



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 06:57 AM EDT

PDB ID : 5VO8
Title : X-ray crystal structure of a bacterial reiterative transcription complex of pyrG promoter
Authors : Murakami, K.S.; Shin, Y.; Turnbough Jr, C.L.; Molodtsov, V.
Deposited on : 2017-05-02
Resolution : 3.30 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (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

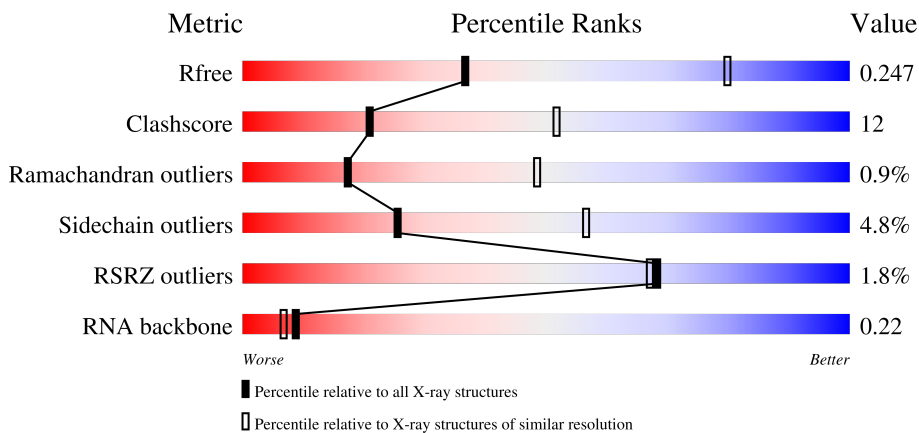
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.






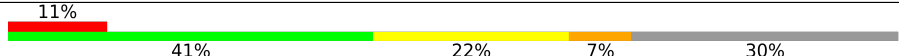
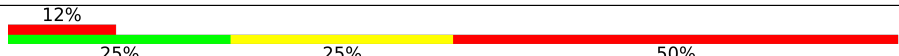
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	A	315	51% 19% • 28%
1	B	315	51% 19% • 29%
2	C	1119	% 69% 28% ••
3	D	1524	% 68% 27% ••

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	99	
5	F	423	
6	G	22	
7	H	27	
8	I	8	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	MG	B	1001	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 28534 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
			Total	C	N	O	S			
1	A	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	224	Total	C	N	O	S	0	0	0
			1767	1129	307	329	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1107	Total	C	N	O	S	0	0	0
			8726	5523	1551	1628	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1484	Total	C	N	O	S	0	0	0
			11722	7431	2065	2191	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			Total	C	N	O	S			
5	F	346	Total	C	N	O	S	0	0	0
			2790	1760	508	518	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	G	19	386	183	75	109	19	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
7	H	19	394	188	76	112	18	0	0	0

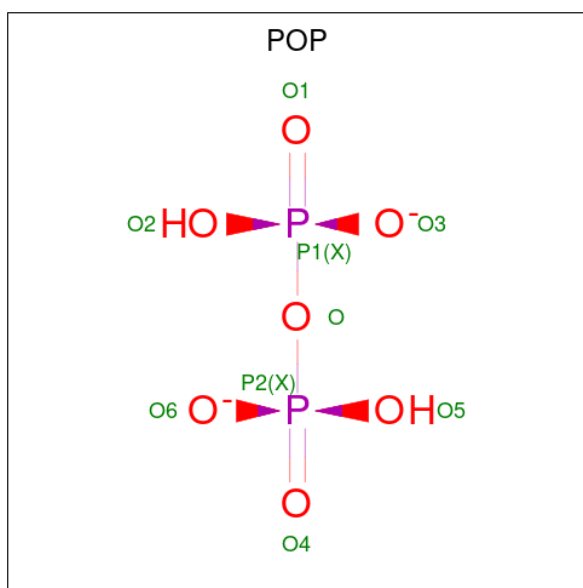
- Molecule 8 is a RNA chain called RNA (5'-D(*(GTP))-R(P*GP*GP*GP*GP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	I	8	193	80	40	63	10	0	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Mg 1 1	0	0
9	D	1	Total Mg 1 1	0	0

- Molecule 10 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H₂O₇P₂).



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

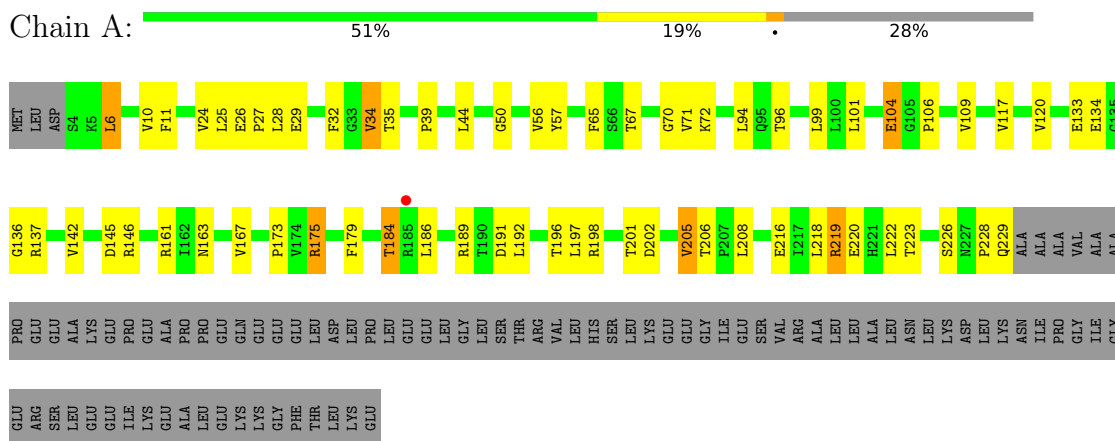
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

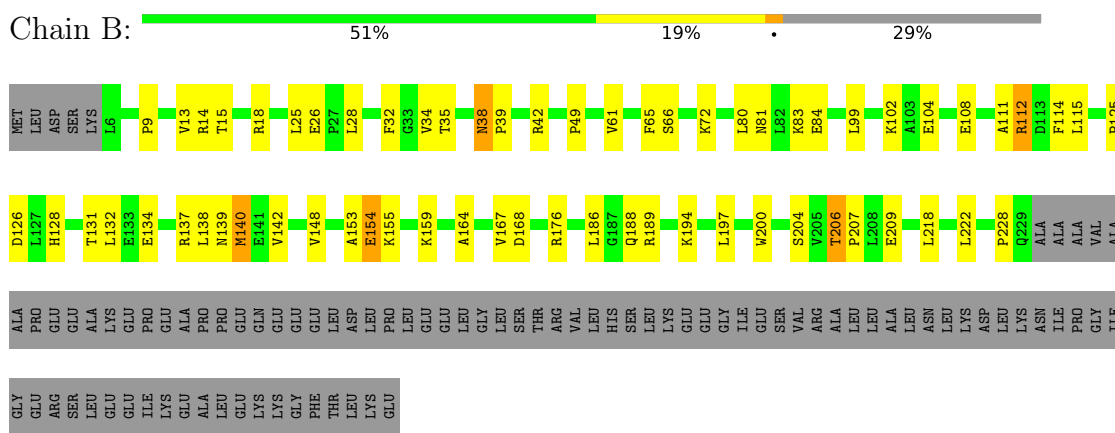
3 Residue-property plots i

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.

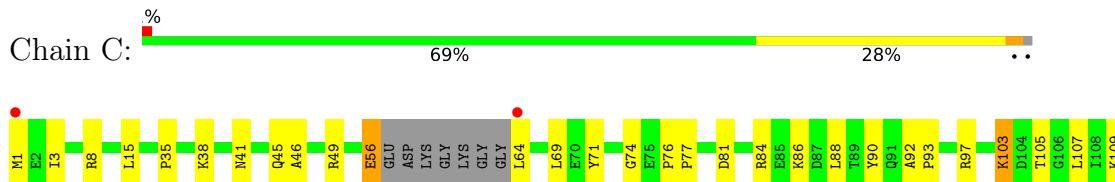
- Molecule 1: DNA-directed RNA polymerase subunit alpha

