



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:29 AM UTC

PDB ID : 1F6D / pdb_00001f6d
Title : THE STRUCTURE OF UDP-N-ACETYLGLUCOSAMINE 2-EPIMERASE FROM E. COLI.
Authors : Campbell, R.E.; Mosimann, S.C.; Tanner, M.E.; Strynadka, N.C.J.
Deposited on : 2000-06-21
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

<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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

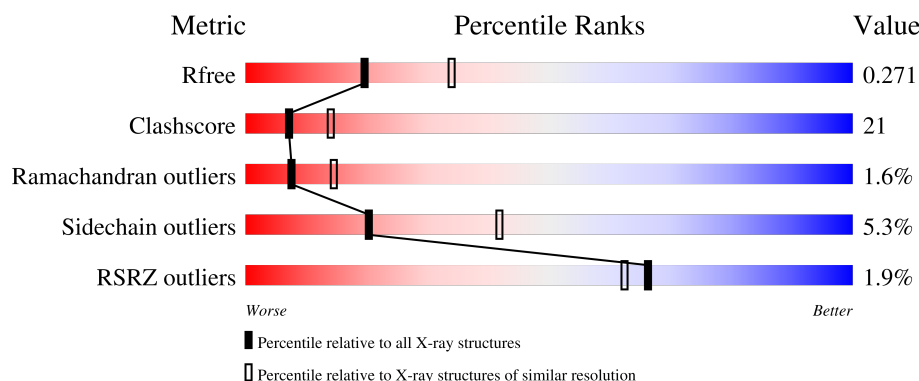
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	376	0% 72% 24% .
1	B	376	2% 62% 34% ..
1	C	376	3% 60% 32% 5% .
1	D	376	2% 65% 31% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12674 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-N-ACETYLGLUCOSAMINE 2-EPIMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	Se	0	1	0
			2977	1888	522	553	4	10			
1	B	372	Total	C	N	O	S	Se	0	4	0
			2968	1882	524	549	4	9			
1	C	367	Total	C	N	O	S	Se	0	0	0
			2899	1841	509	536	4	9			
1	D	374	Total	C	N	O	S	Se	0	0	0
			2957	1876	520	547	4	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P27828
A	16	MSE	MET	modified residue	UNP P27828
A	42	MSE	MET	modified residue	UNP P27828
A	61	MSE	MET	modified residue	UNP P27828
A	143	MSE	MET	modified residue	UNP P27828
A	185	MSE	MET	modified residue	UNP P27828
A	207	MSE	MET	modified residue	UNP P27828
A	280	MSE	MET	modified residue	UNP P27828
A	307	MSE	MET	modified residue	UNP P27828
A	349	MSE	MET	modified residue	UNP P27828
B	1	MSE	MET	modified residue	UNP P27828
B	16	MSE	MET	modified residue	UNP P27828
B	42	MSE	MET	modified residue	UNP P27828
B	61	MSE	MET	modified residue	UNP P27828
B	143	MSE	MET	modified residue	UNP P27828
B	185	MSE	MET	modified residue	UNP P27828
B	207	MSE	MET	modified residue	UNP P27828
B	280	MSE	MET	modified residue	UNP P27828
B	307	MSE	MET	modified residue	UNP P27828
B	349	MSE	MET	modified residue	UNP P27828
C	1	MSE	MET	modified residue	UNP P27828

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Chain	Residue	Modelled	Actual	Comment	Reference
C	16	MSE	MET	modified residue	UNP P27828
C	42	MSE	MET	modified residue	UNP P27828
C	61	MSE	MET	modified residue	UNP P27828
C	143	MSE	MET	modified residue	UNP P27828
C	185	MSE	MET	modified residue	UNP P27828
C	207	MSE	MET	modified residue	UNP P27828
C	280	MSE	MET	modified residue	UNP P27828
C	307	MSE	MET	modified residue	UNP P27828
C	349	MSE	MET	modified residue	UNP P27828
D	1	MSE	MET	modified residue	UNP P27828
D	16	MSE	MET	modified residue	UNP P27828
D	42	MSE	MET	modified residue	UNP P27828
D	61	MSE	MET	modified residue	UNP P27828
D	143	MSE	MET	modified residue	UNP P27828
D	185	MSE	MET	modified residue	UNP P27828
D	207	MSE	MET	modified residue	UNP P27828
D	280	MSE	MET	modified residue	UNP P27828
D	307	MSE	MET	modified residue	UNP P27828
D	349	MSE	MET	modified residue	UNP P27828

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

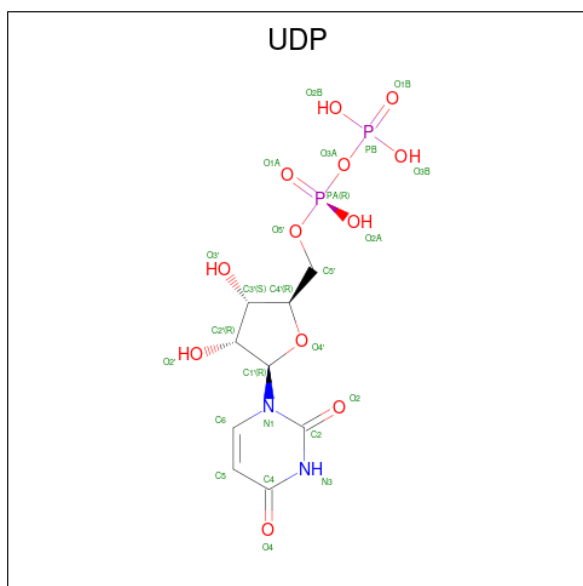
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0

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

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



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

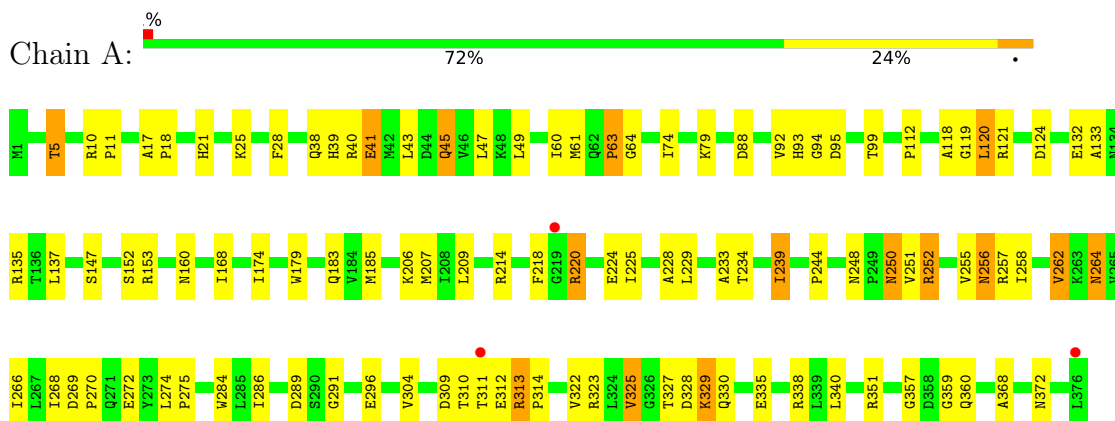
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	229	Total O 229 229	0	0
5	B	216	Total O 216 216	0	0
5	C	140	Total O 140 140	0	0
5	D	180	Total O 180 180	0	0

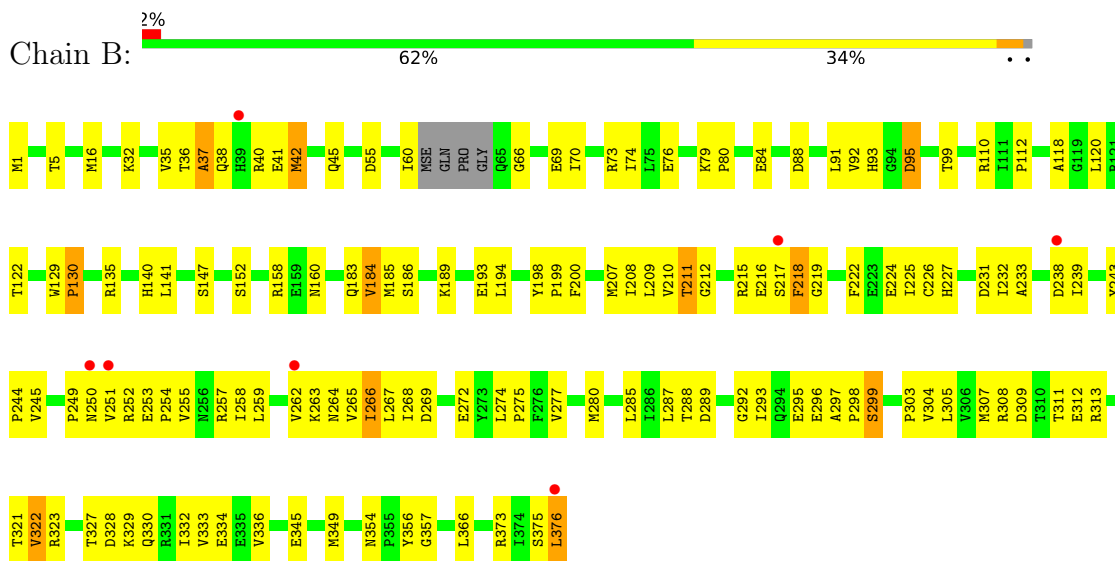
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

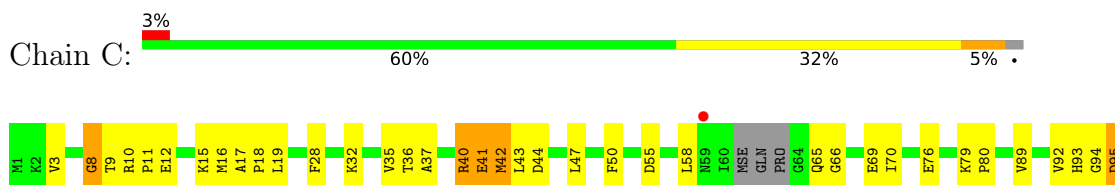
• Molecule 1: UDP-N-ACETYLGLUCOSAMINE 2-EPIMERASE

