Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:19 AM GMT

PDB ID	:	2GN9
Title	:	Crystal structure of UDP-GlcNAc inverting 4,6-dehydratase in complex with NADP and UDP-Glc
Authors	:	Ishiyama, N.; Creuzenet, C.; Lam, J.S.; Berghuis, A.M.
Deposited on	:	2006-04-09
Resolution	:	2.80 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:

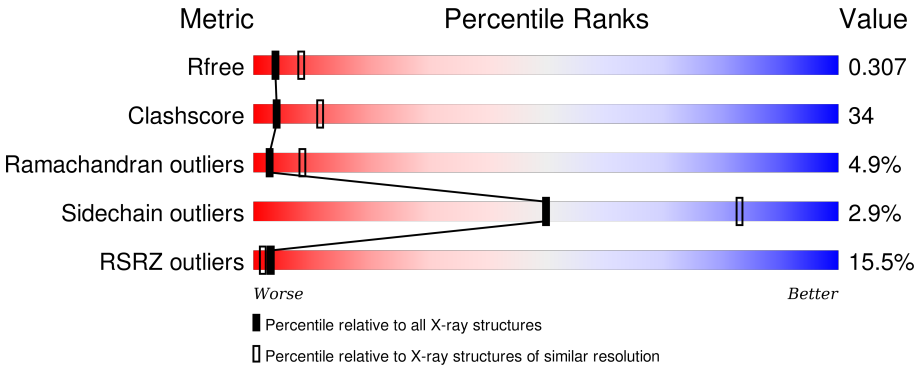
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	344	16% 44% 47% 5% .
1	B	344	14% 44% 46% 5% 5%

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
4	MES	B	336	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5419 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.

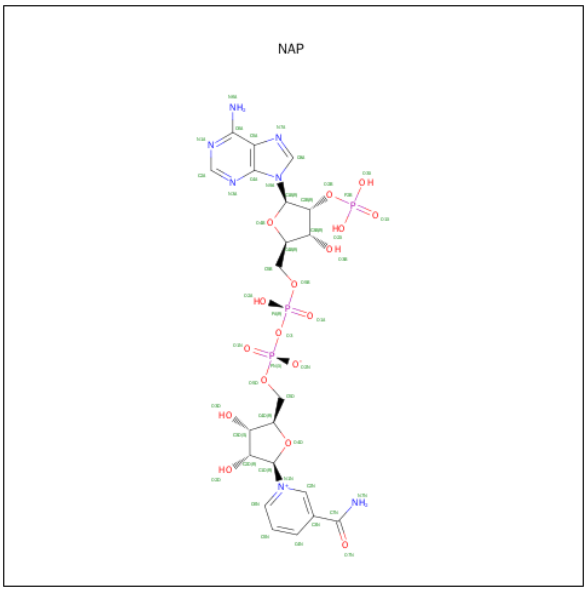
- Molecule 1 is a protein called UDP-GlcNAc C6 dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2590	1656	440	479	15			
1	B	327	Total	C	N	O	S	0	0	0
			2573	1647	436	475	15			

There are 22 discrepancies between the modelled and reference sequences:

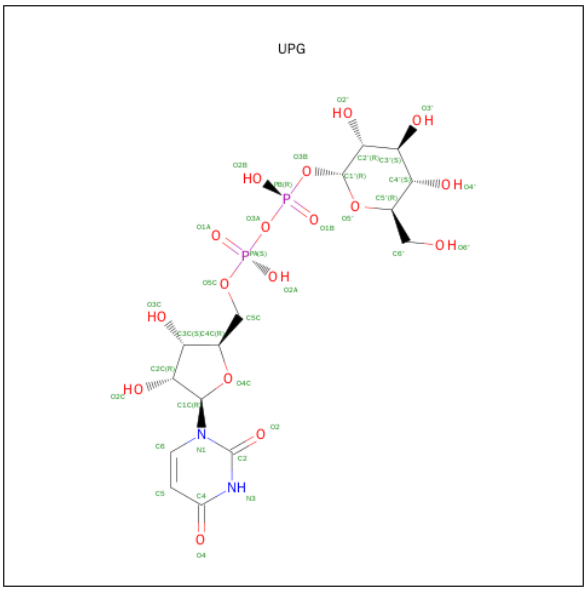
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	CLONING ARTIFACT	UNP O25511
A	-9	HIS	-	EXPRESSION TAG	UNP O25511
A	-8	HIS	-	EXPRESSION TAG	UNP O25511
A	-7	HIS	-	EXPRESSION TAG	UNP O25511
A	-6	HIS	-	EXPRESSION TAG	UNP O25511
A	-5	HIS	-	EXPRESSION TAG	UNP O25511
A	-4	HIS	-	EXPRESSION TAG	UNP O25511
A	-3	GLY	-	CLONING ARTIFACT	UNP O25511
A	-2	SER	-	CLONING ARTIFACT	UNP O25511
A	-1	MET	-	CLONING ARTIFACT	UNP O25511
A	0	SER	-	CLONING ARTIFACT	UNP O25511
B	-10	MET	-	CLONING ARTIFACT	UNP O25511
B	-9	HIS	-	EXPRESSION TAG	UNP O25511
B	-8	HIS	-	EXPRESSION TAG	UNP O25511
B	-7	HIS	-	EXPRESSION TAG	UNP O25511
B	-6	HIS	-	EXPRESSION TAG	UNP O25511
B	-5	HIS	-	EXPRESSION TAG	UNP O25511
B	-4	HIS	-	EXPRESSION TAG	UNP O25511
B	-3	GLY	-	CLONING ARTIFACT	UNP O25511
B	-2	SER	-	CLONING ARTIFACT	UNP O25511
B	-1	MET	-	CLONING ARTIFACT	UNP O25511
B	0	SER	-	CLONING ARTIFACT	UNP O25511

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	11	0
			36	15	2	17	2		

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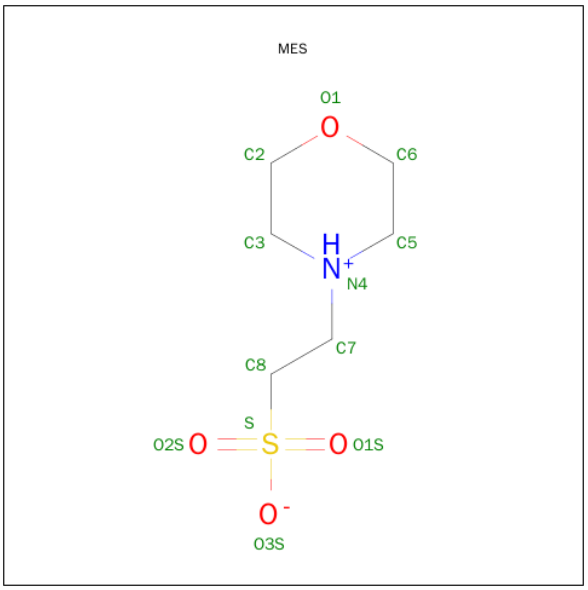
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	11	0
			36	15	2	17	2		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is water.

