



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 04:51 am BST

PDB ID : 6OVY  
Title : X-ray crystal structure of a bacterial reiterative transcription complex of pyrG promoter variant -1C  
Authors : Shin, Y.; Murakami, K.S.  
Deposited on : 2019-05-08  
Resolution : 3.00 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

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

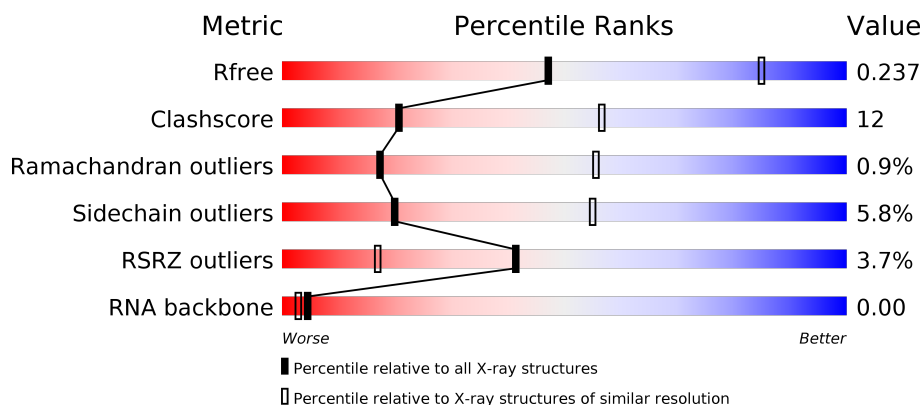
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 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	A	315	<div> <div>4%</div> <div>51% 19% . 28%</div> </div>
1	B	315	<div> <div>46% 23% . 30%</div> </div>
2	C	1119	<div> <div>4%</div> <div>65% 30% . .</div> </div>
3	D	1524	<div> <div>3%</div> <div>69% 26% . .</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	99	<div><div></div><div>3%</div><div>75%</div><div>18%</div><div>• 5%</div></div>
5	F	423	<div><div></div><div>5%</div><div>54%</div><div>23%</div><div>• 20%</div></div>
6	G	22	<div><div></div><div>5%</div><div>18%</div><div>36%</div><div>14%</div><div>32%</div></div>
7	H	27	<div><div></div><div>26%</div><div>33%</div><div>41%</div></div>
8	I	4	<div><div></div><div>25%</div><div>25%</div><div>25%</div><div>25%</div></div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28273 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8760	5543	1561	1632	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1485	Total	C	N	O	S	0	0	0
			11726	7432	2065	2194	35			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	338	Total	C	N	O	S	0	0	0
			2747	1736	500	507	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	46	THR	ALA	conflict	UNP Q72L95

- Molecule 6 is a DNA chain called DNA (5'-D(P\*CP\*AP\*TP\*CP\*AP\*GP\*AP\*GP\*CP\*CP\*CP\*CP\*AP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	15	Total	C	N	O	P	0	0	0
			304	144	60	85	15			

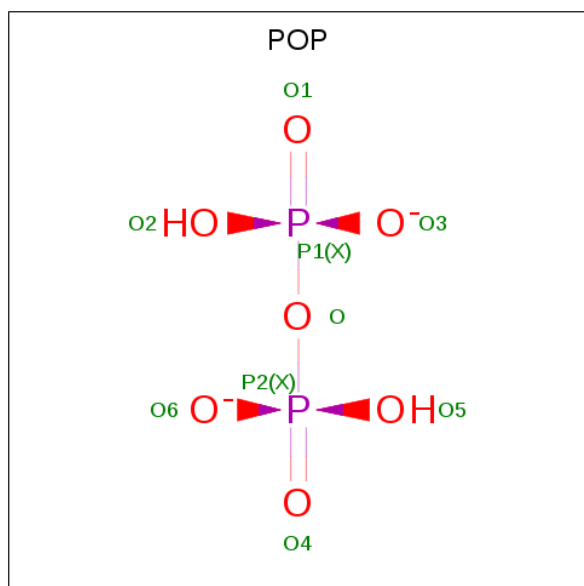
- Molecule 7 is a DNA chain called DNA (5'-D(\*TP\*AP\*TP\*AP\*AP\*TP\*GP\*GP\*GP\*TP\*CP\*TP\*GP\*AP\*TP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	16	Total	C	N	O	P	0	0	0
			330	159	60	96	15			

- Molecule 8 is a RNA chain called RNA (5'-D(\*(GTP))-R(P\*GP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	4	Total	C	N	O	P	0	0	0
			101	40	20	35	6			

- Molecule 9 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H<sub>2</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	O	P	0	0
			9	7	2		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	1	Total	Mg	0	0
			1	1		

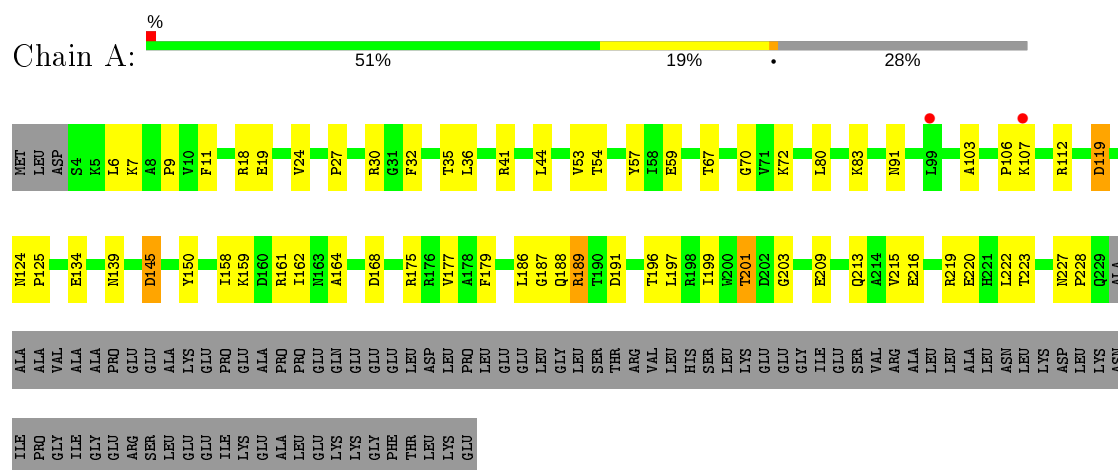
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total	Zn	0	0
			2	2		

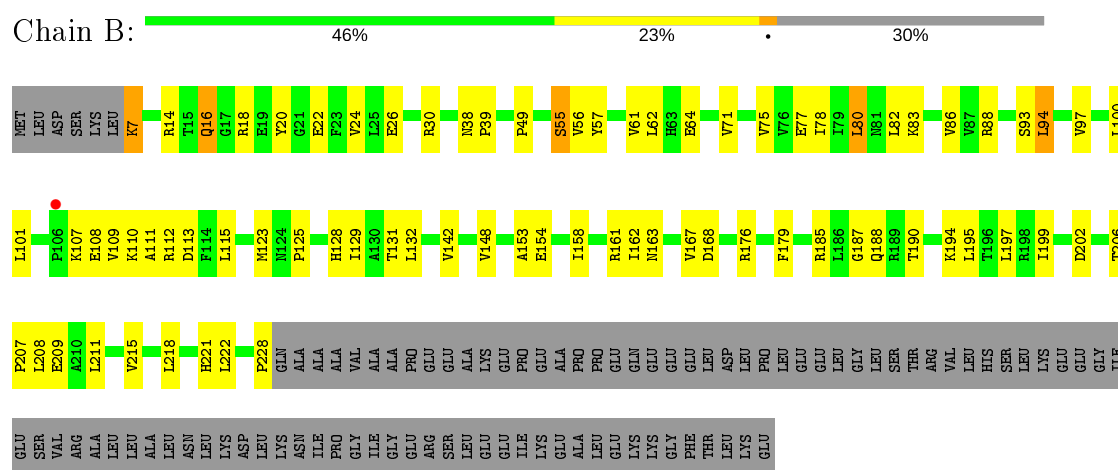
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

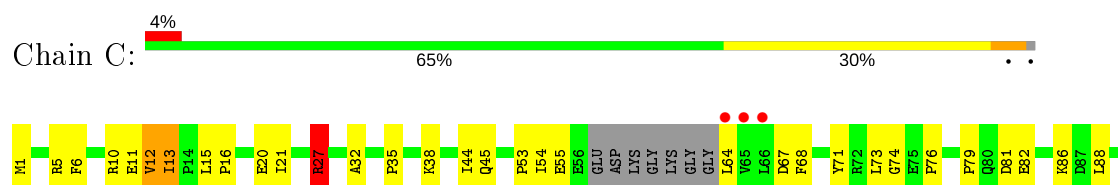
- Molecule 1: DNA-directed RNA polymerase subunit alpha