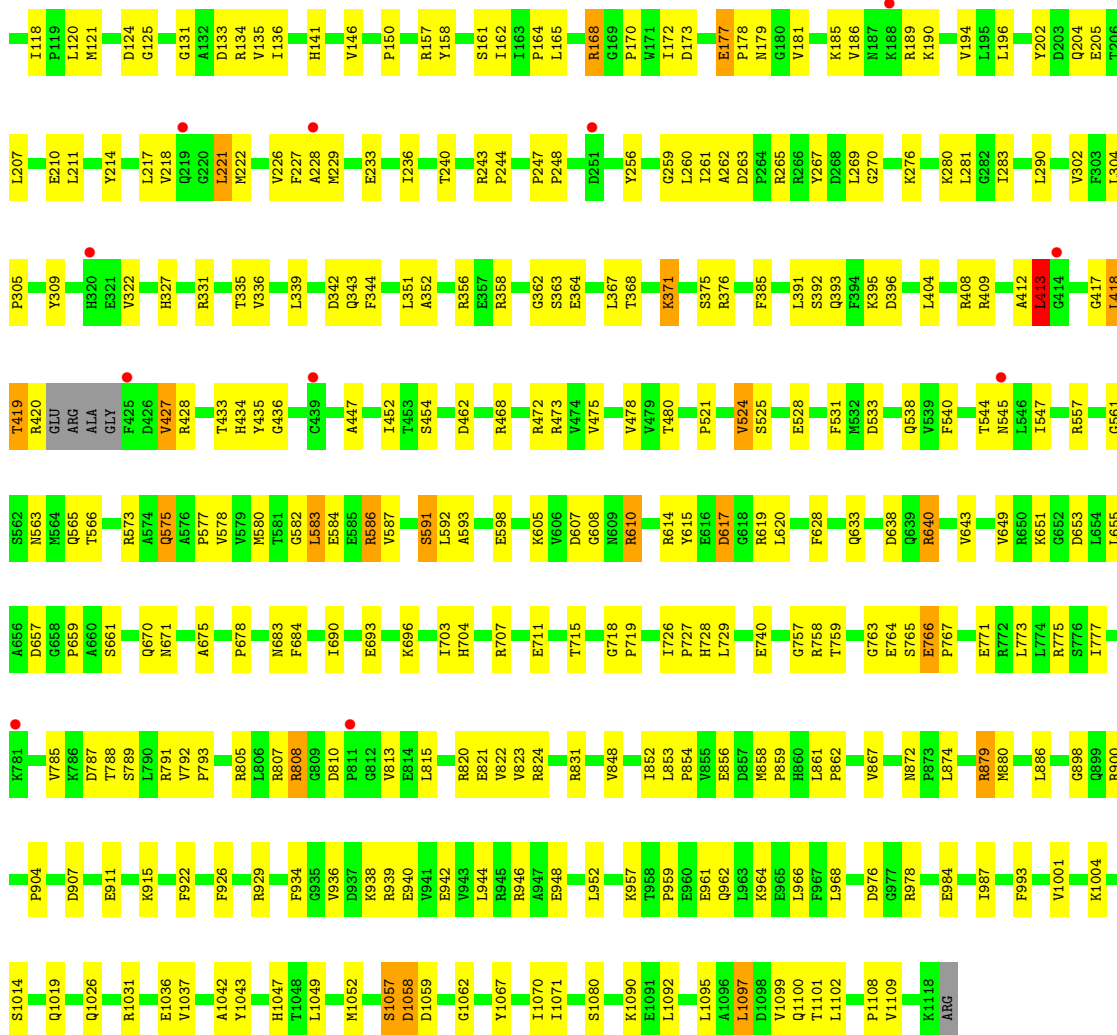


- Molecule 1: DNA-directed RNA polymerase subunit alpha

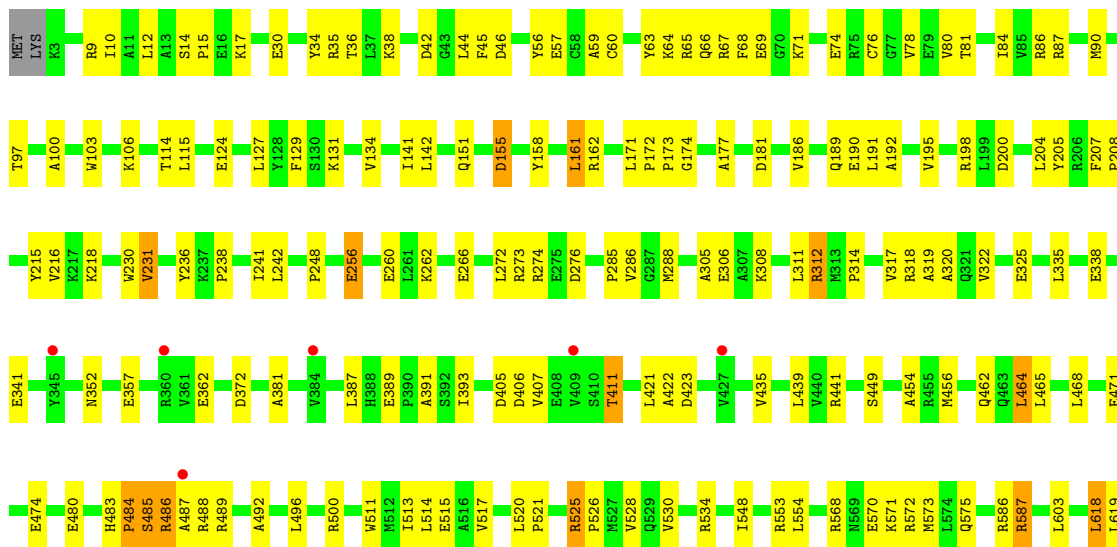


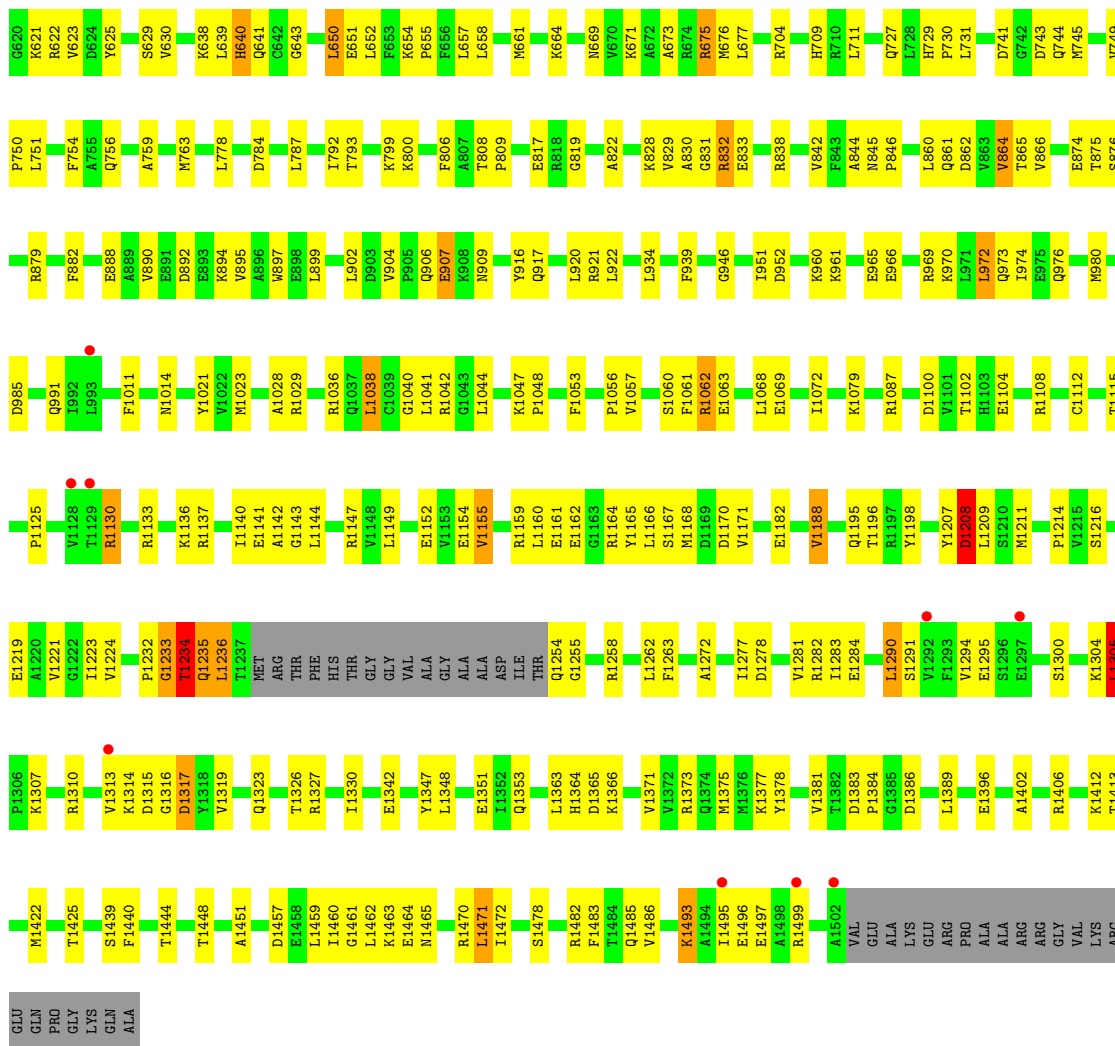
- Molecule 2: DNA-directed RNA polymerase subunit beta





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

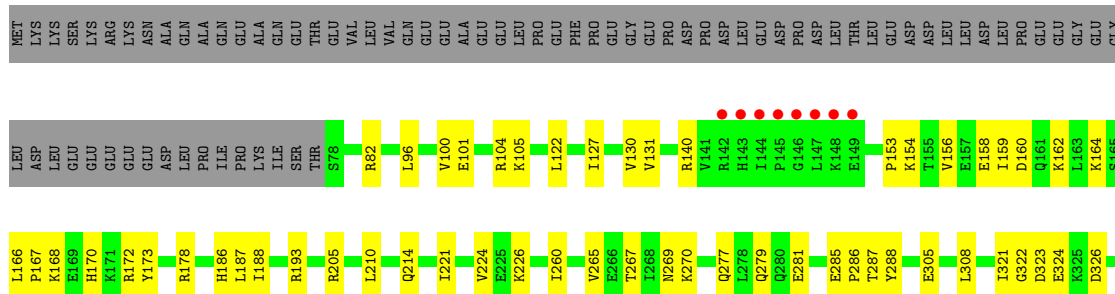


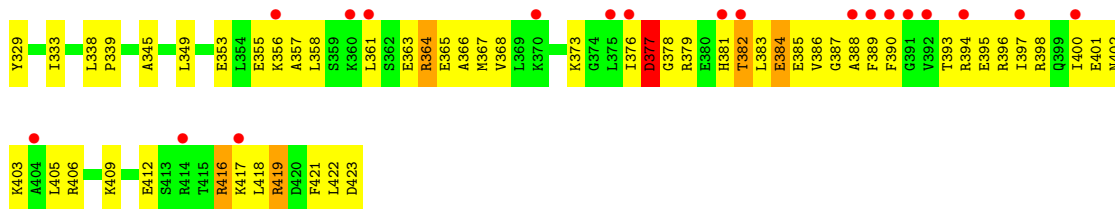


• Molecule 4: DNA-directed RNA polymerase subunit omega

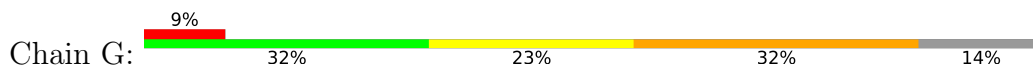


• Molecule 5: RNA polymerase sigma factor SigA

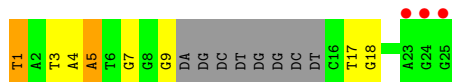
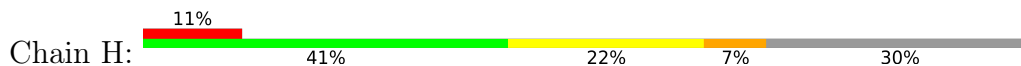




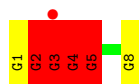
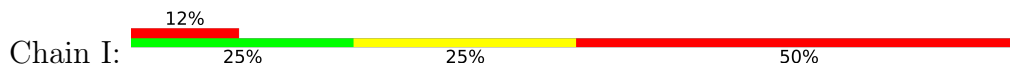
- Molecule 6: DNA (5'-D(P*GP*GP*TP*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*A P*AP*AP*A)-3')



- Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*CP*TP*GP*AP*TP*GP*CP*AP*CP*C)-3')



- Molecule 8: RNA (5'-D(*(GTP))-R(P*GP*GP*GP*GP*GP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.54Å 101.98Å 296.11Å 90.00° 98.56° 90.00°	Depositor
Resolution (Å)	29.88 – 3.30 29.88 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.2 (29.88-3.30) 94.2 (29.88-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.31Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.185 , 0.246 0.185 , 0.247	Depositor DCC
R_{free} test set	1999 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	89.9	Xtrriage
Anisotropy	0.773	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 69.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28534	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: ZN, MG, POP, GTP

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	0.58	1/1814 (0.1%)	0.82	1/2466 (0.0%)
1	B	0.60	2/1799 (0.1%)	0.90	1/2447 (0.0%)
2	C	0.53	0/8892	0.81	4/12028 (0.0%)
3	D	0.59	0/11928	0.86	13/16127 (0.1%)
4	E	0.50	0/775	0.76	0/1045
5	F	0.50	0/2835	0.81	1/3816 (0.0%)
6	G	1.35	4/433 (0.9%)	1.30	8/664 (1.2%)
7	H	1.03	1/442 (0.2%)	1.03	3/680 (0.4%)
8	I	1.06	0/181	2.00	10/283 (3.5%)
All	All	0.60	8/29099 (0.0%)	0.86	41/39556 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
5	F	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	154	GLU	CB-CG	7.78	1.67	1.52
1	B	154	GLU	CG-CD	6.08	1.61	1.51
6	G	19	DA	P-O5'	6.06	1.65	1.59
7	H	1	DT	C1'-N1	5.55	1.56	1.49
6	G	12	DG	C3'-O3'	-5.36	1.36	1.44
6	G	20	DA	N9-C4	5.34	1.41	1.37
1	A	175	ARG	CG-CD	5.24	1.65	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	14	DG	C3'-O3'	-5.20	1.37	1.44