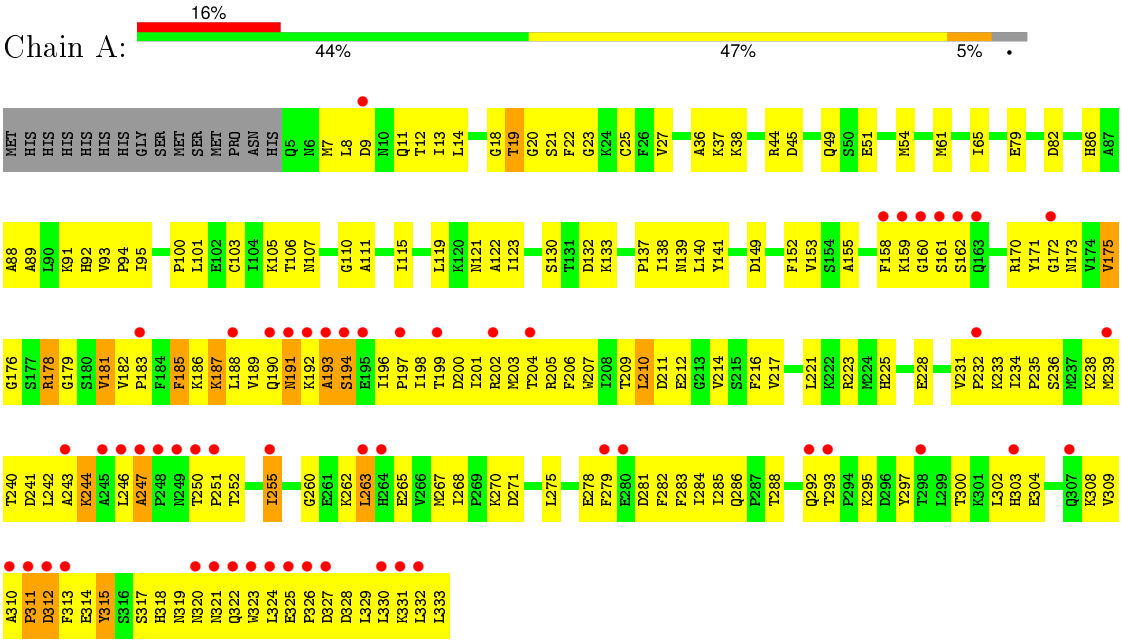
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	34	Total	O	0	0
			34	34		
5	B	42	Total	O	0	0
			42	42		

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.

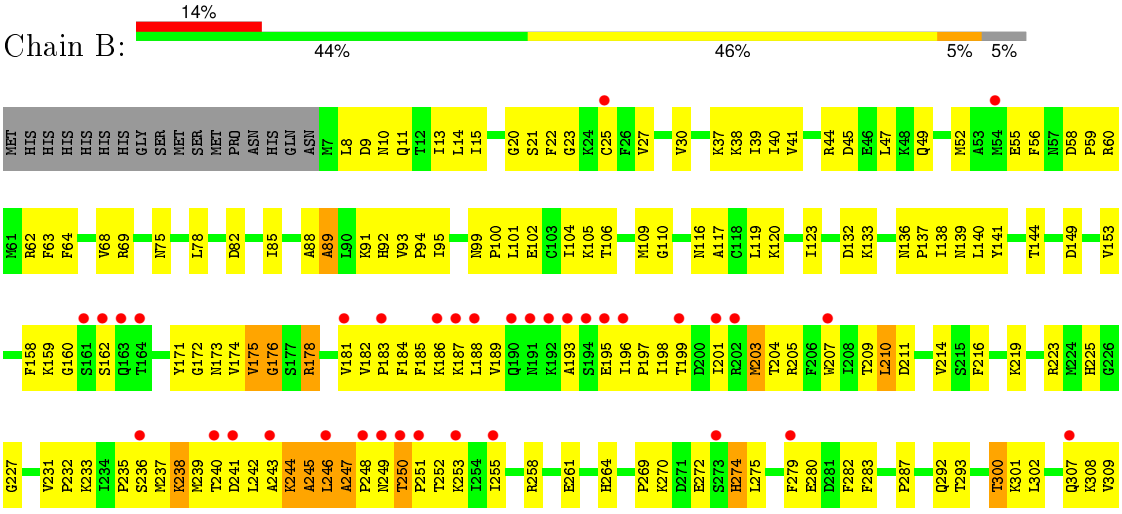
- Molecule 1: UDP-GlcNAc C6 dehydratase

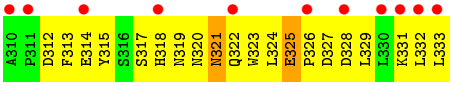
Chain A:



- Molecule 1: UDP-GlcNAc C6 dehydratase

Chain B:




A310
P311
D312
F313
E314
Y315
S316
S317
H318
N319
N320
N321
Q322
W323
L324
E325
P326
D327
D328
L329
L330
K331
L332
L333

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	112.38Å 112.38Å 107.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.78 – 2.81	Depositor EDS
% Data completeness (in resolution range)	96.1 (50.00-2.80) 97.0 (49.78-2.81)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.46 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.307 0.221 , 0.307	Depositor DCC
R_{free} test set	1802 reflections (9.84%)	DCC
Wilson B-factor (Å^2)	47.0	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 83.7	EDS
Estimated twinning fraction	0.057 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 18825 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5419	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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: UPG, NAP, MES

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	0.34	0/2641	0.60	0/3568
1	B	0.33	0/2624	0.61	0/3545
All	All	0.33	0/5265	0.61	0/7113

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	2590	0	2641	172	0
1	B	2573	0	2627	198	0
2	A	48	0	25	2	0
2	B	48	0	25	3	0
3	A	36	0	22	1	0
3	B	36	0	22	2	0
4	B	12	0	13	1	0
5	A	34	0	0	3	0
5	B	42	0	0	7	0
All	All	5419	0	5375	367	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 34.

