Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 10:01 PM GMT

PDB ID	:	1RPN
Title	:	Crystal Structure of GDP-D-mannose 4,6-dehydratase in complexes with GDP and NADPH
Authors	:	Webb, N.A.; Mulichak, A.M.; Lam, J.S.; Rocchetta, H.L.; Garavito, R.M.
Deposited on	:	2003-12-03
Resolution	:	2.15 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:

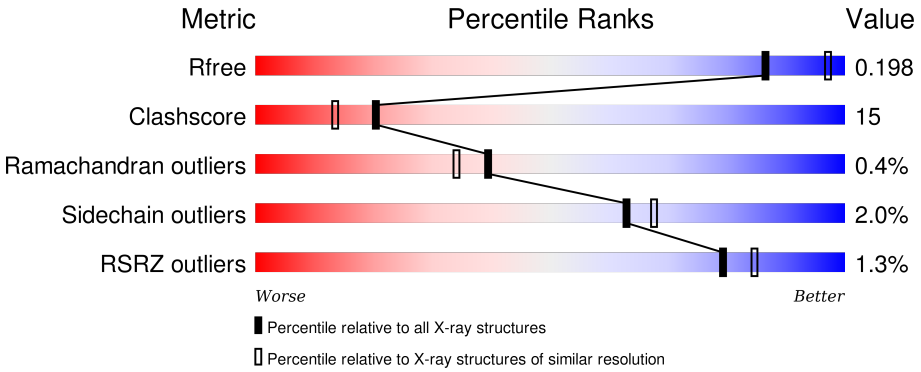
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	335	2% 66% 28%
1	B	335	64% 30%
1	C	335	68% 27%
1	D	335	64% 30%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NDP	A	1501	X	-	-	-
2	NDP	B	1502	X	-	-	-
2	NDP	C	1503	X	-	-	-
2	NDP	D	1504	X	-	-	-
3	GDP	A	1601	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11005 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 GDP-mannose 4,6-dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2503	1582	439	473	9			
1	B	321	Total	C	N	O	S	0	0	0
			2489	1576	435	469	9			
1	C	322	Total	C	N	O	S	0	0	0
			2508	1586	438	475	9			
1	D	322	Total	C	N	O	S	0	0	0
			2508	1587	441	471	9			

There are 48 discrepancies between the modelled and reference sequences:

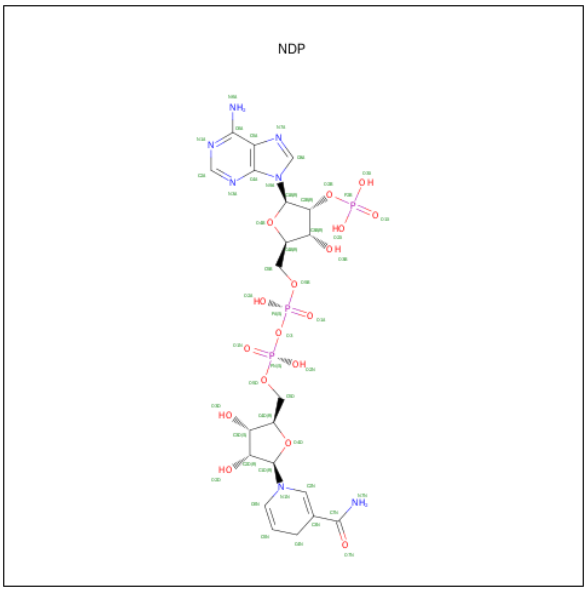
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	cloning artifact	UNP Q51366
A	-10	ARG	-	cloning artifact	UNP Q51366
A	-9	GLY	-	cloning artifact	UNP Q51366
A	-8	SER	-	cloning artifact	UNP Q51366
A	-7	HIS	-	EXPRESSION TAG	UNP Q51366
A	-6	HIS	-	EXPRESSION TAG	UNP Q51366
A	-5	HIS	-	EXPRESSION TAG	UNP Q51366
A	-4	HIS	-	EXPRESSION TAG	UNP Q51366
A	-3	HIS	-	EXPRESSION TAG	UNP Q51366
A	-2	HIS	-	EXPRESSION TAG	UNP Q51366
A	-1	GLY	-	cloning artifact	UNP Q51366
A	0	SER	-	cloning artifact	UNP Q51366
B	-11	MET	-	cloning artifact	UNP Q51366
B	-10	ARG	-	cloning artifact	UNP Q51366
B	-9	GLY	-	cloning artifact	UNP Q51366
B	-8	SER	-	cloning artifact	UNP Q51366
B	-7	HIS	-	EXPRESSION TAG	UNP Q51366
B	-6	HIS	-	EXPRESSION TAG	UNP Q51366
B	-5	HIS	-	EXPRESSION TAG	UNP Q51366
B	-4	HIS	-	EXPRESSION TAG	UNP Q51366
B	-3	HIS	-	EXPRESSION TAG	UNP Q51366

Continued on next page...

Continued from previous page...

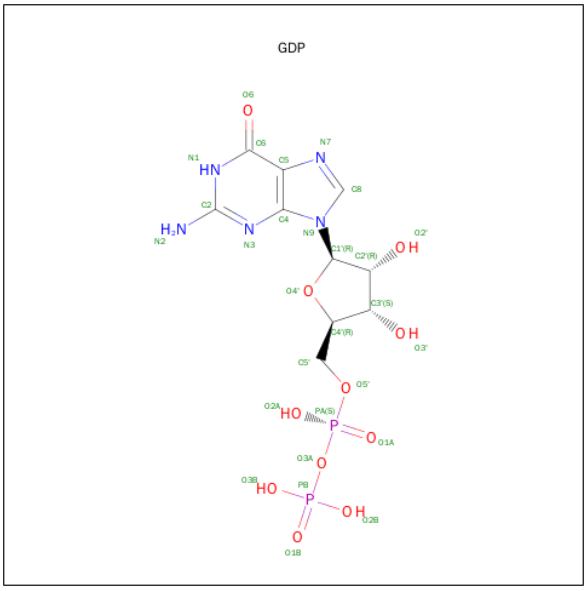
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	EXPRESSION TAG	UNP Q51366
B	-1	GLY	-	cloning artifact	UNP Q51366
B	0	SER	-	cloning artifact	UNP Q51366
C	-11	MET	-	cloning artifact	UNP Q51366
C	-10	ARG	-	cloning artifact	UNP Q51366
C	-9	GLY	-	cloning artifact	UNP Q51366
C	-8	SER	-	cloning artifact	UNP Q51366
C	-7	HIS	-	EXPRESSION TAG	UNP Q51366
C	-6	HIS	-	EXPRESSION TAG	UNP Q51366
C	-5	HIS	-	EXPRESSION TAG	UNP Q51366
C	-4	HIS	-	EXPRESSION TAG	UNP Q51366
C	-3	HIS	-	EXPRESSION TAG	UNP Q51366
C	-2	HIS	-	EXPRESSION TAG	UNP Q51366
C	-1	GLY	-	cloning artifact	UNP Q51366
C	0	SER	-	cloning artifact	UNP Q51366
D	-11	MET	-	cloning artifact	UNP Q51366
D	-10	ARG	-	cloning artifact	UNP Q51366
D	-9	GLY	-	cloning artifact	UNP Q51366
D	-8	SER	-	cloning artifact	UNP Q51366
D	-7	HIS	-	EXPRESSION TAG	UNP Q51366
D	-6	HIS	-	EXPRESSION TAG	UNP Q51366
D	-5	HIS	-	EXPRESSION TAG	UNP Q51366
D	-4	HIS	-	EXPRESSION TAG	UNP Q51366
D	-3	HIS	-	EXPRESSION TAG	UNP Q51366
D	-2	HIS	-	EXPRESSION TAG	UNP Q51366
D	-1	GLY	-	cloning artifact	UNP Q51366
D	0	SER	-	cloning artifact	UNP Q51366

