



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:53 PM UTC

PDB ID : 3KLH / pdb_00003klh
Title : Crystal structure of AZT-Resistant HIV-1 Reverse Transcriptase crosslinked to post-translocation AZTMP-Terminated DNA (COMPLEX P)
Authors : Tu, X.; Sarafianos, S.G.; Arnold, E.
Deposited on : 2009-11-07
Resolution : 2.90 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

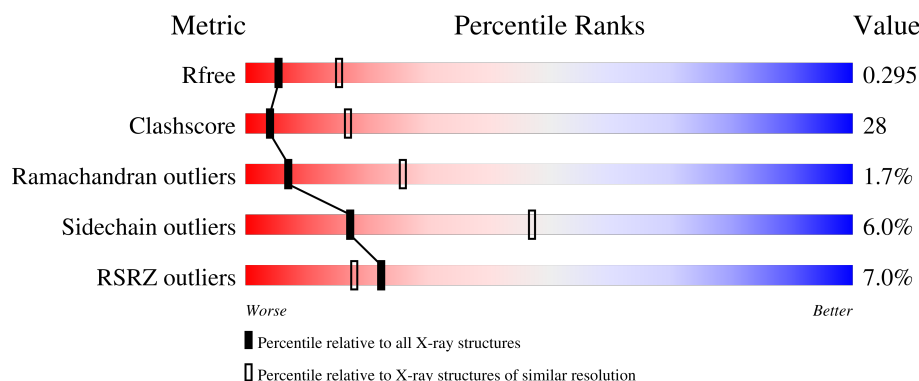
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	564	
2	B	437	
3	C	211	
4	D	225	
5	E	27	

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Mol	Chain	Length	Quality of chain
6	F	21	 29% 52% 19%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12472 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4545	2942	760	836	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	41	LEU	MET	engineered mutation	UNP P03366
A	67	ASN	ASP	engineered mutation	UNP P03366
A	70	ARG	LYS	engineered mutation	UNP P03366
A	215	TYR	THR	engineered mutation	UNP P03366
A	219	GLN	LYS	engineered mutation	UNP P03366
A	258	CYS	GLN	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
A	561	VAL	PHE	SEE REMARK 999	UNP P03366

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	0	0
			3538	2305	586	640	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
B	429	GLY	-	expression tag	UNP P03366
B	430	GLY	-	expression tag	UNP P03366
B	431	HIS	-	expression tag	UNP P03366
B	432	HIS	-	expression tag	UNP P03366
B	433	HIS	-	expression tag	UNP P03366

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Chain	Residue	Modelled	Actual	Comment	Reference
B	434	HIS	-	expression tag	UNP P03366
B	435	HIS	-	expression tag	UNP P03366
B	436	HIS	-	expression tag	UNP P03366
B	437	HIS	-	expression tag	UNP P03366

- Molecule 3 is a protein called monoclonal antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	211	Total	C	N	O	S	0	0	0
			1643	1025	270	342	6			

- Molecule 4 is a protein called monoclonal antibody, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	225	Total	C	N	O	S	0	0	0
			1685	1060	276	340	9			

- Molecule 5 is a DNA chain called DNA (5'-D(*AP*T*GP*CP*TP*AP*GP*GP*CP*GP*C
P*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	24	Total	C	N	O	P	0	0	0
			493	233	97	140	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	21	Total	C	N	O	P	0	0	0
			429	205	77	126	20			

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		

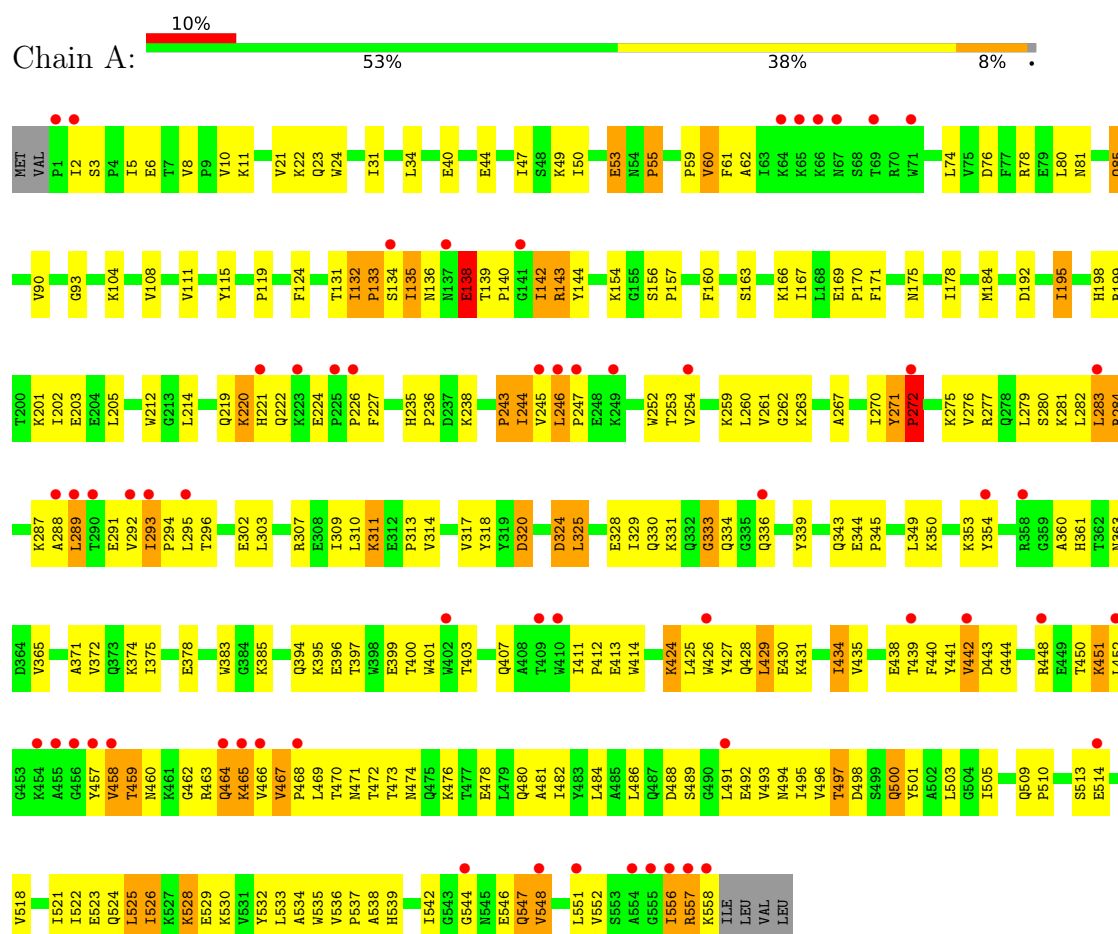
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	41	Total 41	O 41	0	0
8	B	37	Total 37	O 37	0	0
8	C	22	Total 22	O 22	0	0
8	D	25	Total 25	O 25	0	0
8	E	5	Total 5	O 5	0	0
8	F	8	Total 8	O 8	0	0

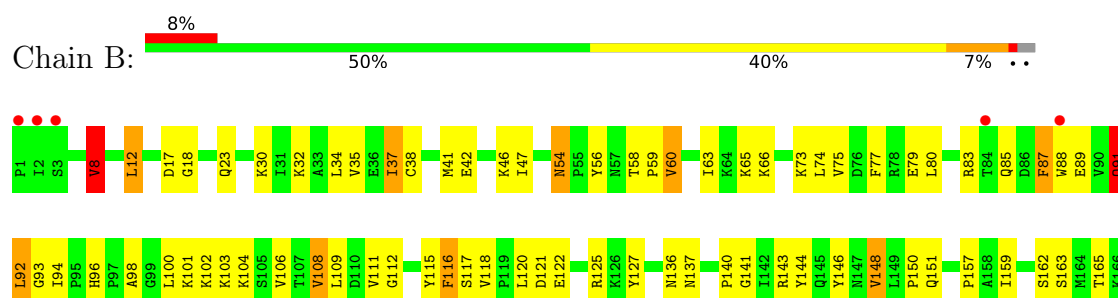
3 Residue-property plots

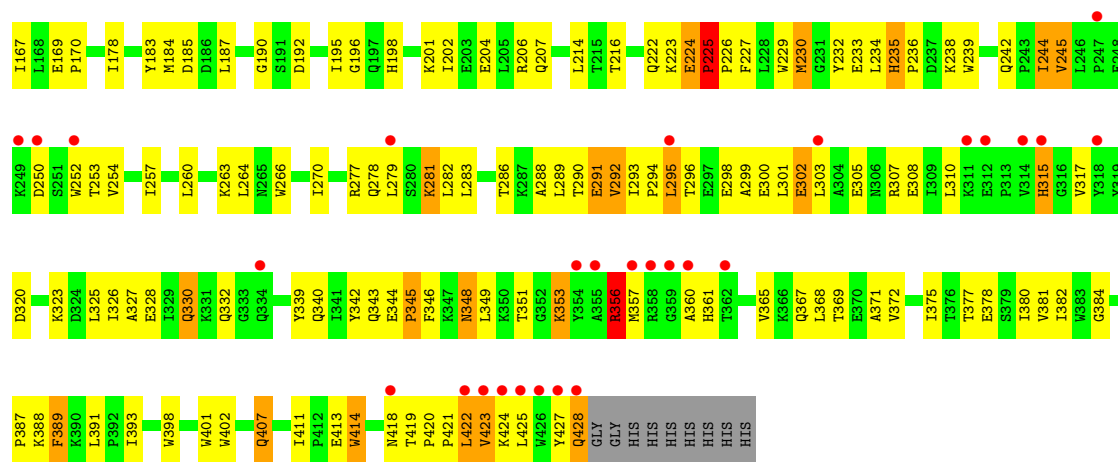
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Reverse transcriptase/ribonuclease H