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	17	DC	O4'-C4'-C3'	-9.24	100.46	106.00
6	G	19	DA	O4'-C4'-C3'	-9.14	100.52	106.00
6	G	16	DC	O5'-P-OP2	-8.29	98.23	105.70
2	C	879	ARG	NE-CZ-NH2	-7.70	116.45	120.30
3	D	1363	LEU	CB-CG-CD2	-7.02	99.06	111.00
3	D	1234	THR	C-N-CA	6.62	138.26	121.70
8	I	4	G	N3-C4-C5	6.54	131.87	128.60
3	D	464	LEU	CB-CG-CD2	-6.43	100.07	111.00
8	I	5	G	O5'-P-OP1	-6.33	100.00	105.70
3	D	1170	ASP	CB-CG-OD2	6.28	123.95	118.30
8	I	8	G	N3-C2-N2	6.22	124.25	119.90
8	I	4	G	N3-C4-N9	-6.17	122.30	126.00
1	A	44	LEU	CB-CG-CD1	-6.05	100.71	111.00
6	G	19	DA	O4'-C1'-N9	6.05	112.23	108.00
8	I	8	G	O5'-P-OP2	5.92	117.80	110.70
3	D	1305	LEU	CA-CB-CG	5.91	128.88	115.30
2	C	1097	LEU	CB-CG-CD2	-5.86	101.04	111.00
3	D	711	LEU	CA-CB-CG	-5.84	101.87	115.30
3	D	1373	ARG	NE-CZ-NH2	-5.82	117.39	120.30
6	G	20	DA	O4'-C1'-N9	5.76	112.03	108.00
8	I	2	G	O4'-C1'-N9	-5.74	103.61	108.20
8	I	3	G	C5-C6-N1	5.74	114.37	111.50
2	C	413	LEU	CA-CB-CG	5.72	128.45	115.30
7	H	1	DT	O4'-C1'-N1	5.60	111.92	108.00
6	G	16	DC	OP1-P-OP2	5.55	127.92	119.60
3	D	621	LYS	CD-CE-NZ	5.54	124.43	111.70
3	D	1471	LEU	CB-CG-CD2	-5.45	101.74	111.00
8	I	8	G	N1-C2-N2	-5.42	111.33	116.20
6	G	15	DC	OP1-P-OP2	5.39	127.69	119.60
3	D	1115	THR	OG1-CB-CG2	-5.39	97.61	110.00
3	D	1208	ASP	CB-CG-OD1	5.32	123.08	118.30
2	C	371	LYS	CA-CB-CG	5.31	125.08	113.40
7	H	5	DA	O4'-C1'-N9	5.26	111.69	108.00
8	I	3	G	C2-N3-C4	5.25	114.53	111.90
3	D	1038	LEU	CB-CG-CD2	-5.23	102.11	111.00
7	H	1	DT	N3-C4-O4	5.12	122.97	119.90
5	F	361	LEU	N-CA-C	-5.11	97.20	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	18	DA	O5'-P-OP1	5.06	116.77	110.70
1	B	28	LEU	CA-CB-CG	5.05	126.91	115.30
3	D	1363	LEU	CA-CB-CG	5.04	126.89	115.30
8	I	8	G	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	766	GLU	Peptide
5	F	389	PHE	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	A	1782	0	1834	44	0
1	B	1767	0	1816	45	0
2	C	8726	0	8814	243	0
3	D	11722	0	11950	309	1
4	E	761	0	778	21	0
5	F	2790	0	2854	79	0
6	G	386	0	212	14	0
7	H	394	0	217	8	0
8	I	193	0	88	8	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	C	9	0	0	0	0
11	D	2	0	0	0	0
All	All	28534	0	28563	694	1