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is water.

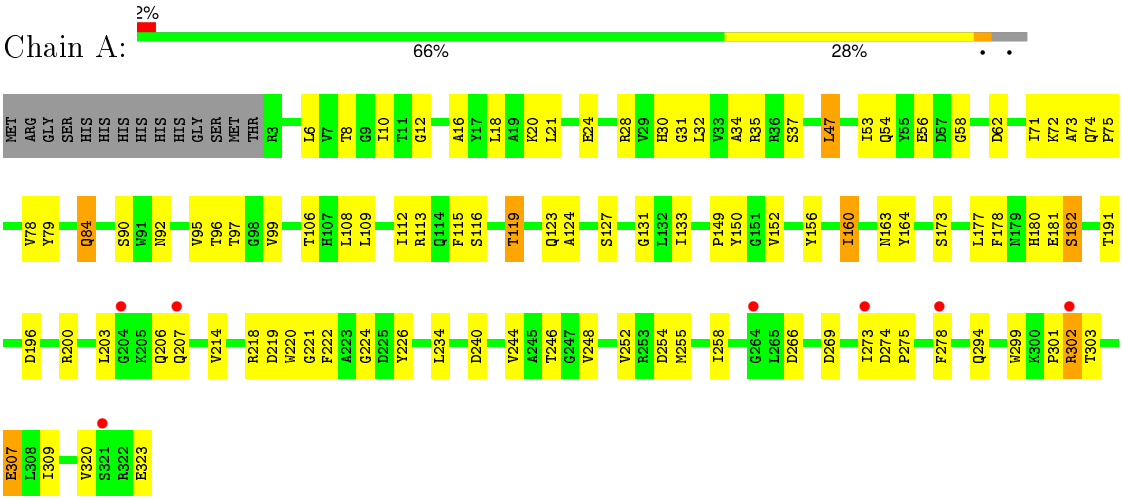
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	176	Total	O	0	0
			176	176		
4	B	155	Total	O	0	0
			155	155		
4	C	179	Total	O	0	0
			179	179		
4	D	183	Total	O	0	0
			183	183		

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.

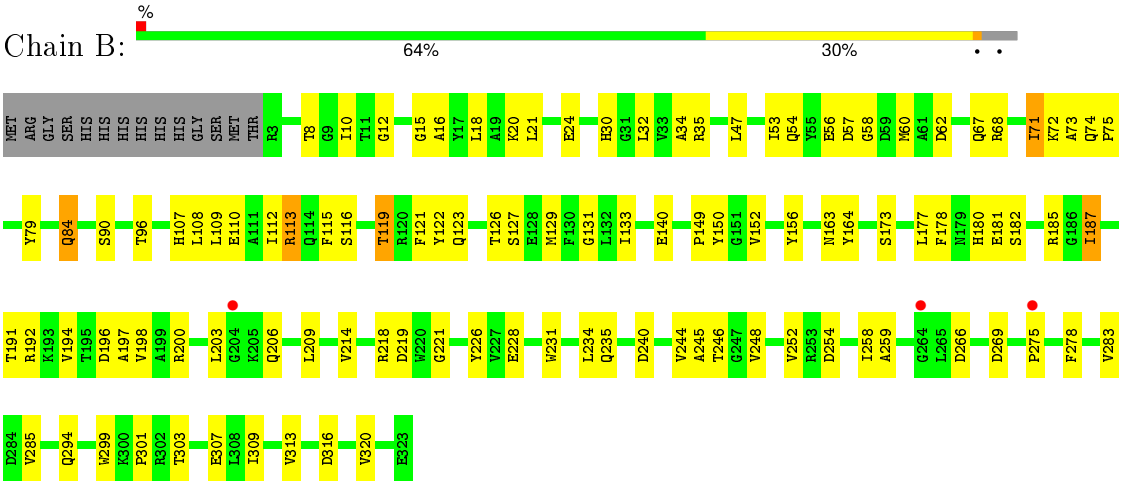
- Molecule 1: GDP-mannose 4,6-dehydratase

Chain A:



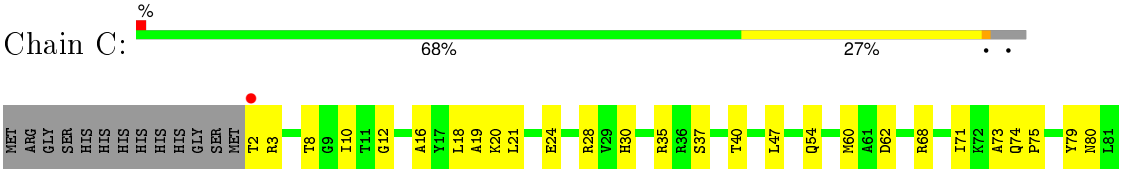
- Molecule 1: GDP-mannose 4,6-dehydratase

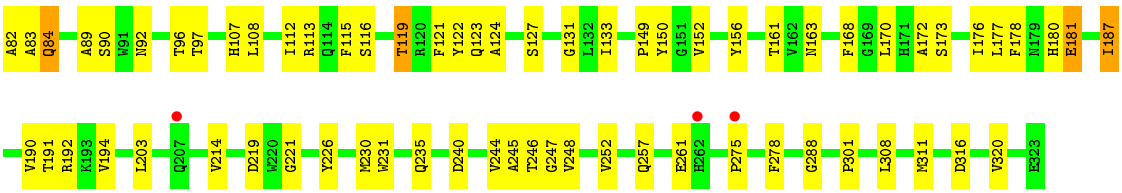
Chain B:



