



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2023 – 07:55 PM EDT

PDB ID : 4I3H
Title : A three-gate structure of topoisomerase IV from *Streptococcus pneumoniae*
Authors : Laponogov, I.; Veselkov, D.A.; Pan, X.-S.; Crevel, I.; Fisher, L.M.; Sanderson, M.R.
Deposited on : 2012-11-26
Resolution : 3.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

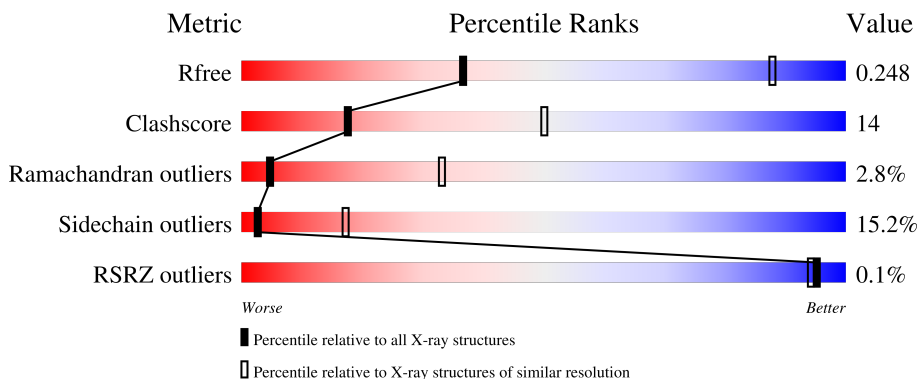
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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

Mol	Chain	Length	Quality of chain
1	E	34	
1	G	34	
2	F	34	
2	H	34	
3	A	1144	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	B	1144	 62% 24% 10%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 16228 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 DNA chain called DNA (5'-D(*CP*AP*AP*AP*GP*GP*CP*GP*GP*TP*AP*AP*TP*AP*CP*GP*GP*TP*TP*AP*TP*CP*CP*AP*CP*AP*GP*AP*AP*TP*CP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	14	Total 282	C 133	N 52	O 83	P 14	0	0	0
1	G	20	Total 407	C 191	N 77	O 119	P 20	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*AP*TP*TP*CP*TP*GP*TP*GP*GP*AP*TP*AP*AP*CP*CP*GP*TP*AP*TP*TP*AP*CP*CP*GP*CP*CP*TP*TP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	F	14	Total 283	C 133	N 51	O 85	P 14	0	0	0
2	H	20	Total 402	C 189	N 72	O 121	P 20	0	0	0

- Molecule 3 is a protein called Topoisomerase IV subunit B, DNA topoisomerase 4 subunit A chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	1037	Total 7477	C 4740	N 1286	O 1430	S 21	0	0	0
3	B	1035	Total 7372	C 4657	N 1280	O 1413	S 22	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1000	HIS	-	linker	UNP Q3HZ71
B	1000	HIS	-	linker	UNP Q3HZ71

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	2	Total O 2 2	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA (5'-D(*CP*AP*AP*AP*GP*GP*CP*GP*GP*TP*AP*AP*TP*AP*CP*GP*GP*TP*TP*AP*TP*CP*CP*AP*CP*AP*GP*AP*AP*TP*CP*AP*GP*G)-3')

Chain E: 



- Molecule 1: DNA (5'-D(*CP*AP*AP*AP*GP*GP*CP*GP*GP*TP*AP*AP*TP*AP*CP*GP*GP*TP*TP*AP*TP*CP*CP*AP*CP*AP*GP*AP*AP*TP*CP*AP*GP*G)-3')

Chain G: 




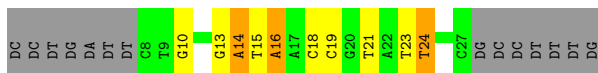
- Molecule 2: DNA (5'-D(*CP*CP*TP*GP*AP*TP*TP*CP*TP*GP*TP*GP*GP*AP*TP*AP*AP*CP*CP*GP*TP*AP*TP*TP*AP*CP*CP*GP*CP*CP*TP*TP*TP*G)-3')

Chain F: 



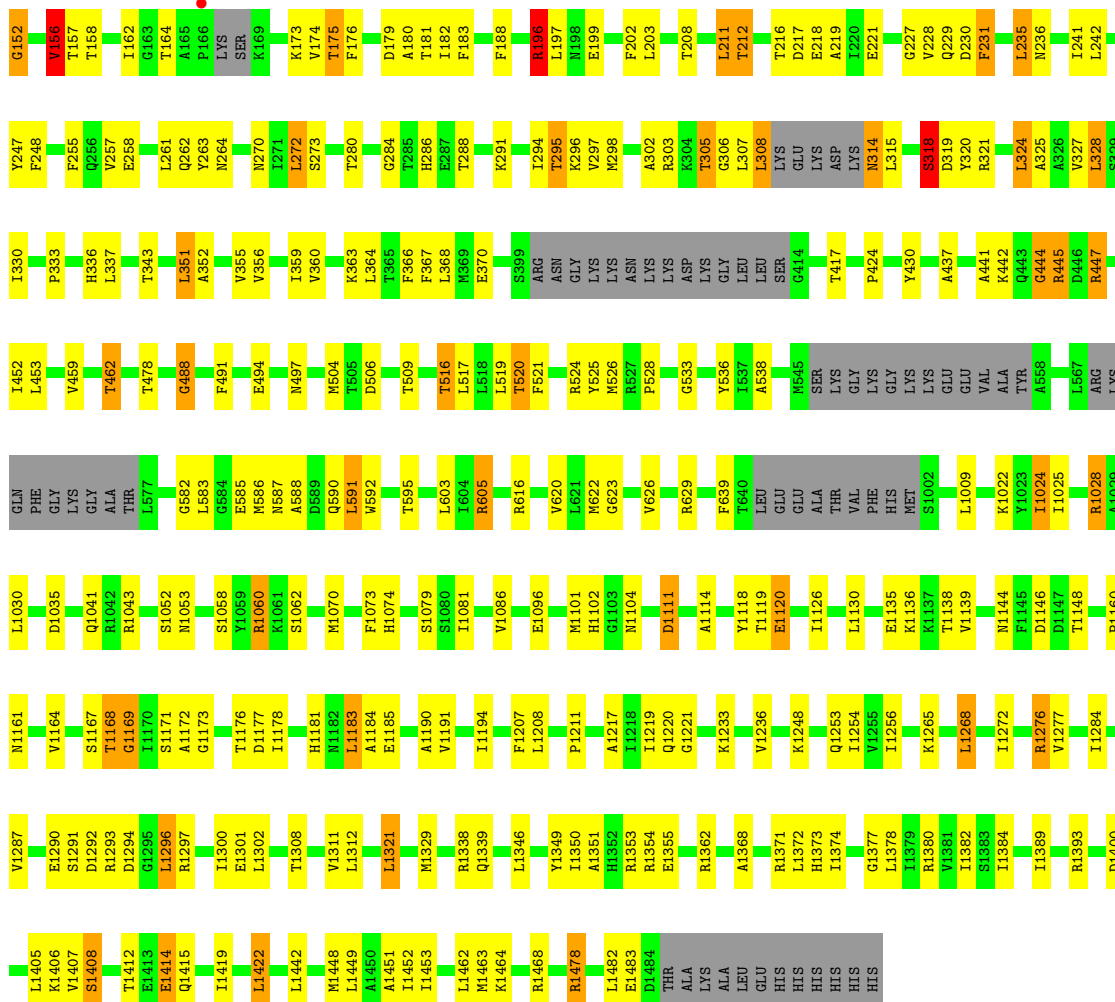
- Molecule 2: DNA (5'-D(*CP*CP*TP*GP*AP*TP*TP*CP*TP*GP*TP*GP*GP*AP*TP*AP*AP*CP*CP*GP*TP*AP*TP*TP*AP*CP*CP*GP*CP*CP*TP*TP*TP*G)-3')