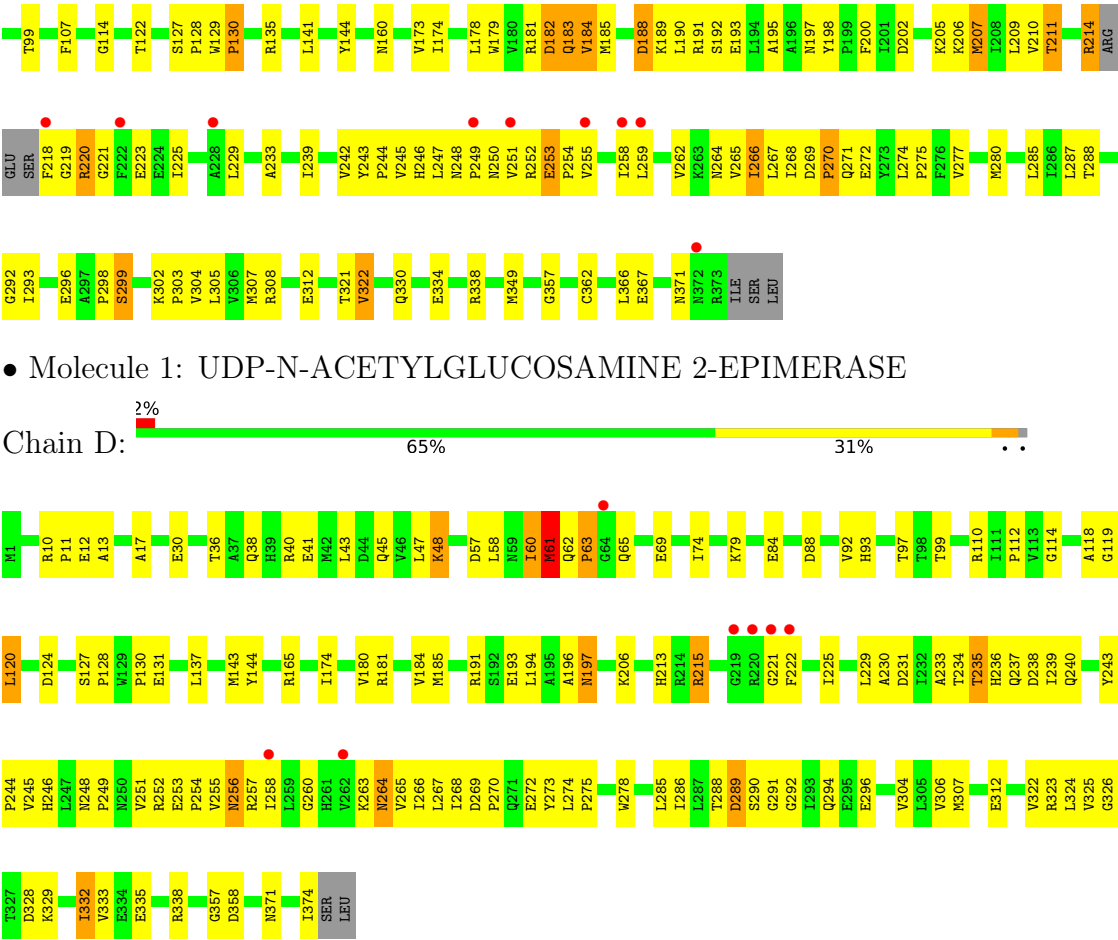


• Molecule 1: UDP-N-ACETYLGLUCOSAMINE 2-EPIMERASE



• Molecule 1: UDP-N-ACETYLGLUCOSAMINE 2-EPIMERASE





● Molecule 1: UDP-N-ACETYLGLUCOSAMINE 2-EPIMERASE

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.01Å 94.54Å 100.97Å 90.00° 109.13° 90.00°	Depositor
Resolution (Å)	30.32 – 2.50 30.32 – 2.50	Depositor EDS
% Data completeness (in resolution range)	87.6 (30.32-2.50) 87.7 (30.32-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.20 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.198 , 0.271 0.198 , 0.271	Depositor DCC
R_{free} test set	5121 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12674	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1284e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, NA, 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	0.61	0/3035	1.00	7/4112 (0.2%)
1	B	0.60	0/3037	0.98	3/4113 (0.1%)
1	C	0.54	0/2951	0.95	3/3999 (0.1%)
1	D	0.57	0/3011	0.95	4/4081 (0.1%)
All	All	0.58	0/12034	0.97	17/16305 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	THR	N-CA-C	-7.87	104.16	114.31
1	D	358	ASP	N-CA-CB	-6.78	102.03	110.98
1	C	95	ASP	N-CA-C	6.47	119.17	110.88
1	B	356	TYR	N-CA-C	6.18	119.85	112.93
1	B	122	THR	N-CA-C	-6.17	106.07	113.97
1	A	325	VAL	CA-C-N	-5.72	116.61	122.27
1	A	325	VAL	C-N-CA	-5.72	116.61	122.27
1	B	95	ASP	N-CA-C	5.71	119.36	111.71
1	D	131	GLU	N-CA-C	5.68	117.14	111.07
1	D	258	ILE	CB-CA-C	-5.51	107.03	111.71
1	C	94	GLY	N-CA-C	5.47	121.20	111.02
1	A	327	THR	N-CA-C	-5.10	105.75	112.94
1	A	359	GLY	N-CA-C	-5.08	108.32	115.32
1	D	332	ILE	CB-CA-C	-5.05	105.51	111.97
1	A	257	ARG	N-CA-C	-5.04	105.91	111.71
1	A	313	ARG	CA-C-N	5.01	124.61	119.05
1	A	313	ARG	C-N-CA	5.01	124.61	119.05

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	2977	0	2998	108	0
1	B	2968	0	2992	144	0
1	C	2899	0	2919	120	0
1	D	2957	0	2980	124	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	25	0	11	1	0
4	B	25	0	11	1	0
4	C	25	0	11	1	0
4	D	25	0	11	2	0
5	A	229	0	0	14	0
5	B	216	0	0	11	0
5	C	140	0	0	5	0
5	D	180	0	0	7	0
All	All	12674	0	11933	495	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 21.