- Molecule 1: GDP-mannose 4,6-dehydratase

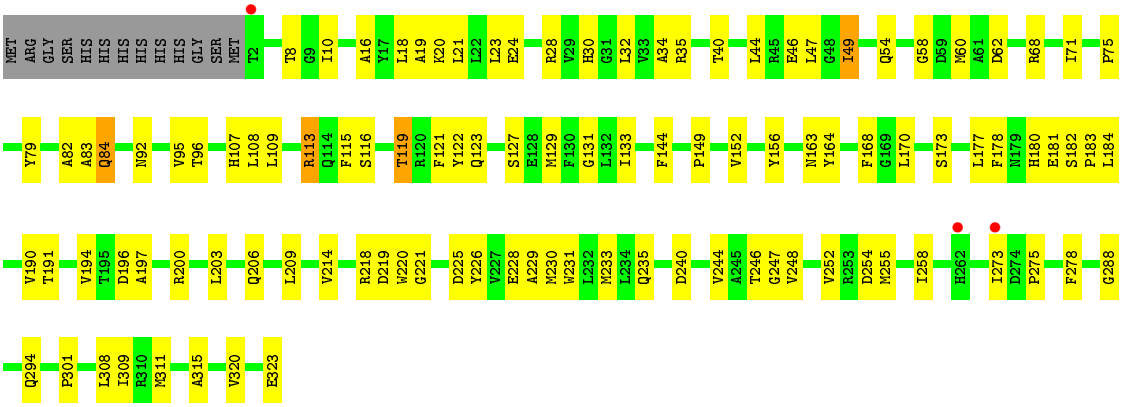
Chain C:





• Molecule 1: GDP-mannose 4,6-dehydratase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	125.73Å 125.73Å 220.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.15 29.92 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-2.15) 97.6 (29.92-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	14.00 (at 2.16Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.174 , 0.196 0.175 , 0.198	Depositor DCC
R_{free} test set	5399 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 49.3	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 108143 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11005	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.01% 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: GDP, NDP

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	0.31	0/2556	0.59	2/3471 (0.1%)
1	B	0.31	0/2542	0.59	1/3453 (0.0%)
1	C	0.33	0/2561	0.61	2/3478 (0.1%)
1	D	0.33	0/2561	0.61	2/3476 (0.1%)
All	All	0.32	0/10220	0.60	7/13878 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	84	GLN	N-CA-C	-7.64	90.38	111.00
1	A	84	GLN	N-CA-C	-7.55	90.62	111.00
1	C	84	GLN	N-CA-C	-7.39	91.03	111.00
1	B	84	GLN	N-CA-C	-7.32	91.25	111.00
1	C	28	ARG	N-CA-C	-5.96	94.90	111.00
1	A	28	ARG	N-CA-C	-5.80	95.35	111.00
1	D	28	ARG	N-CA-C	-5.75	95.46	111.00

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	2503	0	2413	77	0
1	B	2489	0	2397	88	0
1	C	2508	0	2420	67	0
1	D	2508	0	2427	80	0
2	A	48	0	26	3	0
2	B	48	0	26	3	0
2	C	48	0	26	3	0
2	D	48	0	26	2	0
3	A	28	0	12	0	0
3	B	28	0	12	0	0
3	C	28	0	12	0	0
3	D	28	0	12	0	0
4	A	176	0	0	2	0
4	B	155	0	0	5	0
4	C	179	0	0	5	0
4	D	183	0	0	4	0
All	All	11005	0	9809	293	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 15.

