



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:09 AM GMT

PDB ID : 4E5Y  
Title : Structure of human FX protein, the key enzyme in the biosynthesis of GDP-L-fucose  
Authors : Zhou, H.; He, J.H.  
Deposited on : 2012-03-15  
Resolution : 2.37 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

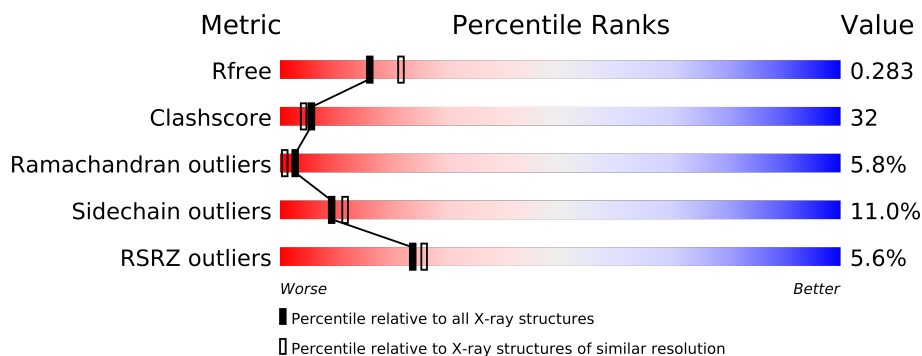
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.37 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))
$R_{free}$	66092	2963 (2.40-2.36)
Clashscore	79885	3668 (2.40-2.36)
Ramachandran outliers	78287	3600 (2.40-2.36)
Sidechain outliers	78261	3602 (2.40-2.36)
RSRZ outliers	66119	2966 (2.40-2.36)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	321	
1	B	321	
1	C	321	
1	D	321	

## 2 Entry composition i

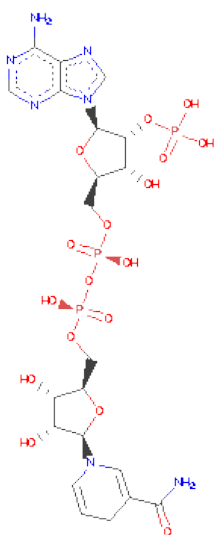
There are 3 unique types of molecules in this entry. The entry contains 9903 atoms, of which 0 are hydrogen and 0 are deuterium.

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-L-fucose synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2433	1555	418	450	10			
1	B	309	Total	C	N	O	S	0	0	0
			2452	1566	421	455	10			
1	C	290	Total	C	N	O	S	0	0	0
			2295	1462	392	431	10			
1	D	318	Total	C	N	O	S	0	0	0
			2509	1601	431	467	10			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (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		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 water.

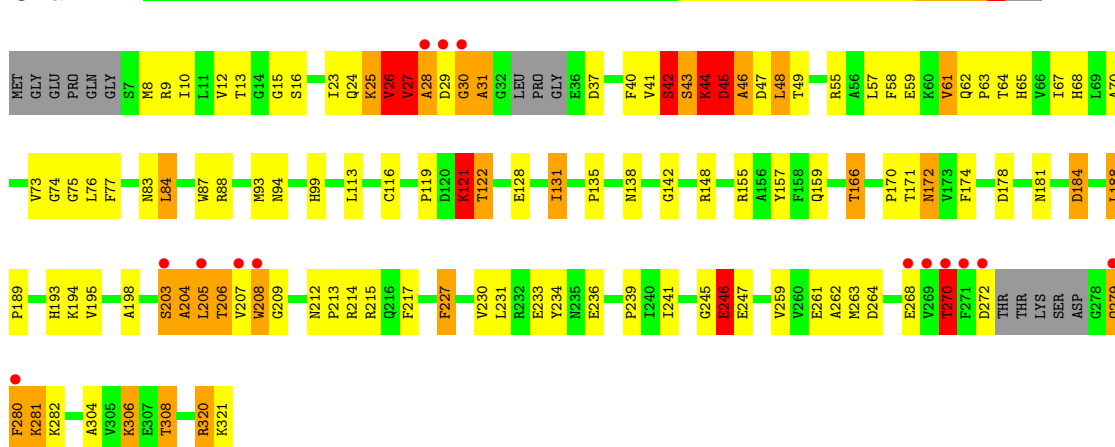
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	5	Total	O	0	0
			5	5		
3	C	6	Total	O	0	0
			6	6		
3	D	8	Total	O	0	0
			8	8		

### 3 Residue-property plots

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.

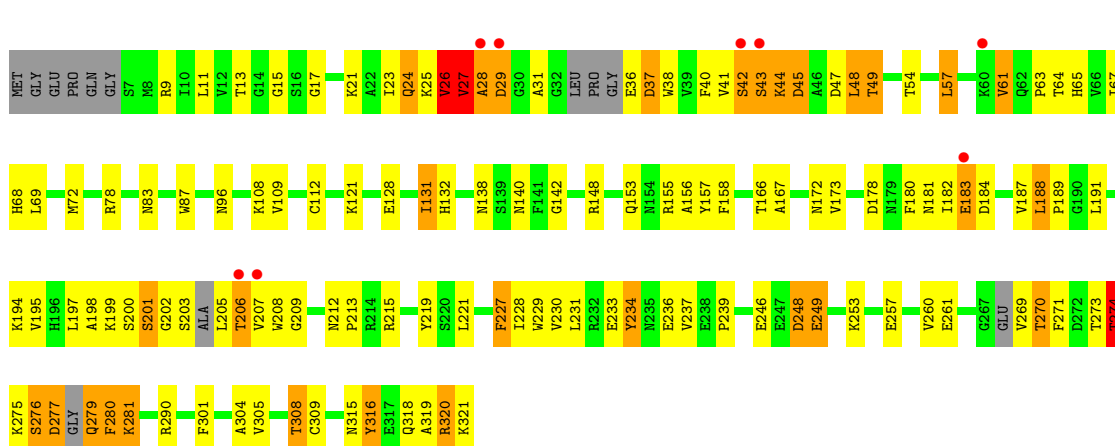
#### • Molecule 1: GDP-L-fucose synthase

Chain A:



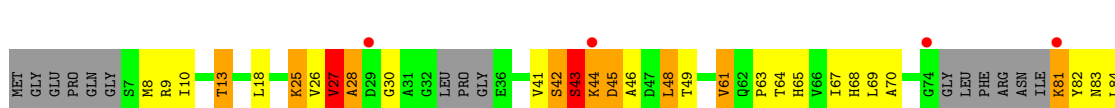
#### • Molecule 1: GDP-L-fucose synthase

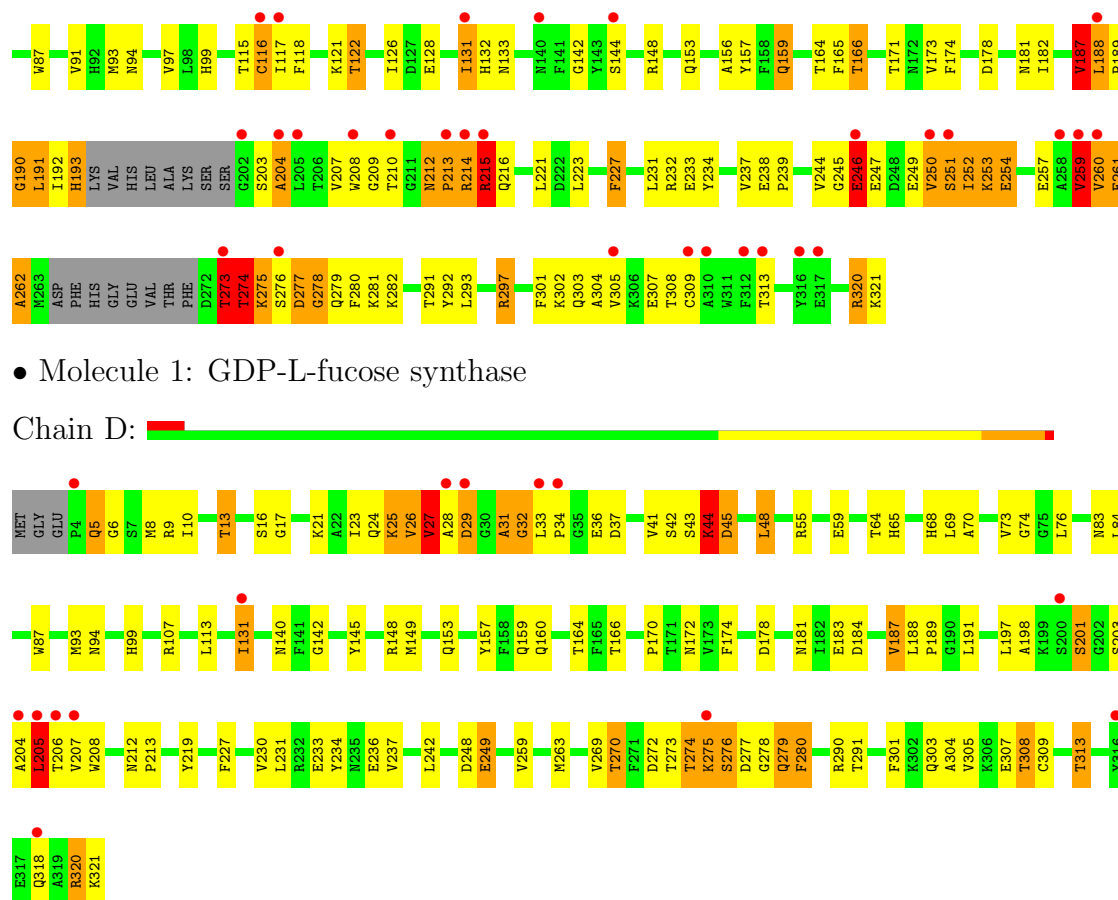
Chain B:



#### • Molecule 1: GDP-L-fucose synthase

Chain C:





