



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:34 PM GMT

PDB ID : 1XPU
Title : Structural mechanism of inhibition of the Rho transcription termination factor by the antibiotic 5a-(3-formylphenylsulfanyl)-dihydrobicyclomycin (FPDB)
Authors : Skordalakes, E.; Brogan, A.P.; Park, B.S.; Kohn, H.; Berger, J.M.
Deposited on : 2004-10-09
Resolution : 3.05 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

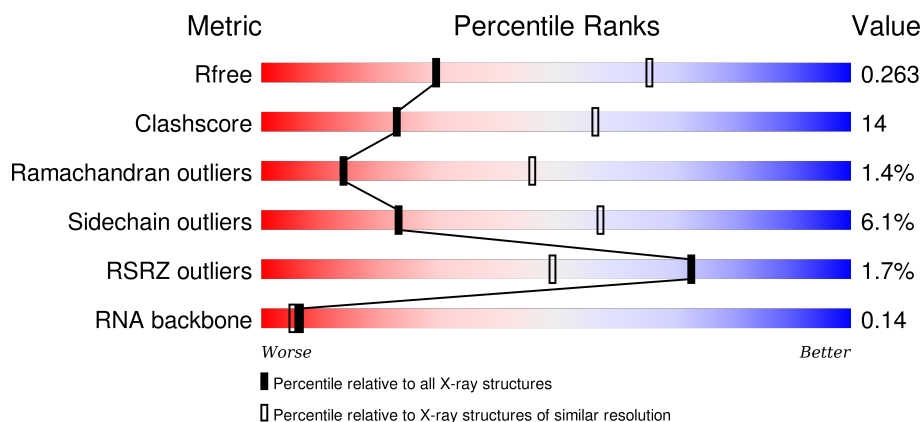
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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}	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)
RNA backbone	2183	1035 (3.50-2.62)

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. 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	G	8	
1	H	8	
1	J	8	
1	K	8	

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Mol	Chain	Length	Quality of chain
1	L	8	
1	M	8	
2	A	419	
2	B	419	
2	C	419	
2	D	419	
2	E	419	
2	F	419	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	D	4601	-	-	-	X
3	MG	E	5601	-	-	-	X
4	AGS	E	5600	-	-	X	-
5	FPD	B	2701	-	-	-	X
5	FPD	C	3701	-	-	X	X
5	FPD	D	4701	-	-	-	X
5	FPD	E	5701	-	-	X	X
5	FPD	F	6701	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19873 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 RNA chain called 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	M	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	H	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	J	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	K	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	L	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			

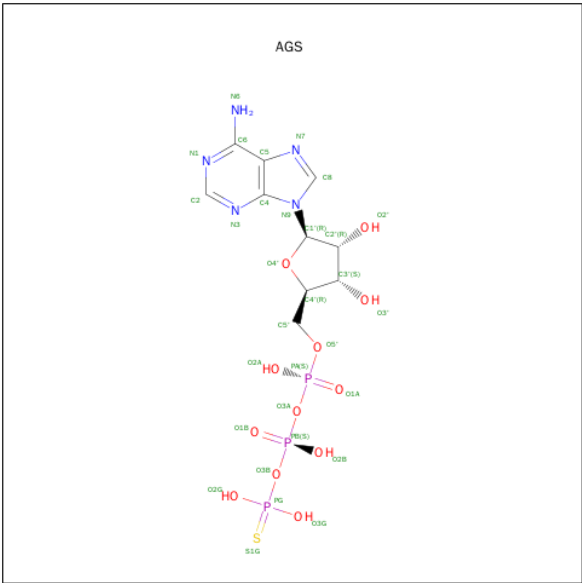
- Molecule 2 is a protein called Rho transcription termination factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			
2	B	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			
2	C	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			
2	D	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			
2	E	407	Total	C	N	O	S	0	0	0
			3206	2023	563	603	17			
2	F	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



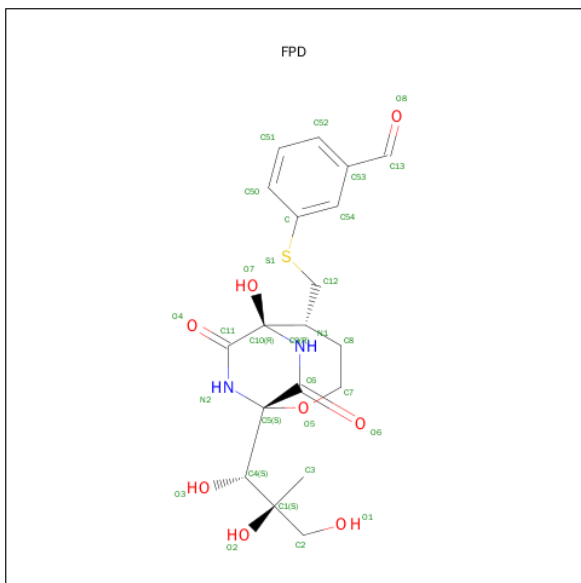
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 31 10 5 12 3 1	0	0
4	B	1	Total C N O P S 31 10 5 12 3 1	0	0
4	C	1	Total C N O P S 31 10 5 12 3 1	0	0
4	D	1	Total C N O P S 31 10 5 12 3 1	0	0
4	E	1	Total C N O P S 31 10 5 12 3 1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 5 is 5A-(3-FORMYLPHENYLSULFANYL)-DIHYDROBICYCLOMYCIN (three-letter code: FPD) (formula: C₁₉H₂₄N₂O₈S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 30	C 19	N 2	O 8	S 1	0	0
5	C	1	Total 30	C 19	N 2	O 8	S 1	0	0
5	D	1	Total 30	C 19	N 2	O 8	S 1	0	0
5	E	1	Total 30	C 19	N 2	O 8	S 1	0	0
5	F	1	Total 30	C 19	N 2	O 8	S 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total O 2 2	0	0
6	B	5	Total O 5 5	0	0
6	C	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	4	Total 4	O 4	0	0
6	E	3	Total 3	O 3	0	0
6	F	1	Total 1	O 1	0	0
6	G	1	Total 1	O 1	0	0
6	H	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'



- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'



- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'



- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

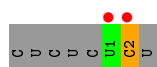


- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

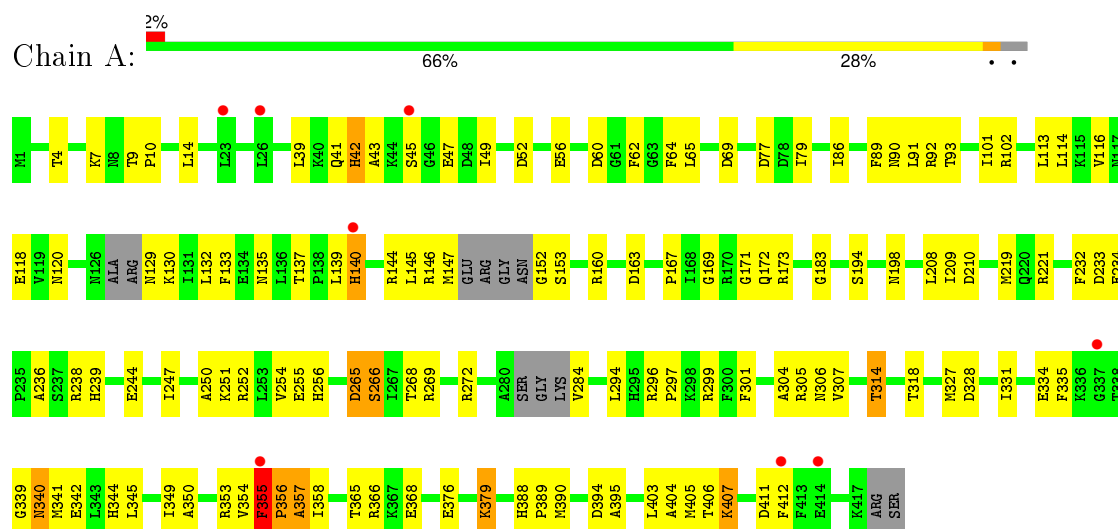


- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

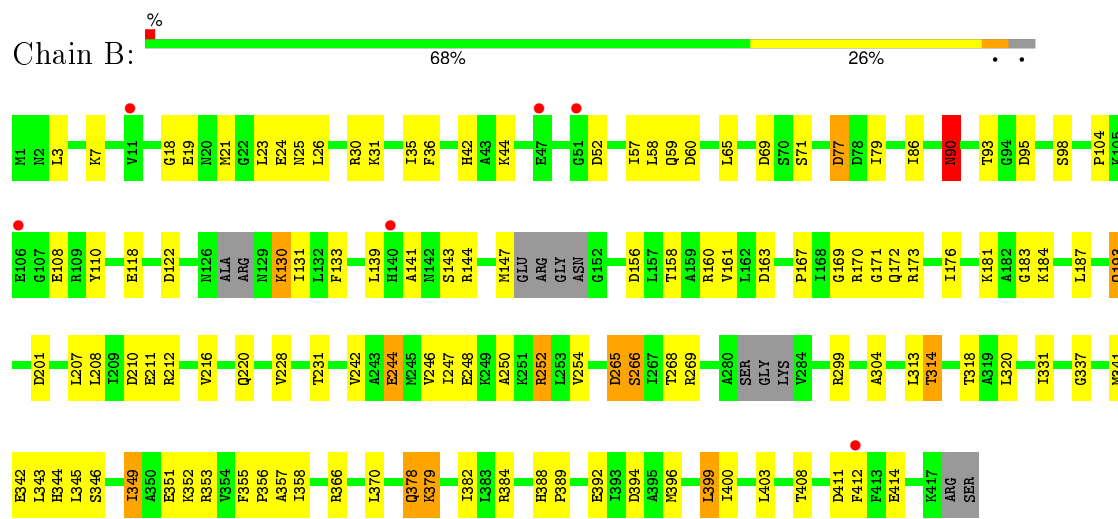




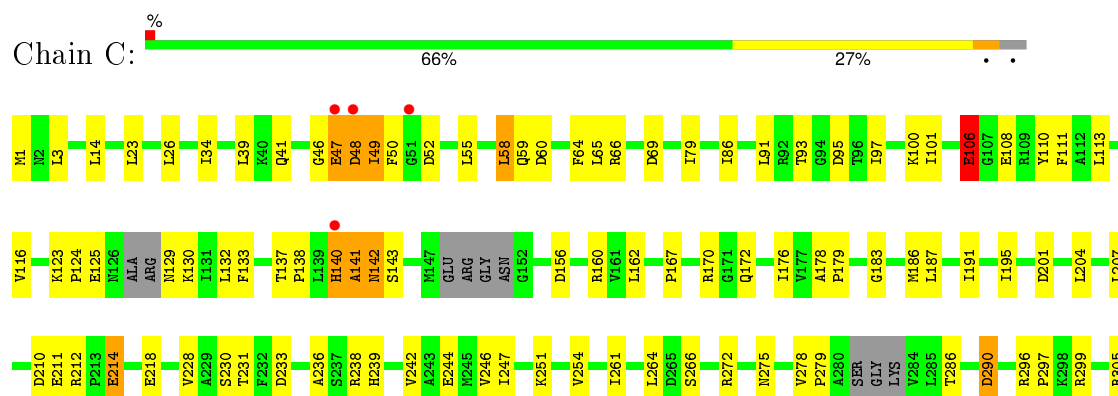
• Molecule 2: Rho transcription termination factor



• Molecule 2: Rho transcription termination factor

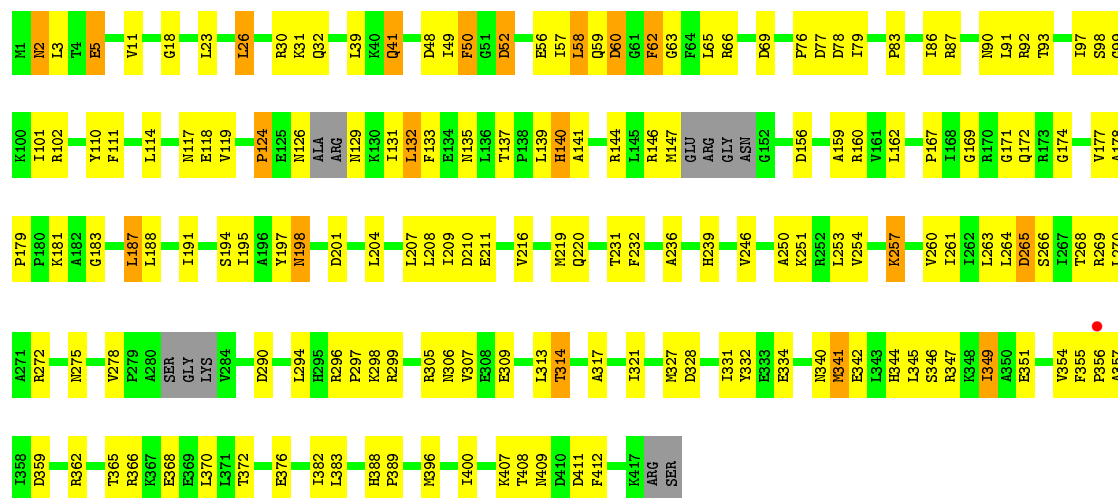


• Molecule 2: Rho transcription termination factor

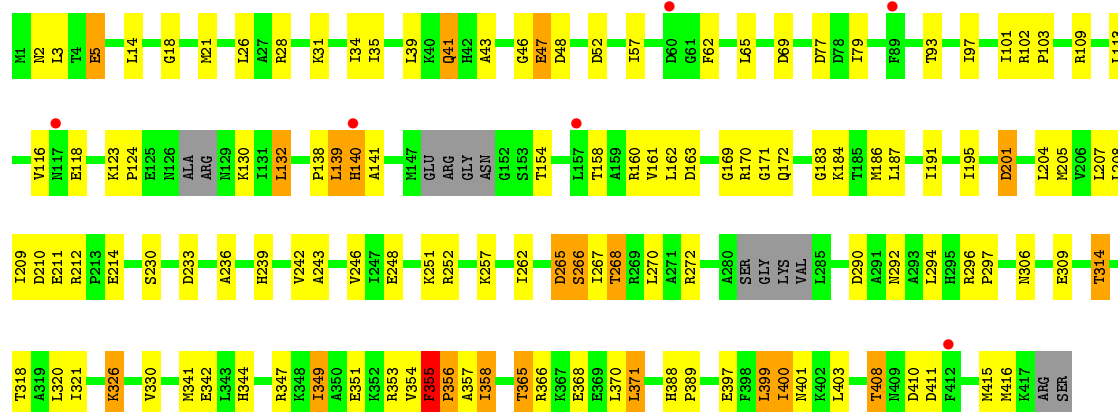




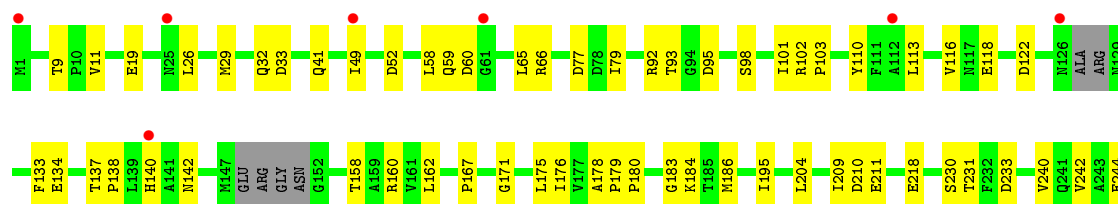
• Molecule 2: Rho transcription termination factor