Chain H: 



- Molecule 3: Topoisomerase IV subunit B, DNA topoisomerase 4 subunit A chimera

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	160.60Å 160.60Å 280.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.82 – 3.70 71.82 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (71.82-3.70) 99.7 (71.82-3.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 3.67Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.185 , 0.248 0.183 , 0.248	Depositor DCC
R_{free} test set	2006 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	95.5	Xtrriage
Anisotropy	0.205	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 82.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16228	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	E	0.83	1/316 (0.3%)	1.85	12/483 (2.5%)
1	G	0.96	0/457	1.94	12/701 (1.7%)
2	F	0.80	0/317	1.91	10/485 (2.1%)
2	H	0.86	0/450	1.83	13/689 (1.9%)
3	A	0.45	0/7600	0.67	2/10359 (0.0%)
3	B	0.43	0/7491	0.65	2/10214 (0.0%)
All	All	0.50	1/16631 (0.0%)	0.87	51/22931 (0.2%)

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
3	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	4	DT	C1'-N1	5.18	1.55	1.49

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	20	DA	O4'-C1'-N9	15.76	119.03	108.00
2	H	16	DA	O4'-C4'-C3'	-10.97	99.42	106.00
1	G	24	DA	O4'-C1'-N9	-8.97	101.72	108.00
2	H	21	DT	O4'-C4'-C3'	-8.15	101.11	106.00
2	H	24	DT	O4'-C1'-N1	-8.15	102.30	108.00
2	F	4	DG	N3-C4-C5	7.50	132.35	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4	DT	N3-C2-O2	-7.35	117.89	122.30
1	G	25	DC	O4'-C1'-C2'	-7.04	100.27	105.90
2	F	15	DT	N3-C4-O4	6.99	124.09	119.90
1	G	20	DA	N9-C1'-C2'	-6.98	99.34	112.60
1	E	4	DT	O4'-C1'-N1	6.83	112.78	108.00
1	G	13	DT	O4'-C1'-C2'	-6.82	100.44	105.90
2	F	6	DT	N3-C4-O4	6.65	123.89	119.90
2	H	13	DG	O4'-C1'-C2'	-6.64	100.59	105.90
2	H	14	DA	O4'-C4'-C3'	-6.58	101.87	104.50
3	A	102	LEU	CA-CB-CG	6.56	130.38	115.30
2	H	21	DT	C4'-C3'-C2'	-6.52	97.23	103.10
1	E	14	DC	C3'-C2'-C1'	-6.39	94.83	102.50
2	F	4	DG	N3-C4-N9	-6.22	122.27	126.00
1	E	9	DT	N3-C4-O4	6.08	123.55	119.90
2	F	6	DT	C5-C4-O4	-6.04	120.67	124.90
1	G	19	DT	N3-C4-O4	6.04	123.52	119.90
1	G	21	DT	O4'-C4'-C3'	-6.00	102.10	104.50
2	F	13	DA	N3-C4-N9	-5.98	122.62	127.40
2	F	13	DA	N1-C2-N3	5.96	132.28	129.30
2	H	21	DT	C5-C4-O4	-5.95	120.73	124.90
1	G	18	DT	N3-C4-O4	5.94	123.47	119.90
1	E	4	DT	N3-C4-O4	5.89	123.44	119.90
1	E	10	DT	N3-C4-O4	5.83	123.40	119.90
2	H	21	DT	N3-C4-O4	5.76	123.36	119.90
1	G	20	DA	O4'-C4'-C3'	5.71	109.42	106.00
1	E	9	DT	C5-C4-O4	-5.66	120.94	124.90
3	B	44	LEU	CA-CB-CG	5.54	128.05	115.30
1	G	25	DC	C3'-C2'-C1'	-5.52	95.88	102.50
2	F	9	DC	N1-C2-O2	5.45	122.17	118.90
3	A	364	LEU	CA-CB-CG	5.42	127.77	115.30
1	G	13	DT	N3-C2-O2	-5.42	119.05	122.30
2	H	13	DG	O4'-C1'-N9	5.36	111.75	108.00
2	H	23	DT	C5-C4-O4	-5.33	121.17	124.90
2	F	13	DA	N9-C4-C5	5.29	107.92	105.80
2	H	15	DT	N3-C4-O4	5.28	123.07	119.90
1	G	9	DG	O4'-C1'-C2'	5.28	110.12	105.90
2	H	14	DA	O4'-C1'-N9	5.24	111.67	108.00
1	E	14	DC	C6-N1-C2	5.20	122.38	120.30
1	E	13	DC	N1-C2-O2	5.14	121.99	118.90
2	H	13	DG	N7-C8-N9	5.14	115.67	113.10
1	E	4	DT	C5-C4-O4	-5.12	121.32	124.90
2	F	3	DG	C3'-C2'-C1'	-5.11	96.37	102.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	196	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	E	4	DT	C6-N1-C2	-5.04	118.78	121.30
1	E	3	DA	O4'-C1'-N9	5.04	111.52	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	102	LEU	Peptide

5.2 Too-close contacts [i](#)

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	E	282	0	147	8	0
1	G	407	0	211	10	0
2	F	283	0	145	11	0
2	H	402	0	209	8	0
3	A	7477	0	6788	217	0
3	B	7372	0	6577	186	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	H	1	0	0	0	0
5	E	2	0	0	0	0
All	All	16228	0	14077	414	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 14.