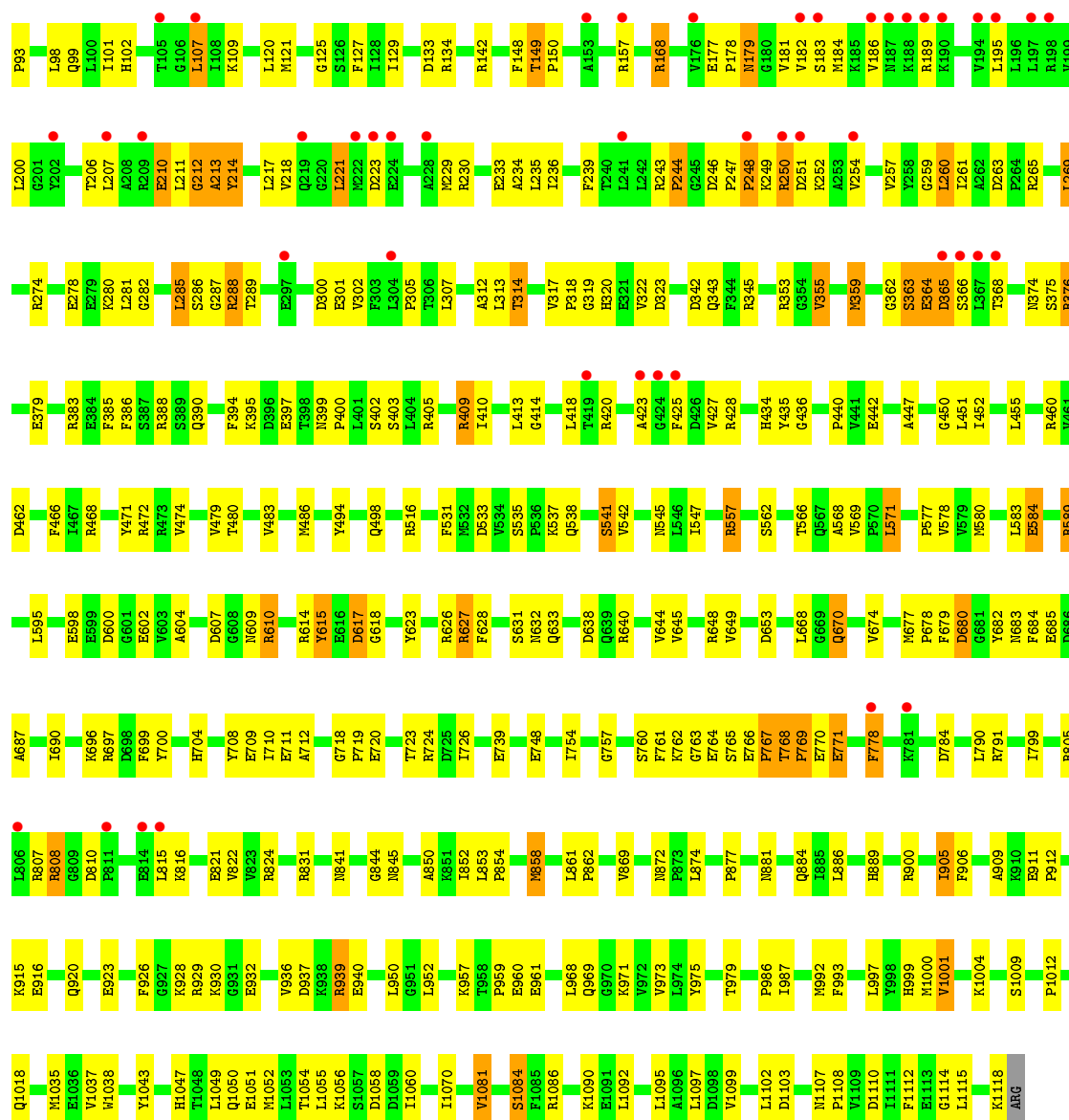


- Molecule 1: DNA-directed RNA polymerase subunit alpha

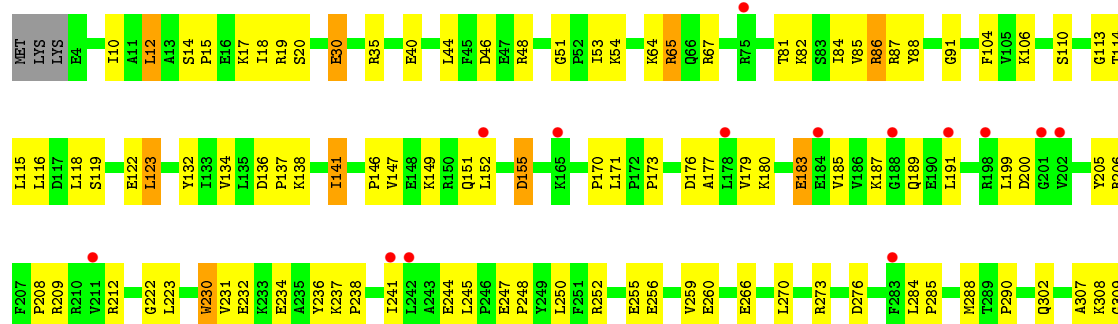


- Molecule 2: DNA-directed RNA polymerase subunit beta

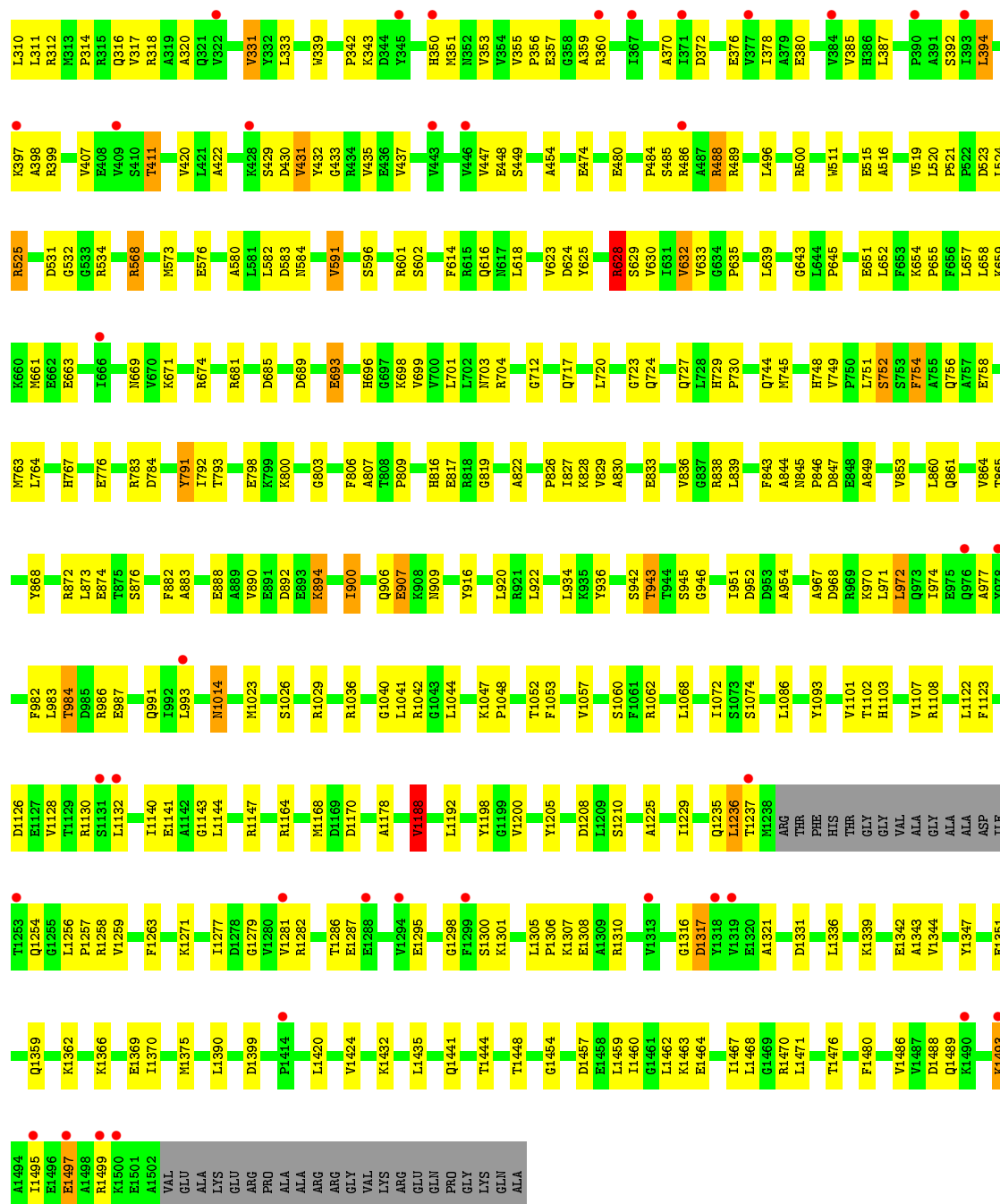




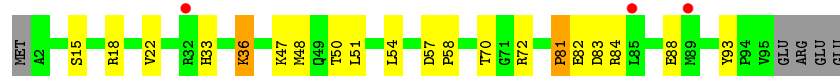
• Molecule 3: DNA-directed RNA polymerase subunit beta'







- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor SigA





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.83Å 102.48Å 295.60Å 90.00° 98.80° 90.00°	Depositor
Resolution (Å)	45.66 – 3.00 45.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (45.66-3.00) 96.7 (45.66-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.213 , 0.237 0.213 , 0.237	Depositor DCC
$R_{free}$ test set	1987 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.3	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	28273	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: GTP, ZN, MG, POP

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	0.57	0/1814	0.81	1/2466 (0.0%)
1	B	0.60	1/1782 (0.1%)	0.86	1/2424 (0.0%)
2	C	0.57	0/8927	0.83	8/12075 (0.1%)
3	D	0.60	1/11932 (0.0%)	0.84	10/16134 (0.1%)
4	E	0.51	0/775	0.80	0/1045
5	F	0.49	0/2791	0.73	1/3754 (0.0%)
6	G	1.21	2/341 (0.6%)	1.09	4/522 (0.8%)
7	H	1.06	1/369 (0.3%)	1.11	1/567 (0.2%)
8	I	1.32	1/77 (1.3%)	1.59	1/119 (0.8%)
All	All	0.60	6/28808 (0.0%)	0.84	27/39106 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	1	DT	C1'-N1	8.54	1.60	1.49
6	G	14	DC	O3'-P	-6.70	1.53	1.61
6	G	10	DG	C2-N3	5.50	1.37	1.32
3	D	791	TYR	CE2-CZ	5.45	1.45	1.38
1	B	154	GLU	CG-CD	5.34	1.59	1.51
8	I	4	G	O3'-P	-5.24	1.54	1.61

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	35	ARG	NE-CZ-NH1	-12.50	114.05	120.30
3	D	35	ARG	NE-CZ-NH2	11.03	125.81	120.30
2	C	409	ARG	CG-CD-NE	7.70	127.97	111.80
3	D	12	LEU	CB-CG-CD2	-7.70	97.91	111.00
3	D	1493	LYS	CD-CE-NZ	-7.50	94.46	111.70
2	C	816	LYS	CD-CE-NZ	-7.21	95.13	111.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	107	LEU	CA-CB-CG	7.19	131.83	115.30
6	G	12	DC	O5'-P-OP2	-6.76	99.62	105.70
2	C	27	ARG	NE-CZ-NH2	6.68	123.64	120.30
6	G	10	DG	O4'-C4'-C3'	-6.29	101.99	104.50
7	H	5	DA	O4'-C1'-N9	6.07	112.25	108.00
3	D	583	ASP	CB-CG-OD2	-5.99	112.91	118.30
8	I	3	G	O5'-P-OP1	-5.79	100.49	105.70
1	B	100	LEU	CB-CG-CD2	5.76	120.79	111.00
3	D	1462	LEU	CA-CB-CG	5.70	128.41	115.30
3	D	1029	ARG	NE-CZ-NH2	-5.63	117.49	120.30
2	C	383	ARG	NE-CZ-NH1	5.58	123.09	120.30
5	F	271	LEU	CA-CB-CG	5.42	127.77	115.30
2	C	383	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	80	LEU	CB-CG-CD2	-5.25	102.08	111.00
2	C	5	ARG	CG-CD-NE	5.22	122.76	111.80
6	G	12	DC	O4'-C4'-C3'	-5.21	102.42	104.50
2	C	13	ILE	CG1-CB-CG2	5.18	122.80	111.40
3	D	993	LEU	CA-CB-CG	5.18	127.21	115.30
3	D	1188	VAL	CG1-CB-CG2	5.13	119.11	110.90
6	G	13	DC	O5'-P-OP1	5.07	116.78	110.70
3	D	628	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1782	0	1834	42	0
1	B	1750	0	1797	61	0
2	C	8760	0	8859	275	0
3	D	11726	0	11949	303	0
4	E	761	0	778	15	0
5	F	2747	0	2831	69	0
6	G	304	0	167	10	0
7	H	330	0	185	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	101	0	43	5	0
9	D	9	0	0	0	0
10	D	1	0	0	0	0
11	D	2	0	0	0	0
All	All	28273	0	28443	696	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 12.