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 (694) 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:218:LYS:HG2	3:D:338:GLU:HG2	1.48	0.92
2:C:367:LEU:HA	2:C:371:LYS:HE2	1.49	0.92
2:C:418:LEU:O	2:C:419:THR:OG1	1.88	0.91
5:F:358:LEU:HB3	5:F:366:ALA:HB1	1.49	0.90
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.53	0.89
2:C:428:ARG:NH2	2:C:447:ALA:O	2.08	0.86
3:D:1281:VAL:HG22	3:D:1317:ASP:H	1.41	0.85
2:C:211:LEU:HD11	2:C:304:LEU:HD11	1.58	0.84
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.60	0.84
3:D:34:TYR:OH	3:D:35:ARG:NH1	2.10	0.84
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.61	0.82
5:F:322:GLY:O	5:F:324:GLU:N	2.14	0.81
1:B:206:THR:HG22	1:B:209:GLU:H	1.45	0.80
1:A:56:VAL:HG22	1:A:142:VAL:HG12	1.64	0.79
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.61	0.79
3:D:1294:VAL:O	3:D:1300:SER:OG	2.00	0.79
2:C:911:GLU:OE2	3:D:1062:ARG:NH1	2.17	0.78
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.64	0.77
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.67	0.77
5:F:326:ASP:O	6:G:19:DA:N6	2.17	0.77
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.18	0.76
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.67	0.76
3:D:97:THR:HG23	3:D:554:LEU:HD21	1.67	0.76
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.69	0.75
5:F:376:ILE:O	5:F:377:ASP:HB3	1.87	0.75
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.69	0.74
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.68	0.74
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.69	0.73
5:F:363:GLU:O	5:F:367:MET:N	2.21	0.73
2:C:56:GLU:HB2	2:C:64:LEU:HB2	1.70	0.73
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.70	0.72
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.71	0.72
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.70	0.72
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.22	0.71
3:D:1290:LEU:HB3	3:D:1305:LEU:HD23	1.73	0.71
2:C:214:TYR:O	2:C:218:VAL:HG23	1.90	0.71
6:G:18:DA:H2'	6:G:19:DA:H5'	1.71	0.71
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.72	0.70
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.73	0.70
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.23	0.70
2:C:649:VAL:HG13	2:C:653:ASP:HB2	1.73	0.70
2:C:758:ARG:HH21	2:C:788:THR:HB	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.73	0.70
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.74	0.70
2:C:109:LYS:HG2	2:C:368:THR:HG22	1.72	0.70
5:F:265:VAL:O	5:F:269:ASN:ND2	2.23	0.70
5:F:397:ILE:HD13	5:F:400:ILE:HD11	1.71	0.70
3:D:520:LEU:O	3:D:525:ARG:NH1	2.25	0.69
3:D:845:ASN:HB2	3:D:846:PRO:HD2	1.75	0.69
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.73	0.68
3:D:640:HIS:CD2	3:D:641:GLN:HG3	2.27	0.68
3:D:1281:VAL:CG2	3:D:1317:ASP:H	2.06	0.68
3:D:485:SER:O	3:D:487:ALA:N	2.25	0.68
2:C:393:GLN:HB3	8:I:5:G:C6	2.29	0.68
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.76	0.68
5:F:377:ASP:OD1	5:F:378:GLY:N	2.26	0.68
5:F:405:LEU:O	5:F:409:LYS:HG3	1.94	0.67
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.29	0.67
2:C:726:ILE:HG23	2:C:787:ASP:HB2	1.77	0.67
3:D:1234:THR:HB	3:D:1235:GLN:HB2	1.78	0.66
2:C:524:VAL:HG23	2:C:528:GLU:HB2	1.77	0.66
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.30	0.66
3:D:248:PRO:HG3	3:D:308:LYS:HG3	1.77	0.66
3:D:1209:LEU:HD11	3:D:1364:HIS:HD2	1.58	0.66
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.13	0.66
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.31	0.65
8:I:2:G:N3	8:I:2:G:H2'	2.08	0.65
2:C:987:ILE:HD11	3:D:946:GLY:HA2	1.78	0.65
3:D:1499:ARG:HH22	4:E:81:PRO:HG2	1.60	0.65
3:D:1364:HIS:CD2	3:D:1366:LYS:HE3	2.32	0.65
1:A:70:GLY:N	2:C:607:ASP:OD1	2.29	0.64
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.31	0.64
3:D:669:ASN:HB3	5:F:417:LYS:HE2	1.79	0.64
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.30	0.64
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.80	0.64
2:C:210:GLU:HB3	2:C:211:LEU:HD12	1.80	0.64
2:C:168:ARG:NH2	2:C:265:ARG:O	2.31	0.63
3:D:842:VAL:HG22	3:D:865:THR:HB	1.79	0.63
3:D:231:VAL:O	3:D:236:TYR:OH	2.15	0.63
6:G:12:DG:N2	7:H:17:DT:O2	2.31	0.63
2:C:573:ARG:HB2	2:C:670:GLN:NE2	2.13	0.63
1:A:99:LEU:HB2	1:A:142:VAL:HG23	1.80	0.63
1:A:191:ASP:OD1	2:C:938:LYS:NZ	2.25	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1004:LYS:HD3	3:D:744:GLN:NE2	2.14	0.63
3:D:619:LEU:HD11	3:D:1439:SER:HB2	1.81	0.63
3:D:973:GLN:HG2	3:D:974:ILE:HD13	1.81	0.62
3:D:1236:LEU:N	3:D:1236:LEU:HD12	2.14	0.62
5:F:386:VAL:HG13	5:F:390:PHE:CE1	2.33	0.62
1:B:18:ARG:NH1	1:B:204:SER:O	2.33	0.62
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.63	0.62
2:C:767:PRO:CB	2:C:771:GLU:HG2	2.30	0.62
2:C:715:THR:OG1	2:C:718:GLY:O	2.18	0.62
5:F:338:LEU:HD23	5:F:339:PRO:HD2	1.82	0.61
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.82	0.61
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.81	0.61
2:C:189:ARG:HH12	2:C:244:PRO:HD3	1.65	0.61
3:D:570:GLU:OE2	5:F:214:GLN:NE2	2.32	0.61
3:D:1319:VAL:HG12	3:D:1323:GLN:NE2	2.15	0.61
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.82	0.61
3:D:208:PRO:HG3	3:D:387:LEU:HD22	1.83	0.61
3:D:673:ALA:HA	3:D:676:MET:HE2	1.83	0.60
2:C:580:MET:HB3	2:C:584:GLU:CD	2.22	0.60
2:C:3:ILE:HD13	2:C:900:ARG:HB2	1.82	0.60
2:C:1059:ASP:OD1	2:C:1062:GLY:HA3	2.00	0.60
1:A:175:ARG:HE	1:A:202:ASP:HB3	1.67	0.60
1:B:80:LEU:HD22	3:D:844:ALA:HA	1.82	0.60
3:D:181:ASP:HB2	3:D:205:TYR:CG	2.37	0.60
8:I:2:G:O2'	8:I:3:G:N7	2.35	0.60
3:D:45:PHE:O	3:D:86:ARG:NH2	2.35	0.59
3:D:1209:LEU:HD11	3:D:1364:HIS:CD2	2.37	0.59
5:F:154:LYS:O	5:F:158:GLU:HG3	2.01	0.59
3:D:1149:LEU:HG	3:D:1166:LEU:HD21	1.84	0.59
2:C:244:PRO:O	5:F:82:ARG:NH1	2.36	0.59
3:D:1087:ARG:NE	3:D:1234:THR:O	2.33	0.59
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.32	0.59
2:C:1067:TYR:CE1	2:C:1071:ILE:HD13	2.38	0.59
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	1.85	0.59
2:C:853:LEU:HB2	2:C:858:MET:CE	2.32	0.58
3:D:750:PRO:O	3:D:756:GLN:NE2	2.36	0.58
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.84	0.58
3:D:1236:LEU:HD12	3:D:1236:LEU:H	1.67	0.58
3:D:1378:TYR:CE1	3:D:1396:GLU:HG2	2.38	0.58
3:D:1330:ILE:HD13	3:D:1347:TYR:CE1	2.38	0.58
1:A:222:LEU:HD11	1:B:218:LEU:HD23	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.86	0.58
2:C:419:THR:HG22	8:I:3:G:O2'	2.03	0.58
5:F:193:ARG:HB3	7:H:7:DG:H5'	1.84	0.58
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.85	0.58
1:A:6:LEU:HD21	1:A:27:PRO:HG2	1.85	0.58
2:C:64:LEU:HD11	2:C:364:GLU:HG2	1.86	0.57
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.85	0.57
2:C:874:LEU:HD12	3:D:784:ASP:OD1	2.04	0.57
3:D:1152:GLU:OE1	3:D:1159:ARG:NH1	2.36	0.57
6:G:5:DT:H2''	6:G:6:DG:C8	2.39	0.57
1:B:18:ARG:O	1:B:207:PRO:HD3	2.05	0.57
2:C:764:GLU:C	2:C:766:GLU:H	2.04	0.57
3:D:1258:ARG:CZ	3:D:1262:LEU:HD21	2.34	0.57
1:A:72:LYS:HE3	2:C:643:VAL:O	2.04	0.57
2:C:472:ARG:HD2	2:C:480:THR:O	2.05	0.57
3:D:1314:LYS:H	3:D:1314:LYS:HD2	1.69	0.57
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.86	0.57
2:C:767:PRO:HB2	2:C:771:GLU:HG2	1.86	0.57
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.08	0.57
4:E:14:ASP:OD2	4:E:18:ARG:NH1	2.38	0.57
2:C:587:VAL:O	2:C:591:SER:HB3	2.04	0.57
3:D:407:VAL:HG12	5:F:172:ARG:HH12	1.70	0.57
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.87	0.56
3:D:1386:ASP:CG	3:D:1413:THR:HG22	2.25	0.56
2:C:331:ARG:HH22	2:C:427:VAL:HG12	1.69	0.56
2:C:409:ARG:HD2	2:C:452:ILE:HG22	1.87	0.56
2:C:607:ASP:HB3	2:C:610:ARG:H	1.70	0.56
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	1.87	0.56
5:F:122:LEU:HB2	5:F:127:ILE:HD11	1.87	0.56
2:C:573:ARG:HB2	2:C:670:GLN:HE21	1.71	0.56
3:D:799:LYS:NZ	3:D:1014:ASN:HA	2.21	0.56
3:D:741:ASP:OD1	3:D:743:ASP:OD1	2.23	0.55
1:B:102:LYS:HG2	1:B:139:ASN:OD1	2.05	0.55
2:C:475:VAL:O	2:C:478:VAL:HG12	2.06	0.55
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	1.88	0.55
3:D:658:LEU:HD23	3:D:661:MET:HE3	1.88	0.55
5:F:326:ASP:CB	6:G:19:DA:H61	2.19	0.55
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.25	0.55
3:D:1232:PRO:O	3:D:1235:GLN:HB3	2.06	0.55
3:D:1277:ILE:HG13	3:D:1278:ASP:H	1.71	0.55
3:D:671:LYS:HE3	5:F:421:PHE:HA	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:757:GLY:HA2	2:C:789:SER:OG	2.06	0.54
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.38	0.54
2:C:243:ARG:NH2	7:H:9:DG:O6	2.41	0.54
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.88	0.54
3:D:474:GLU:OE2	3:D:500:ARG:NE	2.41	0.54
3:D:256:GLU:O	3:D:274:ARG:NH1	2.40	0.54
3:D:480:GLU:OE2	3:D:492:ALA:HB2	2.08	0.54
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.08	0.54
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.43	0.54
5:F:277:GLN:O	5:F:281:GLU:HG2	2.08	0.54
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.42	0.54
2:C:376:ARG:NH1	5:F:279:GLN:OE1	2.40	0.54
2:C:591:SER:O	2:C:592:LEU:HB2	2.07	0.54
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.89	0.54
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.41	0.54
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.73	0.54
3:D:622:ARG:NH1	6:G:17:DC:OP1	2.38	0.54
6:G:18:DA:N6	6:G:19:DA:C5	2.76	0.54
3:D:1386:ASP:OD2	3:D:1412:LYS:HD2	2.08	0.53
5:F:383:LEU:HB3	5:F:394:ARG:HH22	1.73	0.53
2:C:524:VAL:CG2	2:C:528:GLU:HB2	2.39	0.53
3:D:1142:ALA:O	3:D:1364:HIS:ND1	2.42	0.53
3:D:65:ARG:HB3	5:F:377:ASP:HA	1.90	0.53
7:H:17:DT:H2''	7:H:18:DG:H5'	1.91	0.53
3:D:100:ALA:HB3	3:D:575:GLN:HE22	1.72	0.53
3:D:1291:SER:OG	3:D:1304:LYS:HG2	2.08	0.53
4:E:75:PHE:H	4:E:75:PHE:HD2	1.56	0.53
5:F:345:ALA:O	5:F:349:LEU:HG	2.09	0.53
3:D:1263:PHE:O	3:D:1375:MET:HE2	2.08	0.53
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.24	0.53
2:C:617:ASP:OD2	2:C:619:ARG:NE	2.26	0.53
6:G:13:DA:N6	8:I:2:G:O2'	2.42	0.53
2:C:202:TYR:CD2	2:C:207:LEU:HD21	2.44	0.53
3:D:171:LEU:HD21	3:D:177:ALA:HB2	1.90	0.53
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.89	0.53
1:A:96:THR:HB	1:A:145:ASP:OD1	2.09	0.53
1:B:80:LEU:HD22	3:D:844:ALA:CA	2.39	0.53
1:B:188:GLN:CD	1:B:188:GLN:H	2.13	0.53
2:C:41:ASN:OD1	2:C:46:ALA:HA	2.09	0.53
2:C:861:LEU:HB3	2:C:862:PRO:HD2	1.91	0.53
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:97:THR:CG2	3:D:554:LEU:HD21	2.38	0.52
3:D:1258:ARG:NH2	3:D:1262:LEU:HD21	2.24	0.52
2:C:946:ARG:NH1	2:C:984:GLU:OE2	2.42	0.52
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.44	0.52
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.90	0.52
1:A:70:GLY:HA3	1:A:136:GLY:HA2	1.90	0.52
3:D:241:ILE:HG12	3:D:312:ARG:HH12	1.74	0.52
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.91	0.52
3:D:103:TRP:HB3	3:D:1448:THR:CG2	2.39	0.52
3:D:1495:ILE:HG12	4:E:88:GLU:CG	2.38	0.52
5:F:398:ARG:O	5:F:401:GLU:HB3	2.10	0.52
3:D:799:LYS:HZ1	3:D:1014:ASN:HA	1.75	0.52
2:C:267:TYR:CE1	2:C:290:LEU:HG	2.44	0.52
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.92	0.52
3:D:1108:ARG:HD2	3:D:1198:TYR:O	2.09	0.52
2:C:598:GLU:HB2	2:C:615:TYR:CE2	2.44	0.52
3:D:1378:TYR:CD2	3:D:1422:MET:SD	3.03	0.52
2:C:582:GLY:N	2:C:584:GLU:OE2	2.42	0.52
3:D:573:MET:SD	5:F:210:LEU:HB3	2.50	0.52
5:F:168:LYS:O	5:F:172:ARG:HG2	2.10	0.52
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.10	0.51
4:E:70:THR:OG1	4:E:72:ARG:HG3	2.09	0.51
3:D:288:MET:HA	3:D:306:GLU:O	2.10	0.51
3:D:658:LEU:HD23	3:D:661:MET:CE	2.40	0.51
3:D:1459:LEU:HD23	3:D:1464:GLU:HB3	1.92	0.51
5:F:160:ASP:OD2	5:F:164:LYS:HE3	2.10	0.51
5:F:353:GLU:HG2	5:F:418:LEU:HD11	1.91	0.51
2:C:185:LYS:HZ3	2:C:190:LYS:HD2	1.75	0.51
3:D:838:ARG:HD3	3:D:874:GLU:CD	2.31	0.51
3:D:1386:ASP:OD2	3:D:1413:THR:HG22	2.11	0.51
2:C:1095:LEU:HG	3:D:603:LEU:HD23	1.93	0.51
1:A:25:LEU:HB3	1:A:28:LEU:HD11	1.93	0.51
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.20	0.51
2:C:404:LEU:O	2:C:408:ARG:HG3	2.11	0.51
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.76	0.51
3:D:36:THR:HB	3:D:38:LYS:HD2	1.92	0.51
5:F:383:LEU:HB3	5:F:394:ARG:NH2	2.25	0.51
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.92	0.51
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.11	0.51
3:D:800:LYS:NZ	3:D:819:GLY:O	2.44	0.51
5:F:168:LYS:HG3	5:F:172:ARG:HH21	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:64:LEU:N	2:C:103:LYS:HB3	2.25	0.51
2:C:124:ASP:HB3	2:C:592:LEU:HD22	1.92	0.51
3:D:285:PRO:HG3	3:D:311:LEU:HD13	1.93	0.51
3:D:405:ASP:CG	3:D:406:ASP:H	2.14	0.51
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.93	0.51
2:C:280:LYS:HE3	2:C:309:TYR:CZ	2.46	0.50
3:D:1100:ASP:OD2	3:D:1463:LYS:NZ	2.22	0.50
2:C:226:VAL:O	2:C:229:MET:HG2	2.11	0.50
3:D:1310:ARG:HB2	3:D:1327:ARG:HB2	1.93	0.50
4:E:30:LEU:HB3	4:E:35:PHE:CD1	2.45	0.50
2:C:135:VAL:HG23	2:C:395:LYS:HG3	1.94	0.50
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.92	0.50
2:C:767:PRO:HB3	2:C:771:GLU:HG2	1.92	0.50
3:D:1216:SER:OG	4:E:16:LYS:HG2	2.11	0.50
3:D:860:LEU:O	3:D:876:SER:HB2	2.11	0.50
1:A:34:VAL:HG22	1:B:42:ARG:CZ	2.42	0.50
1:A:50:GLY:HA3	1:A:173:PRO:HD3	1.94	0.50
1:A:201:THR:HG21	1:A:205:VAL:O	2.12	0.50
2:C:957:LYS:HD3	2:C:961:GLU:HB3	1.93	0.50
8:I:3:G:N3	8:I:4:G:N2	2.59	0.50
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.93	0.50
2:C:563:ASN:O	2:C:566:THR:HB	2.12	0.50
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.11	0.50
2:C:807:ARG:HB2	2:C:810:ASP:OD2	2.12	0.50
3:D:134:VAL:HG22	3:D:151:GLN:H	1.77	0.50
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.94	0.50
3:D:553:ARG:HD3	5:F:214:GLN:HB3	1.94	0.50
3:D:231:VAL:HG13	3:D:242:LEU:O	2.12	0.49
3:D:462:GLN:HB2	3:D:513:ILE:HG21	1.94	0.49
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.46	0.49
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.94	0.49
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.93	0.49
3:D:241:ILE:HG12	3:D:312:ARG:NH1	2.27	0.49
3:D:1486:VAL:HG22	4:E:22:VAL:HG13	1.95	0.49
1:A:104:GLU:HB3	1:A:137:ARG:HD3	1.94	0.49
1:A:184:THR:O	1:A:192:LEU:HB2	2.12	0.49
2:C:76:PRO:HG3	2:C:120:LEU:HD12	1.93	0.49
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.48	0.49
3:D:1133:ARG:HH12	3:D:1136:LYS:HE3	1.76	0.49
2:C:858:MET:HG2	2:C:867:VAL:O	2.12	0.49
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:33:HIS:NE2	4:E:89:MET:HB3	2.28	0.49
5:F:368:VAL:HG22	5:F:390:PHE:HD2	1.78	0.49
5:F:394:ARG:NH1	5:F:395:GLU:OE2	2.46	0.49
2:C:150:PRO:HA	2:C:158:TYR:CD2	2.48	0.49
2:C:1052:MET:HG3	3:D:623:VAL:HG11	1.95	0.49
3:D:1143:GLY:O	3:D:1147:ARG:HD2	2.13	0.49
2:C:436:GLY:HA2	2:C:538:GLN:O	2.13	0.49
2:C:773:LEU:O	2:C:777:ILE:HG13	2.13	0.49
3:D:675:ARG:HH12	5:F:423:ASP:HA	1.78	0.49
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.13	0.49
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.95	0.49
2:C:773:LEU:HD13	5:F:373:LYS:HG3	1.94	0.48
3:D:216:VAL:CG1	3:D:218:LYS:HE2	2.43	0.48
2:C:1047:HIS:CE1	3:D:1471:LEU:HD11	2.48	0.48
3:D:56:TYR:HE1	3:D:69:GLU:HG3	1.78	0.48
3:D:155:ASP:OD1	3:D:568:ARG:NH1	2.40	0.48
3:D:357:GLU:HB2	3:D:387:LEU:HD12	1.95	0.48
2:C:165:LEU:HD11	2:C:270:GLY:HA2	1.94	0.48
3:D:322:VAL:HG22	3:D:335:LEU:CD2	2.43	0.48
1:B:176:ARG:HB3	1:B:200:TRP:CE3	2.48	0.48
3:D:792:ILE:HG13	3:D:793:THR:HG23	1.95	0.48
5:F:173:TYR:CD1	5:F:173:TYR:N	2.81	0.48
1:A:117:VAL:O	1:A:120:VAL:HG22	2.14	0.48
1:B:65:PHE:CE2	3:D:809:PRO:HB2	2.48	0.48
1:B:197:LEU:HA	1:B:197:LEU:HD23	1.62	0.48
3:D:131:LYS:N	3:D:456:MET:HE2	2.28	0.48
3:D:1386:ASP:HB2	3:D:1412:LYS:HB3	1.95	0.48
2:C:236:ILE:HG23	2:C:248:PRO:HB2	1.96	0.48
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.95	0.48
3:D:526:PRO:HB2	3:D:528:VAL:HG13	1.95	0.48
6:G:12:DG:H5''	6:G:12:DG:H8	1.78	0.48
3:D:174:GLY:HA2	3:D:389:GLU:OE2	2.14	0.48
3:D:1485:GLN:O	4:E:75:PHE:HA	2.14	0.48
1:A:94:LEU:O	1:A:146:ARG:NH1	2.46	0.48
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.95	0.48
1:B:32:PHE:HA	1:B:35:THR:HB	1.95	0.48
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.96	0.48
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.29	0.48
3:D:1353:GLN:NE2	3:D:1365:ASP:OD1	2.39	0.48
3:D:1281:VAL:HG23	3:D:1316:GLY:N	2.29	0.48
6:G:15:DC:H2'	6:G:16:DC:C6	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:SER:O	1:A:228:PRO:HD3	2.14	0.47
2:C:259:GLY:HA2	2:C:263:ASP:HB2	1.96	0.47
2:C:617:ASP:OD1	2:C:617:ASP:N	2.46	0.47
3:D:71:LYS:O	3:D:80:VAL:HG22	2.14	0.47
3:D:103:TRP:HB3	3:D:1448:THR:HG21	1.96	0.47
3:D:1125:PRO:HB2	3:D:1130:ARG:HH22	1.79	0.47
