



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:35 am GMT

PDB ID : 1ND5  
Title : Crystal Structures of Human Prostatic Acid Phosphatase in Complex with a Phosphate Ion and alpha-Benzylaminobenzylphosphonic Acid Update the Mechanistic Picture and Offer New Insights into Inhibitor Design  
Authors : Ortlund, E.; LaCount, M.W.; Lebioda, L.  
Deposited on : 2002-12-07  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : NOT EXECUTED  
EDS : NOT EXECUTED  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

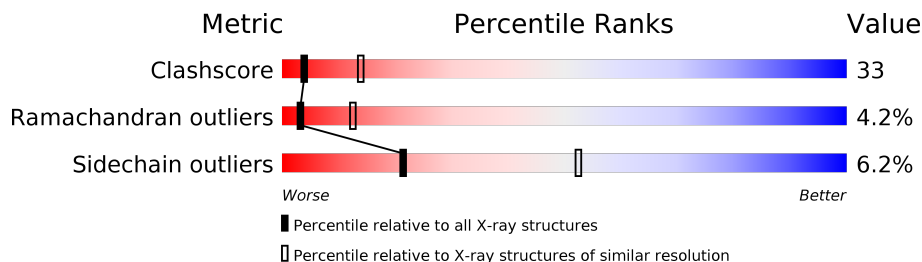
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	354	
1	B	354	
1	C	354	
1	D	354	

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	NAG	A	5001	X	-	-	-
2	NAG	A	5002	X	-	-	-
2	NAG	B	5005	X	-	X	-
2	NAG	C	5007	X	-	X	-
2	NAG	C	5008	X	-	-	-
3	NDG	B	5004	-	-	X	-
4	NAG	D	5009	X	-	-	-
5	NAG	D	5010	X	-	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11727 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.

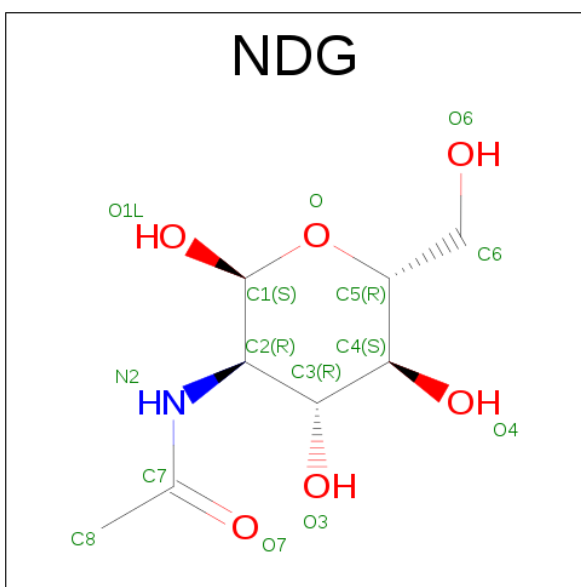
- Molecule 1 is a protein called prostatic acid phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2800	1807	461	516	16			
1	B	342	Total	C	N	O	S	0	0	0
			2796	1802	461	517	16			
1	C	342	Total	C	N	O	S	0	0	0
			2800	1807	461	516	16			
1	D	342	Total	C	N	O	S	0	0	0
			2800	1807	461	516	16			

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

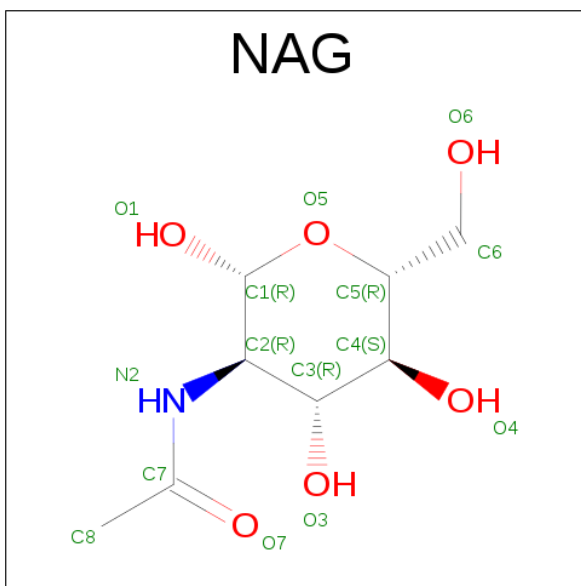
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			30	16	2	12		
2	A	2	Total	C	N	O	0	0
			30	16	2	12		
2	B	2	Total	C	N	O	0	0
			30	16	2	12		
2	C	2	Total	C	N	O	0	0
			30	16	2	12		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

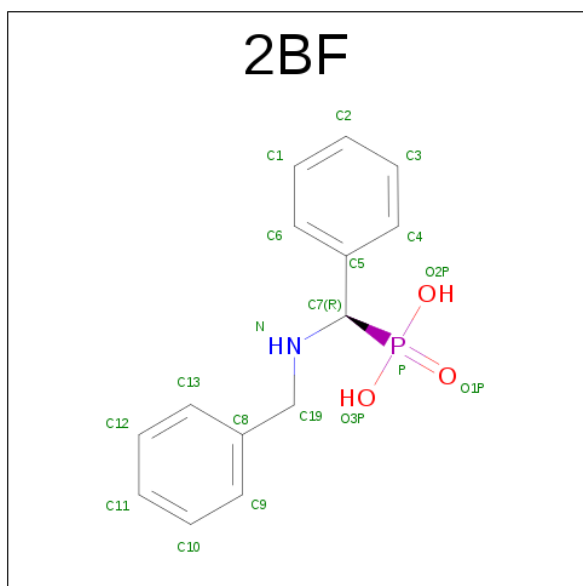


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

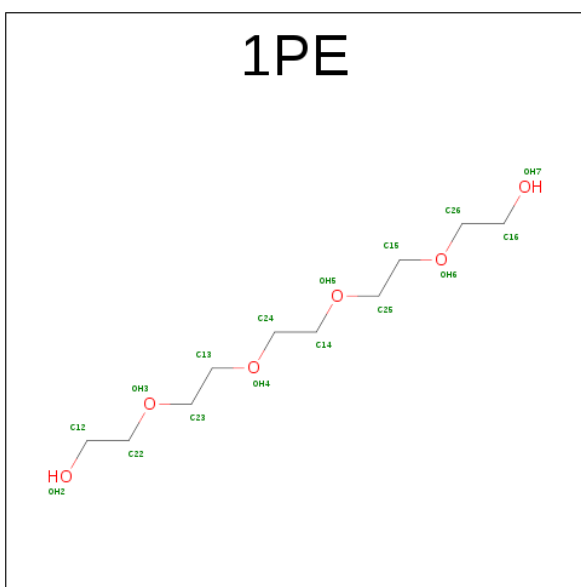
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	3	Total	C	N	O	0	0
			42	22	2	18		

- Molecule 6 is ALPHA-BENZYL-AMINOBENZYL-PHOSPHONIC ACID (three-letter code: 2BF) (formula:  $C_{14}H_{16}NO_3P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			19	14	1	3	1		
6	B	1	Total	C	N	O	P	0	0
			19	14	1	3	1		
6	C	1	Total	C	N	O	P	0	0
			19	14	1	3	1		
6	D	1	Total	C	N	O	P	0	0
			19	14	1	3	1		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



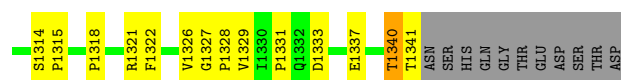
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	10	6		
7	B	1	Total	C	O	0	0
			16	10	6		
7	C	1	Total	C	O	0	0
			16	10	6		
7	D	1	Total	C	O	0	0
			16	10	6		
7	A	1	Total	C	O	0	0
			16	10	6		
7	B	1	Total	C	O	0	0
			16	10	6		
7	C	1	Total	C	O	0	0
			16	10	6		
7	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	47	Total	O	0	0
			47	47		
8	B	35	Total	O	0	0
			35	35		
8	C	22	Total	O	0	0
			22	22		
8	D	31	Total	O	0	0
			31	31		

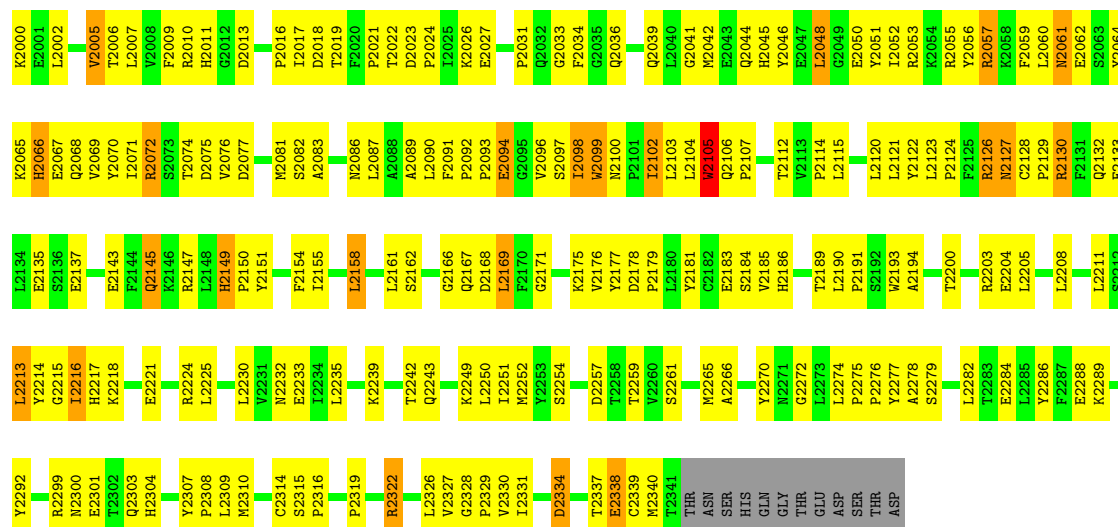






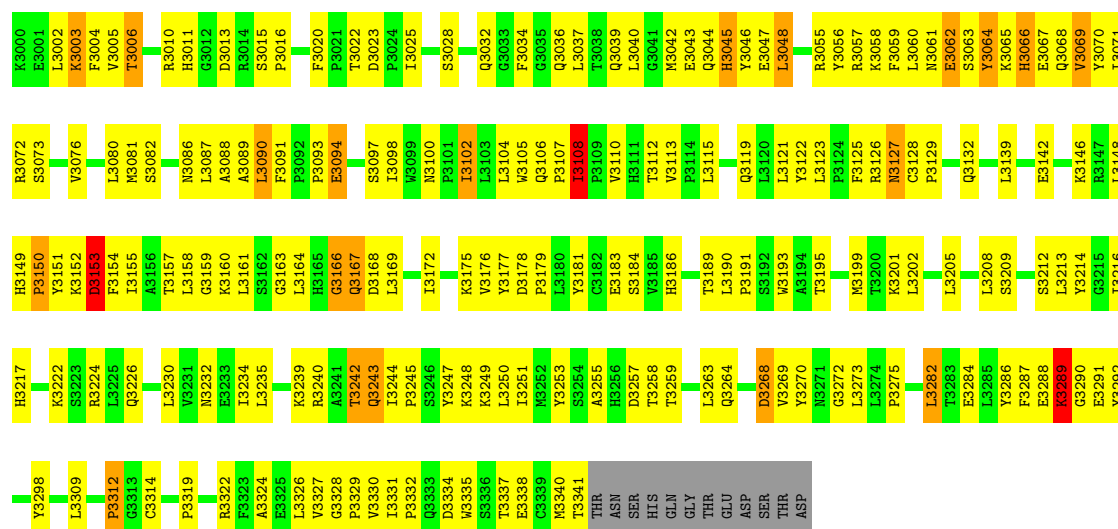
• Molecule 1: prostatic acid phosphatase

Chain C: 42% 49% 6%



• Molecule 1: prostatic acid phosphatase

Chain D: 43% 47% 6%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.10 Å   204.86 Å   71.22 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	77.94 – 2.90	Depositor
% Data completeness (in resolution range)	78.9 (77.94-2.90)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.205 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11727	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2BF, MAN, NAG, NDG, 1PE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.38	0/2882	0.64	0/3914
1	B	0.39	0/2876	0.64	0/3905
1	C	0.39	0/2882	0.64	0/3914
1	D	0.39	0/2882	0.62	0/3914
All	All	0.39	0/11522	0.64	0/15647

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	2	0
2	B	1	0
2	C	2	0
5	D	1	0
All	All	6	0

There are no bond length outliers.

There are no bond angle outliers.