• Molecule 1: GDP-L-fucose synthase

Chain D: ■ ■ ■ ■

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.77Å 136.44Å 139.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.27 – 2.37 39.27 – 2.37	Depositor EDS
% Data completeness (in resolution range)	93.6 (39.27-2.37) 92.6 (39.27-2.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.87 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, $R_{free}$	0.232 , 0.291 0.231 , 0.283	Depositor DCC
$R_{free}$ test set	1839 reflections (2.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 27.4	EDS
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 67181 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9903	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	0/2493	0.64	1/3379 (0.0%)
1	B	0.44	0/2510	0.58	0/3399
1	C	0.48	0/2348	0.69	2/3182 (0.1%)
1	D	0.47	0/2573	0.63	0/3491
All	All	0.46	0/9924	0.64	3/13451 (0.0%)

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
1	A	0	3
1	C	0	3
1	D	0	1
All	All	0	7

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	274	THR	N-CA-C	5.50	125.86	111.00
1	A	75	GLY	N-CA-C	-5.42	99.56	113.10
1	C	273	THR	N-CA-C	5.05	124.64	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	184	ASP	Peptide
1	A	42	SER	Peptide
1	A	44	LYS	Peptide
1	C	209	GLY	Peptide
1	C	273	THR	Peptide
1	C	43	SER	Peptide
1	D	44	LYS	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2433	0	2364	140	0
1	B	2452	0	2384	159	0
1	C	2295	0	2228	210	0
1	D	2509	0	2442	139	0
2	A	48	0	26	2	0
2	B	48	0	26	5	0
2	C	48	0	26	3	0
2	D	48	0	26	1	0
3	A	3	0	0	0	0
3	B	5	0	0	0	0
3	C	6	0	0	0	0
3	D	8	0	0	0	0
All	All	9903	0	9522	619	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

All (619) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:42:SER:HA	1:B:43:SER:O	1.39	1.20
1:A:64:THR:HG23	1:A:65:HIS:HD2	1.00	1.14
1:C:214:ARG:HG2	1:C:214:ARG:HH11	1.13	1.13
1:A:64:THR:HG23	1:A:65:HIS:CD2	1.85	1.11
1:C:64:THR:HG23	1:C:65:HIS:HD2	1.05	1.09