5:F:400:ILE:HG22	5:F:403:LYS:HE2	1.95	0.47
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.53	0.47
3:D:657:LEU:HG	3:D:661:MET:HE1	1.95	0.47
3:D:1161:GLU:CD	3:D:1164:ARG:HB2	2.34	0.47
2:C:136:ILE:HD13	2:C:392:SER:HA	1.97	0.47
2:C:886:LEU:HD11	3:D:951:ILE:HD13	1.95	0.47
3:D:57:GLU:HG3	3:D:64:LYS:HG3	1.97	0.47
3:D:66:GLN:HB3	5:F:376:ILE:CG2	2.44	0.47
3:D:407:VAL:HG23	3:D:422:ALA:HB2	1.95	0.47
3:D:1165:TYR:CZ	3:D:1214:PRO:HB3	2.50	0.47
3:D:1478:SER:O	3:D:1482:ARG:HB2	2.15	0.47
5:F:393:THR:HG22	5:F:394:ARG:N	2.30	0.47
3:D:828:LYS:HG2	3:D:833:GLU:HG2	1.97	0.47
3:D:899:LEU:HD21	3:D:921:ARG:HD3	1.95	0.47
6:G:13:DA:H5''	6:G:14:DG:OP1	2.14	0.47
2:C:170:PRO:HD2	2:C:267:TYR:CE2	2.49	0.47
2:C:179:ASN:OD1	2:C:181:VAL:HG12	2.14	0.47
3:D:215:TYR:HE1	3:D:381:ALA:H	1.62	0.47
3:D:411:THR:HA	3:D:435:VAL:HG12	1.97	0.47
3:D:890:VAL:HG23	3:D:892:ASP:H	1.79	0.47
1:B:80:LEU:HD23	1:B:80:LEU:HA	1.65	0.47
2:C:575:GLN:HG3	2:C:670:GLN:HA	1.95	0.47
2:C:628:PHE:H	2:C:638:ASP:HB2	1.79	0.47
2:C:859:PRO:O	2:C:867:VAL:HG22	2.15	0.47
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.46	0.47
3:D:1154:GLU:HG2	3:D:1159:ARG:HA	1.96	0.47
4:E:50:THR:HG23	4:E:53:GLY:O	2.15	0.47
5:F:158:GLU:O	5:F:162:LYS:HD3	2.15	0.47
1:A:57:TYR:CE1	1:A:163:ASN:HB2	2.50	0.47
2:C:150:PRO:HG3	2:C:322:VAL:HG21	1.97	0.47
3:D:59:ALA:HB2	3:D:78:VAL:HG21	1.97	0.47
3:D:177:ALA:CB	3:D:393:ILE:HD11	2.45	0.47
3:D:629:SER:OG	3:D:630:VAL:N	2.48	0.47
3:D:830:ALA:O	3:D:832:ARG:N	2.48	0.47
3:D:1499:ARG:HH12	4:E:81:PRO:HD2	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:586:ARG:O	3:D:586:ARG:NH1	2.47	0.47
3:D:1378:TYR:HE1	3:D:1396:GLU:HG2	1.78	0.47
3:D:1381:VAL:HG21	3:D:1389:LEU:HD23	1.97	0.47
3:D:1486:VAL:CG2	4:E:22:VAL:HG13	2.45	0.47
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.69	0.47
2:C:598:GLU:O	2:C:651:LYS:HG3	2.14	0.47
2:C:605:LYS:HB3	2:C:610:ARG:NH1	2.29	0.47
3:D:129:PHE:CD2	3:D:456:MET:HB3	2.49	0.47
2:C:690:ILE:HD11	2:C:852:ILE:HD13	1.96	0.46
2:C:727:PRO:HB2	2:C:728:HIS:HD2	1.79	0.46
3:D:1347:TYR:CE2	3:D:1351:GLU:HG3	2.50	0.46
5:F:287:THR:HG22	5:F:288:TYR:H	1.80	0.46
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.98	0.46
2:C:578:VAL:HG13	2:C:671:ASN:CG	2.36	0.46
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	1.97	0.46
3:D:514:LEU:HD13	3:D:517:VAL:HG22	1.98	0.46
5:F:364:ARG:NH2	5:F:365:GLU:HA	2.29	0.46
2:C:693:GLU:HA	2:C:696:LYS:HD2	1.98	0.46
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.97	0.46
2:C:74:GLY:HA3	2:C:93:PRO:HG2	1.98	0.46
2:C:1019:GLN:HG2	2:C:1058:ASP:OD2	2.15	0.46
2:C:1059:ASP:OD2	2:C:1080:SER:HB3	2.16	0.46
3:D:1047:LYS:HB3	3:D:1048:PRO:HD2	1.96	0.46
2:C:640:ARG:O	2:C:657:ASP:N	2.49	0.46
3:D:1330:ILE:HD13	3:D:1347:TYR:HE1	1.80	0.46
2:C:952:LEU:HA	2:C:952:LEU:HD23	1.65	0.46
7:H:17:DT:H2'	7:H:18:DG:C8	2.51	0.46
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.51	0.46
2:C:413:LEU:HD23	8:I:4:G:H8	1.81	0.46
3:D:625:TYR:CD2	3:D:751:LEU:HD11	2.51	0.46
3:D:907:GLU:OE2	3:D:909:ASN:N	2.49	0.46
5:F:226:LYS:HD2	7:H:1:DT:H73	1.97	0.46
3:D:10:ILE:HG23	3:D:1451:ALA:HA	1.98	0.45
3:D:1011:PHE:HB3	3:D:1021:TYR:CD1	2.50	0.45
5:F:329:TYR:CE2	5:F:333:ILE:HD11	2.51	0.45
5:F:364:ARG:NH2	5:F:400:ILE:HD12	2.32	0.45
2:C:417:GLY:O	2:C:418:LEU:O	2.34	0.45
2:C:690:ILE:HD11	2:C:852:ILE:CD1	2.46	0.45
5:F:267:THR:O	5:F:270:LYS:HB3	2.16	0.45
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.97	0.45
2:C:86:LYS:HB2	2:C:88:LEU:HG	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:261:ILE:HG22	2:C:262:ALA:N	2.31	0.45
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.52	0.45
3:D:207:PHE:HB2	3:D:391:ALA:HB2	1.99	0.45
3:D:1140:ILE:CG2	3:D:1144:LEU:HD12	2.47	0.45
3:D:1263:PHE:HD2	3:D:1375:MET:CE	2.30	0.45
5:F:377:ASP:OD2	5:F:379:ARG:HB2	2.16	0.45
2:C:412:ALA:O	2:C:417:GLY:HA3	2.16	0.45
2:C:957:LYS:HB3	2:C:961:GLU:HB2	1.99	0.45
3:D:934:LEU:HA	3:D:934:LEU:HD23	1.72	0.45
3:D:1102:THR:CG2	3:D:1371:VAL:HG22	2.46	0.45
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.99	0.45
1:B:99:LEU:HB3	1:B:114:PHE:CD1	2.52	0.45
1:B:159:LYS:HE3	1:B:164:ALA:O	2.16	0.45
2:C:170:PRO:HD2	2:C:267:TYR:HE2	1.81	0.45
2:C:331:ARG:HH22	2:C:427:VAL:CG1	2.29	0.45
2:C:614:ARG:HE	2:C:620:LEU:HD13	1.81	0.45
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.52	0.45
3:D:186:VAL:HG12	3:D:189:GLN:HB2	1.98	0.45
3:D:288:MET:HE3	3:D:305:ALA:HB3	1.99	0.45
1:A:101:LEU:HD21	1:A:109:VAL:HG11	1.99	0.45
3:D:65:ARG:HD3	5:F:377:ASP:H	1.82	0.45
3:D:90:MET:SD	3:D:521:PRO:HD3	2.57	0.45
3:D:806:PHE:O	3:D:829:VAL:HA	2.17	0.45
3:D:916:TYR:CZ	3:D:920:LEU:HD21	2.52	0.45
3:D:1141:GLU:OE2	3:D:1168:MET:HE1	2.16	0.45
4:E:75:PHE:N	4:E:75:PHE:CD2	2.82	0.45
5:F:101:GLU:HG2	5:F:105:LYS:HE3	1.97	0.45
2:C:136:ILE:CB	2:C:336:VAL:HG13	2.46	0.45
2:C:763:GLY:C	2:C:765:SER:H	2.20	0.45
3:D:216:VAL:HG12	3:D:218:LYS:HE2	1.97	0.45
3:D:961:LYS:O	3:D:965:GLU:HG3	2.17	0.45
2:C:327:HIS:NE2	2:C:433:THR:HG21	2.31	0.45
3:D:784:ASP:HB2	3:D:939:PHE:CE1	2.52	0.45
2:C:327:HIS:CE1	2:C:433:THR:HG21	2.52	0.45
3:D:127:LEU:HD23	3:D:127:LEU:HA	1.73	0.45
3:D:312:ARG:NH1	3:D:312:ARG:HB3	2.31	0.45
3:D:876:SER:OG	3:D:879:ARG:HG3	2.17	0.45
3:D:1112:CYS:HB3	3:D:1196:THR:OG1	2.17	0.45
1:A:10:VAL:HG22	1:A:26:GLU:O	2.16	0.45
1:A:65:PHE:CE2	2:C:703:ILE:HD13	2.51	0.45
1:A:218:LEU:HG	1:B:222:LEU:HD11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3:ILE:CD1	2:C:900:ARG:HB2	2.47	0.45
3:D:976:GLN:O	3:D:980:MET:HB2	2.17	0.45
5:F:187:LEU:HD23	5:F:224:VAL:HG13	1.99	0.45
3:D:465:LEU:HD23	3:D:465:LEU:HA	1.83	0.44
5:F:382:THR:HG22	5:F:383:LEU:HG	1.99	0.44
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.48	0.44
1:A:220:GLU:O	1:A:223:THR:OG1	2.21	0.44
2:C:134:ARG:NH1	2:C:392:SER:O	2.50	0.44
2:C:240:THR:HG22	2:C:248:PRO:HG3	1.99	0.44
2:C:1057:SER:HB3	2:C:1058:ASP:H	1.50	0.44
3:D:638:LYS:HA	3:D:638:LYS:HD3	1.75	0.44
4:E:57:ASP:O	4:E:63:TRP:NE1	2.41	0.44
1:B:9:PRO:HB2	1:B:25:LEU:HD11	2.00	0.44
2:C:49:ARG:CZ	2:C:49:ARG:HB3	2.47	0.44
2:C:719:PRO:HB3	2:C:820:ARG:HE	1.82	0.44
3:D:1425:THR:HG23	3:D:1440:PHE:CE2	2.53	0.44
3:D:162:ARG:O	3:D:449:SER:HB2	2.18	0.44
3:D:1198:TYR:CZ	3:D:1460:ILE:HD13	2.52	0.44
1:B:153:ALA:HB2	1:B:167:VAL:C	2.38	0.44
3:D:471:GLU:H	3:D:471:GLU:HG2	1.43	0.44
1:B:61:VAL:HG13	1:B:66:SER:HB2	1.98	0.44
2:C:185:LYS:HG3	2:C:190:LYS:HG2	2.00	0.44
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.80	0.44
2:C:759:THR:HB	2:C:785:VAL:HB	2.00	0.44
1:B:153:ALA:C	1:B:155:LYS:H	2.21	0.44
2:C:150:PRO:HD3	2:C:322:VAL:CG1	2.46	0.44
2:C:204:GLN:HG3	2:C:222:MET:SD	2.58	0.44
2:C:854:PRO:HB2	2:C:856:GLU:OE1	2.17	0.44
3:D:439:LEU:HD23	3:D:439:LEU:HA	1.76	0.44
3:D:468:LEU:HA	3:D:468:LEU:HD23	1.65	0.44
2:C:1:MET:HB2	2:C:898:GLY:O	2.18	0.44
2:C:593:ALA:HB1	2:C:659:PRO:HD2	2.00	0.44
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.77	0.43
3:D:972:LEU:HD13	3:D:972:LEU:HA	1.60	0.43
3:D:1036:ARG:NH2	3:D:1042:ARG:O	2.51	0.43
3:D:1295:GLU:HA	3:D:1300:SER:HB2	1.99	0.43
3:D:1378:TYR:HD2	3:D:1422:MET:SD	2.41	0.43
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.85	0.43
2:C:161:SER:HA	2:C:172:ILE:O	2.18	0.43
2:C:807:ARG:HG2	2:C:821:GLU:OE1	2.18	0.43
2:C:929:ARG:NH2	2:C:940:GLU:OE2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.75	0.43
1:A:11:PHE:O	1:B:228:PRO:HA	2.18	0.43
1:B:99:LEU:HB2	1:B:142:VAL:HG22	1.99	0.43
2:C:263:ASP:O	2:C:265:ARG:N	2.50	0.43
2:C:605:LYS:HB3	2:C:610:ARG:HH12	1.82	0.43
2:C:853:LEU:HB2	2:C:858:MET:HE2	2.00	0.43
2:C:879:ARG:HD2	2:C:879:ARG:N	2.32	0.43
3:D:464:LEU:HD23	3:D:464:LEU:HA	1.79	0.43
3:D:1044:LEU:CD2	3:D:1056:PRO:HB3	2.45	0.43
3:D:1233:GLY:O	3:D:1234:THR:OG1	2.30	0.43
1:A:32:PHE:HA	1:A:35:THR:HB	1.99	0.43
1:A:56:VAL:HG23	1:A:167:VAL:HG21	2.00	0.43
1:B:115:LEU:HD23	1:B:115:LEU:HA	1.75	0.43
2:C:214:TYR:HB3	2:C:217:LEU:HD12	2.00	0.43
2:C:911:GLU:O	2:C:915:LYS:HG2	2.17	0.43
2:C:1036:GLU:OE2	2:C:1036:GLU:N	2.50	0.43
2:C:1042:ALA:HB1	3:D:1224:VAL:HG22	1.99	0.43
3:D:177:ALA:HB2	3:D:393:ILE:HD11	1.99	0.43
3:D:352:ASN:HB3	5:F:104:ARG:CZ	2.49	0.43
3:D:652:LEU:HB3	3:D:749:VAL:HG21	2.00	0.43
2:C:540:PHE:CD1	2:C:544:THR:HG21	2.53	0.43
2:C:1067:TYR:HE1	2:C:1071:ILE:HD13	1.84	0.43
3:D:480:GLU:OE1	3:D:488:ARG:HD2	2.17	0.43
3:D:651:GLU:O	3:D:654:LYS:HB2	2.19	0.43
3:D:1208:ASP:OD2	3:D:1211:MET:HE2	2.18	0.43
4:E:69:LEU:HD23	4:E:69:LEU:HA	1.87	0.43
5:F:167:PRO:HG2	5:F:170:HIS:HB2	2.00	0.43
5:F:173:TYR:N	5:F:173:TYR:HD1	2.16	0.43
2:C:886:LEU:HD12	2:C:886:LEU:H	1.82	0.43
3:D:115:LEU:HD23	3:D:115:LEU:HA	1.85	0.43
1:B:72:LYS:HB3	1:B:131:THR:OG1	2.18	0.43
1:B:176:ARG:HG2	1:B:200:TRP:CZ3	2.54	0.43
2:C:269:LEU:HA	2:C:269:LEU:HD12	1.66	0.43
2:C:586:ARG:HD2	2:C:586:ARG:HA	1.74	0.43
2:C:880:MET:HB3	3:D:1061:PHE:CE2	2.54	0.43
3:D:669:ASN:ND2	5:F:417:LYS:HG2	2.34	0.43
3:D:1104:GLU:O	3:D:1108:ARG:NH2	2.50	0.43
7:H:3:DT:H2''	7:H:4:DA:H5'	2.01	0.43
1:A:65:PHE:HE2	2:C:703:ILE:HD13	1.84	0.43
2:C:90:TYR:CE2	2:C:120:LEU:HB2	2.54	0.43
2:C:283:ILE:HD13	2:C:305:PRO:HG2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1140:ILE:HG22	3:D:1144:LEU:HD12	2.01	0.43
4:E:40:LEU:HD23	4:E:72:ARG:HH12	1.83	0.43
5:F:384:GLU:O	5:F:387:GLY:N	2.41	0.43
2:C:473:ARG:HA	2:C:531:PHE:CD1	2.53	0.43
2:C:1097:LEU:HD23	2:C:1097:LEU:HA	1.66	0.43
3:D:84:ILE:CD1	3:D:87:ARG:HD3	2.48	0.43
3:D:1057:VAL:HG13	3:D:1069:GLU:CD	2.39	0.43
3:D:1383:ASP:HA	3:D:1384:PRO:HD3	1.88	0.43
5:F:412:GLU:OE2	5:F:416:ARG:HA	2.19	0.43
1:A:117:VAL:HB	1:A:120:VAL:HG21	2.01	0.43
1:A:206:THR:HG22	1:A:208:LEU:H	1.83	0.43
2:C:164:PRO:HA	2:C:269:LEU:HD12	2.01	0.43
5:F:308:LEU:HD23	5:F:308:LEU:HA	1.69	0.43
2:C:76:PRO:HA	2:C:77:PRO:HD3	1.90	0.42
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.86	0.42
3:D:1028:ALA:O	3:D:1029:ARG:HG2	2.18	0.42
3:D:1155:VAL:HG12	3:D:1182:GLU:HG2	2.00	0.42
2:C:134:ARG:NH2	6:G:21:DA:OP2	2.51	0.42
3:D:974:ILE:HD12	3:D:991:GLN:OE1	2.19	0.42
3:D:1087:ARG:HE	3:D:1234:THR:C	2.19	0.42
3:D:1130:ARG:HA	3:D:1130:ARG:NE	2.33	0.42
3:D:1444:THR:O	3:D:1448:THR:HG23	2.20	0.42
1:A:106:PRO:CG	1:A:134:GLU:HG2	2.42	0.42
2:C:419:THR:HB	2:C:420:ARG:H	1.53	0.42
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.54	0.42
3:D:134:VAL:CG2	3:D:151:GLN:H	2.32	0.42
3:D:161:LEU:HD12	3:D:161:LEU:HA	1.84	0.42
3:D:286:VAL:O	3:D:311:LEU:HA	2.19	0.42
3:D:966:GLU:HG2	3:D:969:ARG:NH1	2.33	0.42
3:D:1149:LEU:HD11	3:D:1160:LEU:HB3	2.01	0.42
3:D:1167:SER:O	3:D:1171:VAL:HG23	2.18	0.42
3:D:1272:ALA:HA	3:D:1326:THR:HB	2.01	0.42
5:F:355:GLU:C	5:F:357:ALA:H	2.23	0.42
2:C:352:ALA:O	2:C:356:ARG:HG3	2.20	0.42
3:D:618:LEU:HD13	3:D:618:LEU:HA	1.89	0.42
3:D:1216:SER:HB3	4:E:15:SER:OG	2.20	0.42
3:D:1348:LEU:HD23	3:D:1348:LEU:HA	1.85	0.42
3:D:1402:ALA:O	3:D:1406:ARG:HG3	2.20	0.42
2:C:684:PHE:CE2	3:D:730:PRO:HB3	2.55	0.42
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.53	0.42
3:D:15:PRO:HB3	3:D:515:GLU:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:172:PRO:HA	3:D:173:PRO:HD3	1.96	0.42
3:D:322:VAL:HG22	3:D:335:LEU:HD23	2.01	0.42
3:D:759:ALA:HA	3:D:763:MET:HB2	2.00	0.42
4:E:39:VAL:HG23	4:E:72:ARG:HH11	1.84	0.42
2:C:84:ARG:HA	2:C:131:GLY:HA2	2.02	0.42
2:C:729:LEU:HD23	2:C:729:LEU:HA	1.76	0.42
3:D:60:CYS:SG	3:D:76:CYS:HB3	2.59	0.42
3:D:864:VAL:HG12	3:D:866:VAL:HG23	2.02	0.42
3:D:1038:LEU:HA	3:D:1038:LEU:HD23	1.78	0.42
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.53	0.42
2:C:263:ASP:C	2:C:265:ARG:H	2.23	0.42
2:C:351:LEU:HD12	2:C:375:SER:HA	2.02	0.42
3:D:44:LEU:O	3:D:525:ARG:NH2	2.45	0.42
3:D:650:LEU:HD11	3:D:677:LEU:HD13	2.02	0.42
3:D:658:LEU:HA	3:D:661:MET:HE2	2.02	0.42
5:F:127:ILE:O	5:F:131:VAL:HG23	2.19	0.42
6:G:17:DC:H2'	6:G:18:DA:C8	2.54	0.42
1:B:218:LEU:HD12	1:B:218:LEU:HA	1.85	0.42
3:D:1282:ARG:NH2	3:D:1295:GLU:OE2	2.53	0.42
3:D:1290:LEU:HD23	3:D:1307:LYS:HA	2.02	0.42
7:H:4:DA:C6	7:H:5:DA:N1	2.88	0.42
2:C:69:LEU:HB2	2:C:97:ARG:O	2.19	0.42
3:D:1277:ILE:HG13	3:D:1278:ASP:N	2.35	0.42
3:D:1457:ASP:OD1	3:D:1464:GLU:HG2	2.20	0.42
2:C:196:LEU:HD22	2:C:196:LEU:O	2.19	0.42
2:C:598:GLU:N	2:C:615:TYR:OH	2.46	0.42
3:D:731:LEU:HD23	3:D:731:LEU:HA	1.83	0.42
3:D:1232:PRO:O	3:D:1234:THR:N	2.53	0.42
5:F:140:ARG:HE	5:F:140:ARG:HB2	1.65	0.42
2:C:227:PHE:C	2:C:229:MET:H	2.24	0.41
2:C:926:PHE:HE1	2:C:929:ARG:HH11	1.65	0.41
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.55	0.41
3:D:236:TYR:H	3:D:319:ALA:HB3	1.85	0.41
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.55	0.41
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.78	0.41
5:F:419:ARG:O	5:F:422:LEU:HB2	2.20	0.41
2:C:304:LEU:HB3	2:C:305:PRO:HD3	2.02	0.41
2:C:1043:TYR:CE2	3:D:763:MET:HE3	2.54	0.41
3:D:787:LEU:HA	3:D:787:LEU:HD12	1.81	0.41
5:F:358:LEU:HB3	5:F:366:ALA:CB	2.36	0.41
2:C:210:GLU:HG2	2:C:304:LEU:HD21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:134:ARG:HH11	2:C:134:ARG:HD3	1.72	0.41
2:C:227:PHE:O	2:C:229:MET:N	2.46	0.41
2:C:948:GLU:OE2	2:C:962:GLN:NE2	2.47	0.41
3:D:42:ASP:N	3:D:46:ASP:OD2	2.27	0.41
5:F:394:ARG:HG3	5:F:395:GLU:N	2.34	0.41
2:C:207:LEU:HD13	2:C:221:LEU:HD11	2.02	0.41
2:C:678:PRO:HA	2:C:683:ASN:HD22	1.86	0.41
3:D:480:GLU:O	3:D:480:GLU:HG2	2.20	0.41
3:D:899:LEU:HD22	3:D:917:GLN:HB3	2.03	0.41
5:F:130:VAL:HG11	5:F:159:ILE:HG22	2.02	0.41
2:C:121:MET:SD	2:C:125:GLY:HA2	2.61	0.41
2:C:331:ARG:NH2	2:C:427:VAL:HG12	2.34	0.41
2:C:1100:GLN:HG3	3:D:9:ARG:NH2	2.36	0.41
3:D:84:ILE:HD11	3:D:87:ARG:HD3	2.03	0.41
3:D:97:THR:HG21	3:D:571:LYS:HE3	2.02	0.41
3:D:97:THR:HG21	3:D:571:LYS:HG2	2.03	0.41
3:D:1125:PRO:HB2	3:D:1130:ARG:NH2	2.35	0.41
1:B:132:LEU:HD21	1:B:138:LEU:HB2	2.02	0.41
2:C:367:LEU:HD23	2:C:371:LYS:HE2	2.03	0.41
2:C:904:PRO:HD2	2:C:907:ASP:O	2.20	0.41
2:C:952:LEU:HB3	2:C:966:LEU:HD21	2.03	0.41
3:D:17:LYS:HE2	3:D:17:LYS:HB2	1.75	0.41
3:D:411:THR:O	5:F:178:ARG:NH1	2.50	0.41
3:D:622:ARG:HH12	6:G:17:DC:P	2.42	0.41
3:D:960:LYS:NZ	3:D:1063:GLU:OE1	2.54	0.41
5:F:188:ILE:HD13	5:F:221:ILE:HG12	2.02	0.41
1:A:29:GLU:O	1:A:32:PHE:HB2	2.21	0.41
1:B:13:VAL:HG12	1:B:15:THR:HG23	2.01	0.41
1:B:104:GLU:OE1	1:B:137:ARG:NH1	2.53	0.41
2:C:547:ILE:HG21	2:C:547:ILE:HD13	1.85	0.41
2:C:561:GLY:O	2:C:565:GLN:HG3	2.21	0.41
2:C:655:LEU:HD23	2:C:655:LEU:HA	1.85	0.41
3:D:897:TRP:CH2	3:D:902:LEU:HD22	2.56	0.41
5:F:402:ASN:O	5:F:406:ARG:N	2.47	0.41
1:A:71:VAL:O	2:C:608:GLY:N	2.54	0.41
1:A:104:GLU:HB3	1:A:137:ARG:CD	2.51	0.41
1:A:206:THR:HG22	1:A:208:LEU:N	2.36	0.41
2:C:243:ARG:HD2	2:C:256:TYR:CE2	2.55	0.41
2:C:276:LYS:HE2	2:C:276:LYS:HB3	1.95	0.41
2:C:335:THR:O	2:C:339:LEU:HG	2.21	0.41
2:C:420:ARG:HA	8:I:4:G:O6	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:707:ARG:NE	2:C:824:ARG:HD2	2.35	0.41
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.56	0.41
3:D:483:HIS:HA	3:D:484:PRO:HD3	2.00	0.41
3:D:534:ARG:HE	3:D:534:ARG:HB3	1.62	0.41
3:D:882:PHE:CE2	3:D:906:GLN:HG3	2.55	0.41
3:D:895:VAL:HG11	3:D:922:LEU:HD21	2.03	0.41
3:D:916:TYR:CE1	3:D:920:LEU:HD11	2.56	0.41
3:D:1482:ARG:NH2	3:D:1483:PHE:CZ	2.89	0.41
2:C:45:GLN:HG2	2:C:71:TYR:HE2	1.86	0.41
2:C:260:LEU:O	2:C:261:ILE:HD12	2.21	0.41
3:D:1283:ILE:HG12	3:D:1315:ASP:CG	2.41	0.41
1:B:112:ARG:HG3	1:B:125:PRO:O	2.21	0.40
1:B:112:ARG:CG	1:B:125:PRO:HB2	2.51	0.40
1:B:138:LEU:HD21	1:B:140:MET:CE	2.51	0.40
2:C:944:LEU:HD23	2:C:944:LEU:HA	1.84	0.40
3:D:486:ARG:HA	3:D:489:ARG:NH2	2.36	0.40
3:D:862:ASP:O	3:D:876:SER:HA	2.21	0.40
3:D:1014:ASN:OD1	3:D:1014:ASN:N	2.54	0.40
1:B:112:ARG:HG3	1:B:125:PRO:HB2	2.03	0.40
2:C:35:PRO:HG2	2:C:38:LYS:HD3	2.03	0.40
2:C:302:VAL:O	2:C:305:PRO:HD2	2.22	0.40
2:C:1031:ARG:HB2	3:D:622:ARG:NH1	2.35	0.40
3:D:1207:TYR:O	3:D:1366:LYS:NZ	2.54	0.40
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.56	0.40
2:C:56:GLU:OE2	2:C:103:LYS:HE2	2.21	0.40
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.98	0.40
2:C:1042:ALA:HB2	3:D:1223:ILE:HG22	2.02	0.40
5:F:96:LEU:O	5:F:100:VAL:HG23	2.21	0.40
5:F:260:ILE:HG22	5:F:265:VAL:HG23	2.04	0.40
1:B:81:ASN:O	1:B:84:GLU:HB2	2.21	0.40
2:C:926:PHE:O	2:C:929:ARG:HB3	2.22	0.40
1:B:128:HIS:NE2	1:B:131:THR:HG23	2.37	0.40
2:C:598:GLU:H	2:C:615:TYR:HH	1.63	0.40
2:C:640:ARG:N	2:C:657:ASP:O	2.40	0.40
3:D:204:LEU:HD22	3:D:441:ARG:CZ	2.51	0.40
3:D:262:LYS:HD3	3:D:341:GLU:OE1	2.21	0.40
5:F:397:ILE:HA	5:F:400:ILE:HG12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:985:ASP:N	3:D:1497:GLU:OE1[1_545]	2.11	0.09