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	5001	NAG	C1
2	A	5002	NAG	C1
2	B	5005	NAG	C1
2	C	5007	NAG	C1
2	C	5008	NAG	C1
5	D	5010	NAG	C1

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	2800	0	2749	200	0
1	B	2796	0	2745	180	0
1	C	2800	0	2747	196	0
1	D	2800	0	2746	195	0
2	A	60	0	55	8	0
2	B	30	0	28	9	0
2	C	30	0	27	8	0
3	B	15	0	15	10	0
4	D	15	0	14	6	0
5	D	42	0	38	4	0
6	A	19	0	14	3	0
6	B	19	0	14	2	0
6	C	19	0	14	2	0
6	D	19	0	14	0	0
7	A	48	0	66	3	0
7	B	32	0	44	5	0
7	C	32	0	44	2	0
7	D	16	0	22	1	0
8	A	47	0	0	4	0
8	B	35	0	0	4	0
8	C	22	0	0	1	0
8	D	31	0	0	8	0
All	All	11727	0	11396	767	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 33.

All (767) 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)
5:D:5010:NAG:H61	5:D:5011:NAG:H82	1.37	1.07
1:B:1145:LYS:HA	1:B:1145:LYS:HE3	1.32	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1186:ASN:HD21	3:B:5004:NDG:H1	1.22	1.03
1:B:1299:ASN:ND2	2:B:5005:NAG:H1	1.74	1.02
1:B:1299:ASN:HD21	2:B:5005:NAG:H1	1.23	0.98
1:C:2007:LEU:HD22	1:C:2282:LEU:HD22	1.43	0.97
1:D:3100:ASN:HD21	1:D:3102:ILE:HB	1.29	0.97
1:A:66:LYS:HD3	1:B:1032:GLN:HE22	1.30	0.96
2:A:5000:NAG:H61	2:A:5001:NAG:H82	1.49	0.94
1:B:1186:ASN:ND2	3:B:5004:NDG:H1	1.81	0.94
1:B:1007:LEU:HD13	1:B:1052:ILE:HD13	1.50	0.93
1:B:1199:THR:O	1:B:1203:GLU:HG3	1.68	0.91
1:B:1299:ASN:HD21	2:B:5005:NAG:C1	1.83	0.91
1:C:2307:TYR:CE1	2:C:5007:NAG:O1	2.24	0.91
1:A:148:ARG:O	1:A:151:PRO:HD2	1.73	0.89
1:A:150:HIS:HB3	1:A:151:PRO:HD3	1.55	0.89
1:B:1127:ASN:HD22	1:B:1127:ASN:H	0.92	0.88
1:B:1064:TYR:O	1:B:1065:LYS:HG3	1.75	0.86
1:C:2145:GLN:HA	1:C:2145:GLN:HE21	1.39	0.86
1:A:180:PRO:O	1:A:184:GLU:HG3	1.73	0.86
1:B:1127:ASN:H	1:B:1127:ASN:ND2	1.74	0.86
1:D:3032:GLN:HB3	1:D:3036:GLN:HG2	1.56	0.86
1:A:135:LEU:O	1:A:139:THR:HG23	1.77	0.85
1:B:1299:ASN:CG	2:B:5005:NAG:H1	1.98	0.84
1:D:3087:LEU:HB3	1:D:3108:ILE:HD12	1.56	0.84
1:B:1094:GLU:HA	1:B:1098:ILE:HD11	1.61	0.83
1:B:1148:HIS:HB3	1:B:1149:PRO:HD3	1.61	0.83
1:C:2288:GLU:HG3	1:C:2289:LYS:H	1.44	0.83
1:C:2149:HIS:HB3	1:C:2150:PRO:HD3	1.61	0.82
1:D:3340:MET:HE2	1:D:3341:THR:HG22	1.61	0.82
1:B:1299:ASN:OD1	2:B:5005:NAG:H1	1.80	0.82
1:C:2098:ILE:HG21	1:C:2104:LEU:HD22	1.61	0.81
1:D:3065:LYS:HB2	1:D:3068:GLN:HG3	1.63	0.80
1:C:2190:LEU:HB3	1:C:2191:PRO:HD2	1.63	0.80
1:C:2288:GLU:HG3	1:C:2289:LYS:HG2	1.62	0.80
1:B:1275:PRO:HD2	1:B:1278:SER:HB3	1.63	0.80
1:B:1010:ARG:HD2	1:B:1256:ASP:HB3	1.61	0.80
1:C:2050:GLU:HG3	1:C:2089:ALA:HB1	1.64	0.79
1:A:56:ARG:HG2	1:A:57:TYR:CD2	2.18	0.79
1:D:3003:LYS:HG3	1:D:3292:TYR:HE2	1.47	0.79
1:D:3025:ILE:HD12	1:D:3025:ILE:H	1.47	0.79
1:B:1185:HIS:HA	3:B:5004:NDG:H8C3	1.62	0.78
1:B:1125:PHE:H	1:B:1225:GLN:HE22	1.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2081:MET:HG2	1:D:3107:PRO:HB2	1.65	0.78
1:A:139:THR:HG22	1:A:218:HIS:HB3	1.65	0.78
1:C:2090:LEU:HD13	1:C:2091:PHE:CE1	2.19	0.77
1:B:1186:ASN:HD21	3:B:5004:NDG:C1	1.95	0.76
2:C:5007:NAG:H61	2:C:5008:NAG:H2	1.66	0.76
1:D:3166:GLY:O	1:D:3168:ASP:N	2.17	0.75
1:A:245:ILE:HD12	1:A:246:PRO:CD	2.17	0.75
1:A:6:VAL:HG22	1:A:285:GLU:HG2	1.67	0.75
1:A:8:LEU:HD23	1:A:283:LEU:HB3	1.69	0.75
1:A:181:LEU:HD23	1:A:191:LEU:HD22	1.68	0.75
1:B:1267:ASP:OD2	1:B:1311:PRO:HG3	1.87	0.74
1:A:41:LEU:O	1:A:45:GLN:HG3	1.88	0.74
1:D:3149:HIS:HB3	1:D:3150:PRO:HD3	1.68	0.74
1:B:1045:HIS:HD2	1:B:1086:ASN:HD22	1.35	0.74
1:D:3155:ILE:HG21	1:D:3167:GLN:HG3	1.68	0.74
1:C:2176:VAL:O	1:C:2179:PRO:HD2	1.87	0.74
1:D:3289:LYS:H	1:D:3289:LYS:HD2	1.51	0.74
1:D:3322:ARG:HG2	1:D:3322:ARG:HH11	1.53	0.73
4:D:5009:NAG:O1	4:D:5009:NAG:O7	2.06	0.73
1:A:61:LEU:O	1:A:63:GLU:N	2.21	0.73
1:A:63:GLU:HG2	8:A:4111:HOH:O	1.89	0.73
1:C:2288:GLU:HG3	1:C:2289:LYS:N	2.04	0.73
1:D:3169:LEU:O	8:D:4122:HOH:O	2.06	0.72
1:B:1127:ASN:N	1:B:1127:ASN:HD22	1.73	0.72
1:A:316:SER:HB2	1:A:317:PRO:HD2	1.70	0.72
1:D:3004:PHE:HZ	1:D:3251:ILE:HD12	1.54	0.72
1:C:2007:LEU:CD2	1:C:2282:LEU:HD22	2.20	0.71
1:D:3115:LEU:HD22	1:D:3122:TYR:CE1	2.25	0.71
1:C:2007:LEU:HD22	1:C:2282:LEU:CD2	2.20	0.71
1:C:2145:GLN:HA	1:C:2145:GLN:NE2	2.06	0.71
1:B:1281:LEU:HD23	1:B:1281:LEU:H	1.54	0.70
1:A:66:LYS:CD	1:B:1032:GLN:HE22	2.02	0.70
1:B:1163:LEU:HD11	1:B:1174:LYS:CB	2.21	0.70
1:D:3172:ILE:N	8:D:4122:HOH:O	2.23	0.70
1:A:212:LEU:HD12	1:A:217:ILE:HG13	1.72	0.70
1:D:3268:ASP:HB3	1:D:3312:PRO:HG3	1.74	0.70
1:D:3040:LEU:O	1:D:3044:GLN:HG3	1.92	0.70
1:D:3125:PHE:H	1:D:3226:GLN:HE22	1.39	0.70
1:B:1123:LEU:HD12	1:B:1258:THR:HA	1.75	0.69
1:D:3062:GLU:CD	1:D:3062:GLU:H	1.95	0.69
1:A:49:LEU:HD13	1:A:87:ASN:HD21	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1007:LEU:CD1	1:B:1052:ILE:HD13	2.21	0.69
1:B:1077:ASP:O	1:B:1081:MET:HG3	1.93	0.69
1:B:1239:ARG:HD2	1:B:1246:TYR:HE2	1.58	0.69
1:C:2191:PRO:HG2	1:C:2194:ALA:HB2	1.74	0.69
1:B:1011:HIS:NE2	1:B:1078:ARG:HD2	2.08	0.68
1:B:1306:TYR:CE2	2:B:5005:NAG:H5	2.29	0.68
1:A:82:MET:HA	1:A:85:MET:HE2	1.76	0.68
1:D:3288:GLU:O	1:D:3290:GLY:N	2.25	0.68
1:D:3224:ARG:HA	1:D:3330:VAL:O	1.94	0.68
5:D:5010:NAG:C6	5:D:5011:NAG:H82	2.21	0.68
1:B:1297:TYR:HB2	1:B:1308:LEU:HD11	1.76	0.68
1:B:1045:HIS:CD2	1:B:1086:ASN:HD22	2.12	0.67
5:D:5010:NAG:H61	5:D:5011:NAG:C8	2.21	0.67
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.58	0.67
1:C:2319:PRO:HG2	1:C:2322:ARG:HB2	1.77	0.67
1:D:3127:ASN:HD22	1:D:3127:ASN:H	1.42	0.67
1:D:3169:LEU:HB3	1:D:3209:SER:HB2	1.76	0.67
1:C:2120:LEU:HD23	1:C:2120:LEU:O	1.94	0.66
1:D:3100:ASN:ND2	1:D:3102:ILE:HB	2.08	0.66
1:C:2068:GLN:HG3	1:C:2249:LYS:HG3	1.78	0.66
1:D:3055:ARG:HG2	1:D:3056:TYR:CE2	2.31	0.66
1:B:1163:LEU:HD11	1:B:1174:LYS:HB2	1.78	0.66
1:B:1281:LEU:HD23	1:B:1281:LEU:N	2.11	0.66
1:B:1186:ASN:CG	3:B:5004:NDG:H1	2.16	0.66
1:B:1119:GLN:HB3	7:B:7001:1PE:H142	1.78	0.66
1:C:2130:ARG:HD3	1:C:2221:GLU:OE2	1.95	0.66
1:C:2005:VAL:HG22	1:C:2250:LEU:HD12	1.76	0.65
1:D:3232:ASN:HB2	1:D:3331:ILE:HG23	1.78	0.65
1:A:54:ARG:HG3	1:A:91:LEU:HD22	1.78	0.65
1:B:1015:SER:HB2	1:B:1016:PRO:HD2	1.79	0.65
1:C:2200:THR:O	1:C:2204:GLU:HG3	1.96	0.65
1:A:49:LEU:O	1:A:53:ILE:HG22	1.96	0.65
1:C:2232:ASN:HD22	1:C:2331:ILE:HD13	1.61	0.65
1:B:1004:PHE:HZ	1:B:1250:ILE:HD12	1.62	0.64
1:A:258:ASP:OD2	6:A:6000:2BF:H7	1.97	0.64
1:B:1011:HIS:CD2	1:B:1078:ARG:HD2	2.31	0.64
1:B:1298:ARG:HH12	1:B:1301:THR:HG22	1.62	0.64
1:D:3148:LEU:HD21	1:D:3167:GLN:NE2	2.13	0.64
1:C:2098:ILE:HG22	1:C:2099:TRP:H	1.63	0.64
1:A:283:LEU:HD23	1:A:283:LEU:N	2.13	0.63
1:B:1129:PRO:O	1:B:1131:GLN:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3324:ALA:HA	1:D:3327:VAL:HG12	1.79	0.63
1:A:130:PRO:HD2	1:A:340:CYS:HB3	1.81	0.62
1:C:2100:ASN:O	1:C:2104:LEU:HD23	1.97	0.62
1:C:2176:VAL:C	1:C:2179:PRO:HD2	2.20	0.62
1:D:3322:ARG:HH21	1:D:3326:LEU:HD21	1.64	0.62
1:B:1275:PRO:HD2	1:B:1278:SER:CB	2.29	0.62
1:A:8:LEU:HD11	1:A:53:ILE:HD13	1.81	0.62
1:A:74:SER:HB2	1:A:255:SER:HB3	1.82	0.62
1:A:182:TYR:O	1:A:185:SER:HB3	1.98	0.62
1:D:3242:THR:HG22	1:D:3243:GLN:HG2	1.81	0.62
1:B:1098:ILE:HG22	1:B:1098:ILE:O	1.99	0.62
1:B:1078:ARG:NH2	6:B:6001:2BF:O3P	2.33	0.62
1:D:3172:ILE:HB	8:D:4122:HOH:O	2.00	0.62
1:D:3224:ARG:HG2	1:D:3330:VAL:HA	1.81	0.62
1:C:2114:PRO:HD3	1:D:3113:VAL:HG22	1.82	0.61
1:C:2169:LEU:HD11	1:C:2208:LEU:HD23	1.81	0.61
2:C:5008:NAG:H3	2:C:5008:NAG:H83	1.82	0.61
1:B:1056:TYR:HB3	1:B:1060:LEU:HD23	1.82	0.61
1:C:2098:ILE:O	1:C:2099:TRP:HB3	2.00	0.61
1:C:2178:ASP:HB3	1:C:2179:PRO:HD3	1.82	0.61
1:C:2112:THR:HG22	1:D:3112:THR:HG22	1.80	0.61
1:A:139:THR:HG21	1:A:223:LYS:NZ	2.15	0.61
1:C:2120:LEU:HD22	1:C:2121:LEU:HG	1.81	0.61
1:D:3107:PRO:O	1:D:3108:ILE:HG23	1.99	0.61
1:D:3289:LYS:HD2	1:D:3289:LYS:N	2.14	0.61
1:B:1186:ASN:OD1	3:B:5004:NDG:H1	2.00	0.61
1:D:3045:HIS:CD2	1:D:3086:ASN:HD22	2.18	0.61
1:A:312:LEU:HD23	1:A:327:LEU:HD12	1.80	0.61
1:A:187:HIS:HA	2:A:5000:NAG:H82	1.81	0.61
1:A:135:LEU:HD13	1:A:223:LYS:CG	2.30	0.61
1:D:3158:LEU:HD23	1:D:3172:ILE:HD12	1.81	0.61
1:D:3322:ARG:NH2	1:D:3326:LEU:HD21	2.16	0.61
1:D:3127:ASN:ND2	1:D:3127:ASN:H	1.99	0.61
1:B:1340:THR:HG23	1:B:1341:THR:H	1.65	0.60
1:C:2130:ARG:NH1	1:C:2221:GLU:OE1	2.34	0.60
1:D:3169:LEU:C	8:D:4122:HOH:O	2.39	0.60
1:B:1196:ASP:HB2	8:B:4046:HOH:O	2.00	0.60
1:C:2061:ASN:N	1:C:2061:ASN:HD22	1.99	0.60
1:D:3282:LEU:HD23	1:D:3282:LEU:N	2.16	0.60
1:A:225:ARG:HA	1:A:331:VAL:O	2.00	0.60
1:D:3106:GLN:HB2	1:D:3107:PRO:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PRO:C	1:A:109:ILE:HD12	2.22	0.60
1:C:2018:ASP:OD2	1:C:2175:LYS:HD3	2.01	0.60
1:D:3010:ARG:HD2	1:D:3257:ASP:HB3	1.84	0.60
1:C:2328:GLY:N	1:C:2329:PRO:HD2	2.17	0.59
1:A:114:VAL:HG13	1:A:115:PRO:HD2	1.84	0.59
1:A:155:PHE:HE1	1:A:199:THR:HG22	1.65	0.59
1:B:1214:GLY:O	1:B:1215:ILE:HB	2.01	0.59
1:A:135:LEU:HD13	1:A:223:LYS:HG2	1.84	0.59
1:A:11:ARG:HD2	6:A:6000:2BF:O3P	2.02	0.59
1:D:3176:VAL:O	1:D:3179:PRO:HD2	2.02	0.59
1:A:245:ILE:HD12	1:A:246:PRO:HD2	1.84	0.59
1:D:3069:VAL:HG13	1:D:3250:LEU:HB3	1.84	0.59
1:A:10:PHE:CE1	1:A:255:SER:HA	2.38	0.59