All (293) 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:67:GLN:O	1:B:71:ILE:HD13	1.75	0.85
1:D:196:ASP:O	1:D:200:ARG:HG3	1.77	0.85
1:B:67:GLN:HE21	1:B:71:ILE:HD11	1.42	0.84
1:B:196:ASP:O	1:B:200:ARG:HG3	1.77	0.83
1:B:67:GLN:HE21	1:B:71:ILE:CD1	1.91	0.83
1:B:67:GLN:NE2	1:B:71:ILE:HD11	1.95	0.81
1:A:196:ASP:O	1:A:200:ARG:HG3	1.81	0.80
1:D:49:ILE:H	1:D:49:ILE:HD13	1.48	0.78
1:B:108:LEU:O	1:B:112:ILE:HD13	1.88	0.73
1:D:44:LEU:O	1:D:49:ILE:HD13	1.89	0.72
1:B:116:SER:O	1:B:119:THR:HG23	1.91	0.70
1:A:116:SER:O	1:A:119:THR:HG23	1.91	0.70
1:A:56:GLU:OE1	1:A:72:LYS:HD3	1.92	0.70
1:D:116:SER:O	1:D:119:THR:HG23	1.92	0.69
1:C:60:MET:O	1:C:107:HIS:HD2	1.76	0.69
1:B:113:ARG:HD3	4:B:1732:HOH:O	1.93	0.68
1:C:133:ILE:O	1:C:133:ILE:HD12	1.95	0.67
1:C:116:SER:O	1:C:119:THR:HG23	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ILE:HD11	1:C:19:ALA:HB2	1.77	0.67
1:A:109:LEU:HD12	1:A:160:ILE:HD13	1.78	0.65
1:D:60:MET:O	1:D:107:HIS:HD2	1.78	0.65
1:D:10:ILE:HD11	1:D:19:ALA:HB2	1.78	0.64
1:C:257:GLN:O	1:C:261:GLU:HG3	1.97	0.64
1:C:163:ASN:HD21	1:D:149:PRO:HD3	1.63	0.64
1:D:20:LYS:O	1:D:24:GLU:HG3	1.98	0.64
1:A:133:ILE:O	1:A:133:ILE:HD12	1.98	0.64
1:B:60:MET:O	1:B:107:HIS:HD2	1.80	0.64
1:C:20:LYS:O	1:C:24:GLU:HG3	1.98	0.63
1:D:133:ILE:HD12	1:D:133:ILE:O	1.99	0.63
1:A:275:PRO:HA	1:A:278:PHE:CD1	2.34	0.63
1:B:181:GLU:HG3	1:B:191:THR:HG21	1.81	0.62
1:A:302:ARG:HD2	1:A:302:ARG:N	2.14	0.62
1:B:56:GLU:OE1	1:B:72:LYS:HD3	1.99	0.62
1:D:181:GLU:HG3	1:D:191:THR:HG21	1.81	0.62
1:C:176:ILE:HD12	1:C:176:ILE:N	2.14	0.61
1:C:181:GLU:HG3	1:C:191:THR:HG21	1.80	0.61
1:C:275:PRO:HA	1:C:278:PHE:CD1	2.36	0.60
1:B:275:PRO:HA	1:B:278:PHE:CD1	2.37	0.60
1:A:106:THR:OG1	1:A:160:ILE:HD12	2.02	0.60
1:D:273:ILE:N	1:D:273:ILE:HD12	2.17	0.59
1:A:255:MET:HG2	1:A:309:ILE:HD11	1.84	0.59
1:A:273:ILE:HD12	1:A:273:ILE:N	2.17	0.59
1:C:18:LEU:HD21	1:C:79:TYR:CG	2.37	0.59
1:C:21:LEU:C	1:C:21:LEU:HD23	2.22	0.59
1:D:49:ILE:HD13	1:D:49:ILE:N	2.18	0.57
1:A:18:LEU:HD21	1:A:79:TYR:CG	2.39	0.57
1:D:18:LEU:HD21	1:D:79:TYR:CG	2.40	0.57
1:B:113:ARG:CZ	1:D:68:ARG:NH2	2.68	0.57
1:D:71:ILE:HA	1:D:115:PHE:CE2	2.39	0.57
1:B:21:LEU:C	1:B:21:LEU:HD23	2.25	0.56
1:D:246:THR:HA	1:D:301:PRO:HG3	1.88	0.56
1:C:187:ILE:HD11	4:C:1660:HOH:O	2.04	0.55
1:B:96:THR:OG1	1:C:62:ASP:HB2	2.05	0.55
1:A:62:ASP:HB2	1:D:96:THR:OG1	2.06	0.55
1:C:246:THR:HA	1:C:301:PRO:HG3	1.89	0.55
1:B:18:LEU:HD21	1:B:79:TYR:CG	2.42	0.55
1:A:181:GLU:HG3	1:A:191:THR:HG21	1.88	0.55
1:A:35:ARG:HD3	1:A:35:ARG:C	2.27	0.55
1:D:16:ALA:HB1	1:D:47:LEU:HD22	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:LEU:HD23	1:D:21:LEU:C	2.27	0.54
1:A:21:LEU:HD23	1:A:21:LEU:C	2.27	0.54
1:D:47:LEU:HB3	1:D:49:ILE:HD12	1.90	0.54
1:C:187:ILE:HD13	4:C:1653:HOH:O	2.06	0.54
1:A:10:ILE:HD13	1:A:31:GLY:HA3	1.88	0.54
1:B:246:THR:HA	1:B:301:PRO:HG3	1.90	0.54
1:C:149:PRO:HD3	1:D:163:ASN:HD21	1.72	0.54
1:A:10:ILE:HD11	1:A:53:ILE:HD13	1.90	0.53
1:D:113:ARG:HD3	4:D:1729:HOH:O	2.06	0.53
1:A:20:LYS:O	1:A:24:GLU:HG3	2.07	0.53
1:D:75:PRO:O	1:D:119:THR:HB	2.08	0.53
1:A:273:ILE:HD12	1:A:273:ILE:H	1.74	0.53
1:A:112:ILE:HD12	1:A:119:THR:OG1	2.08	0.52
1:B:309:ILE:O	1:B:313:VAL:HG23	2.09	0.52
1:B:266:ASP:HB3	1:B:269:ASP:OD2	2.10	0.52
1:B:219:ASP:OD1	1:B:245:ALA:HB1	2.09	0.52
1:B:62:ASP:HB2	1:C:96:THR:OG1	2.10	0.52
1:B:20:LYS:O	1:B:24:GLU:HG3	2.10	0.52
1:B:24:GLU:HB2	4:B:1754:HOH:O	2.09	0.52
1:D:30:HIS:HA	1:D:54:GLN:O	2.09	0.52
1:A:177:LEU:HG	1:A:244:VAL:HB	1.91	0.52
1:D:308:LEU:O	1:D:311:MET:HG2	2.09	0.52
1:A:246:THR:HA	1:A:301:PRO:HG3	1.91	0.51
1:A:163:ASN:HD21	1:B:149:PRO:HD3	1.75	0.51
1:C:156:TYR:CD1	1:D:152:VAL:HG12	2.45	0.51
1:B:71:ILE:CD1	1:B:71:ILE:N	2.73	0.51
1:B:177:LEU:O	2:B:1502:NDP:H5N	2.11	0.51
1:B:177:LEU:HG	1:B:244:VAL:HB	1.92	0.51
1:B:35:ARG:HD3	1:B:35:ARG:C	2.31	0.51
1:C:35:ARG:HD3	1:C:35:ARG:C	2.31	0.51
1:C:8:THR:HG1	1:C:80:ASN:HA	1.76	0.51
1:A:149:PRO:HD3	1:B:163:ASN:HD21	1.76	0.51
1:B:187:ILE:HD13	4:B:1665:HOH:O	2.11	0.51
1:D:40:THR:HG21	4:D:1684:HOH:O	2.11	0.51
1:A:266:ASP:HB3	1:A:269:ASP:OD2	2.11	0.51
1:D:230:MET:HA	1:D:233:MET:HE3	1.93	0.51
1:C:177:LEU:O	2:C:1503:NDP:H5N	2.11	0.51
1:C:40:THR:HG21	4:C:1696:HOH:O	2.10	0.51
1:D:177:LEU:HG	1:D:244:VAL:HB	1.92	0.50
1:A:173:SER:HB3	1:A:240:ASP:O	2.12	0.50