All (696) 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)
3:D:260:GLU:OE1	3:D:273:ARG:NH1	1.86	1.07
6:G:17:DA:C8	6:G:17:DA:H5"	1.94	1.01
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.35	0.91
3:D:1256:LEU:O	3:D:1257:PRO:C	2.10	0.89
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.07	0.86
3:D:343:LYS:NZ	3:D:380:GLU:OE2	2.10	0.85
2:C:571:LEU:HD22	2:C:700:TYR:HA	1.57	0.85
2:C:247:PRO:O	2:C:249:LYS:N	2.11	0.82
6:G:17:DA:H8	6:G:17:DA:H5"	1.39	0.82
2:C:674:VAL:HG23	2:C:869:VAL:HB	1.62	0.82
2:C:109:LYS:HG2	2:C:368:THR:HG22	1.61	0.81
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.63	0.80
2:C:1112:PHE:HD2	3:D:88:TYR:HD2	1.30	0.80
2:C:236:ILE:HG23	2:C:248:PRO:HB2	1.64	0.79
3:D:952:ASP:HA	3:D:1062:ARG:HH21	1.49	0.78
2:C:905:ILE:HG23	2:C:906:PHE:HD1	1.49	0.78
2:C:409:ARG:HD3	2:C:452:ILE:CG2	2.14	0.78
3:D:1093:TYR:OH	3:D:1441:GLN:NE2	2.15	0.78
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.67	0.77
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.68	0.76
2:C:274:ARG:HD2	2:C:288:ARG:HG2	1.65	0.76
2:C:235:LEU:HD21	2:C:254:VAL:HG22	1.67	0.76
3:D:654:LYS:HG2	3:D:674:ARG:HH12	1.51	0.76
2:C:541:SER:OG	2:C:542:VAL:N	2.18	0.75
2:C:999:HIS:HB3	2:C:1004:LYS:HZ1	1.51	0.75
3:D:1236:LEU:HD12	3:D:1359:GLN:HG3	1.67	0.75
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.69	0.74
2:C:926:PHE:CE2	2:C:960:GLU:HG3	2.23	0.73
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.71	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:954:ALA:HB3	3:D:1062:ARG:HG3	1.71	0.72
1:B:185:ARG:NH1	1:B:187:GLY:O	2.23	0.72
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.71	0.72
2:C:853:LEU:HB2	2:C:858:MET:CE	2.20	0.71
2:C:649:VAL:HG13	2:C:653:ASP:HB2	1.73	0.71
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.73	0.71
2:C:498:GLN:HE21	3:D:1068:LEU:HD22	1.55	0.71
2:C:547:ILE:O	2:C:905:ILE:HD11	1.91	0.71
2:C:709:GLU:HG3	2:C:824:ARG:HG2	1.71	0.71
2:C:313:LEU:HB2	2:C:320:HIS:HB3	1.73	0.71
2:C:1112:PHE:HD2	3:D:88:TYR:CD2	2.09	0.70
2:C:805:ARG:HH21	2:C:807:ARG:HD3	1.56	0.70
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.74	0.69
1:B:77:GLU:HG2	3:D:872:ARG:HH11	1.58	0.69
3:D:1305:LEU:HD12	3:D:1306:PRO:HD2	1.75	0.69
3:D:231:VAL:O	3:D:236:TYR:OH	2.11	0.69
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.27	0.69
3:D:1068:LEU:O	3:D:1072:ILE:HG12	1.93	0.68
1:A:216:GLU:OE1	1:A:219:ARG:NH2	2.27	0.68
3:D:807:ALA:O	3:D:830:ALA:HB2	1.92	0.68
3:D:132:TYR:OH	3:D:568:ARG:NH2	2.26	0.68
2:C:1052:MET:HG3	3:D:623:VAL:HG11	1.74	0.68
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.29	0.68
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.76	0.68
3:D:1236:LEU:CD1	3:D:1359:GLN:HG3	2.25	0.67
3:D:433:GLY:HA2	3:D:449:SER:O	1.94	0.67
2:C:614:ARG:NH2	2:C:618:GLY:O	2.28	0.67
3:D:284:LEU:HD22	3:D:288:MET:HG2	1.77	0.67
2:C:45:GLN:HG2	2:C:71:TYR:HE2	1.60	0.66
3:D:1281:VAL:HG22	3:D:1317:ASP:H	1.60	0.66
2:C:181:VAL:HG23	2:C:221:LEU:HA	1.76	0.66
1:B:80:LEU:HG	3:D:844:ALA:HA	1.77	0.66
5:F:392:VAL:HG22	5:F:396:ARG:HD2	1.76	0.66
5:F:129:GLU:HG2	5:F:144:ILE:HG13	1.77	0.66
1:B:88:ARG:NH1	1:B:123:MET:SD	2.68	0.66
3:D:657:LEU:HG	3:D:661:MET:HE2	1.77	0.66
5:F:91:VAL:O	5:F:193:ARG:NH2	2.27	0.66
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.78	0.66
3:D:1499:ARG:HH12	4:E:81:PRO:HD2	1.59	0.66
2:C:13:ILE:HD13	2:C:483:VAL:HG11	1.78	0.66
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.76	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:420:ARG:NH2	8:I:2:GTP:O1B	2.28	0.65
2:C:150:PRO:HD3	2:C:322:VAL:CG1	2.26	0.65
2:C:207:LEU:O	2:C:211:LEU:HB2	1.96	0.65
2:C:428:ARG:NH2	2:C:447:ALA:O	2.30	0.65
2:C:409:ARG:HD3	2:C:452:ILE:HG21	1.79	0.65
2:C:1004:LYS:HD3	3:D:744:GLN:NE2	2.12	0.65
2:C:937:ASP:OD1	2:C:939:ARG:HG2	1.96	0.65
2:C:1112:PHE:CD2	3:D:88:TYR:HD2	2.14	0.65
2:C:189:ARG:HH22	2:C:244:PRO:HD2	1.62	0.65
3:D:171:LEU:HD13	3:D:392:SER:HA	1.79	0.65
2:C:27:ARG:CZ	2:C:27:ARG:HB3	2.28	0.64
3:D:1256:LEU:O	3:D:1258:ARG:N	2.29	0.64
2:C:286:SER:OG	2:C:301:GLU:OE1	2.16	0.64
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.79	0.64
3:D:573:MET:SD	5:F:210:LEU:HB3	2.36	0.64
2:C:1018:GLN:HG3	2:C:1060:ILE:HD11	1.80	0.64
5:F:112:ALA:O	5:F:116:LEU:HB2	1.98	0.64
2:C:474:VAL:HG22	2:C:479:VAL:HG22	1.79	0.63
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.80	0.63
5:F:163:LEU:HB3	5:F:174:LEU:HD22	1.80	0.63
3:D:288:MET:SD	3:D:307:ALA:HB2	2.38	0.63
2:C:886:LEU:HD11	3:D:951:ILE:HG12	1.81	0.63
3:D:187:LYS:N	3:D:200:ASP:OD2	2.31	0.63
1:B:86:VAL:HG21	1:B:202:ASP:HB2	1.80	0.62
2:C:157:ARG:HH11	2:C:314:THR:HG21	1.63	0.62
2:C:363:SER:O	2:C:365:ASP:N	2.31	0.62
5:F:392:VAL:HG13	5:F:396:ARG:HB2	1.79	0.62
5:F:392:VAL:CG1	5:F:396:ARG:HB2	2.29	0.62
2:C:1035:MET:HG2	2:C:1038:TRP:CZ3	2.35	0.62
1:A:186:LEU:O	1:A:188:GLN:N	2.29	0.62
2:C:1051:GLU:OE2	3:D:752:SER:HB3	2.00	0.62
2:C:471:TYR:OH	2:C:516:ARG:NH2	2.32	0.62
3:D:984:THR:HG23	3:D:987:GLU:OE2	1.99	0.62
2:C:313:LEU:O	2:C:313:LEU:HG	1.99	0.61
3:D:843:PHE:HE2	3:D:864:VAL:HG11	1.65	0.61
5:F:392:VAL:HG12	5:F:397:ILE:HG12	1.81	0.61
1:A:201:THR:HG23	1:A:203:GLY:H	1.65	0.61
2:C:243:ARG:NH2	7:H:9:DG:O6	2.33	0.61
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.83	0.61
3:D:828:LYS:HG3	3:D:833:GLU:OE2	2.00	0.61
2:C:764:GLU:HB2	3:D:54:LYS:HE3	1.82	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:537:LYS:HD3	2:C:583:LEU:HD11	1.83	0.61
3:D:1489:GLN:HG3	3:D:1493:LYS:HE3	1.82	0.61
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.83	0.60
3:D:1295:GLU:HA	3:D:1300:SER:HB2	1.84	0.60
3:D:614:PHE:HA	3:D:618:LEU:HD23	1.83	0.60
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.36	0.60
3:D:952:ASP:HA	3:D:1062:ARG:NH2	2.17	0.60
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.36	0.60
3:D:616:GLN:HG3	3:D:616:GLN:O	2.00	0.60
2:C:269:LEU:O	2:C:288:ARG:HB3	2.01	0.60
3:D:1486:VAL:HG22	4:E:22:VAL:HG13	1.83	0.60
3:D:212:ARG:HD3	3:D:342:PRO:HB2	1.84	0.60
3:D:658:LEU:HA	3:D:661:MET:HE3	1.82	0.60
2:C:763:GLY:O	2:C:766:GLU:HG2	2.02	0.60
3:D:689:ASP:OD2	4:E:51:LEU:HD11	2.02	0.60
2:C:602:GLU:HB2	2:C:648:ARG:HH11	1.66	0.59
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.84	0.59
3:D:87:ARG:HB2	3:D:88:TYR:CE1	2.37	0.59
6:G:8:DG:H5'	6:G:8:DG:H8	1.68	0.59
2:C:230:ARG:HB2	2:C:233:GLU:HG2	1.85	0.59
2:C:987:ILE:HD11	3:D:946:GLY:HA2	1.83	0.59
3:D:357:GLU:HB2	3:D:387:LEU:HD23	1.84	0.59
5:F:127:ILE:O	5:F:131:VAL:HG23	2.03	0.59
8:I:3:G:C2'	8:I:4:G:H5'	2.33	0.59
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.85	0.59