All (414) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:DA:N6	2:F:13:DA:N6	2.20	0.89
1:E:3:DA:N1	2:F:13:DA:N1	2.21	0.89
3:A:520:THR:HG21	3:A:622:MET:HG3	1.56	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:48:ILE:HG12	3:B:127:VAL:HG21	1.60	0.82
1:E:3:DA:N6	2:F:13:DA:C6	2.47	0.82
3:A:623:GLY:O	3:A:629:ARG:NH2	2.14	0.79
1:E:11:DA:C2	2:F:7:DA:C2	2.72	0.78
3:B:196:ARG:HG2	3:B:196:ARG:HH11	1.49	0.78
3:B:34:GLY:O	3:B:36:THR:N	2.17	0.77
3:B:132:SER:HB3	3:B:179:ASP:HB3	1.65	0.77
3:A:436:SER:HB2	3:B:1114:ALA:HA	1.66	0.76
3:A:259:VAL:HG22	3:A:328:LEU:HD23	1.68	0.75
3:B:623:GLY:O	3:B:629:ARG:NH2	2.20	0.75
3:A:524:ARG:HH11	3:A:524:ARG:HB3	1.52	0.74
3:A:304:LYS:O	3:A:306:GLY:N	2.21	0.74
3:B:99:PHE:O	3:B:101:ILE:N	2.23	0.72
3:A:51:ASN:ND2	3:A:99:PHE:O	2.22	0.72
3:B:520:THR:HG21	3:B:622:MET:HG3	1.70	0.72
3:A:256:GLN:HB3	3:A:331:LEU:HB2	1.70	0.72
3:A:301:TYR:HD2	3:A:379:ILE:HD11	1.55	0.72
3:A:1059:TYR:HB3	3:A:1120:GLU:HB3	1.72	0.72
3:A:1397:ASN:O	3:A:1399:ALA:N	2.23	0.72
1:E:3:DA:C6	2:F:13:DA:N1	2.58	0.71
3:A:332:VAL:HG12	3:A:334:GLU:H	1.56	0.71
3:A:1220:GLN:HB2	3:A:1237:VAL:HG12	1.72	0.71
3:A:1382:ILE:HD12	3:A:1432:VAL:HG23	1.74	0.69
3:A:201:ALA:HB2	3:A:209:LEU:HD11	1.74	0.69
3:A:67:THR:HB	3:A:75:THR:HG23	1.74	0.68
3:A:1075:PRO:HG3	3:A:1145:PHE:CD1	2.28	0.68
3:A:626:VAL:HG21	1:G:24:DA:H3'	1.75	0.68
3:B:506:ASP:HB3	3:B:582:GLY:HA2	1.76	0.68
3:A:75:THR:HB	3:A:175:THR:HB	1.75	0.67
3:B:639:PHE:HA	3:B:1022:LYS:HE3	1.74	0.67
3:A:33:ILE:HD11	3:A:44:LEU:HB3	1.76	0.67
3:B:318:SER:O	3:B:320:TYR:N	2.22	0.67
3:A:543:TYR:HB2	3:A:558:ALA:HB3	1.75	0.67
3:A:294:ILE:HA	3:A:297:VAL:HG12	1.77	0.67
3:B:1118:TYR:OH	2:H:16:DA:OP1	2.12	0.67
3:B:22:LEU:HG	3:B:124:SER:H	1.60	0.66
3:A:132:SER:O	3:A:151:ASN:N	2.25	0.65
3:B:1272:ILE:HG22	3:B:1287:VAL:HG21	1.79	0.65
3:A:1139:VAL:HG22	3:A:1154:VAL:HG13	1.79	0.65
3:B:135:GLU:HG3	3:B:148:ARG:HB3	1.78	0.65
3:A:1144:ASN:HD21	3:A:1148:THR:HG23	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1268:LEU:HD11	3:B:1321:LEU:HD23	1.78	0.65
1:E:3:DA:C6	2:F:13:DA:N6	2.65	0.65
3:A:1254:ILE:HD13	3:A:1312:LEU:HD13	1.78	0.64
3:B:1373:HIS:CD2	3:B:1414:GLU:HG3	2.33	0.64
3:B:227:GLY:O	3:B:230:ASP:N	2.29	0.64
3:B:516:THR:O	3:B:520:THR:HG23	1.97	0.64
1:E:3:DA:C6	2:F:13:DA:C6	2.86	0.63
3:A:265:ASP:HB2	3:A:421:SER:HB2	1.81	0.63
3:B:1178:ILE:HG12	3:B:1329:MET:HG2	1.79	0.62
3:A:104:ALA:O	3:A:106:GLY:N	2.31	0.62
3:B:491:PHE:CD1	3:B:528:PRO:HG2	2.34	0.62
3:A:447:ARG:HD3	3:B:1290:GLU:HA	1.82	0.62
3:A:102:LEU:HD21	3:A:127:VAL:HG22	1.82	0.62
3:B:75:THR:OG1	3:B:175:THR:HB	2.00	0.62
3:A:1211:PRO:O	3:A:1478:ARG:NH2	2.33	0.62
3:B:356:VAL:O	3:B:360:VAL:HG12	2.00	0.62
3:B:1164:VAL:HG21	3:B:1183:LEU:HD23	1.82	0.61
3:B:199:GLU:HA	3:B:202:PHE:HD2	1.66	0.61
3:B:1171:SER:OG	3:B:1172:ALA:N	2.31	0.61
3:A:102:LEU:HD23	3:A:126:VAL:HG22	1.83	0.61
3:A:139:THR:HG23	3:A:144:VAL:HB	1.82	0.60
3:A:301:TYR:CD2	3:A:379:ILE:HD11	2.36	0.60
3:A:1169:GLY:HA3	3:A:1176:THR:O	2.02	0.60
3:B:1144:ASN:HD21	3:B:1148:THR:HG22	1.66	0.60
2:H:18:DC:H2'	2:H:19:DC:C6	2.36	0.60
3:A:459:VAL:HG21	3:A:518:LEU:HD21	1.84	0.60
3:B:134:LEU:HD12	3:B:176:PHE:HB3	1.82	0.60
3:B:1024:ILE:HD11	3:B:1028:ARG:NH2	2.17	0.60
3:A:1369:GLU:HG3	3:A:1446:ILE:HD13	1.84	0.59
3:A:1008:SER:HB3	3:A:1011:ASP:OD2	2.02	0.59
3:A:1350:ILE:HA	3:A:1463:MET:HE3	1.84	0.59
3:A:592:TRP:CE2	3:A:597:ASN:HB2	2.37	0.59
3:A:1063:ALA:HB2	3:A:1116:MET:HG3	1.83	0.59
3:A:51:ASN:HD21	3:A:99:PHE:HA	1.67	0.59
3:A:1146:ASP:HB3	3:A:1148:THR:HG22	1.84	0.59
3:A:1290:GLU:HB2	3:A:1297:ARG:HG2	1.84	0.59
3:A:48:ILE:HD11	3:A:127:VAL:HG11	1.85	0.59
3:B:1362:ARG:HG2	3:B:1453:ILE:HD13	1.83	0.59
3:B:1181:HIS:CD2	3:B:1211:PRO:HA	2.37	0.58
3:A:1181:HIS:CD2	3:A:1211:PRO:HA	2.38	0.58
3:A:486:GLY:O	3:A:491:PHE:HD2	1.87	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1025:ILE:HG23	3:B:1030:LEU:HD12	1.85	0.58
3:A:1171:SER:OG	3:A:1172:ALA:N	2.32	0.58
3:A:134:LEU:HD12	3:A:176:PHE:HB3	1.86	0.58
3:B:42:HIS:HA	3:B:45:VAL:HG13	1.85	0.57
3:A:1006:ASN:OD1	3:A:1006:ASN:N	2.29	0.57
3:B:1219:ILE:HB	3:B:1482:LEU:HD23	1.86	0.57
3:A:474:GLU:O	3:A:478:THR:HG23	2.04	0.57
3:A:271:ILE:HD11	3:A:324:LEU:HD13	1.86	0.57
3:A:1362:ARG:HG2	3:A:1453:ILE:HD13	1.86	0.57
3:A:1114:ALA:HB3	3:A:1119:THR:HG23	1.87	0.56
3:A:1175:ALA:O	3:A:1328:ASN:ND2	2.39	0.56
3:B:136:VAL:HG22	3:B:174:VAL:HG22	1.87	0.56
3:B:212:THR:HB	3:B:219:ALA:HB2	1.87	0.56
3:A:515:GLN:OE1	3:A:1016:ARG:NE	2.37	0.56
3:A:1034:ARG:HH21	3:A:1154:VAL:HG11	1.70	0.56
3:B:1254:ILE:HG21	3:B:1312:LEU:HD13	1.87	0.56
3:A:216:THR:HB	3:A:218:GLU:HG2	1.87	0.56
3:A:1117:ARG:NH1	1:G:16:DG:OP2	2.38	0.56
