



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:03 pm BST

PDB ID : 5ZE0
Title : Hairpin Forming Complex, RAG1/2-Nicked(with Dideoxy) 12RSS/23RSS complex in Mg²⁺
Authors : Kim, M.S.; Chuenchor, W.; Chen, X.; Gellert, M.; Yang, W.
Deposited on : 2018-02-25
Resolution : 2.75 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 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

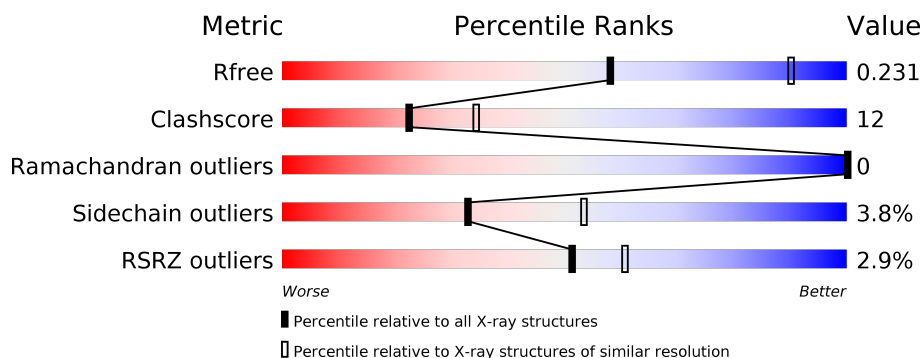
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 ≥ 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	627	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 75%, yellow 22%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 75% 22% .. </div> </div>
1	C	627	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 78%, yellow 21%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 78% 21% .. </div> </div>
2	B	389	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 63%, yellow 24%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 63% 24% • 13% </div> </div>
2	D	389	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, green 55%, yellow 30%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 4% 55% 30% • 13% </div> </div>
3	N	163	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 12%, green 62%, yellow 9%, grey 28%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 12% 62% 9% • 28% </div> </div>
4	F	45	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 36%, yellow 58%, orange 7%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 36% 58% 7% </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	I	16	<div><div></div><div>6%</div><div>50%</div><div>38%</div><div>13%</div></div>
6	J	16	<div><div></div><div>13%</div><div>56%</div><div>31%</div><div>13%</div></div>
7	G	54	<div><div></div><div>6%</div><div>54%</div><div>43%</div><div></div></div>
8	L	30	<div><div></div><div></div><div>50%</div><div>43%</div><div>7%</div></div>
9	M	39	<div><div></div><div>3%</div><div>56%</div><div>38%</div><div>5%</div></div>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 20394 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 mouse RAG1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	618	Total	C	N	O	S	0	0	0
			4964	3124	883	923	34			
1	C	623	Total	C	N	O	S	0	0	0
			5010	3152	897	927	34			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	GLY	-	cloning artifact	UNP P15919
A	383	PRO	-	cloning artifact	UNP P15919
C	382	GLY	-	cloning artifact	UNP P15919
C	383	PRO	-	cloning artifact	UNP P15919

- Molecule 2 is a protein called mouse RAG2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	340	Total	C	N	O	S	0	0	0
			2650	1694	448	490	18			
2	D	340	Total	C	N	O	S	0	1	0
			2659	1700	451	490	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	cloning artifact	UNP P21784
B	0	PRO	-	cloning artifact	UNP P21784
B	1	VAL	MET	engineered mutation	UNP P21784
D	-1	GLY	-	cloning artifact	UNP P21784
D	0	PRO	-	cloning artifact	UNP P21784
D	1	VAL	MET	engineered mutation	UNP P21784

- Molecule 3 is a protein called HMGB1 A-B box.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	118	Total	C	N	O	S	0	0	0
			833	529	142	155	7			

- Molecule 4 is a DNA chain called DNA (45-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	45	Total	C	N	O	P	0	0	0
			928	443	169	272	44			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	16	Total	C	N	O	P	0	0	0
			321	156	54	96	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	16	Total	C	N	O	P	0	0	0
			320	156	51	98	15			

- Molecule 7 is a DNA chain called DNA (54-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	54	Total	C	N	O	P	0	0	0
			1106	529	191	332	54			

- Molecule 8 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	L	30	Total	C	N	O	P	0	0	0
			611	290	118	173	30			

- Molecule 9 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	M	39	Total	C	N	O	P	0	0	0
			805	381	162	223	39			

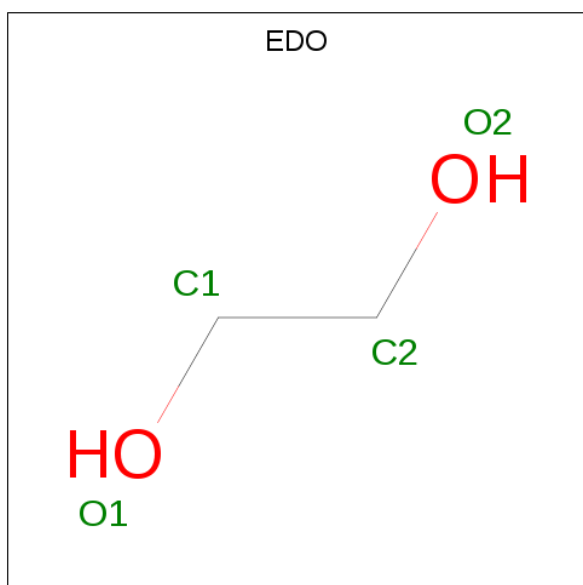
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Mg 1 1	0	0
10	C	1	Total Mg 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total Zn 1 1	0	0
11	C	1	Total Zn 1 1	0	0

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 4 2 2	0	0
12	A	1	Total C O 4 2 2	0	0
12	C	1	Total C O 4 2 2	0	0

- Molecule 13 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total K 1 1	0	0
13	C	1	Total K 1 1	0	0

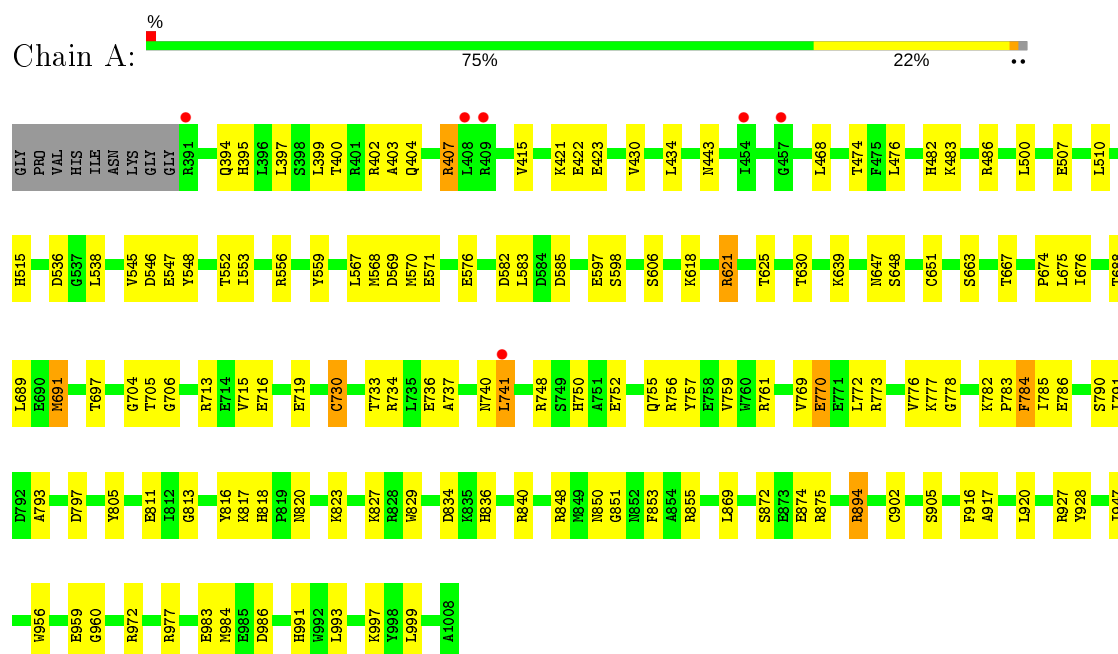
- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	50	Total O 50 50	0	0
14	B	8	Total O 8 8	0	0
14	C	47	Total O 47 47	0	0
14	D	9	Total O 9 9	0	0
14	F	16	Total O 16 16	0	0
14	I	4	Total O 4 4	0	0
14	J	4	Total O 4 4	0	0
14	G	14	Total O 14 14	0	0
14	L	10	Total O 10 10	0	0
14	M	7	Total O 7 7	0	0