All (495) 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:264:ASN:HA	5:A:1463:HOH:O	1.51	1.10
1:C:16:MSE:HE1	1:C:19:LEU:HD23	1.36	1.08
1:D:288:THR:HG22	1:D:290:SER:H	1.15	1.04
1:D:307:MSE:HE3	1:D:332:ILE:HG21	1.41	1.01
1:A:325:VAL:HG12	1:A:335:GLU:HG3	1.42	1.01
1:A:323:ARG:NH2	1:A:338:ARG:HH12	1.60	0.97
1:B:268:ILE:HG22	1:B:269:ASP:H	1.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:GLN:HG2	1:C:69:GLU:HG2	1.50	0.92
1:B:280:MSE:HE3	1:B:293:ILE:HG23	1.55	0.86
1:C:233:ALA:HB1	1:C:264:ASN:HB2	1.57	0.86
1:A:220:ARG:NH1	1:A:220:ARG:HB2	1.91	0.84
1:B:37:ALA:HB1	1:B:40:ARG:HB2	1.58	0.84
1:C:207:MSE:HE2	1:C:242:VAL:HG21	1.57	0.84
1:B:218:PHE:HB2	1:B:251:VAL:HG13	1.57	0.83
1:B:268:ILE:HG22	1:B:269:ASP:N	1.94	0.82
1:C:95:ASP:HB3	1:C:135:ARG:HB3	1.62	0.82
1:B:304:VAL:HB	1:B:322:VAL:HG22	1.61	0.81
1:D:60:ILE:HD11	1:D:74:ILE:HD11	1.61	0.81
1:D:40:ARG:HH11	1:D:40:ARG:HG2	1.45	0.80
1:A:118:ALA:HA	5:A:1444:HOH:O	1.82	0.80
1:B:232:ILE:HG22	1:B:239:ILE:HD11	1.62	0.80
1:C:304:VAL:HB	1:C:322:VAL:HG22	1.64	0.79
1:B:189:LYS:O	1:B:193:GLU:HG3	1.83	0.79
1:B:16:MSE:HE1	1:B:93:HIS:CD2	2.18	0.78
1:D:12:GLU:HG2	5:D:4420:HOH:O	1.82	0.78
1:B:280:MSE:CE	1:B:293:ILE:HG23	2.13	0.78
1:C:247:LEU:HB3	1:C:251:VAL:HG23	1.66	0.78
1:A:256:ASN:HD22	1:A:256:ASN:H	1.31	0.78
1:A:233:ALA:HB1	1:A:264:ASN:HB3	1.66	0.77
1:B:226:CYS:HB3	1:B:259:LEU:HD11	1.66	0.77
1:D:120:LEU:HD12	1:D:120:LEU:N	2.00	0.77
1:D:197:ASN:N	1:D:197:ASN:HD22	1.82	0.77
1:D:233:ALA:HB1	1:D:264:ASN:HB2	1.66	0.77
1:D:213:HIS:HB2	1:D:215:ARG:NH2	1.99	0.76
1:A:325:VAL:CG1	1:A:335:GLU:HG3	2.16	0.75
1:A:250:ASN:HD22	1:A:250:ASN:H	1.35	0.75
1:A:323:ARG:CZ	1:A:338:ARG:HH12	1.98	0.75
1:B:272:GLU:O	1:B:275:PRO:HD2	1.87	0.74
1:B:251:VAL:HG12	1:B:251:VAL:O	1.87	0.74
1:C:253:GLU:H	1:C:254:PRO:HD2	1.51	0.74
1:A:286:ILE:HB	1:A:304:VAL:HG22	1.68	0.74
1:D:291:GLY:HA2	1:D:294:GLN:HE21	1.51	0.74
1:D:221:GLY:O	1:D:225:ILE:HD13	1.87	0.73
1:B:252:ARG:HG3	1:B:253:GLU:H	1.52	0.73
1:C:233:ALA:HB1	1:C:264:ASN:CB	2.18	0.73
1:A:174:ILE:HD12	1:A:357:GLY:HA3	1.68	0.72
1:C:259:LEU:HD11	1:C:267:LEU:HD11	1.71	0.72
1:D:274:LEU:HB3	1:D:275:PRO:HD3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:O	1:A:132:GLU:HG2	1.89	0.72
1:B:36:THR:HG22	1:B:36:THR:O	1.87	0.72
1:B:38:GLN:HA	1:B:60:ILE:C	2.14	0.72
1:A:239:ILE:C	1:A:239:ILE:HD12	2.15	0.72
1:B:1:MSE:HE1	1:B:373:ARG:HG3	1.71	0.72
1:C:178:LEU:O	1:C:182:ASP:HB2	1.90	0.72
1:D:338:ARG:HH11	1:D:338:ARG:HG2	1.55	0.72
1:C:37:ALA:HB3	1:C:40:ARG:HD2	1.72	0.71
1:B:212:GLY:HA2	1:B:289:ASP:OD1	1.90	0.71
1:B:42:MSE:HE2	1:B:45:GLN:HE22	1.55	0.71
1:C:214:ARG:H	1:C:214:ARG:HD3	1.54	0.71
1:D:243:TYR:CE1	1:D:245:VAL:HB	2.25	0.71
1:A:60:ILE:HD11	1:A:74:ILE:HD11	1.73	0.70
1:D:92:VAL:HB	1:D:99:THR:HG23	1.73	0.70
1:A:220:ARG:HB2	1:A:220:ARG:CZ	2.20	0.70
1:A:309:ASP:O	1:A:310:THR:HG23	1.89	0.70
1:B:243:TYR:CE1	1:B:245:VAL:HB	2.26	0.70
1:B:211:THR:HG22	1:B:288:THR:OG1	1.91	0.70
1:D:291:GLY:HA2	1:D:294:GLN:NE2	2.07	0.70
1:D:328:ASP:O	1:D:332:ILE:HG12	1.91	0.70
1:A:250:ASN:HD22	1:A:250:ASN:N	1.89	0.69
1:D:60:ILE:O	1:D:60:ILE:HG22	1.92	0.69
1:D:288:THR:HG22	1:D:289:ASP:N	2.07	0.69
1:B:287:LEU:HD23	1:B:305:LEU:HB2	1.73	0.69
1:B:268:ILE:CG2	1:B:269:ASP:H	2.05	0.69
1:B:194:LEU:HD21	1:B:274:LEU:HD23	1.73	0.68
1:D:307:MSE:CE	1:D:332:ILE:HG21	2.22	0.68
1:C:36:THR:HG22	1:C:58:LEU:HD12	1.75	0.68
1:B:357:GLY:HA2	5:B:2558:HOH:O	1.92	0.68
1:D:263:LYS:HG3	1:D:264:ASN:N	2.09	0.68
1:D:325:VAL:CG1	1:D:335:GLU:HG3	2.24	0.68
1:A:256:ASN:HD22	1:A:256:ASN:N	1.92	0.67
1:B:252:ARG:HG3	1:B:253:GLU:N	2.08	0.67
1:C:220:ARG:HD2	1:C:221:GLY:N	2.10	0.67
1:A:248:ASN:O	1:A:252:ARG:HG3	1.94	0.67
1:B:233:ALA:HB1	1:B:264:ASN:HB3	1.77	0.67
1:C:292:GLY:O	1:C:296:GLU:HG3	1.95	0.67
1:D:325:VAL:HG12	1:D:335:GLU:HG3	1.77	0.67
1:B:227:HIS:HB3	1:B:329:LYS:HD2	1.78	0.66
1:D:286:ILE:HB	1:D:304:VAL:HG22	1.78	0.66
1:C:274:LEU:HB3	1:C:275:PRO:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:LEU:HD23	1:C:305:LEU:HB2	1.77	0.66
1:A:120:LEU:HB3	5:A:1593:HOH:O	1.96	0.66
1:B:227:HIS:CB	1:B:329:LYS:HD2	2.26	0.65
1:C:304:VAL:HB	1:C:322:VAL:CG2	2.26	0.65
1:D:288:THR:HG22	1:D:289:ASP:H	1.60	0.65
1:B:253:GLU:N	1:B:254:PRO:HD2	2.10	0.65
1:C:251:VAL:C	1:C:253:GLU:H	2.05	0.65
1:B:250:ASN:ND2	1:B:251:VAL:HG23	2.11	0.65
1:B:265:VAL:C	1:B:266:ILE:HD12	2.22	0.65
1:D:174:ILE:HD13	1:D:357:GLY:HA3	1.78	0.65
1:C:225:ILE:O	1:C:229:LEU:HD13	1.97	0.65
1:C:92:VAL:HB	1:C:99:THR:HG23	1.80	0.64
1:A:120:LEU:N	1:A:120:LEU:HD12	2.12	0.64
1:A:133:ALA:O	1:A:137:LEU:HG	1.97	0.64
1:A:153:ARG:HB2	1:A:168:ILE:HD11	1.80	0.64
1:D:253:GLU:N	1:D:254:PRO:HD2	2.12	0.64
1:B:35:VAL:HG12	1:B:37:ALA:H	1.62	0.64
1:C:9:THR:OG1	1:C:12:GLU:HB2	1.98	0.64
1:D:120:LEU:N	1:D:120:LEU:CD1	2.61	0.64
1:B:329:LYS:O	1:B:333:VAL:HG23	1.99	0.63
1:C:262:VAL:HG12	1:C:264:ASN:H	1.61	0.63
1:C:266:ILE:O	1:C:266:ILE:HG22	1.98	0.63
1:D:118:ALA:HA	5:D:4492:HOH:O	1.97	0.63
1:A:239:ILE:HD12	1:A:239:ILE:O	1.99	0.63
1:D:36:THR:HB	1:D:60:ILE:HD11	1.79	0.63
1:D:307:MSE:HE3	1:D:332:ILE:CG2	2.23	0.63
1:D:265:VAL:C	1:D:266:ILE:HD12	2.24	0.63
1:D:43:LEU:O	1:D:47:LEU:HG	1.99	0.63
1:A:291:GLY:HA3	1:A:313:ARG:NH1	2.14	0.63
1:A:258:ILE:N	1:A:258:ILE:HD12	2.13	0.62
1:B:266:ILE:HD12	1:B:266:ILE:N	2.14	0.62
1:D:63:PRO:C	1:D:65:GLN:H	2.06	0.62
1:A:5:THR:HG23	5:A:1393:HOH:O	1.98	0.62
1:B:330:GLN:O	1:B:334:GLU:HG3	1.99	0.62
1:C:211:THR:O	1:C:288:THR:HA	2.00	0.62
1:D:180:VAL:HG21	1:D:273:TYR:CE2	2.34	0.62
1:A:258:ILE:HD12	1:A:258:ILE:H	1.65	0.62
1:B:16:MSE:HE1	1:B:93:HIS:CG	2.34	0.62
1:D:143:MSE:HB3	1:D:374:ILE:HG13	1.82	0.62
1:A:311:THR:HG22	1:A:312:GLU:N	2.15	0.61
1:B:66:GLY:O	1:B:70:ILE:HG13	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ILE:HD12	1:B:239:ILE:HD12	1.81	0.61
1:D:40:ARG:HG2	1:D:40:ARG:NH1	2.09	0.61
1:D:292:GLY:HA3	4:D:4377:UDP:O2B	2.01	0.61
1:A:272:GLU:O	1:A:275:PRO:HD2	2.00	0.61
1:C:214:ARG:HH11	1:C:214:ARG:HG3	1.66	0.61
1:C:218:PHE:HB2	1:C:251:VAL:CG1	2.31	0.61
1:A:45:GLN:HE22	1:A:274:LEU:CB	2.13	0.61
1:A:38:GLN:OE1	1:A:63:PRO:HA	2.01	0.61
1:A:224:GLU:HG3	1:A:329:LYS:NZ	2.16	0.61
1:C:40:ARG:HG2	1:C:40:ARG:HH11	1.65	0.60
1:D:243:TYR:CZ	1:D:245:VAL:HB	2.35	0.60
1:D:180:VAL:HG21	1:D:273:TYR:HE2	1.66	0.60
1:D:245:VAL:HG22	1:D:246:HIS:N	2.17	0.60
1:D:338:ARG:HG2	1:D:338:ARG:NH1	2.16	0.60
1:A:311:THR:HB	5:A:1486:HOH:O	2.02	0.60
1:C:246:HIS:HB2	1:C:270:PRO:HG2	1.84	0.60
1:B:222:PHE:HE2	1:B:255:VAL:HG21	1.67	0.59
1:D:63:PRO:C	1:D:65:GLN:N	2.56	0.59
1:B:92:VAL:HB	1:B:99:THR:HG23	1.83	0.59
1:C:303:PRO:HB3	1:C:349:MSE:HB3	1.84	0.59
1:B:267:LEU:HD12	1:B:267:LEU:H	1.68	0.59
1:A:43:LEU:O	1:A:47:LEU:HG	2.03	0.59
1:A:49:LEU:O	1:A:179:TRP:HZ3	1.86	0.58
1:B:1:MSE:CE	1:B:373:ARG:HG3	2.32	0.58
1:D:165:ARG:CZ	1:D:374:ILE:HD11	2.33	0.58
1:A:174:ILE:CD1	1:A:357:GLY:HA3	2.32	0.58
1:D:296:GLU:OE2	4:D:4377:UDP:H3'	2.03	0.58
1:A:323:ARG:CZ	1:A:338:ARG:NH1	2.65	0.58
1:B:16:MSE:CE	1:B:93:HIS:HB2	2.34	0.58
1:B:232:ILE:CG2	1:B:239:ILE:HD11	2.33	0.58
1:C:243:TYR:CE1	1:C:245:VAL:HB	2.39	0.58
1:A:323:ARG:HH22	1:A:338:ARG:HH12	1.49	0.58