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%)	219 (98%)	5 (2%)	0	100	100
1	B	222/315 (70%)	210 (95%)	11 (5%)	1 (0%)	29	61
2	C	1101/1119 (98%)	1065 (97%)	29 (3%)	7 (1%)	25	57
3	D	1480/1524 (97%)	1439 (97%)	30 (2%)	11 (1%)	22	54
4	E	92/99 (93%)	89 (97%)	2 (2%)	1 (1%)	14	45
5	F	344/423 (81%)	316 (92%)	18 (5%)	10 (3%)	4	24
All	All	3463/3795 (91%)	3338 (96%)	95 (3%)	30 (1%)	17	48

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	363	SER
2	C	418	LEU
2	C	419	THR
3	D	484	PRO
3	D	486	ARG
3	D	664	LYS
3	D	1235	GLN
5	F	323	ASP
5	F	377	ASP
5	F	388	ALA
2	C	228	ALA
2	C	362	GLY
3	D	1233	GLY
3	D	1255	GLY
5	F	384	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	385	GLU
5	F	416	ARG
2	C	105	THR
2	C	391	LEU
5	F	356	LYS
5	F	381	HIS
3	D	485	SER
3	D	1234	THR
1	B	154	GLU
5	F	382	THR
3	D	320	ALA
4	E	94	PRO
3	D	831	GLY
5	F	321	ILE
3	D	530	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/273 (73%)	188 (94%)	11 (6%)	21	52
1	B	197/273 (72%)	187 (95%)	10 (5%)	24	54
2	C	931/941 (99%)	888 (95%)	43 (5%)	27	58
3	D	1250/1279 (98%)	1182 (95%)	68 (5%)	22	53
4	E	83/88 (94%)	80 (96%)	3 (4%)	35	63
5	F	296/371 (80%)	290 (98%)	6 (2%)	55	76
All	All	2956/3225 (92%)	2815 (95%)	141 (5%)	25	56