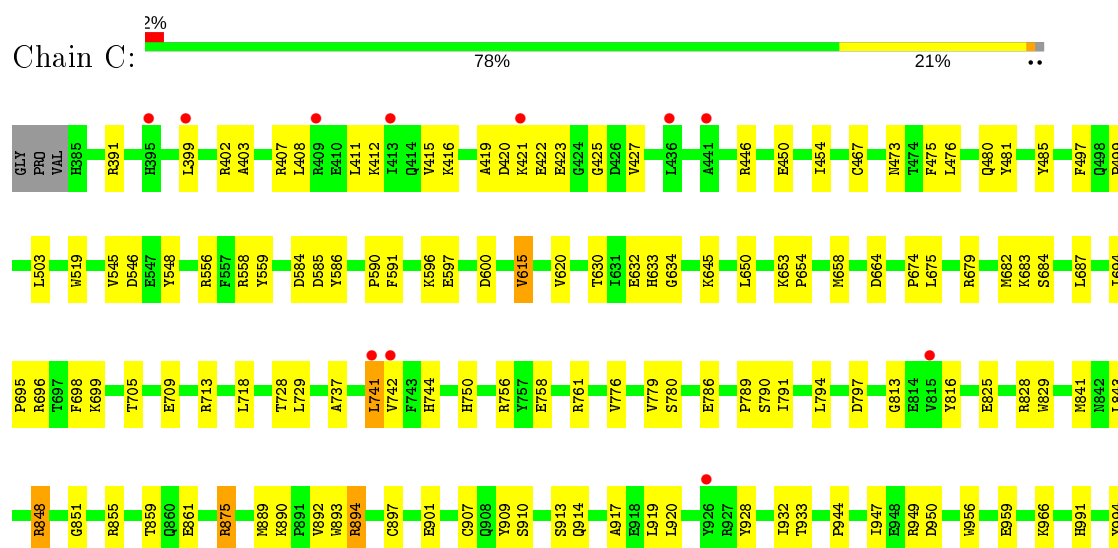
3 Residue-property plots

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: mouse RAG1

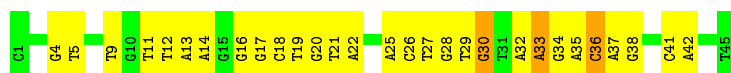


• Molecule 1: mouse RAG1





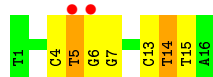
- Molecule 4: DNA (45-MER)



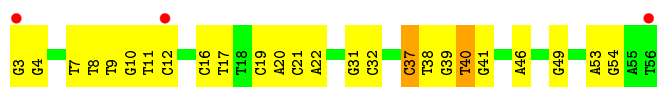
- Molecule 5: DNA (5'-D(*AP*AP*TP*CP*TP*GP*GP*CP*CP*TP*GP*TP*CP*TP*TP*A)-3')



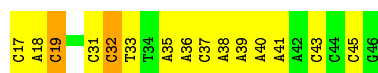
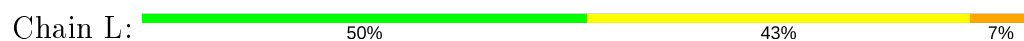
- Molecule 6: DNA (5'-D(*TP*AP*TP*CP*TP*GP*GP*CP*CP*TP*GP*TP*CP*TP*TP*A)-3')



- Molecule 7: DNA (54-MER)



- Molecule 8: DNA (30-MER)



- Molecule 9: DNA (39-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.44Å 109.03Å 156.85Å 90.00° 114.43° 90.00°	Depositor
Resolution (Å)	34.80 – 2.75 86.66 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.4 (34.80-2.75) 89.3 (86.66-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.199 , 0.234 0.199 , 0.231	Depositor DCC
R_{free} test set	5086 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20394	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.56	1/5067 (0.0%)	0.68	0/6826
1	C	0.56	1/5114 (0.0%)	0.68	1/6887 (0.0%)
2	B	0.47	0/2717	0.62	0/3686
2	D	0.45	0/2727	0.62	0/3700
3	N	0.37	0/847	0.45	0/1135
4	F	1.29	5/1041 (0.5%)	1.34	14/1608 (0.9%)
5	I	1.07	1/358 (0.3%)	1.17	2/550 (0.4%)
6	J	1.22	1/356 (0.3%)	1.20	3/547 (0.5%)
7	G	1.06	0/1237	1.20	5/1908 (0.3%)
8	L	1.25	3/686 (0.4%)	1.17	4/1052 (0.4%)
9	M	1.03	2/907 (0.2%)	1.04	3/1395 (0.2%)
All	All	0.71	14/21057 (0.1%)	0.82	32/29294 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	17	DC	OP3-P	-11.24	1.47	1.61
9	M	17	DC	OP3-P	-10.17	1.49	1.61
9	M	21	DG	C3'-O3'	-7.34	1.34	1.44
4	F	27	DT	C3'-O3'	-7.28	1.34	1.44
4	F	36	DC	O5'-C5'	-7.13	1.24	1.42
4	F	36	DC	C3'-O3'	-6.92	1.34	1.44
8	L	19	DC	C3'-O3'	-6.65	1.35	1.44
4	F	36	DC	C5'-C4'	-6.10	1.44	1.51
4	F	28	DG	C3'-O3'	-5.84	1.36	1.44
5	I	13	DC	C3'-O3'	-5.41	1.36	1.44
8	L	17	DC	C3'-O3'	-5.32	1.37	1.44
1	A	730	CYS	CB-SG	-5.28	1.73	1.81
1	C	615	VAL	CB-CG2	-5.26	1.41	1.52
6	J	13	DC	C3'-O3'	-5.23	1.37	1.44

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	36	DC	O5'-P-OP1	-13.32	93.71	105.70
4	F	28	DG	O5'-P-OP2	-8.98	97.62	105.70
7	G	41	DG	O5'-P-OP1	-8.50	98.05	105.70
8	L	32	DC	O4'-C4'-C3'	-7.82	101.31	106.00
9	M	17	DC	O5'-P-OP1	-7.69	98.78	105.70
4	F	36	DC	OP1-P-OP2	7.43	130.75	119.60
6	J	14	DT	O4'-C4'-C3'	-7.21	101.62	104.50
7	G	40	DT	O4'-C4'-C3'	-6.82	101.77	104.50
8	L	45	DC	O5'-P-OP2	-6.64	99.72	105.70
4	F	33	DA	O5'-P-OP1	-6.30	100.03	105.70
6	J	14	DT	O5'-P-OP2	-6.29	100.04	105.70
4	F	9	DT	C1'-O4'-C4'	-6.17	103.93	110.10
8	L	17	DC	O4'-C1'-N1	6.10	112.27	108.00
7	G	40	DT	O5'-P-OP1	6.02	117.93	110.70
4	F	25	DA	OP1-P-O3'	-6.01	91.98	105.20
4	F	27	DT	OP2-P-O3'	5.96	118.32	105.20
8	L	43	DC	O4'-C4'-C3'	-5.94	102.12	104.50
7	G	37	DC	O5'-P-OP2	-5.89	100.39	105.70
1	C	741	LEU	CB-CG-CD1	5.64	120.58	111.00
4	F	30	DG	O4'-C1'-N9	5.63	111.94	108.00
4	F	25	DA	OP2-P-O3'	5.63	117.58	105.20
5	I	15	DT	O5'-P-OP1	5.55	117.36	110.70
9	M	22	DT	N3-C4-O4	5.55	123.23	119.90
4	F	29	DT	C5-C4-O4	-5.47	121.07	124.90
4	F	29	DT	O5'-P-OP1	5.40	117.19	110.70
7	G	41	DG	O4'-C4'-C3'	-5.37	102.35	104.50
4	F	29	DT	N3-C4-O4	5.34	123.11	119.90
4	F	26	DC	O4'-C1'-N1	5.33	111.73	108.00
4	F	36	DC	O4'-C1'-N1	5.20	111.64	108.00
5	I	10	DT	N3-C4-O4	5.20	123.02	119.90
9	M	22	DT	O4'-C4'-C3'	-5.17	102.43	104.50
6	J	5	DT	N3-C4-O4	5.06	122.94	119.90