3:B:272:LEU:H	3:B:272:LEU:HD12	1.71	0.56
3:A:48:ILE:HD11	3:A:127:VAL:HG21	1.87	0.56
3:A:257:VAL:HB	3:A:330:ILE:HG22	1.87	0.56
3:A:1241:LYS:HB3	3:A:1258:GLU:HG3	1.88	0.56
3:B:1169:GLY:HA3	3:B:1176:THR:O	2.06	0.56
3:A:1028:ARG:NH1	2:H:14:DA:H4'	2.22	0.55
3:A:190:TYR:CD2	3:A:213:ASP:HB2	2.42	0.55
3:B:1419:ILE:HA	3:B:1422:LEU:HD12	1.87	0.55
3:B:491:PHE:CE1	3:B:528:PRO:HG2	2.41	0.55
3:B:352:ALA:HA	3:B:355:VAL:HG22	1.88	0.55
3:B:1060:ARG:HH11	3:B:1060:ARG:HB2	1.72	0.55
3:B:1146:ASP:HB3	3:B:1148:THR:HB	1.89	0.55
3:B:297:VAL:HG11	3:B:364:LEU:HG	1.89	0.55
3:B:1276:ARG:HH21	3:B:1277:VAL:HG23	1.71	0.55
3:B:298:MET:O	3:B:302:ALA:N	2.39	0.55
3:B:1292:ASP:O	3:B:1294:ASP:N	2.40	0.55
3:A:373:GLU:C	3:A:375:ALA:H	2.10	0.54
3:A:1333:ASP:HB3	3:A:1338:ARG:HD3	1.88	0.54
3:A:285:THR:HG23	3:A:347:LEU:O	2.08	0.54
3:B:462:THR:HG21	3:B:521:PHE:HD1	1.73	0.54
3:B:1173:GLY:H	2:H:24:DT:H5''	1.72	0.54
3:B:196:ARG:HH11	3:B:196:ARG:CG	2.18	0.53
3:A:373:GLU:O	3:A:375:ALA:N	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:533:GLY:O	3:B:605:ARG:NH1	2.36	0.53
3:A:197:LEU:HD22	3:A:209:LEU:HD22	1.90	0.53
3:A:1095:ARG:HA	3:A:1214:PRO:HB3	1.90	0.53
3:B:1043:ARG:HD3	3:B:1073:PHE:HB3	1.91	0.53
3:B:22:LEU:H	3:B:129:ALA:HB2	1.73	0.53
3:B:364:LEU:O	3:B:368:LEU:HB2	2.08	0.53
3:A:483:ILE:HD13	3:A:526:MET:HE1	1.90	0.53
3:A:321:ARG:HG2	3:A:324:LEU:HD12	1.91	0.53
3:A:96:GLU:HG2	3:A:138:ILE:HD11	1.91	0.53
3:A:1245:GLU:OE2	3:A:1297:ARG:NH2	2.42	0.53
3:B:587:ASN:HB2	3:B:590:GLN:NE2	2.24	0.52
3:A:1162:LEU:HD21	3:A:1178:ILE:HD12	1.91	0.52
3:B:491:PHE:CD2	3:B:526:MET:HG2	2.44	0.52
3:A:52:ALA:HB2	3:A:99:PHE:CE1	2.44	0.52
3:A:1118:TYR:OH	1:G:16:DG:OP1	2.20	0.52
3:A:139:THR:O	3:A:170:THR:HA	2.10	0.52
3:A:443:GLN:NE2	3:B:1111:ASP:OD2	2.43	0.52
3:B:1265:LYS:HD3	3:B:1296:LEU:HD11	1.92	0.52
3:B:488:GLY:N	3:B:525:TYR:O	2.33	0.52
3:A:1178:ILE:HG12	3:A:1329:MET:HG2	1.92	0.51
3:A:1273:ASP:O	3:A:1277:VAL:HG23	2.11	0.51
3:B:148:ARG:HG3	3:B:156:VAL:HG12	1.90	0.51
3:B:247:TYR:OH	3:B:258:GLU:OE2	2.20	0.51
3:B:1191:VAL:HG13	3:B:1464:LYS:HG2	1.93	0.51
3:B:459:VAL:O	3:B:517:LEU:HD13	2.10	0.51
3:B:29:PRO:O	3:B:33:ILE:HG22	2.11	0.51
3:A:253:ASN:O	3:A:253:ASN:ND2	2.38	0.51
3:A:1126:ILE:HG13	3:A:1474:PHE:CD1	2.46	0.51
3:A:54:ASP:OD1	3:A:107:LYS:HA	2.11	0.51
3:A:1025:ILE:HG23	3:A:1030:LEU:HD12	1.91	0.51
3:B:129:ALA:HA	3:B:152:GLY:O	2.11	0.51
3:B:26:ARG:O	3:B:29:PRO:HD3	2.11	0.50
3:B:151:ASN:OD1	3:B:152:GLY:N	2.44	0.50
3:A:420:GLN:HB3	3:A:448:LYS:HA	1.93	0.50
3:B:1024:ILE:HD11	3:B:1028:ARG:CZ	2.42	0.50
3:A:617:ARG:HA	3:A:620:VAL:HG23	1.93	0.50
3:B:437:ALA:HB1	3:B:583:LEU:HB2	1.92	0.50
3:B:107:LYS:O	3:B:109:GLY:N	2.45	0.50
3:A:1272:ILE:HG22	3:A:1287:VAL:HG21	1.92	0.50
3:B:1028:ARG:HD3	1:G:14:DA:O5'	2.11	0.50
3:A:1372:LEU:HA	3:A:1442:LEU:HD13	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:351:LEU:O	3:B:355:VAL:HG13	2.12	0.50
3:B:1104:ASN:HB3	3:B:1114:ALA:HB2	1.93	0.50
3:A:1371:ARG:HG3	3:A:1442:LEU:HD11	1.93	0.49
3:A:263:TYR:CE2	3:A:378:LEU:HD21	2.47	0.49
3:B:257:VAL:HB	3:B:330:ILE:HG22	1.93	0.49
3:B:150:GLU:O	3:B:152:GLY:N	2.37	0.49
3:B:1253:GLN:HG3	3:B:1301:GLU:HA	1.93	0.49
3:A:43:HIS:O	3:A:47:GLU:HG2	2.12	0.49
3:A:463:ALA:HA	3:A:524:ARG:NH2	2.28	0.49
3:B:45:VAL:HG22	3:B:46:TRP:CE3	2.48	0.49
3:B:135:GLU:HG3	3:B:148:ARG:CB	2.42	0.49
3:A:1024:ILE:HD11	3:A:1028:ARG:HE	1.77	0.49
3:B:128:ASN:HB2	3:B:134:LEU:HD22	1.93	0.49
3:B:261:LEU:HB2	3:B:324:LEU:HD21	1.95	0.49
3:B:305:THR:O	3:B:307:LEU:N	2.46	0.49
3:A:360:VAL:O	3:A:364:LEU:HD12	2.13	0.48
3:B:1372:LEU:HA	3:B:1442:LEU:HD13	1.95	0.48
1:E:3:DA:N1	2:F:13:DA:C2	2.80	0.48
3:A:303:ARG:NH1	3:A:310:GLU:HA	2.28	0.48
3:A:304:LYS:C	3:A:306:GLY:H	2.16	0.48
3:A:451:ALA:O	3:A:452:ILE:HD13	2.13	0.48
3:B:1185:GLU:HB3	3:B:1207:PHE:O	2.12	0.48
3:B:444:GLY:N	3:B:588:ALA:HB1	2.28	0.48
3:A:513:HIS:HB2	3:A:1020:TYR:CD1	2.49	0.48
3:B:1168:THR:HA	3:B:1176:THR:O	2.13	0.48
3:A:640:THR:HA	3:A:641:LEU:HA	1.53	0.48
3:B:37:ASP:HA	3:B:38:GLY:HA2	1.49	0.48
3:B:1449:LEU:O	3:B:1453:ILE:HG13	2.12	0.48
1:G:26:DA:H2'	1:G:27:DG:C8	2.49	0.48
3:A:132:SER:N	3:A:177:MET:O	2.43	0.48
3:B:66:VAL:O	3:B:211:LEU:HA	2.14	0.48
3:A:583:LEU:HD13	3:A:591:LEU:HD21	1.96	0.47
3:B:1389:ILE:O	3:B:1393:ARG:HG3	2.14	0.47
3:B:44:LEU:HD23	3:B:130:LEU:HD23	1.97	0.47
3:B:74:LEU:HB2	3:B:188:PHE:CE2	2.50	0.47
3:A:351:LEU:HD22	3:A:355:VAL:HG13	1.96	0.47
3:A:594:THR:OG1	3:A:595:THR:HG22	2.13	0.47
3:A:1096:GLU:HG2	3:A:1126:ILE:HD12	1.96	0.47
3:A:234:TYR:CE2	3:B:1248:LYS:HG2	2.50	0.47
3:A:255:PHE:CE2	3:A:332:VAL:HG22	2.50	0.47
3:A:1101:MET:HG3	3:A:1121:ALA:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1190:ALA:O	3:A:1194:ILE:HG13	2.14	0.47