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	34	VAL
1	A	67	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	104	GLU
1	A	133	GLU
1	A	184	THR
1	A	186	LEU
1	A	189	ARG
1	A	205	VAL
1	A	219	ARG
1	A	229	GLN
1	B	14	ARG
1	B	34	VAL
1	B	38	ASN
1	B	112	ARG
1	B	126	ASP
1	B	134	GLU
1	B	140	MET
1	B	186	LEU
1	B	189	ARG
1	B	206	THR
2	C	8	ARG
2	C	15	LEU
2	C	56	GLU
2	C	81	ASP
2	C	103	LYS
2	C	107	LEU
2	C	133	ASP
2	C	141	HIS
2	C	168	ARG
2	C	177	GLU
2	C	194	VAL
2	C	205	GLU
2	C	221	LEU
2	C	342	ASP
2	C	358	ARG
2	C	413	LEU
2	C	427	VAL
2	C	434	HIS
2	C	454	SER
2	C	524	VAL
2	C	525	SER
2	C	557	ARG
2	C	575	GLN
2	C	583	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	586	ARG
2	C	591	SER
2	C	610	ARG
2	C	617	ASP
2	C	640	ARG
2	C	661	SER
2	C	775	ARG
2	C	808	ARG
2	C	813	VAL
2	C	815	LEU
2	C	848	VAL
2	C	939	ARG
2	C	942	GLU
2	C	968	LEU
2	C	1001	VAL
2	C	1014	SER
2	C	1026	GLN
2	C	1057	SER
2	C	1058	ASP
3	D	30	GLU
3	D	67	ARG
3	D	68	PHE
3	D	81	THR
3	D	106	LYS
3	D	114	THR
3	D	141	ILE
3	D	142	LEU
3	D	155	ASP
3	D	161	LEU
3	D	190	GLU
3	D	191	LEU
3	D	198	ARG
3	D	200	ASP
3	D	230	TRP
3	D	231	VAL
3	D	256	GLU
3	D	272	LEU
3	D	276	ASP
3	D	312	ARG
3	D	325	GLU
3	D	362	GLU
3	D	372	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	411	THR
3	D	421	LEU
3	D	423	ASP
3	D	525	ARG
3	D	548	ILE
3	D	572	ARG
3	D	587	ARG
3	D	618	LEU
3	D	640	HIS
3	D	650	LEU
3	D	675	ARG
3	D	709	HIS
3	D	754	PHE
3	D	778	LEU
3	D	808	THR
3	D	817	GLU
3	D	832	ARG
3	D	861	GLN
3	D	864	VAL
3	D	875	THR
3	D	894	LYS
3	D	904	VAL
3	D	907	GLU
3	D	970	LYS
3	D	972	LEU
3	D	1041	LEU
3	D	1062	ARG
3	D	1079	LYS
3	D	1130	ARG
3	D	1155	VAL
3	D	1162	GLU
3	D	1188	VAL
3	D	1195	GLN
3	D	1208	ASP
3	D	1219	GLU
3	D	1221	VAL
3	D	1236	LEU
3	D	1284	GLU
3	D	1290	LEU
3	D	1305	LEU
3	D	1313	VAL
3	D	1317	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	1470	ARG
3	D	1493	LYS
3	D	1496	GLU
4	E	50	THR
4	E	66	LYS
4	E	75	PHE
5	F	186	HIS
5	F	205	ARG
5	F	364	ARG
5	F	377	ASP
5	F	396	ARG
5	F	419	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	390	GLN
2	C	683	ASN
2	C	728	HIS
3	D	640	HIS
3	D	744	GLN
5	F	411	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	8/8 (100%)	3 (37%)	3 (37%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	3	G
8	I	4	G
8	I	5	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	I	1	GTP
8	I	2	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	I	4	G