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	4964	0	4933	103	0
1	C	5010	0	4989	96	0
2	B	2650	0	2592	68	0
2	D	2659	0	2595	125	0
3	N	833	0	703	9	0
4	F	928	0	511	21	0
5	I	321	0	182	7	0
6	J	320	0	183	6	0
7	G	1106	0	614	19	0
8	L	611	0	335	11	0
9	M	805	0	435	14	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
11	A	1	0	0	0	0
11	C	1	0	0	0	0
12	A	8	0	12	1	0
12	C	4	0	6	0	0
13	A	1	0	0	0	0
13	C	1	0	0	0	0
14	A	50	0	0	5	0
14	B	8	0	0	1	0
14	C	47	0	0	1	0
14	D	9	0	0	0	0
14	F	16	0	0	0	0
14	G	14	0	0	0	0
14	I	4	0	0	0	0
14	J	4	0	0	0	0
14	L	10	0	0	0	0
14	M	7	0	0	0	0
All	All	20394	0	18090	443	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 (443) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:LEU:HG	1:A:917:ALA:HB1	1.53	0.91
1:C:848:ARG:HG2	1:C:848:ARG:HH11	1.34	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:263:LEU:HD21	2:D:271:PHE:HD2	1.38	0.88
2:D:95:GLY:HA2	2:D:104:SER:O	1.73	0.87
2:D:233:LEU:HD21	2:D:297:ILE:HD11	1.58	0.85
2:D:269:ASP:OD1	2:D:292:LEU:HB2	1.78	0.84
2:D:229:ARG:HD3	2:D:259:SER:OG	1.78	0.83
2:B:197:LEU:HD23	2:B:249:CYS:HB2	1.57	0.83
2:B:212:ARG:HH12	2:B:294:ASP:HA	1.43	0.82
1:C:737:ALA:O	1:C:741:LEU:HD23	1.82	0.80
2:D:8:VAL:HG11	2:D:12:ILE:HG13	1.64	0.79
1:A:552:THR:HG21	1:A:667:THR:HG21	1.66	0.78
2:D:163:PRO:HG2	2:D:166:GLN:HB2	1.64	0.78
7:G:10:DG:H2'	7:G:11:DT:C6	2.20	0.77
2:B:278:GLN:HE21	2:B:284:ARG:HG3	1.51	0.75
2:D:115:LYS:HG3	2:D:120:VAL:HG12	1.68	0.75
1:A:972:ARG:NH1	1:A:983:GLU:OE2	2.20	0.74
2:D:329:LEU:H	2:D:329:LEU:HD23	1.52	0.74
4:F:35:DA:H2''	4:F:36:DC:H5''	1.69	0.74
2:D:283:LYS:HD2	2:D:317:TRP:CD1	2.23	0.74
1:C:859:THR:HG22	1:C:861:GLU:H	1.52	0.73
6:J:4:DC:H2''	6:J:5:DT:H71	1.71	0.72
2:D:235:ARG:NH1	2:D:250:THR:OG1	2.23	0.72
1:C:709:GLU:OE1	1:C:713:ARG:NH2	2.22	0.72
2:D:274:VAL:HG11	2:D:327:ILE:HG13	1.72	0.71
2:D:298:GLU:HA	2:D:298:GLU:OE1	1.91	0.70
2:D:292:LEU:HD22	2:D:297:ILE:HG22	1.71	0.70
2:D:310:ASP:OD2	2:D:310:ASP:N	2.17	0.70
1:A:977:ARG:HG3	1:A:986:ASP:OD1	1.92	0.69
4:F:36:DC:H2''	4:F:37:DA:C8	2.28	0.69
1:A:730:CYS:O	1:A:748:ARG:NH1	2.26	0.68
2:D:53:ASN:HD22	2:D:53:ASN:N	1.89	0.68
2:B:7:THR:OG1	2:B:54:HIS:ND1	2.23	0.68
2:B:256:ILE:HD11	2:B:299:ILE:HG21	1.76	0.68
2:D:263:LEU:C	2:D:263:LEU:HD23	2.14	0.68
1:C:419:ALA:O	1:C:423:GLU:N	2.21	0.68
2:D:292:LEU:HD22	2:D:297:ILE:CG2	2.24	0.68
1:C:776:VAL:HG12	1:C:779:VAL:H	1.59	0.67
9:M:50:DA:H2'	9:M:51:DA:C8	2.29	0.67
4:F:11:DT:H2'	4:F:12:DT:C6	2.30	0.67
2:B:105:ASP:HB3	2:B:136:PRO:HG3	1.77	0.66
2:D:199:GLU:OE1	2:D:199:GLU:N	2.27	0.66
2:D:156:PHE:CD1	2:D:218:ILE:CD1	2.79	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:CYS:HB2	1:A:905:SER:HB2	1.78	0.65
1:A:399:LEU:HB3	1:A:403:ALA:HB3	1.77	0.65
4:F:13:DA:H2''	4:F:14:DA:C8	2.32	0.65
8:L:37:DC:H2''	8:L:38:DA:H5'	1.79	0.64
2:D:141:SER:OG	2:D:207:HIS:NE2	2.25	0.64
9:M:51:DA:H2'	9:M:52:DA:C8	2.34	0.63
1:A:688:THR:HG22	1:A:697:THR:HG22	1.79	0.63
2:B:168:THR:HG22	2:B:170:GLU:H	1.64	0.63
2:D:297:ILE:O	2:D:297:ILE:HG13	1.97	0.63
1:A:894:ARG:NH2	1:A:959:GLU:OE1	2.32	0.63
1:A:811:GLU:OE2	1:A:875:ARG:NE	2.20	0.63
2:D:162:MET:HE1	2:D:176:ALA:HB2	1.80	0.63
1:C:556:ARG:HD2	1:C:675:LEU:HD21	1.80	0.62
5:I:2:DA:H2'	5:I:3:DT:C6	2.35	0.62
1:C:758:GLU:OE1	1:C:761:ARG:NH1	2.32	0.62
2:D:217:TYR:CZ	2:D:297:ILE:HG23	2.35	0.62
2:D:156:PHE:CD1	2:D:218:ILE:HD13	2.34	0.62
2:B:266:THR:HG21	2:B:272:VAL:HG23	1.80	0.61
1:C:412:LYS:HE3	1:C:416:LYS:NZ	2.15	0.61
1:C:596:LYS:HE2	1:C:956:TRP:HA	1.81	0.61
1:A:817:LYS:HD2	1:A:818:HIS:NE2	2.15	0.61
1:A:545:VAL:HG23	2:B:316:ILE:HG22	1.83	0.61
2:D:263:LEU:HD21	2:D:271:PHE:CD2	2.28	0.61
1:A:476:LEU:HD21	1:C:476:LEU:HG	1.81	0.61
1:C:632:GLU:HG2	1:C:634:GLY:H	1.66	0.61
2:D:263:LEU:HD12	2:D:273:ILE:HG22	1.83	0.61
2:D:229:ARG:CD	2:D:259:SER:OG	2.48	0.60
2:B:237:ARG:NH2	2:B:295:ASN:OD1	2.34	0.60
2:D:166:GLN:N	2:D:166:GLN:OE1	2.34	0.60
2:B:212:ARG:NH1	2:B:294:ASP:HA	2.16	0.60
1:A:597:GLU:HB2	1:A:704:GLY:HA2	1.84	0.60
2:B:283:LYS:HD2	2:B:317:TRP:CE2	2.37	0.60
1:C:683:LYS:NZ	1:C:786:GLU:OE2	2.27	0.59
2:D:269:ASP:OD1	2:D:292:LEU:O	2.20	0.59