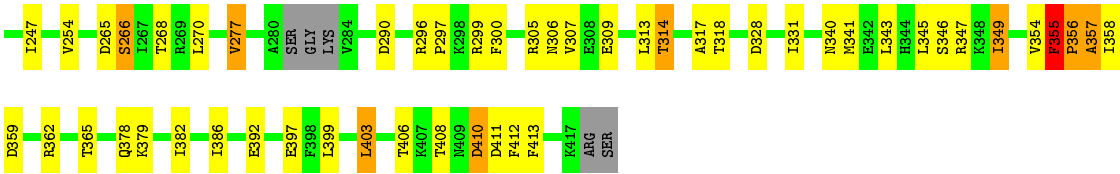


• Molecule 2: Rho transcription termination factor



• Molecule 2: Rho transcription termination factor





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.48Å 206.94Å 148.61Å 90.00° 96.95° 90.00°	Depositor
Resolution (Å)	20.00 – 3.05 45.05 – 2.74	Depositor EDS
% Data completeness (in resolution range)	86.5 (20.00-3.05) 65.0 (45.05-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.276 , 0.295 0.267 , 0.263	Depositor DCC
R_{free} test set	2945 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	92.4	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 60868 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19873	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: FPD, MG, AGS

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	G	0.72	0/43	1.27	1/64 (1.6%)
1	H	0.88	0/43	1.42	1/64 (1.6%)
1	J	0.70	0/43	1.22	0/64
1	K	0.90	0/43	1.60	2/64 (3.1%)
1	L	0.67	0/43	1.08	0/64
1	M	0.81	0/43	1.21	0/64
2	A	0.30	0/3259	0.65	7/4387 (0.2%)
2	B	0.30	0/3259	0.67	12/4387 (0.3%)
2	C	0.30	0/3259	0.65	9/4387 (0.2%)
2	D	0.30	0/3259	0.65	9/4387 (0.2%)
2	E	0.30	0/3252	0.67	11/4377 (0.3%)
2	F	0.30	0/3259	0.64	11/4387 (0.3%)
All	All	0.31	0/19805	0.67	63/26696 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1
2	E	0	1
2	F	0	1
All	All	0	3