1:A:56:ARG:HG2	1:A:57:TYR:CE2	2.37	0.59
1:C:2239:LYS:O	1:C:2243:GLN:HG3	2.02	0.59
1:D:3179:PRO:O	1:D:3183:GLU:HG2	2.02	0.59
1:D:3070:TYR:HB2	1:D:3248:LYS:HE2	1.84	0.59
1:A:175:SER:O	1:A:180:PRO:HD3	2.03	0.59
1:D:3142:GLU:O	1:D:3146:LYS:HD3	2.02	0.59
1:D:3334:ASP:O	1:D:3338:GLU:HG3	2.03	0.59
4:D:5009:NAG:HO1	4:D:5009:NAG:C7	2.13	0.59
1:B:1239:ARG:HD2	1:B:1246:TYR:CE2	2.38	0.59
1:C:2098:ILE:HG21	1:C:2104:LEU:CD2	2.32	0.59
1:C:2100:ASN:ND2	1:C:2103:LEU:HB3	2.18	0.59
1:C:2161:LEU:HD13	1:C:2193:TRP:CB	2.33	0.59
1:C:2232:ASN:ND2	1:C:2331:ILE:HG21	2.18	0.59
1:D:3167:GLN:HG2	1:D:3167:GLN:O	2.02	0.59
1:D:3224:ARG:O	1:D:3332:PRO:HD3	2.02	0.59
1:C:2048:LEU:O	1:C:2052:ILE:HG13	2.02	0.59
1:C:2056:TYR:O	1:C:2059:PHE:N	2.36	0.59
1:C:2214:TYR:HB2	1:C:2265:MET:HG3	1.85	0.58
1:D:3340:MET:CE	1:D:3341:THR:HG22	2.33	0.58
1:B:1060:LEU:C	1:B:1062:GLU:H	2.06	0.58
1:B:1139:LYS:O	1:B:1140:SER:C	2.41	0.58
1:C:2169:LEU:HD21	1:C:2205:LEU:HB3	1.84	0.58
1:A:170:LEU:HB3	1:A:210:SER:HB2	1.85	0.58
1:B:1340:THR:HG23	1:B:1341:THR:N	2.19	0.58
1:C:2071:ILE:HG13	1:C:2252:MET:HB2	1.83	0.58
1:C:2089:ALA:O	1:C:2092:PRO:HD3	2.04	0.58
1:C:2041:GLY:HA2	1:C:2044:GLN:OE1	2.03	0.58
1:C:2151:TYR:CG	1:C:2205:LEU:HD21	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLU:OE1	1:A:322:GLU:HA	2.03	0.58
1:B:1309:MET:HE2	1:B:1315:PRO:HG3	1.86	0.58
1:D:3127:ASN:HD22	1:D:3127:ASN:N	1.99	0.58
1:D:3172:ILE:O	1:D:3176:VAL:HB	2.03	0.58
1:A:11:ARG:HD3	1:A:258:ASP:HB3	1.86	0.58
1:A:302:GLU:OE1	2:A:5002:NAG:O1	2.21	0.58
1:C:2072:ARG:HD3	1:C:2121:LEU:HD12	1.86	0.58
1:C:2217:HIS:CD2	1:C:2218:LYS:HD3	2.38	0.58
1:A:268:LEU:O	1:A:269:ASP:HB2	2.03	0.57
1:C:2048:LEU:HD13	1:C:2052:ILE:HD11	1.86	0.57
1:D:3115:LEU:HD22	1:D:3122:TYR:CD1	2.39	0.57
1:B:1163:LEU:HD21	1:B:1174:LYS:HD3	1.86	0.57
1:C:2314:CYS:HB2	1:C:2326:LEU:CD1	2.34	0.57
1:D:3072:ARG:O	1:D:3253:TYR:HA	2.04	0.57
1:C:2181:TYR:O	1:C:2185:VAL:HG23	2.04	0.57
1:D:3004:PHE:CZ	1:D:3251:ILE:HD12	2.39	0.57
1:D:3186:HIS:HA	4:D:5009:NAG:C8	2.35	0.57
1:C:2232:ASN:HD22	1:C:2331:ILE:HG21	1.70	0.57
1:C:2310:MET:CE	1:C:2316:PRO:HD3	2.35	0.57
1:D:3045:HIS:HD2	1:D:3086:ASN:ND2	2.02	0.57
1:C:2161:LEU:HD13	1:C:2193:TRP:HB2	1.86	0.57
1:D:3148:LEU:HD21	1:D:3167:GLN:HE21	1.69	0.57
1:A:268:LEU:HD22	1:A:312:LEU:HD11	1.86	0.57
1:C:2065:LYS:O	1:C:2068:GLN:N	2.38	0.57
1:A:127:ARG:HH11	1:A:127:ARG:CG	2.18	0.57
1:D:3314:CYS:HB2	1:D:3326:LEU:CD1	2.34	0.57
1:A:177:VAL:C	1:A:180:PRO:HD2	2.24	0.57
1:C:2166:GLY:O	1:C:2168:ASP:N	2.38	0.57
1:C:2007:LEU:CD1	1:C:2052:ILE:HD13	2.35	0.57
1:C:2053:ARG:NH1	1:C:2092:PRO:HG3	2.20	0.57
1:C:2183:GLU:HB3	1:C:2190:LEU:HD21	1.87	0.57
1:D:3169:LEU:HD11	1:D:3208:LEU:HD23	1.87	0.57
1:A:66:LYS:HD3	1:B:1032:GLN:NE2	2.10	0.56
1:B:1010:ARG:O	1:B:1277:ALA:HA	2.04	0.56
1:B:1189:LEU:HG	1:B:1190:PRO:HD2	1.87	0.56
1:D:3065:LYS:O	1:D:3067:GLU:N	2.38	0.56
1:D:3172:ILE:CB	8:D:4122:HOH:O	2.53	0.56
1:A:181:LEU:CD2	1:A:191:LEU:HD22	2.33	0.56
1:B:1243:ILE:HG22	1:B:1244:PRO:O	2.05	0.56
1:A:120:GLN:HB3	7:A:7000:1PE:H152	1.86	0.56
1:C:2026:LYS:HA	1:C:2026:LYS:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:5000:NAG:H81	8:A:4117:HOH:O	2.06	0.56
1:A:277:PRO:HD2	1:A:280:SER:HB3	1.86	0.56
1:A:334:GLN:HA	1:A:334:GLN:NE2	2.20	0.56
1:D:3107:PRO:C	1:D:3108:ILE:HG12	2.25	0.56
1:C:2301:GLU:OE2	1:C:2304:HIS:HD2	1.88	0.56
1:A:159:LEU:HD13	1:A:159:LEU:C	2.26	0.56
1:B:1080:LEU:O	1:B:1084:MET:HG3	2.06	0.56
1:D:3157:THR:O	1:D:3161:LEU:HG	2.06	0.56
1:D:3055:ARG:HG2	1:D:3056:TYR:CD2	2.41	0.56
1:A:312:LEU:HD23	1:A:327:LEU:CD1	2.35	0.55
1:B:1327:GLY:N	1:B:1328:PRO:HD2	2.21	0.55
1:C:2274:LEU:HG	8:C:4100:HOH:O	2.06	0.55
1:C:2310:MET:CE	1:C:2315:SER:HA	2.35	0.55
1:A:11:ARG:CD	1:A:258:ASP:HB3	2.36	0.55
1:B:1146:ARG:O	1:B:1149:PRO:HD2	2.07	0.55
1:B:1210:LEU:HD13	1:B:1215:ILE:HG12	1.88	0.55
1:B:1177:ASP:HB3	1:B:1178:PRO:HD3	1.89	0.55
1:C:2010:ARG:HD2	1:C:2257:ASP:N	2.21	0.55
1:C:2097:SER:HB3	1:C:2106:GLN:NE2	2.21	0.55
1:D:3060:LEU:O	1:D:3062:GLU:N	2.40	0.55
1:A:204:ARG:O	1:A:208:GLU:HG3	2.06	0.55
1:C:2104:LEU:O	1:C:2105:TRP:HB3	2.05	0.55
1:D:3230:LEU:HD23	1:D:3263:LEU:HB2	1.89	0.55
1:C:2211:LEU:HD13	1:C:2211:LEU:O	2.07	0.55
1:D:3002:LEU:HD23	1:D:3059:PHE:CG	2.41	0.55
1:A:304:GLN:HG3	1:A:305:HIS:CE1	2.42	0.55
1:B:1180:TYR:O	1:B:1184:VAL:HG23	2.07	0.55
1:C:2288:GLU:CG	1:C:2289:LYS:N	2.69	0.55
1:A:150:HIS:C	1:A:152:TYR:H	2.09	0.54
1:D:3178:ASP:HB3	1:D:3179:PRO:HD3	1.87	0.54
1:B:1169:PHE:CD1	7:B:7005:1PE:H222	2.41	0.54
1:A:107:GLN:HG3	1:A:109:ILE:HD11	1.89	0.54
1:A:113:THR:HG22	1:B:1112:THR:HG22	1.90	0.54
1:A:139:THR:CG2	1:A:218:HIS:HB3	2.36	0.54
1:C:2010:ARG:O	1:C:2278:ALA:HA	2.08	0.54
1:A:213:SER:HB3	1:A:217:ILE:HD12	1.88	0.54
1:B:1014:ARG:HH22	1:B:1177:ASP:CG	2.10	0.54
1:D:3186:HIS:HA	4:D:5009:NAG:H81	1.88	0.54
1:A:143:GLU:O	1:A:147:LYS:HB2	2.07	0.54
1:A:281:CYS:SG	1:A:283:LEU:HD22	2.48	0.54
1:B:1010:ARG:O	1:B:1045:HIS:HE1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3087:LEU:CB	1:D:3108:ILE:HD12	2.34	0.54
1:B:1306:TYR:CZ	2:B:5005:NAG:O1	2.60	0.54
1:D:3167:GLN:HB2	8:D:4124:HOH:O	2.06	0.54
1:A:152:TYR:O	1:A:155:PHE:N	2.40	0.54
1:B:1306:TYR:CE1	2:B:5005:NAG:O1	2.59	0.54
1:D:3287:PHE:CZ	1:D:3290:GLY:HA2	2.42	0.54
1:B:1229:LEU:O	1:B:1232:GLU:HB3	2.08	0.54
1:D:3151:TYR:O	1:D:3153:ASP:N	2.42	0.54
1:D:3199:MET:O	1:D:3202:LEU:HB2	2.08	0.54
1:A:233:ASN:HB2	1:A:332:ILE:HG23	1.90	0.53
1:A:54:ARG:HG3	1:A:91:LEU:O	2.08	0.53
1:C:2127:ASN:H	1:C:2127:ASN:HD22	1.56	0.53
1:D:3020:PHE:CE2	1:D:3023:ASP:HB2	2.44	0.53
1:B:1295:MET:HG3	8:B:4065:HOH:O	2.09	0.53
1:A:245:ILE:HD12	1:A:246:PRO:N	2.23	0.53
1:C:2065:LYS:HG2	1:C:2067:GLU:HG2	1.90	0.53
1:C:2130:ARG:HG2	1:C:2225:LEU:HD11	1.90	0.53
1:D:3065:LYS:O	1:D:3068:GLN:N	2.35	0.53
1:D:3230:LEU:CD2	1:D:3263:LEU:HD22	2.38	0.53
1:A:137:SER:O	1:A:140:LEU:HB2	2.08	0.53
1:D:3022:THR:HG22	1:D:3022:THR:O	2.07	0.53
1:D:3128:CYS:HB2	1:D:3335:TRP:CZ2	2.42	0.53
1:A:213:SER:HA	1:A:217:ILE:HD12	1.91	0.53
1:B:1299:ASN:HD21	2:B:5005:NAG:C2	2.21	0.53
1:A:58:ARG:NH1	1:A:58:ARG:HG2	2.23	0.53
1:A:179:ASP:HB3	1:A:180:PRO:HD3	1.89	0.53
1:B:1275:PRO:HG2	1:B:1299:ASN:HB2	1.90	0.53
1:C:2133:GLU:O	1:C:2137:GLU:HG3	2.08	0.53
1:B:1298:ARG:NH1	1:B:1301:THR:HG22	2.23	0.53
1:A:316:SER:HB2	1:A:317:PRO:CD	2.37	0.52
1:C:2056:TYR:O	1:C:2057:ARG:C	2.48	0.52
1:C:2130:ARG:HH11	1:C:2221:GLU:CD	2.12	0.52
1:A:274:LEU:HD12	2:A:5002:NAG:H2	1.91	0.52
1:D:3322:ARG:CG	1:D:3322:ARG:HH11	2.22	0.52
1:A:50:GLY:O	1:A:53:ILE:HG23	2.09	0.52
1:D:3047:GLU:C	1:D:3047:GLU:OE2	2.48	0.52
1:A:127:ARG:HH11	1:A:127:ARG:CB	2.22	0.52
1:C:2010:ARG:O	1:C:2045:HIS:HE1	1.92	0.52
1:C:2151:TYR:O	1:C:2155:ILE:HG13	2.09	0.52
4:D:5009:NAG:O1	4:D:5009:NAG:C7	2.56	0.52
1:D:3060:LEU:O	1:D:3062:GLU:OE2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3045:HIS:ND1	1:D:3082:SER:HB3	2.24	0.52
1:A:139:THR:HG21	1:A:223:LYS:HZ1	1.74	0.52
1:A:6:VAL:HG12	1:A:7:THR:N	2.24	0.52
1:B:1056:TYR:CB	1:B:1060:LEU:HD23	2.40	0.52
1:B:1216:HIS:O	1:B:1221:LYS:HE3	2.10	0.52
1:A:152:TYR:O	1:A:154:ASP:N	2.43	0.52
1:B:1011:HIS:CE1	1:B:1078:ARG:HD2	2.45	0.52
1:B:1112:THR:OG1	1:B:1113:VAL:N	2.43	0.52
1:C:2074:THR:O	1:C:2076:VAL:N	2.38	0.52
1:C:2090:LEU:HD22	1:C:2091:PHE:CZ	2.45	0.52
1:A:11:ARG:O	1:A:46:HIS:HE1	1.93	0.52
1:D:3046:TYR:CD1	1:D:3089:ALA:HB2	2.44	0.52
1:D:3193:TRP:O	1:D:3195:THR:HG23	2.10	0.52
1:B:1007:LEU:HD13	1:B:1052:ILE:CD1	2.32	0.52
1:A:106:TRP:HB2	1:B:1103:LEU:HD11	1.92	0.52
1:A:132:PHE:O	1:A:133:GLN:C	2.48	0.52
1:A:68:GLU:CD	1:A:68:GLU:H	2.12	0.52
1:B:1138:LEU:HD22	1:B:1138:LEU:N	2.25	0.52
1:B:1244:PRO:O	1:B:1246:TYR:N	2.43	0.52
1:A:37:GLN:HE21	1:A:37:GLN:N	2.09	0.51
1:D:3025:ILE:HD12	1:D:3025:ILE:N	2.21	0.51
1:A:302:GLU:OE2	1:A:305:HIS:HD2	1.92	0.51
1:C:2016:PRO:HG2	1:C:2034:PHE:CE2	2.46	0.51
1:C:2169:LEU:CD2	1:C:2205:LEU:HB3	2.40	0.51
1:B:1000:LYS:HB2	1:B:1287:GLU:OE1	2.10	0.51
1:C:2098:ILE:HG22	1:C:2099:TRP:N	2.26	0.51
1:D:3090:LEU:HD13	1:D:3091:PHE:CE1	2.45	0.51
1:A:100:TRP:HA	8:A:4034:HOH:O	2.10	0.51
1:D:3068:GLN:HE21	1:D:3249:LYS:HE3	1.75	0.51
1:C:2000:LYS:HG3	1:C:2286:TYR:HB3	1.93	0.51
1:C:2056:TYR:HB3	1:C:2059:PHE:HB3	1.93	0.51
1:C:2098:ILE:O	1:C:2099:TRP:CB	2.59	0.51
1:D:3212:SER:HA	1:D:3216:ILE:HG13	1.91	0.51
1:A:150:HIS:O	1:A:152:TYR:N	2.44	0.51
2:C:5007:NAG:H61	2:C:5008:NAG:C2	2.37	0.51
1:A:127:ARG:HE	7:A:7004:1PE:H262	1.76	0.51
1:B:1126:ARG:NH1	1:B:1126:ARG:HG2	2.26	0.51
1:C:2061:ASN:H	1:C:2061:ASN:HD22	1.59	0.51
1:A:28:GLU:HA	1:A:35:PHE:CE2	2.46	0.50
1:B:1100:ASN:ND2	1:B:1103:LEU:HB3	2.25	0.50
1:B:1128:CYS:O	1:B:1131:GLN:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1144:GLN:HA	1:B:1144:GLN:NE2	2.26	0.50
1:D:3040:LEU:O	1:D:3043:GLU:HB2	2.11	0.50
1:D:3163:GLY:O	1:D:3164:LEU:HD23	2.10	0.50
1:A:159:LEU:HD13	1:A:159:LEU:O	2.10	0.50
1:A:287:TYR:O	1:A:293:TYR:HA	2.11	0.50
1:A:49:LEU:HD13	1:A:87:ASN:ND2	2.23	0.50