2:B:115:LYS:HG3	2:B:120:VAL:HG22	1.84	0.59
2:D:79:SER:OG	2:D:89:HIS:NE2	2.28	0.59
1:A:848:ARG:HD2	5:I:16:DA:C6	2.38	0.59
2:B:233:LEU:HD21	2:B:297:ILE:HD13	1.85	0.59
2:D:292:LEU:CD2	2:D:297:ILE:HG22	2.31	0.59
2:D:263:LEU:HD12	2:D:273:ILE:CG2	2.33	0.59
1:C:467:CYS:HB2	1:C:503:LEU:HD21	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:653:LYS:HG2	1:C:995:THR:HG21	1.85	0.58
2:D:217:TYR:CZ	2:D:297:ILE:CG2	2.86	0.58
2:D:219:LEU:HD22	2:D:256:ILE:HG12	1.85	0.58
1:A:977:ARG:NH2	9:M:24:DA:H5'	2.18	0.58
2:B:78:CYS:HB2	2:B:142:ILE:HG23	1.84	0.58
3:N:98:PRO:HB3	3:N:151:LEU:HD13	1.85	0.58
2:D:215:THR:HG23	2:D:235:ARG:HD3	1.85	0.58
7:G:53:DA:H2''	7:G:54:DG:C8	2.38	0.58
1:C:741:LEU:CD1	1:C:917:ALA:HB1	2.34	0.58
7:G:3:DG:H2''	7:G:4:DG:H5'	1.86	0.58
1:A:547:GLU:OE1	2:B:159:ARG:NH1	2.35	0.58
1:C:890:LYS:HA	1:C:893:TRP:CZ3	2.39	0.58
2:D:7:THR:HB	2:D:54:HIS:ND1	2.19	0.58
1:A:486:ARG:HD3	1:C:1006:HIS:CG	2.39	0.57
1:A:434:LEU:HD21	1:C:415:VAL:HG21	1.86	0.57
7:G:16:DC:H2''	7:G:17:DT:H5'	1.85	0.57
1:A:618:LYS:NZ	14:A:2102:HOH:O	2.38	0.57
2:B:266:THR:CG2	2:B:272:VAL:HG23	2.35	0.57
2:D:262:ILE:HD12	2:D:262:ILE:N	2.19	0.57
2:D:321:ASN:OD1	2:D:323:GLY:N	2.37	0.57
9:M:54:DC:H2'	9:M:55:DC:C5	2.39	0.57
1:A:394:GLN:O	1:A:407:ARG:NH2	2.38	0.57
2:B:326:THR:HG22	2:B:349:ARG:HG3	1.85	0.56
2:D:1:VAL:O	2:D:1:VAL:HG12	2.05	0.56
2:D:292:LEU:CD2	2:D:297:ILE:CG2	2.83	0.56
2:B:1:VAL:HA	2:B:349:ARG:O	2.05	0.56
2:D:283:LYS:HD2	2:D:317:TRP:NE1	2.19	0.56
2:D:264:THR:CG2	2:D:325:GLY:HA2	2.35	0.56
7:G:37:DC:H2'	7:G:38:DT:C7	2.35	0.56
1:A:991:HIS:HE1	14:A:2124:HOH:O	1.87	0.56
2:D:137:ARG:HH11	2:D:157:GLY:HA2	1.69	0.56
2:D:171:LYS:HB3	2:D:174:SER:OG	2.05	0.56
7:G:9:DT:H2''	7:G:10:DG:H5''	1.87	0.56
1:A:606:SER:O	1:A:972:ARG:NH2	2.36	0.56
7:G:38:DT:H2'	7:G:39:DG:C8	2.41	0.56
6:J:6:DG:H2''	6:J:7:DG:C8	2.41	0.56
1:A:482:HIS:HB2	1:A:500:LEU:HD11	1.88	0.55
3:N:102:PHE:O	3:N:106:CYS:HB2	2.06	0.55
2:B:274:VAL:HG12	2:B:287:CYS:SG	2.46	0.55
5:I:1:DA:H2''	5:I:2:DA:O4'	2.06	0.55
1:C:519:TRP:CH2	1:C:682:MET:HE3	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:590:PRO:HB2	1:C:699:LYS:HE2	1.88	0.55
1:C:825:GLU:HG2	1:C:828:ARG:HH22	1.71	0.55
1:A:625:THR:HG23	1:A:651:CYS:O	2.06	0.55
1:C:654:PRO:HG3	1:C:991:HIS:HB3	1.87	0.55
1:A:713:ARG:HD3	1:A:719:GLU:O	2.05	0.54
1:A:733:THR:HG23	1:A:736:GLU:H	1.72	0.54
1:A:813:GLY:HA3	1:A:829:TRP:CE2	2.42	0.54
2:D:169:THR:HA	2:D:172:TRP:HB2	1.89	0.54
3:N:98:PRO:HD2	3:N:155:TYR:HB2	1.89	0.54
2:D:219:LEU:HD22	2:D:256:ILE:CD1	2.38	0.54
2:D:308:THR:O	2:D:312:LYS:HG3	2.07	0.54
2:D:269:ASP:OD1	2:D:292:LEU:CB	2.54	0.54
1:A:770:GLU:H	1:A:770:GLU:CD	2.09	0.54
2:B:262:ILE:HG22	2:B:263:LEU:H	1.73	0.54
7:G:11:DT:H2'	7:G:12:DC:C6	2.43	0.54
9:M:51:DA:H2'	9:M:52:DA:H8	1.71	0.54
1:C:848:ARG:HG2	1:C:848:ARG:NH1	2.12	0.54
1:A:548:TYR:OH	2:B:34:LYS:HE3	2.08	0.53
1:A:770:GLU:OE1	1:A:770:GLU:N	2.32	0.53
2:B:41:CYS:HB2	2:B:59:PRO:HB3	1.90	0.53
1:C:653:LYS:NZ	1:C:995:THR:HG22	2.22	0.53
2:B:311:ILE:HD11	2:B:346:TYR:CE1	2.43	0.53
2:B:51:LYS:NZ	2:B:52:GLN:HG3	2.23	0.53
2:B:5:MET:HG2	2:B:346:TYR:CE2	2.43	0.53
6:J:5:DT:H2''	6:J:6:DG:C8	2.42	0.53
2:D:290:VAL:HG22	2:D:299:ILE:HG12	1.90	0.53
2:B:150:LYS:HG3	2:B:240:LEU:HD13	1.90	0.53
1:C:548:TYR:OH	2:D:34:LYS:HE2	2.09	0.53
4:F:20:DG:H1'	4:F:21:DT:H5'	1.91	0.53
1:A:805:TYR:OH	1:A:834:ASP:OD1	2.22	0.52
1:A:991:HIS:HD2	14:A:2106:HOH:O	1.92	0.52
1:C:420:ASP:OD1	1:C:421:LYS:N	2.42	0.52
2:D:145:VAL:HG21	2:D:238:VAL:HG21	1.90	0.52
1:A:719:GLU:HG3	1:A:778:GLY:O	2.09	0.52
1:A:443:ASN:ND2	4:F:17:DG:H1'	2.25	0.52
6:J:4:DC:H2''	6:J:5:DT:C7	2.37	0.52
2:D:210:ILE:CG2	2:D:217:TYR:HB2	2.40	0.52
2:D:331:ILE:HG22	2:D:332:PRO:O	2.10	0.52
1:C:741:LEU:HD13	1:C:917:ALA:HB1	1.92	0.52
1:C:897:CYS:O	1:C:901:GLU:HG3	2.09	0.52
2:D:271:PHE:O	2:D:290:VAL:N	2.28	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:816:TYR:OH	1:C:875:ARG:HD3	2.09	0.52
2:D:265:GLN:HB3	2:D:271:PHE:CE2	2.44	0.52
2:D:80:TYR:O	2:D:89:HIS:HD2	1.92	0.52
1:C:790:SER:OG	1:C:791:ILE:N	2.42	0.51
9:M:53:DA:H2''	9:M:54:DC:C6	2.44	0.51
1:C:416:LYS:HG2	1:C:427:VAL:HG21	1.92	0.51