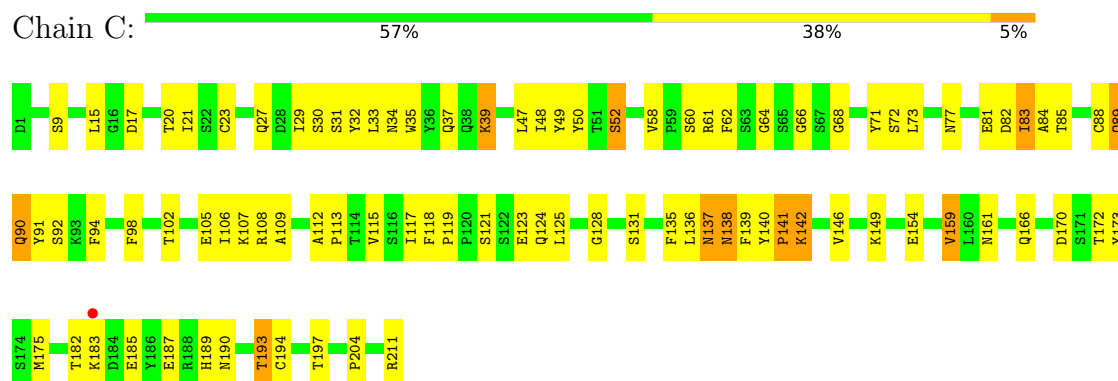


• Molecule 2: p51 RT





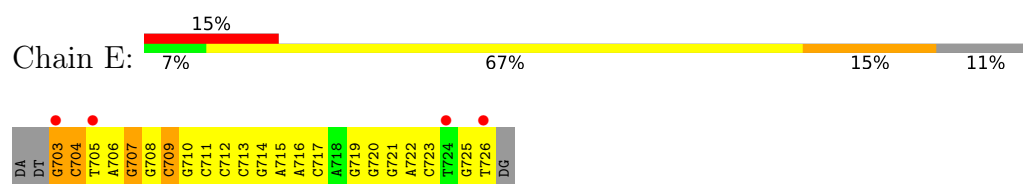
• Molecule 3: monoclonal antibody, heavy chain



• Molecule 4: monoclonal antibody, light chain



• Molecule 5: DNA (5'-D(*AP*T*GP*CP*TP*AP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3')



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

Chain F: 29% 52% 19%

A802	G815
C803	G816
A804	G817
G805	C818
T806	G819
C807	C820
C808	C821
	T822

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	166.47Å 166.47Å 220.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.79 – 2.90 24.79 – 2.91	Depositor EDS
% Data completeness (in resolution range)	86.5 (24.79-2.90) 86.5 (24.79-2.91)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.90Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.260 , 0.294 0.260 , 0.295	Depositor DCC
R_{free} test set	2742 reflections (4.11%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12472	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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: ATM, MRG, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	0/4664	1.04	20/6336 (0.3%)
2	B	0.73	0/3643	1.09	27/4952 (0.5%)
3	C	0.61	0/1681	1.08	14/2283 (0.6%)
4	D	0.66	0/1729	1.05	5/2372 (0.2%)
5	E	0.35	0/554	0.88	3/854 (0.4%)
6	F	0.35	0/424	0.84	2/649 (0.3%)
All	All	0.64	0/12695	1.05	71/17446 (0.4%)

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
5	E	0	1

There are no bond length outliers.

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	138	ASN	N-CA-C	10.66	124.34	111.02
3	C	9	SER	N-CA-C	9.25	122.69	111.40
1	A	320	ASP	CA-C-N	8.66	128.24	119.24
1	A	320	ASP	C-N-CA	8.66	128.24	119.24
2	B	382	ILE	N-CA-C	8.51	118.59	110.42
2	B	91	GLN	N-CA-C	8.47	121.35	111.02
2	B	225	PRO	N-CA-C	8.06	120.53	110.70
1	A	289	LEU	N-CA-C	8.04	121.66	108.08
1	A	542	ILE	N-CA-C	7.75	119.25	107.77
1	A	458	VAL	N-CA-C	-7.67	96.35	107.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	VAL	N-CA-C	-7.41	99.81	107.89
3	C	115	VAL	N-CA-C	7.27	118.49	108.89
3	C	137	ASN	N-CA-C	6.69	120.95	110.32
3	C	52	SER	N-CA-C	6.69	119.62	110.06
2	B	66	LYS	N-CA-C	-6.46	105.38	113.20
1	A	349	LEU	N-CA-C	-6.45	104.10	112.68
3	C	94	PHE	N-CA-C	-6.41	100.88	110.24
4	D	34	ILE	N-CA-C	6.33	117.36	110.21
1	A	442	VAL	CB-CA-C	-6.31	101.79	111.31
1	A	271	TYR	CA-C-N	6.29	127.71	119.84
1	A	271	TYR	C-N-CA	6.29	127.71	119.84
2	B	356	ARG	N-CA-C	6.27	117.97	110.19
2	B	46	LYS	N-CA-C	-6.25	104.71	112.90
2	B	224	GLU	CA-C-N	6.12	126.68	120.38
2	B	224	GLU	C-N-CA	6.12	126.68	120.38
4	D	32	SER	N-CA-C	6.07	121.38	111.37
1	A	203	GLU	N-CA-C	-6.05	104.69	111.28
1	A	245	VAL	N-CA-C	6.03	115.30	106.55
2	B	87	PHE	N-CA-C	5.99	117.50	110.97
2	B	424	LYS	N-CA-C	-5.96	102.40	110.68
1	A	542	ILE	CB-CA-C	-5.88	102.49	110.42
1	A	138	GLU	N-CA-C	5.84	120.09	111.04
2	B	54	ASN	CA-C-N	5.83	125.93	119.87
2	B	54	ASN	C-N-CA	5.83	125.93	119.87
6	F	821	DC	C2'-C3'-O3'	-5.82	102.76	111.50
2	B	343	GLN	N-CA-C	-5.79	106.75	113.88
2	B	391	LEU	N-CA-C	5.79	117.29	109.24
3	C	9	SER	CB-CA-C	-5.78	101.07	110.79
2	B	245	VAL	N-CA-C	5.78	116.61	108.17
3	C	193	THR	N-CA-C	5.75	117.89	108.52
3	C	142	LYS	N-CA-C	5.74	117.54	111.28
2	B	414	TRP	N-CA-C	5.74	118.42	109.52
3	C	139	PHE	N-CA-CB	-5.67	102.41	111.43
1	A	458	VAL	CB-CA-C	5.64	117.80	110.12
2	B	8	VAL	CA-C-N	5.58	127.10	120.23
2	B	8	VAL	C-N-CA	5.58	127.10	120.23
2	B	389	PHE	N-CA-C	5.53	118.84	109.76
6	F	820	DC	C2'-C3'-O3'	-5.51	103.23	111.50
1	A	219	GLN	N-CA-C	-5.49	104.78	112.25
5	E	704	DC	C2'-C3'-O3'	-5.49	103.27	111.50
1	A	8	VAL	CA-C-N	5.48	125.65	119.90
1	A	8	VAL	C-N-CA	5.48	125.65	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	159	VAL	N-CA-C	5.41	115.58	107.51
4	D	127	THR	CA-C-N	5.40	125.94	120.38
4	D	127	THR	C-N-CA	5.40	125.94	120.38
5	E	709	DC	C2'-C3'-O3'	-5.38	103.44	111.50
1	A	288	ALA	N-CA-C	5.37	118.47	110.14
2	B	230	MET	N-CA-C	-5.27	106.85	113.28
2	B	235	HIS	CA-C-N	5.21	126.35	119.84
2	B	235	HIS	C-N-CA	5.21	126.35	119.84
4	D	12	VAL	N-CA-C	5.20	115.61	108.12
3	C	72	SER	N-CA-C	5.20	117.89	109.06
1	A	431	LYS	N-CA-C	-5.18	105.70	112.23
2	B	198	HIS	N-CA-C	-5.18	105.08	111.40
3	C	138	ASN	CB-CA-C	-5.15	102.82	112.30
2	B	89	GLU	N-CA-C	5.13	116.73	111.03
2	B	202	ILE	N-CA-C	-5.12	105.71	110.53
2	B	91	GLN	CB-CA-C	-5.10	102.81	110.92
2	B	291	GLU	N-CA-C	5.09	115.73	107.23
5	E	703	DG	C2'-C3'-O3'	-5.04	103.94	111.50
3	C	48	ILE	N-CA-C	5.03	115.72	108.48

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	707	DG	Sidechain

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	4545	0	4607	295	0
2	B	3538	0	3576	213	0
3	C	1643	0	1565	73	0
4	D	1685	0	1640	80	0
5	E	493	0	269	30	0
6	F	429	0	242	23	0
7	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	41	0	0	12	0
8	B	37	0	0	17	0
8	C	22	0	0	6	0
8	D	25	0	0	6	0
8	E	5	0	0	3	0
8	F	8	0	0	2	0
All	All	12472	0	11899	677	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 28.