1:D:275:PRO:HA	1:D:278:PHE:CD1	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ALA:HB1	1:A:47:LEU:HD22	1.93	0.50
1:A:96:THR:OG1	1:D:62:ASP:HB2	2.11	0.50
1:D:123:GLN:HA	1:D:123:GLN:NE2	2.26	0.50
1:B:123:GLN:HA	1:B:123:GLN:NE2	2.27	0.50
1:D:219:ASP:HA	1:D:248:VAL:O	2.12	0.50
1:C:16:ALA:HB1	1:C:47:LEU:HD22	1.92	0.50
1:B:187:ILE:HD11	4:B:1679:HOH:O	2.11	0.50
1:B:140:GLU:CD	1:B:140:GLU:H	2.15	0.50
1:D:46:GLU:HG2	1:D:184:LEU:HD21	1.94	0.50
1:C:92:ASN:ND2	4:C:1611:HOH:O	2.46	0.49
1:C:75:PRO:O	1:C:119:THR:HB	2.12	0.49
1:B:16:ALA:HB1	1:B:47:LEU:HD22	1.94	0.49
1:D:35:ARG:C	1:D:35:ARG:HD3	2.32	0.49
1:A:113:ARG:CZ	1:C:68:ARG:NH2	2.75	0.49
1:C:108:LEU:HD13	1:C:121:PHE:HE1	1.77	0.49
1:B:75:PRO:O	1:B:119:THR:HB	2.13	0.49
1:B:68:ARG:NH2	1:D:113:ARG:CZ	2.76	0.49
1:D:123:GLN:HA	1:D:123:GLN:HE21	1.77	0.49
1:B:173:SER:HB3	1:B:240:ASP:O	2.13	0.49
1:D:92:ASN:ND2	4:D:1669:HOH:O	2.46	0.49
1:B:197:ALA:CB	1:B:209:LEU:HD13	2.43	0.49
1:A:214:VAL:HA	1:A:252:VAL:HB	1.95	0.49
1:A:177:LEU:O	2:A:1501:NDP:H5N	2.12	0.49
1:A:294:GLN:NE2	4:A:1738:HOH:O	2.46	0.49
1:C:316:ASP:O	1:C:320:VAL:HG23	2.13	0.49
1:C:71:ILE:HA	1:C:115:PHE:CE2	2.48	0.49
1:C:177:LEU:HG	1:C:244:VAL:HB	1.95	0.48
1:C:247:GLY:HA2	1:C:288:GLY:O	2.12	0.48
1:B:10:ILE:HD13	1:B:53:ILE:HG21	1.94	0.48
1:B:123:GLN:HA	1:B:123:GLN:HE21	1.78	0.48
1:B:110:GLU:OE1	1:D:68:ARG:NH2	2.38	0.48
1:B:67:GLN:HE21	1:B:71:ILE:HD13	1.74	0.48
1:B:303:THR:HG23	1:B:307:GLU:CG	2.44	0.48
1:A:92:ASN:ND2	4:A:1674:HOH:O	2.47	0.48
1:B:32:LEU:HD11	1:B:58:GLY:HA3	1.96	0.47
1:A:10:ILE:HD13	1:A:53:ILE:HG21	1.97	0.47
1:B:219:ASP:HA	1:B:248:VAL:O	2.14	0.47
1:A:8:THR:HA	1:A:32:LEU:HB3	1.96	0.47
1:A:71:ILE:HA	1:A:115:PHE:CE2	2.50	0.47
1:C:308:LEU:O	1:C:311:MET:HG2	2.15	0.47
1:D:177:LEU:O	2:D:1504:NDP:H5N	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:MET:HG2	1:D:309:ILE:HD11	1.97	0.47
1:A:219:ASP:HA	1:A:248:VAL:O	2.15	0.47
1:D:197:ALA:CB	1:D:209:LEU:HD13	2.45	0.47
1:D:108:LEU:HD13	1:D:121:PHE:HE1	1.78	0.47
1:A:200:ARG:HD3	1:A:206:GLN:OE1	2.14	0.47
1:D:254:ASP:O	1:D:258:ILE:HG12	2.15	0.47
1:A:294:GLN:HA	1:A:299:TRP:O	2.14	0.46
1:B:79:TYR:CZ	1:B:234:LEU:HD22	2.50	0.46
1:B:194:VAL:HG22	1:B:209:LEU:HD21	1.97	0.46
1:C:152:VAL:HG12	1:D:156:TYR:CD1	2.50	0.46
1:D:122:TYR:CZ	1:D:230:MET:HG2	2.50	0.46
1:A:37:SER:HB3	2:D:1504:NDP:H3B	1.98	0.46
1:B:294:GLN:HA	1:B:299:TRP:O	2.15	0.46
1:A:160:ILE:HD11	1:A:164:TYR:CE1	2.50	0.46
1:C:180:HIS:HA	1:C:221:GLY:O	2.15	0.46
1:D:47:LEU:CB	1:D:49:ILE:HD12	2.45	0.46
1:C:10:ILE:CD1	1:C:19:ALA:HB2	2.44	0.46
1:D:273:ILE:H	1:D:273:ILE:HD12	1.80	0.46
1:C:231:TRP:O	1:C:235:GLN:HG2	2.14	0.46
1:D:8:THR:HA	1:D:32:LEU:HB3	1.97	0.46
1:C:127:SER:OG	1:C:178:PHE:HA	2.16	0.46
1:A:255:MET:HG2	1:A:309:ILE:CD1	2.44	0.46
1:C:219:ASP:HA	1:C:248:VAL:O	2.15	0.46
1:A:73:ALA:O	1:A:74:GLN:C	2.54	0.46
1:C:12:GLY:HA3	2:C:1503:NDP:O5B	2.16	0.46
1:C:161:THR:HG23	1:C:172:ALA:HB1	1.97	0.46
1:A:180:HIS:HA	1:A:221:GLY:O	2.16	0.46
1:B:316:ASP:O	1:B:320:VAL:HG23	2.15	0.45
1:C:112:ILE:HD12	1:C:119:THR:OG1	2.16	0.45
1:B:10:ILE:HD11	1:B:53:ILE:HD13	1.98	0.45
1:D:200:ARG:HD3	1:D:206:GLN:OE1	2.17	0.45
1:D:23:LEU:CD1	1:D:49:ILE:HB	2.47	0.45
1:C:127:SER:HB3	1:C:178:PHE:CD1	2.51	0.45
1:B:30:HIS:HA	1:B:54:GLN:O	2.17	0.45
1:D:183:PRO:HB3	1:D:315:ALA:CB	2.46	0.45
1:B:126:THR:O	1:B:129:MET:HG3	2.17	0.45
1:A:181:GLU:O	1:A:182:SER:HB3	2.16	0.45
1:C:30:HIS:HA	1:C:54:GLN:O	2.17	0.45
1:B:12:GLY:HA3	2:B:1502:NDP:O5B	2.17	0.45
1:D:173:SER:HB3	1:D:240:ASP:O	2.17	0.45
1:A:156:TYR:CD1	1:B:152:VAL:HG12	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:LEU:HD11	1:B:228:GLU:HA	1.99	0.45
1:A:123:GLN:HA	1:A:123:GLN:HE21	1.82	0.45
1:A:123:GLN:HA	1:A:123:GLN:NE2	2.32	0.45
1:C:82:ALA:O	1:C:83:ALA:HB2	2.15	0.45
1:C:173:SER:HB3	1:C:240:ASP:O	2.17	0.45
1:D:225:ASP:O	1:D:228:GLU:HB2	2.17	0.45
1:C:214:VAL:HA	1:C:252:VAL:HB	1.97	0.45
1:A:299:TRP:CZ3	1:A:301:PRO:HD3	2.52	0.44
1:D:214:VAL:HA	1:D:252:VAL:HB	1.99	0.44
1:B:122:TYR:HB2	1:B:234:LEU:HD11	1.99	0.44
1:A:78:VAL:HG21	1:A:112:ILE:HD11	1.97	0.44
1:B:200:ARG:HD3	1:B:206:GLN:OE1	2.17	0.44
1:B:34:ALA:HA	1:B:58:GLY:O	2.17	0.44
1:B:180:HIS:HA	1:B:221:GLY:O	2.17	0.44
1:D:180:HIS:HA	1:D:221:GLY:O	2.18	0.44
1:A:6:LEU:HB3	1:A:78:VAL:HG22	2.00	0.44
1:C:123:GLN:NE2	1:C:123:GLN:HA	2.33	0.44
1:D:226:TYR:CD1	1:D:226:TYR:N	2.85	0.44
1:D:200:ARG:NH1	1:D:323:GLU:OE1	2.51	0.44