1:C:41:GLU:C	1:C:43:LEU:H	2.12	0.58
1:D:272:GLU:O	1:D:275:PRO:HD2	2.04	0.58
1:B:226:CYS:HB3	1:B:259:LEU:CD1	2.32	0.57
1:D:266:ILE:HD12	1:D:266:ILE:N	2.19	0.57
1:B:112:PRO:HD2	1:B:376:LEU:HD23	1.85	0.57
1:B:218:PHE:HB2	1:B:251:VAL:CG1	2.31	0.57
1:A:291:GLY:HA3	1:A:313:ARG:HH12	1.70	0.57
1:B:110[A]:ARG:HD2	5:B:2587:HOH:O	2.05	0.57
1:B:307:MSE:O	1:B:308:ARG:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:ILE:C	1:D:239:ILE:HD12	2.30	0.57
1:D:244:PRO:HB3	1:D:268:ILE:HD11	1.86	0.57
1:B:66:GLY:HA3	1:B:69[A]:GLU:OE1	2.03	0.57
1:C:362:CYS:O	1:C:366:LEU:HG	2.05	0.57
1:B:118:ALA:HB1	5:B:2409:HOH:O	2.04	0.57
1:C:251:VAL:C	1:C:254:PRO:HD2	2.30	0.56
1:C:367:GLU:HG2	5:C:3418:HOH:O	2.03	0.56
1:A:224:GLU:HG3	1:A:329:LYS:CE	2.35	0.56
1:D:257:ARG:HG2	1:D:257:ARG:HH11	1.69	0.56
1:A:120:LEU:N	1:A:120:LEU:CD1	2.69	0.56
1:A:262:VAL:HG12	1:A:264:ASN:HB2	1.87	0.56
1:B:252:ARG:C	1:B:254:PRO:HD2	2.30	0.56
1:C:185:MSE:HE1	1:C:277:VAL:HG12	1.88	0.56
1:D:288:THR:HG22	1:D:290:SER:N	2.01	0.56
1:B:218:PHE:CE2	1:B:254:PRO:HB2	2.41	0.56
1:B:274:LEU:HB3	1:B:275:PRO:HD3	1.88	0.56
1:B:292:GLY:O	1:B:296:GLU:HG3	2.06	0.55
1:C:211:THR:HG22	1:C:288:THR:OG1	2.07	0.55
1:D:234:THR:HA	1:D:237:GLN:HE22	1.70	0.55
1:D:255:VAL:C	1:D:257:ARG:H	2.15	0.55
1:A:323:ARG:NH2	1:A:338:ARG:NH1	2.42	0.55
1:B:88:ASP:HA	1:B:376:LEU:HD11	1.86	0.55
1:C:245:VAL:HG22	1:C:246:HIS:N	2.22	0.55
1:D:248:ASN:HA	5:D:4527:HOH:O	2.07	0.55
1:C:3:VAL:HG22	1:C:89:VAL:CG1	2.37	0.54
1:D:45:GLN:HB3	5:D:4496:HOH:O	2.07	0.54
1:C:245:VAL:C	1:C:270:PRO:HD3	2.33	0.54
1:B:323:ARG:HH12	1:B:345:GLU:CD	2.15	0.54
1:C:371:ASN:HD22	1:C:371:ASN:N	2.05	0.54
1:A:45:GLN:HE22	1:A:274:LEU:HB2	1.70	0.54
1:B:5:THR:HG22	1:B:91:LEU:HD12	1.89	0.54
1:A:220:ARG:HB2	1:A:220:ARG:HH11	1.72	0.54
1:B:373:ARG:HD3	5:B:2444:HOH:O	2.08	0.54
1:C:239:ILE:HD12	1:C:239:ILE:O	2.08	0.53
1:D:62:GLN:O	1:D:65:GLN:HB2	2.08	0.53
1:A:233:ALA:HB1	1:A:264:ASN:CB	2.36	0.53
1:A:296:GLU:OE2	4:A:1377:UDP:H3'	2.07	0.53
1:C:251:VAL:O	1:C:254:PRO:HD2	2.09	0.53
1:C:209:LEU:HD12	1:C:242:VAL:O	2.08	0.53
1:A:21:HIS:HE1	5:A:1487:HOH:O	1.91	0.53
1:A:266:ILE:N	1:A:266:ILE:HD12	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:ILE:CD1	1:D:357:GLY:HA3	2.38	0.53
1:C:218:PHE:HB2	1:C:251:VAL:HG11	1.90	0.53
1:B:285:LEU:HD21	1:B:305:LEU:HD11	1.91	0.53
1:D:215:ARG:HD3	1:D:222:PHE:HE2	1.74	0.53
1:C:44:ASP:HA	1:C:47:LEU:HD12	1.89	0.52
1:C:265:VAL:O	1:C:266:ILE:HG13	2.09	0.52
1:A:218:PHE:HD1	1:A:251:VAL:HG23	1.72	0.52
1:B:332:ILE:O	1:B:336:VAL:HG23	2.08	0.52
1:D:215:ARG:HD3	1:D:222:PHE:CE2	2.45	0.52
1:C:174:ILE:HD13	1:C:357:GLY:O	2.09	0.52
1:B:287:LEU:CD2	1:B:305:LEU:HB2	2.40	0.52
1:C:266:ILE:O	1:C:268:ILE:HG23	2.09	0.52
1:C:35:VAL:HG12	1:C:37:ALA:H	1.74	0.52
1:D:114:GLY:HA2	1:D:144:TYR:HB2	1.91	0.52
1:B:218:PHE:CB	1:B:251:VAL:HG13	2.36	0.52
1:B:262:VAL:C	1:B:264:ASN:H	2.17	0.52
1:B:280:MSE:CE	1:B:297:ALA:HB2	2.40	0.52
1:A:38:GLN:HG2	1:A:60:ILE:CG2	2.40	0.52
1:C:265:VAL:C	1:C:266:ILE:HG13	2.35	0.52
1:D:63:PRO:O	1:D:65:GLN:N	2.44	0.51
1:A:368:ALA:O	1:A:372:ASN:HB2	2.10	0.51
1:C:189:LYS:O	1:C:193:GLU:HG3	2.11	0.51
1:B:233:ALA:O	1:B:264:ASN:ND2	2.42	0.51
1:A:137:LEU:HD11	1:B:141:LEU:HD21	1.93	0.51
1:A:284:TRP:CH2	1:A:340:LEU:HG	2.46	0.51
1:C:206:LYS:HB2	1:C:239:ILE:HG22	1.92	0.51
1:C:259:LEU:C	1:C:259:LEU:HD12	2.35	0.51
1:D:79:LYS:HE3	5:D:4556:HOH:O	2.10	0.51
1:D:267:LEU:HD12	1:D:267:LEU:N	2.25	0.51
1:B:249:PRO:HA	1:B:252:ARG:CD	2.41	0.51
1:B:376:LEU:HB2	5:B:2535:HOH:O	2.10	0.51
1:C:307:MSE:O	1:C:308:ARG:HG2	2.10	0.51
1:B:249:PRO:HA	1:B:252:ARG:NE	2.26	0.51
1:C:211:THR:HG22	1:C:288:THR:HG1	1.75	0.51
1:A:274:LEU:HB3	1:A:275:PRO:HD3	1.93	0.51
1:C:10:ARG:HB3	1:C:11:PRO:CD	2.41	0.51
1:B:5:THR:HG22	1:B:91:LEU:HB2	1.92	0.50
1:C:210:VAL:O	1:C:244:PRO:HD2	2.11	0.50
1:D:230:ALA:O	1:D:234:THR:HG23	2.10	0.50
1:B:323:ARG:HD3	1:C:338:ARG:NH2	2.25	0.50
1:A:45:GLN:HB2	5:A:1537:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:MSE:CA	1:B:16:MSE:HE2	2.41	0.50
1:B:198:TYR:HB3	1:B:200:PHE:CE1	2.46	0.50
1:C:114:GLY:HA2	1:C:144:TYR:HB2	1.93	0.50
1:B:120:LEU:HD12	1:B:120:LEU:N	2.27	0.50
1:D:197:ASN:N	1:D:197:ASN:ND2	2.51	0.50
1:A:225:ILE:O	1:A:228:ALA:HB3	2.11	0.50
1:B:267:LEU:HD12	1:B:267:LEU:N	2.26	0.50
1:C:79:LYS:HB3	1:C:80:PRO:CD	2.42	0.49
1:D:252:ARG:C	1:D:254:PRO:HD2	2.37	0.49
1:C:218:PHE:HB2	1:C:251:VAL:HG12	1.94	0.49
1:D:119:GLY:C	1:D:120:LEU:HD12	2.37	0.49
1:A:311:THR:CG2	1:A:312:GLU:N	2.76	0.49
1:B:194:LEU:HD21	1:B:274:LEU:CD2	2.42	0.49
1:B:218:PHE:HE2	1:B:254:PRO:HB2	1.77	0.49
1:C:247:LEU:HB3	1:C:251:VAL:CG2	2.39	0.49
1:D:306:VAL:HB	1:D:324:LEU:HD23	1.94	0.49
1:A:119:GLY:C	1:A:120:LEU:HD12	2.38	0.49
1:C:253:GLU:C	1:C:255:VAL:H	2.19	0.49
1:B:16:MSE:HE1	1:B:93:HIS:HB2	1.94	0.49
1:C:223:GLU:HG2	1:C:258:ILE:HD11	1.93	0.49
1:D:60:ILE:CD1	1:D:74:ILE:HD11	2.40	0.49
1:B:207:MSE:CE	1:B:209:LEU:HB2	2.43	0.49
1:B:258:ILE:HB	1:B:259:LEU:HD12	1.95	0.49
1:B:280:MSE:HE2	1:B:297:ALA:HB2	1.95	0.49
1:A:64:GLY:N	5:A:1558:HOH:O	2.46	0.48
1:D:245:VAL:CG2	1:D:246:HIS:N	2.76	0.48
1:A:93:HIS:CG	1:A:94:GLY:N	2.80	0.48
1:A:250:ASN:CG	1:A:251:VAL:H	2.21	0.48
1:A:214:ARG:HD3	1:A:214:ARG:H	1.78	0.48
1:B:296:GLU:O	1:B:299:SER:HB2	2.13	0.48
1:A:250:ASN:N	1:A:250:ASN:ND2	2.59	0.48
1:B:60:ILE:HD12	1:B:73:ARG:HB3	1.95	0.48
1:B:227:HIS:HB2	1:B:329:LYS:HD2	1.94	0.48
1:B:298:PRO:HB3	1:B:321:THR:HB	1.95	0.48
1:C:40:ARG:HG2	1:C:40:ARG:NH1	2.29	0.48
1:D:254:PRO:O	1:D:257:ARG:HB3	2.13	0.48
1:D:263:LYS:C	1:D:265:VAL:H	2.21	0.48
1:C:184:VAL:O	1:C:190:LEU:HD23	2.12	0.48
1:C:272:GLU:O	1:C:275:PRO:HD2	2.13	0.48
1:B:376:LEU:HD22	1:B:376:LEU:OXT	2.14	0.48
1:C:17:ALA:N	1:C:18:PRO:HD2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:VAL:O	1:B:244:PRO:HD2	2.13	0.48
1:C:107:PHE:HA	5:C:3401:HOH:O	2.14	0.48
1:D:185:MSE:HA	1:D:191:ARG:NH1	2.29	0.48
1:D:263:LYS:HG3	1:D:264:ASN:H	1.79	0.48
1:D:256:ASN:C	1:D:256:ASN:HD22	2.21	0.47
1:A:25:LYS:HE2	5:A:1510:HOH:O	2.13	0.47
1:B:288:THR:OG1	1:B:289:ASP:N	2.46	0.47
1:B:38:GLN:HB2	5:B:2479:HOH:O	2.14	0.47
4:B:2377:UDP:O2B	4:B:2377:UDP:H5'2	2.14	0.47
1:C:28:PHE:O	1:C:28:PHE:CD1	2.67	0.47
1:A:313:ARG:HG3	1:A:313:ARG:HH11	1.79	0.47
1:B:243:TYR:CD1	1:B:243:TYR:C	2.92	0.47
1:B:259:LEU:HD12	1:B:259:LEU:N	2.29	0.47
1:B:285:LEU:HD21	1:B:305:LEU:CD1	2.44	0.47
1:C:251:VAL:O	1:C:253:GLU:N	2.47	0.47
1:D:60:ILE:O	1:D:61:MSE:C	2.58	0.47
1:D:253:GLU:N	1:D:254:PRO:CD	2.78	0.47
1:C:214:ARG:HG3	1:C:214:ARG:NH1	2.28	0.47
1:D:322:VAL:CG1	1:D:323:ARG:N	2.77	0.47
1:B:272:GLU:C	1:B:275:PRO:HD2	2.39	0.47
1:C:243:TYR:HB3	1:C:267:LEU:HD23	1.96	0.47
1:D:184:VAL:O	1:D:191:ARG:NH1	2.48	0.47
1:D:248:ASN:CG	1:D:249:PRO:HD2	2.40	0.47
1:D:269:ASP:O	1:D:270:PRO:C	2.56	0.47
1:A:225:ILE:O	1:A:229:LEU:HG	2.15	0.47
1:B:185:MSE:HE1	1:B:277:VAL:HB	1.97	0.47
1:C:259:LEU:HD11	1:C:267:LEU:CD1	2.41	0.46
1:B:36:THR:HG21	1:B:74:ILE:HD11	1.98	0.46
1:C:272:GLU:C	1:C:275:PRO:HD2	2.40	0.46
1:B:211:THR:O	1:B:288:THR:HA	2.15	0.46
1:B:304:VAL:HB	1:B:322:VAL:CG2	2.36	0.46
1:D:38:GLN:OE1	1:D:63:PRO:HB3	2.15	0.46
1:A:39:HIS:HB3	1:A:41:GLU:OE2	2.15	0.46