2:D:98:THR:HB	2:D:99:PRO:HD2	1.92	0.51
4:F:41:DC:H2''	4:F:42:DA:C8	2.45	0.51
1:A:430:VAL:HG23	1:C:408:LEU:HD21	1.91	0.51
1:C:422:GLU:HG3	1:C:422:GLU:O	2.10	0.51
2:D:103:LEU:HD12	2:D:161:TYR:CD2	2.46	0.51
8:L:37:DC:H2'	8:L:38:DA:C8	2.45	0.51
4:F:37:DA:H2''	4:F:38:DG:C8	2.46	0.51
1:A:823:LYS:O	1:A:827:LYS:HG2	2.11	0.51
7:G:49:DG:H2'	7:G:49:DG:OP2	2.11	0.51
1:C:794:LEU:HD13	1:C:959:GLU:OE1	2.11	0.51
1:C:851:GLY:O	1:C:855:ARG:HG3	2.11	0.51
1:A:773:ARG:NH2	2:B:39:ARG:HH21	2.09	0.51
2:B:268:ASN:N	2:B:268:ASN:OD1	2.43	0.51
2:D:94:HIS:CD2	2:D:155:LEU:HD11	2.46	0.51
5:I:14:DT:H2'	5:I:15:DT:C6	2.46	0.51
2:D:76:ALA:HB2	2:D:140:HIS:CD2	2.46	0.50
7:G:37:DC:H2'	7:G:38:DT:H72	1.92	0.50
6:J:14:DT:H2'	6:J:15:DT:C6	2.47	0.50
2:D:283:LYS:HE3	2:D:317:TRP:CD2	2.46	0.50
1:A:474:THR:HA	1:C:480:GLN:OE1	2.12	0.50
2:D:219:LEU:HD22	2:D:256:ILE:HD11	1.92	0.50
1:C:889:MET:HE1	1:C:913:SER:HB3	1.93	0.50
2:D:305:PRO:HG2	2:D:307:TRP:CE2	2.46	0.50
2:B:240:LEU:HD23	2:B:245:PRO:HB3	1.93	0.50
1:C:558:ARG:NH1	2:D:170:GLU:OE2	2.41	0.50
2:D:272:VAL:HG23	2:D:302:MET:SD	2.52	0.50
2:D:219:LEU:HD22	2:D:256:ILE:CG1	2.42	0.49
1:A:816:TYR:CE2	1:A:875:ARG:HD2	2.47	0.49
2:B:200:LEU:HD11	2:B:236:ILE:HD11	1.94	0.49
1:A:648:SER:HB2	8:L:19:DC:H5''	1.94	0.49
8:L:32:DC:H2'	8:L:33:DT:C6	2.47	0.49
1:C:597:GLU:OE1	1:C:679:ARG:NE	2.45	0.49
2:D:147:SER:O	2:D:148:ARG:C	2.50	0.49
1:A:536:ASP:OD1	1:A:538:LEU:HB2	2.13	0.49
1:A:486:ARG:HD3	1:C:1006:HIS:ND1	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:31:DG:H1'	7:G:32:DC:H5'	1.95	0.49
7:G:9:DT:H2''	7:G:10:DG:O4'	2.13	0.49
1:A:582:ASP:O	1:A:583:LEU:HD23	2.13	0.49
1:C:694:ILE:HG22	1:C:695:PRO:O	2.13	0.49
2:D:264:THR:HG22	2:D:325:GLY:HA2	1.94	0.48
2:D:210:ILE:HD11	2:D:271:PHE:CD1	2.47	0.48
2:B:275:GLY:HA2	2:B:317:TRP:CZ2	2.48	0.48
1:A:855:ARG:NH2	4:F:30:DG:O6	2.46	0.48
2:B:279:LEU:HB2	2:B:282:GLN:HB3	1.96	0.48
2:B:314:SER:OG	2:B:316:ILE:O	2.31	0.48
1:C:750:HIS:CD2	1:C:786:GLU:HB2	2.49	0.48
7:G:19:DC:H2''	7:G:20:DA:C8	2.48	0.48
1:A:556:ARG:HD2	1:A:675:LEU:HD21	1.94	0.48
1:A:400:THR:O	1:A:404:GLN:HG2	2.14	0.48
2:D:263:LEU:CD1	2:D:273:ILE:HG22	2.44	0.48
1:A:772:LEU:O	1:A:776:VAL:HG22	2.14	0.48
2:B:141:SER:OG	2:B:207:HIS:NE2	2.31	0.48
1:C:481:TYR:OH	1:C:497:PHE:HB3	2.13	0.48
1:A:571:GLU:HG3	1:A:691:MET:HG2	1.96	0.47
2:B:274:VAL:HG21	2:B:327:ILE:HD12	1.96	0.47
2:D:123:ARG:HG2	2:D:125:THR:HG23	1.96	0.47
2:D:274:VAL:HG23	2:D:274:VAL:O	2.14	0.47
8:L:31:DC:H2'	8:L:32:DC:C6	2.49	0.47
3:N:98:PRO:CD	3:N:155:TYR:HB2	2.44	0.47
2:D:94:HIS:HD2	2:D:140:HIS:NE2	2.11	0.47
4:F:4:DG:H1'	4:F:5:DT:H5'	1.96	0.47
1:A:855:ARG:NH1	8:L:18:DA:OP2	2.46	0.47
1:A:755:GLN:O	1:A:759:VAL:HG23	2.15	0.47
1:C:412:LYS:HE3	1:C:416:LYS:HZ2	1.78	0.47
2:D:263:LEU:CG	2:D:273:ILE:HG22	2.45	0.47
1:A:618:LYS:NZ	4:F:32:DA:H5''	2.29	0.47
1:C:586:TYR:HA	1:C:694:ILE:HD13	1.95	0.47
2:D:270:GLU:HG2	2:D:289:LEU:HD11	1.96	0.47
8:L:39:DA:H2''	8:L:40:DA:H8	1.78	0.47
1:A:647:ASN:O	1:A:960:GLY:HA2	2.14	0.47
2:B:167:ARG:NH2	2:B:172:TRP:O	2.34	0.47
2:B:263:LEU:HD12	2:B:272:VAL:O	2.15	0.47
2:D:150:LYS:HB3	2:D:240:LEU:HD23	1.97	0.47
2:D:53:ASN:ND2	2:D:53:ASN:N	2.60	0.47
2:D:120:VAL:O	2:D:120:VAL:HG23	2.13	0.47
2:D:307:TRP:HB2	2:D:312:LYS:HE2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:329:LEU:HD23	2:D:329:LEU:N	2.21	0.47
2:D:47[A]:HIS:HE1	2:D:49:ASP:OD2	1.97	0.47
9:M:54:DC:H2'	9:M:55:DC:C6	2.50	0.47
1:C:966:LYS:HA	7:G:40:DT:H5'	1.96	0.46
1:A:598:SER:OG	1:A:706:GLY:HA3	2.15	0.46
1:A:750:HIS:CD2	1:A:786:GLU:HG3	2.50	0.46
1:A:741:LEU:CG	1:A:917:ALA:HB1	2.36	0.46
1:C:475:PHE:HA	14:C:2124:HOH:O	2.15	0.46
2:D:167:ARG:NH2	2:D:172:TRP:NE1	2.63	0.46
3:N:113:ILE:HD12	3:N:129:LEU:HG	1.96	0.46
1:A:733:THR:CG2	1:A:736:GLU:H	2.28	0.46
2:D:144:VAL:O	2:D:144:VAL:HG23	2.16	0.46
1:A:567:LEU:HD23	1:A:570:MET:HE3	1.97	0.46
2:B:278:GLN:HG3	2:B:284:ARG:HB2	1.96	0.46
9:M:53:DA:H2''	9:M:54:DC:H6	1.80	0.46
1:A:545:VAL:O	12:A:2003:EDO:H11	2.14	0.46
2:B:130:VAL:O	2:B:191:CYS:HA	2.16	0.46
2:B:170:GLU:O	2:B:171:LYS:HD3	2.15	0.46
3:N:19:PHE:HZ	3:N:48:ARG:HB3	1.80	0.46