All (367) 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:B:184:PHE:HA	1:B:187:LYS:HE2	1.39	1.03
1:A:189:VAL:HG21	1:A:247:ALA:HB2	1.38	1.02
1:B:321:ASN:HD22	1:B:322:GLN:N	1.73	0.87
1:A:223:ARG:HB2	1:A:300:THR:HB	1.56	0.85
1:B:269:PRO:HB2	1:B:272:GLU:HG2	1.57	0.85
1:B:159:LYS:NZ	1:B:292:GLN:HB2	1.90	0.85
1:B:250:THR:HG22	1:B:251:PRO:HD2	1.57	0.84
1:B:238:LYS:HE2	1:B:239:MET:H	1.43	0.84
1:B:38:LYS:HZ1	1:B:62:ARG:HH11	1.27	0.81
1:B:132:ASP:OD2	1:B:172:GLY:HA2	1.81	0.81
1:B:38:LYS:NZ	1:B:62:ARG:HH11	1.78	0.81
1:B:270:LYS:HB2	1:B:314:GLU:OE1	1.82	0.80
1:A:209:THR:OG1	1:A:212:GLU:HB2	1.83	0.78
1:B:8:LEU:HD11	1:B:13:ILE:HD11	1.65	0.78
1:B:119:LEU:HD22	1:B:158:PHE:CD2	2.18	0.77
1:B:75:ASN:HD22	1:B:120:LYS:HD3	1.47	0.77
1:B:237:MET:HE3	1:B:324:LEU:HD23	1.66	0.77
1:B:238:LYS:HD3	1:B:240:THR:H	1.50	0.77
1:A:194:SER:O	1:A:251:PRO:HG2	1.85	0.77
1:B:20:GLY:HA2	1:B:178:ARG:NH1	2.00	0.76
1:B:174:VAL:HG11	1:B:210:LEU:HD22	1.67	0.76
1:B:75:ASN:ND2	1:B:120:LYS:HD3	2.01	0.75
1:B:325:GLU:HB2	1:B:328:ASP:OD2	1.85	0.75
1:A:25:CYS:SG	1:A:214:VAL:HG21	2.27	0.75
1:A:231:VAL:HB	1:A:283:PHE:HB2	1.68	0.75
1:B:38:LYS:HE2	1:B:40:ILE:HD11	1.67	0.74
1:B:193:ALA:O	1:B:250:THR:HG21	1.87	0.74
1:B:225:HIS:HA	1:B:301:LYS:HE2	1.69	0.74
1:A:178:ARG:HD3	1:B:47:LEU:HG	1.67	0.74
1:A:7:MET:SD	1:A:9:ASP:HB3	2.28	0.74
1:B:198:ILE:HD11	1:B:243:ALA:HB2	1.70	0.73
1:B:159:LYS:HZ1	1:B:293:THR:N	1.86	0.72
1:B:238:LYS:HE2	1:B:239:MET:N	2.04	0.72
1:A:92:HIS:CE1	1:A:94:PRO:HG2	2.25	0.71
1:B:321:ASN:HD22	1:B:322:GLN:H	1.36	0.71
1:A:182:VAL:HG13	1:A:246:LEU:HD11	1.72	0.70
1:B:269:PRO:HD2	1:B:272:GLU:HG3	1.73	0.68
1:B:196:ILE:O	1:B:252:THR:HA	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:LEU:HD13	1:B:78:LEU:HD23	1.76	0.68
1:A:268:ILE:HG12	1:A:285:ILE:HD11	1.76	0.68
1:A:250:THR:HG23	1:A:251:PRO:HD2	1.76	0.67
1:B:88:ALA:O	1:B:89:ALA:HB2	1.93	0.67
1:B:89:ALA:HB2	5:B:368:HOH:O	1.94	0.67
1:B:182:VAL:HG23	1:B:183:PRO:HD3	1.77	0.66
1:B:21:SER:HB3	1:B:210:LEU:HD21	1.78	0.66
1:B:149:ASP:O	1:B:153:VAL:HG23	1.96	0.66
1:B:324:LEU:HD21	1:B:329:LEU:HD13	1.76	0.66
1:B:203:MET:O	1:B:239:MET:HB2	1.95	0.65
1:B:58:ASP:OD1	1:B:60:ARG:HG2	1.97	0.65
1:B:204:THR:O	1:B:205:ARG:HG2	1.97	0.65
1:A:7:MET:HG3	1:A:9:ASP:H	1.63	0.64
1:B:264:HIS:HB3	1:B:317:SER:OG	1.97	0.64
1:B:119:LEU:HD22	1:B:158:PHE:HD2	1.61	0.64
1:B:184:PHE:HA	1:B:187:LYS:CE	2.22	0.64
1:B:159:LYS:HZ2	1:B:292:GLN:HB2	1.63	0.63
1:B:236:SER:O	1:B:323:TRP:HA	1.98	0.63
1:A:186:LYS:HG2	1:A:246:LEU:HD22	1.81	0.63
1:B:239:MET:HE3	1:B:242:LEU:HD23	1.80	0.63
1:B:68:VAL:HG22	2:B:334:NAP:N1A	2.14	0.62
1:A:241:ASP:HA	1:A:244:LYS:HD2	1.81	0.62
1:B:196:ILE:HB	1:B:252:THR:HG22	1.81	0.62
1:A:197:PRO:HB2	3:A:335:UPG:HN3	1.64	0.62
1:A:20:GLY:HA2	1:A:178:ARG:HH21	1.65	0.62
1:B:293:THR:HG23	1:B:293:THR:O	2.00	0.62
1:B:223:ARG:HG2	1:B:302:LEU:HD12	1.82	0.62
1:B:23:GLY:O	1:B:27:VAL:HG23	1.99	0.62
1:B:136:ASN:HD21	1:B:269:PRO:HB3	1.63	0.61
1:B:92:HIS:ND1	1:B:94:PRO:HD2	2.15	0.61
1:B:188:LEU:C	1:B:193:ALA:HB2	2.21	0.61
1:A:327:ASP:HA	1:A:330:LEU:HG	1.81	0.61
1:A:333:LEU:O	1:A:333:LEU:HD23	2.00	0.61
1:B:242:LEU:HD13	1:B:329:LEU:HD23	1.82	0.61
1:B:100:PRO:HA	1:B:140:LEU:CD2	2.30	0.61
1:A:9:ASP:O	1:A:11:GLN:HG3	2.00	0.61
1:B:197:PRO:HB2	1:B:255:ILE:HD13	1.81	0.61
1:A:189:VAL:HA	1:A:193:ALA:HB2	1.82	0.61
1:B:13:ILE:HD12	1:B:30:VAL:HG11	1.83	0.61
1:A:18:GLY:HA2	1:A:23:GLY:HA3	1.83	0.60
1:A:160:GLY:C	1:A:162:SER:H	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:VAL:HG21	1:B:247:ALA:CB	2.31	0.60
1:B:38:LYS:HE3	1:B:62:ARG:HD2	1.83	0.60
1:A:133:LYS:HE3	5:A:366:HOH:O	2.01	0.60
1:A:122:ALA:HA	1:A:162:SER:OG	2.00	0.60
1:B:324:LEU:CD2	1:B:329:LEU:HD13	2.32	0.60
1:A:239:MET:SD	1:A:242:LEU:HD23	2.42	0.60
1:B:188:LEU:HB3	1:B:193:ALA:HB2	1.82	0.60
1:A:313:PHE:CZ	1:A:315:TYR:HB2	2.37	0.59
1:A:194:SER:C	1:A:251:PRO:HG2	2.22	0.59
1:A:327:ASP:O	1:A:331:LYS:HG3	2.03	0.59
1:A:238:LYS:HE2	1:A:240:THR:CG2	2.32	0.59
1:A:206:PHE:HB3	1:A:234:ILE:CD1	2.33	0.58