All (677) 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)
2:B:225:PRO:HB2	2:B:226:PRO:HD3	1.16	1.12
1:A:139:THR:HG23	1:A:140:PRO:HD2	1.20	1.11
1:A:556:ILE:HG22	1:A:557:ARG:H	0.98	1.08
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.33	1.08
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.35	1.07
1:A:139:THR:CG2	1:A:140:PRO:HD2	1.83	1.07
1:A:557:ARG:HH21	1:A:557:ARG:HB2	0.92	1.05
1:A:142:ILE:HD12	1:A:142:ILE:H	1.23	1.03
1:A:557:ARG:HB2	1:A:557:ARG:NH2	1.75	1.00
1:A:138:GLU:HG2	1:A:139:THR:N	1.74	1.00
2:B:224:GLU:HB3	2:B:225:PRO:HD2	1.41	1.00
2:B:356:ARG:C	2:B:356:ARG:HD2	1.84	1.00
2:B:12:LEU:HD12	2:B:12:LEU:H	1.27	0.98
1:A:556:ILE:HG22	1:A:557:ARG:N	1.76	0.95
1:A:459:THR:CG2	1:A:463:ARG:HB3	1.96	0.95
1:A:556:ILE:CG2	1:A:557:ARG:H	1.82	0.93
4:D:166:SER:H	4:D:206:ASN:HD21	1.12	0.92
1:A:3:SER:HB3	1:A:5:ILE:HD13	1.48	0.92
2:B:225:PRO:HB2	2:B:226:PRO:CD	1.99	0.91
1:A:557:ARG:HH21	1:A:557:ARG:CB	1.83	0.89
3:C:146:VAL:HG21	3:C:175:MET:HE1	1.52	0.89
4:D:3:THR:HA	8:D:247:HOH:O	1.71	0.89
2:B:344:GLU:HB3	2:B:345:PRO:HD2	1.53	0.88
3:C:142:LYS:HG2	8:C:221:HOH:O	1.74	0.88
1:A:11:LYS:H	1:A:85:GLN:HE21	1.21	0.87
1:A:143:ARG:HG3	1:A:143:ARG:HH11	1.40	0.87
1:A:142:ILE:HD12	1:A:142:ILE:N	1.89	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:SER:HB3	1:A:5:ILE:CD1	2.05	0.86
4:D:92:THR:HG23	4:D:120:THR:HA	1.58	0.86
1:A:434:ILE:HG22	1:A:494:ASN:HD21	1.42	0.85
1:A:132:ILE:HD13	1:A:132:ILE:O	1.77	0.85
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.56	0.84
4:D:166:SER:N	4:D:206:ASN:HD21	1.76	0.84
3:C:128:GLY:HA3	8:C:232:HOH:O	1.76	0.84
2:B:244:ILE:HD13	2:B:244:ILE:H	1.41	0.83
1:A:396:GLU:HG3	8:A:573:HOH:O	1.78	0.83
2:B:281:LYS:HE3	2:B:281:LYS:HA	1.60	0.83
2:B:263:LYS:HD3	8:B:454:HOH:O	1.81	0.81
1:A:498:ASP:CB	1:A:538:ALA:HB2	2.08	0.81
1:A:74:LEU:HD21	5:E:704:DC:H1'	1.63	0.81
3:C:33:LEU:HD21	3:C:88:CYS:HB2	1.60	0.81
1:A:142:ILE:H	1:A:142:ILE:CD1	1.94	0.81
1:A:354:TYR:CE2	1:A:374:LYS:HG2	2.15	0.80
1:A:439:THR:HG21	2:B:289:LEU:H	1.46	0.80
5:E:723:DC:H4'	8:E:99:HOH:O	1.80	0.80
1:A:424:LYS:NZ	1:A:424:LYS:H	1.79	0.80
1:A:500:GLN:H	1:A:500:GLN:HE21	1.30	0.79
2:B:87:PHE:O	2:B:91:GLN:HB3	1.82	0.79
3:C:211:ARG:HG3	8:C:215:HOH:O	1.83	0.79
1:A:465:LYS:HD2	1:A:467:VAL:HG13	1.63	0.78
2:B:226:PRO:HD2	8:B:448:HOH:O	1.81	0.78
2:B:222:GLN:HE21	2:B:224:GLU:HG3	1.48	0.78
1:A:275:LYS:HB3	1:A:336:GLN:HE22	1.49	0.78
5:E:704:DC:H3'	8:E:136:HOH:O	1.83	0.78
1:A:22:LYS:H	1:A:22:LYS:HD3	1.48	0.78
5:E:706:DA:H2'	5:E:707:DG:C8	2.19	0.77
1:A:501:TYR:O	1:A:505:ILE:HG13	1.84	0.77
1:A:143:ARG:HG3	1:A:143:ARG:NH1	1.95	0.77
3:C:34:ASN:HD22	3:C:89:GLN:HE22	1.33	0.76
1:A:281:LYS:HD2	1:A:284:ARG:HD2	1.67	0.76
2:B:60:VAL:CG1	2:B:75:VAL:HG22	2.15	0.76
5:E:710:DG:H2''	5:E:711:DC:H5'	1.66	0.76
4:D:65:LEU:HD22	4:D:68:ARG:HH21	1.50	0.76
5:E:707:DG:H2''	5:E:708:DG:H5'	1.66	0.75
1:A:81:ASN:HB2	8:A:572:HOH:O	1.85	0.75
2:B:361:HIS:HB3	8:B:453:HOH:O	1.85	0.75
3:C:105:GLU:HG2	3:C:173:TYR:OH	1.87	0.74
5:E:705:DT:H2'	5:E:706:DA:C8	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:4:LEU:HD23	4:D:24:PHE:HB3	1.68	0.74
2:B:222:GLN:HG3	2:B:224:GLU:H	1.52	0.74
2:B:12:LEU:HD11	2:B:127:TYR:CE2	2.22	0.73
1:A:11:LYS:H	1:A:85:GLN:NE2	1.85	0.73
3:C:85:THR:HG21	8:C:223:HOH:O	1.87	0.73
1:A:459:THR:HG21	1:A:463:ARG:HB3	1.69	0.73
2:B:93:GLY:HA2	8:B:451:HOH:O	1.89	0.73
2:B:428:GLN:CD	2:B:428:GLN:H	1.98	0.71
2:B:12:LEU:HD11	2:B:127:TYR:CZ	2.25	0.71
1:A:427:TYR:CZ	1:A:525:LEU:HD23	2.25	0.71
1:A:131:THR:OG1	1:A:143:ARG:HD3	1.89	0.71
1:A:246:LEU:HD23	1:A:246:LEU:H	1.55	0.71
2:B:106:VAL:HG13	2:B:234:LEU:HB2	1.73	0.71
1:A:281:LYS:HD2	1:A:284:ARG:CD	2.21	0.71
2:B:224:GLU:HB3	2:B:225:PRO:CD	2.21	0.70
1:A:371:ALA:O	1:A:375:ILE:HG12	1.92	0.70
2:B:266:TRP:CD1	2:B:425:LEU:HD22	2.27	0.70
1:A:10:VAL:HA	1:A:85:GLN:NE2	2.07	0.70
1:A:311:LYS:HA	1:A:311:LYS:NZ	2.07	0.70
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.72	0.70
4:D:88:GLU:HB2	8:D:246:HOH:O	1.90	0.69
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.74	0.69
6:F:818:DC:H2''	6:F:819:DG:H5'	1.72	0.69
1:A:139:THR:CG2	1:A:140:PRO:CD	2.69	0.69
2:B:422:LEU:HD23	2:B:422:LEU:H	1.55	0.69
6:F:820:DC:H2''	6:F:821:DC:H5'	1.75	0.69
1:A:350:LYS:NZ	1:A:378:GLU:OE1	2.26	0.69
1:A:2:ILE:HG22	1:A:3:SER:H	1.58	0.69
2:B:402:TRP:HH2	2:B:411:ILE:HD13	1.58	0.69
3:C:149:LYS:HA	3:C:154:GLU:HA	1.75	0.69
1:A:220:LYS:HE2	1:A:222:GLN:HB3	1.75	0.69
2:B:301:LEU:O	2:B:305:GLU:HB2	1.92	0.68
4:D:141:GLN:HE22	4:D:199:PRO:HD3	1.58	0.68
4:D:187:LEU:C	4:D:187:LEU:HD12	2.18	0.68
4:D:103:THR:HB	4:D:107:ASP:HB2	1.76	0.68
4:D:69:LEU:HD21	4:D:84:MET:HE2	1.75	0.68
1:A:430:GLU:HB2	1:A:532:TYR:HB2	1.76	0.68
1:A:458:VAL:HG22	1:A:464:GLN:CG	2.22	0.68
3:C:83:ILE:HG21	3:C:106:ILE:HG13	1.74	0.68
3:C:21:ILE:HD12	3:C:102:THR:HG21	1.74	0.67
2:B:330:GLN:HE22	2:B:340:GLN:NE2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TRP:HZ2	8:A:564:HOH:O	1.75	0.67
1:A:450:THR:O	1:A:451:LYS:HB3	1.94	0.67
2:B:163:SER:O	2:B:167:ILE:HG13	1.95	0.66
1:A:143:ARG:HH11	1:A:143:ARG:CG	2.08	0.66
1:A:275:LYS:HB3	1:A:336:GLN:NE2	2.10	0.66
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.31	0.66
3:C:89:GLN:HB2	3:C:98:PHE:CD1	2.31	0.66
1:A:3:SER:CB	1:A:5:ILE:HD13	2.25	0.66
1:A:261:VAL:HG11	6:F:817:MRG:H231	1.76	0.66
3:C:108:ARG:HG2	3:C:109:ALA:N	2.11	0.66
4:D:73:LYS:HE2	4:D:75:THR:HG23	1.78	0.66
4:D:129:PRO:HB3	4:D:155:TYR:HB3	1.78	0.66
1:A:272:PRO:HB2	1:A:309:ILE:HD11	1.78	0.66
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.30	0.66
4:D:107:ASP:OD2	4:D:107:ASP:N	2.29	0.65
6:F:818:DC:H2'	6:F:819:DG:H8	1.61	0.65
1:A:135:ILE:HG12	1:A:136:ASN:N	2.10	0.65
1:A:353:LYS:HD2	1:A:353:LYS:O	1.97	0.65
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.77	0.65
1:A:394:GLN:HB2	1:A:397:THR:OG1	1.97	0.65
1:A:277:ARG:HB3	1:A:336:GLN:NE2	2.12	0.65
1:A:108:VAL:HB	1:A:221:HIS:HB2	1.79	0.64
4:D:53:ILE:HD13	4:D:73:LYS:HB3	1.79	0.64
1:A:424:LYS:H	1:A:424:LYS:HZ2	1.43	0.64
4:D:125:LYS:O	4:D:127:THR:HG23	1.97	0.64
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.32	0.64
2:B:118:VAL:O	2:B:148:VAL:HG23	1.97	0.64
4:D:59:ASN:O	4:D:60:ARG:HD3	1.98	0.64
1:A:11:LYS:N	1:A:85:GLN:HE21	1.92	0.64
3:C:37:GLN:HB2	3:C:47:LEU:HD11	1.80	0.64
2:B:34:LEU:HD11	2:B:73:LYS:HG3	1.81	0.63
2:B:266:TRP:CH2	2:B:422:LEU:HB2	2.34	0.63
3:C:81:GLU:CD	3:C:81:GLU:H	2.05	0.63
4:D:164:TRP:CZ3	4:D:205:CYS:HB2	2.33	0.63
6:F:803:DC:H2''	6:F:804:DA:C8	2.33	0.63
2:B:320:ASP:OD2	2:B:323:LYS:HG3	1.97	0.63
2:B:245:VAL:HG13	2:B:427:TYR:HB3	1.81	0.63
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.80	0.63
1:A:310:LEU:HD23	1:A:310:LEU:O	1.98	0.63
2:B:330:GLN:HE22	2:B:340:GLN:HE22	1.44	0.63
4:D:161:THR:HB	4:D:208:ALA:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:THR:HA	1:A:494:ASN:HB2	1.81	0.63
2:B:270:ILE:HD13	2:B:346:PHE:HB3	1.81	0.63
3:C:33:LEU:HD23	3:C:34:ASN:N	2.14	0.62
1:A:295:LEU:HD12	1:A:295:LEU:H	1.64	0.62
3:C:61:ARG:HG2	3:C:61:ARG:HH11	1.64	0.62
1:A:526:ILE:HD13	1:A:526:ILE:O	2.00	0.62
1:A:47:ILE:HD12	1:A:144:TYR:CD1	2.35	0.62
1:A:363:ASN:HB3	1:A:510:PRO:HA	1.81	0.62
1:A:469:LEU:HD21	1:A:480:GLN:HG2	1.82	0.62
1:A:500:GLN:H	1:A:500:GLN:NE2	1.96	0.62
1:A:444:GLY:HA2	1:A:552:VAL:HG11	1.82	0.62
2:B:104:LYS:O	2:B:235:HIS:HD2	1.82	0.62
5:E:722:DA:H2''	5:E:723:DC:OP2	1.98	0.62
1:A:424:LYS:HE2	1:A:426:TRP:CZ2	2.35	0.62
4:D:13:GLN:HG2	8:D:237:HOH:O	1.98	0.62
4:D:73:LYS:HE2	4:D:75:THR:CG2	2.30	0.62
1:A:22:LYS:HD3	1:A:22:LYS:N	2.16	0.61