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:33:LEU:HG	1:D:34:PRO:HA	1.28	1.08
1:B:181:ASN:HD21	1:B:183:GLU:HG2	0.94	1.08
1:D:13:THR:HG21	1:D:68:HIS:HD2	1.18	1.03
1:C:64:THR:HG23	1:C:65:HIS:CD2	1.94	1.02
1:D:33:LEU:CG	1:D:34:PRO:HA	1.90	1.01
1:B:181:ASN:ND2	1:B:183:GLU:HG2	1.75	1.01
1:B:279:GLN:N	1:B:280:PHE:HA	1.74	1.00
1:B:26:VAL:HG12	1:B:27:VAL:HG22	1.44	1.00
1:A:27:VAL:HA	1:A:28:ALA:C	1.82	1.00
1:C:43:SER:HB2	1:C:45:ASP:HB2	1.41	0.99
1:C:13:THR:HG21	1:C:68:HIS:CD2	2.00	0.96
1:D:32:GLY:HA3	1:D:33:LEU:HD13	1.48	0.96
1:C:191:LEU:HB3	1:C:192:ILE:HG13	1.46	0.95
1:D:205:LEU:HA	1:D:206:THR:OG1	1.67	0.93
1:C:13:THR:HG21	1:C:68:HIS:HD2	1.29	0.93
1:C:249:GLU:O	1:C:250:VAL:HG22	1.69	0.93
1:A:121:LYS:CG	1:A:122:THR:H	1.80	0.93
1:C:187:VAL:O	1:C:188:LEU:HD13	1.67	0.93
1:A:64:THR:CG2	1:A:65:HIS:HD2	1.80	0.92
1:D:13:THR:HG21	1:D:68:HIS:CD2	2.04	0.92
1:C:9:ARG:H	1:C:64:THR:HG22	1.32	0.92
1:D:269:VAL:HG13	1:D:270:THR:H	1.35	0.91
1:D:181:ASN:HD21	1:D:183:GLU:HG2	1.33	0.91
1:C:13:THR:HG22	1:C:69:LEU:H	1.34	0.91
1:D:33:LEU:HD11	1:D:36:GLU:H	1.31	0.91
1:C:214:ARG:HG2	1:C:214:ARG:NH1	1.83	0.90
1:B:207:VAL:HG22	1:B:208:TRP:H	1.36	0.90
1:D:27:VAL:N	1:D:28:ALA:HB3	1.87	0.90
1:C:214:ARG:HA	1:C:215:ARG:CB	1.99	0.90
1:C:43:SER:CB	1:C:45:ASP:HB2	2.02	0.90
1:D:27:VAL:H	1:D:28:ALA:HB3	1.37	0.89
1:A:121:LYS:H	1:A:121:LYS:HZ3	1.19	0.88
1:A:61:VAL:HG22	1:A:63:PRO:HD3	1.56	0.88
1:B:158:PHE:HZ	1:C:273:THR:HG23	1.39	0.88
1:B:27:VAL:HA	1:B:28:ALA:O	1.74	0.87
1:B:166:THR:HG22	1:B:167:ALA:H	1.39	0.86
1:D:83:ASN:HD22	1:D:142:GLY:H	1.24	0.86
1:B:181:ASN:HD22	1:B:184:ASP:H	1.24	0.86
1:B:237:VAL:H	1:C:274:THR:HG21	1.39	0.85
1:C:212:ASN:N	1:C:213:PRO:HD3	1.90	0.85
1:C:249:GLU:HG3	1:C:250:VAL:HG13	1.58	0.84
1:A:166:THR:HG21	1:A:234:TYR:HE2	1.42	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:181:ASN:HD21	1:B:183:GLU:CG	1.87	0.83
1:C:208:TRP:HD1	1:C:277:ASP:HA	1.42	0.83
1:C:246:GLU:H	1:C:246:GLU:CD	1.79	0.83
1:C:116:CYS:HB2	1:C:282:LYS:NZ	1.94	0.83
1:A:194:LYS:HZ3	1:A:207:VAL:HG23	1.42	0.82
1:D:205:LEU:HB3	1:D:206:THR:O	1.80	0.82
1:C:116:CYS:HB2	1:C:282:LYS:HZ3	1.45	0.81
1:C:213:PRO:HA	1:C:214:ARG:HB3	1.61	0.81
1:C:27:VAL:HA	1:C:28:ALA:O	1.79	0.81
1:D:43:SER:OG	1:D:44:LYS:HA	1.80	0.81
1:A:121:LYS:HG3	1:A:122:THR:H	1.44	0.81
1:B:42:SER:HA	1:B:43:SER:C	1.99	0.81
1:B:269:VAL:HG13	1:B:270:THR:H	1.43	0.81
1:C:260:VAL:HG12	1:C:261:GLU:H	1.45	0.81
1:C:64:THR:CG2	1:C:65:HIS:HD2	1.93	0.80
1:B:158:PHE:CZ	1:C:273:THR:HG23	2.15	0.80
1:C:44:LYS:HA	1:C:46:ALA:N	1.96	0.80
1:D:26:VAL:O	1:D:27:VAL:HG22	1.83	0.79
1:D:83:ASN:ND2	1:D:142:GLY:H	1.79	0.79
1:A:121:LYS:HE3	1:A:135:PRO:HD2	1.64	0.79
1:D:31:ALA:C	1:D:33:LEU:HB2	2.03	0.78
1:D:248:ASP:O	1:D:249:GLU:HB2	1.83	0.78
1:D:181:ASN:ND2	1:D:184:ASP:H	1.81	0.78
1:B:276:SER:O	1:B:277:ASP:HB2	1.84	0.78
1:A:121:LYS:NZ	1:A:121:LYS:H	1.82	0.77
1:C:83:ASN:HB2	1:D:159:GLN:NE2	2.00	0.76
1:A:8:MET:HB2	1:A:64:THR:HG21	1.66	0.76
1:C:273:THR:OG1	1:C:274:THR:HG22	1.85	0.76
1:D:206:THR:HB	1:D:207:VAL:HA	1.68	0.76
1:B:237:VAL:HG22	1:C:274:THR:HG23	1.66	0.75
1:A:119:PRO:HB3	1:A:121:LYS:HE2	1.68	0.75
1:D:13:THR:HG22	1:D:70:ALA:H	1.51	0.75
1:C:259:VAL:HA	1:C:260:VAL:C	2.07	0.75
1:A:121:LYS:CG	1:A:122:THR:N	2.50	0.74
1:D:73:VAL:HG22	1:D:74:GLY:H	1.53	0.74
1:D:32:GLY:CA	1:D:33:LEU:HD13	2.18	0.74
1:C:131:ILE:HD12	1:C:148:ARG:HG2	1.70	0.74
1:C:208:TRP:CD1	1:C:277:ASP:HA	2.23	0.73
1:C:83:ASN:H	1:D:159:GLN:HE22	1.35	0.73
1:A:55:ARG:O	1:A:59:GLU:HG2	1.88	0.73
1:C:214:ARG:HA	1:C:215:ARG:HB2	1.68	0.73
1:C:191:LEU:HB3	1:C:192:ILE:CG1	2.18	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:279:GLN:N	1:B:280:PHE:CA	2.52	0.73
1:A:155:ARG:HH21	1:B:138:ASN:HD21	1.37	0.73
1:D:33:LEU:CD1	1:D:36:GLU:H	2.02	0.73
1:C:44:LYS:HA	1:C:46:ALA:H	1.54	0.73
1:A:43:SER:HB3	1:A:46:ALA:H	1.53	0.73
1:C:13:THR:CG2	1:C:70:ALA:H	2.02	0.72
1:B:24:GLN:O	1:B:25:LYS:HG3	1.90	0.72
1:B:27:VAL:HA	1:B:28:ALA:C	2.09	0.72
1:D:181:ASN:HD22	1:D:184:ASP:H	1.35	0.72
1:B:25:LYS:HA	1:B:27:VAL:H	1.52	0.72
1:C:13:THR:HG22	1:C:69:LEU:N	2.05	0.72
1:D:33:LEU:CD1	1:D:36:GLU:HB2	2.19	0.72
1:D:13:THR:CG2	1:D:70:ALA:H	2.02	0.72
1:B:207:VAL:HG22	1:B:208:TRP:N	2.03	0.71
1:C:257:GLU:C	1:C:259:VAL:H	1.93	0.71
1:B:248:ASP:O	1:B:249:GLU:HB3	1.91	0.71
1:B:24:GLN:C	1:B:25:LYS:HG3	2.11	0.70
1:B:269:VAL:HG13	1:B:270:THR:N	2.06	0.70
1:A:166:THR:HG23	1:A:236:GLU:O	1.91	0.70
1:C:212:ASN:O	1:C:212:ASN:ND2	2.25	0.70
1:C:42:SER:H	1:C:43:SER:HB3	1.55	0.70
1:C:42:SER:N	1:C:43:SER:HB3	2.06	0.70
1:B:273:THR:O	1:B:274:THR:HB	1.89	0.70
1:C:260:VAL:HG12	1:C:261:GLU:N	2.06	0.70
1:C:214:ARG:HB2	1:C:281:LYS:HA	1.73	0.70
1:B:43:SER:HA	2:B:401:NDP:O2X	1.92	0.70
1:A:138:ASN:HD21	1:B:155:ARG:HH21	1.38	0.70
1:D:73:VAL:HG23	1:D:76:LEU:HD22	1.73	0.70
1:D:32:GLY:HA3	1:D:33:LEU:CD1	2.22	0.70
1:A:43:SER:HB3	1:A:44:LYS:C	2.12	0.70
1:D:304:ALA:O	1:D:308:THR:HG23	1.91	0.69
1:A:215:ARG:HD3	1:A:279:GLN:HE22	1.57	0.69
1:A:27:VAL:HA	1:A:28:ALA:O	1.91	0.69
1:D:33:LEU:HD11	1:D:36:GLU:HB2	1.74	0.69
1:B:237:VAL:H	1:C:274:THR:CG2	2.05	0.69
1:C:83:ASN:ND2	1:C:142:GLY:H	1.91	0.69
1:C:42:SER:CA	1:C:43:SER:HB3	2.22	0.69
1:C:128:GLU:HG2	1:C:239:PRO:O	1.93	0.69
1:D:33:LEU:HD11	1:D:36:GLU:N	2.06	0.68
1:C:250:VAL:HB	1:C:251:SER:CB	2.23	0.68
1:C:9:ARG:H	1:C:64:THR:CG2	2.06	0.68
1:C:309:CYS:O	1:C:313:THR:HG23	1.94	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:181:ASN:ND2	1:B:184:ASP:H	1.90	0.68
1:A:204:ALA:O	1:A:205:LEU:HB2	1.94	0.68
1:A:23:ILE:O	1:A:26:VAL:HB	1.94	0.68
1:D:206:THR:CB	1:D:207:VAL:HA	2.24	0.68
1:D:269:VAL:HG13	1:D:270:THR:N	2.08	0.68
1:B:248:ASP:O	1:B:249:GLU:CB	2.41	0.68
1:C:61:VAL:O	1:C:63:PRO:HD3	1.94	0.68
1:D:279:GLN:N	1:D:280:PHE:HA	2.09	0.67
1:C:191:LEU:HB3	1:C:192:ILE:HA	1.75	0.67
1:C:203:SER:HB3	1:C:204:ALA:HB3	1.76	0.67
1:D:8:MET:O	1:D:36:GLU:O	2.12	0.67
1:C:70:ALA:HB1	1:C:93:MET:CE	2.24	0.67
1:C:203:SER:HA	1:C:204:ALA:HB3	1.75	0.67
1:B:29:ASP:OD2	1:B:31:ALA:HB2	1.95	0.67
1:A:178:ASP:O	1:A:320:ARG:HG3	1.95	0.67
1:B:9:ARG:HB2	1:B:9:ARG:NH1	2.10	0.67
1:B:178:ASP:O	1:B:320:ARG:HG3	1.94	0.66
1:D:248:ASP:O	1:D:249:GLU:CB	2.43	0.66
1:C:166:THR:HG21	1:C:234:TYR:HE2	1.59	0.66
1:B:9:ARG:HB2	1:B:9:ARG:CZ	2.25	0.66
1:A:194:LYS:HE2	1:A:206:THR:O	1.96	0.66
1:B:187:VAL:HG13	1:B:188:LEU:N	2.11	0.66
1:C:213:PRO:HB2	1:C:251:SER:HA	1.78	0.66
1:C:250:VAL:HB	1:C:251:SER:HB3	1.78	0.65
1:A:178:ASP:OD2	1:A:189:PRO:HG3	1.96	0.65
1:C:214:ARG:HD2	1:C:279:GLN:O	1.96	0.65
1:B:274:THR:HG22	1:B:275:LYS:HG2	1.77	0.65
1:C:245:GLY:C	1:C:247:GLU:H	2.00	0.65
1:A:279:GLN:HB2	1:A:281:LYS:N	2.11	0.65
1:D:36:GLU:O	1:D:37:ASP:HB3	1.96	0.65
1:A:194:LYS:NZ	1:A:207:VAL:HA	2.12	0.65
1:C:182:ILE:HD11	1:C:190:GLY:HA2	1.79	0.65
1:C:118:PHE:CE2	1:C:131:ILE:HG22	2.32	0.65
1:A:43:SER:HA	1:A:44:LYS:O	1.97	0.65
1:C:208:TRP:HA	1:C:276:SER:O	1.97	0.64
1:C:68:HIS:HE1	1:C:94:ASN:OD1	1.79	0.64
1:C:261:GLU:O	1:C:262:ALA:CB	2.46	0.64
1:D:74:GLY:C	1:D:76:LEU:H	2.00	0.64
1:D:17:GLY:O	1:D:21:LYS:HG2	1.97	0.64
1:C:181:ASN:ND2	1:C:321:LYS:HD3	2.12	0.64
1:B:215:ARG:HH22	1:B:279:GLN:N	1.96	0.64
1:C:203:SER:CA	1:C:204:ALA:HB3	2.28	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:197:LEU:O	1:D:201:SER:HB3	1.98	0.64
1:A:25:LYS:HA	1:A:26:VAL:HG12	1.80	0.64
1:A:23:ILE:O	1:A:25:LYS:N	2.31	0.64
1:D:73:VAL:HG23	1:D:76:LEU:CD2	2.28	0.64
1:B:206:THR:CB	1:B:207:VAL:HA	2.28	0.63
1:D:13:THR:HG22	1:D:69:LEU:H	1.63	0.63
1:C:278:GLY:HA2	1:C:279:GLN:C	2.19	0.63
1:C:188:LEU:HD12	1:C:189:PRO:HD3	1.80	0.63
1:D:205:LEU:HA	1:D:206:THR:CB	2.27	0.63
1:A:83:ASN:ND2	1:A:142:GLY:H	1.96	0.63
1:A:84:LEU:HD22	1:A:88:ARG:HG3	1.79	0.63
1:D:73:VAL:HG22	1:D:74:GLY:N	2.13	0.63
1:C:42:SER:HB2	1:C:43:SER:HA	1.79	0.63
1:C:273:THR:OG1	1:C:274:THR:N	2.31	0.63
1:A:67:ILE:HD11	1:A:231:LEU:HD22	1.79	0.62
1:C:304:ALA:O	1:C:308:THR:HG22	2.00	0.62
1:C:212:ASN:O	1:C:212:ASN:CG	2.38	0.62
1:C:83:ASN:HB2	1:D:159:GLN:HE21	1.61	0.62
1:C:48:LEU:HD22	2:C:401:NDP:H2A	1.81	0.62
1:D:272:ASP:OD1	1:D:274:THR:HB	1.99	0.62
1:C:67:ILE:HD11	1:C:231:LEU:HD22	1.81	0.62
1:B:237:VAL:N	1:C:274:THR:HG21	2.13	0.62
1:C:191:LEU:HB3	1:C:192:ILE:CA	2.29	0.62
1:D:206:THR:O	1:D:270:THR:O	2.17	0.62
1:A:8:MET:CB	1:A:64:THR:HG21	2.29	0.62
1:C:42:SER:OG	1:C:43:SER:HB3	1.99	0.61
1:B:253:LYS:HE3	1:B:257:GLU:OE2	2.00	0.61
1:C:208:TRP:HD1	1:C:277:ASP:CA	2.13	0.61
1:A:166:THR:HG21	1:A:234:TYR:CE2	2.31	0.61
1:B:212:ASN:N	1:B:213:PRO:HD2	2.15	0.61
1:D:28:ALA:O	1:D:29:ASP:HB2	1.99	0.61
1:C:25:LYS:HA	1:C:26:VAL:C	2.21	0.61
1:B:83:ASN:HD21	1:B:140:ASN:HA	1.65	0.61
1:B:207:VAL:CG2	1:B:208:TRP:H	2.10	0.61
1:A:215:ARG:HD3	1:A:279:GLN:NE2	2.15	0.61
1:A:73:VAL:HG23	1:A:76:LEU:HD22	1.81	0.61
1:A:159:GLN:NE2	1:B:83:ASN:H	1.98	0.61
1:D:13:THR:HG23	1:D:70:ALA:CB	2.31	0.61
1:A:279:GLN:H	1:A:280:PHE:HA	1.66	0.60
1:A:159:GLN:HE22	1:B:83:ASN:H	1.46	0.60
1:B:131:ILE:HD11	1:B:132:HIS:CE1	2.36	0.60
1:C:277:ASP:O	1:C:278:GLY:O	2.18	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:25:LYS:HA	1:B:27:VAL:N	2.15	0.60
1:D:33:LEU:HD12	1:D:34:PRO:C	2.21	0.60
1:A:48:LEU:HD22	2:A:401:NDP:H2A	1.83	0.60
1:C:203:SER:HA	1:C:204:ALA:CB	2.32	0.60
1:D:13:THR:HG23	1:D:70:ALA:HB2	1.82	0.60
1:A:26:VAL:O	1:A:26:VAL:HG13	2.02	0.60
1:B:25:LYS:N	1:B:26:VAL:HB	2.16	0.60
1:B:155:ARG:HD2	1:C:275:LYS:HE3	1.84	0.60
1:C:212:ASN:N	1:C:213:PRO:CD	2.64	0.60
1:A:23:ILE:C	1:A:25:LYS:H	2.04	0.60
1:C:26:VAL:O	1:C:27:VAL:HG13	2.01	0.60
1:C:13:THR:HG23	1:C:70:ALA:HB2	1.84	0.59
1:B:47:ASP:OD1	1:B:49:THR:HB	2.02	0.59
1:A:138:ASN:ND2	1:B:155:ARG:HH21	2.00	0.59
1:A:43:SER:HB3	1:A:45:ASP:HB3	1.83	0.59
1:C:252:ILE:C	1:C:254:GLU:H	2.04	0.59
1:D:178:ASP:OD2	1:D:189:PRO:HG3	2.02	0.59
1:B:207:VAL:O	1:B:271:PHE:O	2.19	0.58
1:A:43:SER:CB	1:A:45:ASP:HB3	2.32	0.58
1:B:194:LYS:HD2	1:B:206:THR:OG1	2.02	0.58
1:C:116:CYS:CB	1:C:282:LYS:NZ	2.64	0.58
1:C:214:ARG:HA	1:C:215:ARG:CG	2.32	0.58
1:C:116:CYS:CB	1:C:282:LYS:HZ2	2.16	0.58
1:C:70:ALA:HB1	1:C:93:MET:HE2	1.85	0.58
1:A:83:ASN:HD22	1:A:142:GLY:H	1.50	0.58
1:A:87:TRP:HZ3	1:B:153:GLN:NE2	2.01	0.58
1:B:206:THR:O	1:B:270:THR:O	2.22	0.58
1:B:199:LYS:C	1:B:201:SER:H	2.07	0.58
1:D:26:VAL:O	1:D:26:VAL:HG12	2.03	0.57
1:D:68:HIS:HE1	1:D:94:ASN:OD1	1.87	0.57
1:C:42:SER:CA	1:C:43:SER:CB	2.80	0.57
1:D:64:THR:OG1	1:D:65:HIS:HD2	1.87	0.57
1:D:70:ALA:C	1:D:93:MET:HE1	2.25	0.57
1:A:215:ARG:HD3	1:A:279:GLN:OE1	2.04	0.57
1:D:43:SER:HA	1:D:44:LYS:C	2.22	0.57
1:D:43:SER:HA	1:D:45:ASP:N	2.20	0.57
1:C:13:THR:HG23	1:C:70:ALA:CB	2.35	0.57
1:A:304:ALA:O	1:A:308:THR:HG23	2.05	0.57
1:B:208:TRP:CE3	1:B:275:LYS:HG3	2.40	0.56
1:A:87:TRP:HZ3	1:B:153:GLN:HE21	1.51	0.56
1:B:301:PHE:O	1:B:305:VAL:HG23	2.05	0.56
1:A:27:VAL:CA	1:A:28:ALA:C	2.66	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:203:SER:CB	1:C:204:ALA:HB3	2.35	0.56
1:B:304:ALA:O	1:B:308:THR:HG23	2.06	0.56
1:A:47:ASP:OD1	1:A:49:THR:HB	2.07	0.55
1:C:191:LEU:HB3	1:C:192:ILE:CB	2.35	0.55
1:C:166:THR:HG21	1:C:234:TYR:CE2	2.41	0.55
1:B:131:ILE:HD12	1:B:148:ARG:HG2	1.89	0.55
1:A:68:HIS:HE1	1:A:94:ASN:OD1	1.89	0.55
1:C:99:HIS:HD2	1:C:157:TYR:OH	1.89	0.55
1:A:43:SER:HB3	1:A:46:ALA:N	2.20	0.55
1:D:230:VAL:O	1:D:233:GLU:O	2.23	0.55
1:B:166:THR:HG22	1:B:167:ALA:N	2.16	0.55
1:D:99:HIS:HD2	1:D:157:TYR:OH	1.89	0.55
1:B:36:GLU:O	1:B:37:ASP:CB	2.54	0.55
1:D:301:PHE:O	1:D:305:VAL:HG23	2.07	0.55
1:D:83:ASN:HD22	1:D:142:GLY:N	2.00	0.55
1:C:116:CYS:HA	1:C:282:LYS:HD3	1.88	0.55
1:C:42:SER:CB	1:C:43:SER:HB3	2.37	0.55
1:C:13:THR:HG23	1:C:70:ALA:H	1.69	0.55
1:D:26:VAL:C	1:D:27:VAL:HG22	2.28	0.55
1:D:27:VAL:HA	1:D:28:ALA:C	2.27	0.55
1:D:33:LEU:HD13	1:D:36:GLU:HB2	1.89	0.54
1:B:230:VAL:O	1:B:233:GLU:O	2.25	0.54
1:B:191:LEU:HD21	1:B:207:VAL:HB	1.89	0.54
1:B:269:VAL:CG1	1:B:270:THR:H	2.17	0.54
1:D:23:ILE:O	1:D:25:LYS:N	2.41	0.54
1:B:15:GLY:N	1:B:42:SER:O	2.41	0.54
1:C:251:SER:O	1:C:253:LYS:N	2.41	0.54
1:D:269:VAL:CG1	1:D:270:THR:H	2.16	0.54
1:A:10:ILE:HG12	1:A:231:LEU:HD21	1.88	0.54
1:C:254:GLU:CA	1:C:254:GLU:OE1	2.56	0.54
1:C:214:ARG:HB2	1:C:280:PHE:O	2.08	0.54
1:A:15:GLY:N	1:A:42:SER:OG	2.41	0.54
1:B:273:THR:O	1:B:274:THR:CB	2.57	0.53
1:A:58:PHE:O	1:A:61:VAL:O	2.26	0.53
1:B:112:CYS:SG	1:B:227:PHE:HZ	2.30	0.53
1:B:128:GLU:HG2	1:B:239:PRO:O	2.08	0.53
1:C:303:GLN:O	1:C:307:GLU:HG3	2.08	0.53
1:C:8:MET:HB2	1:C:64:THR:HG21	1.89	0.53
1:D:204:ALA:O	1:D:205:LEU:HB2	2.08	0.53
1:C:181:ASN:HD22	1:C:321:LYS:HD3	1.72	0.53
1:A:48:LEU:HD22	2:A:401:NDP:C2A	2.37	0.53
1:B:48:LEU:HD22	2:B:401:NDP:C2A	2.38	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:159:GLN:HE21	1:B:83:ASN:HB2	1.73	0.53
1:B:45:ASP:C	1:B:45:ASP:OD1	2.45	0.53
1:C:276:SER:OG	1:C:277:ASP:N	2.42	0.53
1:A:246:GLU:CD	1:A:246:GLU:H	2.11	0.53
1:C:257:GLU:H	1:C:257:GLU:CD	2.12	0.53
1:C:249:GLU:O	1:C:250:VAL:CG2	2.52	0.53
1:A:194:LYS:HZ1	1:A:207:VAL:HA	1.72	0.53
1:B:131:ILE:CD1	1:B:148:ARG:HG2	2.39	0.53
1:D:26:VAL:O	1:D:26:VAL:CG1	2.56	0.53
1:C:10:ILE:N	1:C:10:ILE:HD12	2.24	0.53
1:B:206:THR:HB	1:B:207:VAL:HA	1.91	0.52
1:A:99:HIS:HD2	1:A:157:TYR:OH	1.91	0.52
1:C:252:ILE:C	1:C:254:GLU:N	2.60	0.52
1:D:23:ILE:C	1:D:25:LYS:H	2.12	0.52