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 5 ligands modelled in this entry, 4 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	$\# Z > 2$
10	POP	C	1201	2	6,8,8	0.59	0	13,13,13	1.02	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	POP	C	1201	2	-	0/6/6/6	-

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

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, 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	A	226/315 (71%)	-0.36	1 (0%) 92 93	86, 127, 163, 192	0
1	B	224/315 (71%)	-0.42	0 100 100	73, 114, 162, 206	0
2	C	1107/1119 (98%)	-0.24	13 (1%) 79 78	47, 116, 201, 261	0
3	D	1484/1524 (97%)	-0.28	15 (1%) 82 82	46, 105, 183, 273	0
4	E	94/99 (94%)	-0.34	0 100 100	67, 121, 193, 216	0
5	F	346/423 (81%)	0.03	27 (7%) 13 12	82, 136, 247, 282	0
6	G	19/22 (86%)	0.39	2 (10%) 6 6	68, 117, 257, 289	0
7	H	19/27 (70%)	0.11	3 (15%) 2 2	119, 141, 268, 271	0
8	I	7/8 (87%)	0.52	1 (14%) 2 2	88, 104, 219, 238	0
All	All	3526/3852 (91%)	-0.25	62 (1%) 68 67	46, 117, 199, 289	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	375	LEU	5.0
5	F	148	LYS	4.8
2	C	188	LYS	4.8
3	D	1313	VAL	4.0
5	F	391	GLY	3.8
5	F	143	HIS	3.7
5	F	388	ALA	3.6
3	D	1128	VAL	3.6
5	F	356	LYS	3.6
5	F	376	ILE	3.6
5	F	414	ARG	3.5
7	H	25	DG	3.4
5	F	389	PHE	3.4
5	F	397	ILE	3.3
5	F	404	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	F	392	VAL	3.2
6	G	3	DC	3.2
3	D	1502	ALA	3.2
2	C	228	ALA	3.1
5	F	145	PRO	3.1
5	F	144	ILE	3.0
2	C	545	ASN	3.0
5	F	381	HIS	2.9
2	C	219	GLN	2.9
2	C	414	GLY	2.9
8	I	3	G	2.9
3	D	1129	THR	2.8
2	C	251	ASP	2.8
5	F	146	GLY	2.8
5	F	390	PHE	2.6
3	D	384	VAL	2.6
3	D	1292	VAL	2.6
2	C	439	CYS	2.6
7	H	24	DG	2.6
3	D	345	TYR	2.6
5	F	394	ARG	2.5
5	F	382	THR	2.5
5	F	149	GLU	2.4
3	D	1495	ILE	2.4
2	C	64	LEU	2.3
3	D	409	VAL	2.3
3	D	1297	GLU	2.3
2	C	1	MET	2.3
3	D	1499	ARG	2.3
5	F	400	ILE	2.3
2	C	811	PRO	2.2
3	D	993	LEU	2.2
7	H	23	DA	2.2
5	F	417	LYS	2.2
5	F	361	LEU	2.1
2	C	425	PHE	2.1
6	G	8	DA	2.1
5	F	370	LYS	2.1
5	F	142	ARG	2.1
5	F	360	LYS	2.1
3	D	427	VAL	2.1
5	F	147	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	781	LYS	2.1
2	C	320	HIS	2.1
1	A	185	ARG	2.0
3	D	360	ARG	2.0
3	D	487	ALA	2.0

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
9	MG	B	1001	1/1	0.53	0.40	80,80,80,80	0
10	POP	C	1201	9/9	0.94	0.11	94,111,146,148	0
11	ZN	D	2002	1/1	0.96	0.09	134,134,134,134	0
9	MG	D	2001	1/1	0.97	0.14	46,46,46,46	0
11	ZN	D	2003	1/1	0.98	0.23	123,123,123,123	0

6.5 Other polymers [i](#)

There are no such residues in this entry.