1:C:188:ASP:OD1	1:C:191:ARG:NH1	2.49	0.46
1:B:79:LYS:HE2	5:B:2434:HOH:O	2.16	0.46
1:D:257:ARG:HG2	1:D:257:ARG:NH1	2.31	0.46
1:C:268:ILE:HD12	1:C:271:GLN:NE2	2.31	0.46
1:D:222:PHE:CD1	1:D:222:PHE:C	2.94	0.46
1:B:199:PRO:HA	5:B:2575:HOH:O	2.16	0.46
1:D:124:ASP:HB3	1:D:127:SER:O	2.15	0.46
1:D:225:ILE:O	1:D:229:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:GLN:HE21	1:D:266:ILE:HD11	1.81	0.46
1:C:298:PRO:HB3	1:C:321:THR:HB	1.98	0.46
1:D:97:THR:HG23	5:D:4401:HOH:O	2.17	0.46
1:D:231:ASP:O	1:D:235:THR:OG1	2.33	0.46
1:B:88:ASP:HA	1:B:376:LEU:HD21	1.97	0.45
1:C:80:PRO:HA	5:C:3493:HOH:O	2.15	0.45
1:B:253:GLU:N	1:B:254:PRO:CD	2.78	0.45
1:C:285:LEU:HD11	1:C:305:LEU:HG	1.99	0.45
1:D:243:TYR:CD1	1:D:243:TYR:C	2.92	0.45
1:D:326:GLY:O	1:D:332:ILE:HD11	2.16	0.45
1:A:256:ASN:H	1:A:256:ASN:ND2	2.09	0.45
1:B:217:SER:O	1:B:219:GLY:N	2.50	0.45
1:D:193:GLU:O	1:D:196:ALA:HB3	2.17	0.45
1:A:45:GLN:HE22	1:A:274:LEU:HB3	1.80	0.45
1:A:313:ARG:HH11	1:A:313:ARG:CG	2.28	0.45
1:B:328:ASP:O	1:B:332:ILE:HG13	2.16	0.45
1:D:180:VAL:O	1:D:184:VAL:HG23	2.16	0.45
1:B:189:LYS:HE2	5:B:2594:HOH:O	2.17	0.45
1:C:16:MSE:CE	1:C:19:LEU:HD23	2.26	0.45
1:A:95:ASP:HB3	1:A:135:ARG:HB3	1.98	0.45
1:B:252:ARG:CG	1:B:253:GLU:N	2.78	0.45
5:C:3446:HOH:O	1:D:69:GLU:HG2	2.17	0.45
1:A:49:LEU:O	1:A:179:TRP:CZ3	2.68	0.45
1:A:118:ALA:HB1	5:A:1383:HOH:O	2.16	0.45
1:A:147:SER:HB3	1:A:152:SER:OG	2.17	0.45
1:A:244:PRO:HA	1:A:268:ILE:HG13	1.99	0.45
1:B:35:VAL:HG12	1:B:37:ALA:N	2.32	0.45
1:D:194:LEU:HD13	1:D:278:TRP:HB2	1.98	0.45
1:A:38:GLN:NE2	1:A:63:PRO:HB3	2.32	0.45
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.82	0.45
1:A:250:ASN:ND2	1:A:251:VAL:H	2.14	0.45
1:C:211:THR:HG21	1:C:293:ILE:CD1	2.47	0.44
1:A:153:ARG:CB	1:A:168:ILE:HD11	2.47	0.44
1:B:258:ILE:HB	1:B:259:LEU:CD1	2.47	0.44
1:D:288:THR:CG2	1:D:289:ASP:H	2.29	0.44
1:C:66:GLY:O	1:C:70:ILE:HG13	2.17	0.44
1:D:38:GLN:HB3	1:D:63:PRO:HD3	2.00	0.44
1:B:16:MSE:CE	1:B:93:HIS:CB	2.95	0.44
1:B:32:LYS:HA	1:B:55:ASP:OD2	2.17	0.44
1:B:252:ARG:CG	1:B:253:GLU:H	2.24	0.44
1:C:107:PHE:HB2	5:C:3402:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:3377:UDP:O2B	4:C:3377:UDP:H5'2	2.18	0.44
1:D:325:VAL:HG23	1:D:332:ILE:CD1	2.47	0.44
1:C:16:MSE:HE3	1:C:19:LEU:HB3	2.00	0.44
1:C:269:ASP:O	1:C:270:PRO:C	2.61	0.44
1:D:325:VAL:HG23	1:D:332:ILE:HD12	1.99	0.44
1:A:256:ASN:N	1:A:256:ASN:ND2	2.65	0.44
1:B:249:PRO:HA	1:B:252:ARG:HD3	2.00	0.44
1:D:255:VAL:C	1:D:257:ARG:N	2.73	0.44
1:C:192:SER:O	1:C:195:ALA:HB3	2.17	0.44
1:C:280:MSE:O	1:C:302:LYS:HE3	2.18	0.44
1:D:127:SER:HA	1:D:128:PRO:HA	1.89	0.44
1:A:28:PHE:CD1	1:A:28:PHE:C	2.96	0.44
1:C:16:MSE:SE	1:C:93:HIS:HB2	2.68	0.44
1:D:251:VAL:O	1:D:255:VAL:HG23	2.17	0.44
1:B:251:VAL:O	1:B:251:VAL:CG1	2.59	0.43
1:C:15:LYS:HE2	1:C:173:VAL:HB	1.99	0.43
1:C:179:TRP:CZ3	1:C:184:VAL:HG21	2.53	0.43
1:C:259:LEU:HD22	1:C:265:VAL:HG11	1.99	0.43
1:D:48:LYS:O	1:D:48:LYS:HD3	2.18	0.43
1:A:93:HIS:ND1	1:A:94:GLY:N	2.65	0.43
1:A:95:ASP:HB3	1:A:135:ARG:HD3	1.99	0.43
1:B:16:MSE:HE1	1:B:93:HIS:CB	2.48	0.43
1:B:208:ILE:CD1	1:B:239:ILE:HD12	2.46	0.43
1:C:218:PHE:CD1	1:C:219:GLY:N	2.85	0.43
1:B:184:VAL:C	1:B:186:SER:H	2.26	0.43
1:D:10:ARG:N	1:D:11:PRO:HD2	2.34	0.43
1:D:45:GLN:N	5:D:4496:HOH:O	2.51	0.43
1:A:207:MSE:HE3	1:A:209:LEU:HB2	1.99	0.43
1:B:79:LYS:N	1:B:80:PRO:HD2	2.33	0.43
1:B:158[A]:ARG:NH2	5:B:2400:HOH:O	2.52	0.43
1:B:224:GLU:HG2	1:B:327:THR:O	2.17	0.43
1:C:141:LEU:HD21	1:D:137:LEU:HD11	1.99	0.43
1:D:312:GLU:O	1:D:312:GLU:HG2	2.17	0.43
1:D:329:LYS:O	1:D:333:VAL:HG23	2.18	0.43
1:A:132:GLU:HB3	5:A:1387:HOH:O	2.17	0.43
1:A:311:THR:HG22	1:A:313:ARG:N	2.34	0.43
1:D:236:HIS:O	1:D:239:ILE:HG13	2.18	0.43
1:A:88:ASP:O	1:A:112:PRO:HG2	2.19	0.43
1:B:120:LEU:N	1:B:120:LEU:CD1	2.81	0.43
1:A:313:ARG:N	1:A:314:PRO:CD	2.82	0.43
1:A:224:GLU:CG	1:A:329:LYS:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:PRO:HD2	1:B:376:LEU:CD2	2.48	0.42
1:A:179:TRP:O	1:A:183:GLN:HB2	2.20	0.42
1:A:250:ASN:CG	1:A:251:VAL:N	2.77	0.42
1:B:225:ILE:HD11	1:B:327:THR:HG22	2.01	0.42
1:C:40:ARG:NH1	1:C:44:ASP:OD1	2.52	0.42
1:C:93:HIS:ND1	1:C:93:HIS:C	2.77	0.42
1:D:13:ALA:O	1:D:17:ALA:HB2	2.18	0.42
1:B:200:PHE:CE2	1:B:266:ILE:HG21	2.54	0.42
1:B:266:ILE:N	1:B:266:ILE:CD1	2.81	0.42
1:A:250:ASN:H	1:A:250:ASN:ND2	2.10	0.42
1:A:251:VAL:O	1:A:255:VAL:HG23	2.20	0.42
1:A:262:VAL:C	1:A:264:ASN:N	2.78	0.42
1:B:147:SER:HB3	1:B:152:SER:HB2	2.02	0.42
1:B:215:ARG:NH1	1:B:222:PHE:CD1	2.88	0.42
1:C:181:ARG:C	1:C:183:GLN:H	2.27	0.42
1:D:88:ASP:O	1:D:112:PRO:HG2	2.20	0.42
1:D:253:GLU:O	1:D:257:ARG:HB2	2.19	0.42
1:C:330:GLN:O	1:C:334:GLU:HB2	2.19	0.42
1:A:10:ARG:N	1:A:11:PRO:HD2	2.35	0.42
1:B:40:ARG:O	1:B:40:ARG:HG2	2.20	0.42
1:B:200:PHE:CD2	1:B:266:ILE:HG12	2.55	0.42
1:D:285:LEU:HD12	1:D:286:ILE:H	1.84	0.42
5:A:1445:HOH:O	1:B:140:HIS:CE1	2.72	0.41
1:B:95:ASP:HB3	1:B:135:ARG:HB3	2.02	0.41
1:D:93:HIS:ND1	1:D:93:HIS:C	2.78	0.41
1:D:194:LEU:HD22	1:D:275:PRO:HA	2.02	0.41
1:B:303:PRO:HB3	1:B:349:MSE:CB	2.49	0.41
1:C:202:ASP:OD2	1:C:205:LYS:HG3	2.19	0.41
1:D:45:GLN:CD	1:D:272:GLU:HB3	2.45	0.41
1:D:60:ILE:O	1:D:61:MSE:O	2.37	0.41
1:D:236:HIS:HB3	1:D:238:ASP:OD1	2.20	0.41
1:B:303:PRO:HB3	1:B:349:MSE:HB2	2.01	0.41
1:C:41:GLU:C	1:C:43:LEU:N	2.78	0.41
1:C:245:VAL:CG2	1:C:246:HIS:N	2.83	0.41
1:D:206:LYS:HB2	1:D:239:ILE:HG22	2.01	0.41
1:A:121:ARG:O	1:A:312:GLU:OE2	2.38	0.41
1:A:312:GLU:O	1:A:312:GLU:HG2	2.20	0.41
1:C:28:PHE:CD1	1:C:28:PHE:C	2.98	0.41
1:C:32:LYS:HE3	1:C:55:ASP:OD2	2.20	0.41
1:C:210:VAL:HG21	1:C:229:LEU:HD21	2.02	0.41
1:D:213:HIS:CD2	1:D:290:SER:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:PRO:HA	1:B:257:ARG:HD2	2.01	0.41
1:A:206:LYS:HD3	1:A:284:TRP:CD2	2.56	0.41
1:A:269:ASP:O	1:A:270:PRO:C	2.62	0.41
1:B:298:PRO:HG2	1:B:354:ASN:ND2	2.36	0.41
1:D:213:HIS:HB2	1:D:215:ARG:HH21	1.81	0.41
1:B:129:TRP:HA	1:B:130:PRO:HA	1.87	0.41
1:C:127:SER:HA	1:C:128:PRO:HA	1.89	0.41
1:A:79:LYS:HE3	5:A:1580:HOH:O	2.21	0.41
1:A:92:VAL:HB	1:A:99:THR:HG23	2.02	0.41
1:C:253:GLU:HB2	1:C:254:PRO:CD	2.51	0.41
1:D:36:THR:HG22	1:D:58:LEU:HB2	2.02	0.41
1:A:360:GLN:HA	5:A:1413:HOH:O	2.21	0.41
1:B:1:MSE:HE1	1:B:373:ARG:CG	2.45	0.41
1:B:258:ILE:C	1:B:259:LEU:HD12	2.45	0.41
1:C:214:ARG:HD3	1:C:214:ARG:N	2.29	0.41
1:C:296:GLU:O	1:C:299:SER:HB2	2.20	0.41
1:C:200:PHE:CD1	1:C:266:ILE:HD13	2.55	0.41
1:C:225:ILE:O	1:C:225:ILE:CG2	2.69	0.41
1:C:233:ALA:O	1:C:264:ASN:ND2	2.54	0.41
1:C:248:ASN:O	1:C:250:ASN:N	2.54	0.41
1:B:295:GLU:OE2	1:B:313:ARG:NE	2.37	0.40
1:C:251:VAL:C	1:C:253:GLU:N	2.72	0.40
1:B:189:LYS:HB3	5:B:2594:HOH:O	2.21	0.40
1:C:248:ASN:C	1:C:250:ASN:H	2.28	0.40
1:D:288:THR:CG2	1:D:289:ASP:N	2.76	0.40
1:A:206:LYS:HD3	1:A:284:TRP:CE2	2.56	0.40
1:B:262:VAL:O	1:B:264:ASN:N	2.54	0.40
1:C:8:GLY:O	1:C:43:LEU:HD22	2.21	0.40
1:C:243:TYR:C	1:C:243:TYR:CD1	3.00	0.40
1:A:17:ALA:N	1:A:18:PRO:HD2	2.35	0.40
1:C:17:ALA:HB1	1:C:50:PHE:CG	2.56	0.40
1:C:129:TRP:HA	1:C:130:PRO:HA	1.92	0.40
1:B:88:ASP:HA	1:B:376:LEU:CG	2.52	0.40
1:B:211:THR:HG22	1:B:288:THR:HG1	1.85	0.40
1:D:263:LYS:C	1:D:265:VAL:N	2.79	0.40