2:C:1058:ASP:OD2	2:C:1084:SER:HB2	2.03	0.58
3:D:1499:ARG:HG2	4:E:84:ARG:NH2	2.18	0.58
3:D:480:GLU:OE1	3:D:488:ARG:HD2	2.03	0.58
3:D:1263:PHE:HA	3:D:1375:MET:HE1	1.84	0.58
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.39	0.58
1:B:128:HIS:HE1	1:B:131:THR:HG22	1.68	0.58
2:C:627:ARG:O	2:C:628:PHE:HB2	2.03	0.58
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.85	0.58
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.37	0.58
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.86	0.58
3:D:1144:LEU:O	3:D:1147:ARG:HG3	2.04	0.58
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.86	0.58
2:C:189:ARG:NH2	2:C:244:PRO:HD2	2.18	0.58
2:C:425:PHE:CE2	3:D:1086:LEU:HD12	2.39	0.57
2:C:748:GLU:HA	2:C:799:ILE:HD13	1.86	0.57
3:D:800:LYS:NZ	3:D:819:GLY:O	2.35	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:136:ASP:OD2	3:D:138:LYS:HE3	2.03	0.57
3:D:1444:THR:O	3:D:1448:THR:HG23	2.03	0.57
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.39	0.57
3:D:977:ALA:HB3	3:D:983:LEU:HD12	1.87	0.57
2:C:177:GLU:HG3	2:C:183:SER:HB3	1.86	0.57
3:D:64:LYS:O	3:D:65:ARG:HD2	2.05	0.57
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.86	0.57
2:C:708:TYR:HB3	2:C:790:LEU:HD21	1.85	0.57
3:D:1205:TYR:CZ	3:D:1366:LYS:HE2	2.40	0.57
3:D:1286:THR:HG22	3:D:1287:GLU:H	1.70	0.57
3:D:809:PRO:HB3	3:D:839:LEU:HD13	1.85	0.57
2:C:1054:THR:OG1	2:C:1055:LEU:N	2.37	0.57
4:E:70:THR:OG1	4:E:72:ARG:HG3	2.04	0.57
3:D:1235:GLN:O	3:D:1235:GLN:HG3	2.05	0.57
2:C:375:SER:OG	2:C:379:GLU:OE1	2.14	0.57
3:D:1126:ASP:O	3:D:1130:ARG:HA	2.04	0.56
5:F:358:LEU:HD22	5:F:366:ALA:HB1	1.86	0.56
2:C:680:ASP:OD1	3:D:943:THR:HG21	2.05	0.56
7:H:3:DT:H2'	7:H:4:DA:C8	2.40	0.56
1:B:185:ARG:NH2	3:D:689:ASP:OD1	2.33	0.56
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.87	0.56
1:A:70:GLY:H	2:C:607:ASP:CG	2.09	0.56
3:D:485:SER:O	3:D:486:ARG:HB2	2.05	0.56
3:D:798:GLU:OE1	3:D:822:ALA:HB1	2.04	0.56
2:C:212:GLY:H	2:C:218:VAL:HG11	1.69	0.56
2:C:394:PHE:CE2	2:C:632:ASN:HB3	2.41	0.56
3:D:1047:LYS:HB3	3:D:1048:PRO:HD2	1.88	0.56
5:F:415:THR:HB	5:F:417:LYS:HE3	1.86	0.56
5:F:377:ASP:CG	5:F:381:HIS:HE2	2.08	0.56
1:A:112:ARG:HG2	1:A:125:PRO:HB3	1.86	0.55
3:D:87:ARG:HB2	3:D:88:TYR:CD1	2.41	0.55
7:H:19:DT:H2''	7:H:20:DC:H5'	1.87	0.55
1:A:159:LYS:HG2	1:A:164:ALA:HB3	1.88	0.55
2:C:214:TYR:O	2:C:217:LEU:N	2.37	0.55
3:D:411:THR:HA	3:D:435:VAL:HG12	1.88	0.55
8:I:3:G:C3'	8:I:4:G:H5'	2.35	0.55
3:D:669:ASN:ND2	5:F:420:ASP:OD2	2.36	0.55
2:C:748:GLU:O	3:D:681:ARG:NH2	2.40	0.55
3:D:173:PRO:HA	3:D:209:ARG:HH12	1.72	0.55
3:D:671:LYS:HE3	5:F:421:PHE:HA	1.87	0.55
1:B:57:TYR:CG	1:B:161:ARG:HD2	2.42	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:148:PHE:O	2:C:322:VAL:HG13	2.07	0.55
7:H:25:DG:H5'	7:H:25:DG:C8	2.43	0.54
5:F:360:LYS:HD3	5:F:411:HIS:CE1	2.43	0.54
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.36	0.54
2:C:928:LYS:O	2:C:932:GLU:HB2	2.07	0.54
3:D:1143:GLY:O	3:D:1147:ARG:HD2	2.07	0.54
8:I:3:G:H2'	8:I:4:G:H5'	1.90	0.54
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.42	0.54
2:C:390:GLN:OE1	2:C:414:GLY:HA2	2.06	0.54
2:C:604:ALA:O	2:C:645:VAL:HG13	2.08	0.54
3:D:1486:VAL:CG2	4:E:22:VAL:HG13	2.38	0.54
3:D:170:PRO:HA	3:D:392:SER:HB3	1.90	0.54
3:D:486:ARG:HA	3:D:489:ARG:HH21	1.73	0.54
4:E:36:LYS:HB3	4:E:93:TYR:HB3	1.90	0.54
1:A:44:LEU:HD13	1:A:199:ILE:HD12	1.90	0.53
2:C:557:ARG:HG3	2:C:844:GLY:HA3	1.90	0.53
2:C:678:PRO:HA	2:C:683:ASN:HD22	1.73	0.53
3:D:1281:VAL:CG2	3:D:1317:ASP:H	2.21	0.53
1:A:220:GLU:O	1:A:223:THR:OG1	2.26	0.53
1:B:101:LEU:HD21	1:B:109:VAL:HG11	1.89	0.53
3:D:752:SER:OG	3:D:754:PHE:N	2.41	0.53
1:A:222:LEU:HD22	1:B:215:VAL:HG23	1.89	0.53
2:C:249:LYS:HB3	2:C:252:LYS:HB2	1.90	0.53
3:D:1282:ARG:NH2	3:D:1295:GLU:OE2	2.20	0.53
3:D:1014:ASN:OD1	3:D:1014:ASN:N	2.41	0.53
5:F:338:LEU:HD23	5:F:339:PRO:HD2	1.90	0.53
1:A:30:ARG:HD2	1:A:191:ASP:OD2	2.08	0.53
1:B:57:TYR:CD1	1:B:161:ARG:HD2	2.44	0.53
2:C:214:TYR:O	2:C:218:VAL:N	2.40	0.53
2:C:280:LYS:NZ	2:C:323:ASP:OD1	2.38	0.53
3:D:1101:VAL:HG11	3:D:1424:VAL:HG12	1.91	0.53
3:D:696:HIS:ND1	4:E:57:ASP:OD1	2.42	0.53
3:D:350:HIS:CD2	5:F:232:ARG:HG2	2.43	0.53
3:D:65:ARG:HD3	5:F:378:GLY:HA2	1.89	0.53
2:C:20:GLU:OE1	2:C:460:ARG:NH2	2.41	0.53
2:C:53:PRO:HB3	2:C:67:ASP:OD1	2.09	0.53
3:D:122:GLU:HG2	3:D:152:LEU:HD11	1.89	0.53
3:D:18:ILE:HG21	3:D:516:ALA:O	2.08	0.53
3:D:1141:GLU:HG2	3:D:1168:MET:CE	2.38	0.53
3:D:259:VAL:HG13	3:D:270:LEU:HD21	1.91	0.53
5:F:384:GLU:HG2	5:F:394:ARG:CZ	2.39	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:184:MET:HE2	2:C:186:VAL:HG21	1.91	0.53
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.90	0.53
2:C:568:ALA:CB	2:C:668:LEU:HB3	2.38	0.53
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.90	0.53
3:D:860:LEU:O	3:D:876:SER:HB2	2.09	0.53
3:D:1198:TYR:CE2	3:D:1460:ILE:HD13	2.44	0.52
1:B:71:VAL:HG22	1:B:132:LEU:CD1	2.38	0.52
2:C:580:MET:HB3	2:C:584:GLU:CD	2.30	0.52
5:F:350:LEU:HD13	5:F:421:PHE:CD1	2.43	0.52
3:D:1321:ALA:O	3:D:1339:LYS:HG3	2.10	0.52
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.91	0.52
2:C:285:LEU:HD21	2:C:302:VAL:HG22	1.90	0.52
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	1.90	0.52
1:B:206:THR:HG22	1:B:208:LEU:H	1.75	0.52
5:F:96:LEU:O	5:F:100:VAL:HG23	2.10	0.52
2:C:312:ALA:HB3	2:C:320:HIS:NE2	2.25	0.52
2:C:362:GLY:O	2:C:363:SER:OG	2.26	0.52
6:G:7:DA:H2"	6:G:8:DG:OP2	2.10	0.52
1:A:222:LEU:HB3	1:B:215:VAL:HG23	1.91	0.52
2:C:690:ILE:HD11	2:C:852:ILE:HG12	1.92	0.52
3:D:398:ALA:HB2	3:D:447:VAL:HA	1.91	0.52
3:D:699:VAL:N	3:D:756:GLN:OE1	2.41	0.52
3:D:864:VAL:HG12	3:D:865:THR:N	2.25	0.52
3:D:88:TYR:CD1	3:D:88:TYR:N	2.77	0.52
5:F:420:ASP:O	5:F:422:LEU:N	2.42	0.52
3:D:520:LEU:O	3:D:525:ARG:NH1	2.40	0.52
3:D:693:GLU:HG3	4:E:48:MET:HE1	1.91	0.52
2:C:74:GLY:HA3	2:C:93:PRO:HG2	1.92	0.51
6:G:15:DA:C2	8:I:2:GTP:C2	2.98	0.51
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.91	0.51
2:C:999:HIS:CD2	2:C:1004:LYS:HZ1	2.28	0.51
2:C:440:PRO:HB2	3:D:1074:SER:OG	2.10	0.51
3:D:44:LEU:O	3:D:525:ARG:NH2	2.34	0.51
1:A:41:ARG:HG3	1:A:177:VAL:CG1	2.41	0.51
1:B:111:ALA:HA	1:B:129:ILE:HD11	1.93	0.51
2:C:76:PRO:HG3	2:C:120:LEU:HD12	1.92	0.51
2:C:27:ARG:NH1	2:C:27:ARG:HB3	2.25	0.51
3:D:185:VAL:HG13	3:D:189:GLN:HB3	1.93	0.51
3:D:288:MET:O	3:D:290:PRO:HD3	2.11	0.51
3:D:658:LEU:HD23	3:D:661:MET:HE1	1.91	0.51
5:F:109:GLY:O	5:F:113:ILE:HG13	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:402:SER:HA	2:C:566:THR:HG23	1.92	0.51
3:D:407:VAL:HG23	3:D:422:ALA:HB2	1.92	0.51