1:B:108:LEU:HD13	1:B:121:PHE:HE1	1.81	0.44
1:C:190:VAL:O	1:C:194:VAL:HG23	2.18	0.44
1:D:168:PHE:HB2	1:D:170:LEU:HG	1.99	0.44
1:A:218:ARG:HB2	1:A:220:TRP:CZ2	2.53	0.44
1:A:222:PHE:CE2	1:A:224:GLY:HA3	2.53	0.44
1:A:74:GLN:N	1:A:75:PRO:CD	2.81	0.43
1:A:152:VAL:HG12	1:B:156:TYR:CD1	2.53	0.43
1:C:90:SER:HB3	1:C:150:TYR:HB2	2.00	0.43
1:D:129:MET:HE3	1:D:144:PHE:CE1	2.53	0.43
1:A:207:GLN:HE21	1:A:207:GLN:HA	1.83	0.43
1:B:90:SER:HB3	1:B:150:TYR:HB2	2.00	0.43
1:A:254:ASP:O	1:A:258:ILE:HG12	2.19	0.43
1:D:226:TYR:HD1	1:D:226:TYR:N	2.16	0.43
1:B:218:ARG:NH1	1:B:283:VAL:HB	2.33	0.43
1:C:226:TYR:N	1:C:226:TYR:CD1	2.86	0.43
1:D:229:ALA:O	1:D:233:MET:HG3	2.18	0.43
1:C:127:SER:HB3	1:C:178:PHE:CG	2.54	0.43
1:A:34:ALA:HA	1:A:58:GLY:O	2.19	0.43
1:A:301:PRO:C	1:A:302:ARG:HD2	2.39	0.43
1:D:181:GLU:O	1:D:182:SER:HB3	2.19	0.42
1:A:203:LEU:HD12	1:A:320:VAL:CG1	2.49	0.42
1:B:203:LEU:HD12	1:B:320:VAL:HB	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ASP:CG	1:D:95:VAL:HB	2.39	0.42
1:B:10:ILE:CD1	1:B:53:ILE:HD13	2.49	0.42
1:A:8:THR:HG21	1:A:108:LEU:HD11	2.01	0.42
1:A:79:TYR:CZ	1:A:234:LEU:HD22	2.54	0.42
1:B:10:ILE:HA	1:B:15:GLY:HA3	2.02	0.42
1:C:226:TYR:N	1:C:226:TYR:HD1	2.17	0.42
1:D:231:TRP:O	1:D:235:GLN:HG2	2.19	0.42
1:C:73:ALA:O	1:C:74:GLN:C	2.56	0.42
1:B:71:ILE:HA	1:B:115:PHE:CE2	2.54	0.42
1:B:294:GLN:HB2	4:B:1680:HOH:O	2.19	0.42
1:D:218:ARG:HB2	1:D:220:TRP:CZ2	2.54	0.42
1:B:254:ASP:O	1:B:258:ILE:HG12	2.19	0.42
1:B:214:VAL:HA	1:B:252:VAL:HB	2.02	0.42
1:B:8:THR:HA	1:B:32:LEU:HB3	2.01	0.42
1:D:247:GLY:HA2	1:D:288:GLY:O	2.18	0.42
1:B:122:TYR:HB2	1:B:234:LEU:CD1	2.50	0.42
2:B:1502:NDP:H3B	1:C:37:SER:HB3	2.01	0.42
1:C:97:THR:HG21	1:C:150:TYR:HA	2.02	0.42
1:A:109:LEU:HB3	1:A:164:TYR:CD2	2.55	0.42
1:B:275:PRO:HA	1:B:278:PHE:HD1	1.80	0.42
1:B:226:TYR:N	1:B:226:TYR:CD1	2.86	0.42
1:C:176:ILE:CD1	1:C:176:ILE:N	2.83	0.42
1:B:185:ARG:O	1:B:192:ARG:HG2	2.20	0.42
1:A:226:TYR:N	1:A:226:TYR:CD1	2.88	0.42
1:B:127:SER:OG	1:B:178:PHE:HA	2.20	0.42
1:D:109:LEU:HB3	1:D:164:TYR:CD2	2.55	0.42
1:D:127:SER:OG	1:D:178:PHE:HA	2.20	0.42
1:D:127:SER:HB3	1:D:178:PHE:CG	2.56	0.41
1:D:34:ALA:HA	1:D:58:GLY:O	2.21	0.41
1:D:49:ILE:CD1	1:D:49:ILE:N	2.83	0.41
1:D:116:SER:OG	1:D:119:THR:CG2	2.68	0.41
1:D:10:ILE:CD1	1:D:19:ALA:HB2	2.49	0.41
1:C:124:ALA:HB1	2:C:1503:NDP:O4D	2.21	0.41
1:C:219:ASP:OD1	1:C:245:ALA:HB1	2.20	0.41
1:D:127:SER:HB3	1:D:178:PHE:CD1	2.55	0.41
1:D:203:LEU:HD12	1:D:320:VAL:CG1	2.51	0.41
1:C:2:THR:HG23	1:C:3:ARG:N	2.35	0.41
1:B:133:ILE:CD1	1:B:285:VAL:HG13	2.51	0.41
1:B:112:ILE:CD1	1:B:112:ILE:N	2.83	0.41
1:A:75:PRO:O	1:A:119:THR:HB	2.20	0.41
1:B:181:GLU:O	1:B:182:SER:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ALA:HB1	2:A:1501:NDP:O4D	2.20	0.41
1:C:168:PHE:HB2	1:C:170:LEU:HG	2.02	0.41
1:D:190:VAL:O	1:D:194:VAL:HG23	2.20	0.41
1:B:200:ARG:HA	1:B:320:VAL:HG11	2.02	0.41
1:C:163:ASN:ND2	1:D:149:PRO:HD3	2.32	0.41
1:C:192:ARG:HH11	1:C:192:ARG:HG2	1.84	0.41
1:B:73:ALA:O	1:B:74:GLN:C	2.57	0.41
1:B:127:SER:HB3	1:B:178:PHE:CD1	2.56	0.41
1:A:90:SER:HB3	1:A:150:TYR:HB2	2.03	0.41
1:B:226:TYR:HD1	1:B:226:TYR:N	2.18	0.41
1:D:82:ALA:O	1:D:83:ALA:HB2	2.21	0.41
1:A:127:SER:HB3	1:A:178:PHE:CG	2.56	0.41
1:A:30:HIS:HA	1:A:54:GLN:O	2.19	0.41
1:B:57:ASP:OD2	1:C:89:ALA:HA	2.21	0.41
1:B:109:LEU:HB3	1:B:164:TYR:CD2	2.55	0.41
1:B:231:TRP:O	1:B:235:GLN:HG2	2.21	0.41
1:A:200:ARG:NH1	1:A:323:GLU:OE1	2.54	0.41
1:A:97:THR:HG21	1:A:150:TYR:HA	2.03	0.41
1:A:95:VAL:O	1:A:99:VAL:HG23	2.21	0.41
1:A:12:GLY:HA3	2:A:1501:NDP:O5B	2.21	0.40
1:A:10:ILE:CD1	1:A:53:ILE:HD13	2.52	0.40
1:B:198:VAL:HG21	1:B:259:ALA:HB1	2.03	0.40
1:A:303:THR:HG23	1:A:307:GLU:HB3	2.03	0.40
1:C:203:LEU:HD12	1:C:320:VAL:CG1	2.51	0.40
1:D:294:GLN:NE2	4:D:1708:HOH:O	2.55	0.40
1:C:122:TYR:CZ	1:C:230:MET:HG2	2.56	0.40
1:B:112:ILE:N	1:B:112:ILE:HD12	2.37	0.40
1:C:107:HIS:CE1	4:C:1698:HOH:O	2.74	0.40
1:A:274:ASP:HA	1:A:275:PRO:HD2	1.95	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	319/335 (95%)	311 (98%)	6 (2%)	2 (1%)	30 21
1	B	319/335 (95%)	313 (98%)	5 (2%)	1 (0%)	46 42
1	C	320/335 (96%)	315 (98%)	4 (1%)	1 (0%)	46 42
1	D	320/335 (96%)	313 (98%)	6 (2%)	1 (0%)	46 42
All	All	1278/1340 (95%)	1252 (98%)	21 (2%)	5 (0%)	39 34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	GLY
1	B	131	GLY
1	C	131	GLY
1	D	131	GLY
1	A	182	SER