There are no symmetry-related clashes.

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	375/376 (100%)	350 (93%)	23 (6%)	2 (0%)	24	43
1	B	372/376 (99%)	347 (93%)	18 (5%)	7 (2%)	6	11
1	C	361/376 (96%)	318 (88%)	34 (9%)	9 (2%)	4	7
1	D	372/376 (99%)	340 (91%)	27 (7%)	5 (1%)	9	18
All	All	1480/1504 (98%)	1355 (92%)	102 (7%)	23 (2%)	7	14

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	37	ALA
1	D	61	MSE
1	A	61	MSE
1	B	218	PHE
1	B	263	LYS
1	C	40	ARG
1	C	182	ASP
1	B	375	SER
1	C	252	ARG
1	C	266	ILE
1	D	63	PRO
1	D	264	ASN
1	B	184	VAL
1	C	253	GLU
1	B	41	GLU
1	B	183	GLN
1	C	249	PRO
1	C	42	MSE
1	D	60	ILE
1	D	260	GLY
1	A	63	PRO
1	C	184	VAL
1	C	8	GLY

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	328/317 (104%)	309 (94%)	19 (6%)	18	38
1	B	328/317 (104%)	311 (95%)	17 (5%)	21	42
1	C	318/317 (100%)	301 (95%)	17 (5%)	20	42
1	D	325/317 (102%)	309 (95%)	16 (5%)	22	45
All	All	1299/1268 (102%)	1230 (95%)	69 (5%)	20	42

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	41	GLU
1	A	45	GLN
1	A	120	LEU
1	A	185	MSE
1	A	220	ARG
1	A	234	THR
1	A	239	ILE
1	A	250	ASN
1	A	252	ARG
1	A	256	ASN
1	A	262	VAL
1	A	264	ASN
1	A	289	ASP
1	A	322	VAL
1	A	328	ASP
1	A	329	LYS
1	A	330	GLN
1	A	351	ARG
1	B	42	MSE
1	B	76	GLU
1	B	84	GLU
1	B	130	PRO
1	B	160	ASN

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Mol	Chain	Res	Type
1	B	211	THR
1	B	216	GLU
1	B	231	ASP
1	B	238	ASP
1	B	266	ILE
1	B	299	SER
1	B	309	ASP
1	B	311	THR
1	B	312	GLU
1	B	322	VAL
1	B	366	LEU
1	B	376	LEU
1	C	41	GLU
1	C	42	MSE
1	C	76	GLU
1	C	130	PRO
1	C	160	ASN
1	C	183	GLN
1	C	188	ASP
1	C	197	ASN
1	C	198	TYR
1	C	207	MSE
1	C	211	THR
1	C	214	ARG
1	C	220	ARG
1	C	270	PRO
1	C	299	SER
1	C	312	GLU
1	C	322	VAL
1	D	30	GLU
1	D	41	GLU
1	D	48	LYS
1	D	57	ASP
1	D	61	MSE
1	D	84	GLU
1	D	110	ARG
1	D	120	LEU
1	D	130	PRO
1	D	181	ARG
1	D	197	ASN
1	D	215	ARG
1	D	235	THR

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Mol	Chain	Res	Type
1	D	256	ASN
1	D	289	ASP
1	D	371	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	45	GLN
1	A	197	ASN
1	A	227	HIS
1	A	250	ASN
1	A	256	ASN
1	A	271	GLN
1	A	294	GLN
1	B	45	GLN
1	B	160	ASN
1	B	183	GLN
1	B	344	ASN
1	B	354	ASN
1	C	197	ASN
1	C	227	HIS
1	C	236	HIS
1	C	237	GLN
1	C	248	ASN
1	C	264	ASN
1	C	271	GLN
1	C	281	ASN
1	C	371	ASN
1	D	21	HIS
1	D	59	ASN
1	D	197	ASN
1	D	213	HIS
1	D	227	HIS
1	D	237	GLN
1	D	256	ASN
1	D	271	GLN
1	D	294	GLN
1	D	371	ASN
1	D	372	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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$
4	UDP	A	1377	-	25,26,26	0.74	1 (4%)	38,40,40	1.06	3 (7%)
4	UDP	C	3377	-	25,26,26	0.88	1 (4%)	38,40,40	1.01	3 (7%)
4	UDP	D	4377	-	25,26,26	0.74	1 (4%)	38,40,40	1.06	3 (7%)
4	UDP	B	2377	-	25,26,26	0.84	1 (4%)	38,40,40	0.84	1 (2%)

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
4	UDP	A	1377	-	-	3/16/32/32	0/2/2/2
4	UDP	C	3377	-	-	1/16/32/32	0/2/2/2
4	UDP	D	4377	-	-	3/16/32/32	0/2/2/2
4	UDP	B	2377	-	-	1/16/32/32	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3377	UDP	O4'-C1'	2.48	1.47	1.42
4	A	1377	UDP	O4'-C1'	2.37	1.47	1.42
4	D	4377	UDP	O4'-C1'	2.36	1.47	1.42
4	B	2377	UDP	O4'-C1'	2.19	1.47	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4377	UDP	O4'-C1'-N1	3.44	116.16	108.36
4	A	1377	UDP	O4'-C1'-N1	3.42	116.11	108.36
4	C	3377	UDP	O4'-C1'-N1	2.73	114.54	108.36
4	C	3377	UDP	O3A-PB-O1B	-2.44	98.21	111.04
4	A	1377	UDP	O3B-PB-O2B	2.33	116.53	107.80
4	D	4377	UDP	O3B-PB-O2B	2.32	116.49	107.80
4	B	2377	UDP	O3B-PB-O2B	2.29	116.38	107.80
4	C	3377	UDP	O3B-PB-O2B	2.17	115.94	107.80
4	A	1377	UDP	C5'-C4'-C3'	-2.14	107.52	115.21
4	D	4377	UDP	C5'-C4'-C3'	-2.13	107.55	115.21

There are no chirality outliers.