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1	U	P-O3'-C3'	6.60	127.61	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	77	ASP	CB-CG-OD2	6.21	123.89	118.30
2	D	77	ASP	CB-CG-OD2	6.21	123.89	118.30
2	F	233	ASP	CB-CG-OD2	6.08	123.77	118.30
2	F	290	ASP	CB-CG-OD2	6.04	123.73	118.30
2	B	156	ASP	CB-CG-OD2	6.03	123.72	118.30
2	E	77	ASP	CB-CG-OD2	6.02	123.72	118.30
2	F	77	ASP	CB-CG-OD2	5.99	123.69	118.30
2	E	233	ASP	CB-CG-OD2	5.99	123.69	118.30
2	E	210	ASP	CB-CG-OD2	5.96	123.66	118.30
1	G	1	U	P-O3'-C3'	5.79	126.65	119.70
2	E	163	ASP	CB-CG-OD2	5.77	123.49	118.30
2	B	77	ASP	CB-CG-OD2	5.75	123.47	118.30
2	C	52	ASP	CB-CG-OD2	5.75	123.47	118.30
1	K	1	U	P-O3'-C3'	5.73	126.57	119.70
2	D	156	ASP	CB-CG-OD2	5.70	123.43	118.30
2	B	163	ASP	CB-CG-OD2	5.63	123.37	118.30
2	C	290	ASP	CB-CG-OD2	5.61	123.34	118.30
2	B	265	ASP	CB-CG-OD2	5.37	123.13	118.30
2	A	233	ASP	CB-CG-OD2	5.37	123.13	118.30
2	B	122	ASP	CB-CG-OD2	5.37	123.13	118.30
2	B	394	ASP	CB-CG-OD2	5.34	123.11	118.30
1	K	1	U	C3'-C2'-C1'	5.34	105.77	101.50
2	E	355	PHE	CB-CA-C	5.31	121.02	110.40
2	E	411	ASP	CB-CG-OD2	5.29	123.06	118.30
2	E	201	ASP	CB-CG-OD2	5.25	123.02	118.30
2	C	201	ASP	CB-CG-OD2	5.24	123.01	118.30
2	E	265	ASP	CB-CG-OD2	5.24	123.01	118.30
2	F	265	ASP	CB-CG-OD2	5.22	123.00	118.30
2	B	201	ASP	CB-CG-OD2	5.21	122.98	118.30
2	F	328	ASP	CB-CG-OD2	5.18	122.96	118.30
2	D	60	ASP	CB-CG-OD2	5.17	122.95	118.30
2	A	52	ASP	CB-CG-OD2	5.17	122.95	118.30
2	B	52	ASP	CB-CG-OD2	5.15	122.94	118.30
2	D	201	ASP	CB-CG-OD2	5.15	122.94	118.30
2	A	394	ASP	CB-CG-OD2	5.14	122.93	118.30
2	A	265	ASP	CB-CG-OD2	5.14	122.92	118.30
2	C	95	ASP	CB-CG-OD2	5.13	122.92	118.30
2	D	78	ASP	CB-CG-OD2	5.13	122.92	118.30
2	C	411	ASP	CB-CG-OD2	5.11	122.90	118.30
2	A	328	ASP	CB-CG-OD2	5.11	122.90	118.30
2	B	69	ASP	CB-CG-OD2	5.11	122.90	118.30
2	E	290	ASP	CB-CG-OD2	5.10	122.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	33	ASP	CB-CG-OD2	5.09	122.89	118.30
2	F	52	ASP	CB-CG-OD2	5.09	122.88	118.30
2	D	328	ASP	CB-CG-OD2	5.08	122.87	118.30
2	B	95	ASP	CB-CG-OD2	5.08	122.87	118.30
2	F	411	ASP	CB-CG-OD2	5.08	122.87	118.30
2	B	60	ASP	CB-CG-OD2	5.07	122.86	118.30
2	C	60	ASP	CB-CG-OD2	5.06	122.85	118.30
2	D	265	ASP	CB-CG-OD2	5.05	122.85	118.30
2	C	48	ASP	CB-CG-OD2	5.05	122.85	118.30
2	E	52	ASP	CB-CG-OD2	5.05	122.85	118.30
2	F	122	ASP	CB-CG-OD2	5.05	122.84	118.30
2	D	411	ASP	CB-CG-OD2	5.05	122.84	118.30
2	D	52	ASP	CB-CG-OD2	5.04	122.84	118.30
2	B	411	ASP	CB-CG-OD2	5.02	122.82	118.30
2	F	60	ASP	CB-CG-OD2	5.02	122.81	118.30
2	C	156	ASP	CB-CG-OD2	5.01	122.81	118.30
2	C	233	ASP	CB-CG-OD2	5.01	122.81	118.30
2	E	410	ASP	CB-CG-OD2	5.01	122.81	118.30
2	F	95	ASP	CB-CG-OD2	5.01	122.81	118.30
2	A	69	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	355	PHE	Peptide
2	E	355	PHE	Peptide
2	F	355	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	40	0	22	0	0
1	H	40	0	22	2	0
1	J	40	0	22	3	0
1	K	40	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	40	0	22	2	0
1	M	40	0	22	0	0
2	A	3213	0	3289	106	0
2	B	3213	0	3288	76	0
2	C	3213	0	3289	81	0
2	D	3213	0	3289	118	0
2	E	3206	0	3279	87	0
2	F	3213	0	3288	62	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	31	0	12	4	0
4	B	31	0	12	6	0
4	C	31	0	12	7	0
4	D	31	0	12	5	0
4	E	62	0	24	16	0
5	B	30	0	24	6	0
5	C	30	0	24	9	0
5	D	30	0	24	8	0
5	E	30	0	24	11	0
5	F	30	0	24	3	0
6	A	2	0	0	0	0
6	B	5	0	0	1	0
6	C	3	0	0	0	0
6	D	4	0	0	1	0
6	E	3	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
All	All	19873	0	20046	539	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (539) 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:C:366:ARG:NE	4:D:4600:AGS:S1G	2.12	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:366:ARG:NE	4:B:2600:AGS:S1G	2.13	1.20
2:D:356:PRO:HG3	2:D:400:ILE:HD11	1.26	1.15
2:B:366:ARG:NE	4:C:3600:AGS:S1G	2.23	1.11
2:D:366:ARG:NE	4:E:5600:AGS:S1G	2.24	1.11
2:A:183:GLY:HA2	4:A:1600:AGS:H8	1.35	1.08
2:A:140:HIS:CE1	2:A:172:GLN:HG2	1.94	1.02
1:J:2:C:H42	2:D:66:ARG:HH12	1.22	0.86
2:D:349:ILE:HG22	2:D:354:VAL:HB	1.58	0.85
2:D:98:SER:HB3	2:D:118:GLU:HB2	1.58	0.84
2:E:208:LEU:HB3	2:E:211:GLU:HG3	1.56	0.84
2:A:272:ARG:HG3	2:A:272:ARG:HH11	1.44	0.81
2:E:140:HIS:HA	2:E:306:ASN:HB2	1.63	0.80
2:D:140:HIS:HA	2:D:306:ASN:HD22	1.47	0.80
2:B:171:GLY:H	2:B:314:THR:HG22	1.46	0.80
2:A:140:HIS:HA	2:A:306:ASN:HB2	1.62	0.79
2:C:133:PHE:HB3	2:D:30:ARG:HH22	1.47	0.79