1:C:2005:VAL:HG22	1:C:2250:LEU:CD1	2.41	0.50
1:C:2266:ALA:O	1:C:2330:VAL:HG11	2.12	0.50
1:D:3235:LEU:HD11	1:D:3324:ALA:HB2	1.93	0.50
1:B:1145:LYS:CE	1:B:1145:LYS:HA	2.21	0.50
1:C:2126:ARG:HG3	7:C:7006:1PE:H122	1.94	0.50
1:D:3056:TYR:HB3	1:D:3059:PHE:HB3	1.93	0.50
1:D:3071:ILE:HG22	1:D:3110:VAL:HG13	1.93	0.50
1:A:155:PHE:CE1	1:A:199:THR:HG22	2.45	0.50
1:D:3181:TYR:O	1:D:3184:SER:HB3	2.11	0.50
1:A:236:LEU:O	1:A:240:LYS:HG2	2.12	0.50
1:B:1124:PRO:HD2	7:B:7005:1PE:H131	1.93	0.50
1:B:1184:VAL:O	3:B:5004:NDG:C8	2.60	0.50
1:C:2013:ASP:N	1:C:2044:GLN:OE1	2.37	0.50
1:B:1163:LEU:HD11	1:B:1174:LYS:HB3	1.94	0.50
1:C:2017:ILE:HD11	6:C:6002:2BF:O1P	2.12	0.50
1:A:40:GLN:HG2	1:B:1099:TRP:HB3	1.92	0.49
1:C:2070:TYR:C	1:C:2071:ILE:HD12	2.33	0.49
1:D:3098:ILE:HG23	1:D:3104:LEU:HD21	1.94	0.49
1:A:57:TYR:HB3	1:A:61:LEU:HD13	1.93	0.49
1:B:1210:LEU:CD1	1:B:1215:ILE:HG12	2.43	0.49
1:A:114:VAL:CG1	1:A:115:PRO:HD2	2.41	0.49
1:D:3062:GLU:O	1:D:3064:TYR:N	2.45	0.49
1:B:1060:LEU:HD22	1:B:1060:LEU:N	2.27	0.49
1:D:3016:PRO:HG2	1:D:3034:PHE:CE2	2.46	0.49
1:D:3322:ARG:HG2	1:D:3322:ARG:NH1	2.24	0.49
1:A:116:LEU:HD22	1:A:123:TYR:CE1	2.47	0.49
1:A:6:VAL:CG1	1:A:7:THR:N	2.75	0.49
1:B:1002:LEU:HD13	1:B:1285:TYR:CE2	2.48	0.49
1:C:2048:LEU:HD23	1:C:2299:ARG:NH2	2.28	0.49
1:C:2096:VAL:O	1:C:2096:VAL:HG22	2.13	0.49
1:D:3070:TYR:C	1:D:3071:ILE:HD12	2.33	0.49
1:A:109:ILE:HD12	1:A:109:ILE:N	2.27	0.49
1:C:2071:ILE:HG12	1:C:2087:LEU:HD21	1.95	0.49
1:C:2215:GLY:O	1:C:2216:ILE:HB	2.13	0.49
1:B:1070:TYR:HB2	1:B:1247:LYS:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2009:PHE:CE1	1:C:2254:SER:HA	2.47	0.49
1:D:3217:HIS:O	1:D:3222:LYS:HE3	2.13	0.49
1:A:172:GLY:O	1:A:176:LYS:HB2	2.13	0.49
1:B:1070:TYR:CE1	1:B:1111:HIS:CD2	3.01	0.49
1:B:1163:LEU:HD11	1:B:1174:LYS:HD3	1.94	0.49
1:B:1256:ASP:OD2	6:B:6001:2BF:H7	2.13	0.49
1:A:124:LEU:HB3	1:A:125:PRO:HA	1.95	0.48
1:B:1171:ILE:O	1:B:1175:VAL:HB	2.13	0.48
1:B:1194:THR:O	1:B:1197:THR:N	2.46	0.48
1:C:2071:ILE:N	1:C:2071:ILE:HD12	2.28	0.48
1:C:2022:THR:HG23	1:C:2162:SER:O	2.13	0.48
1:A:125:PRO:HD2	7:A:7004:1PE:H131	1.95	0.48
1:C:2061:ASN:H	1:C:2061:ASN:ND2	2.11	0.48
1:B:1007:LEU:HD23	1:B:1281:LEU:HB3	1.95	0.48
1:C:2083:ALA:O	1:C:2087:LEU:HG	2.13	0.48
1:D:3257:ASP:OD2	1:D:3258:THR:N	2.46	0.48
1:A:213:SER:CA	1:A:217:ILE:HD12	2.44	0.48
1:D:3159:GLY:HA3	1:D:3164:LEU:O	2.14	0.48
1:D:3289:LYS:HG2	1:D:3289:LYS:O	2.14	0.48
1:A:165:LEU:HD11	1:A:176:LYS:HD2	1.95	0.48
1:B:1281:LEU:CD2	1:B:1281:LEU:N	2.77	0.48
1:C:2235:LEU:HD13	1:C:2235:LEU:C	2.34	0.48
1:D:3155:ILE:HG22	8:D:4124:HOH:O	2.14	0.48
1:D:3286:TYR:O	1:D:3292:TYR:HA	2.14	0.48
1:B:1016:PRO:HG2	1:B:1034:PHE:CE2	2.49	0.48
1:B:1093:PRO:HB3	1:B:1106:GLN:HB3	1.95	0.48
1:B:1157:LEU:HD23	1:B:1171:ILE:HD12	1.96	0.48
1:C:2104:LEU:O	1:C:2105:TRP:CB	2.61	0.48
1:B:1238:LYS:HE3	8:B:4058:HOH:O	2.14	0.48
1:C:2127:ASN:ND2	1:C:2127:ASN:H	2.11	0.48
1:C:2128:CYS:SG	1:C:2225:LEU:HD13	2.53	0.48
1:A:97:VAL:O	1:B:1039:GLN:NE2	2.47	0.48
1:B:1036:GLN:HE22	1:B:1077:ASP:HB2	1.79	0.48
1:D:3322:ARG:NH1	1:D:3322:ARG:CG	2.77	0.48
1:A:148:ARG:C	1:A:151:PRO:HD2	2.34	0.48
1:A:19:ASP:OD2	1:A:176:LYS:HG2	2.14	0.48
1:B:1019:THR:OG1	1:B:1020:PHE:N	2.46	0.48
1:D:3148:LEU:HD11	1:D:3155:ILE:CD1	2.44	0.48
1:C:2105:TRP:CZ2	1:C:2107:PRO:HB3	2.49	0.47
1:D:3270:TYR:CE2	1:D:3272:GLY:HA2	2.48	0.47
1:A:135:LEU:HD13	1:A:223:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:SER:CB	1:A:255:SER:HB3	2.42	0.47
1:B:1087:LEU:HD13	1:B:1108:ILE:CG2	2.44	0.47
1:D:3123:LEU:HD12	1:D:3123:LEU:N	2.29	0.47
1:A:64:SER:HB2	1:A:95:GLU:OE2	2.15	0.47
1:B:1210:LEU:C	1:B:1210:LEU:HD13	2.34	0.47
1:D:3115:LEU:HD22	1:D:3122:TYR:CZ	2.49	0.47
1:D:3055:ARG:NH2	1:D:3284:GLU:OE1	2.45	0.47
1:A:113:THR:OG1	1:A:114:VAL:N	2.47	0.47
1:C:2334:ASP:O	1:C:2338:GLU:HG3	2.14	0.47
1:D:3025:ILE:CD1	1:D:3025:ILE:H	2.23	0.47
1:D:3090:LEU:HD22	1:D:3091:PHE:CE2	2.49	0.47
1:D:3093:PRO:HB2	1:D:3098:ILE:HG12	1.95	0.47
1:B:1200:LYS:HE2	8:B:4039:HOH:O	2.14	0.47
1:A:88:LEU:HD13	1:A:109:ILE:CG2	2.45	0.47
1:A:152:TYR:O	1:A:153:LYS:C	2.53	0.47
1:B:1239:ARG:HB3	1:B:1246:TYR:CE2	2.49	0.47
1:A:328:VAL:O	1:A:331:VAL:HG22	2.15	0.47
1:B:1006:THR:HG22	1:B:1006:THR:O	2.15	0.47
1:D:3048:LEU:HD13	1:D:3086:ASN:HD21	1.79	0.47
1:D:3177:TYR:HB2	1:D:3202:LEU:HB3	1.95	0.47
1:D:3337:THR:O	1:D:3340:MET:HB2	2.14	0.47
1:A:301:ASN:O	1:A:302:GLU:HG3	2.14	0.47
1:C:2337:THR:HA	1:C:2340:MET:CE	2.45	0.47
1:D:3193:TRP:O	1:D:3195:THR:N	2.40	0.47
1:D:3239:LYS:O	1:D:3242:THR:HG22	2.14	0.47
1:D:3232:ASN:HB2	1:D:3331:ILE:CG2	2.42	0.47
1:A:150:HIS:HB3	1:A:151:PRO:CD	2.35	0.47
1:A:115:PRO:HD3	1:B:1113:VAL:HG22	1.97	0.47
1:C:2010:ARG:NH2	6:C:6002:2BF:O2P	2.46	0.47
1:B:1126:ARG:HG2	1:B:1126:ARG:HH11	1.80	0.46
1:B:1163:LEU:CD2	1:B:1174:LYS:HD3	2.45	0.46
1:C:2061:ASN:N	1:C:2061:ASN:ND2	2.63	0.46
1:C:2120:LEU:HD11	1:C:2233:GLU:HG2	1.96	0.46
1:D:3071:ILE:HD12	1:D:3071:ILE:N	2.30	0.46
1:D:3298:TYR:HB2	1:D:3309:LEU:HD11	1.97	0.46
1:A:24:ASP:OD1	1:A:26:ILE:N	2.47	0.46
1:A:51:GLU:HG3	1:A:90:ALA:HB1	1.97	0.46
1:C:2145:GLN:CA	1:C:2145:GLN:HE21	2.11	0.46
1:D:3071:ILE:CG2	1:D:3110:VAL:HG13	2.45	0.46
1:C:2006:THR:O	1:C:2007:LEU:HD23	2.15	0.46
1:C:2123:LEU:HD22	1:C:2259:THR:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2224:ARG:HH11	1:C:2224:ARG:HG3	1.80	0.46
1:C:2099:TRP:HH2	1:D:3046:TYR:CD1	2.33	0.46
1:C:2288:GLU:OE2	1:C:2288:GLU:HA	2.16	0.46
1:D:3045:HIS:HD2	1:D:3086:ASN:HD22	1.54	0.46
1:A:245:ILE:HD12	1:A:246:PRO:CG	2.45	0.46
1:D:3046:TYR:CE1	1:D:3089:ALA:HB2	2.49	0.46
1:C:2310:MET:HE3	1:C:2316:PRO:HD3	1.98	0.46
1:A:88:LEU:HD13	1:A:109:ILE:HB	1.98	0.46
1:A:200:MET:O	1:A:203:LEU:HB2	2.16	0.46
1:A:246:PRO:HG2	1:A:247:SER:H	1.80	0.46
2:A:5000:NAG:C6	2:A:5001:NAG:H82	2.32	0.46
1:B:1056:TYR:HB3	1:B:1060:LEU:CD2	2.44	0.46
1:C:2124:PRO:HG3	1:C:2213:LEU:HD21	1.96	0.46
1:C:2127:ASN:HD21	7:C:7002:1PE:H242	1.80	0.46
1:D:3235:LEU:HD21	1:D:3324:ALA:HB1	1.98	0.46
1:A:127:ARG:NH1	1:A:127:ARG:HG2	2.30	0.46
1:A:178:TYR:CE1	1:A:204:ARG:HB2	2.51	0.46
1:A:121:LEU:HD21	1:A:234:GLU:HG2	1.97	0.46
1:C:2235:LEU:HD13	1:C:2235:LEU:O	2.15	0.46
1:C:2000:LYS:HE2	1:C:2286:TYR:CE2	2.51	0.46
1:D:3020:PHE:CD2	1:D:3023:ASP:HB2	2.51	0.46
1:D:3068:GLN:HE21	1:D:3249:LYS:CE	2.29	0.46
1:D:3190:LEU:HD12	1:D:3190:LEU:N	2.30	0.46
1:A:241:ARG:HD2	1:A:248:TYR:OH	2.16	0.46
1:B:1002:LEU:HD23	1:B:1059:PHE:CG	2.52	0.46
1:C:2126:ARG:NH1	1:C:2132:GLN:OE1	2.47	0.46
1:C:2270:TYR:CE2	1:C:2272:GLY:HA2	2.51	0.46
1:D:3002:LEU:HD13	1:D:3286:TYR:CZ	2.51	0.46
1:D:3190:LEU:HB3	1:D:3191:PRO:HD2	1.98	0.46
1:A:212:LEU:HD12	1:A:217:ILE:CG1	2.42	0.45
1:A:308:TYR:CE2	2:A:5002:NAG:H5	2.51	0.45
1:C:2002:LEU:HD23	1:C:2059:PHE:CG	2.51	0.45
1:D:3032:GLN:HB3	1:D:3036:GLN:CG	2.38	0.45
1:D:3076:VAL:O	1:D:3080:LEU:HG	2.16	0.45
1:B:1090:LEU:HD13	1:B:1091:PHE:CE1	2.51	0.45
1:C:2055:ARG:NH2	1:C:2284:GLU:OE1	2.50	0.45
1:C:2070:TYR:HB3	1:C:2251:ILE:HG12	1.98	0.45
1:D:3149:HIS:O	1:D:3151:TYR:N	2.49	0.45
1:C:2288:GLU:CG	1:C:2289:LYS:H	2.14	0.45
1:C:2315:SER:HB2	1:C:2316:PRO:CD	2.47	0.45
1:A:12:HIS:NE2	6:A:6000:2BF:P	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:THR:HG21	1:A:235:ILE:HG12	1.98	0.45
1:D:3057:ARG:HG3	1:D:3058:LYS:N	2.32	0.45
1:D:3060:LEU:HD11	1:D:3250:LEU:HD22	1.99	0.45
1:A:204:ARG:NH1	1:A:208:GLU:OE1	2.49	0.45
1:A:213:SER:CB	1:A:217:ILE:HD12	2.46	0.45
1:A:245:ILE:HD11	1:A:247:SER:O	2.16	0.45
1:A:5:PHE:CZ	1:A:238:HIS:HB3	2.51	0.45
1:A:64:SER:HB2	1:A:95:GLU:CD	2.37	0.45
1:B:1065:LYS:HB3	1:B:1067:GLU:CD	2.37	0.45
1:B:1010:ARG:CD	1:B:1256:ASP:HB3	2.39	0.45
1:C:2120:LEU:HD23	1:C:2120:LEU:C	2.37	0.45
1:D:3129:PRO:O	1:D:3132:GLN:HB2	2.16	0.45
1:B:1244:PRO:O	1:B:1245:SER:C	2.55	0.45
1:C:2107:PRO:O	1:D:3081:MET:HG2	2.16	0.45
1:D:3264:GLN:HE21	1:D:3270:TYR:HA	1.81	0.45
1:A:127:ARG:CG	1:A:127:ARG:NH1	2.76	0.45
1:A:315:CYS:HB2	1:A:327:LEU:CD1	2.46	0.45
1:C:2242:THR:HB	1:C:2292:TYR:CE1	2.52	0.45
1:D:3062:GLU:OE2	1:D:3068:GLN:NE2	2.43	0.45
1:D:3094:GLU:H	1:D:3097:SER:HB2	1.82	0.45
1:A:239:MET:O	1:A:243:THR:HG23	2.17	0.45
1:A:61:LEU:HD23	1:A:92:PHE:CE2	2.52	0.45
1:A:71:TYR:HB2	1:A:249:LYS:HE2	1.99	0.45
1:B:1145:LYS:CA	1:B:1145:LYS:HE3	2.21	0.45
1:C:2056:TYR:HB2	1:C:2060:LEU:HD23	1.99	0.45
1:C:2161:LEU:HD13	1:C:2193:TRP:CG	2.52	0.45
1:A:150:HIS:HA	1:A:153:LYS:HG3	1.99	0.44
1:A:301:ASN:OD1	2:A:5002:NAG:O1	2.35	0.44
1:B:1186:ASN:HD21	3:B:5004:NDG:C2	2.29	0.44
1:D:3175:LYS:O	1:D:3179:PRO:HG2	2.18	0.44
1:A:107:GLN:HG3	1:A:109:ILE:CD1	2.48	0.44
1:A:288:PHE:CE1	1:A:291:GLY:HA2	2.53	0.44
1:D:3212:SER:HA	1:D:3216:ILE:CG1	2.46	0.44
1:A:301:ASN:C	1:A:302:GLU:HG3	2.37	0.44
1:B:1223:ARG:NH2	1:B:1331:PRO:HA	2.32	0.44
1:C:2115:LEU:HD13	1:C:2122:TYR:CE1	2.52	0.44
1:C:2013:ASP:OD1	1:C:2186:HIS:HE1	2.00	0.44
1:C:2337:THR:O	1:C:2339:CYS:N	2.50	0.44
1:D:3154:PHE:CD1	1:D:3201:LYS:HD2	2.52	0.44
1:D:3328:GLY:N	1:D:3329:PRO:HD2	2.33	0.44
