2.52	0.44
1:A:339:VAL:O	1:A:343:VAL:HG23	2.17	0.44
1:C:127:LYS:HG2	1:C:128:SER:H	1.83	0.44
1:A:339:VAL:HG11	1:A:449:MET:HE2	1.98	0.44
1:A:91:HIS:O	1:A:95:ARG:HG2	2.18	0.44
1:C:91:HIS:O	1:C:95:ARG:HG2	2.18	0.43
1:C:7:MET:HG2	1:C:41:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:ASN:HD22	1:C:407:LEU:HD21	1.83	0.43
1:D:91:HIS:CE1	1:D:95:ARG:HH11	2.36	0.43
1:B:98:ASN:ND2	1:B:114:ILE:HG13	2.33	0.43
1:A:116:THR:HG23	1:A:118:THR:OG1	2.19	0.43
1:D:91:HIS:O	1:D:95:ARG:HG2	2.18	0.43
1:A:91:HIS:CE1	1:A:95:ARG:HH11	2.36	0.43
1:A:127:LYS:HG2	1:A:128:SER:H	1.84	0.43
1:B:91:HIS:CE1	1:B:95:ARG:HH11	2.37	0.43
1:C:333:ILE:HG23	1:C:336:LEU:HD23	2.01	0.43
1:B:193:VAL:CG1	1:B:200:PHE:HE1	2.31	0.43
1:C:140:ARG:HD2	1:C:161:ASN:OD1	2.19	0.43
1:B:312:PRO:HG3	1:B:391:GLU:HG2	2.00	0.43
1:D:398:SER:HB3	1:D:421:ALA:HB2	2.00	0.43
1:D:169:TYR:HA	1:D:174:TYR:O	2.18	0.42
1:D:7:MET:HG2	1:D:41:PHE:CZ	2.54	0.42
1:C:332:ARG:HH11	1:C:401:GLN:HE22	1.67	0.42
1:D:113:ASP:CB	1:D:116:THR:HG22	2.49	0.42
1:D:47:TYR:CZ	1:D:66:MET:HE1	2.54	0.42
1:C:344:VAL:HG21	1:C:373:LEU:HD22	2.01	0.42
1:B:234:MET:HG2	1:B:244:LYS:HD3	2.01	0.42
1:B:135:PHE:CE2	1:B:140:ARG:HB2	2.53	0.42
1:D:325:SER:HB2	1:D:331:LYS:HD2	2.00	0.42
1:D:101:GLU:HG3	1:D:111:TYR:CE1	2.55	0.42
1:C:98:ASN:HD21	1:C:115:THR:HG22	1.84	0.42
1:C:41:PHE:HA	1:C:69:VAL:HG12	2.00	0.42
1:A:84:SER:HB3	1:A:86:LYS:HE3	2.01	0.42
1:C:91:HIS:CE1	1:C:95:ARG:HH11	2.38	0.42
1:D:41:PHE:HA	1:D:69:VAL:HG12	2.01	0.42
1:D:11:LEU:HD12	1:D:66:MET:HE2	2.01	0.42
1:B:102:ILE:HD12	1:B:112:PHE:CD1	2.55	0.42
1:C:312:PRO:HG3	1:C:391:GLU:HG2	2.02	0.42
1:A:77:SER:CB	1:A:195:VAL:HG11	2.49	0.42
1:C:26:SER:OG	1:C:64:THR:HB	2.20	0.42
1:B:26:SER:OG	1:B:64:THR:HB	2.20	0.42
1:B:91:HIS:O	1:B:95:ARG:HG2	2.20	0.42
1:C:234:MET:HG2	1:C:244:LYS:HD3	2.01	0.42
1:B:98:ASN:HD21	1:B:115:THR:HG22	1.85	0.41
1:C:113:ASP:HB2	1:C:120:ILE:HD11	2.02	0.41
1:D:312:PRO:HG3	1:D:391:GLU:HG2	2.01	0.41
1:B:339:VAL:HG21	1:B:449:MET:CE	2.51	0.41
1:A:87:LEU:HA	1:A:87:LEU:HD23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLU:HB3	1:B:108:ILE:HG22	2.02	0.41
1:A:332:ARG:HG3	1:A:401:GLN:HE21	1.86	0.41
1:A:344:VAL:HG21	1:A:373:LEU:HD22	2.03	0.41
1:D:298:ASN:HA	1:D:298:ASN:HD22	1.70	0.41
1:B:103:GLU:HG2	1:B:109:SER:OG	2.21	0.41
1:D:89:TYR:CZ	1:D:151:VAL:HG12	2.54	0.41
1:D:140:ARG:HD2	1:D:161:ASN:OD1	2.20	0.41
1:A:26:SER:OG	1:A:64:THR:HB	2.20	0.41
1:C:298:ASN:HA	1:C:298:ASN:HD22	1.70	0.41
1:A:89:TYR:CZ	1:A:151:VAL:HG12	2.55	0.41
1:A:178:SER:HB3	1:A:194:LEU:HD11	2.03	0.41
1:B:77:SER:HA	1:B:195:VAL:HG11	2.03	0.41
1:D:337:ILE:HD11	1:D:364:ILE:HG23	2.03	0.41
1:B:344:VAL:HG21	1:B:373:LEU:HD22	2.02	0.41
1:C:89:TYR:CZ	1:C:151:VAL:HG12	2.56	0.41
1:A:234:MET:HG2	1:A:244:LYS:HD3	2.03	0.40
1:B:89:TYR:CZ	1:B:151:VAL:HG12	2.57	0.40
1:B:127:LYS:HG2	1:B:128:SER:N	2.37	0.40
1:C:116:THR:HG23	1:C:118:THR:H	1.86	0.40
1:D:344:VAL:HG21	1:D:373:LEU:HD22	2.02	0.40
1:D:127:LYS:HG2	1:D:128:SER:N	2.36	0.40
1:C:11:LEU:HD12	1:C:66:MET:HE2	2.02	0.40
1:B:47:TYR:CZ	1:B:66:MET:HE1	2.57	0.40
1:B:363:LYS:H	1:B:363:LYS:HG2	1.71	0.40
1:A:239:HIS:HB3	1:A:242:ALA:HB3	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	491/493 (100%)	457 (93%)	33 (7%)	1 (0%)	52 88