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	256/278 (92%)	250 (98%)	6 (2%)	58 62
1	B	253/278 (91%)	248 (98%)	5 (2%)	63 67
1	C	257/278 (92%)	252 (98%)	5 (2%)	65 69
1	D	256/278 (92%)	252 (98%)	4 (2%)	70 76
All	All	1022/1112 (92%)	1002 (98%)	20 (2%)	63 67

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	84	GLN
1	A	119	THR
1	A	160	ILE
1	A	302	ARG
1	A	307	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	71	ILE
1	B	84	GLN
1	B	113	ARG
1	B	119	THR
1	B	187	ILE
1	C	84	GLN
1	C	113	ARG
1	C	119	THR
1	C	181	GLU
1	C	187	ILE
1	D	49	ILE
1	D	84	GLN
1	D	113	ARG
1	D	119	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	80	ASN
1	A	92	ASN
1	A	93	GLN
1	A	123	GLN
1	A	207	GLN
1	A	294	GLN
1	B	67	GLN
1	B	80	ASN
1	B	92	ASN
1	B	93	GLN
1	B	107	HIS
1	B	123	GLN
1	B	163	ASN
1	C	54	GLN
1	C	80	ASN
1	C	92	ASN
1	C	93	GLN
1	C	107	HIS
1	C	123	GLN
1	C	163	ASN
1	C	294	GLN
1	D	74	GLN
1	D	80	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	92	ASN
1	D	93	GLN
1	D	107	HIS
1	D	123	GLN
1	D	163	ASN
1	D	294	GLN