1:A:49:LEU:HA	1:A:300:ARG:HH22	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:HG3	1:A:69:GLN:NE2	2.32	0.44
1:B:1134:GLU:O	1:B:1138:LEU:HD23	2.17	0.44
1:C:2184:SER:O	1:C:2185:VAL:C	2.55	0.44
1:D:3149:HIS:C	1:D:3151:TYR:H	2.21	0.44
1:D:3230:LEU:HD23	1:D:3263:LEU:HD22	1.99	0.44
1:A:40:GLN:OE1	1:B:1097:SER:HA	2.18	0.44
1:A:201:THR:O	1:A:205:GLU:HG3	2.18	0.44
1:A:53:ILE:CD1	1:A:57:TYR:CD1	3.01	0.44
1:B:1023:ASP:HA	1:B:1024:PRO:HD3	1.82	0.44
1:C:2093:PRO:HB2	1:C:2104:LEU:HB3	2.00	0.44
1:D:3169:LEU:HD21	1:D:3205:LEU:HD22	1.99	0.44
1:A:72:ILE:N	1:A:72:ILE:HD12	2.33	0.44
1:B:1214:GLY:HA3	1:B:1264:MET:HE1	2.00	0.44
1:C:2061:ASN:O	1:C:2062:GLU:HG3	2.18	0.44
1:A:49:LEU:HD22	1:A:53:ILE:HG22	2.00	0.44
1:A:82:MET:HA	1:A:85:MET:CE	2.45	0.44
1:A:142:SER:O	1:A:146:GLN:HG2	2.18	0.43
1:C:2303:GLN:HG3	1:C:2304:HIS:CD2	2.53	0.43
1:B:1165:GLY:C	1:B:1167:ASP:H	2.21	0.43
1:B:1318:PRO:HG2	1:B:1321:ARG:CB	2.49	0.43
1:C:2086:ASN:ND2	1:C:2252:MET:CE	2.81	0.43
1:C:2149:HIS:HB3	1:C:2150:PRO:CD	2.41	0.43
1:C:2310:MET:HE2	1:C:2315:SER:HA	1.99	0.43
1:D:3154:PHE:CZ	1:D:3201:LYS:HB2	2.53	0.43
1:D:3287:PHE:HA	1:D:3291:GLU:O	2.18	0.43
1:A:127:ARG:HH11	1:A:127:ARG:HB3	1.83	0.43
1:B:1321:ARG:NH1	1:B:1321:ARG:HG2	2.33	0.43
1:D:3094:GLU:HG3	1:D:3094:GLU:O	2.18	0.43
1:C:2190:LEU:HB3	1:C:2191:PRO:CD	2.40	0.43
1:C:2276:PRO:HD2	1:C:2279:SER:HB3	2.00	0.43
1:A:18:ILE:O	1:A:18:ILE:HG22	2.17	0.43
1:B:1075:ASP:HB2	1:B:1113:VAL:O	2.18	0.43
1:B:1175:VAL:C	1:B:1178:PRO:HD2	2.38	0.43
1:B:1326:VAL:O	1:B:1329:VAL:HG22	2.16	0.43
1:C:2224:ARG:NH1	1:C:2224:ARG:HG3	2.34	0.43
1:D:3160:LYS:HA	1:D:3160:LYS:HD2	1.89	0.43
1:A:177:VAL:O	1:A:180:PRO:HD2	2.19	0.43
1:B:1230:VAL:HG11	1:B:1326:VAL:CG2	2.48	0.43
1:C:2261:SER:O	1:C:2265:MET:HG2	2.19	0.43
1:D:3062:GLU:HB2	1:D:3065:LYS:HD2	2.00	0.43
1:D:3006:THR:HG21	1:D:3234:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3121:LEU:HD11	1:D:3253:TYR:HD2	1.83	0.43
1:A:100:TRP:CE3	1:A:101:ASN:HB2	2.53	0.43
1:A:124:LEU:HD12	1:A:260:THR:HA	2.01	0.43
1:C:2169:LEU:HD23	1:C:2169:LEU:HA	1.82	0.43
1:C:2257:ASP:HB2	1:C:2275:PRO:HD2	2.01	0.43
1:D:3273:LEU:HD12	5:D:5010:NAG:H2	2.01	0.43
1:B:1216:HIS:CE1	1:B:1217:LYS:HG3	2.53	0.43
1:C:2126:ARG:NH1	1:C:2126:ARG:HG2	2.34	0.43
1:D:3088:ALA:HA	1:D:3105:TRP:HE1	1.84	0.43
1:D:3240:ARG:HB3	1:D:3247:TYR:CE2	2.54	0.43
1:A:17:PRO:HG2	1:A:35:PHE:CE2	2.53	0.43
1:C:2130:ARG:HB3	1:C:2339:CYS:HA	2.01	0.43
1:C:2154:PHE:O	1:C:2158:LEU:HB2	2.19	0.43
1:A:245:ILE:HD12	1:A:246:PRO:HG2	2.00	0.43
1:D:3013:ASP:O	1:D:3037:LEU:HD12	2.19	0.43
1:A:17:PRO:HB3	1:A:180:PRO:HA	2.01	0.42
1:A:178:TYR:HD1	1:A:203:LEU:HB3	1.84	0.42
1:A:218:HIS:CE1	1:A:219:LYS:HE3	2.54	0.42
1:A:24:ASP:HA	1:A:25:PRO:HD3	1.93	0.42
1:B:1060:LEU:O	1:B:1062:GLU:N	2.51	0.42
1:B:1168:LEU:HD22	1:B:1204:LEU:HD22	2.01	0.42
1:C:2168:ASP:OD2	1:C:2171:GLY:N	2.43	0.42
1:C:2217:HIS:NE2	1:C:2218:LYS:HD3	2.33	0.42
1:D:3269:VAL:HB	1:D:3309:LEU:HD22	1.99	0.42
1:B:1038:THR:O	1:B:1042:MET:HG3	2.18	0.42
1:B:1138:LEU:CD2	1:B:1138:LEU:N	2.82	0.42
1:B:1115:LEU:HD22	1:B:1122:TYR:CD2	2.54	0.42
1:B:1322:PHE:O	1:B:1326:VAL:HG12	2.19	0.42
1:B:1184:VAL:O	3:B:5004:NDG:H8C3	2.19	0.42
1:C:2310:MET:HE1	1:C:2316:PRO:HD3	2.01	0.42
1:D:3045:HIS:CE1	1:D:3082:SER:HB3	2.54	0.42
1:D:3319:PRO:HG2	1:D:3322:ARG:HB3	2.01	0.42
1:B:1166:GLN:HB2	1:B:1166:GLN:HE21	1.67	0.42
1:B:1184:VAL:O	3:B:5004:NDG:H8C1	2.19	0.42
1:C:2013:ASP:HA	1:C:2277:TYR:CE1	2.55	0.42
1:C:2051:TYR:CE2	1:C:2299:ARG:HD2	2.54	0.42
1:D:3213:LEU:HD23	1:D:3214:TYR:CE1	2.54	0.42
1:B:1069:VAL:HG12	1:B:1070:TYR:N	2.35	0.42
1:C:2018:ASP:CG	1:C:2019:THR:H	2.23	0.42
1:C:2327:VAL:O	1:C:2327:VAL:HG12	2.19	0.42
1:D:3119:GLN:HA	1:D:3125:PHE:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3169:LEU:HD23	1:D:3169:LEU:HA	1.89	0.42
1:A:311:MET:HG2	1:A:317:PRO:HD3	2.01	0.42
1:B:1068:GLN:O	1:B:1247:LYS:HG3	2.20	0.42
1:C:2027:GLU:HB2	1:C:2034:PHE:CE1	2.55	0.42
1:C:2301:GLU:OE1	2:C:5007:NAG:H83	2.19	0.42
1:D:3208:LEU:O	1:D:3212:SER:HB3	2.20	0.42
1:A:323:ARG:HD2	1:A:323:ARG:HA	1.79	0.42
1:A:232:VAL:HG11	1:A:328:VAL:CG2	2.50	0.42
1:B:1216:HIS:CE1	1:B:1217:LYS:HE3	2.54	0.42
1:D:3167:GLN:HA	8:D:4127:HOH:O	2.19	0.42
1:A:216:GLY:O	1:A:217:ILE:HB	2.19	0.42
1:B:1063:SER:O	1:B:1064:TYR:O	2.38	0.42
1:B:1210:LEU:O	1:B:1210:LEU:HD13	2.20	0.42
1:B:1321:ARG:HH11	1:B:1321:ARG:HG2	1.85	0.42
1:C:2064:TYR:OH	1:C:2066:HIS:HB3	2.19	0.42
1:C:2090:LEU:HD22	1:C:2091:PHE:CE1	2.54	0.42
1:D:3230:LEU:HD21	1:D:3263:LEU:HD22	2.01	0.42
1:D:3065:LYS:C	1:D:3067:GLU:N	2.72	0.42
1:A:312:LEU:O	1:A:313:PRO:C	2.56	0.42
1:B:1150:TYR:O	1:B:1154:ILE:HG23	2.20	0.42
1:B:1023:ASP:OD2	1:B:1182:GLU:OE2	2.37	0.42
1:B:1056:TYR:OH	1:B:1283:GLU:OE1	2.29	0.42
1:B:1169:PHE:CE1	7:B:7005:1PE:H222	2.55	0.42
1:B:1089:ALA:O	1:B:1092:PRO:HD3	2.20	0.41
1:C:2191:PRO:HB2	1:C:2193:TRP:NE1	2.35	0.41
1:C:2319:PRO:HG2	1:C:2322:ARG:CB	2.48	0.41
1:A:215:TYR:CE1	1:A:263:GLY:HA2	2.54	0.41
1:C:2093:PRO:O	1:C:2094:GLU:HB3	2.20	0.41
1:C:2126:ARG:HH11	1:C:2126:ARG:CG	2.33	0.41
1:A:122:LEU:HD11	1:A:254:TYR:HD2	1.86	0.41
1:A:313:PRO:HD3	8:A:4028:HOH:O	2.18	0.41
1:B:1071:ILE:HG12	1:B:1087:LEU:HD21	2.02	0.41
1:B:1229:LEU:HD23	1:B:1262:LEU:HB2	2.03	0.41
1:D:3269:VAL:CG2	1:D:3309:LEU:HD13	2.50	0.41
1:A:122:LEU:O	1:A:124:LEU:N	2.53	0.41
1:A:245:ILE:HG13	1:A:248:TYR:HB2	2.01	0.41
1:A:8:LEU:CD2	1:A:283:LEU:HB3	2.43	0.41
1:C:2076:VAL:O	1:C:2077:ASP:C	2.58	0.41
1:C:2115:LEU:HD13	1:C:2122:TYR:CZ	2.55	0.41
1:C:2154:PHE:CE1	1:C:2158:LEU:HD23	2.55	0.41
1:C:2235:LEU:HD11	1:C:2239:LYS:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3064:TYR:OH	1:D:3066:HIS:HB3	2.19	0.41
1:D:3093:PRO:O	1:D:3094:GLU:HB3	2.20	0.41
1:A:176:LYS:C	1:A:180:PRO:HG2	2.41	0.41
1:A:315:CYS:HB2	1:A:327:LEU:HD11	2.03	0.41
1:C:2307:TYR:HA	1:C:2308:PRO:HD3	1.85	0.41
1:C:2307:TYR:CD1	2:C:5007:NAG:O1	2.67	0.41
1:D:3176:VAL:C	1:D:3179:PRO:HD2	2.40	0.41
1:A:176:LYS:O	1:A:180:PRO:HG2	2.20	0.41
1:B:1060:LEU:C	1:B:1062:GLU:N	2.73	0.41
1:B:1176:TYR:CE1	1:B:1202:ARG:HB2	2.55	0.41
1:C:2120:LEU:CD2	1:C:2121:LEU:HG	2.48	0.41
1:C:2169:LEU:HD11	1:C:2208:LEU:CD2	2.50	0.41
1:C:2039:GLN:O	1:C:2042:MET:HB2	2.20	0.41
1:C:2310:MET:HE3	1:C:2315:SER:HA	2.03	0.41
1:D:3119:GLN:HB3	7:D:7003:1PE:OH4	2.21	0.41
1:A:116:LEU:HD22	1:A:123:TYR:CD1	2.55	0.41
1:A:41:LEU:HD12	1:A:41:LEU:O	2.21	0.41
1:A:70:VAL:HG12	1:A:71:TYR:N	2.35	0.41
1:C:2023:ASP:HA	1:C:2024:PRO:HD3	1.96	0.41
1:D:3073:SER:OG	1:D:3080:LEU:HD23	2.21	0.41
1:B:1333:ASP:O	1:B:1337:GLU:HG3	2.21	0.41
1:C:2177:TYR:CE1	1:C:2203:ARG:HB2	2.56	0.41
1:C:2086:ASN:HD22	1:C:2252:MET:HE1	1.85	0.41
1:D:3186:HIS:HA	4:D:5009:NAG:H83	2.03	0.41
1:A:4:LYS:O	1:A:4:LYS:HD3	2.20	0.41
1:B:1225:GLN:HA	1:B:1225:GLN:NE2	2.36	0.41
1:C:2013:ASP:H	1:C:2041:GLY:HA2	1.85	0.41
1:C:2143:GLU:O	1:C:2147:ARG:HG3	2.20	0.41
1:D:3119:GLN:HA	1:D:3125:PHE:CE1	2.56	0.41
1:D:3282:LEU:N	1:D:3282:LEU:CD2	2.84	0.41
1:A:149:LEU:HD11	1:A:156:ILE:HD11	2.03	0.41
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.86	0.41
1:A:301:ASN:O	1:A:302:GLU:CG	2.68	0.41
1:B:1055:ARG:HG2	1:B:1056:TYR:CE2	2.56	0.41
1:C:2098:ILE:CG2	1:C:2099:TRP:H	2.29	0.41
1:C:2068:GLN:CG	1:C:2249:LYS:HG3	2.47	0.41
1:C:2099:TRP:CH2	1:D:3046:TYR:CD1	3.09	0.41
1:A:20:THR:OG1	1:A:21:PHE:N	2.55	0.40
1:A:11:ARG:HG3	1:A:257:HIS:HA	2.04	0.40
1:A:53:ILE:HD12	1:A:57:TYR:CD1	2.55	0.40
1:A:54:ARG:CB	1:A:91:LEU:HD23	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1004:PHE:CZ	1:B:1236:HIS:HB3	2.56	0.40
1:B:1126:ARG:HH21	7:B:7005:1PE:H121	1.85	0.40
1:B:1175:VAL:O	1:B:1178:PRO:HD2	2.20	0.40
1:C:2042:MET:O	1:C:2046:TYR:HB2	2.20	0.40
1:A:150:HIS:C	1:A:152:TYR:N	2.73	0.40
1:B:1147:LEU:O	1:B:1148:HIS:C	2.60	0.40
1:C:2309:LEU:HD23	1:C:2309:LEU:HA	1.91	0.40
1:D:3224:ARG:NH2	1:D:3332:PRO:HA	2.36	0.40
1:A:179:ASP:N	1:A:180:PRO:CD	2.84	0.40
1:B:1048:LEU:HD22	1:B:1052:ILE:CD1	2.51	0.40
2:C:5007:NAG:C6	2:C:5008:NAG:O5	2.69	0.40
1:D:3015:SER:HB2	1:D:3016:PRO:HD2	2.02	0.40
1:D:3148:LEU:HD11	1:D:3155:ILE:HD11	2.03	0.40
1:D:3244:ILE:HG22	1:D:3245:PRO:O	2.22	0.40
1:A:141:LYS:N	1:A:141:LYS:HD2	2.36	0.40
1:B:1014:ARG:HH11	1:B:1014:ARG:HG3	1.85	0.40
1:B:1069:VAL:CG1	1:B:1070:TYR:N	2.84	0.40
1:C:2177:TYR:OH	1:C:2203:ARG:HD3	2.21	0.40
1:C:2300:ASN:CG	2:C:5007:NAG:HN2	2.24	0.40
1:D:3010:ARG:NH1	1:D:3275:PRO:O	2.55	0.40
1:A:149:LEU:HD11	1:A:156:ILE:CD1	2.52	0.40
1:A:8:LEU:HD12	1:A:253:MET:HG2	2.03	0.40
1:B:1005:VAL:HG21	1:B:1056:TYR:CZ	2.57	0.40
1:C:2057:ARG:HA	1:C:2057:ARG:HD2	1.99	0.40
1:C:2099:TRP:HB3	1:D:3039:GLN:HG3	2.02	0.40
1:B:1242:GLN:NE2	1:D:3189:THR:OG1	2.47	0.40
1:D:3255:ALA:HB1	1:D:3259:THR:OG1	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	340/354 (96%)	288 (85%)	39 (12%)	13 (4%)	4	15
1	B	338/354 (96%)	284 (84%)	43 (13%)	11 (3%)	4	18
1	C	340/354 (96%)	282 (83%)	41 (12%)	17 (5%)	2	8
1	D	340/354 (96%)	287 (84%)	37 (11%)	16 (5%)	3	10
All	All	1358/1416 (96%)	1141 (84%)	160 (12%)	57 (4%)	3	12