3:A:1334:ASN:O	3:A:1336:THR:HG23	2.15	0.47
3:B:96:GLU:O	3:B:99:PHE:HB3	2.14	0.47
3:B:273:SER:HA	3:B:328:LEU:O	2.15	0.47
3:B:616:ARG:O	3:B:620:VAL:HG23	2.14	0.47
3:B:1406:LYS:O	3:B:1408:SER:N	2.39	0.47
3:A:340:GLU:HB3	3:A:341:GLY:H	1.51	0.47
3:B:445:ARG:HE	3:B:447:ARG:HA	1.80	0.47
3:A:179:ASP:OD1	3:A:182:ILE:HG23	2.14	0.47
2:F:3:DG:H2''	2:F:4:DG:N7	2.30	0.46
3:B:1086:VAL:HG22	3:B:1101:MET:SD	2.55	0.46
3:B:1464:LYS:HB3	3:B:1468:ARG:HH12	1.80	0.46
3:B:231:PHE:HB3	3:B:327:VAL:HG21	1.97	0.46
3:B:1350:ILE:HA	3:B:1463:MET:HE3	1.96	0.46
3:A:1030:LEU:HD12	3:A:1332:ILE:HD11	1.97	0.46
3:B:1096:GLU:HG2	3:B:1126:ILE:HD13	1.97	0.46
3:B:197:LEU:HD12	3:B:211:LEU:HB2	1.97	0.46
3:B:355:VAL:O	3:B:359:ILE:HD13	2.16	0.46
1:G:17:DG:H2''	1:G:18:DT:H5'	1.97	0.46
3:A:246:LEU:O	3:A:260:ALA:HA	2.15	0.46
3:A:334:GLU:HA	3:A:337:LEU:HB2	1.98	0.46
3:A:361:ALA:O	3:A:365:THR:OG1	2.33	0.46
3:A:1164:VAL:HG21	3:A:1183:LEU:HD23	1.97	0.46
3:A:1264:ASN:HB3	3:A:1267:ASN:HB2	1.96	0.46
3:A:1423:GLN:O	3:A:1426:ARG:HB2	2.16	0.46
3:A:25:VAL:HB	3:A:32:TYR:CZ	2.50	0.46
3:A:543:TYR:HA	3:A:578:GLN:O	2.16	0.46
3:A:1449:LEU:O	3:A:1453:ILE:HG13	2.15	0.46
3:A:1090:GLN:HB3	3:A:1092:TRP:CH2	2.51	0.46
3:B:248:PHE:HB3	3:B:363:LYS:HG2	1.98	0.46
3:B:424:PRO:HA	3:B:497:ASN:O	2.14	0.46
3:B:1256:ILE:HD13	3:B:1321:LEU:HD21	1.99	0.46
3:A:1103:GLY:HA3	3:B:585:GLU:HA	1.97	0.45
3:B:216:THR:O	3:B:218:GLU:N	2.48	0.45
3:B:291:LYS:O	3:B:295:THR:HG23	2.16	0.45
3:A:41:LEU:HD11	3:A:178:PRO:HG3	1.98	0.45
3:A:1126:ILE:HG13	3:A:1474:PHE:CE1	2.51	0.45
3:B:366:PHE:C	3:B:368:LEU:H	2.19	0.45
3:B:1351:ALA:O	3:B:1354:ARG:HB3	2.16	0.45
3:A:75:THR:HB	3:A:175:THR:CB	2.44	0.45
3:A:341:GLY:O	3:A:343:THR:N	2.43	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1160:PRO:HG3	3:B:1349:TYR:CE2	2.51	0.45
3:B:1233:LYS:HG3	3:B:1339:GLN:NE2	2.32	0.45
3:A:1338:ARG:HH21	3:A:1340:VAL:HG12	1.82	0.45
3:B:263:TYR:CE1	3:B:324:LEU:HG	2.51	0.45
3:B:236:ASN:HB2	3:B:262:GLN:HE21	1.81	0.45
3:B:272:LEU:HD13	3:B:327:VAL:HG13	1.97	0.45
3:B:519:LEU:HD23	3:B:519:LEU:HA	1.67	0.45
3:B:1024:ILE:HA	3:B:1024:ILE:HD12	1.63	0.45
3:B:1053:ASN:ND2	3:B:1060:ARG:HD2	2.32	0.45
3:B:444:GLY:O	3:B:592:TRP:HB2	2.16	0.45
3:A:263:TYR:CZ	3:A:378:LEU:HD21	2.51	0.45
3:A:1111:ASP:OD1	3:A:1111:ASP:N	2.48	0.45
3:A:544:LYS:HE3	3:A:580:TYR:OH	2.17	0.45
3:A:26:ARG:HD2	3:A:129:ALA:O	2.17	0.45
3:A:1194:ILE:HD11	3:A:1463:MET:HE1	1.98	0.45
3:A:1294:ASP:N	3:A:1294:ASP:OD1	2.50	0.45
3:A:547:LYS:H	3:A:548:GLY:HA2	1.81	0.45
3:A:1075:PRO:HG3	3:A:1145:PHE:CG	2.52	0.45
3:A:1442:LEU:O	3:A:1446:ILE:HG13	2.16	0.45
3:B:1291:SER:HB3	3:B:1296:LEU:HA	1.99	0.45
3:A:234:TYR:CE1	3:B:1248:LYS:HE2	2.53	0.44
3:A:297:VAL:HG11	3:A:364:LEU:HD11	1.99	0.44
3:A:1260:PRO:HB2	3:A:1263:ILE:HG13	1.99	0.44
3:A:1424:LEU:HD12	3:B:1422:LEU:HB2	1.99	0.44
3:B:437:ALA:CB	3:B:583:LEU:HB2	2.47	0.44
3:B:1185:GLU:OE2	3:B:1478:ARG:NH1	2.50	0.44
3:A:307:LEU:HD13	3:A:307:LEU:N	2.33	0.44
3:A:513:HIS:O	3:A:516:THR:HB	2.18	0.44
3:B:308:LEU:HD23	3:B:308:LEU:HA	1.79	0.44
3:A:100:THR:O	3:A:102:LEU:HD13	2.17	0.44
3:A:190:TYR:HD2	3:A:213:ASP:HB2	1.80	0.44
3:B:314:ASN:N	3:B:314:ASN:HD22	2.15	0.44
3:B:1074:HIS:HB3	3:B:1081:ILE:HD11	2.00	0.44
3:B:1371:ARG:HG3	3:B:1442:LEU:HD11	1.99	0.44
3:A:37:ASP:HA	3:A:38:GLY:HA2	1.72	0.44
3:A:1086:VAL:O	3:A:1089:SER:OG	2.26	0.44
3:B:199:GLU:HA	3:B:202:PHE:CD2	2.48	0.44
3:B:366:PHE:O	3:B:368:LEU:N	2.50	0.44
3:B:255:PHE:CG	3:B:355:VAL:HG21	2.53	0.44
3:B:305:THR:C	3:B:307:LEU:H	2.21	0.44
3:A:374:LEU:O	3:A:378:LEU:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:416:LEU:HD12	3:A:417:THR:N	2.32	0.44
3:B:1035:ASP:O	3:B:1161:ASN:HB3	2.18	0.44
1:G:25:DC:H42	2:H:10:DG:H1	1.66	0.44
3:A:30:GLY:HA2	3:A:35:SER:H	1.83	0.43
3:B:77:GLN:HB3	3:B:173:LYS:CB	2.48	0.43
3:B:506:ASP:CB	3:B:582:GLY:HA2	2.48	0.43
3:B:1114:ALA:HB3	3:B:1119:THR:HG23	1.99	0.43
3:B:1220:GLN:HA	3:B:1483:GLU:O	2.18	0.43
3:B:1353:ARG:HB2	3:B:1463:MET:HE3	2.00	0.43
3:A:491:PHE:CE1	3:A:528:PRO:HB2	2.53	0.43
3:B:63:ARG:NH2	3:B:221:GLU:OE1	2.51	0.43
3:B:1190:ALA:HA	3:B:1346:LEU:HD22	1.99	0.43
3:A:538:ALA:O	3:A:540:PRO:HD3	2.19	0.43
3:A:1130:LEU:HD23	3:A:1130:LEU:HA	1.78	0.43
3:B:1302:LEU:HD21	3:B:1311:VAL:HG11	1.99	0.43
3:B:504:MET:HG2	3:B:583:LEU:HD11	2.00	0.43
3:A:337:LEU:HD23	3:A:337:LEU:HA	1.83	0.43
3:B:591:LEU:HD23	3:B:591:LEU:HA	1.91	0.43
3:A:154:LYS:HA	3:A:155:PRO:HD2	1.86	0.43
3:A:500:LYS:HD3	3:A:536:TYR:CZ	2.53	0.43
3:A:1245:GLU:CD	3:A:1297:ARG:HH22	2.21	0.43
3:A:1353:ARG:HA	3:A:1353:ARG:HD2	1.76	0.43
3:A:1455:ASP:HB3	3:A:1458:THR:HB	2.01	0.43
3:A:1111:ASP:HA	3:A:1112:PRO:HD3	1.91	0.43