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	491/493 (100%)	462 (94%)	28 (6%)	1 (0%)	52 88
1	C	491/493 (100%)	461 (94%)	29 (6%)	1 (0%)	52 88
1	D	491/493 (100%)	456 (93%)	34 (7%)	1 (0%)	52 88
All	All	1964/1972 (100%)	1836 (94%)	124 (6%)	4 (0%)	52 88

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	ASN
1	B	298	ASN
1	C	298	ASN
1	D	298	ASN

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	449/449 (100%)	407 (91%)	42 (9%)	11 41
1	B	449/449 (100%)	409 (91%)	40 (9%)	12 44
1	C	449/449 (100%)	408 (91%)	41 (9%)	12 42
1	D	449/449 (100%)	409 (91%)	40 (9%)	12 44
All	All	1796/1796 (100%)	1633 (91%)	163 (9%)	12 42

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	LYS
1	A	24	ASN
1	A	47	TYR
1	A	51	ILE
1	A	64	THR
1	A	66	MET

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Mol	Chain	Res	Type
1	A	83	LYS
1	A	96	LEU
1	A	103	GLU
1	A	106	LYS
1	A	115	THR
1	A	116	THR
1	A	127	LYS
1	A	131	VAL
1	A	136	LYS
1	A	139	LYS
1	A	140	ARG
1	A	149	ASN
1	A	155	GLU
1	A	171	GLU
1	A	190	LYS
1	A	193	VAL
1	A	240	LYS
1	A	258	ASP
1	A	259	THR
1	A	265	SER
1	A	296	VAL
1	A	298	ASN
1	A	308	ILE
1	A	363	LYS
1	A	364	ILE
1	A	366	LYS
1	A	384	THR
1	A	388	LYS
1	A	401	GLN
1	A	429	SER
1	A	435	ASN
1	A	457	VAL
1	A	459	ASN
1	A	462	LEU
1	A	465	GLU
1	B	3	LYS
1	B	24	ASN
1	B	47	TYR
1	B	51	ILE
1	B	64	THR
1	B	66	MET
1	B	83	LYS

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Mol	Chain	Res	Type
1	B	97	LYS
1	B	106	LYS
1	B	114	ILE
1	B	115	THR
1	B	127	LYS
1	B	131	VAL
1	B	136	LYS
1	B	139	LYS
1	B	140	ARG
1	B	149	ASN
1	B	171	GLU
1	B	190	LYS
1	B	193	VAL
1	B	195	VAL
1	B	202	ASN
1	B	240	LYS
1	B	258	ASP
1	B	259	THR
1	B	265	SER
1	B	296	VAL
1	B	298	ASN
1	B	308	ILE
1	B	363	LYS
1	B	364	ILE
1	B	366	LYS
1	B	384	THR
1	B	388	LYS
1	B	429	SER
1	B	435	ASN
1	B	457	VAL
1	B	459	ASN
1	B	462	LEU
1	B	465	GLU
1	C	1	MET
1	C	3	LYS
1	C	24	ASN
1	C	47	TYR
1	C	51	ILE
1	C	64	THR
1	C	66	MET
1	C	83	LYS
1	C	97	LYS