1:A:283:LEU:HD22	6:F:817:MRG:S24	2.40	0.61
2:B:371:ALA:O	2:B:375:ILE:HG13	2.01	0.61
1:A:452:LEU:HB3	1:A:470:THR:HA	1.82	0.61
1:A:535:TRP:CH2	8:B:447:HOH:O	2.51	0.61
4:D:165:ASN:HB2	4:D:169:LEU:HD13	1.82	0.61
1:A:259:LYS:O	1:A:263:LYS:HG3	2.00	0.61
2:B:101:LYS:HG3	2:B:102:LYS:HG3	1.81	0.61
2:B:225:PRO:CB	2:B:226:PRO:HD3	2.10	0.61
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.81	0.61
1:A:472:THR:CG2	1:A:476:LYS:HB2	2.31	0.60
2:B:356:ARG:HD2	2:B:357:MET:N	2.16	0.60
1:A:424:LYS:NZ	1:A:424:LYS:N	2.48	0.60
1:A:424:LYS:HE2	1:A:426:TRP:CE2	2.36	0.60
2:B:281:LYS:HE3	2:B:281:LYS:CA	2.32	0.60
4:D:157:PRO:HD2	4:D:211:ALA:CB	2.31	0.60
1:A:438:GLU:OE2	1:A:463:ARG:NH2	2.34	0.60
4:D:126:THR:HG22	4:D:157:PRO:HD3	1.83	0.60
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.82	0.60
1:A:557:ARG:O	1:A:558:LYS:O	2.20	0.60
3:C:15:LEU:HD12	3:C:15:LEU:H	1.67	0.59
2:B:162:SER:O	2:B:165:THR:HG22	2.02	0.59
3:C:23:CYS:SG	3:C:33:LEU:HD11	2.41	0.59
1:A:317:VAL:HG22	1:A:318:TYR:N	2.16	0.59
4:D:34:ILE:CG2	4:D:35:GLY:N	2.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:713:DC:H2''	5:E:714:DG:C8	2.36	0.59
5:E:703:DG:N3	5:E:703:DG:H2'	2.17	0.59
6:F:808:DC:H5'	6:F:808:DC:H6	1.68	0.59
1:A:131:THR:OG1	1:A:143:ARG:CD	2.50	0.59
1:A:434:ILE:HG22	1:A:494:ASN:ND2	2.14	0.59
2:B:356:ARG:C	2:B:356:ARG:CD	2.69	0.59
3:C:118:PHE:HZ	4:D:147:THR:O	1.86	0.59
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.38	0.59
1:A:497:THR:HG22	1:A:498:ASP:H	1.67	0.59
4:D:10:GLY:HA2	4:D:118:SER:O	2.03	0.59
5:E:708:DG:H2'	5:E:709:DC:C6	2.38	0.59
1:A:395:LYS:HD3	1:A:414:TRP:CH2	2.38	0.58
1:A:533:LEU:HD12	1:A:533:LEU:N	2.17	0.58
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.38	0.58
1:A:3:SER:HB2	1:A:119:PRO:HD3	1.86	0.58
2:B:12:LEU:HD12	2:B:12:LEU:N	2.09	0.58
1:A:452:LEU:HB2	1:A:469:LEU:O	2.04	0.58
2:B:342:TYR:HB3	2:B:348:ASN:HB3	1.84	0.58
5:E:709:DC:H2''	5:E:710:DG:H5'	1.86	0.58
4:D:98:ALA:HB1	4:D:112:HIS:O	2.04	0.58
2:B:244:ILE:HG22	2:B:425:LEU:O	2.04	0.57
3:C:105:GLU:HG2	3:C:173:TYR:HH	1.67	0.57
1:A:397:THR:HG21	1:A:424:LYS:HA	1.87	0.57
2:B:330:GLN:HE22	2:B:340:GLN:CD	2.12	0.57
1:A:424:LYS:H	1:A:424:LYS:HZ3	1.52	0.57
3:C:20:THR:HA	3:C:73:LEU:O	2.03	0.57
2:B:263:LYS:HB3	8:B:454:HOH:O	2.03	0.57
3:C:159:VAL:HG12	3:C:161:ASN:HD21	1.69	0.57
4:D:53:ILE:HB	4:D:71:VAL:HG11	1.86	0.57
4:D:68:ARG:O	4:D:84:MET:HA	2.05	0.57
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.34	0.57
2:B:344:GLU:HB3	2:B:345:PRO:CD	2.33	0.57
1:A:311:LYS:HA	1:A:311:LYS:HZ2	1.68	0.57
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.87	0.57
1:A:22:LYS:H	1:A:22:LYS:CD	2.16	0.56
1:A:93:GLY:HA3	2:B:137:ASN:ND2	2.20	0.56
1:A:279:LEU:HD22	1:A:302:GLU:HG2	1.87	0.56
1:A:546:GLU:HA	8:A:591:HOH:O	2.05	0.56
1:A:400:THR:O	1:A:403:THR:HG22	2.04	0.56
1:A:521:ILE:O	1:A:525:LEU:HD13	2.06	0.56
2:B:238:LYS:CB	8:B:440:HOH:O	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:LYS:CE	4:D:58:ASP:HB3	2.35	0.56
1:A:472:THR:HG22	1:A:476:LYS:HB2	1.88	0.56
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.88	0.56
6:F:805:DG:H1'	6:F:806:DT:H5''	1.88	0.56
2:B:239:TRP:CZ2	2:B:378:GLU:HG2	2.41	0.56
1:A:311:LYS:O	1:A:313:PRO:HD3	2.06	0.56
2:B:65:LYS:HA	2:B:407:GLN:OE1	2.06	0.56
1:A:462:GLY:O	1:A:464:GLN:NE2	2.39	0.56
1:A:473:THR:O	1:A:476:LYS:N	2.38	0.56
2:B:141:GLY:HA2	8:B:467:HOH:O	2.05	0.55
1:A:244:ILE:HD13	1:A:244:ILE:C	2.32	0.55
1:A:132:ILE:O	1:A:133:PRO:C	2.49	0.55
1:A:493:VAL:HG22	1:A:494:ASN:N	2.20	0.55
2:B:229:TRP:HA	2:B:232:TYR:CE1	2.41	0.55
3:C:39:LYS:NZ	3:C:39:LYS:HB3	2.21	0.55
1:A:450:THR:O	1:A:451:LYS:CB	2.55	0.55
3:C:34:ASN:OD1	3:C:49:TYR:HA	2.07	0.55
2:B:224:GLU:CB	2:B:225:PRO:HD2	2.17	0.55
3:C:47:LEU:HA	3:C:58:VAL:HG21	1.89	0.55
1:A:222:GLN:O	1:A:224:GLU:HG3	2.06	0.55
1:A:220:LYS:O	1:A:220:LYS:HD3	2.07	0.55
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.42	0.54
1:A:538:ALA:HB1	1:A:539:HIS:HD2	1.72	0.54
4:D:53:ILE:HB	4:D:71:VAL:CG1	2.37	0.54
5:E:705:DT:H2''	5:E:706:DA:H5'	1.90	0.54
1:A:441:TYR:O	1:A:548:VAL:HG11	2.07	0.54
1:A:439:THR:HG21	2:B:289:LEU:N	2.19	0.54
1:A:295:LEU:HD12	1:A:295:LEU:N	2.22	0.54
4:D:126:THR:HA	4:D:156:PHE:O	2.06	0.54
6:F:817:MRG:H2''	6:F:818:DC:C6	2.43	0.54
2:B:195:ILE:HG23	2:B:196:GLY:N	2.22	0.54
2:B:225:PRO:HD3	3:C:92:SER:HA	1.89	0.54
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.88	0.54
4:D:18:PHE:CD2	4:D:87:VAL:HG11	2.42	0.54
4:D:219:LYS:HD2	8:D:248:HOH:O	2.08	0.54
1:A:23:GLN:HE22	1:A:60:VAL:H	1.56	0.54
1:A:163:SER:O	1:A:167:ILE:HG12	2.08	0.54
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.43	0.54
4:D:68:ARG:HD2	4:D:85:MET:O	2.07	0.54
2:B:234:LEU:HD21	2:B:377:THR:HG21	1.90	0.54
2:B:238:LYS:HB2	8:B:440:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:GLN:NE2	2:B:353:LYS:HD2	2.22	0.54
1:A:50:ILE:HG13	1:A:143:ARG:HB3	1.89	0.53
2:B:184:MET:HE2	8:B:444:HOH:O	2.07	0.53
2:B:295:LEU:HD22	2:B:300:GLU:HB2	1.90	0.53
4:D:150:CYS:HB2	4:D:164:TRP:CH2	2.43	0.53
5:E:716:DA:H2''	5:E:717:DC:H5'	1.89	0.53
1:A:202:ILE:HB	8:A:581:HOH:O	2.08	0.53
1:A:407:GLN:HE22	2:B:418:ASN:HA	1.71	0.53
4:D:69:LEU:HD22	4:D:82:LEU:HD11	1.90	0.53
1:A:293:ILE:HD13	1:A:294:PRO:N	2.24	0.53
1:A:324:ASP:HA	1:A:385:LYS:HZ3	1.72	0.53
1:A:424:LYS:HZ2	1:A:424:LYS:N	2.04	0.53
1:A:115:TYR:CE1	1:A:156:SER:HB3	2.43	0.53
2:B:115:TYR:C	2:B:117:SER:H	2.16	0.53
1:A:10:VAL:HA	1:A:85:GLN:HE21	1.74	0.53
1:A:132:ILE:O	1:A:132:ILE:CD1	2.55	0.53
1:A:518:VAL:O	1:A:522:ILE:HG13	2.09	0.53
2:B:104:LYS:O	2:B:235:HIS:CD2	2.62	0.53
2:B:296:THR:HB	2:B:299:ALA:CB	2.38	0.53
2:B:325:LEU:HB3	2:B:387:PRO:HA	1.91	0.53
4:D:89:THR:HA	4:D:121:VAL:HB	1.91	0.53
6:F:818:DC:H2'	6:F:819:DG:C8	2.43	0.53
2:B:103:LYS:O	2:B:236:PRO:HD2	2.07	0.53
2:B:244:ILE:HG13	2:B:310:LEU:HD22	1.91	0.53
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.90	0.53
3:C:149:LYS:HB2	3:C:193:THR:HB	1.90	0.53
4:D:202:THR:HG22	4:D:219:LYS:HE3	1.90	0.53
1:A:428:GLN:HG3	1:A:429:LEU:H	1.74	0.53
1:A:167:ILE:O	1:A:170:PRO:HD2	2.08	0.52
3:C:141:PRO:HB2	8:C:221:HOH:O	2.10	0.52
4:D:14:PRO:O	4:D:15:SER:HB2	2.09	0.52
1:A:271:TYR:CE1	1:A:314:VAL:HG22	2.44	0.52
2:B:223:LYS:HE2	4:D:58:ASP:HB3	1.90	0.52
2:B:326:ILE:HG22	2:B:327:ALA:N	2.24	0.52
2:B:281:LYS:HA	2:B:281:LYS:CE	2.36	0.52
2:B:101:LYS:O	2:B:236:PRO:HB2	2.10	0.52
1:A:198:HIS:HD2	1:A:199:ARG:HD2	1.75	0.52
3:C:117:ILE:HD12	3:C:194:CYS:HB2	1.90	0.52
2:B:428:GLN:CD	2:B:428:GLN:N	2.66	0.52
1:A:78:ARG:HA	8:A:572:HOH:O	2.10	0.52
1:A:537:PRO:HB3	8:B:447:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:HIS:HB2	1:A:238:LYS:O	2.10	0.52
4:D:18:PHE:HD2	4:D:87:VAL:HG11	1.74	0.52
1:A:220:LYS:HD3	1:A:220:LYS:C	2.35	0.52
2:B:222:GLN:NE2	2:B:224:GLU:HG3	2.20	0.52
2:B:360:ALA:HB1	2:B:367:GLN:HG2	1.92	0.52
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.91	0.51
2:B:365:VAL:O	2:B:369:THR:HG23	2.10	0.51
6:F:802:DA:H2''	6:F:803:DC:O5'	2.10	0.51
1:A:270:ILE:HG12	1:A:270:ILE:O	2.10	0.51
2:B:279:LEU:HD11	2:B:302:GLU:CB	2.40	0.51
2:B:183:TYR:CD2	2:B:380:ILE:HD13	2.46	0.51
2:B:414:TRP:CD1	2:B:414:TRP:C	2.88	0.51
3:C:211:ARG:CG	8:C:215:HOH:O	2.51	0.51
1:A:277:ARG:HB3	1:A:336:GLN:CD	2.36	0.51
1:A:329:ILE:N	1:A:329:ILE:HD12	2.26	0.51
2:B:332:GLN:HG2	2:B:428:GLN:HG3	1.91	0.51
2:B:420:PRO:O	2:B:422:LEU:N	2.43	0.51
6:F:815:DG:C5'	8:F:122:HOH:O	2.57	0.51
1:A:320:ASP:H	1:A:343:GLN:HE22	1.57	0.51
2:B:279:LEU:HD11	2:B:302:GLU:HB3	1.93	0.51
3:C:89:GLN:HB2	3:C:98:PHE:CE1	2.46	0.51
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.91	0.51