1:A:100:PRO:HA	1:A:140:LEU:CD2	2.33	0.58
1:A:235:PRO:HG3	1:A:322:GLN:NE2	2.19	0.58
1:B:159:LYS:HZ3	1:B:293:THR:HB	1.68	0.58
1:B:239:MET:CE	1:B:242:LEU:HD23	2.34	0.58
1:B:8:LEU:HD23	1:B:9:ASP:N	2.19	0.58
1:B:301:LYS:HD2	5:B:365:HOH:O	2.03	0.58
1:A:228:GLU:HG3	1:A:297:TYR:CD2	2.38	0.58
1:A:241:ASP:HA	1:A:244:LYS:CD	2.34	0.58
1:B:69:ARG:NH2	1:B:102:GLU:OE1	2.36	0.57
1:A:159:LYS:HD2	1:A:292:GLN:OE1	2.05	0.57
1:A:88:ALA:O	1:A:89:ALA:HB2	2.04	0.57
1:A:318:HIS:CE1	1:A:319:ASN:HB3	2.40	0.57
1:B:101:LEU:HG	1:B:105:LYS:HE3	1.86	0.57
1:A:325:GLU:C	1:A:327:ASP:H	2.07	0.57
1:B:258:ARG:HD3	1:B:261:GLU:OE2	2.04	0.56
1:A:225:HIS:HB3	1:A:295:LYS:HD3	1.86	0.56
1:A:188:LEU:C	1:A:190:GLN:H	2.07	0.56
1:B:60:ARG:HH11	1:B:60:ARG:HG3	1.71	0.56
1:A:8:LEU:HD23	1:A:13:ILE:HD11	1.88	0.56
1:A:300:THR:C	1:A:302:LEU:H	2.08	0.56
1:B:181:VAL:HG23	3:B:335:UPG:O2A	2.06	0.56
1:A:12:THR:HG23	1:A:38:LYS:CG	2.36	0.56
1:B:38:LYS:NZ	1:B:62:ARG:NH1	2.51	0.55
1:A:22:PHE:CZ	1:A:217:VAL:HG21	2.40	0.55
1:B:30:VAL:CG1	1:B:39:ILE:HD11	2.37	0.55
1:A:130:SER:O	2:A:334:NAP:H6N	2.06	0.55
1:A:209:THR:C	1:A:211:ASP:H	2.10	0.54
1:B:22:PHE:HA	1:B:210:LEU:HD11	1.89	0.54
1:B:199:THR:HG22	1:B:255:ILE:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ASN:HD22	1:B:173:ASN:N	2.04	0.54
1:B:25:CYS:SG	1:B:214:VAL:HG21	2.48	0.54
1:A:189:VAL:HG13	1:A:193:ALA:HB2	1.90	0.54
1:A:19:THR:HG22	2:A:334:NAP:O3B	2.08	0.54
1:A:106:THR:O	1:A:110:GLY:HA3	2.08	0.54
1:A:278:GLU:HB2	1:A:309:VAL:HG12	1.90	0.54
1:A:242:LEU:HD13	1:A:329:LEU:CD2	2.38	0.54
1:A:240:THR:O	1:A:243:ALA:HB3	2.09	0.53
1:A:100:PRO:HB3	1:A:140:LEU:HD22	1.89	0.53
1:A:182:VAL:O	1:A:246:LEU:HD13	2.09	0.53
1:B:9:ASP:H	1:B:11:GLN:HG2	1.74	0.53
1:A:235:PRO:HB2	1:A:324:LEU:HG	1.91	0.53
1:B:238:LYS:HD3	1:B:240:THR:HB	1.90	0.53
1:B:328:ASP:HA	1:B:331:LYS:HD2	1.89	0.53
1:B:93:VAL:HB	1:B:94:PRO:HD3	1.90	0.53
1:A:270:LYS:HB2	1:A:314:GLU:OE2	2.09	0.53
1:B:245:ALA:HB2	1:B:326:PRO:O	2.09	0.53
1:B:309:VAL:HG21	1:B:313:PHE:CD2	2.43	0.53
1:B:160:GLY:C	1:B:162:SER:H	2.11	0.53
1:B:30:VAL:HG12	1:B:39:ILE:HD11	1.90	0.52
1:B:207:TRP:CD1	1:B:237:MET:HB3	2.43	0.52
1:B:246:LEU:O	1:B:247:ALA:HB2	2.09	0.52
1:B:60:ARG:NH1	5:B:350:HOH:O	2.42	0.52
1:A:197:PRO:O	1:A:198:ILE:HD13	2.09	0.52
1:A:173:ASN:N	1:A:173:ASN:HD22	2.07	0.52
1:A:302:LEU:O	1:A:303:HIS:HB2	2.09	0.52
1:B:195:GLU:OE2	1:B:253:LYS:HD2	2.10	0.52
1:A:190:GLN:HG2	1:A:190:GLN:O	2.10	0.52
1:B:196:ILE:N	1:B:251:PRO:O	2.43	0.52
1:B:138:ILE:HG13	1:B:139:ASN:N	2.24	0.52
1:B:38:LYS:HE2	1:B:40:ILE:CD1	2.38	0.52
1:B:209:THR:CG2	1:B:332:LEU:HD21	2.40	0.52
1:B:209:THR:HG22	1:B:332:LEU:HD21	1.91	0.52
1:A:45:ASP:O	1:A:49:GLN:HG3	2.10	0.52
1:A:198:ILE:HG22	1:A:199:THR:N	2.25	0.51
1:B:91:LYS:HA	1:B:141:TYR:CE1	2.44	0.51
1:B:159:LYS:HZ1	1:B:292:GLN:HB2	1.73	0.51
1:B:8:LEU:HD11	1:B:13:ILE:CD1	2.37	0.51
1:A:242:LEU:HD12	1:A:242:LEU:O	2.10	0.51
1:A:325:GLU:O	1:A:327:ASP:N	2.43	0.51
1:B:175:VAL:HA	1:B:207:TRP:CZ3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASP:O	1:A:153:VAL:HG23	2.10	0.51
1:B:49:GLN:OE1	1:B:63:PHE:HB3	2.11	0.51
1:A:329:LEU:O	1:A:332:LEU:HB2	2.10	0.51
1:B:159:LYS:HZ1	1:B:293:THR:H	1.59	0.51
1:B:189:VAL:HG21	1:B:247:ALA:HB2	1.93	0.51
1:B:237:MET:SD	1:B:329:LEU:HD22	2.50	0.51
1:B:11:GLN:HA	1:B:82:ASP:OD1	2.11	0.50
1:A:279:PHE:HB2	1:A:282:PHE:O	2.11	0.50
1:A:182:VAL:N	1:A:183:PRO:HD2	2.26	0.50
1:B:182:VAL:CG2	1:B:183:PRO:HD3	2.41	0.50
1:A:235:PRO:HG3	1:A:322:GLN:HE21	1.76	0.50
1:B:133:LYS:O	1:B:137:PRO:HB3	2.11	0.50
1:B:244:LYS:O	1:B:245:ALA:C	2.50	0.50
1:B:181:VAL:HG21	3:B:335:UPG:O4C	2.11	0.50
1:A:7:MET:CG	1:A:9:ASP:HB3	2.42	0.50
1:A:223:ARG:HB3	1:A:302:LEU:HG	1.94	0.50
1:B:250:THR:CG2	1:B:251:PRO:HD2	2.35	0.50
1:A:91:LYS:HA	1:A:141:TYR:CE1	2.47	0.50
1:B:116:ASN:HB2	4:B:336:MES:O1	2.12	0.50
1:A:160:GLY:O	1:A:162:SER:N	2.43	0.50
1:A:216:PHE:CE2	1:A:232:PRO:HD3	2.46	0.50
1:A:171:TYR:HB3	1:A:232:PRO:CG	2.42	0.50
1:B:159:LYS:CE	1:B:292:GLN:HB2	2.40	0.49
1:A:194:SER:HA	1:A:251:PRO:HD2	1.94	0.49