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	65	TYR
1	B	1064	TYR
1	B	1245	SER
1	C	2099	TRP
1	C	2105	TRP
1	C	2167	GLN
1	D	3061	ASN
1	D	3063	SER
1	D	3152	LYS
1	D	3167	GLN
1	A	123	TYR
1	A	153	LYS
1	B	1140	SER
1	B	1340	THR
1	C	2031	PRO
1	C	2033	GLY
1	C	2057	ARG
1	C	2066	HIS
1	C	2098	ILE
1	C	2149	HIS
1	C	2334	ASP
1	C	2338	GLU
1	D	3011	HIS
1	D	3066	HIS
1	D	3094	GLU
1	D	3102	ILE
1	D	3289	LYS
1	A	117	SER
1	A	151	PRO
1	A	246	PRO
1	A	335	ASP
1	B	1027	GLU

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Mol	Chain	Res	Type
1	B	1061	ASN
1	C	2094	GLU
1	B	1148	HIS
1	C	2011	HIS
1	D	3064	TYR
1	D	3150	PRO
1	D	3153	ASP
1	A	64	SER
1	B	1063	SER
1	C	2075	ASP
1	C	2216	ILE
1	D	3028	SER
1	D	3166	GLY
1	A	269	ASP
1	B	1300	GLU
1	C	2021	PRO
1	D	3108	ILE
1	A	330	PRO
1	C	2102	ILE
1	A	228	GLY
1	B	1215	ILE
1	A	32	PRO
1	B	1031	PRO
1	D	3312	PRO