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

8 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	NDP	A	1501	-	42,52,52	1.26	3 (7%)	55,80,80	1.19	6 (10%)
3	GDP	A	1601	-	23,30,30	1.03	1 (4%)	30,47,47	2.39	4 (13%)
2	NDP	B	1502	-	42,52,52	1.28	2 (4%)	55,80,80	1.17	7 (12%)
3	GDP	B	1602	-	23,30,30	1.02	2 (8%)	30,47,47	2.60	7 (23%)
2	NDP	C	1503	-	42,52,52	1.28	2 (4%)	55,80,80	1.18	7 (12%)
3	GDP	C	1603	-	23,30,30	1.09	1 (4%)	30,47,47	2.54	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NDP	D	1504	-	42,52,52	1.28	2 (4%)	55,80,80	1.18	7 (12%)
3	GDP	D	1604	-	23,30,30	1.10	2 (8%)	30,47,47	2.58	7 (23%)

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	NDP	A	1501	-	1/1/14/17	0/30/77/77	0/5/5/5
3	GDP	A	1601	-	-	0/12/32/32	0/3/3/3
2	NDP	B	1502	-	1/1/14/17	0/30/77/77	0/5/5/5
3	GDP	B	1602	-	-	0/12/32/32	0/3/3/3
2	NDP	C	1503	-	1/1/14/17	0/30/77/77	0/5/5/5
3	GDP	C	1603	-	-	0/12/32/32	0/3/3/3
2	NDP	D	1504	-	1/1/14/17	0/30/77/77	0/5/5/5
3	GDP	D	1604	-	-	0/12/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1504	NDP	C4N-C5N	-5.42	1.37	1.49
2	B	1502	NDP	C4N-C5N	-5.37	1.37	1.49
2	A	1501	NDP	C4N-C5N	-5.36	1.37	1.49
2	C	1503	NDP	C4N-C5N	-5.35	1.37	1.49
2	C	1503	NDP	P2B-O2B	-4.00	1.47	1.60
2	D	1504	NDP	P2B-O2B	-3.99	1.47	1.60
2	B	1502	NDP	P2B-O2B	-3.86	1.48	1.60
2	A	1501	NDP	P2B-O2B	-3.76	1.48	1.60
3	D	1604	GDP	C8-N7	-2.05	1.30	1.34
3	B	1602	GDP	C8-N7	-2.05	1.30	1.34
2	A	1501	NDP	O4B-C1B	2.02	1.43	1.41
3	B	1602	GDP	C6-N1	3.13	1.38	1.33
3	A	1601	GDP	C6-N1	3.38	1.39	1.33
3	D	1604	GDP	C6-N1	3.44	1.39	1.33
3	C	1603	GDP	C6-N1	3.52	1.39	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1604	GDP	C5-C6-N1	-9.10	111.15	123.59
3	B	1602	GDP	C5-C6-N1	-9.01	111.27	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1603	GDP	C5-C6-N1	-8.97	111.32	123.59
3	A	1601	GDP	C5-C6-N1	-8.76	111.61	123.59
2	D	1504	NDP	O4B-C4B-C3B	-2.53	100.04	105.15
3	D	1604	GDP	N3-C2-N1	-2.51	123.62	127.44
2	B	1502	NDP	O4B-C4B-C3B	-2.45	100.20	105.15
3	B	1602	GDP	N3-C2-N1	-2.42	123.75	127.44
2	A	1501	NDP	O4B-C4B-C3B	-2.39	100.34	105.15
3	A	1601	GDP	N3-C2-N1	-2.34	123.89	127.44
3	C	1603	GDP	N3-C2-N1	-2.32	123.91	127.44
2	C	1503	NDP	O4B-C4B-C3B	-2.30	100.51	105.15
2	D	1504	NDP	O3-PN-O5D	-2.29	96.85	102.94
2	C	1503	NDP	O3-PN-O5D	-2.17	97.17	102.94
2	A	1501	NDP	C2B-C3B-C4B	-2.17	96.72	101.85
2	B	1502	NDP	C2B-C3B-C4B	-2.10	96.89	101.85
2	A	1501	NDP	O3-PN-O5D	-2.09	97.38	102.94
2	B	1502	NDP	O3-PN-O5D	-2.09	97.39	102.94
2	C	1503	NDP	C2B-C3B-C4B	-2.07	96.95	101.85
2	B	1502	NDP	O2N-PN-O3	-2.07	95.70	105.09
2	D	1504	NDP	C2B-C3B-C4B	-2.06	96.98	101.85
2	D	1504	NDP	O2N-PN-O5D	2.03	118.68	108.46
2	A	1501	NDP	O2N-PN-O5D	2.03	118.71	108.46
2	B	1502	NDP	O2N-PN-O5D	2.03	118.72	108.46
2	C	1503	NDP	O2N-PN-O5D	2.04	118.74	108.46
3	B	1602	GDP	O3'-C3'-C2'	2.13	118.75	111.83
2	D	1504	NDP	O5D-PN-O1N	2.13	117.89	109.62
3	B	1602	GDP	O3'-C3'-C4'	2.16	117.54	111.05
2	C	1503	NDP	O5D-PN-O1N	2.17	118.04	109.62
2	C	1503	NDP	C2D-C1D-N1N	2.18	119.22	113.34
2	A	1501	NDP	O5D-PN-O1N	2.21	118.18	109.62
2	B	1502	NDP	O5D-PN-O1N	2.21	118.18	109.62
3	D	1604	GDP	O3'-C3'-C2'	2.24	119.10	111.83
2	D	1504	NDP	C2D-C1D-N1N	2.28	119.51	113.34
3	D	1604	GDP	O3B-PB-O2B	2.42	116.59	107.38
3	B	1602	GDP	O3B-PB-O2B	2.43	116.62	107.38
3	C	1603	GDP	O3B-PB-O2B	2.44	116.67	107.38
3	A	1601	GDP	O3B-PB-O2B	2.46	116.75	107.38
2	D	1504	NDP	C5N-C4N-C3N	2.53	119.48	112.52
2	B	1502	NDP	C5N-C4N-C3N	2.55	119.53	112.52
2	C	1503	NDP	C5N-C4N-C3N	2.56	119.58	112.52
2	A	1501	NDP	C5N-C4N-C3N	2.57	119.61	112.52
3	C	1603	GDP	O3'-C3'-C2'	2.67	120.52	111.83
3	D	1604	GDP	O3'-C3'-C4'	2.68	119.10	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1603	GDP	O3'-C3'-C4'	3.16	120.52	111.05
3	C	1603	GDP	C2'-C1'-N9	4.31	120.88	114.29
3	D	1604	GDP	C2'-C1'-N9	4.67	121.42	114.29
3	B	1602	GDP	C2'-C1'-N9	5.06	122.02	114.29
3	A	1601	GDP	C6-N1-C2	6.61	125.12	115.94
3	C	1603	GDP	C6-N1-C2	6.64	125.16	115.94
3	D	1604	GDP	C6-N1-C2	6.96	125.59	115.94
3	B	1602	GDP	C6-N1-C2	7.03	125.69	115.94

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	1504	NDP	C4B
2	C	1503	NDP	C4B
2	B	1502	NDP	C4B
2	A	1501	NDP	C4B

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1501	NDP	3	0
2	B	1502	NDP	3	0
2	C	1503	NDP	3	0
2	D	1504	NDP	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	321/335 (95%)	-0.16	7 (2%)	65	73	11, 19, 35, 48	0
1	B	321/335 (95%)	-0.09	3 (0%)	85	89	11, 20, 40, 51	0
1	C	322/335 (96%)	-0.28	4 (1%)	81	85	9, 18, 32, 49	0
1	D	322/335 (96%)	-0.27	3 (0%)	85	89	8, 17, 33, 47	0
All	All	1286/1340 (95%)	-0.20	17 (1%)	79	84	8, 19, 35, 51	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	THR	5.1
1	D	2	THR	4.4
1	B	204	GLY	3.2
1	B	264	GLY	3.1
1	C	262	HIS	2.8
1	A	207	GLN	2.7
1	C	207	GLN	2.7
1	A	321	SER	2.6
1	A	302	ARG	2.6
1	A	278	PHE	2.5
1	A	204	GLY	2.4
1	C	275	PRO	2.4
1	A	273	ILE	2.2
1	A	264	GLY	2.1
1	B	275	PRO	2.1
1	D	262	HIS	2.1
1	D	273	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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
3	GDP	A	1601	28/28	0.95	0.22	4.02	37,42,45,46	0
2	NDP	D	1504	48/48	0.97	0.11	0.26	10,12,15,15	0
2	NDP	A	1501	48/48	0.96	0.11	0.16	11,14,15,16	0
2	NDP	C	1503	48/48	0.97	0.11	0.14	9,12,15,16	0
2	NDP	B	1502	48/48	0.97	0.11	0.03	11,14,17,18	0
3	GDP	D	1604	28/28	0.98	0.10	-0.18	14,20,22,26	0
3	GDP	C	1603	28/28	0.98	0.10	-0.21	14,19,21,24	0
3	GDP	B	1602	28/28	0.97	0.10	-0.61	20,24,27,28	0

6.5 Other polymers (i)

There are no such residues in this entry.