1:C:164:THR:HG22	1:C:164:THR:O	2.09	0.52
1:B:202:GLY:O	1:B:203:SER:C	2.47	0.52
1:D:33:LEU:CD1	1:D:34:PRO:HA	2.38	0.52
1:A:16:SER:N	1:A:42:SER:OG	2.41	0.52
1:A:279:GLN:HG3	1:A:280:PHE:C	2.30	0.52
1:A:304:ALA:O	1:A:308:THR:CG2	2.58	0.52
1:A:194:LYS:NZ	1:A:207:VAL:HG23	2.18	0.52
1:C:189:PRO:O	1:C:190:GLY:C	2.47	0.52
1:A:116:CYS:HB3	1:A:282:LYS:NZ	2.24	0.52
1:A:230:VAL:O	1:A:233:GLU:O	2.27	0.52
1:C:276:SER:O	1:C:277:ASP:HB3	2.10	0.52
1:D:198:ALA:HB2	1:D:204:ALA:HB3	1.92	0.52
1:A:113:LEU:O	1:A:170:PRO:HD2	2.10	0.52
1:A:26:VAL:C	1:A:27:VAL:HG22	2.29	0.51
1:D:303:GLN:O	1:D:307:GLU:HG3	2.11	0.51
1:C:254:GLU:HA	1:C:254:GLU:OE1	2.09	0.51
1:D:32:GLY:N	1:D:33:LEU:HB2	2.24	0.51
1:C:187:VAL:C	1:C:188:LEU:HD13	2.29	0.51
1:C:261:GLU:O	1:C:262:ALA:HB3	2.10	0.51
1:C:42:SER:CB	1:C:43:SER:CA	2.88	0.51
1:A:205:LEU:CB	1:A:206:THR:HA	2.39	0.51
1:A:131:ILE:CD1	1:A:148:ARG:HG2	2.40	0.51
1:C:213:PRO:HB3	1:C:252:ILE:HG12	1.92	0.51
1:D:206:THR:HG22	1:D:208:TRP:CH2	2.45	0.51
1:A:121:LYS:HG2	1:A:122:THR:N	2.26	0.51
1:A:8:MET:HB2	1:A:64:THR:CG2	2.40	0.50
1:C:131:ILE:HD11	1:C:132:HIS:CE1	2.46	0.50
1:D:31:ALA:O	1:D:33:LEU:HB2	2.10	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:26:VAL:O	1:B:29:ASP:HA	2.10	0.50
1:A:84:LEU:HA	1:B:156:ALA:HB1	1.93	0.50
1:B:83:ASN:ND2	1:B:142:GLY:H	2.10	0.50
1:B:195:VAL:O	1:B:198:ALA:HB3	2.12	0.50
1:B:27:VAL:CA	1:B:28:ALA:C	2.77	0.50
1:A:203:SER:O	1:A:204:ALA:HB3	2.11	0.50
1:B:57:LEU:HD12	1:B:57:LEU:O	2.12	0.50
1:A:23:ILE:C	1:A:25:LYS:N	2.64	0.50
1:A:204:ALA:O	1:A:205:LEU:HD13	2.11	0.50
1:D:43:SER:HA	1:D:45:ASP:H	1.76	0.50
1:C:203:SER:CA	1:C:204:ALA:CB	2.90	0.50
1:C:245:GLY:C	1:C:247:GLU:N	2.64	0.50
1:D:32:GLY:N	1:D:33:LEU:HD13	2.27	0.49
1:C:171:THR:HB	1:C:216:GLN:O	2.11	0.49
1:C:68:HIS:CD2	1:C:97:VAL:HG11	2.48	0.49
1:A:188:LEU:HB3	1:A:189:PRO:HD3	1.93	0.49
1:A:214:ARG:HH11	1:A:214:ARG:HG2	1.77	0.49
1:D:273:THR:HG22	1:D:273:THR:O	2.12	0.49
1:B:43:SER:C	1:B:45:ASP:H	2.16	0.49
1:D:10:ILE:HG12	1:D:231:LEU:HD21	1.94	0.49
1:A:16:SER:OG	1:A:42:SER:HB3	2.11	0.49
1:C:42:SER:HB2	1:C:43:SER:CA	2.42	0.49
1:B:194:LYS:HD2	1:B:206:THR:HG1	1.77	0.49
1:B:205:LEU:HB3	1:B:269:VAL:O	2.13	0.49
1:B:173:VAL:HG23	2:B:401:NDP:H42N	1.94	0.49
1:B:23:ILE:C	1:B:25:LYS:H	2.15	0.49
1:C:216:GLN:HG3	1:C:249:GLU:CB	2.43	0.49
1:B:23:ILE:HG22	1:B:40:PHE:HZ	1.78	0.49
1:C:99:HIS:CD2	1:C:157:TYR:OH	2.65	0.49
1:C:207:VAL:O	1:C:208:TRP:HB2	2.12	0.49
1:A:279:GLN:N	1:A:280:PHE:HA	2.27	0.49
1:D:145:TYR:O	1:D:149:MET:HG2	2.12	0.49
1:C:65:HIS:HB3	1:C:231:LEU:HD11	1.95	0.49
1:C:259:VAL:HA	1:C:260:VAL:O	2.11	0.49
1:C:214:ARG:HA	1:C:215:ARG:HG3	1.95	0.49
1:D:74:GLY:C	1:D:76:LEU:N	2.66	0.49
1:C:193:HIS:ND1	1:C:193:HIS:N	2.59	0.49
1:B:65:HIS:HB3	1:B:231:LEU:HD11	1.95	0.49
1:A:77:PHE:HB2	1:A:184:ASP:O	2.13	0.49
1:B:199:LYS:O	1:B:201:SER:N	2.46	0.48
1:D:113:LEU:O	1:D:170:PRO:HD2	2.12	0.48
1:B:279:GLN:HA	1:B:279:GLN:OE1	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:233:GLU:O	1:A:234:TYR:HB3	2.13	0.48
1:B:23:ILE:O	1:B:25:LYS:N	2.42	0.48
1:A:212:ASN:N	1:A:213:PRO:CD	2.76	0.48
1:B:41:VAL:HG13	1:B:42:SER:HB2	1.95	0.48
1:A:9:ARG:O	1:A:64:THR:HG22	2.13	0.48
1:B:23:ILE:HG22	1:B:40:PHE:CZ	2.49	0.48
1:B:209:GLY:O	1:B:271:PHE:HB3	2.14	0.48
1:B:305:VAL:HG12	1:B:309:CYS:SG	2.54	0.48
1:C:207:VAL:O	1:C:208:TRP:CE3	2.66	0.48
1:C:215:ARG:HD2	1:C:216:GLN:OE1	2.14	0.48
1:B:25:LYS:CA	1:B:27:VAL:H	2.25	0.48
1:D:204:ALA:O	1:D:205:LEU:HD12	2.14	0.48
1:B:41:VAL:HG22	1:B:42:SER:N	2.29	0.47
1:C:252:ILE:O	1:C:254:GLU:N	2.47	0.47
1:A:207:VAL:O	1:A:208:TRP:CD1	2.67	0.47
1:C:48:LEU:HD22	2:C:401:NDP:C2A	2.43	0.47
1:B:26:VAL:O	1:B:27:VAL:HG13	2.15	0.47
1:D:73:VAL:CG2	1:D:74:GLY:H	2.24	0.47
1:A:209:GLY:H	1:A:272:ASP:C	2.17	0.47
1:C:257:GLU:C	1:C:259:VAL:N	2.62	0.47
1:B:320:ARG:HG2	1:B:320:ARG:H	1.54	0.47
1:B:187:VAL:CG1	1:B:188:LEU:N	2.77	0.47
1:B:67:ILE:HD11	1:B:231:LEU:HD22	1.96	0.47
1:C:44:LYS:HB3	1:C:44:LYS:HE3	1.70	0.47
1:A:43:SER:HB2	1:A:46:ALA:O	2.14	0.47
1:C:244:VAL:HG22	1:C:245:GLY:H	1.79	0.47
1:D:178:ASP:O	1:D:320:ARG:HG3	2.14	0.47
1:D:99:HIS:CD2	1:D:157:TYR:OH	2.67	0.47
1:B:112:CYS:HG	1:B:227:PHE:HZ	1.61	0.47
1:C:214:ARG:CG	1:C:214:ARG:HH11	2.00	0.47
1:B:205:LEU:HA	1:B:206:THR:OG1	2.15	0.47
1:B:166:THR:HG21	1:B:234:TYR:HE2	1.80	0.47
1:B:304:ALA:O	1:B:308:THR:CG2	2.62	0.47
1:A:9:ARG:HD3	1:A:37:ASP:OD2	2.15	0.47
1:D:32:GLY:HA2	1:D:36:GLU:CD	2.35	0.47
1:C:191:LEU:CB	1:C:192:ILE:HA	2.44	0.47
1:D:205:LEU:CB	1:D:206:THR:O	2.58	0.47
1:B:212:ASN:HB2	1:D:291:THR:OG1	2.15	0.47
1:B:64:THR:OG1	1:B:65:HIS:HD2	1.97	0.47
1:C:83:ASN:H	1:D:159:GLN:NE2	2.10	0.47
1:B:319:ALA:O	1:B:321:LYS:HG3	2.15	0.47
1:D:36:GLU:O	1:D:37:ASP:CB	2.58	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:219:TYR:CZ	1:B:221:LEU:HD23	2.50	0.46
1:C:156:ALA:HB1	1:D:84:LEU:CA	2.45	0.46
1:C:8:MET:HB2	1:C:64:THR:CG2	2.45	0.46
1:A:172:ASN:C	1:A:172:ASN:HD22	2.19	0.46
1:D:275:LYS:CG	1:D:276:SER:H	2.28	0.46
1:A:28:ALA:O	1:A:29:ASP:HB2	2.15	0.46
1:B:206:THR:CB	1:B:207:VAL:CA	2.93	0.46
1:C:27:VAL:HA	1:C:28:ALA:C	2.36	0.46
1:D:259:VAL:O	1:D:263:MET:HG3	2.15	0.46
1:D:33:LEU:HD12	1:D:33:LEU:HA	1.47	0.46
1:D:70:ALA:O	1:D:93:MET:HE1	2.15	0.46
1:C:215:ARG:HB3	1:C:216:GLN:H	1.33	0.46
1:C:181:ASN:HA	1:C:321:LYS:HG2	1.97	0.46
1:A:9:ARG:H	1:A:64:THR:HG22	1.81	0.46
1:C:207:VAL:O	1:C:208:TRP:CB	2.62	0.46
1:A:29:ASP:OD2	1:A:31:ALA:HB2	2.16	0.46
1:A:207:VAL:O	1:A:208:TRP:CG	2.68	0.46
1:B:61:VAL:HG22	1:B:63:PRO:HD3	1.97	0.46
1:C:292:TYR:O	1:C:293:LEU:HD23	2.16	0.46
1:D:8:MET:HG3	1:D:65:HIS:CD2	2.50	0.46
1:C:257:GLU:N	1:C:257:GLU:CD	2.69	0.46
1:C:182:ILE:HD11	1:C:190:GLY:CA	2.45	0.45
1:A:99:HIS:CD2	1:A:157:TYR:OH	2.68	0.45
1:D:275:LYS:O	1:D:276:SER:HB3	2.16	0.45
1:D:55:ARG:O	1:D:59:GLU:HG2	2.16	0.45
1:C:214:ARG:CG	1:C:214:ARG:NH1	2.62	0.45
1:B:206:THR:OG1	1:B:207:VAL:HA	2.17	0.45
1:C:210:THR:HG22	1:C:253:LYS:HG3	1.99	0.45
1:A:26:VAL:O	1:A:27:VAL:HG22	2.16	0.45
1:D:206:THR:CB	1:D:207:VAL:CA	2.94	0.45
1:C:221:LEU:HD13	1:C:221:LEU:HA	1.71	0.45
1:D:174:PHE:CG	1:D:188:LEU:HD23	2.52	0.45
1:D:48:LEU:HB3	1:D:93:MET:HG2	1.97	0.45
1:B:236:GLU:HA	1:C:274:THR:HG21	1.98	0.45
1:A:42:SER:C	1:A:43:SER:OG	2.53	0.45
1:A:320:ARG:H	1:A:320:ARG:HG2	1.56	0.45
1:D:8:MET:HG2	1:D:10:ILE:HD11	1.98	0.45
1:C:118:PHE:CG	1:C:126:ILE:HD12	2.52	0.45
1:B:205:LEU:N	1:B:205:LEU:HD23	2.32	0.45
1:B:194:LYS:HD3	1:B:206:THR:HG21	1.99	0.45
1:C:131:ILE:O	1:C:132:HIS:HB2	2.17	0.45
1:C:164:THR:O	1:C:165:PHE:HD1	2.00	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:9:ARG:H	1:A:64:THR:CG2	2.30	0.44
1:D:83:ASN:HD21	1:D:140:ASN:HA	1.83	0.44
1:D:212:ASN:N	1:D:213:PRO:CD	2.80	0.44
1:D:33:LEU:CB	1:D:34:PRO:HA	2.42	0.44
1:A:207:VAL:C	1:A:208:TRP:CG	2.90	0.44
1:A:155:ARG:HH21	1:B:138:ASN:ND2	2.10	0.44
1:D:290:ARG:HA	1:D:290:ARG:HD3	1.73	0.44
1:B:290:ARG:HD3	1:B:290:ARG:HA	1.74	0.44
1:D:5:GLN:HA	1:D:6:GLY:HA3	1.80	0.44
1:D:198:ALA:HB2	1:D:204:ALA:CB	2.46	0.44
1:D:25:LYS:HA	1:D:26:VAL:C	2.37	0.44
1:C:27:VAL:CA	1:C:28:ALA:O	2.59	0.44
1:B:108:LYS:HG2	1:B:109:VAL:N	2.32	0.44
1:C:70:ALA:CB	1:C:93:MET:HE2	2.48	0.44
1:B:131:ILE:HG13	1:B:132:HIS:CD2	2.53	0.44
1:C:87:TRP:CE2	1:C:91:VAL:HG21	2.53	0.44
1:C:213:PRO:HA	1:C:214:ARG:CB	2.30	0.44
1:A:205:LEU:HB3	1:A:206:THR:HA	1.99	0.44
1:C:173:VAL:HG23	2:C:401:NDP:H42N	1.99	0.44
1:B:212:ASN:N	1:B:213:PRO:CD	2.81	0.44
1:A:174:PHE:CE1	1:A:217:PHE:HB3	2.53	0.44
1:A:245:GLY:C	1:A:247:GLU:H	2.21	0.44
1:C:275:LYS:HA	1:C:276:SER:HA	1.63	0.44
1:D:204:ALA:O	1:D:205:LEU:CB	2.66	0.44
1:A:204:ALA:O	1:A:205:LEU:CB	2.63	0.44
1:B:9:ARG:CB	1:B:9:ARG:CZ	2.95	0.44
1:D:33:LEU:HD11	1:D:36:GLU:CB	2.44	0.44
1:D:13:THR:HG22	1:D:69:LEU:N	2.31	0.44
1:B:54:THR:HG21	1:B:96:ASN:HB3	1.99	0.44
1:B:48:LEU:HD22	2:B:401:NDP:H2A	1.98	0.44
1:B:38:TRP:HB3	1:B:40:PHE:CE1	2.52	0.44
1:C:115:THR:OG1	1:C:215:ARG:NH1	2.51	0.43
1:A:70:ALA:HB1	1:A:93:MET:HE1	1.98	0.43
1:C:121:LYS:O	1:C:122:THR:O	2.36	0.43
1:D:93:MET:HB3	1:D:93:MET:HE3	1.71	0.43
1:C:173:VAL:HG12	1:C:174:PHE:N	2.34	0.43
1:B:131:ILE:HG13	1:B:132:HIS:N	2.31	0.43
1:C:215:ARG:HD3	1:C:282:LYS:C	2.38	0.43
1:B:205:LEU:HA	1:B:206:THR:C	2.38	0.43
1:A:84:LEU:HD11	1:B:157:TYR:CE1	2.53	0.43
1:A:128:GLU:HG3	1:A:241:ILE:HG13	2.00	0.43
1:B:173:VAL:H	2:B:401:NDP:H71N	1.66	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:43:SER:OG	1:C:45:ASP:HB2	2.19	0.43
1:C:188:LEU:HD12	1:C:189:PRO:CD	2.46	0.43
1:C:223:LEU:O	1:C:227:PHE:HB2	2.18	0.43
1:A:215:ARG:HD3	1:A:279:GLN:CD	2.38	0.43
1:A:116:CYS:CB	1:A:282:LYS:NZ	2.82	0.43
1:C:26:VAL:O	1:C:26:VAL:HG12	2.18	0.43
1:A:87:TRP:CZ3	1:B:153:GLN:HG2	2.53	0.43
1:C:215:ARG:HD3	1:C:282:LYS:HG3	2.01	0.43
1:B:78:ARG:HH11	1:B:183:GLU:HB2	1.84	0.43
1:C:26:VAL:O	1:C:27:VAL:HG22	2.19	0.43
1:D:277:ASP:HB3	1:D:278:GLY:H	1.68	0.43
1:C:117:ILE:HG22	1:C:144:SER:HA	1.99	0.43
1:B:315:ASN:O	1:B:316:TYR:C	2.57	0.43
1:C:260:VAL:CG1	1:C:261:GLU:N	2.77	0.43
1:C:43:SER:OG	1:C:45:ASP:CB	2.67	0.43
1:D:207:VAL:HG22	1:D:208:TRP:N	2.34	0.43
1:D:164:THR:O	1:D:164:THR:HG22	2.18	0.43
1:B:17:GLY:O	1:B:21:LYS:HG2	2.19	0.43
1:C:191:LEU:CB	1:C:192:ILE:CA	2.97	0.42
1:B:182:ILE:HD12	1:B:194:LYS:HG3	2.01	0.42
1:B:233:GLU:HB3	1:B:234:TYR:H	1.74	0.42
1:C:41:VAL:HG13	1:C:45:ASP:HB3	2.02	0.42
1:C:30:GLY:HA2	1:C:232:ARG:HH22	1.83	0.42
1:B:24:GLN:HG2	1:B:40:PHE:CE2	2.54	0.42
1:C:188:LEU:HB3	1:C:189:PRO:HD2	2.00	0.42
1:B:206:THR:HA	1:B:207:VAL:O	2.20	0.42
1:A:280:PHE:CD2	1:A:280:PHE:C	2.92	0.42
1:A:74:GLY:H	1:A:76:LEU:HB2	1.84	0.42
1:C:238:GLU:HG3	1:C:239:PRO:HD2	2.02	0.42
1:D:275:LYS:O	1:D:276:SER:CB	2.68	0.42
1:B:281:LYS:HG2	1:B:281:LYS:O	2.18	0.42
1:D:191:LEU:HD21	1:D:207:VAL:CG2	2.50	0.42
1:C:178:ASP:O	1:C:320:ARG:HG3	2.19	0.42
1:B:41:VAL:HG22	1:B:42:SER:H	1.82	0.42
1:C:81:LYS:C	1:C:82:TYR:CD2	2.93	0.42
1:C:82:TYR:CD2	1:C:82:TYR:N	2.86	0.42
1:A:9:ARG:N	1:A:64:THR:HG22	2.35	0.42
1:C:131:ILE:HG13	1:C:132:HIS:N	2.33	0.42
1:C:81:LYS:C	1:C:82:TYR:HD2	2.23	0.42
1:B:44:LYS:HB3	1:B:44:LYS:HE2	1.90	0.42
1:C:131:ILE:HG13	1:C:132:HIS:CG	2.55	0.42
1:C:10:ILE:HD12	1:C:10:ILE:H	1.83	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:128:GLU:HG2	1:A:239:PRO:O	2.20	0.42
1:D:269:VAL:CG1	1:D:270:THR:N	2.79	0.42
1:C:84:LEU:HB3	1:D:160:GLN:OE1	2.19	0.42
1:C:9:ARG:N	1:C:64:THR:HG22	2.16	0.42
1:A:121:LYS:O	1:A:122:THR:HG22	2.18	0.42
1:D:28:ALA:O	1:D:29:ASP:CB	2.68	0.42
1:D:234:TYR:CZ	1:D:236:GLU:HB2	2.55	0.42
1:A:8:MET:CA	1:A:64:THR:HG21	2.49	0.41
1:C:187:VAL:O	1:C:187:VAL:HG22	2.19	0.41
1:A:87:TRP:CZ3	1:B:153:GLN:CG	3.04	0.41
1:C:18:LEU:HD22	1:C:178:ASP:OD1	2.19	0.41
1:D:131:ILE:HD12	1:D:148:ARG:HG2	2.00	0.41
1:D:31:ALA:O	1:D:32:GLY:C	2.58	0.41
1:B:276:SER:OG	1:B:277:ASP:N	2.53	0.41
1:B:180:PHE:HB2	1:B:320:ARG:O	2.20	0.41
1:B:87:TRP:HD1	1:B:142:GLY:O	2.03	0.41
1:B:13:THR:OG1	1:B:68:HIS:HD2	2.04	0.41
1:C:153:GLN:HG2	1:D:87:TRP:CZ3	2.54	0.41
1:A:57:LEU:O	1:A:61:VAL:HG13	2.20	0.41
1:C:18:LEU:HD22	1:C:178:ASP:CG	2.40	0.41
1:A:198:ALA:CB	1:A:204:ALA:HB3	2.50	0.41
1:C:301:PHE:O	1:C:305:VAL:HG23	2.21	0.41
1:D:187:VAL:O	1:D:191:LEU:HG	2.20	0.41
1:B:205:LEU:CD1	1:B:269:VAL:HA	2.51	0.41
1:C:260:VAL:CG1	1:C:261:GLU:H	2.20	0.41
1:B:13:THR:HG1	1:B:68:HIS:HA	1.85	0.41
1:A:181:ASN:HB2	1:A:321:LYS:HB3	2.01	0.41
1:A:195:VAL:HG21	1:A:259:VAL:HG12	2.01	0.41
1:C:131:ILE:HG13	1:C:132:HIS:CD2	2.56	0.41
1:B:188:LEU:HB3	1:B:189:PRO:HD3	2.03	0.41
1:B:41:VAL:O	1:B:42:SER:O	2.38	0.41
1:A:9:ARG:HH21	1:A:62:GLN:HB2	1.85	0.41
1:A:13:THR:HG1	1:A:70:ALA:H	1.68	0.41
1:B:11:LEU:HD11	1:B:41:VAL:CG1	2.50	0.41
1:C:216:GLN:HG3	1:C:249:GLU:HB3	2.03	0.41
1:B:280:PHE:C	1:B:280:PHE:CD2	2.94	0.41
1:D:206:THR:HG22	1:D:208:TRP:CZ3	2.55	0.41
1:A:45:ASP:O	1:A:46:ALA:HB2	2.21	0.41
1:B:198:ALA:HA	1:B:203:SER:O	2.21	0.41
1:D:170:PRO:HA	1:D:242:LEU:O	2.20	0.41
1:B:228:ILE:HG22	1:B:229:TRP:N	2.35	0.41
1:A:203:SER:O	1:A:204:ALA:CB	2.69	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:25:LYS:CD	1:C:25:LYS:N	2.84	0.41
1:A:259:VAL:O	1:A:263:MET:HG3	2.21	0.41
1:D:309:CYS:O	1:D:313:THR:HG23	2.20	0.41
1:C:8:MET:CB	1:C:64:THR:HG21	2.51	0.40
1:A:44:LYS:HA	1:A:46:ALA:H	1.86	0.40
1:C:254:GLU:N	1:C:254:GLU:OE1	2.54	0.40
1:A:30:GLY:O	1:A:31:ALA:HB3	2.21	0.40
1:C:42:SER:N	1:C:43:SER:CB	2.80	0.40
1:C:42:SER:CB	1:C:43:SER:HA	2.46	0.40
1:D:25:LYS:HA	1:D:27:VAL:N	2.37	0.40
1:B:166:THR:CG2	1:B:167:ALA:H	2.19	0.40
1:A:214:ARG:NH1	1:A:214:ARG:HG2	2.36	0.40
1:B:13:THR:O	1:B:69:LEU:HB2	2.21	0.40
1:D:16:SER:OG	2:D:401:NDP:O3B	2.28	0.40
1:C:159:GLN:HE21	1:C:159:GLN:HB3	1.70	0.40
1:A:262:ALA:O	1:A:306:LYS:HE3	2.21	0.40
1:B:78:ARG:NH1	1:B:183:GLU:HB2	2.37	0.40
1:B:24:GLN:O	1:B:25:LYS:CG	2.63	0.40
1:D:205:LEU:HB3	1:D:206:THR:C	2.41	0.40
1:D:219:TYR:HE1	1:D:308:THR:HG22	1.86	0.40
1:A:12:VAL:HG21	1:A:40:PHE:CE2	2.56	0.40
1:A:166:THR:CG2	1:A:236:GLU:O	2.66	0.40
1:A:67:ILE:HG23	1:A:227:PHE:CE1	2.56	0.40
1:C:297:ARG:HD3	1:C:297:ARG:HA	1.62	0.40
1:D:321:LYS:HB2	1:D:321:LYS:HE3	1.89	0.40
1:A:268:GLU:OE1	1:A:270:THR:HG22	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	301/321 (94%)	265 (88%)	17 (6%)	19 (6%)	2 1
1	B	299/321 (93%)	252 (84%)	31 (10%)	16 (5%)	3 1