2:A:355:PHE:HB3	2:A:356:PRO:CD	2.11	0.79
2:E:169:GLY:H	2:E:172:GLN:HG3	1.48	0.78
2:A:183:GLY:HA2	4:A:1600:AGS:C8	2.13	0.78
2:D:356:PRO:HG3	2:D:400:ILE:CD1	2.10	0.78
2:C:341:MET:HG2	2:C:365:THR:HG22	1.65	0.77
1:K:1:U:H4'	1:K:2:C:OP2	1.84	0.77
4:E:6600:AGS:H8	2:F:183:GLY:HA2	1.67	0.77
2:D:83:PRO:O	2:D:87:ARG:HG3	1.86	0.76
2:B:183:GLY:HA2	4:B:2600:AGS:H8	1.68	0.76
2:A:366:ARG:CZ	4:B:2600:AGS:S1G	2.73	0.76
2:A:173:ARG:NH2	2:B:212:ARG:HB3	2.01	0.76
1:L:2:C:H42	2:F:66:ARG:HH12	1.32	0.76
2:C:141:ALA:O	2:C:370:LEU:HB3	1.85	0.75
2:E:183:GLY:HA2	4:E:5600:AGS:H8	1.67	0.75
2:D:174:GLY:HA2	2:D:341:MET:HG3	1.68	0.74
2:A:366:ARG:NH2	4:B:2600:AGS:S1G	2.60	0.73
2:C:46:GLY:O	2:C:47:GLU:HB2	1.87	0.73
2:E:132:LEU:HD22	2:E:251:LYS:HG2	1.70	0.73
2:B:104:PRO:HB3	2:B:108:GLU:O	1.87	0.73
2:C:183:GLY:HA2	4:C:3600:AGS:H8	1.69	0.73
2:D:65:LEU:HD21	2:D:97:ILE:HB	1.71	0.73
2:D:408:THR:HG23	2:D:409:ASN:H	1.55	0.72
2:D:257:LYS:HD2	2:D:309:GLU:O	1.89	0.72
2:A:183:GLY:CA	4:A:1600:AGS:H8	2.16	0.72
2:F:171:GLY:H	2:F:314:THR:HG22	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:355:PHE:CZ	4:E:5600:AGS:H1'	2.24	0.72
2:D:65:LEU:HB2	2:D:79:ILE:HB	1.72	0.71
2:B:57:ILE:H	2:B:93:THR:HG22	1.55	0.71
2:D:32:GLN:HB3	2:D:76:PRO:HD2	1.72	0.71
2:F:341:MET:HG2	2:F:365:THR:HG22	1.70	0.71
2:D:169:GLY:H	2:D:172:GLN:HG3	1.56	0.71
2:A:173:ARG:H	2:A:340:ASN:HD21	1.39	0.71
2:D:92:ARG:HH12	2:D:131:ILE:HG23	1.56	0.71
2:B:169:GLY:H	2:B:172:GLN:HG3	1.54	0.71
2:D:388:HIS:HB3	2:D:389:PRO:HD3	1.72	0.70
2:B:355:PHE:CZ	4:B:2600:AGS:H1'	2.27	0.70
2:D:132:LEU:HD22	2:D:251:LYS:HG2	1.74	0.69
2:B:379:LYS:HD3	2:B:412:PHE:HB2	1.72	0.69
2:E:347:ARG:O	2:E:351:GLU:HG2	1.92	0.69
2:E:65:LEU:HD21	2:E:97:ILE:HD12	1.74	0.69
2:D:372:THR:HB	2:D:376:GLU:HB3	1.74	0.69
2:E:21:MET:HB3	2:E:41:GLN:HE22	1.56	0.69
2:E:140:HIS:HA	2:E:306:ASN:CB	2.22	0.69
2:C:275:ASN:HD21	2:C:290:ASP:H	1.41	0.69
2:C:369:GLU:HG2	2:C:370:LEU:HD12	1.73	0.69
2:A:350:ALA:HB2	2:A:357:ALA:HB2	1.72	0.69
2:A:265:ASP:O	2:A:318:THR:HB	1.92	0.69
2:A:169:GLY:H	2:A:172:GLN:HG3	1.58	0.68
2:C:140:HIS:HA	2:C:306:ASN:HB2	1.76	0.68
2:D:236:ALA:HA	2:D:239:HIS:CD2	2.28	0.67
2:E:138:PRO:HD2	2:E:306:ASN:O	1.93	0.67
2:C:141:ALA:HB1	2:C:370:LEU:HB2	1.76	0.67
2:D:62:PHE:H	2:D:62:PHE:HD2	1.41	0.67
2:C:138:PRO:HD2	2:C:306:ASN:O	1.95	0.67
2:E:320:LEU:HD11	5:E:5701:FPD:H4	1.77	0.67
2:D:102:ARG:HD3	2:D:114:LEU:HD13	1.76	0.66
2:D:160:ARG:HH11	2:D:408:THR:HB	1.59	0.66
2:D:140:HIS:CE1	2:D:172:GLN:HG2	2.31	0.66
2:D:268:THR:HA	2:D:331:ILE:HG21	1.78	0.66
2:D:3:LEU:HD13	2:D:39:LEU:HD11	1.77	0.66
2:C:3:LEU:HD13	2:C:39:LEU:HD11	1.76	0.66
2:A:140:HIS:HA	2:A:306:ASN:CB	2.25	0.66
2:F:140:HIS:CE1	2:F:305:ARG:HB2	2.31	0.66
2:D:346:SER:HB3	2:D:349:ILE:HG12	1.78	0.66
2:B:216:VAL:HG12	2:B:220:GLN:HE21	1.60	0.65
2:C:320:LEU:HD21	5:C:3701:FPD:H4	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:388:HIS:HB3	2:A:389:PRO:HD3	1.78	0.65
2:E:140:HIS:CA	2:E:306:ASN:HB2	2.26	0.65
2:E:3:LEU:HD13	2:E:39:LEU:HD11	1.78	0.65
2:A:355:PHE:HB3	2:A:356:PRO:HD2	1.79	0.65
2:A:173:ARG:HD2	2:A:301:PHE:O	1.98	0.64
2:E:349:ILE:HG13	2:E:357:ALA:O	1.96	0.64
2:D:140:HIS:HB2	2:D:306:ASN:HB2	1.78	0.64
2:E:341:MET:HG3	2:E:365:THR:HB	1.78	0.64
2:F:406:THR:HB	2:F:410:ASP:HB2	1.78	0.64
2:D:236:ALA:HA	2:D:239:HIS:HD2	1.62	0.64
2:B:346:SER:HB3	2:B:349:ILE:HG12	1.79	0.64
2:A:297:PRO:HB2	2:A:335:PHE:HZ	1.61	0.63
2:B:171:GLY:H	2:B:314:THR:CG2	2.11	0.63
2:F:345:LEU:HA	2:F:357:ALA:O	1.97	0.63
2:F:79:ILE:HG12	2:F:101:ILE:HG21	1.80	0.63
2:D:57:ILE:H	2:D:93:THR:HB	1.62	0.63
2:C:130:LYS:HE3	2:D:11:VAL:HB	1.79	0.63
2:B:141:ALA:HB1	2:B:370:LEU:HB2	1.80	0.62
2:A:41:GLN:C	2:A:43:ALA:H	2.01	0.62
2:A:379:LYS:HD3	2:A:412:PHE:HB2	1.80	0.62
2:B:193:GLN:HE21	2:B:193:GLN:HA	1.64	0.62
2:D:261:ILE:HG12	2:D:314:THR:HG23	1.81	0.62
2:F:379:LYS:HD3	2:F:412:PHE:HB3	1.80	0.62
2:A:355:PHE:CB	2:A:356:PRO:HD2	2.30	0.62
2:E:140:HIS:CB	2:E:306:ASN:HB2	2.30	0.61
2:D:131:ILE:HG22	2:D:133:PHE:H	1.65	0.61
2:B:254:VAL:HG21	2:B:313:LEU:HB2	1.81	0.61
2:A:268:THR:O	2:A:272:ARG:HG2	2.00	0.61
2:F:354:VAL:HG11	2:F:397:GLU:HG3	1.82	0.61
2:D:183:GLY:HA2	4:D:4600:AGS:H8	1.82	0.61
2:A:120:ASN:HB2	2:A:256:HIS:CE1	2.35	0.61
2:A:140:HIS:NE2	2:A:172:GLN:HG2	2.16	0.61
2:A:147:MET:HB3	2:A:194:SER:HB3	1.83	0.61
2:E:18:GLY:HA3	2:E:26:LEU:HD11	1.83	0.61
2:C:141:ALA:HB1	2:C:370:LEU:CB	2.31	0.60
2:D:169:GLY:H	2:D:172:GLN:CG	2.14	0.60