### 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	314/325 (97%)	293 (93%)	21 (7%)	19	48
1	B	314/325 (97%)	297 (95%)	17 (5%)	26	59
1	C	314/325 (97%)	293 (93%)	21 (7%)	19	48
1	D	314/325 (97%)	295 (94%)	19 (6%)	22	53
All	All	1256/1300 (97%)	1178 (94%)	78 (6%)	21	52

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	37	GLN
1	A	46	HIS
1	A	49	LEU
1	A	53	ILE
1	A	58	ARG
1	A	91	LEU
1	A	127	ARG
1	A	144	GLU
1	A	147	LYS
1	A	154	ASP
1	A	197	GLU
1	A	212	LEU
1	A	214	LEU
1	A	231	LEU
1	A	240	LYS
1	A	245	ILE
1	A	269	ASP
1	A	283	LEU
1	A	315	CYS
1	A	317	PRO
1	B	1006	THR
1	B	1009	PHE
1	B	1027	GLU
1	B	1036	GLN
1	B	1045	HIS
1	B	1048	LEU
1	B	1063	SER
1	B	1078	ARG
1	B	1090	LEU
1	B	1127	ASN
1	B	1145	LYS
1	B	1166	GLN
1	B	1168	LEU
1	B	1212	LEU
1	B	1241	THR
1	B	1281	LEU
1	B	1314	SER
1	C	2005	VAL
1	C	2036	GLN
1	C	2048	LEU
1	C	2061	ASN

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Mol	Chain	Res	Type
1	C	2069	VAL
1	C	2072	ARG
1	C	2082	SER
1	C	2102	ILE
1	C	2105	TRP
1	C	2126	ARG
1	C	2127	ASN
1	C	2129	PRO
1	C	2130	ARG
1	C	2135	GLU
1	C	2145	GLN
1	C	2158	LEU
1	C	2169	LEU
1	C	2189	THR
1	C	2213	LEU
1	C	2230	LEU
1	C	2322	ARG
1	D	3003	LYS
1	D	3005	VAL
1	D	3006	THR
1	D	3042	MET
1	D	3045	HIS
1	D	3048	LEU
1	D	3062	GLU
1	D	3069	VAL
1	D	3090	LEU
1	D	3108	ILE
1	D	3126	ARG
1	D	3127	ASN
1	D	3139	LEU
1	D	3153	ASP
1	D	3242	THR
1	D	3243	GLN
1	D	3268	ASP
1	D	3282	LEU
1	D	3289	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	46	HIS

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Mol	Chain	Res	Type
1	A	67	HIS
1	A	87	ASN
1	A	120	GLN
1	A	233	ASN
1	A	237	ASN
1	A	265	GLN
1	A	305	HIS
1	A	334	GLN
1	B	1032	GLN
1	B	1036	GLN
1	B	1045	HIS
1	B	1068	GLN
1	B	1127	ASN
1	B	1131	GLN
1	B	1144	GLN
1	B	1166	GLN
1	B	1185	HIS
1	B	1186	ASN
1	B	1225	GLN
1	B	1231	ASN
1	B	1263	GLN
1	C	2061	ASN
1	C	2086	ASN
1	C	2106	GLN
1	C	2127	ASN
1	C	2145	GLN
1	C	2186	HIS
1	C	2232	ASN
1	C	2264	GLN
1	C	2304	HIS
1	D	3045	HIS
1	D	3061	ASN
1	D	3068	GLN
1	D	3086	ASN
1	D	3100	ASN
1	D	3127	ASN
1	D	3226	GLN
1	D	3232	ASN
1	D	3236	ASN
1	D	3264	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 ⓘ

11 carbohydrates 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	NAG	A	5000	1,2	15,15,15	0.52	0	21,21,21	0.90	1 (4%)
2	NAG	A	5001	2	15,15,15	0.43	0	21,21,21	0.50	0
2	NAG	A	5002	1,2	15,15,15	0.42	0	21,21,21	0.67	0
2	NAG	A	5003	2	15,15,15	0.44	0	21,21,21	1.06	2 (9%)
2	NAG	B	5005	2	15,15,15	0.42	0	21,21,21	0.58	0
2	NAG	B	5006	2	15,15,15	0.49	0	21,21,21	0.99	1 (4%)
2	NAG	C	5007	1,2	15,15,15	0.74	0	21,21,21	1.04	1 (4%)
2	NAG	C	5008	2	15,15,15	0.44	0	21,21,21	0.88	1 (4%)
5	NAG	D	5010	1,5	15,15,15	0.54	0	21,21,21	0.56	0
5	NAG	D	5011	5	15,15,15	0.46	0	21,21,21	1.04	1 (4%)
5	MAN	D	5012	5	12,12,12	0.60	0	17,17,17	0.56	0