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	280/321 (87%)	221 (79%)	37 (13%)	22 (8%)	1	0
1	D	316/321 (98%)	270 (85%)	34 (11%)	12 (4%)	5	3
All	All	1196/1284 (93%)	1008 (84%)	119 (10%)	69 (6%)	3	1

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	26	VAL
1	A	27	VAL
1	A	28	ALA
1	A	44	LYS
1	A	121	LYS
1	A	122	THR
1	A	203	SER
1	A	204	ALA
1	A	205	LEU
1	B	28	ALA
1	B	37	ASP
1	B	43	SER
1	B	276	SER
1	C	27	VAL
1	C	28	ALA
1	C	43	SER
1	C	122	THR
1	C	213	PRO
1	C	215	ARG
1	C	259	VAL
1	C	262	ALA
1	C	275	LYS
1	C	277	ASP
1	D	27	VAL
1	D	29	ASP
1	D	249	GLU
1	D	275	LYS
1	A	31	ALA
1	A	45	ASP
1	A	46	ALA
1	A	270	THR
1	B	24	GLN
1	B	27	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	200	SER
1	B	201	SER
1	B	234	TYR
1	B	249	GLU
1	B	274	THR
1	C	191	LEU
1	C	204	ALA
1	C	250	VAL
1	C	252	ILE
1	C	253	LYS
1	C	260	VAL
1	C	278	GLY
1	D	24	GLN
1	D	31	ALA
1	D	32	GLY
1	D	203	SER
1	D	276	SER
1	A	208	TRP
1	B	44	LYS
1	C	246	GLU
1	D	26	VAL
1	A	42	SER
1	A	246	GLU
1	B	26	VAL
1	B	42	SER
1	B	316	TYR
1	C	45	ASP
1	D	270	THR
1	A	171	THR
1	B	270	THR
1	C	133	ASN
1	C	187	VAL
1	D	205	LEU
1	C	190	GLY
1	A	30	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/273 (96%)	234 (90%)	27 (10%)	10	14
1	B	265/273 (97%)	236 (89%)	29 (11%)	9	12
1	C	248/273 (91%)	216 (87%)	32 (13%)	6	7
1	D	270/273 (99%)	243 (90%)	27 (10%)	11	15
All	All	1044/1092 (96%)	929 (89%)	115 (11%)	9	11