1:A:115:ILE:HD13	1:A:155:ALA:HB2	1.95	0.49
1:B:38:LYS:HZ1	1:B:62:ARG:NH1	2.01	0.49
1:B:78:LEU:HD12	1:B:117:ALA:CB	2.42	0.49
1:A:171:TYR:HB3	1:A:232:PRO:HG3	1.95	0.49
1:B:185:PHE:CB	1:B:246:LEU:HD13	2.43	0.49
1:A:186:LYS:O	1:A:190:GLN:N	2.45	0.49
1:A:327:ASP:HA	1:A:330:LEU:CG	2.43	0.49
1:B:244:LYS:C	1:B:248:PRO:HG3	2.33	0.49
1:A:206:PHE:HB3	1:A:234:ILE:HD11	1.95	0.49
1:A:187:LYS:O	1:A:191:ASN:ND2	2.41	0.49
1:A:20:GLY:CA	1:A:178:ARG:HH21	2.26	0.49
1:A:176:GLY:HA2	1:A:183:PRO:HD3	1.95	0.48
1:B:227:GLY:O	1:B:287:PRO:HG3	2.11	0.48
1:B:325:GLU:HB2	1:B:328:ASP:CG	2.32	0.48
1:A:325:GLU:N	1:A:328:ASP:OD2	2.44	0.48
1:B:293:THR:HG21	5:B:351:HOH:O	2.13	0.48
1:B:186:LYS:HZ1	1:B:333:LEU:HD12	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:CD2	1:A:105:LYS:HE3	2.44	0.48
1:A:197:PRO:HB3	1:A:255:ILE:HD12	1.94	0.48
1:A:7:MET:HG3	1:A:9:ASP:HB3	1.96	0.48
1:B:105:LYS:O	1:B:109:MET:HB2	2.13	0.48
1:A:310:ALA:O	1:A:312:ASP:N	2.47	0.48
1:A:189:VAL:HG13	1:A:193:ALA:CB	2.44	0.48
1:B:88:ALA:O	1:B:89:ALA:CB	2.60	0.48
1:B:189:VAL:N	1:B:193:ALA:HB2	2.28	0.48
1:A:332:LEU:O	1:A:333:LEU:C	2.52	0.47
1:B:274:HIS:CD2	1:B:275:LEU:H	2.32	0.47
1:A:11:GLN:N	1:A:37:LYS:H	2.12	0.47
1:A:204:THR:O	1:A:205:ARG:HG2	2.13	0.47
1:B:159:LYS:NZ	1:B:293:THR:HG22	2.29	0.47
1:A:11:GLN:O	1:A:36:ALA:HB1	2.14	0.47
1:B:219:LYS:HB3	1:B:223:ARG:NH1	2.29	0.47
1:B:309:VAL:HG21	1:B:313:PHE:HD2	1.79	0.47
1:B:238:LYS:CE	1:B:239:MET:H	2.21	0.47
1:A:286:GLN:HG2	1:A:297:TYR:CD1	2.50	0.47
1:B:181:VAL:HG11	1:B:239:MET:CE	2.45	0.47
1:B:242:LEU:CD1	1:B:329:LEU:HD23	2.44	0.47
1:A:209:THR:C	1:A:211:ASP:N	2.67	0.47
1:A:86:HIS:HE1	5:A:349:HOH:O	1.97	0.47
1:B:136:ASN:N	1:B:137:PRO:CD	2.77	0.47
1:B:238:LYS:CE	1:B:239:MET:N	2.75	0.47
1:A:318:HIS:ND1	1:A:319:ASN:N	2.63	0.47
1:B:216:PHE:CE2	1:B:232:PRO:HD3	2.50	0.47
1:B:188:LEU:HB3	1:B:193:ALA:CB	2.44	0.47
1:A:92:HIS:HE1	1:A:94:PRO:HG2	1.76	0.47
1:B:188:LEU:CB	1:B:193:ALA:HB2	2.45	0.47
1:B:325:GLU:CB	1:B:328:ASP:OD2	2.60	0.47
1:B:258:ARG:HD3	1:B:261:GLU:CD	2.34	0.46
1:B:176:GLY:HA2	1:B:183:PRO:HD3	1.97	0.46
1:B:92:HIS:CE1	1:B:94:PRO:HD2	2.49	0.46
1:B:185:PHE:CD2	1:B:246:LEU:HD13	2.50	0.46
1:B:238:LYS:HA	1:B:238:LYS:HE2	1.96	0.46
1:B:13:ILE:CD1	1:B:30:VAL:HG11	2.46	0.46
1:A:132:ASP:OD2	1:A:172:GLY:HA2	2.15	0.46
1:B:318:HIS:C	1:B:320:ASN:H	2.18	0.46
1:B:172:GLY:O	2:B:334:NAP:H4N	2.15	0.46
1:A:44:ARG:NH1	1:B:44:ARG:HB3	2.30	0.46
1:B:106:THR:O	1:B:110:GLY:HA3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LYS:HE3	1:B:312:ASP:OD1	2.16	0.46
1:A:100:PRO:CB	1:A:140:LEU:HD22	2.46	0.46
1:A:321:ASN:CG	1:A:322:GLN:N	2.69	0.46
1:B:25:CYS:SG	1:B:210:LEU:HD12	2.56	0.45
1:B:55:GLU:HG3	1:B:56:PHE:CD1	2.51	0.45
1:A:196:ILE:H	1:A:252:THR:HA	1.79	0.45
1:A:231:VAL:CG1	1:A:267:MET:HG3	2.46	0.45
1:B:237:MET:HE3	1:B:329:LEU:HB2	1.97	0.45
1:A:111:ALA:HB1	1:A:152:PHE:CE2	2.52	0.45
1:A:186:LYS:O	1:A:188:LEU:N	2.49	0.45
1:A:12:THR:HG23	1:A:38:LYS:HG3	1.99	0.45
1:A:278:GLU:HB2	1:A:309:VAL:CG1	2.46	0.45
1:A:281:ASP:N	1:A:281:ASP:OD1	2.49	0.45
1:A:103:CYS:SG	1:A:107:ASN:ND2	2.89	0.45
1:B:274:HIS:N	1:B:274:HIS:CD2	2.83	0.45
1:B:181:VAL:C	1:B:183:PRO:HD2	2.37	0.45
1:B:185:PHE:HB2	1:B:246:LEU:HD22	1.98	0.45
1:A:160:GLY:C	1:A:162:SER:N	2.70	0.45
1:A:284:ILE:O	1:A:284:ILE:HG22	2.15	0.45
1:B:238:LYS:HD3	1:B:240:THR:CB	2.46	0.45
1:B:45:ASP:HA	5:B:354:HOH:O	2.16	0.45
1:A:333:LEU:C	1:A:333:LEU:HD23	2.36	0.45
1:A:22:PHE:HZ	1:A:217:VAL:HG21	1.82	0.45
1:B:60:ARG:NH1	1:B:60:ARG:HG3	2.31	0.44
1:B:279:PHE:HB2	1:B:282:PHE:O	2.17	0.44
1:A:93:VAL:HG12	1:A:94:PRO:N	2.31	0.44
1:A:246:LEU:O	1:A:247:ALA:HB2	2.17	0.44
1:B:8:LEU:C	1:B:8:LEU:HD23	2.38	0.44
1:A:235:PRO:CG	1:A:322:GLN:HE21	2.29	0.44
1:A:203:MET:HA	1:A:263:LEU:HD23	1.98	0.44
1:A:119:LEU:HD22	1:A:158:PHE:CE2	2.52	0.44
1:A:175:VAL:HA	1:A:207:TRP:CZ3	2.52	0.44
1:A:51:GLU:HA	1:A:54:MET:CE	2.47	0.44
1:A:236:SER:CB	1:A:320:ASN:HD22	2.30	0.44
1:B:173:ASN:N	1:B:173:ASN:ND2	2.65	0.44
1:A:139:ASN:HB3	1:A:260:GLY:O	2.17	0.44