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	NAG	A	5000	1,2	-	0/6/26/26	0/1/1/1
2	NAG	A	5001	2	1/1/6/7	0/6/26/26	0/1/1/1
2	NAG	A	5002	1,2	1/1/6/7	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	5003	2	-	0/6/26/26	0/1/1/1
2	NAG	B	5005	2	1/1/6/7	0/6/26/26	0/1/1/1
2	NAG	B	5006	2	-	0/6/26/26	0/1/1/1
2	NAG	C	5007	1,2	1/1/6/7	0/6/26/26	0/1/1/1
2	NAG	C	5008	2	1/1/6/7	0/6/26/26	0/1/1/1
5	NAG	D	5010	1,5	1/1/6/7	0/6/26/26	0/1/1/1
5	NAG	D	5011	5	-	0/6/26/26	0/1/1/1
5	MAN	D	5012	5	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5003	NAG	O1-C1-C2	-3.52	101.91	109.22
5	D	5011	NAG	O1-C1-C2	-3.49	101.96	109.22
2	C	5007	NAG	C1-C2-C3	-3.30	106.05	110.54
2	B	5006	NAG	O1-C1-C2	-3.28	102.41	109.22
2	A	5000	NAG	O1-C1-C2	-2.92	103.16	109.22
2	A	5003	NAG	C1-C2-C3	-2.00	107.81	110.54
2	C	5008	NAG	O5-C1-C2	2.60	112.13	109.52

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	5007	NAG	C1
2	B	5005	NAG	C1
2	A	5001	NAG	C1
2	C	5008	NAG	C1
2	A	5002	NAG	C1
5	D	5010	NAG	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5000	NAG	4	0
2	A	5001	NAG	2	0
2	A	5002	NAG	4	0
2	B	5005	NAG	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	5007	NAG	7	0
2	C	5008	NAG	4	0
5	D	5010	NAG	4	0
5	D	5011	NAG	3	0

## 5.6 Ligand geometry

14 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	$\# Z  > 2$
6	2BF	A	6000	-	20,20,20	4.08	15 (75%)	22,27,27	1.32	3 (13%)
7	1PE	A	7000	-	15,15,15	0.90	0	14,14,14	1.47	4 (28%)
7	1PE	A	7004	-	15,15,15	0.80	0	14,14,14	1.50	4 (28%)
7	1PE	A	7007	-	15,15,15	0.96	0	14,14,14	1.48	4 (28%)
3	NDG	B	5004	-	15,15,15	0.30	0	21,21,21	0.63	0
6	2BF	B	6001	-	20,20,20	3.90	16 (80%)	22,27,27	1.34	3 (13%)
7	1PE	B	7001	-	15,15,15	0.72	0	14,14,14	1.43	4 (28%)
7	1PE	B	7005	-	15,15,15	0.84	0	14,14,14	1.49	4 (28%)
6	2BF	C	6002	-	20,20,20	3.96	15 (75%)	22,27,27	1.38	4 (18%)
7	1PE	C	7002	-	15,15,15	0.86	0	14,14,14	1.49	4 (28%)
7	1PE	C	7006	-	15,15,15	0.88	0	14,14,14	1.47	4 (28%)
4	NAG	D	5009	1	15,15,15	0.42	0	21,21,21	0.61	0
6	2BF	D	6003	-	20,20,20	4.09	16 (80%)	22,27,27	1.27	3 (13%)
7	1PE	D	7003	-	15,15,15	0.85	0	14,14,14	1.43	4 (28%)

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
6	2BF	A	6000	-	-	0/15/15/15	0/2/2/2
7	1PE	A	7000	-	-	0/13/13/13	0/0/0/0
7	1PE	A	7004	-	-	0/13/13/13	0/0/0/0
7	1PE	A	7007	-	-	0/13/13/13	0/0/0/0
3	NDG	B	5004	-	-	0/6/26/26	0/1/1/1
6	2BF	B	6001	-	-	0/15/15/15	0/2/2/2
7	1PE	B	7001	-	-	0/13/13/13	0/0/0/0
7	1PE	B	7005	-	-	0/13/13/13	0/0/0/0
6	2BF	C	6002	-	-	0/15/15/15	0/2/2/2
7	1PE	C	7002	-	-	0/13/13/13	0/0/0/0
7	1PE	C	7006	-	-	0/13/13/13	0/0/0/0
4	NAG	D	5009	1	1/1/6/7	0/6/26/26	0/1/1/1
6	2BF	D	6003	-	-	0/15/15/15	0/2/2/2
7	1PE	D	7003	-	-	0/13/13/13	0/0/0/0

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	6001	2BF	P-C7	2.03	1.86	1.83
6	B	6001	2BF	C10-C9	2.03	1.42	1.38
6	D	6003	2BF	C10-C9	2.04	1.42	1.38
6	D	6003	2BF	C2-C1	2.12	1.43	1.38
6	C	6002	2BF	P-C7	2.23	1.86	1.83
6	A	6000	2BF	P-C7	2.23	1.86	1.83
6	A	6000	2BF	C12-C13	2.25	1.43	1.38
6	B	6001	2BF	C11-C10	2.31	1.43	1.38
6	C	6002	2BF	C12-C13	2.36	1.43	1.38
6	B	6001	2BF	C2-C1	2.37	1.43	1.38
6	D	6003	2BF	C12-C13	2.37	1.43	1.38
6	A	6000	2BF	C11-C10	2.38	1.43	1.38
6	C	6002	2BF	C2-C1	2.43	1.43	1.38
6	A	6000	2BF	C2-C1	2.47	1.44	1.38
6	B	6001	2BF	C12-C13	2.48	1.43	1.38
6	D	6003	2BF	C3-C4	2.49	1.43	1.38
6	D	6003	2BF	C11-C10	2.54	1.44	1.38
6	D	6003	2BF	C1-C6	2.62	1.43	1.38
6	A	6000	2BF	C13-C8	2.62	1.44	1.38
6	B	6001	2BF	C13-C8	2.67	1.44	1.38
6	C	6002	2BF	C3-C4	2.77	1.44	1.38
6	B	6001	2BF	C1-C6	2.86	1.44	1.38
6	C	6002	2BF	C1-C6	2.86	1.44	1.38
6	D	6003	2BF	C13-C8	2.89	1.44	1.38
6	A	6000	2BF	C1-C6	2.94	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	6002	2BF	C11-C10	2.94	1.45	1.38
6	B	6001	2BF	C3-C4	2.97	1.44	1.38
6	A	6000	2BF	C3-C4	2.99	1.44	1.38
6	D	6003	2BF	P-C7	3.28	1.88	1.83
6	C	6002	2BF	C13-C8	3.33	1.45	1.38
6	B	6001	2BF	P-O3P	3.34	1.60	1.54
6	D	6003	2BF	C4-C5	3.45	1.44	1.39
6	C	6002	2BF	C4-C5	3.50	1.44	1.39
6	B	6001	2BF	C4-C5	3.65	1.45	1.39
6	A	6000	2BF	C4-C5	3.77	1.45	1.39
6	B	6001	2BF	C6-C5	3.81	1.45	1.39
6	C	6002	2BF	C6-C5	3.84	1.45	1.39
6	C	6002	2BF	P-O3P	3.86	1.61	1.54
6	C	6002	2BF	P-O2P	3.95	1.61	1.54
6	A	6000	2BF	P-O2P	3.96	1.61	1.54
6	D	6003	2BF	P-O3P	4.15	1.61	1.54
6	A	6000	2BF	P-O3P	4.30	1.61	1.54
6	D	6003	2BF	C6-C5	4.43	1.46	1.39
6	A	6000	2BF	C6-C5	4.44	1.46	1.39
6	B	6001	2BF	P-O2P	4.49	1.62	1.54
6	D	6003	2BF	P-O2P	4.61	1.62	1.54
6	B	6001	2BF	P-O1P	5.30	1.59	1.49
6	C	6002	2BF	P-O1P	5.66	1.60	1.49
6	A	6000	2BF	P-O1P	6.10	1.60	1.49
6	D	6003	2BF	P-O1P	6.47	1.61	1.49
6	C	6002	2BF	C3-C2	6.49	1.53	1.38
6	B	6001	2BF	C3-C2	6.64	1.54	1.38
6	D	6003	2BF	C3-C2	6.69	1.54	1.38
6	C	6002	2BF	C12-C11	6.98	1.54	1.38
6	A	6000	2BF	C3-C2	7.00	1.54	1.38
6	D	6003	2BF	C12-C11	7.07	1.55	1.38
6	B	6001	2BF	C12-C11	7.13	1.55	1.38
6	A	6000	2BF	C12-C11	7.26	1.55	1.38
6	B	6001	2BF	C9-C8	8.53	1.56	1.38
6	D	6003	2BF	C9-C8	8.56	1.56	1.38
6	C	6002	2BF	C9-C8	8.66	1.56	1.38
6	A	6000	2BF	C9-C8	8.71	1.56	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	6001	2BF	O1P-P-C7	-4.07	104.03	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	6002	2BF	O1P-P-C7	-3.76	104.56	111.04
6	A	6000	2BF	O1P-P-C7	-3.26	105.42	111.04
6	D	6003	2BF	C8-C19-N	-2.75	105.73	112.69
6	D	6003	2BF	C6-C5-C7	-2.66	117.89	120.72
6	A	6000	2BF	C6-C5-C7	-2.45	118.11	120.72
6	A	6000	2BF	C8-C19-N	-2.39	106.64	112.69
6	C	6002	2BF	C8-C19-N	-2.36	106.71	112.69
6	D	6003	2BF	O1P-P-C7	-2.35	106.99	111.04
6	B	6001	2BF	C6-C5-C7	-2.25	118.33	120.72
6	C	6002	2BF	C6-C5-C7	-2.19	118.39	120.72
6	B	6001	2BF	C8-C19-N	-2.13	107.30	112.69
6	C	6002	2BF	O3P-P-O1P	-2.09	108.10	113.41
7	A	7007	1PE	OH3-C22-C12	2.08	119.75	110.15
7	D	7003	1PE	OH3-C22-C12	2.15	120.06	110.15
7	C	7002	1PE	OH3-C22-C12	2.19	120.27	110.15
7	B	7001	1PE	OH3-C22-C12	2.25	120.52	110.15
7	B	7001	1PE	OH4-C13-C23	2.25	120.74	110.41
7	A	7004	1PE	OH3-C22-C12	2.25	120.54	110.15
7	D	7003	1PE	OH4-C13-C23	2.26	120.80	110.41
7	A	7004	1PE	OH4-C13-C23	2.27	120.84	110.41
7	A	7007	1PE	OH6-C26-C16	2.28	120.66	110.15
7	C	7006	1PE	OH3-C22-C12	2.29	120.72	110.15
7	A	7000	1PE	OH3-C22-C12	2.29	120.72	110.15
7	A	7007	1PE	OH4-C13-C23	2.30	120.96	110.41
7	A	7000	1PE	OH6-C26-C16	2.30	120.78	110.15
7	B	7001	1PE	OH6-C26-C16	2.31	120.79	110.15
7	C	7006	1PE	OH4-C13-C23	2.31	121.00	110.41
7	B	7005	1PE	OH3-C22-C12	2.33	120.91	110.15
7	C	7002	1PE	OH4-C13-C23	2.34	121.16	110.41
7	B	7005	1PE	OH6-C26-C16	2.34	120.96	110.15
7	B	7005	1PE	OH4-C13-C23	2.39	121.38	110.41
7	C	7006	1PE	OH6-C26-C16	2.40	121.21	110.15
7	D	7003	1PE	OH6-C26-C16	2.40	121.22	110.15
7	C	7002	1PE	OH6-C26-C16	2.46	121.51	110.15
7	A	7004	1PE	OH6-C26-C16	2.49	121.62	110.15
7	A	7000	1PE	OH4-C13-C23	2.50	121.88	110.41
7	C	7002	1PE	C25-OH5-C14	2.54	124.32	113.30
7	B	7005	1PE	C25-OH5-C14	2.63	124.71	113.30
7	A	7004	1PE	C25-OH5-C14	2.64	124.72	113.30
7	B	7001	1PE	C25-OH5-C14	2.66	124.81	113.30
7	A	7000	1PE	C25-OH5-C14	2.66	124.82	113.30
7	A	7007	1PE	C25-OH5-C14	2.66	124.84	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	7003	1PE	C25-OH5-C14	2.67	124.88	113.30
7	C	7006	1PE	C25-OH5-C14	2.76	125.26	113.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	5009	NAG	C1

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	6000	2BF	3	0
7	A	7000	1PE	1	0
7	A	7004	1PE	2	0
3	B	5004	NDG	10	0
6	B	6001	2BF	2	0
7	B	7001	1PE	1	0
7	B	7005	1PE	4	0
6	C	6002	2BF	2	0
7	C	7002	1PE	1	0
7	C	7006	1PE	1	0
4	D	5009	NAG	6	0
7	D	7003	1PE	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.