3:A:1428:THR:OG1	3:A:1429:ASN:N	2.51	0.43
3:B:284:GLY:O	3:B:288:THR:HG23	2.19	0.43
3:B:441:ALA:HB1	3:B:452:ILE:HD12	2.01	0.43
3:B:1070:MET:HA	3:B:1074:HIS:O	2.19	0.43
3:A:74:LEU:HB2	3:A:188:PHE:CE2	2.54	0.43
3:A:1358:LEU:HD23	3:A:1358:LEU:HA	1.84	0.43
3:A:417:THR:HA	3:A:418:PRO:HD2	1.75	0.43
3:B:147:GLN:NE2	3:B:157:THR:O	2.36	0.43
3:B:1120:GLU:H	3:B:1120:GLU:HG2	1.64	0.43
2:F:3:DG:H2"	2:F:4:DG:C8	2.54	0.42
3:A:96:GLU:O	3:A:99:PHE:HB3	2.19	0.42
3:A:212:THR:HG22	3:A:219:ALA:HB2	2.01	0.42
3:A:285:THR:OG1	3:A:352:ALA:HB3	2.18	0.42
3:A:297:VAL:HG11	3:A:364:LEU:CD1	2.50	0.42
3:B:21:GLY:O	3:B:123:GLY:HA2	2.19	0.42
3:B:134:LEU:HD12	3:B:176:PHE:CB	2.47	0.42
3:B:236:ASN:OD1	3:B:264:ASN:ND2	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:538:ALA:HA	3:B:603:LEU:HD23	2.02	0.42
3:B:1276:ARG:HG3	3:B:1284:ILE:CB	2.49	0.42
3:A:298:MET:SD	3:A:368:LEU:HD21	2.59	0.42
3:B:586:MET:HG2	3:B:590:GLN:HB2	2.01	0.42
3:A:145:TYR:HA	3:A:160:LYS:O	2.19	0.42
3:A:283:GLY:HA2	3:A:287:GLU:OE1	2.19	0.42
3:A:383:ILE:H	3:A:383:ILE:HG13	1.64	0.42
3:A:459:VAL:HG21	3:A:518:LEU:CD2	2.50	0.42
3:A:1160:PRO:HG2	3:A:1186:VAL:HG12	2.01	0.42
3:A:1187:ILE:HG21	3:A:1471:LYS:HB2	2.00	0.42
3:B:626:VAL:HG21	2:H:24:DT:H3'	2.01	0.42
3:A:1129:TYR:CD2	3:A:1470:VAL:HG22	2.54	0.42
3:A:328:LEU:HD22	3:A:329:SER:N	2.35	0.42
3:A:1334:ASN:O	3:A:1336:THR:N	2.52	0.42
3:B:333:PRO:HG2	3:B:336:HIS:HB2	2.01	0.42
1:G:8:DG:N2	1:G:9:DG:C4	2.87	0.42
3:A:303:ARG:HH12	3:A:310:GLU:HA	1.83	0.42
3:A:591:LEU:HD23	3:A:591:LEU:HA	1.94	0.42
3:A:639:PHE:HA	3:A:1022:LYS:HE3	2.01	0.42
3:A:629:ARG:O	3:A:633:ILE:HD12	2.19	0.42
3:A:629:ARG:NH1	1:G:24:DA:OP1	2.48	0.42
3:B:74:LEU:HB3	3:B:176:PHE:CE1	2.54	0.42
3:B:294:ILE:HD11	3:B:321:ARG:HH11	1.84	0.42
3:B:1135:GLU:OE1	3:B:1135:GLU:N	2.39	0.42
3:A:1462:LEU:O	3:A:1466:GLU:HG3	2.20	0.42
3:B:197:LEU:HD23	3:B:197:LEU:HA	1.83	0.42
3:A:442:LYS:HA	3:A:445:ARG:HD3	2.02	0.41
3:A:491:PHE:HE1	3:A:528:PRO:HB2	1.85	0.41
3:B:1136:LYS:O	3:B:1138:THR:HG23	2.20	0.41
3:B:1373:HIS:CE1	3:B:1412:THR:HG21	2.55	0.41
2:F:14:DT:H1'	2:F:15:DT:H5'	2.02	0.41
3:A:121:GLY:C	3:A:123:GLY:H	2.24	0.41
3:A:1179:PRO:HA	3:A:1180:PRO:HD3	1.90	0.41
3:A:1236:VAL:HG12	3:A:1325:TYR:HB3	2.02	0.41
3:B:1194:ILE:HG13	3:B:1350:ILE:HD13	2.01	0.41
3:A:510:ASP:OD1	3:A:1028:ARG:NH2	2.53	0.41
3:B:44:LEU:O	3:B:48:ILE:HG13	2.21	0.41
3:B:270:ASN:O	3:B:325:ALA:HA	2.20	0.41
3:B:1102:HIS:HB3	3:B:1120:GLU:CG	2.50	0.41
1:G:11:DA:H2	2:H:24:DT:H3	1.61	0.41
3:A:102:LEU:HD21	3:A:127:VAL:HG13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1032:ASP:HB3	3:A:1035:ASP:OD1	2.21	0.41
3:A:165:ALA:HA	3:A:166:PRO:HD3	1.90	0.41
3:A:352:ALA:HA	3:A:355:VAL:HG22	2.03	0.41
3:A:368:LEU:HD12	3:A:368:LEU:HA	1.93	0.41
3:A:1185:GLU:HB3	3:A:1207:PHE:O	2.20	0.41
3:B:235:LEU:HD12	3:B:235:LEU:HA	1.88	0.41
3:B:442:LYS:O	3:B:445:ARG:HD3	2.20	0.41
3:A:547:LYS:N	3:A:548:GLY:HA2	2.35	0.41
3:A:630:ARG:HD3	3:A:1174:TYR:CE1	2.55	0.41
3:A:1462:LEU:HD23	3:A:1462:LEU:HA	1.76	0.41
3:B:25:VAL:HG23	3:B:32:TYR:HB2	2.02	0.41
3:B:247:TYR:HE1	3:B:258:GLU:HG2	1.86	0.41
3:A:388:ALA:HA	3:A:391:ALA:HB3	2.01	0.41
3:B:525:TYR:O	3:B:526:MET:HG3	2.20	0.41
3:B:1346:LEU:O	3:B:1350:ILE:HG13	2.21	0.41
3:A:220:ILE:HG22	3:A:221:GLU:H	1.86	0.41
3:A:283:GLY:O	3:A:286:HIS:HE1	2.04	0.41
3:A:1386:ASP:OD1	3:A:1386:ASP:N	2.54	0.41
3:B:202:PHE:CE1	3:B:231:PHE:HA	2.55	0.41
3:A:66:VAL:HG13	3:A:76:VAL:HG22	2.02	0.41
3:A:1139:VAL:HA	3:A:1140:PRO:HD3	1.86	0.40
3:A:1372:LEU:CA	3:A:1442:LEU:HD13	2.50	0.40
3:B:180:ALA:HA	3:B:183:PHE:O	2.20	0.40
3:A:147:GLN:HB2	3:A:159:LEU:HA	2.02	0.40
3:A:236:ASN:HD21	3:A:264:ASN:HD22	1.70	0.40
3:A:373:GLU:C	3:A:375:ALA:N	2.75	0.40
3:B:143:ALA:HA	3:B:164:THR:HA	2.01	0.40
3:B:318:SER:C	3:B:320:TYR:H	2.15	0.40
3:B:430:TYR:HB2	3:B:452:ILE:HD13	2.02	0.40
3:A:301:TYR:CE2	3:A:375:ALA:HB1	2.56	0.40
3:B:1378:LEU:O	3:B:1382:ILE:HG13	2.22	0.40
3:B:1448:MET:O	3:B:1451:ALA:HB3	2.22	0.40
3:A:99:PHE:CD1	3:A:99:PHE:C	2.94	0.40
3:A:430:TYR:CZ	3:A:502:ILE:HD12	2.56	0.40
3:A:1283:GLY:HA2	3:A:1306:ALA:HB1	2.03	0.40
3:B:1168:THR:HA	3:B:1169:GLY:HA3	1.88	0.40
3:B:1377:GLY:HA3	3:B:1415:GLN:HG2	2.03	0.40
3:A:94:THR:O	3:A:98:ILE:HG22	2.21	0.40
3:A:516:THR:HG22	3:A:622:MET:HE1	2.03	0.40
3:A:1168:THR:HA	3:A:1169:GLY:HA3	1.91	0.40
3:B:1368:ALA:O	3:B:1442:LEU:HD22	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:DC:H2'	2:H:19:DC:C5	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	1017/1144 (89%)	891 (88%)	101 (10%)	25 (2%)	5	35
3	B	1015/1144 (89%)	868 (86%)	115 (11%)	32 (3%)	4	31
All	All	2032/2288 (89%)	1759 (87%)	216 (11%)	57 (3%)	5	33