1:A:621:ARG:NH1	14:A:2106:HOH:O	2.48	0.46
1:A:850:ASN:HB2	1:A:853:PHE:HB2	1.97	0.46
2:B:142:ILE:HA	2:B:154:VAL:O	2.16	0.46
2:B:256:ILE:HD11	2:B:299:ILE:CG2	2.45	0.46
1:C:584:ASP:HB3	1:C:586:TYR:CZ	2.51	0.46
1:C:705:THR:OG1	1:C:956:TRP:HB3	2.16	0.46
9:M:31:DT:H2''	9:M:32:DC:H5'	1.97	0.46
1:C:909:TYR:CD1	1:C:944:PRO:HG3	2.51	0.46
2:D:289:LEU:HB2	2:D:302:MET:CG	2.45	0.46
4:F:21:DT:H1'	4:F:22:DA:H5'	1.98	0.46
4:F:33:DA:H2''	4:F:34:DG:C8	2.50	0.46
2:D:233:LEU:CD2	2:D:297:ILE:HD11	2.40	0.45
2:B:340:SER:OG	2:B:341:GLU:N	2.39	0.45
2:D:145:VAL:CG1	2:D:216:VAL:HG23	2.45	0.45
1:A:630:THR:HG22	1:A:639:LYS:HA	1.99	0.45
1:A:740:ASN:O	1:A:741:LEU:HB2	2.17	0.45
2:D:52:GLN:HA	2:D:52:GLN:OE1	2.16	0.45
1:A:851:GLY:HA3	4:F:30:DG:O6	2.17	0.45
2:B:158:GLY:HA2	2:B:205:SER:HB3	1.98	0.45
2:B:317:TRP:HB3	2:B:331:ILE:HG22	1.99	0.45
2:D:272:VAL:CG2	2:D:302:MET:SD	3.04	0.45
1:C:591:PHE:HB2	1:C:698:PHE:CD2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:TYR:CD2	1:A:782:LYS:HB2	2.52	0.45
1:C:420:ASP:HA	1:C:425:GLY:N	2.31	0.45
9:M:42:DG:C2	9:M:43:DC:C2	3.05	0.45
1:A:674:PRO:HG3	2:B:172:TRP:HB3	1.98	0.45
2:B:65:ASP:OD2	2:B:123:ARG:NH1	2.50	0.45
1:C:729:LEU:N	1:C:729:LEU:HD12	2.31	0.45
1:A:515:HIS:ND1	1:A:568:MET:HG3	2.31	0.45
1:C:519:TRP:CE2	1:C:687:LEU:HD13	2.52	0.45
2:D:71:PRO:HG2	2:D:99:PRO:CG	2.46	0.45
5:I:13:DC:C6	5:I:14:DT:H72	2.52	0.45
1:A:546:ASP:OD2	2:B:229:ARG:NH1	2.48	0.45
1:C:620:VAL:HB	1:C:658:MET:CG	2.47	0.45
8:L:31:DC:H2'	8:L:32:DC:H6	1.81	0.45
2:B:317:TRP:CE3	2:B:329:LEU:HD21	2.52	0.44
1:C:674:PRO:HG3	2:D:172:TRP:HB3	1.99	0.44
14:A:2128:HOH:O	4:F:32:DA:H5'	2.16	0.44
4:F:37:DA:H2''	4:F:38:DG:H8	1.81	0.44
1:A:757:TYR:CE2	1:A:782:LYS:HB2	2.52	0.44
1:A:769:VAL:HG22	2:B:68:TYR:OH	2.17	0.44
2:D:264:THR:HG21	2:D:325:GLY:HA2	2.00	0.44
1:A:676:ILE:HG21	1:A:785:ILE:HG12	2.00	0.44
2:B:71:PRO:O	2:B:99:PRO:HD3	2.17	0.44
1:C:412:LYS:HE3	1:C:416:LYS:HZ1	1.81	0.44
1:C:933:THR:HA	6:J:14:DT:H5''	1.98	0.44
2:D:266:THR:HG23	2:D:351:SER:CB	2.46	0.44
9:M:39:DG:H2''	9:M:40:DA:H8	1.83	0.44
1:A:947:ILE:HD13	1:A:947:ILE:HA	1.70	0.44
1:A:773:ARG:CZ	2:B:39:ARG:HE	2.31	0.44
1:A:483:LYS:NZ	1:C:473:ASN:O	2.51	0.44
2:D:219:LEU:HD21	2:D:299:ILE:HD11	1.99	0.44
7:G:21:DC:H2''	7:G:22:DA:C8	2.52	0.44
1:A:395:HIS:HE1	1:A:397:LEU:HD13	1.83	0.44
1:A:716:GLU:HA	1:A:783:PRO:HB3	2.00	0.44
1:C:794:LEU:HA	1:C:894:ARG:NH2	2.33	0.44
2:D:326:THR:HG23	2:D:349:ARG:HG2	1.99	0.44
1:A:733:THR:HG22	1:A:736:GLU:HB2	2.00	0.43
1:A:927:ARG:HG2	1:A:928:TYR:CZ	2.53	0.43
1:C:709:GLU:O	1:C:713:ARG:HG3	2.17	0.43
1:A:872:SER:OG	1:A:874:GLU:HG2	2.18	0.43
1:C:949:ARG:HD2	1:C:950:ASP:OD1	2.18	0.43
7:G:7:DT:H2''	7:G:8:DT:O5'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:SER:OG	1:A:791:ILE:N	2.50	0.43
1:A:848:ARG:HH11	1:A:848:ARG:HG3	1.83	0.43
2:B:289:LEU:HB2	2:B:302:MET:HE2	2.00	0.43
2:B:272:VAL:HG12	2:B:274:VAL:HG13	2.01	0.43
2:B:34:LYS:HG2	14:B:407:HOH:O	2.19	0.43
2:B:72:LEU:HA	2:B:97:LYS:O	2.18	0.43
1:C:995:THR:HG22	1:C:995:THR:O	2.19	0.43
1:C:997:LYS:HZ2	1:C:997:LYS:HG2	1.76	0.43
2:D:113:ALA:HB2	2:D:123:ARG:HB2	2.00	0.43
1:A:415:VAL:HG22	1:C:411:LEU:HD11	1.99	0.43
1:C:718:LEU:HD12	1:C:728:THR:HG22	2.01	0.43
2:B:216:VAL:HG22	2:B:236:ILE:HB	2.00	0.43
1:C:889:MET:HB3	1:C:909:TYR:CE2	2.53	0.43
1:C:920:LEU:HD22	1:C:928:TYR:CD2	2.53	0.43
3:N:132:MET:O	3:N:136:THR:HG23	2.18	0.43
9:M:42:DG:H1'	9:M:43:DC:H5'	2.01	0.43
1:A:748:ARG:NH2	1:A:777:LYS:O	2.52	0.43
2:B:317:TRP:CD1	2:B:317:TRP:N	2.87	0.43
3:N:125:VAL:HG12	3:N:129:LEU:HD11	2.01	0.43
1:A:836:HIS:CG	1:A:869:LEU:HD11	2.54	0.43
1:A:916:PHE:HE1	1:A:920:LEU:HD11	1.84	0.43
1:C:919:LEU:HD12	1:C:919:LEU:HA	1.84	0.43
1:A:507:GLU:HG2	1:A:993:LEU:HD11	2.01	0.42
1:A:737:ALA:O	1:A:741:LEU:HD13	2.19	0.42
1:C:843:LEU:HD23	1:C:843:LEU:HA	1.86	0.42
1:C:789:PRO:O	1:C:949:ARG:NH2	2.52	0.42
4:F:22:DA:H5'	4:F:22:DA:C8	2.54	0.42
1:A:399:LEU:HD22	7:G:8:DT:H5'	2.01	0.42
1:C:546:ASP:OD1	2:D:260:SER:OG	2.22	0.42
9:M:21:DG:H2'	9:M:22:DT:H72	1.99	0.42
2:B:212:ARG:NE	2:B:269:ASP:OD1	2.51	0.42
1:C:653:LYS:HB3	1:C:653:LYS:HE3	1.71	0.42
2:D:22:MET:HE1	2:D:93:ILE:HD11	2.00	0.42