1:A:206:PHE:CE1	1:A:317:SER:HB3	2.52	0.44
1:A:205:ARG:HD3	1:A:265:GLU:CG	2.47	0.44
1:A:137:PRO:HA	5:A:344:HOH:O	2.18	0.44
1:B:320:ASN:ND2	1:B:322:GLN:O	2.50	0.44
1:A:238:LYS:HE2	1:A:240:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:LEU:HD13	1:B:78:LEU:CD2	2.47	0.44
1:A:202:ARG:O	1:A:204:THR:HG23	2.18	0.44
1:B:186:LYS:NZ	1:B:333:LEU:HD12	2.33	0.44
1:B:95:ILE:HG23	1:B:99:ASN:HD22	1.83	0.44
1:A:318:HIS:CG	1:A:319:ASN:N	2.86	0.43
1:B:45:ASP:OD1	1:B:47:LEU:HB3	2.18	0.43
1:B:45:ASP:OD1	1:B:47:LEU:N	2.51	0.43
1:A:235:PRO:HA	1:A:322:GLN:HG3	2.00	0.43
1:A:173:ASN:N	1:A:173:ASN:ND2	2.66	0.43
1:A:210:LEU:O	1:A:214:VAL:HG23	2.18	0.43
1:B:160:GLY:C	1:B:162:SER:N	2.71	0.43
1:B:171:TYR:O	2:B:334:NAP:H5N	2.17	0.43
1:A:228:GLU:HG3	1:A:297:TYR:CE2	2.53	0.43
1:B:82:ASP:O	1:B:123:ILE:HG23	2.19	0.43
1:A:300:THR:CG2	1:A:304:GLU:HB2	2.47	0.43
1:B:328:ASP:HA	1:B:331:LYS:CD	2.48	0.43
1:A:92:HIS:CE1	1:A:95:ILE:HG13	2.54	0.43
1:B:10:ASN:HA	1:B:37:LYS:HB2	1.99	0.43
1:A:275:LEU:CD1	1:A:288:THR:HG22	2.49	0.43
1:A:300:THR:C	1:A:302:LEU:N	2.71	0.43
1:B:325:GLU:N	1:B:328:ASP:OD2	2.52	0.43
1:B:140:LEU:O	1:B:144:THR:HG23	2.19	0.43
1:A:27:VAL:HG11	1:A:61:MET:CE	2.49	0.43
1:A:188:LEU:C	1:A:190:GLN:N	2.70	0.43
1:A:8:LEU:HD23	1:A:13:ILE:CD1	2.48	0.43
1:B:41:VAL:HG21	1:B:52:MET:CE	2.49	0.43
1:A:191:ASN:C	1:A:192:LYS:HG3	2.39	0.43
1:B:184:PHE:HD1	1:B:187:LYS:NZ	2.17	0.42
1:B:325:GLU:C	1:B:327:ASP:H	2.21	0.42
1:A:330:LEU:C	1:A:332:LEU:H	2.23	0.42
1:A:203:MET:SD	1:A:263:LEU:HA	2.59	0.42
1:B:182:VAL:HG23	1:B:183:PRO:CD	2.47	0.42
1:A:159:LYS:NZ	1:A:293:THR:OG1	2.47	0.42
1:A:235:PRO:CA	1:A:322:GLN:HE21	2.31	0.42
1:B:182:VAL:HG11	1:B:329:LEU:HD21	2.01	0.42
1:B:181:VAL:HG13	1:B:185:PHE:CE1	2.54	0.42
1:A:267:MET:HB3	1:A:315:TYR:CD2	2.55	0.42
1:B:101:LEU:HA	1:B:101:LEU:HD12	1.90	0.42
1:A:176:GLY:HA2	1:A:182:VAL:HB	2.02	0.42
1:B:58:ASP:HA	1:B:59:PRO:HD3	1.82	0.42
1:A:186:LYS:CG	1:A:246:LEU:HD22	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:PRO:HA	1:B:322:GLN:HB2	2.01	0.42
1:B:78:LEU:HD12	1:B:117:ALA:HB3	2.02	0.42
1:B:100:PRO:O	1:B:104:ILE:HD12	2.20	0.42
1:A:321:ASN:OD1	1:A:322:GLN:N	2.50	0.42
1:A:286:GLN:HE21	1:A:297:TYR:HD1	1.68	0.42
1:A:200:ASP:HB3	1:A:203:MET:HB2	2.02	0.42
1:A:36:ALA:O	1:A:37:LYS:C	2.58	0.41
1:A:201:ILE:HG22	1:A:201:ILE:O	2.20	0.41
1:B:182:VAL:N	1:B:183:PRO:HD2	2.35	0.41
1:B:238:LYS:HE2	1:B:238:LYS:CA	2.50	0.41
1:A:194:SER:CA	1:A:251:PRO:HG2	2.49	0.41
1:B:174:VAL:HG21	5:B:360:HOH:O	2.19	0.41
1:A:320:ASN:ND2	1:A:322:GLN:O	2.53	0.41
1:A:275:LEU:HD11	1:A:288:THR:HG22	2.01	0.41
1:B:15:ILE:HA	1:B:85:ILE:O	2.19	0.41
1:B:231:VAL:HB	1:B:283:PHE:HB2	2.01	0.41
1:B:201:ILE:C	1:B:238:LYS:HZ2	2.23	0.41
1:B:321:ASN:ND2	1:B:322:GLN:HG3	2.35	0.41
1:A:194:SER:HA	1:A:251:PRO:CG	2.51	0.41
1:A:130:SER:HB3	1:A:170:ARG:HB2	2.01	0.41
1:B:20:GLY:HA2	1:B:178:ARG:HH12	1.82	0.41
1:B:300:THR:C	1:B:302:LEU:H	2.23	0.41
1:A:65:ILE:HB	1:B:102:GLU:HG3	2.01	0.41
1:A:82:ASP:O	1:A:123:ILE:HG23	2.20	0.41
1:B:242:LEU:HD12	1:B:242:LEU:O	2.21	0.41
1:A:185:PHE:CB	1:A:246:LEU:HD13	2.51	0.41
1:B:237:MET:HE3	1:B:324:LEU:CD2	2.44	0.41
1:B:40:ILE:CG2	1:B:64:PHE:HD2	2.33	0.41
1:A:209:THR:O	1:A:211:ASP:N	2.54	0.41
1:A:194:SER:HA	1:A:251:PRO:HG2	2.03	0.41
1:A:14:LEU:C	1:A:14:LEU:HD23	2.42	0.41
1:A:79:GLU:HA	1:A:121:ASN:OD1	2.21	0.41
1:B:321:ASN:ND2	1:B:322:GLN:N	2.55	0.41
1:B:201:ILE:O	1:B:238:LYS:HD2	2.21	0.41
1:A:51:GLU:HA	1:A:54:MET:HE2	2.02	0.41
1:B:68:VAL:HG21	5:B:344:HOH:O	2.21	0.40
1:B:159:LYS:NZ	1:B:293:THR:HB	2.35	0.40
1:A:233:LYS:HE2	1:A:283:PHE:CE2	2.57	0.40
1:A:322:GLN:C	1:A:323:TRP:CD1	2.94	0.40
1:A:311:PRO:O	1:A:312:ASP:HB3	2.22	0.40
1:A:181:VAL:O	1:A:185:PHE:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LYS:HD2	1:B:280:GLU:O	2.21	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	327/344 (95%)	267 (82%)	40 (12%)	20 (6%)	2 5
1	B	325/344 (94%)	274 (84%)	39 (12%)	12 (4%)	4 14
All	All	652/688 (95%)	541 (83%)	79 (12%)	32 (5%)	3 8