3:D:803:GLY:HA2	3:D:826:PRO:O	2.09	0.51
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.46	0.51
3:D:500:ARG:HH12	3:D:1390:LEU:HD21	1.75	0.51
3:D:652:LEU:HB3	3:D:749:VAL:HG21	1.93	0.51
3:D:654:LYS:HG2	3:D:674:ARG:NH1	2.23	0.51
5:F:88:ILE:HD11	5:F:192:LEU:HD13	1.93	0.51
5:F:194:LEU:HB2	7:H:6:DT:C2	2.45	0.51
3:D:1168:MET:O	3:D:1168:MET:HE3	2.11	0.51
1:B:110:LYS:NZ	1:B:128:HIS:HB2	2.25	0.51
2:C:150:PRO:CD	2:C:322:VAL:HG11	2.40	0.51
2:C:571:LEU:CD2	2:C:700:TYR:HA	2.35	0.51
3:D:91:GLY:O	3:D:519:VAL:N	2.42	0.51
5:F:360:LYS:HD3	5:F:411:HIS:ND1	2.26	0.51
3:D:1256:LEU:O	3:D:1259:VAL:N	2.43	0.51
5:F:155:THR:O	5:F:159:ILE:HG12	2.11	0.51
2:C:274:ARG:NH2	2:C:278:GLU:OE2	2.43	0.50
2:C:35:PRO:HG2	2:C:38:LYS:HD3	1.93	0.50
2:C:861:LEU:HB3	2:C:862:PRO:HD2	1.93	0.50
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.46	0.50
2:C:999:HIS:CB	2:C:1004:LYS:HZ1	2.21	0.50
3:D:30:GLU:HG2	3:D:40:GLU:HG2	1.93	0.50
2:C:617:ASP:OD1	2:C:617:ASP:N	2.45	0.50
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.42	0.50
3:D:843:PHE:CE2	3:D:864:VAL:HG11	2.45	0.50
5:F:202:TYR:HE1	5:F:248:ASN:HD21	1.59	0.50
1:A:32:PHE:HA	1:A:35:THR:HB	1.93	0.50
2:C:182:VAL:HG11	2:C:307:LEU:HD11	1.94	0.50
2:C:129:ILE:HG12	2:C:386:PHE:HB3	1.92	0.50
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.22	0.50
2:C:64:LEU:HD13	2:C:359:MET:HG2	1.94	0.50
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.93	0.50
3:D:1279:GLY:HA3	3:D:1295:GLU:O	2.12	0.50
5:F:313:GLU:OE1	5:F:314:PRO:HD2	2.11	0.50
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.45	0.50
3:D:1256:LEU:HB3	3:D:1257:PRO:HD3	1.94	0.50
3:D:967:ALA:O	3:D:971:LEU:HB2	2.12	0.50
3:D:155:ASP:OD1	3:D:568:ARG:NH1	2.43	0.50
2:C:769:PRO:HG2	5:F:374:GLY:O	2.11	0.50
2:C:712:ALA:HB3	2:C:821:GLU:HG3	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:VAL:CG2	1:B:202:ASP:HB2	2.42	0.49
3:D:237:LYS:HA	3:D:318:ARG:HG3	1.94	0.49
5:F:358:LEU:CD2	5:F:366:ALA:HB1	2.42	0.49
3:D:1495:ILE:HG23	4:E:88:GLU:OE1	2.12	0.49
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	1.93	0.49
3:D:1263:PHE:HD2	3:D:1375:MET:CE	2.26	0.49
2:C:249:LYS:HG2	2:C:251:ASP:OD1	2.13	0.49
2:C:428:ARG:HB3	2:C:450:GLY:HA3	1.93	0.49
3:D:1053:PHE:CZ	3:D:1072:ILE:HD12	2.47	0.49
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.95	0.49
2:C:498:GLN:NE2	3:D:1068:LEU:HB2	2.27	0.49
5:F:157:GLU:O	5:F:161:GLN:HG2	2.12	0.49
2:C:32:ALA:HB2	2:C:73:LEU:HD12	1.93	0.49
3:D:776:GLU:OE2	3:D:1362:LYS:HD3	2.13	0.49
5:F:197:SER:HA	5:F:200:LYS:HE3	1.94	0.49
2:C:239:PHE:HD2	2:C:248:PRO:HA	1.77	0.49
2:C:259:GLY:HA2	2:C:263:ASP:CB	2.43	0.49
2:C:615:TYR:HH	2:C:623:TYR:HH	1.52	0.49
2:C:683:ASN:HB3	2:C:872:ASN:ND2	2.16	0.49
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.48	0.49
2:C:687:ALA:HB1	2:C:850:ALA:HB2	1.94	0.49
5:F:392:VAL:CG1	5:F:397:ILE:HG12	2.43	0.49
2:C:462:ASP:OD1	2:C:466:PHE:N	2.46	0.49
2:C:739:GLU:OE1	2:C:739:GLU:N	2.46	0.49
3:D:1459:LEU:HD23	3:D:1464:GLU:HB3	1.95	0.49
2:C:263:ASP:O	2:C:265:ARG:N	2.40	0.48
2:C:769:PRO:HG2	3:D:65:ARG:NH1	2.28	0.48
5:F:123:ASP:OD1	5:F:125:ASP:HB2	2.13	0.48
2:C:300:ASP:OD1	2:C:301:GLU:N	2.44	0.48
1:B:128:HIS:HE1	1:B:131:THR:CG2	2.27	0.48
1:B:55:SER:HB2	1:B:158:ILE:HD11	1.94	0.48
2:C:86:LYS:HB2	2:C:88:LEU:HG	1.95	0.48
3:D:241:ILE:HD11	3:D:310:LEU:HD23	1.95	0.48
5:F:104:ARG:HH11	5:F:104:ARG:HG2	1.78	0.48
3:D:1399:ASP:OD2	3:D:1432:LYS:NZ	2.46	0.48
3:D:1468:LEU:HB3	3:D:1470:ARG:HG3	1.96	0.48
3:D:703:ASN:HA	3:D:712:GLY:O	2.12	0.48
2:C:1056:LYS:HD2	3:D:751:LEU:HG	1.94	0.48
3:D:248:PRO:HG3	3:D:308:LYS:HE3	1.94	0.48
3:D:629:SER:OG	3:D:630:VAL:N	2.46	0.48
2:C:472:ARG:HD2	2:C:480:THR:O	2.12	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:598:GLU:N	2:C:615:TYR:OH	2.34	0.48
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.96	0.48
3:D:580:ALA:O	3:D:584:ASN:HB2	2.14	0.48
1:B:109:VAL:HG23	1:B:132:LEU:HD23	1.96	0.48
6:G:14:DC:H2'	6:G:15:DA:C8	2.49	0.48
3:D:250:LEU:O	3:D:252:ARG:HG3	2.14	0.47
3:D:860:LEU:HB2	3:D:861:GLN:NE2	2.28	0.47
3:D:764:LEU:HD23	3:D:767:HIS:NE2	2.29	0.47
2:C:1060:ILE:HD13	5:F:338:LEU:HD11	1.96	0.47
3:D:845:ASN:HB2	3:D:846:PRO:HD2	1.95	0.47
6:G:11:DC:H2'	6:G:12:DC:C6	2.49	0.47
5:F:289:GLU:N	5:F:289:GLU:OE1	2.47	0.47
2:C:862:PRO:HA	2:C:975:TYR:CE2	2.49	0.47
3:D:67:ARG:NH1	5:F:377:ASP:OD1	2.47	0.47
1:A:188:GLN:HG2	1:A:189:ARG:HG2	1.97	0.47
1:B:112:ARG:HB3	1:B:125:PRO:CB	2.44	0.47
2:C:54:ILE:HG21	2:C:355:VAL:HG12	1.96	0.47
3:D:15:PRO:O	3:D:19:ARG:HG3	2.15	0.47
3:D:394:LEU:HG	3:D:394:LEU:O	2.15	0.47
3:D:689:ASP:CG	4:E:51:LEU:HD11	2.35	0.47
3:D:82:LYS:HB2	3:D:84:ILE:HG22	1.96	0.47
3:D:693:GLU:HA	4:E:48:MET:HE1	1.96	0.47
1:B:179:PHE:HB3	1:B:197:LEU:HD12	1.97	0.47
1:B:56:VAL:HG23	1:B:142:VAL:HG12	1.97	0.47
2:C:405:ARG:HD2	2:C:442:GLU:OE2	2.14	0.47
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.96	0.47
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.49	0.47
2:C:200:LEU:HD13	2:C:300:ASP:HB2	1.96	0.47
2:C:13:ILE:HG23	2:C:483:VAL:HG21	1.96	0.47
2:C:494:TYR:CD1	2:C:531:PHE:HE2	2.32	0.47
2:C:68:PHE:HA	2:C:98:LEU:HD23	1.97	0.47
5:F:193:ARG:HB2	7:H:6:DT:H1'	1.96	0.47
2:C:6:PHE:CE1	2:C:909:ALA:HB2	2.49	0.47
2:C:850:ALA:HA	3:D:632:VAL:HG22	1.97	0.47
2:C:916:GLU:O	2:C:920:GLN:HG3	2.14	0.47
3:D:645:PRO:HB3	3:D:723:GLY:O	2.15	0.47
3:D:701:LEU:HB2	3:D:748:HIS:HB2	1.97	0.47
3:D:816:HIS:HB2	3:D:836:VAL:HG11	1.95	0.47
2:C:259:GLY:HA2	2:C:263:ASP:HB2	1.97	0.47
2:C:260:LEU:O	2:C:261:ILE:HD12	2.14	0.47
2:C:768:THR:O	2:C:771:GLU:HB2	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:250:ARG:HD3	2:C:250:ARG:O	2.14	0.46
3:D:10:ILE:O	3:D:1454:GLY:HA2	2.15	0.46
3:D:212:ARG:HD3	3:D:342:PRO:CB	2.45	0.46
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.14	0.46
3:D:208:PRO:HG2	3:D:353:VAL:HG21	1.97	0.46
3:D:625:TYR:CD2	3:D:751:LEU:HD21	2.50	0.46
3:D:882:PHE:CE2	3:D:906:GLN:HG3	2.49	0.46
2:C:807:ARG:HB2	2:C:810:ASP:OD2	2.15	0.46
5:F:186:HIS:O	5:F:186:HIS:ND1	2.48	0.46
2:C:13:ILE:CG2	2:C:483:VAL:HG21	2.45	0.46
2:C:578:VAL:HA	2:C:900:ARG:HG2	1.98	0.46
2:C:364:GLU:O	2:C:365:ASP:HB2	2.16	0.46
2:C:468:ARG:HA	2:C:486:MET:O	2.16	0.46
1:A:6:LEU:HD12	1:A:7:LYS:N	2.31	0.46
3:D:580:ALA:HB1	3:D:591:VAL:HG11	1.98	0.46
3:D:907:GLU:OE1	3:D:909:ASN:N	2.49	0.46
5:F:130:VAL:HG22	5:F:156:VAL:HG12	1.98	0.46
2:C:1012:PRO:HB3	5:F:334:PRO:HB3	1.96	0.46
5:F:371:LEU:HD23	5:F:376:ILE:HD12	1.98	0.46
1:B:62:LEU:HD22	1:B:163:ASN:HD21	1.81	0.46
2:C:719:PRO:HD2	2:C:761:PHE:CE1	2.50	0.46
3:D:137:PRO:HB3	3:D:147:VAL:HB	1.98	0.46