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	26	VAL
1	A	27	VAL
1	A	41	VAL
1	A	43	SER
1	A	45	ASP
1	A	48	LEU
1	A	61	VAL
1	A	84	LEU
1	A	121	LYS
1	A	131	ILE
1	A	166	THR
1	A	172	ASN
1	A	188	LEU
1	A	193	HIS
1	A	206	THR
1	A	227	PHE
1	A	246	GLU
1	A	261	GLU
1	A	264	ASP
1	A	270	THR
1	A	279	GLN
1	A	280	PHE
1	A	281	LYS
1	A	306	LYS
1	A	308	THR
1	A	320	ARG
1	B	26	VAL
1	B	27	VAL
1	B	29	ASP
1	B	45	ASP
1	B	48	LEU
1	B	49	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	57	LEU
1	B	61	VAL
1	B	72	MET
1	B	121	LYS
1	B	131	ILE
1	B	172	ASN
1	B	183	GLU
1	B	188	LEU
1	B	197	LEU
1	B	206	THR
1	B	227	PHE
1	B	246	GLU
1	B	248	ASP
1	B	260	VAL
1	B	261	GLU
1	B	274	THR
1	B	277	ASP
1	B	279	GLN
1	B	280	PHE
1	B	281	LYS
1	B	308	THR
1	B	318	GLN
1	B	320	ARG
1	C	13	THR
1	C	25	LYS
1	C	27	VAL
1	C	42	SER
1	C	44	LYS
1	C	48	LEU
1	C	49	THR
1	C	61	VAL
1	C	81	LYS
1	C	116	CYS
1	C	131	ILE
1	C	159	GLN
1	C	166	THR
1	C	187	VAL
1	C	188	LEU
1	C	193	HIS
1	C	212	ASN
1	C	214	ARG
1	C	215	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	227	PHE
1	C	233	GLU
1	C	237	VAL
1	C	246	GLU
1	C	251	SER
1	C	254	GLU
1	C	259	VAL
1	C	261	GLU
1	C	274	THR
1	C	291	THR
1	C	297	ARG
1	C	302	LYS
1	C	320	ARG
1	D	5	GLN
1	D	9	ARG
1	D	13	THR
1	D	25	LYS
1	D	27	VAL
1	D	41	VAL
1	D	42	SER
1	D	44	LYS
1	D	45	ASP
1	D	48	LEU
1	D	107	ARG
1	D	131	ILE
1	D	153	GLN
1	D	166	THR
1	D	172	ASN
1	D	187	VAL
1	D	201	SER
1	D	205	LEU
1	D	227	PHE
1	D	237	VAL
1	D	274	THR
1	D	279	GLN
1	D	280	PHE
1	D	308	THR
1	D	313	THR
1	D	318	GLN
1	D	320	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	65	HIS
1	A	68	HIS
1	A	83	ASN
1	A	99	HIS
1	A	138	ASN
1	A	159	GLN
1	A	172	ASN
1	A	177	HIS
1	B	24	GLN
1	B	65	HIS
1	B	68	HIS
1	B	83	ASN
1	B	99	HIS
1	B	138	ASN
1	B	153	GLN
1	B	172	ASN
1	B	181	ASN
1	B	193	HIS
1	C	65	HIS
1	C	68	HIS
1	C	83	ASN
1	C	99	HIS
1	C	138	ASN
1	C	153	GLN
1	C	159	GLN
1	C	212	ASN
1	D	65	HIS
1	D	68	HIS
1	D	83	ASN
1	D	99	HIS
1	D	159	GLN
1	D	181	ASN
1	D	193	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	401	-	52,52,52	1.88	14 (26%)	80,80,80	1.67	10 (12%)
2	NDP	B	401	-	52,52,52	1.68	9 (17%)	80,80,80	1.64	12 (15%)
2	NDP	C	401	-	52,52,52	1.93	14 (26%)	80,80,80	1.74	15 (18%)
2	NDP	D	401	-	52,52,52	1.81	12 (23%)	80,80,80	1.61	9 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	A	401	-	-	0/35/77/77	0/3/5/5
2	NDP	B	401	-	-	0/35/77/77	0/3/5/5
2	NDP	C	401	-	-	0/35/77/77	0/3/5/5
2	NDP	D	401	-	-	0/35/77/77	0/3/5/5