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	VAL
1	A	255	ILE
1	A	312	ASP
1	B	244	LYS
1	A	21	SER
1	A	161	SER
1	A	179	GLY
1	A	187	LYS
1	A	193	ALA
1	A	308	LYS
1	A	315	TYR
1	B	175	VAL
1	B	176	GLY
1	B	178	ARG
1	B	203	MET
1	B	245	ALA
1	B	247	ALA

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Mol	Chain	Res	Type
1	B	308	LYS
1	A	178	ARG
1	A	191	ASN
1	A	247	ALA
1	A	326	PRO
1	B	89	ALA
1	B	246	LEU
1	B	249	ASN
1	A	262	LYS
1	B	300	THR
1	A	194	SER
1	A	210	LEU
1	A	181	VAL
1	A	138	ILE
1	A	311	PRO

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	290/304 (95%)	284 (98%)	6 (2%)	61 90
1	B	288/304 (95%)	277 (96%)	11 (4%)	40 74
All	All	578/608 (95%)	561 (97%)	17 (3%)	50 83

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	185	PHE
1	A	221	LEU
1	A	244	LYS
1	A	263	LEU
1	A	271	ASP
1	B	210	LEU
1	B	211	ASP

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Mol	Chain	Res	Type
1	B	238	LYS
1	B	241	ASP
1	B	250	THR
1	B	274	HIS
1	B	307	GLN
1	B	315	TYR
1	B	319	ASN
1	B	321	ASN
1	B	325	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	86	HIS
1	A	107	ASN
1	A	125	GLN
1	A	165	GLN
1	A	173	ASN
1	A	286	GLN
1	A	320	ASN
1	A	322	GLN
1	B	35	ASN
1	B	75	ASN
1	B	99	ASN
1	B	136	ASN
1	B	165	GLN
1	B	173	ASN
1	B	274	HIS
1	B	286	GLN
1	B	307	GLN
1	B	320	ASN
1	B	321	ASN

5.3.3 RNA

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)

5 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	NAP	A	334	-	42,52,52	1.56	10 (23%)	54,80,80	1.55	8 (14%)
3	UPG	A	335	-	29,38,38	1.33	3 (10%)	43,58,58	2.26	3 (6%)
2	NAP	B	334	-	42,52,52	1.55	9 (21%)	54,80,80	1.51	10 (18%)
3	UPG	B	335	-	29,38,38	1.30	3 (10%)	43,58,58	2.29	4 (9%)
4	MES	B	336	-	11,12,12	0.58	0	14,16,16	1.49	2 (14%)