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Mol	Chain	Res	Type
1	C	106	LYS
1	C	114	ILE
1	C	116	THR
1	C	127	LYS
1	C	131	VAL
1	C	136	LYS
1	C	139	LYS
1	C	140	ARG
1	C	149	ASN
1	C	171	GLU
1	C	190	LYS
1	C	193	VAL
1	C	195	VAL
1	C	240	LYS
1	C	258	ASP
1	C	259	THR
1	C	265	SER
1	C	296	VAL
1	C	298	ASN
1	C	308	ILE
1	C	363	LYS
1	C	364	ILE
1	C	366	LYS
1	C	384	THR
1	C	388	LYS
1	C	429	SER
1	C	435	ASN
1	C	436	LYS
1	C	457	VAL
1	C	459	ASN
1	C	462	LEU
1	C	465	GLU
1	D	1	MET
1	D	3	LYS
1	D	18	MET
1	D	24	ASN
1	D	47	TYR
1	D	51	ILE
1	D	64	THR
1	D	66	MET
1	D	83	LYS
1	D	97	LYS

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Mol	Chain	Res	Type
1	D	106	LYS
1	D	114	ILE
1	D	115	THR
1	D	127	LYS
1	D	131	VAL
1	D	136	LYS
1	D	139	LYS
1	D	140	ARG
1	D	149	ASN
1	D	155	GLU
1	D	171	GLU
1	D	193	VAL
1	D	197	LYS
1	D	240	LYS
1	D	258	ASP
1	D	259	THR
1	D	265	SER
1	D	296	VAL
1	D	298	ASN
1	D	308	ILE
1	D	363	LYS
1	D	364	ILE
1	D	366	LYS
1	D	384	THR
1	D	388	LYS
1	D	429	SER
1	D	457	VAL
1	D	459	ASN
1	D	462	LEU
1	D	465	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	A	241	ASN
1	A	298	ASN
1	A	444	HIS
1	B	81	HIS
1	B	98	ASN
1	B	203	ASN
1	B	241	ASN

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Mol	Chain	Res	Type
1	B	298	ASN
1	B	401	GLN
1	B	444	HIS
1	C	81	HIS
1	C	98	ASN
1	C	203	ASN
1	C	241	ASN
1	C	298	ASN
1	C	401	GLN
1	D	81	HIS
1	D	98	ASN
1	D	241	ASN
1	D	298	ASN
1	D	437	ASN
1	D	444	HIS

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

3 ligands 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	$\#\|Z\|>2$
2	UDP	A	500	-	18,26,26	0.99	1 (5%)	26,40,40	2.76	3 (11%)
2	UDP	B	500	-	18,26,26	1.07	3 (16%)	26,40,40	2.75	3 (11%)
2	UDP	C	500	-	18,26,26	1.01	2 (11%)	26,40,40	2.80	3 (11%)

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	500	-	-	0/12/32/32	0/2/2/2
2	UDP	B	500	-	-	0/12/32/32	0/2/2/2
2	UDP	C	500	-	-	0/12/32/32	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	UDP	C6-N1	2.05	1.38	1.35
2	C	500	UDP	C6-N1	2.10	1.38	1.35
2	B	500	UDP	PB-O3B	2.25	1.62	1.54
2	A	500	UDP	C4-N3	2.60	1.37	1.33
2	B	500	UDP	C4-N3	2.66	1.38	1.33
2	C	500	UDP	C4-N3	2.73	1.38	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	UDP	C5-C4-N3	-3.28	114.71	123.12
2	B	500	UDP	C5-C4-N3	-3.28	114.72	123.12
2	A	500	UDP	C5-C4-N3	-3.24	114.80	123.12
2	B	500	UDP	O3A-PA-O5'	2.43	109.37	102.94
2	A	500	UDP	O3A-PA-O5'	2.50	109.56	102.94
2	C	500	UDP	O3A-PA-O5'	2.71	110.13	102.94
2	A	500	UDP	C4-N3-C2	12.99	127.01	114.14
2	B	500	UDP	C4-N3-C2	13.05	127.06	114.14
2	C	500	UDP	C4-N3-C2	13.06	127.08	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	UDP	1	0
2	C	500	UDP	1	0