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	305	THR
3	A	373	GLU
3	A	1398	LYS
3	B	35	SER
3	B	99	PHE
3	B	100	THR
3	B	108	PHE
3	B	151	ASN
3	B	217	ASP
3	B	318	SER
3	B	367	PHE
3	B	1058	SER
3	B	1293	ARG
3	A	105	GLY
3	A	122	VAL
3	A	151	ASN
3	A	304	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	374	LEU
3	A	488	GLY
3	A	516	THR
3	A	1217	ALA
3	B	37	ASP
3	B	228	VAL
3	B	306	GLY
3	B	343	THR
3	B	370	GLU
3	B	488	GLY
3	B	1169	GLY
3	B	1407	VAL
3	B	1408	SER
3	A	107	LYS
3	A	227	GLY
3	A	340	GLU
3	A	567	LEU
3	A	1169	GLY
3	A	1250	GLY
3	B	95	VAL
3	B	305	THR
3	B	315	LEU
3	B	1217	ALA
3	A	132	SER
3	A	418	PRO
3	A	1168	THR
3	A	1279	ASN
3	B	1079	SER
3	A	121	GLY
3	B	156	VAL
3	B	319	ASP
3	B	1184	ALA
3	A	487	VAL
3	A	1384	ILE
3	B	106	GLY
3	A	166	PRO
3	B	444	GLY
3	B	1221	GLY
3	B	152	GLY
3	B	1384	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	672/969 (69%)	565 (84%)	107 (16%)	2	16
3	B	640/969 (66%)	548 (86%)	92 (14%)	3	19
All	All	1312/1938 (68%)	1113 (85%)	199 (15%)	3	17