2:D:90:ASN:HD22	2:E:28:ARG:HB2	1.66	0.60
2:D:382:ILE:HB	2:D:412:PHE:HZ	1.65	0.60
2:A:355:PHE:CB	2:A:356:PRO:CD	2.79	0.60
2:F:113:LEU:HD21	2:F:116:VAL:HG22	1.84	0.60
2:F:378:GLN:O	2:F:382:ILE:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:39:LEU:HD22	2:A:49:ILE:HG23	1.84	0.59
2:D:327:MET:O	2:D:331:ILE:HG12	2.02	0.59
2:B:98:SER:HB2	2:B:118:GLU:HB2	1.84	0.59
2:C:65:LEU:HB2	2:C:79:ILE:HB	1.84	0.59
2:B:141:ALA:CB	2:B:370:LEU:HB2	2.32	0.59
2:E:388:HIS:HB3	2:E:389:PRO:HD3	1.84	0.59
2:E:158:THR:HA	2:E:356:PRO:HG3	1.85	0.59
2:A:266:SER:HB2	2:A:269:ARG:H	1.68	0.59
2:C:49:ILE:HD13	2:C:101:ILE:O	2.03	0.58
2:A:42:HIS:HD2	2:A:47:GLU:HB3	1.68	0.58
2:A:152:GLY:HA3	2:A:407:LYS:HE2	1.83	0.58
2:D:183:GLY:CA	4:D:4600:AGS:H8	2.33	0.58
1:J:2:C:N4	2:D:66:ARG:HH12	1.99	0.58
2:D:57:ILE:HA	2:D:63:GLY:HA2	1.84	0.58
2:A:139:LEU:O	2:A:140:HIS:CG	2.56	0.58
2:B:337:GLY:HA3	5:C:3701:FPD:H71	1.86	0.58
2:C:244:GLU:HA	2:C:247:ILE:HG22	1.84	0.58
2:A:42:HIS:CD2	2:A:47:GLU:HB3	2.39	0.58
4:E:6600:AGS:H1'	2:F:355:PHE:CZ	2.38	0.58
2:D:141:ALA:CB	2:D:370:LEU:HB2	2.34	0.58
2:B:160:ARG:NH2	2:B:403:LEU:HD22	2.19	0.57
2:B:356:PRO:HD2	2:B:400:ILE:HD11	1.85	0.57
2:A:140:HIS:CE1	2:A:172:GLN:HE21	2.21	0.57
2:A:349:ILE:O	2:A:354:VAL:HB	2.04	0.57
2:C:349:ILE:HD11	2:C:392:GLU:HB3	1.87	0.57
5:F:6701:FPD:H71	5:F:6701:FPD:C11	2.32	0.57
2:E:349:ILE:O	2:E:354:VAL:HB	2.05	0.57
2:B:355:PHE:CZ	4:B:2600:AGS:C1'	2.88	0.56
2:D:366:ARG:NH2	5:E:5701:FPD:H81	2.19	0.56
5:C:3701:FPD:H71	5:C:3701:FPD:C11	2.34	0.56
2:D:147:MET:C	2:D:159:ALA:HB1	2.25	0.56
2:E:208:LEU:HB3	2:E:211:GLU:CG	2.30	0.56
2:B:173:ARG:HG3	2:B:304:ALA:HB3	1.87	0.56
2:E:130:LYS:HE3	2:F:11:VAL:HB	1.87	0.56
2:E:57:ILE:H	2:E:93:THR:HG22	1.71	0.56
2:D:266:SER:HB3	2:D:269:ARG:HB2	1.87	0.56
2:B:346:SER:HB3	2:B:349:ILE:CG1	2.36	0.56
2:A:101:ILE:HG22	2:A:113:LEU:HA	1.86	0.56
2:A:365:THR:HG23	2:A:368:GLU:HG2	1.88	0.56
2:B:158:THR:HG23	6:B:2705:HOH:O	2.05	0.56
2:C:236:ALA:HA	2:C:239:HIS:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:207:LEU:HD11	2:E:242:VAL:HG12	1.88	0.56
2:D:345:LEU:HD22	2:D:357:ALA:O	2.06	0.56
2:D:275:ASN:HD21	2:D:290:ASP:H	1.54	0.56
2:C:379:LYS:HG3	2:C:412:PHE:CD1	2.40	0.56
2:B:131:ILE:HD12	2:B:133:PHE:HD2	1.71	0.56
2:B:176:ILE:HB	2:B:318:THR:HG22	1.88	0.55
5:D:4701:FPD:C11	5:D:4701:FPD:H71	2.36	0.55
5:B:2701:FPD:C11	5:B:2701:FPD:H71	2.35	0.55
2:A:160:ARG:HH11	2:A:403:LEU:HB3	1.72	0.55
2:F:176:ILE:HB	2:F:318:THR:HG22	1.88	0.55
2:D:183:GLY:O	2:D:187:LEU:HB2	2.07	0.55
2:F:266:SER:HA	2:F:318:THR:O	2.06	0.55
2:E:266:SER:HA	2:E:318:THR:O	2.07	0.55
4:E:6600:AGS:H8	2:F:183:GLY:CA	2.37	0.55
2:E:141:ALA:CB	2:E:370:LEU:HB2	2.36	0.55
2:A:390:MET:HB3	2:A:395:ALA:HB2	1.89	0.54
2:B:207:LEU:HD13	2:B:246:VAL:HG21	1.89	0.54
2:C:296:ARG:HB2	2:C:297:PRO:HD3	1.89	0.54
2:D:356:PRO:CG	2:D:400:ILE:HD11	2.18	0.54
2:E:65:LEU:HB2	2:E:79:ILE:HB	1.90	0.54
2:E:183:GLY:CA	4:E:5600:AGS:H8	2.36	0.54
2:E:160:ARG:HG2	2:E:408:THR:HG23	1.88	0.54
2:C:106:GLU:C	2:C:108:GLU:H	2.10	0.54
2:B:266:SER:OG	2:B:269:ARG:HB2	2.08	0.54
2:A:135:ASN:HD22	2:A:307:VAL:HG11	1.71	0.54
2:C:414:GLU:HG3	2:C:415:MET:N	2.23	0.54
2:C:140:HIS:HA	2:C:306:ASN:CB	2.38	0.53
2:C:55:LEU:HA	2:C:64:PHE:O	2.08	0.53
2:E:186:MET:HG3	4:E:5600:AGS:O2A	2.08	0.53
2:F:138:PRO:HD2	2:F:306:ASN:O	2.08	0.53
2:E:349:ILE:HB	2:E:357:ALA:HA	1.88	0.53
2:A:140:HIS:CA	2:A:306:ASN:HB2	2.34	0.53
2:F:167:PRO:O	2:F:365:THR:HG21	2.09	0.53
2:F:296:ARG:HB2	2:F:297:PRO:HD3	1.91	0.53
2:A:92:ARG:HD3	2:A:252:ARG:CZ	2.39	0.52
2:C:349:ILE:HG21	2:C:357:ALA:HA	1.90	0.52
2:A:350:ALA:HB2	2:A:357:ALA:CB	2.38	0.52
2:C:357:ALA:O	2:C:358:ILE:C	2.46	0.52
2:B:207:LEU:HD11	2:B:242:VAL:HG12	1.92	0.52
2:C:186:MET:HB2	4:C:3600:AGS:N7	2.25	0.52
2:C:347:ARG:O	2:C:351:GLU:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:HIS:C	2:B:44:LYS:H	2.11	0.52
2:C:396:MET:HA	2:C:396:MET:HE3	1.92	0.52
2:C:176:ILE:HB	2:C:318:THR:HG22	1.91	0.52
5:E:5701:FPD:C6	5:E:5701:FPD:C8	2.88	0.52
2:A:268:THR:HA	2:A:331:ILE:HG21	1.92	0.52
2:F:399:LEU:O	2:F:403:LEU:HB2	2.10	0.52
5:E:5701:FPD:C11	5:E:5701:FPD:H71	2.38	0.52
2:F:341:MET:CG	2:F:365:THR:HG22	2.39	0.52
2:E:158:THR:OG1	2:E:356:PRO:HD3	2.10	0.52
2:F:356:PRO:C	2:F:358:ILE:H	2.13	0.52
5:C:3701:FPD:C11	5:C:3701:FPD:C7	2.87	0.51
2:C:187:LEU:O	2:C:191:ILE:HG12	2.10	0.51
2:D:2:ASN:HB2	2:D:50:PHE:HB2	1.91	0.51
2:C:366:ARG:CZ	4:D:4600:AGS:S1G	2.94	0.51