6:G:5:DT:H2"	6:G:6:DC:OP2	2.15	0.46
1:A:209:GLU:O	1:A:213:GLN:HG3	2.16	0.46
2:C:195:LEU:HD12	2:C:234:ALA:HB1	1.96	0.46
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.98	0.46
3:D:1263:PHE:HA	3:D:1375:MET:CE	2.46	0.46
3:D:838:ARG:HD3	3:D:874:GLU:CD	2.36	0.46
2:C:127:PHE:O	2:C:133:ASP:HA	2.14	0.46
2:C:374:ASN:OD1	5:F:276:ARG:HD2	2.15	0.46
2:C:764:GLU:C	2:C:766:GLU:H	2.19	0.46
2:C:999:HIS:HB3	2:C:1004:LYS:NZ	2.27	0.46
3:D:652:LEU:HD22	3:D:749:VAL:HG23	1.97	0.46
2:C:677:MET:O	2:C:683:ASN:ND2	2.49	0.46
2:C:712:ALA:HB3	2:C:821:GLU:CG	2.46	0.46
3:D:244:GLU:HG3	3:D:310:LEU:HG	1.98	0.46
1:A:103:ALA:HB1	1:A:107:LYS:HE2	1.98	0.45
2:C:236:ILE:HG23	2:C:248:PRO:CB	2.40	0.45
2:C:285:LEU:HD12	2:C:287:GLY:O	2.15	0.45
3:D:230:TRP:CD1	3:D:331:VAL:HG21	2.52	0.45
2:C:1047:HIS:HB2	3:D:758:GLU:OE1	2.15	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:868:TYR:HB3	3:D:873:LEU:CD1	2.45	0.45
3:D:1140:ILE:CG2	3:D:1144:LEU:HD12	2.46	0.45
3:D:1300:SER:OG	3:D:1301:LYS:N	2.48	0.45
2:C:884:GLN:HB2	2:C:992:MET:CE	2.47	0.45
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.20	0.45
1:A:91:ASN:HB2	1:A:119:ASP:OD2	2.17	0.45
1:B:153:ALA:HB2	1:B:167:VAL:C	2.37	0.45
2:C:754:ILE:HG12	2:C:791:ARG:HD3	1.98	0.45
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.47	0.45
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.47	0.45
3:D:180:LYS:HA	3:D:205:TYR:OH	2.16	0.45
3:D:892:ASP:OD1	3:D:894:LYS:HD2	2.16	0.45
2:C:16:PRO:HB3	2:C:460:ARG:HE	1.81	0.45
2:C:374:ASN:OD1	2:C:376:ARG:HG2	2.16	0.45
2:C:11:GLU:HG2	2:C:535:SER:HB2	1.98	0.45
3:D:1052:THR:HG22	3:D:1053:PHE:O	2.16	0.45
3:D:500:ARG:NH1	3:D:1390:LEU:HD21	2.31	0.45
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	1.98	0.45
1:A:44:LEU:HB3	1:A:177:VAL:HG21	1.99	0.45
1:B:153:ALA:HB2	1:B:168:ASP:N	2.31	0.45
2:C:322:VAL:HG12	2:C:323:ASP:N	2.30	0.45
2:C:149:THR:HA	2:C:322:VAL:HG13	1.99	0.45
2:C:363:SER:HB2	2:C:366:SER:HB3	1.99	0.45
2:C:997:LEU:HD23	2:C:997:LEU:HA	1.70	0.45
3:D:245:LEU:HD12	3:D:309:GLY:O	2.17	0.45
3:D:628:ARG:HD2	6:G:13:DC:H4'	1.98	0.45
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.99	0.45
1:A:54:THR:HG21	1:A:145:ASP:HB2	1.99	0.45
1:B:86:VAL:HG12	1:B:123:MET:CG	2.47	0.45
1:B:62:LEU:HA	1:B:163:ASN:ND2	2.32	0.45
5:F:361:LEU:HD21	5:F:408:LEU:HG	1.99	0.45
1:B:197:LEU:HD23	1:B:199:ILE:HD11	1.98	0.45
3:D:1036:ARG:NH2	3:D:1042:ARG:O	2.48	0.45
3:D:411:THR:HB	3:D:437:VAL:H	1.82	0.45
3:D:86:ARG:HB2	3:D:523:ASP:OD2	2.17	0.45
5:F:160:ASP:O	5:F:164:LYS:HG3	2.17	0.45
2:C:54:ILE:HG21	2:C:355:VAL:CG1	2.47	0.45
3:D:1141:GLU:HG2	3:D:1168:MET:HE2	1.97	0.45
3:D:1263:PHE:O	3:D:1375:MET:HE2	2.17	0.45
3:D:849:ALA:O	3:D:853:VAL:HG23	2.16	0.45
1:A:59:GLU:OE2	1:A:139:ASN:ND2	2.50	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1081:VAL:HG23	2:C:1086:ARG:NH2	2.32	0.45
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.32	0.45
2:C:679:PHE:CE1	2:C:853:LEU:HD11	2.52	0.45
3:D:110:SER:O	3:D:114:THR:HG23	2.16	0.45
3:D:1164:ARG:NH2	3:D:1170:ASP:OD1	2.50	0.45
3:D:123:LEU:HA	3:D:123:LEU:HD23	1.63	0.45
2:C:317:VAL:HA	2:C:318:PRO:HD3	1.87	0.44
2:C:595:LEU:HD21	2:C:623:TYR:HB3	1.99	0.44
2:C:971:LYS:HB3	2:C:986:PRO:HB2	1.99	0.44
3:D:223:LEU:HD11	3:D:288:MET:HE1	1.99	0.44
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	1.99	0.44
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.99	0.44
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.87	0.44
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.99	0.44
1:B:86:VAL:HG12	1:B:123:MET:HG3	1.99	0.44
2:C:580:MET:SD	2:C:584:GLU:HG3	2.58	0.44
3:D:110:SER:OG	3:D:113:GLY:HA3	2.18	0.44
3:D:1435:LEU:HB2	3:D:1457:ASP:OD2	2.18	0.44
3:D:285:PRO:CG	3:D:311:LEU:HD13	2.47	0.44
5:F:368:VAL:HG21	5:F:400:ILE:HG21	1.99	0.44
2:C:969:GLN:HG2	3:D:952:ASP:OD2	2.17	0.44
5:F:345:ALA:O	5:F:349:LEU:HG	2.17	0.44
5:F:95:THR:HB	5:F:98:GLU:HG2	1.99	0.44
1:A:83:LYS:HD2	1:A:168:ASP:HB2	2.00	0.44
2:C:1097:LEU:HD23	2:C:1097:LEU:HA	1.62	0.44
3:D:659:LYS:NZ	3:D:663:GLU:HB2	2.33	0.44
2:C:569:VAL:HG21	2:C:1000:MET:CE	2.46	0.44
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.33	0.44
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.99	0.44
3:D:1459:LEU:CD2	3:D:1464:GLU:HB3	2.47	0.44
3:D:351:MET:HG2	3:D:370:ALA:HB2	2.00	0.44
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.99	0.44
5:F:284:ARG:NH2	5:F:290:GLU:OE2	2.41	0.44
5:F:396:ARG:HA	5:F:399:GLN:HG2	1.99	0.44
2:C:778:PHE:CE1	5:F:419:ARG:HA	2.52	0.44
2:C:99:GLN:NE2	2:C:101:ILE:HD11	2.32	0.44
3:D:720:LEU:HD23	3:D:720:LEU:HA	1.74	0.44
2:C:1001:VAL:HB	3:D:724:GLN:HB2	2.00	0.44
5:F:228:GLU:OE2	5:F:231:ARG:NE	2.51	0.44
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.99	0.44
1:A:11:PHE:O	1:B:228:PRO:HA	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:274:ARG:NH2	2:C:285:LEU:O	2.34	0.43
1:A:72:LYS:HZ3	2:C:644:VAL:HG22	1.82	0.43
1:B:115:LEU:HA	1:B:115:LEU:HD23	1.84	0.43
3:D:883:ALA:HA	3:D:900:ILE:HD13	2.00	0.43
1:A:201:THR:HG23	1:A:203:GLY:N	2.33	0.43
3:D:1497:GLU:H	3:D:1497:GLU:HG2	1.52	0.43
1:A:67:THR:HG21	2:C:609:ASN:OD1	2.18	0.43
1:B:162:ILE:HD12	1:B:163:ASN:H	1.82	0.43
2:C:710:ILE:HD12	2:C:790:LEU:HB2	2.00	0.43
3:D:1103:HIS:CD2	3:D:1463:LYS:HG3	2.53	0.43
3:D:206:ARG:HG2	3:D:392:SER:O	2.17	0.43
3:D:890:VAL:HB	3:D:922:LEU:HD13	2.00	0.43
4:E:48:MET:SD	4:E:58:PRO:HD3	2.58	0.43
5:F:181:GLU:O	5:F:185:GLN:HG2	2.18	0.43
5:F:372:ARG:HH11	5:F:382:THR:HA	1.84	0.43
2:C:206:THR:O	2:C:210:GLU:HB2	2.18	0.43
2:C:318:PRO:O	2:C:320:HIS:ND1	2.45	0.43
2:C:168:ARG:HE	2:C:345:ARG:HD2	1.83	0.43
2:C:405:ARG:NH2	2:C:409:ARG:NH1	2.66	0.43
2:C:940:GLU:HG2	2:C:973:VAL:HG11	2.01	0.43
1:B:14:ARG:HB3	1:B:22:GLU:HB2	2.00	0.43
2:C:45:GLN:HG2	2:C:71:TYR:CE2	2.49	0.43
3:D:520:LEU:HD11	3:D:524:LEU:HD12	2.01	0.43
4:E:47:LYS:HB3	4:E:54:LEU:HG	1.99	0.43
2:C:418:LEU:HD22	2:C:423:ALA:HB2	2.01	0.43
3:D:951:ILE:HD11	3:D:1062:ARG:HG2	1.99	0.43
3:D:266:GLU:HG3	3:D:314:PRO:HB3	2.01	0.43
2:C:1009:SER:O	3:D:624:ASP:HB3	2.19	0.43
2:C:399:ASN:HB2	2:C:400:PRO:HD2	2.01	0.43
2:C:670:GLN:HG2	2:C:699:PHE:CE2	2.54	0.43
3:D:480:GLU:HG2	3:D:480:GLU:O	2.18	0.43
1:B:7:LYS:HD2	1:B:7:LYS:HA	1.72	0.43
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.18	0.43
1:A:216:GLU:CD	1:A:219:ARG:HH22	2.22	0.43
1:B:190:THR:HG22	1:B:190:THR:O	2.19	0.43
2:C:589:ARG:HG3	2:C:589:ARG:NH1	2.32	0.43
2:C:911:GLU:OE2	3:D:1062:ARG:NH1	2.52	0.43
2:C:950:LEU:HB3	2:C:952:LEU:HD13	2.01	0.43
2:C:957:LYS:HB3	2:C:961:GLU:HB2	2.00	0.43
2:C:278:GLU:O	2:C:282:GLY:N	2.51	0.42