3:C:146:VAL:CG2	3:C:175:MET:HE1	2.32	0.51
6:F:808:DC:H5'	6:F:808:DC:C6	2.46	0.51
5:E:719:DG:H2''	5:E:720:DG:OP2	2.11	0.51
1:A:115:TYR:CD1	1:A:156:SER:HB3	2.46	0.51
1:A:489:SER:HB3	1:A:528:LYS:HZ1	1.74	0.51
1:A:466:VAL:HG21	1:A:551:LEU:HG	1.92	0.51
3:C:66:GLY:HA3	3:C:71:TYR:HA	1.92	0.51
2:B:244:ILE:HD13	2:B:244:ILE:N	2.18	0.50
1:A:448:ARG:HD2	6:F:807:DC:H4'	1.92	0.50
2:B:279:LEU:HD12	2:B:279:LEU:N	2.26	0.50
1:A:131:THR:OG1	1:A:143:ARG:NE	2.45	0.50
1:A:160:PHE:C	1:A:160:PHE:CD2	2.90	0.50
1:A:439:THR:HB	2:B:289:LEU:HG	1.94	0.50
2:B:98:ALA:O	2:B:101:LYS:HG2	2.11	0.50
3:C:15:LEU:HD12	3:C:15:LEU:N	2.27	0.50
2:B:38:CYS:HB3	8:B:458:HOH:O	2.10	0.50
6:F:815:DG:H5''	8:F:122:HOH:O	2.10	0.50
1:A:3:SER:HB3	1:A:5:ILE:HD12	1.90	0.50
1:A:5:ILE:HD12	1:A:5:ILE:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:GLU:O	2:B:345:PRO:C	2.55	0.50
3:C:190:ASN:HD21	3:C:211:ARG:HG3	1.76	0.50
4:D:31:THR:OG1	4:D:34:ILE:HD13	2.12	0.50
4:D:40:ARG:HB2	4:D:50:LEU:HD11	1.92	0.50
1:A:339:TYR:CD2	1:A:375:ILE:HD11	2.47	0.50
2:B:136:ASN:O	2:B:137:ASN:C	2.55	0.50
2:B:296:THR:HB	2:B:299:ALA:HB2	1.93	0.50
5:E:705:DT:H2''	5:E:706:DA:C5'	2.41	0.50
2:B:330:GLN:NE2	2:B:340:GLN:OE1	2.44	0.49
3:C:182:THR:HG22	3:C:183:LYS:H	1.76	0.49
1:A:115:TYR:HE1	1:A:156:SER:C	2.20	0.49
1:A:451:LYS:HE3	1:A:471:ASN:ND2	2.27	0.49
1:A:460:ASN:HA	2:B:286:THR:O	2.12	0.49
1:A:498:ASP:HB2	1:A:538:ALA:CB	2.23	0.49
3:C:27:GLN:O	3:C:29:ILE:HG23	2.12	0.49
1:A:360:ALA:HA	8:A:565:HOH:O	2.12	0.49
1:A:458:VAL:HG22	1:A:464:GLN:HG3	1.95	0.49
2:B:234:LEU:HD21	2:B:377:THR:CG2	2.42	0.49
1:A:328:GLU:HG2	1:A:330:GLN:HE22	1.77	0.49
1:A:333:GLY:O	1:A:334:GLN:C	2.56	0.49
4:D:6:GLU:OE1	4:D:6:GLU:N	2.43	0.49
5:E:715:DA:H2''	5:E:716:DA:H8	1.77	0.49
6:F:820:DC:H2''	6:F:821:DC:C5'	2.43	0.49
1:A:132:ILE:O	1:A:133:PRO:O	2.30	0.49
2:B:253:THR:O	2:B:257:ILE:HG12	2.13	0.49
1:A:31:ILE:HG23	1:A:132:ILE:HD11	1.93	0.49
1:A:535:TRP:HH2	8:B:447:HOH:O	1.91	0.49
3:C:159:VAL:HG12	3:C:161:ASN:ND2	2.27	0.49
4:D:148:LEU:HD21	4:D:198:TRP:CE3	2.48	0.49
1:A:407:GLN:HG3	2:B:393:ILE:HA	1.95	0.49
1:A:441:TYR:CE2	1:A:544:GLY:HA3	2.48	0.49
2:B:12:LEU:H	2:B:12:LEU:CD1	2.10	0.49
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.12	0.49
2:B:206:ARG:HD2	2:B:216:THR:OG1	2.13	0.49
2:B:47:ILE:CG2	2:B:144:TYR:HB3	2.42	0.49
2:B:278:GLN:HG3	2:B:299:ALA:HA	1.94	0.49
4:D:22:CYS:HB3	4:D:80:ALA:HB3	1.93	0.49
5:E:709:DC:H2'	5:E:710:DG:H8	1.78	0.49
1:A:31:ILE:HD13	1:A:134:SER:C	2.38	0.49
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.95	0.49
1:A:279:LEU:HD23	1:A:279:LEU:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.42	0.49
2:B:238:LYS:HG3	8:B:440:HOH:O	2.11	0.49
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.13	0.48
3:C:61:ARG:HG2	3:C:61:ARG:NH1	2.28	0.48
1:A:491:LEU:HB3	1:A:529:GLU:HB3	1.95	0.48
1:A:303:LEU:O	1:A:307:ARG:HG3	2.13	0.48
2:B:303:LEU:HD21	2:B:307:ARG:HH21	1.79	0.48
1:A:115:TYR:HE1	1:A:156:SER:O	1.96	0.48
1:A:138:GLU:CG	1:A:139:THR:N	2.54	0.48
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.13	0.48
4:D:169:LEU:HD12	4:D:169:LEU:N	2.28	0.48
1:A:281:LYS:HD2	1:A:284:ARG:NE	2.29	0.48
2:B:227:PHE:HB2	4:D:105:VAL:HA	1.96	0.48
1:A:10:VAL:HG23	1:A:124:PHE:CD1	2.49	0.48
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.14	0.48
2:B:85:GLN:HG3	2:B:88:TRP:CZ2	2.49	0.48
2:B:225:PRO:HB3	3:C:32:TYR:CE1	2.48	0.48
3:C:17:ASP:O	3:C:77:ASN:HA	2.14	0.48
3:C:137:ASN:HB3	3:C:138:ASN:HD22	1.77	0.48
1:A:135:ILE:HD13	1:A:135:ILE:H	1.77	0.48
2:B:266:TRP:HB3	2:B:425:LEU:HD13	1.95	0.48
4:D:38:TRP:CZ3	4:D:97:CYS:HB3	2.48	0.48
1:A:442:VAL:HG21	1:A:482:ILE:HG12	1.95	0.48
2:B:104:LYS:HG2	2:B:192:ASP:HA	1.95	0.48
4:D:77:ASN:O	4:D:78:ASN:HB2	2.12	0.48
1:A:244:ILE:O	1:A:244:ILE:HG23	2.13	0.48
2:B:79:GLU:O	2:B:83:ARG:HG2	2.14	0.48
2:B:91:GLN:HG3	2:B:92:LEU:HG	1.95	0.48
3:C:121:SER:O	3:C:125:LEU:HG	2.13	0.48
4:D:53:ILE:CD1	4:D:73:LYS:HB3	2.43	0.47
4:D:57:ASP:OD2	4:D:73:LYS:NZ	2.42	0.47
1:A:139:THR:HG22	1:A:140:PRO:HD2	1.87	0.47
1:A:535:TRP:CZ3	8:B:447:HOH:O	2.66	0.47
2:B:47:ILE:HG22	2:B:144:TYR:HD1	1.79	0.47
2:B:342:TYR:HB3	2:B:348:ASN:CB	2.43	0.47
4:D:2:ILE:HD12	4:D:27:PHE:HD1	1.78	0.47
2:B:214:LEU:HD12	2:B:214:LEU:N	2.28	0.47
2:B:230:MET:HB2	4:D:105:VAL:HG22	1.97	0.47
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.94	0.47
3:C:31:SER:O	3:C:50:TYR:CD1	2.67	0.47
4:D:34:ILE:HG23	4:D:35:GLY:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:HG12	2:B:140:PRO:HB3	1.96	0.47
1:A:277:ARG:H	1:A:336:GLN:HE21	1.62	0.47
2:B:317:VAL:HG22	2:B:349:LEU:HD23	1.96	0.47
4:D:37:THR:OG1	4:D:100:SER:HB2	2.15	0.47
1:A:489:SER:HB3	1:A:528:LYS:NZ	2.29	0.47
2:B:87:PHE:HZ	2:B:159:ILE:HG13	1.80	0.47
4:D:20:LEU:HD12	4:D:82:LEU:HD23	1.96	0.47
1:A:317:VAL:HG22	1:A:318:TYR:H	1.79	0.47
1:A:441:TYR:CD2	1:A:544:GLY:CA	2.98	0.47
2:B:18:GLY:H	2:B:56:TYR:HE2	1.62	0.47
2:B:32:LYS:O	2:B:35:VAL:HG12	2.14	0.47
2:B:77:PHE:CD1	2:B:80:LEU:HD23	2.49	0.47
3:C:83:ILE:HD12	3:C:106:ILE:HG12	1.97	0.47
1:A:40:GLU:OE2	1:A:44:GLU:OE2	2.33	0.47
1:A:5:ILE:HD12	1:A:5:ILE:H	1.79	0.47
1:A:74:LEU:CD2	5:E:704:DC:H1'	2.41	0.47
1:A:184:MET:HG2	6:F:822:ATM:H1'	1.97	0.47
1:A:280:SER:OG	5:E:712:DC:H4'	2.15	0.47
2:B:58:THR:HG22	2:B:59:PRO:N	2.30	0.47
1:A:60:VAL:O	1:A:60:VAL:HG13	2.15	0.46
2:B:79:GLU:OE1	2:B:83:ARG:NH1	2.48	0.46
4:D:187:LEU:C	4:D:187:LEU:CD1	2.86	0.46
1:A:132:ILE:CG2	1:A:142:ILE:HB	2.46	0.46
1:A:135:ILE:HD13	1:A:135:ILE:N	2.30	0.46
1:A:259:LYS:HE3	8:A:585:HOH:O	2.15	0.46
1:A:293:ILE:HD13	1:A:294:PRO:CD	2.46	0.46
2:B:75:VAL:HG11	2:B:77:PHE:CE2	2.50	0.46
2:B:342:TYR:CB	2:B:348:ASN:HA	2.45	0.46
4:D:31:THR:HG21	8:D:244:HOH:O	2.15	0.46
1:A:500:GLN:HE21	1:A:500:GLN:N	2.06	0.46
1:A:513:SER:OG	1:A:514:GLU:N	2.46	0.46
1:A:247:PRO:HG2	1:A:260:LEU:HD13	1.96	0.46
1:A:495:ILE:HG22	1:A:496:VAL:N	2.30	0.46
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.50	0.46
2:B:242:GLN:CD	2:B:353:LYS:HD2	2.40	0.46
2:B:368:LEU:O	2:B:372:VAL:HG23	2.15	0.46
4:D:34:ILE:O	4:D:55:TRP:HE3	1.98	0.46
1:A:93:GLY:HA3	2:B:137:ASN:HD21	1.79	0.46
2:B:388:LYS:HA	2:B:413:GLU:O	2.16	0.46
1:A:5:ILE:HG12	1:A:167:ILE:HD11	1.97	0.46
3:C:182:THR:H	3:C:185:GLU:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:VAL:HG21	4:D:18:PHE:HB3	1.97	0.46
4:D:209:HIS:CD2	4:D:212:SER:OG	2.69	0.46
2:B:380:ILE:O	2:B:384:GLY:HA2	2.16	0.46
3:C:82:ASP:O	3:C:84:ALA:N	2.49	0.46
3:C:89:GLN:HE21	3:C:89:GLN:HB3	1.52	0.46
5:E:706:DA:H2'	5:E:707:DG:H8	1.74	0.46
1:A:24:TRP:HZ3	1:A:61:PHE:CD2	2.33	0.46
1:A:267:ALA:HB1	1:A:271:TYR:HD2	1.81	0.46
2:B:342:TYR:HB3	2:B:348:ASN:CA	2.46	0.46
1:A:438:GLU:CD	1:A:463:ARG:HH21	2.23	0.46
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.96	0.45
5:E:715:DA:H2''	5:E:716:DA:C8	2.51	0.45
1:A:252:TRP:CD1	1:A:295:LEU:HD21	2.51	0.45
1:A:276:VAL:HG12	1:A:280:SER:HB2	1.98	0.45
1:A:523:GLU:O	1:A:526:ILE:HG22	2.15	0.45
3:C:90:GLN:HE21	3:C:92:SER:H	1.65	0.45
1:A:171:PHE:CE2	1:A:205:LEU:HD13	2.51	0.45
1:A:253:THR:HA	1:A:292:VAL:HA	1.98	0.45
1:A:276:VAL:O	1:A:277:ARG:C	2.59	0.45
2:B:178:ILE:CD1	2:B:201:LYS:HG2	2.47	0.45
2:B:254:VAL:HB	2:B:289:LEU:O	2.16	0.45
2:B:303:LEU:HD23	2:B:303:LEU:C	2.40	0.45
1:A:279:LEU:HD22	1:A:302:GLU:CG	2.46	0.45
2:B:260:LEU:O	2:B:264:LEU:HD12	2.16	0.45
3:C:91:TYR:CE1	4:D:108:SER:HB3	2.51	0.45
2:B:245:VAL:CG1	2:B:427:TYR:HB3	2.46	0.45
2:B:295:LEU:HD11	2:B:303:LEU:HD13	1.98	0.45
1:A:279:LEU:CD2	1:A:302:GLU:HG2	2.46	0.45
2:B:327:ALA:HA	2:B:340:GLN:O	2.17	0.45
4:D:137:GLY:HA2	4:D:223:ALA:HB2	1.99	0.45
4:D:182:SER:O	4:D:183:ASP:HB2	2.16	0.45