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	NAP	A	334	-	-	0/27/67/67	0/5/5/5
3	UPG	A	335	-	-	0/19/59/59	0/3/3/3
2	NAP	B	334	-	-	0/27/67/67	0/5/5/5
3	UPG	B	335	-	-	0/19/59/59	0/3/3/3
4	MES	B	336	-	-	0/6/14/14	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	334	NAP	P2B-O3X	2.02	1.61	1.54
2	B	334	NAP	C5N-C4N	2.12	1.43	1.38
2	A	334	NAP	P2B-O3X	2.13	1.62	1.54
2	A	334	NAP	C2A-N3A	2.15	1.36	1.32
2	A	334	NAP	C7N-N7N	2.15	1.37	1.33
2	A	334	NAP	C4A-N3A	2.20	1.38	1.35
2	B	334	NAP	C4A-N3A	2.25	1.38	1.35
2	A	334	NAP	C5N-C4N	2.26	1.43	1.38
2	B	334	NAP	C7N-N7N	2.38	1.37	1.33
2	B	334	NAP	C4N-C3N	2.56	1.43	1.39
2	A	334	NAP	PA-O1A	2.71	1.61	1.51
2	A	334	NAP	C4N-C3N	2.71	1.43	1.39
3	B	335	UPG	PA-O1A	2.85	1.61	1.51
2	B	334	NAP	PA-O1A	2.88	1.61	1.51
3	A	335	UPG	PA-O1A	2.90	1.61	1.51
3	B	335	UPG	PB-O1B	2.92	1.61	1.51
3	A	335	UPG	PB-O1B	2.96	1.62	1.51
2	B	334	NAP	PN-O1N	3.04	1.62	1.51
2	B	334	NAP	P2B-O1X	3.05	1.61	1.51
2	A	334	NAP	PN-O1N	3.14	1.62	1.51
2	A	334	NAP	P2B-O1X	3.18	1.61	1.51
2	A	334	NAP	C2A-N1A	3.28	1.40	1.33
2	B	334	NAP	C2A-N1A	3.37	1.40	1.33
3	B	335	UPG	C4-N3	3.68	1.39	1.33
3	A	335	UPG	C4-N3	3.85	1.40	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	335	UPG	O5'-C1'-O3B	-6.71	102.52	111.36
3	A	335	UPG	O5'-C1'-O3B	-6.60	102.67	111.36
2	A	334	NAP	C3N-C7N-N7N	-4.39	113.01	117.82
2	A	334	NAP	C3N-C2N-N1N	-4.07	115.67	120.36
2	B	334	NAP	C3N-C2N-N1N	-3.99	115.77	120.36
2	B	334	NAP	C3N-C7N-N7N	-3.49	114.00	117.82
3	B	335	UPG	C5-C4-N3	-3.30	114.65	123.12
3	A	335	UPG	C5-C4-N3	-3.25	114.78	123.12
4	B	336	MES	O2S-S-C8	-2.94	104.39	106.91
4	B	336	MES	C7-C8-S	-2.87	103.63	112.51
2	A	334	NAP	C1B-N9A-C4A	-2.63	122.98	126.94
2	B	334	NAP	C1B-N9A-C4A	-2.52	123.14	126.94
2	B	334	NAP	N3A-C2A-N1A	-2.35	127.09	128.89
2	A	334	NAP	N3A-C2A-N1A	-2.26	127.17	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	334	NAP	C5N-C6N-N1N	-2.22	116.64	120.47
2	A	334	NAP	C5N-C6N-N1N	-2.11	116.82	120.47
3	B	335	UPG	O4C-C1C-N1	2.00	112.31	108.08
2	B	334	NAP	C4A-C5A-N7A	2.13	111.44	109.48
2	B	334	NAP	N6A-C6A-N1A	2.27	124.08	119.20
2	A	334	NAP	N6A-C6A-N1A	2.28	124.09	119.20
2	B	334	NAP	O4D-C1D-N1N	2.52	110.91	108.13
2	B	334	NAP	O2B-P2B-O1X	2.58	113.56	107.11
2	A	334	NAP	O2B-P2B-O1X	2.64	113.71	107.11
2	B	334	NAP	O7N-C7N-C3N	3.56	123.47	119.59
2	A	334	NAP	O7N-C7N-C3N	3.93	123.88	119.59
3	A	335	UPG	C4-N3-C2	11.62	125.64	114.14
3	B	335	UPG	C4-N3-C2	11.73	125.76	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	334	NAP	2	0
3	A	335	UPG	1	0
2	B	334	NAP	3	0
3	B	335	UPG	2	0
4	B	336	MES	1	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^{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	329/344 (95%)	0.89	55 (16%) 2 1	14, 48, 80, 80	0
1	B	327/344 (95%)	0.79	47 (14%) 3 2	12, 45, 79, 80	0
All	All	656/688 (95%)	0.84	102 (15%) 3 1	12, 46, 80, 80	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	SER	9.9
1	A	161	SER	9.8
1	B	331	LYS	8.7
1	A	248	PRO	8.6
1	B	201	ILE	8.2
1	A	195	GLU	7.8
1	A	191	ASN	7.6
1	A	159	LYS	7.3
1	A	247	ALA	7.0
1	B	162	SER	7.0
1	A	303	HIS	6.8
1	A	250	THR	6.8
1	B	196	ILE	6.5
1	B	240	THR	6.4
1	B	188	LEU	6.4
1	B	195	GLU	6.2
1	B	250	THR	6.2
1	B	163	GLN	6.1
1	A	321	ASN	5.9
1	B	249	ASN	5.8
1	B	191	ASN	5.6
1	A	245	ALA	5.3
1	A	160	GLY	5.2
1	B	330	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	193	ALA	5.0
1	A	255	ILE	5.0
1	B	187	LYS	5.0
1	B	161	SER	4.8
1	B	243	ALA	4.8
1	A	193	ALA	4.8
1	A	249	ASN	4.8
1	A	172	GLY	4.8
1	A	204	THR	4.7
1	A	194	SER	4.6
1	A	183	PRO	4.4
1	A	320	ASN	4.4
1	B	54	MET	4.4
1	A	322	GLN	4.3
1	B	253	LYS	4.3
1	B	333	LEU	4.2
1	B	251	PRO	4.1
1	A	199	THR	4.1
1	B	322	GLN	4.1
1	A	330	LEU	4.1
1	A	327	ASP	4.0
1	A	188	LEU	3.9
1	A	192	LYS	3.9
1	A	251	PRO	3.7
1	A	307	GLN	3.7
1	B	326	PRO	3.7
1	A	190	GLN	3.6
1	A	279	PHE	3.6
1	A	324	LEU	3.5
1	B	248	PRO	3.4
1	B	25	CYS	3.4
1	B	246	LEU	3.4
1	A	310	ALA	3.3
1	B	192	LYS	3.3
1	A	9	ASP	3.3
1	B	241	ASP	3.3
1	A	263	LEU	3.2
1	A	246	LEU	3.2
1	B	186	LYS	3.2
1	B	194	SER	3.2
1	B	307	GLN	3.1
1	A	158	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	292	GLN	3.0
1	A	326	PRO	3.0
1	B	311	PRO	3.0
1	A	202	ARG	3.0
1	A	264	HIS	2.9
1	A	312	ASP	2.7
1	A	331	LYS	2.7
1	B	314	GLU	2.7
1	B	183	PRO	2.7
1	A	323	TRP	2.7
1	B	190	GLN	2.7
1	B	199	THR	2.6
1	A	197	PRO	2.6
1	B	279	PHE	2.6
1	A	311	PRO	2.6
1	B	332	LEU	2.6
1	B	164	THR	2.6
1	A	239	MET	2.5
1	A	293	THR	2.5
1	B	202	ARG	2.5
1	B	181	VAL	2.4
1	B	273	SER	2.4
1	A	232	PRO	2.4
1	B	328	ASP	2.3
1	A	313	PHE	2.3
1	A	332	LEU	2.3
1	A	243	ALA	2.2
1	B	236	SER	2.2
1	B	207	TRP	2.2
1	B	310	ALA	2.2
1	A	280	GLU	2.2
1	B	318	HIS	2.2
1	A	298	THR	2.1
1	A	325	GLU	2.1
1	A	163	GLN	2.0
1	B	255	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
4	MES	B	336	12/12	0.86	0.26	3.39	68,74,80,80	0
2	NAP	B	334	48/48	0.97	0.21	0.19	22,44,77,80	0
3	UPG	B	335	36/36	0.87	0.26	0.12	56,73,78,80	11
2	NAP	A	334	48/48	0.95	0.21	-0.25	23,46,64,68	0
3	UPG	A	335	36/36	0.87	0.21	-0.80	73,80,80,80	11

6.5 Other polymers (i)

There are no such residues in this entry.