All (8) torsion outliers are listed below:

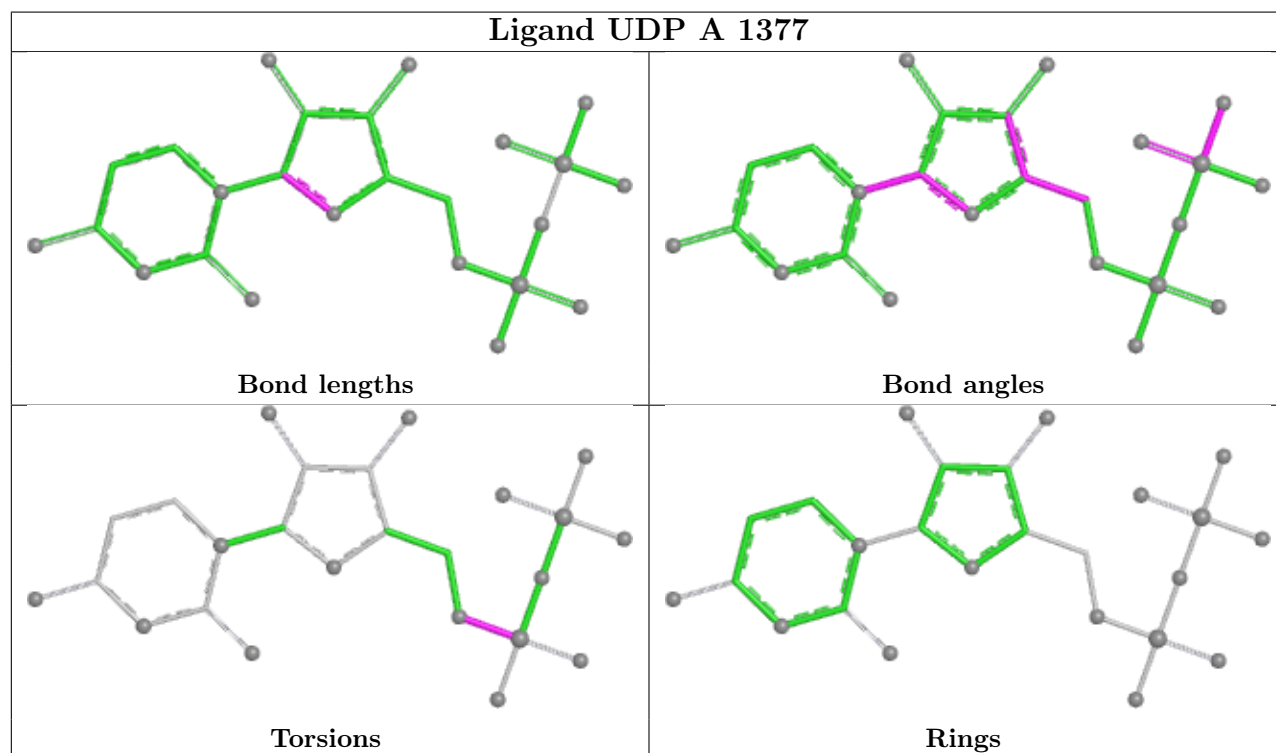
Mol	Chain	Res	Type	Atoms
4	A	1377	UDP	C5'-O5'-PA-O2A
4	A	1377	UDP	C5'-O5'-PA-O3A
4	B	2377	UDP	C5'-O5'-PA-O2A
4	D	4377	UDP	C5'-O5'-PA-O2A
4	D	4377	UDP	C5'-O5'-PA-O3A
4	A	1377	UDP	C5'-O5'-PA-O1A
4	D	4377	UDP	C5'-O5'-PA-O1A
4	C	3377	UDP	C3'-C4'-C5'-O5'

There are no ring outliers.

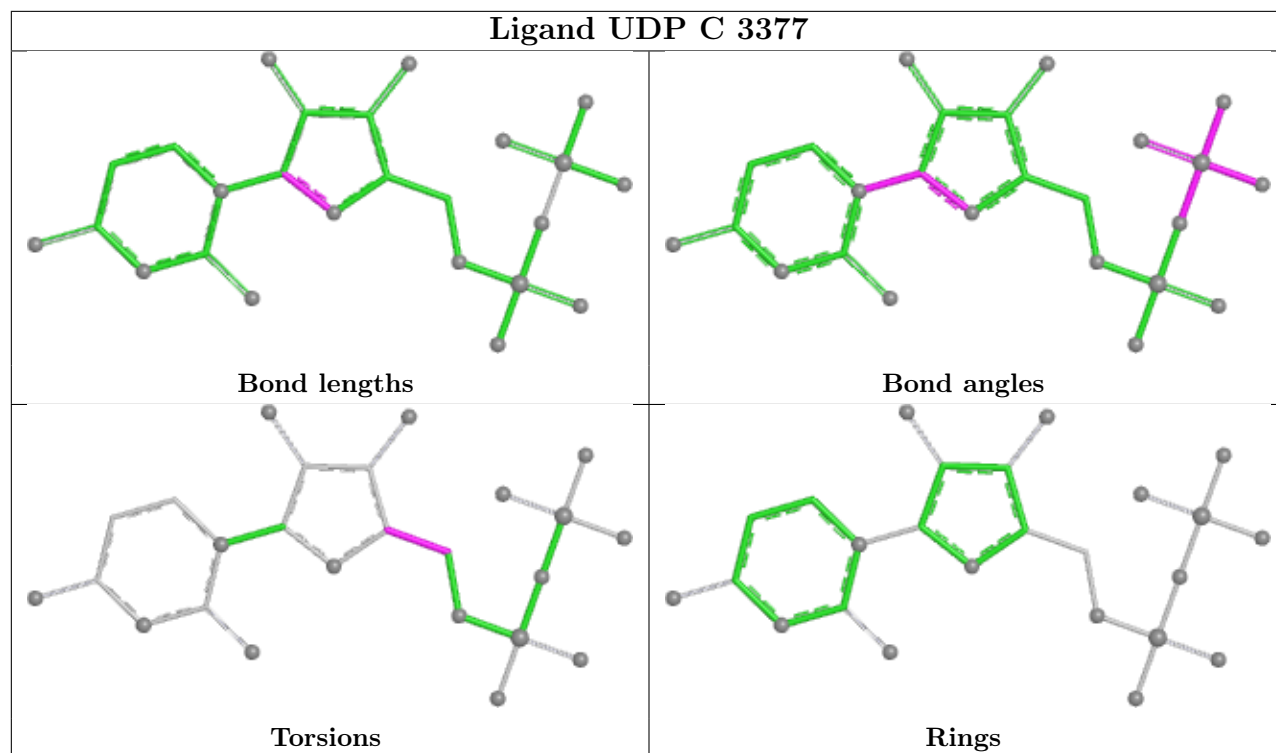
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1377	UDP	1	0
4	C	3377	UDP	1	0
4	D	4377	UDP	2	0
4	B	2377	UDP	1	0

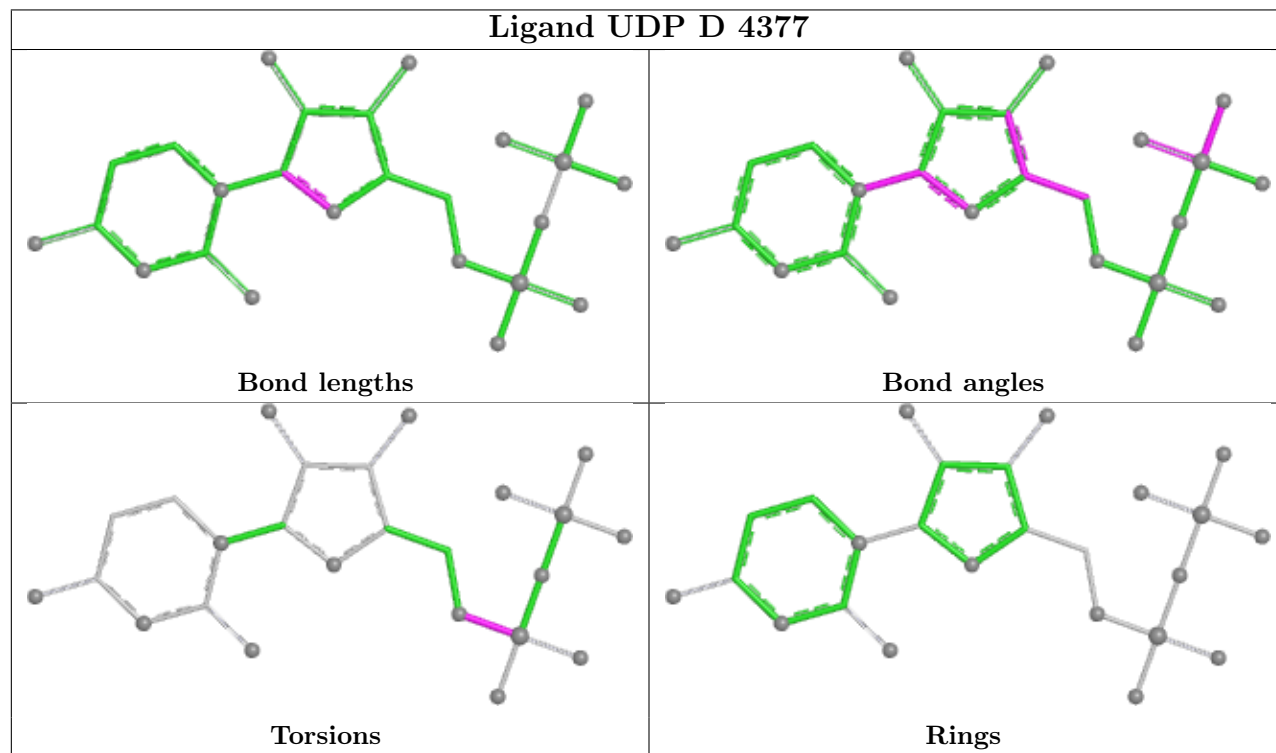
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