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

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^{th} 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	493/493 (100%)	-0.02	3 (0%) 90 84	77, 112, 147, 163	0
1	B	493/493 (100%)	0.03	2 (0%) 93 90	62, 97, 139, 163	0
1	C	493/493 (100%)	0.01	0 100 100	62, 103, 140, 159	0
1	D	493/493 (100%)	1.05	112 (22%) 1 1	67, 148, 269, 277	0
All	All	1972/1972 (100%)	0.27	117 (5%) 26 14	62, 109, 252, 277	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	396	VAL	15.1
1	D	453	ILE	11.7
1	D	337	ILE	9.7
1	D	336	LEU	9.4
1	D	454	LEU	8.9
1	D	449	MET	8.7
1	D	397	VAL	7.4
1	D	447	ASN	7.3
1	D	324	ILE	7.0
1	D	451	ASP	6.9
1	D	432	ILE	6.4
1	D	322	GLY	6.1
1	D	457	VAL	6.0
1	D	456	LEU	6.0
1	D	349	ALA	5.9
1	D	319	LYS	5.9
1	D	450	ALA	5.6
1	D	375	ARG	5.5
1	D	340	ALA	5.4
1	D	466	PHE	5.4
1	D	365	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	419	VAL	5.4
1	D	395	LEU	5.3
1	D	359	SER	5.3
1	D	463	ALA	5.2
1	D	356	GLY	5.1
1	D	333	ILE	5.1
1	D	439	TYR	5.1
1	D	318	GLU	5.1
1	D	428	PRO	5.0
1	D	435	ASN	4.8
1	D	388	LYS	4.6
1	D	330	THR	4.6
1	D	323	HIS	4.5
1	D	420	VAL	4.5
1	D	398	SER	4.5
1	D	418	PRO	4.4
1	D	317	THR	4.2
1	D	341	GLU	4.1
1	D	438	GLY	4.1
1	D	370	ASP	4.0
1	D	343	VAL	4.0
1	D	329	PRO	3.9
1	D	444	HIS	3.8
1	D	410	ILE	3.8
1	D	384	THR	3.8
1	D	421	ALA	3.8
1	D	422	PHE	3.8
1	D	431	PHE	3.8
1	D	458	ASN	3.8
1	D	320	ILE	3.7
1	D	338	GLU	3.7
1	D	474	ILE	3.7
1	D	334	ASP	3.7
1	D	353	HIS	3.6
1	D	392	ASP	3.6
1	D	357	GLU	3.6
1	D	381	GLY	3.5
1	D	308	ILE	3.4
1	D	342	LEU	3.4
1	D	377	VAL	3.4
1	D	354	ILE	3.4
1	D	307	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	372	ASN	3.3
1	D	408	SER	3.3
1	D	386	PRO	3.2
1	D	434	ASP	3.2
1	D	407	LEU	3.2
1	D	351	LYS	3.2
1	D	316	GLN	3.1
1	D	339	VAL	3.0
1	D	455	GLN	3.0
1	D	493	SER	2.9
1	D	411	GLU	2.9
1	D	446	ILE	2.9
1	D	321	VAL	2.9
1	D	369	GLU	2.9
1	D	427	GLY	2.9
1	D	325	SER	2.8
1	D	328	VAL	2.8
1	D	452	LYS	2.7
1	D	424	ILE	2.7
1	D	445	ASN	2.7
1	D	412	ALA	2.6
1	D	374	GLU	2.6
1	D	315	PHE	2.6
1	D	437	ASN	2.6
1	D	448	ASP	2.6
1	D	373	LEU	2.6
1	D	326	ARG	2.5
1	D	440	LEU	2.5
1	D	4	ILE	2.5
1	D	387	GLN	2.5
1	D	391	GLU	2.5
1	D	385	THR	2.4
1	D	290	ILE	2.4
1	A	352	PHE	2.4
1	A	377	VAL	2.4
1	D	382	TYR	2.4
1	D	376	ASN	2.4
1	D	378	PHE	2.3
1	D	405	GLN	2.3
1	D	459	ASN	2.3
1	D	366	LYS	2.3
1	D	400	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	393	PHE	2.2
1	D	415	SER	2.2
1	D	470	ALA	2.2
1	B	320	ILE	2.2
1	D	362	ASP	2.2
1	D	360	VAL	2.2
1	A	456	LEU	2.1
1	D	256	PHE	2.1
1	D	306	VAL	2.1
1	D	327	MET	2.1
1	D	282	LEU	2.0
1	B	324	ILE	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^{th} 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	C	500	25/25	0.94	0.24	0.10	107,122,129,130	0
2	UDP	B	500	25/25	0.92	0.21	-0.31	107,118,124,127	0
2	UDP	A	500	25/25	0.95	0.20	-0.43	117,131,134,140	0

6.5 Other polymers (i)

There are no such residues in this entry.