1:A:93:GLY:CA	2:B:137:ASN:ND2	2.79	0.45
1:A:221:HIS:HB3	1:A:227:PHE:HD2	1.82	0.45
1:A:425:LEU:HD13	1:A:509:GLN:OE1	2.17	0.45
2:B:8:VAL:HG11	2:B:159:ILE:HG12	1.99	0.45
2:B:106:VAL:CG1	2:B:234:LEU:HB2	2.46	0.45
2:B:112:GLY:HA3	2:B:151:GLN:HE21	1.82	0.45
2:B:239:TRP:CH2	2:B:378:GLU:HA	2.52	0.45
2:B:223:LYS:HE3	4:D:58:ASP:HB3	1.97	0.45
2:B:238:LYS:CG	8:B:440:HOH:O	2.64	0.45
2:B:282:LEU:HB3	2:B:293:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:SER:HB3	3:C:64:GLY:O	2.17	0.45
3:C:60:SER:C	3:C:62:PHE:H	2.25	0.45
1:A:195:ILE:O	1:A:199:ARG:HG2	2.17	0.44
2:B:414:TRP:CD1	2:B:414:TRP:O	2.70	0.44
3:C:197:THR:HG22	3:C:204:PRO:HG3	1.98	0.44
1:A:2:ILE:HG22	1:A:3:SER:N	2.30	0.44
1:A:493:VAL:CG2	1:A:494:ASN:N	2.80	0.44
2:B:112:GLY:C	2:B:151:GLN:HE21	2.25	0.44
2:B:242:GLN:HA	2:B:242:GLN:HE21	1.82	0.44
2:B:250:ASP:N	2:B:250:ASP:OD1	2.51	0.44
2:B:353:LYS:HB2	2:B:353:LYS:NZ	2.33	0.44
3:C:30:SER:O	3:C:31:SER:HB2	2.17	0.44
1:A:5:ILE:O	1:A:6:GLU:C	2.61	0.44
1:A:325:LEU:HD21	1:A:383:TRP:CD2	2.52	0.44
1:A:136:ASN:C	1:A:138:GLU:H	2.25	0.44
1:A:365:VAL:HG11	1:A:401:TRP:CD1	2.53	0.44
1:A:365:VAL:HG11	1:A:401:TRP:CG	2.53	0.44
2:B:423:VAL:HG13	2:B:425:LEU:HB2	2.00	0.44
3:C:170:ASP:OD1	3:C:170:ASP:C	2.61	0.44
5:E:707:DG:C2'	5:E:708:DG:H5'	2.44	0.44
1:A:61:PHE:CE1	5:E:703:DG:H2''	2.52	0.44
1:A:254:VAL:HB	1:A:289:LEU:O	2.17	0.44
1:A:536:VAL:HG13	1:A:537:PRO:HD2	1.99	0.44
1:A:49:LYS:HE2	1:A:142:ILE:HG21	2.00	0.44
1:A:154:LYS:O	1:A:157:PRO:HD2	2.18	0.44
1:A:246:LEU:HD23	1:A:246:LEU:N	2.30	0.44
1:A:317:VAL:CG2	1:A:318:TYR:N	2.80	0.44
2:B:328:GLU:O	2:B:339:TYR:HA	2.18	0.44
3:C:124:GLN:NE2	3:C:131:SER:OG	2.51	0.44
3:C:197:THR:HG22	3:C:204:PRO:HB3	2.00	0.44
1:A:135:ILE:CG1	1:A:136:ASN:N	2.78	0.43
2:B:47:ILE:CG2	2:B:144:TYR:CD1	3.01	0.43
2:B:54:ASN:HB3	2:B:143:ARG:HH12	1.83	0.43
2:B:348:ASN:H	2:B:348:ASN:ND2	2.15	0.43
3:C:182:THR:HG22	3:C:183:LYS:N	2.33	0.43
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.53	0.43
1:A:440:PHE:CZ	1:A:488:ASP:O	2.71	0.43
1:A:546:GLU:CB	8:A:591:HOH:O	2.66	0.43
2:B:37:ILE:O	2:B:41:MET:HG3	2.18	0.43
1:A:261:VAL:HG13	1:A:262:GLY:N	2.33	0.43
1:A:427:TYR:CE2	1:A:525:LEU:HD23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:THR:HG22	1:A:473:THR:N	2.32	0.43
2:B:58:THR:HA	2:B:59:PRO:HD3	1.79	0.43
4:D:105:VAL:HG12	4:D:105:VAL:O	2.19	0.43
1:A:473:THR:O	1:A:474:ASN:C	2.62	0.43
3:C:90:GLN:C	3:C:90:GLN:CD	2.86	0.43
6:F:807:DC:C2	6:F:808:DC:C5	3.06	0.43
1:A:40:GLU:OE2	1:A:44:GLU:CD	2.61	0.43
2:B:58:THR:CG2	2:B:59:PRO:CD	2.96	0.43
2:B:63:ILE:HD13	2:B:74:LEU:HD11	1.99	0.43
2:B:223:LYS:HE2	4:D:58:ASP:OD2	2.18	0.43
2:B:317:VAL:HG13	2:B:317:VAL:O	2.18	0.43
1:A:132:ILE:HG23	1:A:142:ILE:HD13	2.00	0.43
1:A:556:ILE:CG2	1:A:557:ARG:N	2.50	0.43
2:B:87:PHE:HZ	2:B:159:ILE:CG1	2.32	0.43
6:F:806:DT:H2''	6:F:807:DC:C6	2.54	0.43
1:A:5:ILE:HD11	1:A:212:TRP:HB3	1.99	0.43
2:B:344:GLU:CB	2:B:345:PRO:CD	2.95	0.43
4:D:156:PHE:HA	4:D:157:PRO:HA	1.65	0.43
1:A:546:GLU:CA	8:A:591:HOH:O	2.66	0.43
3:C:107:LYS:HA	3:C:140:TYR:OH	2.19	0.43
1:A:458:VAL:HG12	2:B:286:THR:HG21	2.00	0.43
1:A:498:ASP:HA	1:A:536:VAL:O	2.19	0.43
3:C:34:ASN:HD22	3:C:89:GLN:NE2	2.09	0.43
1:A:443:ASP:O	1:A:481:ALA:HB2	2.18	0.43
1:A:459:THR:HG22	1:A:463:ARG:HB3	1.92	0.43
1:A:261:VAL:HG23	1:A:276:VAL:CG1	2.49	0.42
1:A:557:ARG:NH2	1:A:557:ARG:CB	2.59	0.42
2:B:116:PHE:C	2:B:148:VAL:HG21	2.43	0.42
1:A:458:VAL:HG23	1:A:548:VAL:HG13	2.01	0.42
2:B:96:HIS:CE1	2:B:381:VAL:O	2.72	0.42
2:B:106:VAL:HA	2:B:190:GLY:HA2	2.01	0.42
1:A:201:LYS:HD2	1:A:201:LYS:HA	1.87	0.42
1:A:460:ASN:HA	2:B:286:THR:OG1	2.19	0.42
2:B:277:ARG:O	2:B:281:LYS:HD2	2.19	0.42
3:C:187:GLU:C	3:C:189:HIS:H	2.27	0.42
4:D:53:ILE:HG13	4:D:59:ASN:ND2	2.35	0.42
5:E:720:DG:H1'	5:E:721:DG:H5''	2.02	0.42
5:E:725:DG:N9	5:E:726:DT:H72	2.34	0.42
3:C:106:ILE:H	3:C:166:GLN:HE22	1.66	0.42
3:C:118:PHE:HA	3:C:119:PRO:HD3	1.82	0.42
4:D:95:TYR:O	4:D:116:GLY:HA2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:802:DA:H1'	6:F:803:DC:O4'	2.20	0.42
1:A:460:ASN:HD22	2:B:288:ALA:HB2	1.84	0.42
1:A:484:LEU:C	1:A:486:LEU:N	2.77	0.42
2:B:17:ASP:CG	2:B:18:GLY:H	2.28	0.42
6:F:816:DG:H2''	6:F:817:MRG:H8	2.01	0.42
1:A:53:GLU:O	1:A:55:PRO:HD3	2.19	0.42
1:A:458:VAL:HG11	1:A:547:GLN:HB3	2.02	0.42
1:A:484:LEU:C	1:A:486:LEU:H	2.28	0.42
2:B:94:ILE:N	2:B:94:ILE:HD12	2.34	0.42
1:A:467:VAL:HG22	1:A:484:LEU:HD11	2.02	0.42
3:C:112:ALA:HB1	3:C:113:PRO:HD2	2.01	0.42
6:F:818:DC:H2''	6:F:819:DG:C5'	2.45	0.42
1:A:246:LEU:H	1:A:246:LEU:CD2	2.27	0.41
1:A:260:LEU:HD21	1:A:303:LEU:HD13	2.01	0.41
1:A:283:LEU:O	1:A:284:ARG:C	2.62	0.41
1:A:442:VAL:HG12	1:A:457:TYR:HB3	2.02	0.41
1:A:491:LEU:HD12	1:A:491:LEU:N	2.34	0.41
2:B:293:ILE:HA	2:B:294:PRO:HD3	1.94	0.41
3:C:33:LEU:HD23	3:C:34:ASN:H	1.85	0.41
1:A:361:HIS:CD2	1:A:505:ILE:HD13	2.55	0.41
1:A:503:LEU:HD22	1:A:535:TRP:HB2	2.01	0.41
2:B:204:GLU:O	2:B:207:GLN:HB2	2.20	0.41
2:B:214:LEU:N	2:B:214:LEU:CD1	2.83	0.41
4:D:4:LEU:N	8:D:247:HOH:O	2.53	0.41
4:D:157:PRO:HD2	4:D:211:ALA:HB2	2.01	0.41
5:E:704:DC:H2''	5:E:705:DT:H5'	2.02	0.41
6:F:817:MRG:H2''	6:F:818:DC:C5	2.54	0.41
1:A:291:GLU:O	1:A:292:VAL:C	2.64	0.41
1:A:486:LEU:HD11	1:A:521:ILE:HG23	2.02	0.41
2:B:225:PRO:HG3	3:C:92:SER:O	2.20	0.41
4:D:169:LEU:N	4:D:169:LEU:CD1	2.83	0.41
1:A:166:LYS:O	1:A:169:GLU:HB3	2.21	0.41
2:B:242:GLN:NE2	2:B:242:GLN:HA	2.35	0.41
3:C:135:PHE:C	3:C:136:LEU:HD12	2.45	0.41
1:A:11:LYS:N	1:A:85:GLN:NE2	2.60	0.41
1:A:412:PRO:O	1:A:413:GLU:C	2.64	0.41
2:B:244:ILE:HG12	2:B:310:LEU:HB3	2.02	0.41
2:B:422:LEU:HD23	2:B:422:LEU:N	2.29	0.41
3:C:146:VAL:HG21	3:C:175:MET:CE	2.36	0.41
1:A:374:LYS:NZ	8:A:588:HOH:O	2.54	0.41
1:A:457:TYR:CD2	1:A:457:TYR:C	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:ALA:O	2:B:361:HIS:ND1	2.53	0.41
1:A:111:VAL:HG11	1:A:214:LEU:HD12	2.03	0.41
1:A:279:LEU:HD23	1:A:279:LEU:N	2.35	0.41
2:B:108:VAL:HA	2:B:187:LEU:O	2.21	0.41
2:B:120:LEU:O	2:B:121:ASP:C	2.64	0.41
2:B:122:GLU:HA	2:B:125:ARG:NE	2.36	0.41
2:B:252:TRP:HB3	2:B:257:ILE:HD11	2.02	0.41
2:B:332:GLN:CG	2:B:428:GLN:HG3	2.51	0.41
2:B:340:GLN:HG3	2:B:351:THR:HG22	2.01	0.41
3:C:91:TYR:OH	4:D:106:THR:O	2.35	0.41
3:C:170:ASP:OD1	3:C:172:THR:HG23	2.21	0.41
5:E:723:DC:C4'	8:E:99:HOH:O	2.54	0.41
1:A:60:VAL:CG1	1:A:131:THR:O	2.69	0.41
1:A:287:LYS:HD3	1:A:291:GLU:OE2	2.21	0.41
1:A:372:VAL:HG11	1:A:411:ILE:HG23	2.02	0.41
1:A:484:LEU:O	1:A:486:LEU:N	2.54	0.41
2:B:253:THR:HA	2:B:292:VAL:HA	2.03	0.41
1:A:10:VAL:CA	1:A:85:GLN:HE21	2.33	0.40
1:A:331:LYS:HD3	1:A:331:LYS:C	2.46	0.40
2:B:38:CYS:CB	8:B:458:HOH:O	2.67	0.40
2:B:47:ILE:HG23	2:B:144:TYR:HB3	2.02	0.40
5:E:716:DA:C2	5:E:717:DC:C2	3.09	0.40
1:A:160:PHE:CD2	1:A:160:PHE:O	2.74	0.40
1:A:280:SER:C	1:A:282:LEU:H	2.30	0.40
2:B:30:LYS:O	2:B:34:LEU:HB2	2.21	0.40
2:B:58:THR:HG23	2:B:59:PRO:CD	2.52	0.40
2:B:223:LYS:HE2	4:D:58:ASP:CB	2.51	0.40
3:C:35:TRP:CZ3	3:C:88:CYS:HB3	2.57	0.40
5:E:720:DG:H2''	5:E:721:DG:OP2	2.20	0.40
1:A:441:TYR:CD2	1:A:544:GLY:C	2.99	0.40
2:B:254:VAL:HG23	2:B:291:GLU:HB3	2.03	0.40
1:A:344:GLU:HB3	8:A:571:HOH:O	2.22	0.40
2:B:56:TYR:O	2:B:143:ARG:NH2	2.55	0.40
4:D:59:ASN:ND2	4:D:59:ASN:N	2.68	0.40
4:D:142:THR:HB	4:D:143:ASN:H	1.63	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	556/564 (99%)	483 (87%)	61 (11%)	12 (2%)	5	20
2	B	426/437 (98%)	377 (88%)	41 (10%)	8 (2%)	6	23
3	C	209/211 (99%)	185 (88%)	22 (10%)	2 (1%)	12	39
4	D	223/225 (99%)	197 (88%)	24 (11%)	2 (1%)	14	41
All	All	1414/1437 (98%)	1242 (88%)	148 (10%)	24 (2%)	7	26