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NDP	C4A-N9A	-6.21	1.28	1.37
2	A	401	NDP	C4A-N9A	-5.89	1.29	1.37
2	D	401	NDP	C4A-N9A	-5.49	1.29	1.37
2	B	401	NDP	C4A-N9A	-5.40	1.29	1.37
2	C	401	NDP	C8A-N9A	-4.09	1.30	1.36
2	D	401	NDP	C8A-N9A	-3.61	1.31	1.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NDP	P2B-O2X	-3.53	1.41	1.54
2	A	401	NDP	C8A-N9A	-3.41	1.31	1.36
2	A	401	NDP	PN-O2N	-3.25	1.40	1.55
2	C	401	NDP	P2B-O2X	-3.17	1.43	1.54
2	D	401	NDP	C4A-N3A	-3.01	1.31	1.35
2	C	401	NDP	P2B-O3X	-3.00	1.43	1.54
2	B	401	NDP	C8A-N9A	-2.98	1.32	1.36
2	A	401	NDP	P2B-O2X	-2.96	1.43	1.54
2	B	401	NDP	PA-O3	-2.85	1.54	1.59
2	A	401	NDP	P2B-O3X	-2.83	1.44	1.54
2	A	401	NDP	C4A-N3A	-2.77	1.31	1.35
2	A	401	NDP	PA-O2A	-2.77	1.42	1.55
2	C	401	NDP	C5A-N7A	-2.73	1.30	1.40
2	A	401	NDP	PN-O3	-2.73	1.54	1.59
2	D	401	NDP	P2B-O3X	-2.69	1.44	1.54
2	D	401	NDP	PA-O2A	-2.66	1.43	1.55
2	B	401	NDP	PN-O3	-2.64	1.55	1.59
2	B	401	NDP	P2B-O3X	-2.62	1.45	1.54
2	C	401	NDP	O7N-C7N	-2.62	1.17	1.24
2	C	401	NDP	C4A-N3A	-2.61	1.31	1.35
2	D	401	NDP	P2B-O1X	-2.56	1.42	1.51
2	B	401	NDP	P2B-O2X	-2.55	1.45	1.54
2	C	401	NDP	PA-O2A	-2.54	1.43	1.55
2	B	401	NDP	PA-O2A	-2.43	1.44	1.55
2	A	401	NDP	PA-O1A	-2.40	1.42	1.51
2	A	401	NDP	O4D-C4D	-2.35	1.39	1.45
2	D	401	NDP	C5A-N7A	-2.35	1.31	1.40
2	A	401	NDP	PN-O1N	-2.34	1.42	1.51
2	A	401	NDP	C5A-N7A	-2.34	1.31	1.40
2	D	401	NDP	C4N-C5N	-2.33	1.44	1.49
2	C	401	NDP	PA-O1A	-2.31	1.42	1.51
2	C	401	NDP	PN-O2N	-2.29	1.44	1.55
2	B	401	NDP	C4N-C5N	-2.29	1.44	1.49
2	C	401	NDP	P2B-O1X	-2.28	1.43	1.51
2	D	401	NDP	PN-O2N	-2.27	1.44	1.55
2	A	401	NDP	O7N-C7N	-2.22	1.18	1.24
2	C	401	NDP	C8A-N7A	-2.19	1.30	1.34
2	A	401	NDP	P2B-O1X	-2.17	1.43	1.51
2	B	401	NDP	PN-O2N	-2.12	1.45	1.55
2	C	401	NDP	PN-O1N	-2.12	1.43	1.51
2	D	401	NDP	C2N-C3N	2.06	1.38	1.34
2	C	401	NDP	PA-O3	-2.03	1.56	1.59