2:C:21:ILE:HD12	2:C:455:LEU:HD22	1.99	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:874:LEU:HA	2:C:874:LEU:HD23	1.78	0.42
2:C:929:ARG:HG2	2:C:930:LYS:N	2.33	0.42
3:D:1281:VAL:HG23	3:D:1316:GLY:H	1.84	0.42
3:D:179:VAL:HB	3:D:183:GLU:OE1	2.19	0.42
5:F:265:VAL:O	5:F:269:ASN:ND2	2.41	0.42
3:D:376:GLU:O	3:D:378:ILE:HG13	2.20	0.42
3:D:916:TYR:CZ	3:D:920:LEU:HD21	2.55	0.42
1:A:19:GLU:O	1:A:201:THR:N	2.53	0.42
2:C:121:MET:SD	2:C:125:GLY:HA2	2.59	0.42
2:C:229:MET:HB2	2:C:233:GLU:HB2	2.02	0.42
2:C:244:PRO:O	5:F:82:ARG:NH1	2.52	0.42
2:C:260:LEU:C	2:C:261:ILE:HD12	2.39	0.42
3:D:1023:MET:HB2	3:D:1023:MET:HE3	1.67	0.42
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.54	0.42
3:D:618:LEU:HG	3:D:1467:ILE:HG23	2.00	0.42
3:D:360:ARG:HB3	3:D:360:ARG:NH2	2.33	0.42
3:D:791:TYR:CZ	3:D:945:SER:HB2	2.53	0.42
1:B:94:LEU:HD21	1:B:97:VAL:CG1	2.50	0.42
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.50	0.42
2:C:247:PRO:HA	2:C:248:PRO:HD2	1.78	0.42
2:C:133:ASP:HB3	2:C:395:LYS:HD2	2.01	0.42
3:D:134:VAL:CG2	3:D:151:GLN:H	2.33	0.42
3:D:317:VAL:HB	3:D:339:TRP:HB3	2.01	0.42
3:D:432:TYR:O	3:D:448:GLU:HA	2.18	0.42
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.99	0.42
3:D:827:ILE:HD12	3:D:829:VAL:HG21	2.01	0.42
3:D:84:ILE:HG13	3:D:88:TYR:CE1	2.54	0.42
3:D:972:LEU:HD13	3:D:972:LEU:O	2.19	0.42
1:B:211:LEU:O	1:B:215:VAL:HG12	2.19	0.42
2:C:1103:ASP:OD1	2:C:1107:ASN:N	2.49	0.42
2:C:213:ALA:H	2:C:218:VAL:HG21	1.83	0.42
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	2.02	0.42
3:D:1192:LEU:HG	3:D:1369:GLU:HB3	2.01	0.42
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.55	0.42
3:D:534:ARG:HB3	3:D:534:ARG:HE	1.71	0.42
2:C:64:LEU:HD12	2:C:364:GLU:HG3	2.01	0.42
2:C:726:ILE:HD11	2:C:757:GLY:CA	2.50	0.42
3:D:222:GLY:HA2	3:D:333:LEU:O	2.19	0.42
3:D:584:ASN:H	3:D:602:SER:CB	2.33	0.42
3:D:698:LYS:HG2	3:D:756:GLN:HG2	2.02	0.42
2:C:886:LEU:CD1	3:D:951:ILE:HG12	2.48	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:276:ARG:O	5:F:280:GLN:HG3	2.20	0.42
1:A:106:PRO:HG3	1:A:134:GLU:HG2	2.01	0.42
1:B:18:ARG:O	1:B:207:PRO:HD3	2.20	0.42
1:B:206:THR:HG22	1:B:208:LEU:N	2.35	0.42
2:C:127:PHE:HB3	2:C:129:ILE:HD13	2.01	0.42
2:C:79:PRO:HG2	2:C:82:GLU:HB2	2.02	0.42
2:C:889:HIS:CD2	3:D:951:ILE:HG22	2.54	0.42
1:A:9:PRO:HB3	1:A:27:PRO:O	2.19	0.42
3:D:134:VAL:HG22	3:D:151:GLN:H	1.83	0.42
3:D:176:ASP:OD1	3:D:177:ALA:N	2.48	0.42
2:C:685:GLU:OE2	3:D:783:ARG:NE	2.52	0.42
2:C:1112:PHE:CD2	3:D:88:TYR:CD2	2.96	0.42
2:C:177:GLU:O	2:C:179:ASN:N	2.52	0.42
3:D:17:LYS:HA	3:D:20:SER:OG	2.20	0.42
3:D:729:HIS:ND1	3:D:730:PRO:HD2	2.35	0.42
1:A:227:ASN:HA	1:A:228:PRO:HD3	1.83	0.42
2:C:720:GLU:HG2	2:C:760:SER:OG	2.20	0.42
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.59	0.42
5:F:102:LEU:O	5:F:106:VAL:HG23	2.20	0.42
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.52	0.41
3:D:1225:ALA:O	3:D:1229:ILE:HG13	2.20	0.41
3:D:230:TRP:CZ2	3:D:232:GLU:HG2	2.55	0.41
1:B:110:LYS:HZ3	1:B:128:HIS:HB2	1.84	0.41
1:B:20:TYR:C	1:B:207:PRO:HG2	2.41	0.41
3:D:1123:PHE:HB3	3:D:1132:LEU:HB3	2.02	0.41
3:D:116:LEU:HB2	3:D:118:LEU:HD12	2.01	0.41
3:D:234:GLU:O	3:D:234:GLU:HG3	2.20	0.41
3:D:355:VAL:HG11	3:D:385:VAL:HG21	2.02	0.41
2:C:452:ILE:HG21	2:C:452:ILE:HD13	1.84	0.41
3:D:1053:PHE:CE2	3:D:1072:ILE:HG23	2.55	0.41
3:D:1271:LYS:HD3	3:D:1331:ASP:HB2	2.02	0.41
3:D:399:ARG:NH1	3:D:431:VAL:HG11	2.34	0.41
3:D:601:ARG:HD3	5:F:318:GLU:HG2	2.02	0.41
1:A:36:LEU:HD11	1:B:221:HIS:HB3	2.02	0.41
3:D:630:VAL:HA	3:D:744:GLN:HG2	2.02	0.41
1:B:206:THR:HB	1:B:209:GLU:HG3	2.01	0.41
2:C:999:HIS:CD2	2:C:1004:LYS:NZ	2.89	0.41
2:C:682:TYR:CE1	3:D:635:PRO:HD2	2.55	0.41
1:A:54:THR:HB	1:A:158:ILE:HD12	2.02	0.41
2:C:1009:SER:HB3	3:D:651:GLU:O	2.19	0.41
3:D:1122:LEU:HD13	3:D:1178:ALA:HB2	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1236:LEU:HD12	3:D:1236:LEU:HA	1.82	0.41
1:A:124:ASN:OD1	1:A:124:ASN:N	2.54	0.41
1:A:70:GLY:N	2:C:607:ASP:OD1	2.54	0.41
2:C:877:PRO:HG3	3:D:1023:MET:HE1	2.02	0.41
2:C:912:PRO:O	2:C:916:GLU:HG3	2.21	0.41
2:C:15:LEU:HA	2:C:16:PRO:HD3	1.84	0.41
2:C:841:ASN:ND2	2:C:845:ASN:HB3	2.36	0.41
3:D:882:PHE:CZ	3:D:906:GLN:HG3	2.56	0.41
2:C:1050:GLN:NE2	3:D:1471:LEU:HD13	2.35	0.41
2:C:287:GLY:O	2:C:289:THR:N	2.49	0.41
2:C:718:GLY:HA3	2:C:761:PHE:CD1	2.56	0.41
5:F:356:LYS:HD3	5:F:417:LYS:HZ2	1.85	0.41
1:B:107:LYS:HE2	1:B:113:ASP:OD2	2.21	0.41
1:B:61:VAL:HG11	1:B:75:VAL:HG21	2.01	0.41
2:C:1037:VAL:HG13	2:C:1049:LEU:CD1	2.51	0.41
2:C:436:GLY:HA2	2:C:538:GLN:O	2.20	0.41
1:B:38:ASN:OD1	2:C:979:THR:HG22	2.21	0.41
3:D:15:PRO:HB3	3:D:515:GLU:HB2	2.02	0.41
3:D:934:LEU:HA	3:D:934:LEU:HD23	1.87	0.41
1:B:64:GLU:O	1:B:75:VAL:HB	2.20	0.41
1:B:78:ILE:O	1:B:82:LEU:HG	2.21	0.41
2:C:1092:LEU:HD12	2:C:1099:VAL:HG21	2.03	0.41
3:D:907:GLU:HB3	3:D:1026:SER:HA	2.03	0.41
3:D:134:VAL:HG23	3:D:149:LYS:HA	2.02	0.41
3:D:791:TYR:CE2	3:D:945:SER:HB2	2.56	0.41
3:D:51:GLY:O	3:D:86:ARG:HD2	2.21	0.41
2:C:44:ILE:HD13	2:C:44:ILE:HA	1.85	0.40
2:C:881:ASN:O	2:C:884:GLN:HG2	2.20	0.40
3:D:936:TYR:CD2	3:D:936:TYR:C	2.95	0.40
2:C:644:VAL:HG12	2:C:645:VAL:N	2.36	0.40
2:C:999:HIS:HD2	2:C:1004:LYS:NZ	2.18	0.40
3:D:134:VAL:HG12	3:D:454:ALA:HB2	2.03	0.40
3:D:431:VAL:HG11	3:D:448:GLU:OE2	2.21	0.40
3:D:792:ILE:HG13	3:D:793:THR:HG23	2.03	0.40
5:F:373:LYS:HA	5:F:373:LYS:HD3	1.95	0.40
1:A:186:LEU:HA	1:A:186:LEU:HD12	1.64	0.40
2:C:627:ARG:HD3	2:C:638:ASP:OD1	2.21	0.40
2:C:723:THR:OG1	2:C:724:ARG:N	2.55	0.40
3:D:1208:ASP:O	3:D:1210:SER:N	2.54	0.40
3:D:259:VAL:HG13	3:D:270:LEU:CD2	2.51	0.40
2:C:684:PHE:HB3	3:D:633:VAL:HG21	2.03	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:645:PRO:HG2	3:D:724:GLN:O	2.21	0.40
3:D:974:ILE:HG12	3:D:991:GLN:HG2	2.03	0.40
2:C:1118:LYS:HE2	3:D:20:SER:O	2.21	0.40
2:C:409:ARG:HG2	2:C:410:ILE:N	2.35	0.40
3:D:141:ILE:HA	3:D:146:PRO:HA	2.03	0.40
3:D:46:ASP:OD2	3:D:48:ARG:HB2	2.22	0.40
6:G:7:DA:C2'	6:G:8:DG:OP2	2.70	0.40
1:B:24:VAL:HA	1:B:195:LEU:O	2.22	0.40
1:B:88:ARG:HH12	1:B:123:MET:CE	2.34	0.40
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.21	0.40
3:D:977:ALA:HB1	3:D:982:PHE:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/315 (71%)	203 (91%)	20 (9%)	1 (0%)	34	72
1	B	220/315 (70%)	201 (91%)	18 (8%)	1 (0%)	29	68
2	C	1107/1119 (99%)	1021 (92%)	71 (6%)	15 (1%)	11	43
3	D	1481/1524 (97%)	1387 (94%)	86 (6%)	8 (0%)	29	68
4	E	92/99 (93%)	87 (95%)	3 (3%)	2 (2%)	6	31
5	F	334/423 (79%)	314 (94%)	16 (5%)	4 (1%)	13	48
All	All	3458/3795 (91%)	3213 (93%)	214 (6%)	31 (1%)	17	55