2:E:79:ILE:HG12	2:E:101:ILE:HG21	1.91	0.51
2:C:65:LEU:HD21	2:C:97:ILE:HD12	1.93	0.51
2:C:160:ARG:HB3	2:C:408:THR:HG23	1.92	0.51
2:E:205:MET:O	2:E:262:ILE:HA	2.11	0.51
2:C:160:ARG:HE	2:C:408:THR:HG23	1.75	0.51
2:E:118:GLU:HA	2:E:124:PRO:HG3	1.93	0.51
2:E:397:GLU:O	2:E:401:ASN:HB2	2.11	0.51
2:F:240:VAL:HG21	2:F:277:VAL:HG11	1.93	0.51
2:F:58:LEU:HG	2:F:59:GLN:H	1.75	0.51
5:D:4701:FPD:C11	5:D:4701:FPD:C7	2.89	0.51
5:D:4701:FPD:C6	5:D:4701:FPD:C8	2.89	0.51
2:D:366:ARG:CZ	4:E:5600:AGS:S1G	2.98	0.51
2:D:99:GLY:HA2	2:D:117:ASN:HB2	1.93	0.51
5:C:3701:FPD:C6	5:C:3701:FPD:C8	2.89	0.50
2:A:272:ARG:HG3	2:A:272:ARG:NH1	2.17	0.50
5:F:6701:FPD:C11	5:F:6701:FPD:C7	2.85	0.50
2:C:132:LEU:HD13	2:C:251:LYS:HG2	1.92	0.50
2:A:327:MET:O	2:A:331:ILE:HG12	2.12	0.50
2:D:23:LEU:HD21	2:D:41:GLN:HG3	1.93	0.50
2:F:101:ILE:HG22	2:F:113:LEU:HA	1.93	0.50
2:D:137:THR:HG23	2:D:305:ARG:HB2	1.93	0.50
2:D:177:VAL:HG13	2:D:321:ILE:HD12	1.93	0.50
2:C:137:THR:HG22	2:C:305:ARG:HD3	1.94	0.50
5:E:5701:FPD:C7	5:E:5701:FPD:C11	2.89	0.50
2:B:244:GLU:O	2:B:248:GLU:HG2	2.12	0.50
2:B:341:MET:HE2	2:B:343:LEU:HB2	1.93	0.50
2:A:144:ARG:NH2	2:A:163:ASP:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:209:ILE:HD13	2:F:270:LEU:HD13	1.94	0.50
4:E:6600:AGS:C1'	2:F:355:PHE:CZ	2.95	0.50
2:E:207:LEU:HD21	2:E:243:ALA:HA	1.94	0.50
2:C:23:LEU:HB3	2:C:26:LEU:HD11	1.92	0.50
2:F:26:LEU:HD22	2:F:29:MET:CE	2.42	0.50
2:A:140:HIS:CE1	2:A:172:GLN:CG	2.82	0.50
2:A:403:LEU:C	2:A:405:MET:H	2.15	0.50
2:A:342:GLU:HG3	2:A:344:HIS:HE1	1.76	0.50
2:B:23:LEU:HB3	2:B:26:LEU:HD23	1.94	0.50
2:B:378:GLN:HE21	2:B:378:GLN:HA	1.77	0.49
2:C:211:GLU:HG3	2:C:212:ARG:H	1.78	0.49
2:B:250:ALA:O	2:B:254:VAL:HG23	2.13	0.49
5:B:2701:FPD:C11	5:B:2701:FPD:C7	2.87	0.49
2:B:244:GLU:HA	2:B:247:ILE:HG22	1.94	0.49
2:C:113:LEU:HD21	2:C:116:VAL:HG22	1.94	0.49
2:B:36:PHE:HB2	2:B:77:ASP:HB3	1.95	0.49
2:A:266:SER:OG	2:A:269:ARG:HB2	2.13	0.49
2:E:207:LEU:HD13	2:E:246:VAL:HG21	1.94	0.49
2:F:158:THR:HA	2:F:356:PRO:HG3	1.93	0.49
2:B:366:ARG:HH21	5:C:3701:FPD:H81	1.77	0.49
2:E:113:LEU:HD21	2:E:116:VAL:HG22	1.94	0.49
2:E:184:LYS:HZ2	5:E:5701:FPD:H22	1.78	0.49
2:D:216:VAL:O	2:D:220:GLN:HB2	2.13	0.49
2:A:160:ARG:HD3	2:A:403:LEU:HD22	1.94	0.49
2:F:180:PRO:HD2	2:F:347:ARG:HH12	1.76	0.49
2:D:356:PRO:O	2:D:396:MET:HG3	2.13	0.48
2:D:48:ASP:O	2:D:49:ILE:HG13	2.12	0.48
2:D:211:GLU:O	2:D:231:THR:HA	2.12	0.48
5:E:5701:FPD:C6	5:E:5701:FPD:H82	2.43	0.48
2:C:195:ILE:HG21	2:C:204:LEU:HD13	1.95	0.48
2:E:171:GLY:H	2:E:314:THR:HB	1.78	0.48
2:B:7:LYS:HB3	2:B:35:ILE:HD13	1.94	0.48
2:A:62:PHE:HE1	2:A:64:PHE:HE2	1.59	0.48
2:A:208:LEU:HD23	2:A:265:ASP:HB2	1.94	0.48
2:C:167:PRO:HG2	2:C:368:GLU:HG2	1.95	0.48
2:B:169:GLY:H	2:B:172:GLN:CG	2.24	0.48
2:B:139:LEU:HD23	2:C:214:GLU:HG3	1.96	0.48
2:A:252:ARG:NH1	2:A:255:GLU:OE2	2.46	0.48
2:D:254:VAL:HG21	2:D:313:LEU:HB2	1.94	0.48
2:F:92:ARG:HH22	2:F:133:PHE:HE2	1.61	0.48
1:H:2:C:N3	2:C:66:ARG:NH2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:139:LEU:O	2:A:140:HIS:CD2	2.66	0.48
2:B:211:GLU:O	2:B:231:THR:HA	2.14	0.48
2:F:268:THR:HA	2:F:331:ILE:HG21	1.96	0.48
2:A:140:HIS:HD1	2:A:140:HIS:C	2.16	0.48
2:D:141:ALA:HB3	2:D:370:LEU:HB2	1.96	0.48
2:A:144:ARG:HG2	2:A:145:LEU:N	2.29	0.48
2:E:186:MET:HB2	4:E:5600:AGS:N7	2.28	0.47
2:A:234:GLU:HB3	2:A:238:ARG:HG2	1.96	0.47
2:D:346:SER:HB3	2:D:349:ILE:CG1	2.44	0.47
2:D:171:GLY:H	2:D:314:THR:HB	1.79	0.47
2:D:141:ALA:HB1	2:D:370:LEU:HB2	1.95	0.47
2:D:56:GLU:OE1	2:D:66:ARG:NE	2.47	0.47
2:D:101:ILE:HD12	2:D:111:PHE:HB3	1.95	0.47
2:F:98:SER:HB2	2:F:118:GLU:HB2	1.95	0.47
2:A:342:GLU:HG3	2:A:344:HIS:CE1	2.50	0.47
2:A:244:GLU:HA	2:A:247:ILE:HG22	1.95	0.47
2:E:326:LYS:O	2:E:330:VAL:HG23	2.13	0.47
2:E:355:PHE:CE1	4:E:5600:AGS:C4	2.97	0.47
2:A:183:GLY:CA	4:A:1600:AGS:C8	2.85	0.47
2:E:139:LEU:O	2:E:141:ALA:N	2.48	0.47
2:A:173:ARG:HH22	2:B:212:ARG:HB3	1.78	0.47
2:C:349:ILE:CG2	2:C:357:ALA:HA	2.45	0.47
2:C:396:MET:CE	2:C:396:MET:HA	2.45	0.47
2:A:146:ARG:NH2	2:A:376:GLU:OE1	2.48	0.47
2:E:195:ILE:HG21	2:E:204:LEU:HD13	1.96	0.47
2:D:340:ASN:ND2	2:E:214:GLU:OE2	2.47	0.47
2:C:58:LEU:HD13	2:C:59:GLN:H	1.79	0.47
2:C:123:LYS:C	2:C:125:GLU:H	2.18	0.47
2:A:140:HIS:CB	2:A:306:ASN:HB2	2.45	0.47
2:E:141:ALA:HB3	2:E:370:LEU:HB2	1.97	0.47
1:K:1:U:H5"	2:E:62:PHE:CE1	2.50	0.47
2:F:140:HIS:ND1	2:F:306:ASN:N	2.59	0.47
2:F:356:PRO:O	2:F:358:ILE:N	2.34	0.47
2:D:209:ILE:HD13	2:D:270:LEU:HD13	1.96	0.47