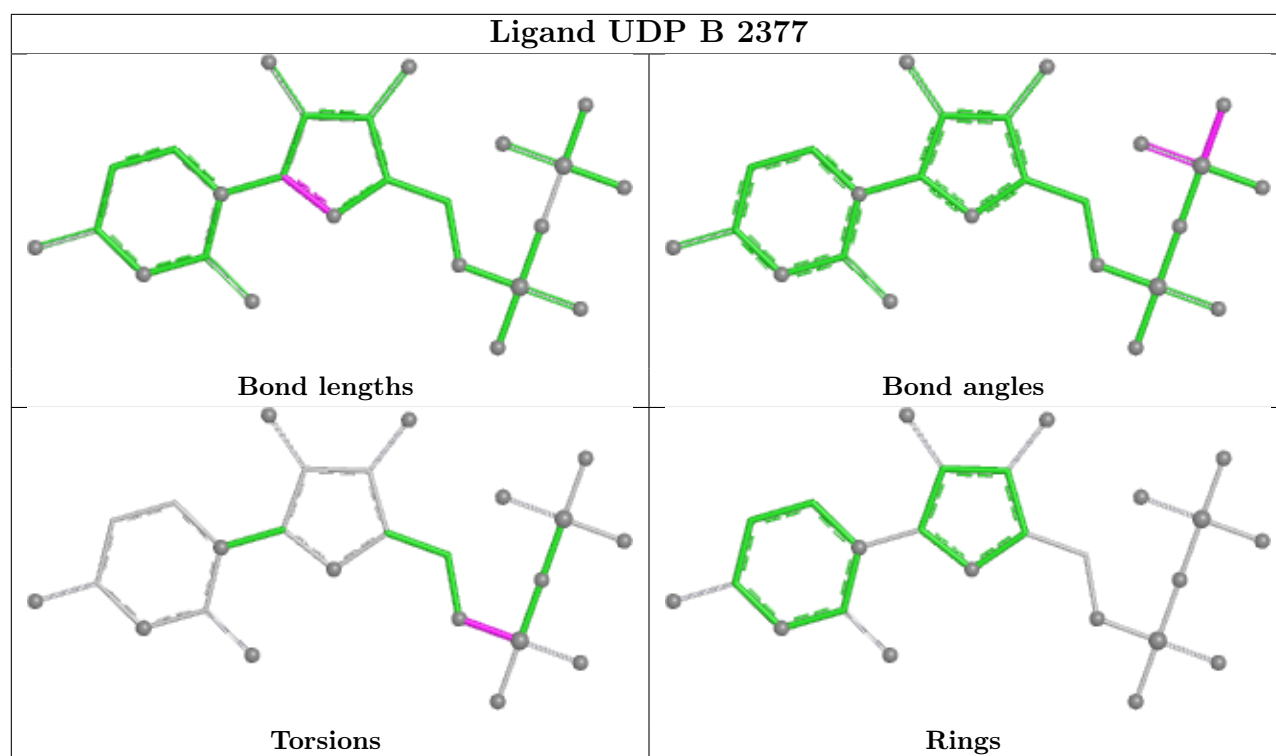


Ligand UDP C 3377



Ligand UDP D 4377





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	366/376 (97%)	-0.30	3 (0%)	82 80	7, 25, 56, 70	1 (0%)
1	B	363/376 (96%)	-0.16	7 (1%)	66 62	7, 26, 67, 84	4 (1%)
1	C	358/376 (95%)	0.08	10 (2%)	55 50	14, 36, 79, 96	0
1	D	364/376 (96%)	0.03	7 (1%)	66 62	11, 32, 80, 88	0
All	All	1451/1504 (96%)	-0.09	27 (1%)	66 62	7, 30, 74, 96	5 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	251	VAL	3.5
1	B	262	VAL	3.2
1	C	259	LEU	3.1
1	C	255	VAL	3.0
1	B	376	LEU	2.9
1	B	217	SER	2.9
1	D	219	GLY	2.8
1	A	376	LEU	2.8
1	A	311	THR	2.7
1	D	221	GLY	2.7
1	D	262	VAL	2.6
1	A	219	GLY	2.4
1	B	39	HIS	2.3
1	C	249	PRO	2.3
1	D	220	ARG	2.3
1	C	228	ALA	2.3
1	C	218	PHE	2.3
1	D	222	PHE	2.3
1	C	222	PHE	2.2
1	D	258	ILE	2.2
1	B	238	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	250	ASN	2.1
1	C	258	ILE	2.1
1	C	251	VAL	2.0
1	C	59	ASN	2.0
1	C	372	ASN	2.0
1	D	64	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

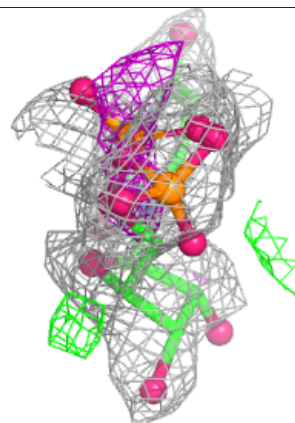
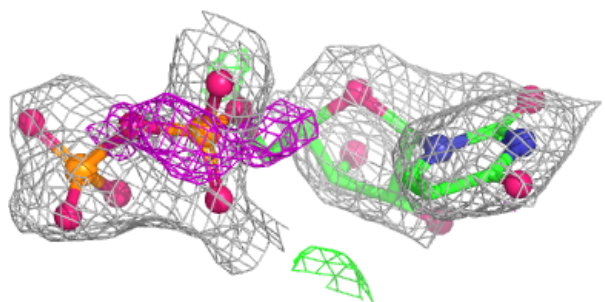
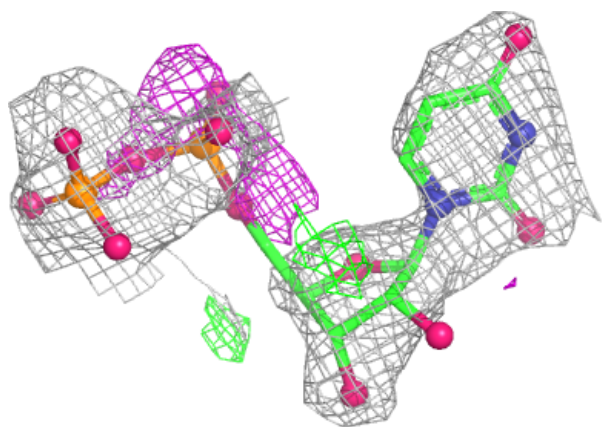
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	UDP	D	4377	25/25	0.67	0.15	64,66,100,100	0
4	UDP	A	1377	25/25	0.78	0.14	59,62,100,100	0
2	NA	C	3378	1/1	0.87	0.14	36,36,36,36	0
2	NA	D	4378	1/1	0.93	0.06	17,17,17,17	0
4	UDP	C	3377	25/25	0.95	0.07	18,24,30,32	0
2	NA	B	2378	1/1	0.95	0.04	25,25,25,25	0
2	NA	A	1378	1/1	0.97	0.05	21,21,21,21	0
4	UDP	B	2377	25/25	0.97	0.05	7,13,25,26	0
3	CL	B	2379	1/1	0.97	0.04	26,26,26,26	0
3	CL	D	4379	1/1	0.97	0.04	28,28,28,28	0
3	CL	A	1379	1/1	0.98	0.03	28,28,28,28	0
3	CL	C	3379	1/1	0.99	0.03	33,33,33,33	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

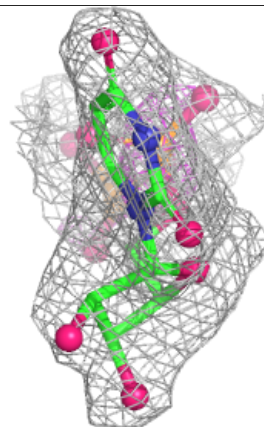
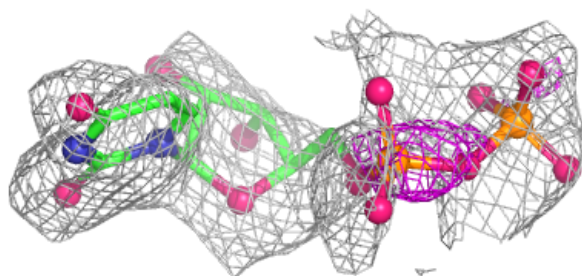
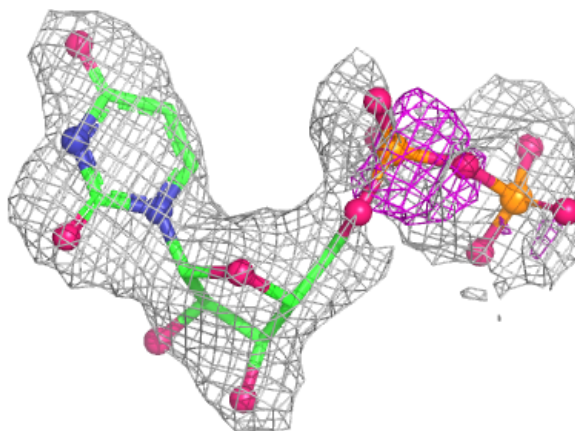
Electron density around UDP D 4377:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



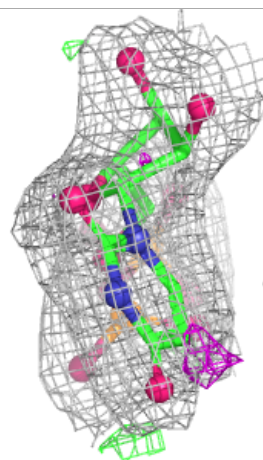
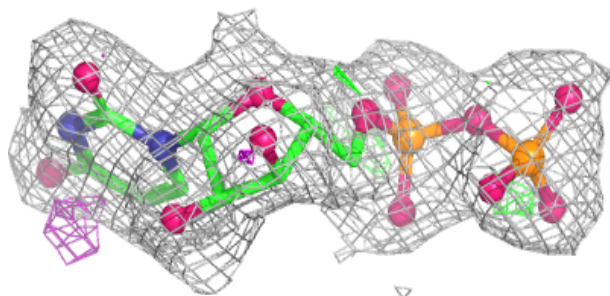
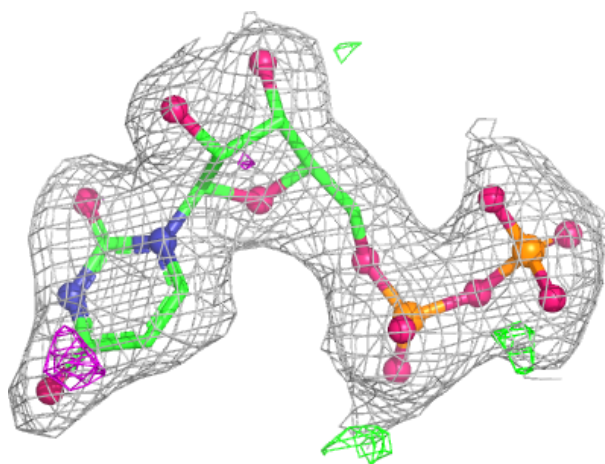
Electron density around UDP A 1377:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



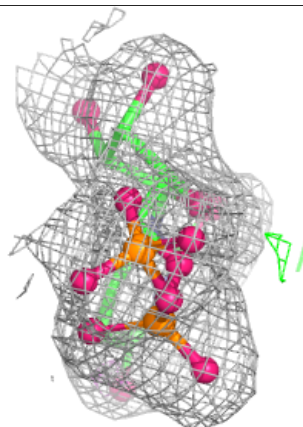
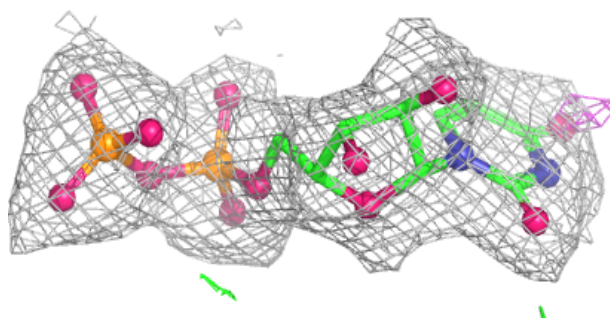
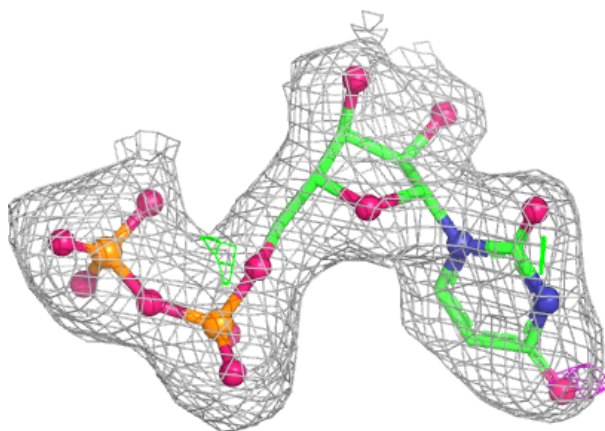
Electron density around UDP C 3377:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UDP B 2377:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.