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	GLY

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	16	GLN
2	C	213	ALA
2	C	248	PRO
2	C	365	ASP
2	C	767	PRO
3	D	320	ALA
3	D	397	LYS
3	D	1307	LYS
4	E	82	GLU
5	F	421	PHE
2	C	12	VAL
2	C	212	GLY
5	F	361	LEU
2	C	178	PRO
2	C	244	PRO
2	C	288	ARG
2	C	319	GLY
2	C	363	SER
2	C	364	GLU
3	D	484	PRO
3	D	532	GLY
3	D	1128	VAL
4	E	83	ASP
2	C	179	ASN
2	C	765	SER
5	F	141	VAL
3	D	431	VAL
5	F	153	PRO
3	D	1298	GLY
2	C	376	ARG

### 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	199/273 (73%)	191 (96%)	8 (4%)	31 68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	195/273 (71%)	188 (96%)	7 (4%)	35	70
2	C	934/941 (99%)	870 (93%)	64 (7%)	15	48
3	D	1251/1279 (98%)	1180 (94%)	71 (6%)	20	56
4	E	83/88 (94%)	78 (94%)	5 (6%)	19	53
5	F	294/371 (79%)	277 (94%)	17 (6%)	20	55
All	All	2956/3225 (92%)	2784 (94%)	172 (6%)	20	55

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	53	VAL
1	A	119	ASP
1	A	145	ASP
1	A	162	ILE
1	A	175	ARG
1	A	189	ARG
1	A	201	THR
1	B	7	LYS
1	B	16	GLN
1	B	55	SER
1	B	80	LEU
1	B	93	SER
1	B	94	LEU
1	B	188	GLN
2	C	1	MET
2	C	10	ARG
2	C	27	ARG
2	C	55	GLU
2	C	81	ASP
2	C	102	HIS
2	C	107	LEU
2	C	134	ARG
2	C	142	ARG
2	C	149	THR
2	C	168	ARG
2	C	210	GLU
2	C	214	TYR
2	C	221	LEU
2	C	223	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	246	ASP
2	C	250	ARG
2	C	257	VAL
2	C	260	LEU
2	C	269	LEU
2	C	285	LEU
2	C	314	THR
2	C	342	ASP
2	C	353	ARG
2	C	355	VAL
2	C	359	MET
2	C	388	ARG
2	C	427	VAL
2	C	434	HIS
2	C	541	SER
2	C	557	ARG
2	C	562	SER
2	C	571	LEU
2	C	584	GLU
2	C	589	ARG
2	C	600	ASP
2	C	610	ARG
2	C	615	TYR
2	C	617	ASP
2	C	626	ARG
2	C	627	ARG
2	C	633	GLN
2	C	640	ARG
2	C	670	GLN
2	C	680	ASP
2	C	697	ARG
2	C	762	LYS
2	C	767	PRO
2	C	768	THR
2	C	769	PRO
2	C	770	GLU
2	C	771	GLU
2	C	778	PHE
2	C	784	ASP
2	C	808	ARG
2	C	815	LEU
2	C	858	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	905	ILE
2	C	923	GLU
2	C	939	ARG
2	C	968	LEU
2	C	1001	VAL
2	C	1081	VAL
2	C	1084	SER
3	D	30	GLU
3	D	53	ILE
3	D	65	ARG
3	D	81	THR
3	D	86	ARG
3	D	106	LYS
3	D	115	LEU
3	D	119	SER
3	D	123	LEU
3	D	141	ILE
3	D	155	ASP
3	D	183	GLU
3	D	191	LEU
3	D	199	LEU
3	D	230	TRP
3	D	247	GLU
3	D	255	GLU
3	D	256	GLU
3	D	276	ASP
3	D	302	GLN
3	D	312	ARG
3	D	316	GLN
3	D	331	VAL
3	D	372	ASP
3	D	394	LEU
3	D	411	THR
3	D	420	VAL
3	D	429	SER
3	D	430	ASP
3	D	488	ARG
3	D	525	ARG
3	D	531	ASP
3	D	568	ARG
3	D	576	GLU
3	D	591	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	D	596	SER
3	D	628	ARG
3	D	632	VAL
3	D	685	ASP
3	D	693	GLU
3	D	717	GLN
3	D	752	SER
3	D	754	PHE
3	D	784	ASP
3	D	817	GLU
3	D	847	ASP
3	D	894	LYS
3	D	900	ILE
3	D	907	GLU
3	D	942	SER
3	D	943	THR
3	D	968	ASP
3	D	970	LYS
3	D	972	LEU
3	D	984	THR
3	D	986	ARG
3	D	1014	ASN
3	D	1041	LEU
3	D	1044	LEU
3	D	1188	VAL
3	D	1236	LEU
3	D	1237	THR
3	D	1254	GLN
3	D	1277	ILE
3	D	1308	GLU
3	D	1310	ARG
3	D	1317	ASP
3	D	1420	LEU
3	D	1476	THR
3	D	1488	ASP
3	D	1497	GLU
4	E	15	SER
4	E	33	HIS
4	E	36	LYS
4	E	50	THR
4	E	81	PRO
5	F	88	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	F	116	LEU
5	F	128	ARG
5	F	141	VAL
5	F	254	GLN
5	F	259	ARG
5	F	272	SER
5	F	303	ARG
5	F	313	GLU
5	F	315	VAL
5	F	336	GLU
5	F	369	LEU
5	F	375	LEU
5	F	382	THR
5	F	383	LEU
5	F	394	ARG
5	F	420	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	A	212	ASN
1	B	163	ASN
2	C	498	GLN
2	C	683	ASN
2	C	969	GLN
2	C	999	HIS
2	C	1050	GLN
3	D	350	HIS
3	D	611	GLN
3	D	744	GLN
3	D	762	GLN
3	D	1124	GLN
3	D	1333	HIS
3	D	1359	GLN
3	D	1441	GLN
5	F	90	GLN
5	F	175	HIS
5	F	248	ASN

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	2/4 (50%)	1 (50%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	4	G

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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
9	POP	D	1601	-	6,8,8	1.32	1 (16%)	13,13,13	1.09	1 (7%)

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
9	POP	D	1601	-	-	0/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	1601	POP	P1-O3	-2.08	1.46	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	1601	POP	O6-P2-O5	2.39	116.77	107.64

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 ⓘ

### 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	226/315 (71%)	-0.03	2 (0%) 84 63	64, 86, 106, 116	0
1	B	222/315 (70%)	-0.01	1 (0%) 91 75	61, 89, 112, 133	0
2	C	1111/1119 (99%)	0.25	48 (4%) 35 13	50, 83, 147, 176	0
3	D	1485/1524 (97%)	0.13	52 (3%) 44 18	42, 79, 137, 179	0
4	E	94/99 (94%)	0.09	3 (3%) 47 20	59, 90, 131, 148	0
5	F	338/423 (79%)	0.31	22 (6%) 18 5	58, 95, 165, 201	0
6	G	15/22 (68%)	-0.25	1 (6%) 17 5	56, 92, 222, 239	0
7	H	16/27 (59%)	-0.48	0 100 100	84, 108, 189, 199	0
8	I	3/4 (75%)	-0.18	0 100 100	58, 58, 66, 71	0
All	All	3510/3848 (91%)	0.16	129 (3%) 41 17	42, 85, 145, 239	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	219	GLN	5.9
5	F	410	TYR	5.8
3	D	1299	PHE	5.6
2	C	778	PHE	5.6
5	F	412	GLU	5.5
2	C	195	LEU	5.5
2	C	365	ASP	5.3
2	C	107	LEU	5.2
2	C	188	LYS	5.0
2	C	194	VAL	5.0
2	C	367	LEU	4.8
5	F	149	GLU	4.8
2	C	224	GLU	4.4
2	C	254	VAL	4.3
2	C	153	ALA	4.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	C	222	MET	4.1
2	C	419	THR	4.0
5	F	413	SER	4.0
2	C	189	ARG	4.0
3	D	384	VAL	3.8
5	F	147	LEU	3.8
2	C	207	LEU	3.5
3	D	978	TYR	3.5
2	C	66	LEU	3.4
2	C	209	ARG	3.4
2	C	811	PRO	3.4
5	F	361	LEU	3.4
3	D	1499	ARG	3.4
5	F	414	ARG	3.4
5	F	391	GLY	3.3
2	C	198	ARG	3.3
2	C	424	GLY	3.3
2	C	814	GLU	3.3
5	F	419	ARG	3.2
2	C	250	ARG	3.2
2	C	64	LEU	3.2
3	D	242	LEU	3.2
5	F	365	GLU	3.1
5	F	394	ARG	3.1
3	D	152	LEU	3.1
2	C	182	VAL	3.1
5	F	390	PHE	3.0
3	D	1288	GLU	3.0
3	D	1237	THR	3.0
4	E	89	MET	3.0
3	D	393	ILE	3.0
5	F	392	VAL	2.9
2	C	423	ALA	2.9
3	D	178	LEU	2.9
3	D	188	GLY	2.9
3	D	1497	GLU	2.9
3	D	1318	TYR	2.8
3	D	367	ILE	2.8
2	C	251	ASP	2.8
2	C	368	THR	2.8
2	C	815	LEU	2.8
3	D	409	VAL	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	C	304	LEU	2.7
2	C	157	ARG	2.7
2	C	186	VAL	2.7
3	D	184	GLU	2.7
3	D	1495	ILE	2.7
2	C	425	PHE	2.6
3	D	360	ARG	2.6
2	C	190	LYS	2.6
3	D	198	ARG	2.6
3	D	371	ILE	2.6
5	F	381	HIS	2.6
2	C	248	PRO	2.6
3	D	1294	VAL	2.6
2	C	187	ASN	2.6
3	D	1131	SER	2.5
5	F	350	LEU	2.5
3	D	350	HIS	2.5
3	D	202	VAL	2.5
2	C	228	ALA	2.5
1	A	99	LEU	2.4
3	D	1490	LYS	2.4
2	C	183	SER	2.4
3	D	322	VAL	2.4
5	F	389	PHE	2.4
3	D	201	GLY	2.4
5	F	420	ASP	2.4
3	D	397	LYS	2.4
2	C	806	LEU	2.4
2	C	202	TYR	2.4
3	D	428	LYS	2.4
3	D	345	TYR	2.4
4	E	32	ARG	2.4
3	D	377	VAL	2.4
3	D	390	PRO	2.3
2	C	241	LEU	2.3
3	D	241	ILE	2.3
3	D	443	VAL	2.3
2	C	105	THR	2.3
3	D	211	VAL	2.3
4	E	85	LEU	2.3
3	D	666	ILE	2.3
3	D	1500	LYS	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	D	191	LEU	2.2
3	D	486	ARG	2.2
3	D	165	LYS	2.2
3	D	446	VAL	2.2
3	D	993	LEU	2.2
5	F	354	LEU	2.2
1	A	107	LYS	2.2
2	C	197	LEU	2.2
5	F	141	VAL	2.2
2	C	781	LYS	2.2
3	D	283	PHE	2.2
2	C	223	ASP	2.2
2	C	366	SER	2.2
3	D	1253	THR	2.1
3	D	1281	VAL	2.1
3	D	1493	LYS	2.1
3	D	1414	PRO	2.1
1	B	106	PRO	2.1
6	G	17	DA	2.1
2	C	176	VAL	2.1
5	F	148	LYS	2.1
3	D	75	ARG	2.1
5	F	415	THR	2.1
2	C	297	GLU	2.1
3	D	1132	LEU	2.1
2	C	65	VAL	2.1
3	D	976	GLN	2.0
5	F	409	LYS	2.0
3	D	1313	VAL	2.0
3	D	1319	VAL	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 [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, 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	POP	D	1601	9/9	0.92	0.17	84,92,116,124	0
10	MG	D	1602	1/1	0.96	0.36	59,59,59,59	0
11	ZN	D	1603	1/1	0.98	0.13	101,101,101,101	0
11	ZN	D	1604	1/1	0.99	0.19	74,74,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.