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	25	VAL
3	A	26	ARG
3	A	33	ILE
3	A	43	HIS
3	A	44	LEU
3	A	45	VAL
3	A	46	TRP
3	A	48	ILE
3	A	49	VAL
3	A	75	THR
3	A	99	PHE
3	A	100	THR
3	A	102	LEU
3	A	108	PHE
3	A	122	VAL
3	A	139	THR
3	A	148	ARG
3	A	158	THR
3	A	182	ILE
3	A	203	LEU
3	A	204	LEU
3	A	208	THR
3	A	209	LEU
3	A	211	LEU
3	A	216	THR
3	A	220	ILE
3	A	231	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	233	SER
3	A	235	LEU
3	A	242	LEU
3	A	245	VAL
3	A	253	ASN
3	A	275	VAL
3	A	286	HIS
3	A	288	THR
3	A	298	MET
3	A	299	ASN
3	A	307	LEU
3	A	324	LEU
3	A	328	LEU
3	A	331	LEU
3	A	337	LEU
3	A	340	GLU
3	A	351	LEU
3	A	363	LYS
3	A	364	LEU
3	A	365	THR
3	A	368	LEU
3	A	378	LEU
3	A	429	LEU
3	A	432	VAL
3	A	453	LEU
3	A	462	THR
3	A	478	THR
3	A	501	ILE
3	A	503	ILE
3	A	520	THR
3	A	524	ARG
3	A	536	TYR
3	A	565	GLU
3	A	583	LEU
3	A	591	LEU
3	A	595	THR
3	A	611	LEU
3	A	620	VAL
3	A	627	GLU
3	A	1006	ASN
3	A	1009	LEU
3	A	1024	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1028	ARG
3	A	1054	THR
3	A	1055	PHE
3	A	1090	GLN
3	A	1111	ASP
3	A	1117	ARG
3	A	1126	ILE
3	A	1138	THR
3	A	1139	VAL
3	A	1148	THR
3	A	1162	LEU
3	A	1168	THR
3	A	1177	ASP
3	A	1183	LEU
3	A	1208	LEU
3	A	1233	LYS
3	A	1236	VAL
3	A	1237	VAL
3	A	1242	THR
3	A	1244	ILE
3	A	1268	LEU
3	A	1279	ASN
3	A	1288	ARG
3	A	1308	THR
3	A	1321	LEU
3	A	1336	THR
3	A	1342	ILE
3	A	1347	SER
3	A	1350	ILE
3	A	1382	ILE
3	A	1385	LEU
3	A	1386	ASP
3	A	1387	GLU
3	A	1430	THR
3	A	1432	VAL
3	A	1457	ARG
3	A	1462	LEU
3	A	1476	THR
3	B	22	LEU
3	B	45	VAL
3	B	46	TRP
3	B	48	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	75	THR
3	B	94	THR
3	B	95	VAL
3	B	99	PHE
3	B	100	THR
3	B	125	SER
3	B	139	THR
3	B	148	ARG
3	B	151	ASN
3	B	156	VAL
3	B	158	THR
3	B	162	ILE
3	B	175	THR
3	B	181	THR
3	B	182	ILE
3	B	196	ARG
3	B	203	LEU
3	B	208	THR
3	B	211	LEU
3	B	212	THR
3	B	229	GLN
3	B	231	PHE
3	B	235	LEU
3	B	241	ILE
3	B	242	LEU
3	B	272	LEU
3	B	280	THR
3	B	286	HIS
3	B	295	THR
3	B	296	LYS
3	B	303	ARG
3	B	308	LEU
3	B	314	ASN
3	B	318	SER
3	B	324	LEU
3	B	328	LEU
3	B	337	LEU
3	B	351	LEU
3	B	417	THR
3	B	445	ARG
3	B	447	ARG
3	B	453	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	462	THR
3	B	478	THR
3	B	494	GLU
3	B	509	THR
3	B	516	THR
3	B	520	THR
3	B	524	ARG
3	B	536	TYR
3	B	591	LEU
3	B	595	THR
3	B	605	ARG
3	B	1009	LEU
3	B	1024	ILE
3	B	1028	ARG
3	B	1041	GLN
3	B	1052	SER
3	B	1060	ARG
3	B	1062	SER
3	B	1111	ASP
3	B	1120	GLU
3	B	1130	LEU
3	B	1139	VAL
3	B	1167	SER
3	B	1168	THR
3	B	1177	ASP
3	B	1183	LEU
3	B	1208	LEU
3	B	1236	VAL
3	B	1268	LEU
3	B	1276	ARG
3	B	1296	LEU
3	B	1297	ARG
3	B	1300	ILE
3	B	1308	THR
3	B	1321	LEU
3	B	1338	ARG
3	B	1355	GLU
3	B	1374	ILE
3	B	1380	ARG
3	B	1400	ASP
3	B	1405	LEU
3	B	1414	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	1422	LEU
3	B	1452	ILE
3	B	1462	LEU
3	B	1478	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	51	ASN
3	A	264	ASN
3	B	264	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	E	14/34 (41%)	-0.60	0	100 100	144, 201, 233, 259	14 (100%)
1	G	20/34 (58%)	-0.50	0	100 100	66, 82, 159, 192	0
2	F	14/34 (41%)	-0.62	0	100 100	138, 196, 225, 254	14 (100%)
2	H	20/34 (58%)	-0.56	0	100 100	60, 85, 168, 199	0
3	A	1037/1144 (90%)	-0.51	1 (0%)	95 94	35, 83, 129, 225	0
3	B	1035/1144 (90%)	-0.49	1 (0%)	95 94	44, 89, 136, 212	0
All	All	2140/2424 (88%)	-0.50	2 (0%)	95 94	35, 86, 142, 259	28 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	166	PRO	3.3
3	A	37	ASP	2.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	B	1700	1/1	0.85	0.07	109,109,109,109	0
4	MG	H	1901	1/1	0.90	0.15	72,72,72,72	0
4	MG	A	1700	1/1	0.92	0.23	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.