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	272	PRO
2	B	225	PRO
2	B	292	VAL
2	B	345	PRO
1	A	133	PRO
1	A	333	GLY
1	A	451	LYS
3	C	83	ILE
1	A	243	PRO
1	A	324	ASP
1	A	528	LYS
2	B	315	HIS
4	D	126	THR
1	A	345	PRO
2	B	116	PHE
2	B	421	PRO
2	B	423	VAL
4	D	142	THR
1	A	195	ILE
1	A	284	ARG
1	A	556	ILE

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Mol	Chain	Res	Type
3	C	68	GLY
2	B	111	VAL

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	498/504 (99%)	463 (93%)	35 (7%)	14	40
2	B	390/397 (98%)	363 (93%)	27 (7%)	14	41
3	C	190/190 (100%)	185 (97%)	5 (3%)	40	73
4	D	196/196 (100%)	187 (95%)	9 (5%)	24	57
All	All	1274/1287 (99%)	1198 (94%)	76 (6%)	17	47

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	55	PRO
1	A	60	VAL
1	A	80	LEU
1	A	132	ILE
1	A	135	ILE
1	A	138	GLU
1	A	142	ILE
1	A	143	ARG
1	A	220	LYS
1	A	243	PRO
1	A	244	ILE
1	A	246	LEU
1	A	272	PRO
1	A	283	LEU
1	A	293	ILE
1	A	296	THR
1	A	311	LYS
1	A	325	LEU