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NDP	C3B-C2B	-2.02	1.48	1.53

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NDP	N3A-C2A-N1A	-7.70	122.27	128.71
2	D	401	NDP	N3A-C2A-N1A	-6.37	123.38	128.71
2	A	401	NDP	O4B-C1B-N9A	5.96	113.98	108.44
2	C	401	NDP	N3A-C4A-N9A	5.87	136.03	125.43
2	C	401	NDP	N3A-C2A-N1A	-5.81	123.85	128.71
2	A	401	NDP	O4B-C1B-C2B	-5.45	101.85	106.95
2	D	401	NDP	N3A-C4A-N9A	5.32	135.04	125.43
2	A	401	NDP	N3A-C2A-N1A	-5.31	124.27	128.71
2	C	401	NDP	C8A-N9A-C4A	5.03	110.74	106.90
2	B	401	NDP	N3A-C4A-N9A	4.77	134.04	125.43
2	A	401	NDP	C4A-C5A-N7A	-4.08	106.03	109.52
2	A	401	NDP	N3A-C4A-N9A	3.99	132.64	125.43
2	D	401	NDP	C4A-C5A-N7A	-3.98	106.11	109.52
2	A	401	NDP	O2X-P2B-O2B	-3.50	97.01	107.09
2	D	401	NDP	O4B-C1B-C2B	-3.38	103.79	106.95
2	B	401	NDP	C8A-N9A-C4A	3.38	109.48	106.90
2	D	401	NDP	C5A-C4A-N3A	-3.33	118.46	125.70
2	B	401	NDP	O4B-C1B-C2B	-2.97	104.17	106.95
2	C	401	NDP	O4D-C1D-N1N	2.95	114.30	108.05
2	C	401	NDP	C3N-C7N-N7N	2.95	123.15	117.48
2	B	401	NDP	O4B-C1B-N9A	2.95	111.18	108.44
2	C	401	NDP	C4A-C5A-N7A	-2.94	107.01	109.52
2	C	401	NDP	C5A-C4A-N3A	-2.92	119.33	125.70
2	A	401	NDP	C5A-C4A-N3A	-2.88	119.43	125.70
2	D	401	NDP	C2A-N3A-C4A	2.85	122.12	114.01
2	D	401	NDP	O2X-P2B-O2B	-2.81	98.99	107.09
2	D	401	NDP	C8A-N9A-C4A	2.75	109.00	106.90
2	C	401	NDP	O4B-C1B-C2B	-2.74	104.39	106.95
2	D	401	NDP	O4B-C1B-N9A	2.68	110.93	108.44
2	C	401	NDP	C1D-N1N-C6N	-2.58	115.08	120.79
2	B	401	NDP	C4A-C5A-N7A	-2.57	107.32	109.52
2	B	401	NDP	C1B-N9A-C4A	-2.55	122.23	126.64
2	B	401	NDP	C5A-C4A-N3A	-2.48	120.29	125.70
2	B	401	NDP	C2A-N3A-C4A	2.44	120.96	114.01
2	B	401	NDP	C6N-N1N-C2N	2.43	122.62	119.44
2	A	401	NDP	O3X-P2B-O2X	2.37	116.84	107.61
2	C	401	NDP	O4B-C1B-N9A	2.37	110.64	108.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NDP	C2A-N1A-C6A	2.36	123.04	118.77
2	A	401	NDP	C2A-N3A-C4A	2.32	120.61	114.01
2	C	401	NDP	C4B-O4B-C1B	-2.24	107.31	109.75
2	A	401	NDP	O7N-C7N-N7N	-2.24	117.28	122.93
2	C	401	NDP	C2N-C3N-C7N	2.23	124.18	118.49
2	C	401	NDP	C2A-N3A-C4A	2.16	120.17	114.01
2	C	401	NDP	O3D-C3D-C2D	-2.04	105.21	111.83
2	C	401	NDP	O7N-C7N-N7N	-2.03	117.79	122.93
2	B	401	NDP	O3D-C3D-C4D	-2.01	105.16	111.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	307/321 (95%)	0.21	14 (4%) 31 33	23, 34, 58, 79	0
1	B	309/321 (96%)	0.32	8 (2%) 53 55	24, 44, 66, 81	0
1	C	290/321 (90%)	0.62	33 (11%) 6 6	24, 39, 69, 84	0
1	D	318/321 (99%)	0.19	14 (4%) 33 35	23, 35, 59, 73	0
All	All	1224/1284 (95%)	0.33	69 (5%) 24 26	23, 38, 64, 84	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	VAL	9.7
1	D	204	ALA	7.1
1	A	208	TRP	6.8
1	C	208	TRP	6.3
1	C	250	VAL	5.1
1	C	310	ALA	4.4
1	A	272	ASP	4.3
1	C	205	LEU	4.2
1	A	30	GLY	4.1
1	A	205	LEU	3.9
1	B	42	SER	3.9
1	C	316	TYR	3.6
1	C	260	VAL	3.6
1	C	44	LYS	3.5
1	C	273	THR	3.5
1	D	28	ALA	3.5
1	D	316	TYR	3.5
1	C	210	THR	3.3
1	C	188	LEU	3.3
1	A	29	ASP	3.1
1	B	29	ASP	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	203	SER	3.1
1	B	206	THR	3.1
1	A	280	PHE	3.0
1	A	28	ALA	3.0
1	C	251	SER	2.9
1	D	34	PRO	2.8
1	B	28	ALA	2.8
1	D	207	VAL	2.8
1	D	275	LYS	2.8
1	A	279	GLN	2.7
1	D	206	THR	2.6
1	C	276	SER	2.6
1	D	200	SER	2.6
1	B	207	VAL	2.6
1	D	205	LEU	2.6
1	C	140	ASN	2.5
1	C	204	ALA	2.5
1	B	43	SER	2.5
1	C	305	VAL	2.5
1	C	215	ARG	2.5
1	A	268	GLU	2.5
1	C	116	CYS	2.5
1	C	313	THR	2.4
1	A	270	THR	2.4
1	C	312	PHE	2.4
1	C	246	GLU	2.4
1	C	29	ASP	2.3
1	C	213	PRO	2.3
1	C	317	GLU	2.3
1	A	269	VAL	2.3
1	C	81	LYS	2.3
1	C	202	GLY	2.3
1	D	318	GLN	2.2
1	C	214	ARG	2.2
1	D	4	PRO	2.2
1	A	271	PHE	2.2
1	D	29	ASP	2.2
1	C	74	GLY	2.2
1	C	144	SER	2.2
1	C	131	ILE	2.2
1	D	33	LEU	2.2
1	C	258	ALA	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	259	VAL	2.1
1	B	60	LYS	2.1
1	C	309	CYS	2.1
1	D	131	ILE	2.0
1	B	183	GLU	2.0
1	C	117	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NDP	B	401	48/48	0.12	-0.92	20,20,20,20	0
2	NDP	D	401	48/48	0.10	-1.08	20,20,20,20	0
2	NDP	C	401	48/48	0.08	-1.30	20,20,20,20	0
2	NDP	A	401	48/48	0.09	-1.41	20,20,20,20	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.