2:D:229:ARG:HH11	2:D:259:SER:CB	2.32	0.42
2:B:270:GLU:HA	2:B:290:VAL:O	2.19	0.42
1:C:892:VAL:HG12	1:C:947:ILE:HD13	2.01	0.42
2:D:215:THR:CG2	2:D:235:ARG:HD3	2.48	0.42
2:D:275:GLY:O	2:D:317:TRP:CZ2	2.73	0.42
1:C:742:VAL:HG21	1:C:914:GLN:HG2	2.01	0.42
1:C:756:ARG:HB3	1:C:776:VAL:HG13	2.01	0.42
2:D:266:THR:CG2	2:D:351:SER:CB	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:ALA:O	1:A:797:ASP:HB2	2.19	0.42
2:B:39:ARG:HD2	2:B:39:ARG:HA	1.82	0.42
2:D:71:PRO:HG2	2:D:99:PRO:HG3	2.02	0.42
1:C:741:LEU:HD21	1:C:932:ILE:HD12	2.01	0.41
2:D:258:VAL:CG2	2:D:261:ALA:HB2	2.50	0.41
1:C:545:VAL:HG22	2:D:280:GLU:OE1	2.20	0.41
2:D:289:LEU:HB2	2:D:302:MET:HG3	2.02	0.41
1:A:705:THR:OG1	1:A:956:TRP:HB3	2.20	0.41
2:B:159:ARG:CZ	2:B:224:LEU:HD22	2.50	0.41
2:B:283:LYS:HE3	2:B:314:SER:O	2.20	0.41
1:A:421:LYS:HG2	1:A:422:GLU:HG2	2.01	0.41
1:A:797:ASP:OD2	1:A:894:ARG:NH1	2.53	0.41
5:I:13:DC:H2'	5:I:14:DT:C7	2.50	0.41
2:D:239:ASP:O	2:D:241:PRO:HD3	2.20	0.41
9:M:49:DA:H2''	9:M:50:DA:C8	2.55	0.41
1:C:841:MET:HE1	1:C:861:GLU:HG3	2.02	0.41
2:D:76:ALA:HB2	2:D:140:HIS:O	2.21	0.41
8:L:35:DA:H2''	8:L:36:DA:OP2	2.19	0.41
2:B:67:CYS:N	2:B:124:CYS:O	2.41	0.41
1:C:450:GLU:O	1:C:454:ILE:HD13	2.20	0.41
1:C:519:TRP:CZ2	1:C:687:LEU:HD13	2.55	0.41
1:C:890:LYS:HA	1:C:893:TRP:CE3	2.54	0.41
2:D:219:LEU:CD2	2:D:256:ILE:HG12	2.50	0.41
4:F:16:DG:H2''	4:F:17:DG:H8	1.85	0.41
1:C:485:TYR:OH	1:C:499:PRO:HG3	2.19	0.41
1:C:650:LEU:HD23	1:C:994:TYR:CE2	2.56	0.41
2:D:263:LEU:HG	2:D:273:ILE:HG22	2.03	0.41
1:A:510:LEU:HD13	1:A:999:LEU:HD11	2.02	0.41
1:A:752:GLU:O	1:A:756:ARG:HG3	2.21	0.41
2:D:292:LEU:HD22	2:D:297:ILE:HG21	2.01	0.41
2:D:271:PHE:O	2:D:289:LEU:HD12	2.21	0.41
3:N:16:TYR:O	3:N:20:VAL:HG23	2.20	0.41
1:C:645:LYS:HE3	1:C:645:LYS:HB2	1.85	0.41
2:D:142:ILE:HA	2:D:154:VAL:O	2.21	0.41
2:D:279:LEU:HA	2:D:279:LEU:HD12	1.74	0.41
2:D:39:ARG:HG3	7:G:46:DA:H3'	2.02	0.41
1:A:468:LEU:HA	1:A:468:LEU:HD12	1.82	0.41
1:A:576:GLU:HG2	1:A:576:GLU:O	2.20	0.41
1:A:984:MET:HE2	1:A:984:MET:HA	2.03	0.41
2:D:94:HIS:ND1	2:D:107:ILE:HG13	2.36	0.41
2:D:142:ILE:HG23	2:D:142:ILE:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:12:DT:H2'	4:F:13:DA:C8	2.55	0.41
1:A:569:ASP:OD2	1:A:997:LYS:N	2.47	0.40
1:A:817:LYS:HD2	1:A:818:HIS:CD2	2.56	0.40
2:B:140:HIS:HB3	2:B:158:GLY:HA3	2.03	0.40
1:A:486:ARG:HD3	1:C:1006:HIS:CE1	2.56	0.40
1:C:585:ASP:O	1:C:696:ARG:NH1	2.49	0.40
1:C:813:GLY:HA3	1:C:829:TRP:CE2	2.56	0.40
1:C:892:VAL:CG1	1:C:947:ILE:HD13	2.51	0.40
2:D:196:ILE:O	2:D:197:LEU:HD23	2.22	0.40
8:L:40:DA:H1'	8:L:41:DA:H5'	2.04	0.40
2:B:252:LEU:N	2:B:252:LEU:HD12	2.36	0.40
1:C:664:ASP:OD1	2:D:34:LYS:NZ	2.54	0.40
1:C:776:VAL:HG11	1:C:779:VAL:O	2.22	0.40
2:D:173:ASN:O	2:D:175:VAL:HG23	2.22	0.40
4:F:18:DC:C6	4:F:19:DT:H72	2.56	0.40
7:G:3:DG:H2''	7:G:4:DG:C8	2.56	0.40
5:I:13:DC:H2'	5:I:14:DT:H72	2.03	0.40
1:A:568:MET:SD	1:A:689:LEU:HD11	2.61	0.40
2:D:269:ASP:CG	2:D:292:LEU:HB2	2.40	0.40
2:D:77:THR:HA	2:D:92:ILE:O	2.20	0.40
1:C:399:LEU:HB3	1:C:403:ALA:HB3	2.03	0.40
1:C:825:GLU:HG2	1:C:828:ARG:NH2	2.36	0.40
4:F:18:DC:H2''	4:F:19:DT:O5'	2.22	0.40
1:A:715:VAL:HG12	1:A:784:PHE:HE1	1.86	0.40
2:B:215:THR:HG22	2:B:237:ARG:HB2	2.03	0.40
1:A:423:GLU:CD	1:C:407:ARG:HH11	2.24	0.40
1:C:446:ARG:O	1:C:450:GLU:HG3	2.22	0.40
2:D:162:MET:HE1	2:D:176:ALA:CB	2.51	0.40
2:D:262:ILE:HB	2:D:274:VAL:CG2	2.51	0.40
2:D:98:THR:HB	2:D:99:PRO:CD	2.51	0.40
8:L:38:DA:H2''	8:L:39:DA:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	616/627 (98%)	596 (97%)	20 (3%)	0	100	100
1	C	621/627 (99%)	598 (96%)	23 (4%)	0	100	100
2	B	334/389 (86%)	322 (96%)	12 (4%)	0	100	100
2	D	335/389 (86%)	323 (96%)	12 (4%)	0	100	100
3	N	108/163 (66%)	107 (99%)	1 (1%)	0	100	100
All	All	2014/2195 (92%)	1946 (97%)	68 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	542/550 (98%)	526 (97%)	16 (3%)	41	61
1	C	547/550 (100%)	530 (97%)	17 (3%)	40	60
2	B	295/344 (86%)	286 (97%)	9 (3%)	40	60
2	D	295/344 (86%)	276 (94%)	19 (6%)	17	31
3	N	68/139 (49%)	63 (93%)	5 (7%)	13	24
All	All	1747/1927 (91%)	1681 (96%)	66 (4%)	33	53