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Mol	Chain	Res	Type
1	A	399	GLU
1	A	424	LYS
1	A	429	LEU
1	A	434	ILE
1	A	459	THR
1	A	464	GLN
1	A	465	LYS
1	A	468	PRO
1	A	478	GLU
1	A	497	THR
1	A	500	GLN
1	A	525	LEU
1	A	526	ILE
1	A	547	GLN
1	A	548	VAL
1	A	557	ARG
2	B	8	VAL
2	B	12	LEU
2	B	37	ILE
2	B	42	GLU
2	B	60	VAL
2	B	91	GLN
2	B	92	LEU
2	B	100	LEU
2	B	108	VAL
2	B	109	LEU
2	B	148	VAL
2	B	233	GLU
2	B	244	ILE
2	B	281	LYS
2	B	295	LEU
2	B	298	GLU
2	B	302	GLU
2	B	308	GLU
2	B	315	HIS
2	B	330	GLN
2	B	348	ASN
2	B	353	LYS
2	B	356	ARG
2	B	407	GLN
2	B	419	THR
2	B	422	LEU

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Mol	Chain	Res	Type
2	B	428	GLN
3	C	39	LYS
3	C	89	GLN
3	C	90	GLN
3	C	123	GLU
3	C	141	PRO
4	D	11	ILE
4	D	29	LEU
4	D	75	THR
4	D	86	THR
4	D	107	ASP
4	D	141	GLN
4	D	142	THR
4	D	187	LEU
4	D	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	85	GLN
1	A	161	GLN
1	A	221	HIS
1	A	235	HIS
1	A	242	GLN
1	A	269	GLN
1	A	330	GLN
1	A	336	GLN
1	A	343	GLN
1	A	373	GLN
1	A	428	GLN
1	A	471	ASN
1	A	494	ASN
1	A	500	GLN
1	A	519	ASN
1	A	539	HIS
1	A	545	ASN
2	B	96	HIS
2	B	137	ASN
2	B	151	GLN
2	B	222	GLN
2	B	235	HIS

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Mol	Chain	Res	Type
2	B	242	GLN
2	B	255	ASN
2	B	258	GLN
2	B	330	GLN
2	B	340	GLN
2	B	348	ASN
2	B	373	GLN
2	B	394	GLN
2	B	418	ASN
3	C	27	GLN
3	C	89	GLN
3	C	90	GLN
3	C	138	ASN
3	C	156	GLN
3	C	157	ASN
3	C	161	ASN
3	C	190	ASN
3	C	198	HIS
3	C	210	ASN
4	D	59	ASN
4	D	79	GLN
4	D	115	GLN
4	D	141	GLN
4	D	181	GLN
4	D	206	ASN
4	D	209	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MRG	F	817	6,5,1	25,28,29	1.26	1 (4%)	32,39,42	2.43	4 (12%)
6	ATM	F	822	6,5	20,23,24	1.10	2 (10%)	26,32,35	0.71	1 (3%)

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
6	MRG	F	817	6,5,1	-	1/12/26/27	0/3/3/3
6	ATM	F	822	6,5	-	3/10/24/25	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	817	MRG	C21-N2	-5.48	1.33	1.46
6	F	822	ATM	N5'-N4'	3.39	1.30	1.23
6	F	822	ATM	N4'-N3'	-2.98	1.16	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	817	MRG	C21-N2-C2	-12.86	99.20	123.36
6	F	817	MRG	C22-C23-S24	2.94	122.09	113.10
6	F	817	MRG	C22-C21-N2	2.15	118.22	112.20
6	F	817	MRG	C2'-C1'-N9	-2.07	108.63	113.81
6	F	822	ATM	C2'-C3'-N3'	2.01	114.07	108.72

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	822	ATM	C3'-N3'-N4'-N5'
6	F	822	ATM	C4'-C3'-N3'-N4'
6	F	817	MRG	N2-C21-C22-C23
6	F	822	ATM	C2'-C3'-N3'-N4'

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	817	MRG	5	0
6	F	822	ATM	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	558/564 (98%)	0.67	58 (10%)	11 10	43, 79, 112, 125	0
2	B	428/437 (97%)	0.43	33 (7%)	19 16	36, 62, 108, 122	0
3	C	211/211 (100%)	0.42	1 (0%)	87 83	52, 69, 102, 109	0
4	D	225/225 (100%)	0.23	7 (3%)	51 42	42, 64, 96, 115	0
5	E	24/27 (88%)	0.72	4 (16%)	4 3	57, 109, 140, 157	0
6	F	19/21 (90%)	0.35	0	100 100	71, 93, 130, 137	0
All	All	1465/1485 (98%)	0.49	103 (7%)	22 18	36, 70, 110, 157	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	TYR	5.7
1	A	456	GLY	5.1
1	A	557	ARG	5.1
2	B	1	PRO	4.8
1	A	466	VAL	4.5
1	A	289	LEU	4.1
2	B	422	LEU	4.1
2	B	2	ILE	4.0
4	D	139	ALA	3.7
4	D	137	GLY	3.6
1	A	458	VAL	3.6
2	B	427	TYR	3.6
2	B	314	VAL	3.5
2	B	315	HIS	3.5
2	B	359	GLY	3.4
4	D	141	GLN	3.4
2	B	354	TYR	3.3
1	A	555	GLY	3.3
2	B	360	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	554	ALA	3.2
1	A	556	ILE	3.2
2	B	425	LEU	3.2
1	A	464	GLN	3.2
2	B	334	GLN	3.1
1	A	558	LYS	3.1
1	A	2	ILE	3.0
2	B	3	SER	3.0
1	A	336	GLN	3.0
2	B	423	VAL	3.0
1	A	455	ALA	3.0
2	B	303	LEU	2.9
1	A	223	LYS	2.9
2	B	88	TRP	2.9
1	A	548	VAL	2.9
1	A	283	LEU	2.9
2	B	357	MET	2.8
2	B	362	THR	2.8
1	A	1	PRO	2.8
1	A	454	LYS	2.8
1	A	247	PRO	2.8
1	A	491	LEU	2.8
2	B	355	ALA	2.7
5	E	703	DG	2.7
1	A	288	ALA	2.6
1	A	551	LEU	2.6
1	A	409	THR	2.6
4	D	223	ALA	2.6
2	B	252	TRP	2.5
1	A	64	LYS	2.5
2	B	312	GLU	2.5
2	B	418	ASN	2.5
1	A	452	LEU	2.5
4	D	140	ALA	2.5
1	A	293	ILE	2.4
1	A	134	SER	2.4
1	A	402	TRP	2.4
1	A	426	TRP	2.4
4	D	138	SER	2.4
4	D	145	MET	2.4
1	A	221	HIS	2.4
1	A	225	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	428	GLN	2.3
1	A	468	PRO	2.3
1	A	292	VAL	2.3
2	B	295	LEU	2.3
1	A	439	THR	2.3
2	B	247	PRO	2.3
1	A	295	LEU	2.3
2	B	426	TRP	2.3
1	A	254	VAL	2.3
1	A	137	ASN	2.2
1	A	246	LEU	2.2
1	A	514	GLU	2.2
1	A	465	LYS	2.2
5	E	726	DT	2.2
1	A	249	LYS	2.2
2	B	311	LYS	2.2
1	A	448	ARG	2.2
1	A	69	THR	2.2
1	A	457	TYR	2.2
1	A	141	GLY	2.2
1	A	65	LYS	2.1
1	A	290	THR	2.1
2	B	424	LYS	2.1
3	C	183	LYS	2.1
2	B	249	LYS	2.1
5	E	705	DT	2.1
1	A	66	LYS	2.1
1	A	442	VAL	2.1
1	A	226	PRO	2.1
2	B	279	LEU	2.1
1	A	71	TRP	2.1
1	A	358	ARG	2.1
2	B	358	ARG	2.1
1	A	67	ASN	2.1
2	B	250	ASP	2.1
1	A	245	VAL	2.0
1	A	272	PRO	2.0
5	E	724	DT	2.0
1	A	544	GLY	2.0
2	B	84	THR	2.0
1	A	410	TRP	2.0
2	B	318	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
6	MRG	F	817	26/27	0.89	0.16	84,95,114,122	0
6	ATM	F	822	22/23	0.91	0.13	84,92,96,100	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
7	MG	A	1001	1/1	0.97	0.11	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.