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	402	ARG
1	A	407	ARG
1	A	553	ILE
1	A	559	TYR
1	A	585	ASP
1	A	621	ARG
1	A	663	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	691	MET
1	A	734	ARG
1	A	741	LEU
1	A	761	ARG
1	A	770	GLU
1	A	784	PHE
1	A	820	ASN
1	A	840	ARG
1	A	894	ARG
2	B	12	ILE
2	B	34	LYS
2	B	58	LYS
2	B	104	SER
2	B	107	ILE
2	B	226	SER
2	B	250	THR
2	B	268	ASN
2	B	317	TRP
1	C	391	ARG
1	C	402	ARG
1	C	559	TYR
1	C	600	ASP
1	C	615	VAL
1	C	630	THR
1	C	633	HIS
1	C	684	SER
1	C	744	HIS
1	C	780	SER
1	C	797	ASP
1	C	848	ARG
1	C	875	ARG
1	C	894	ARG
1	C	907	CYS
1	C	910	SER
1	C	1001	LYS
2	D	8	VAL
2	D	12	ILE
2	D	53	ASN
2	D	80	TYR
2	D	114	CYS
2	D	119	LYS
2	D	162	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	200	LEU
2	D	229	ARG
2	D	235	ARG
2	D	237	ARG
2	D	259	SER
2	D	273	ILE
2	D	278	GLN
2	D	281	ASN
2	D	294	ASP
2	D	304	THR
2	D	310	ASP
2	D	317	TRP
3	N	42	SER
3	N	46	SER
3	N	48	ARG
3	N	73	ARG
3	N	106	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	278	GLN
2	B	282	GLN
2	D	53	ASN
2	D	94	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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
12	EDO	A	2004	-	3,3,3	0.47	0	2,2,2	0.12	0
12	EDO	C	2004	-	3,3,3	0.48	0	2,2,2	0.23	0
12	EDO	A	2003	-	3,3,3	0.50	0	2,2,2	0.42	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
12	EDO	A	2004	-	-	0/1/1/1	-
12	EDO	C	2004	-	-	0/1/1/1	-
12	EDO	A	2003	-	-	0/1/1/1	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	2003	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	618/627 (98%)	0.31	6 (0%) 82 87	37, 56, 90, 143	0
1	C	623/627 (99%)	0.30	11 (1%) 68 76	34, 57, 89, 121	0
2	B	340/389 (87%)	0.27	5 (1%) 73 81	46, 77, 109, 124	0
2	D	340/389 (87%)	0.49	15 (4%) 34 41	40, 70, 110, 130	0
3	N	118/163 (72%)	0.73	20 (16%) 1 1	104, 148, 162, 167	0
4	F	45/45 (100%)	-0.19	0 100 100	37, 65, 112, 129	0
5	I	16/16 (100%)	-0.03	1 (6%) 20 24	42, 92, 125, 125	0
6	J	16/16 (100%)	0.32	2 (12%) 3 4	43, 89, 130, 130	0
7	G	54/54 (100%)	0.26	3 (5%) 24 29	40, 107, 167, 192	0
8	L	30/30 (100%)	-0.12	0 100 100	40, 66, 111, 115	0
9	M	39/39 (100%)	0.15	1 (2%) 56 65	47, 104, 162, 174	0
All	All	2239/2395 (93%)	0.33	64 (2%) 51 61	34, 64, 134, 192	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	113	ILE	6.5
3	N	13	MET	4.8
1	A	408	LEU	4.6
3	N	11	GLY	4.4
3	N	144	TYR	3.5
3	N	105	PHE	3.4
3	N	114	LYS	3.3
2	D	92	ILE	3.3
1	A	391	ARG	3.3
3	N	115	GLY	3.2
1	A	409	ARG	3.2
2	D	119	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	N	17	ALA	3.2
3	N	75	MET	3.1
2	D	93	ILE	3.0
5	I	1	DA	2.9
2	D	292	LEU	2.8
2	D	210	ILE	2.8
3	N	41	PHE	2.8
1	C	395	HIS	2.7
3	N	47	GLU	2.7
7	G	56	DT	2.7
2	B	189	PHE	2.7
3	N	109	TYR	2.7
2	D	297	ILE	2.7
2	D	271	PHE	2.7
3	N	38	PHE	2.7
2	D	80	TYR	2.6
7	G	12	DC	2.6
1	C	742	VAL	2.6
3	N	49	TRP	2.6
2	D	329	LEU	2.5
1	A	457	GLY	2.5
1	C	413	ILE	2.4
2	D	265	GLN	2.4
1	C	741	LEU	2.4
1	C	815	VAL	2.4
3	N	112	LYS	2.4
2	D	109	ILE	2.3
2	B	92	ILE	2.3
3	N	10	ARG	2.3
6	J	5	DT	2.3
2	D	216	VAL	2.3
1	C	926	TYR	2.2
3	N	20	VAL	2.2
1	C	399	LEU	2.2
2	B	155	LEU	2.2
2	D	299	ILE	2.2
9	M	35	DG	2.2
1	C	409	ARG	2.2
1	C	421	LYS	2.2
3	N	12	LYS	2.1
3	N	99	PRO	2.1
1	C	436	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	J	6	DG	2.1
1	A	741	LEU	2.1
1	A	454	ILE	2.0
3	N	16	TYR	2.0
2	B	116	ASN	2.0
2	D	187	PHE	2.0
2	D	258	VAL	2.0
1	C	441	ALA	2.0
2	B	107	ILE	2.0
7	G	3	DG	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 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, 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(Å ²)	Q<0.9
10	MG	C	2001	1/1	0.80	0.17	54,54,54,54	0
10	MG	A	2001	1/1	0.82	0.44	61,61,61,61	0
12	EDO	A	2003	4/4	0.85	0.21	60,61,72,74	0
12	EDO	C	2004	4/4	0.86	0.35	68,73,74,81	0
12	EDO	A	2004	4/4	0.92	0.26	51,52,54,56	0
13	K	C	2003	1/1	0.97	0.13	42,42,42,42	0
13	K	A	2005	1/1	0.97	0.10	49,49,49,49	0
11	ZN	C	2002	1/1	0.99	0.21	54,54,54,54	0
11	ZN	A	2002	1/1	0.99	0.21	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.