2:A:41:GLN:C	2:A:43:ALA:N	2.68	0.47
2:D:321:ILE:HD11	2:D:332:TYR:CE2	2.50	0.47
2:C:355:PHE:CZ	4:C:3600:AGS:H1'	2.50	0.47
2:B:187:LEU:HD22	2:B:345:LEU:HD21	1.97	0.47
2:E:248:GLU:O	2:E:252:ARG:HG2	2.15	0.47
2:C:207:LEU:HD13	2:C:246:VAL:HG21	1.96	0.47
2:E:268:THR:O	2:E:272:ARG:HG2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:169:GLY:HA3	2:E:371:LEU:HD23	1.97	0.46
2:A:173:ARG:CD	2:A:301:PHE:O	2.63	0.46
2:D:23:LEU:HB3	2:D:26:LEU:HD21	1.97	0.46
2:B:23:LEU:HB3	2:B:26:LEU:CD2	2.45	0.46
2:E:212:ARG:HH12	5:E:5701:FPD:H72	1.79	0.46
2:D:126:ASN:HB3	2:D:129:ASN:ND2	2.31	0.46
2:B:208:LEU:HD23	2:B:265:ASP:HB2	1.97	0.46
2:A:356:PRO:C	2:A:358:ILE:H	2.17	0.46
2:A:345:LEU:HA	2:A:357:ALA:O	2.15	0.46
2:F:349:ILE:HG22	2:F:354:VAL:O	2.14	0.46
2:B:86:ILE:O	2:B:90:ASN:HA	2.15	0.46
2:D:211:GLU:HA	5:D:4701:FPD:H32	1.97	0.46
5:B:2701:FPD:H54	5:B:2701:FPD:H122	1.67	0.46
2:A:171:GLY:H	2:A:314:THR:HB	1.81	0.46
2:A:356:PRO:O	2:A:358:ILE:N	2.44	0.46
2:C:228:VAL:HG12	2:C:242:VAL:HG13	1.97	0.46
2:D:58:LEU:HD23	2:D:59:GLN:H	1.80	0.46
5:D:4701:FPD:H82	5:D:4701:FPD:C6	2.46	0.46
2:C:275:ASN:HD21	2:C:290:ASP:N	2.10	0.46
2:F:26:LEU:CD2	2:F:29:MET:CE	2.94	0.46
2:E:365:THR:HG23	2:E:368:GLU:HG2	1.97	0.46
2:A:173:ARG:HB3	2:A:339:GLY:HA2	1.98	0.46
2:C:86:ILE:HA	2:C:91:LEU:HD12	1.98	0.46
2:E:139:LEU:HD12	2:F:218:GLU:HG3	1.98	0.46
2:F:346:SER:HB3	2:F:349:ILE:HG12	1.98	0.46
2:A:140:HIS:ND1	2:A:140:HIS:C	2.68	0.45
2:A:169:GLY:N	2:A:172:GLN:HG3	2.29	0.45
2:F:140:HIS:HE1	2:F:305:ARG:HB2	1.81	0.45
2:C:211:GLU:OE1	5:C:3701:FPD:H31	2.17	0.45
2:D:18:GLY:O	2:D:23:LEU:HB2	2.16	0.45
2:C:172:GLN:H	2:C:314:THR:HB	1.80	0.45
2:A:102:ARG:HG2	2:A:114:LEU:HD13	1.98	0.45
2:C:211:GLU:O	2:C:231:THR:HA	2.17	0.45
2:D:264:LEU:O	2:D:317:ALA:HA	2.17	0.45
1:L:2:C:H5	2:F:110:TYR:HH	1.64	0.45
2:D:174:GLY:CA	2:D:341:MET:HG3	2.41	0.45
2:B:3:LEU:CD2	2:B:79:ILE:HD11	2.47	0.45
2:E:355:PHE:CE1	4:E:5600:AGS:N9	2.84	0.45
2:B:71:SER:HA	2:B:228:VAL:HG13	1.97	0.45
1:J:2:C:H5	2:D:110:TYR:HH	1.62	0.45
2:A:173:ARG:H	2:A:340:ASN:ND2	2.10	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2701:FPD:C8	5:B:2701:FPD:C6	2.94	0.45
2:E:296:ARG:HB2	2:E:297:PRO:HD3	1.98	0.45
2:D:349:ILE:HB	2:D:357:ALA:CB	2.47	0.45
2:E:368:GLU:HA	2:E:371:LEU:HD12	1.98	0.45
2:C:140:HIS:O	2:C:142:ASN:N	2.43	0.45
2:A:250:ALA:O	2:A:254:VAL:HG23	2.16	0.45
5:D:4701:FPD:O4	5:D:4701:FPD:H121	2.16	0.45
2:B:65:LEU:HB2	2:B:79:ILE:HB	1.98	0.45
2:F:230:SER:HB3	2:F:242:VAL:HG21	1.98	0.45
2:C:167:PRO:O	2:C:365:THR:HG21	2.18	0.44
2:B:144:ARG:CZ	2:B:167:PRO:HB3	2.47	0.44
2:D:60:ASP:HB2	2:D:62:PHE:CE2	2.52	0.44
2:D:162:LEU:HD13	2:D:191:ILE:HD11	1.99	0.44
2:D:187:LEU:HD12	2:D:345:LEU:HD11	1.99	0.44
2:D:211:GLU:HA	5:D:4701:FPD:C3	2.48	0.44
5:C:3701:FPD:H82	5:C:3701:FPD:C6	2.47	0.44
2:D:388:HIS:NE2	2:E:351:GLU:OE1	2.51	0.44
2:B:18:GLY:O	2:B:23:LEU:HB2	2.18	0.44
2:C:238:ARG:O	2:C:242:VAL:HG23	2.18	0.44
2:D:265:ASP:O	2:D:266:SER:HB2	2.18	0.44
2:B:378:GLN:O	2:B:382:ILE:HG12	2.17	0.44
2:C:264:LEU:O	2:C:317:ALA:HA	2.17	0.44
2:D:208:LEU:HD11	2:D:219:MET:HG2	1.99	0.44
5:F:6701:FPD:C8	5:F:6701:FPD:C6	2.96	0.44
2:B:248:GLU:OE1	2:B:252:ARG:NH2	2.51	0.44
2:D:210:ASP:OD1	2:D:232:PHE:HA	2.17	0.44
2:A:294:LEU:HD13	2:A:334:GLU:HG3	1.98	0.44
2:C:398:PHE:O	2:C:402:LYS:HG2	2.18	0.44
2:E:267:ILE:HD12	2:E:270:LEU:HD23	2.00	0.44
2:D:341:MET:HB2	2:D:365:THR:HB	1.99	0.44
2:C:162:LEU:HD13	2:C:191:ILE:HD11	2.00	0.44
2:B:139:LEU:HD11	2:C:218:GLU:OE1	2.18	0.44
2:D:135:ASN:HB3	2:D:307:VAL:HG13	2.00	0.44
2:F:307:VAL:HG12	2:F:309:GLU:H	1.81	0.44
2:E:31:LYS:O	2:E:35:ILE:HG12	2.17	0.44
2:C:39:LEU:HB3	2:C:111:PHE:CZ	2.53	0.43
2:F:382:ILE:O	2:F:386:ILE:HG23	2.18	0.43
2:F:349:ILE:HD11	2:F:392:GLU:HB3	2.00	0.43
2:C:26:LEU:HD23	2:C:34:ILE:HG23	1.99	0.43
2:B:351:GLU:C	2:B:353:ARG:H	2.20	0.43
2:E:268:THR:HG21	2:E:320:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:209:ILE:HD11	2:E:243:ALA:HB2	2.00	0.43
2:D:250:ALA:O	2:D:254:VAL:HG23	2.18	0.43
2:D:207:LEU:HD23	2:D:264:LEU:HD13	2.00	0.43
2:A:56:GLU:HA	2:A:93:THR:HG23	2.00	0.43
2:E:400:ILE:HG13	2:E:400:ILE:H	1.53	0.43
2:A:89:PHE:HB2	2:A:91:LEU:HG	1.99	0.43
2:C:355:PHE:CZ	4:C:3600:AGS:C1'	3.01	0.43
2:B:357:ALA:O	2:B:358:ILE:C	2.57	0.43
2:D:347:ARG:O	2:D:351:GLU:HG2	2.18	0.43
2:C:278:VAL:HA	2:C:279:PRO:HD3	1.88	0.43
2:C:211:GLU:HA	5:C:3701:FPD:H31	2.01	0.43
2:F:247:ILE:HB	2:F:300:PHE:CE1	2.54	0.43
2:D:355:PHE:N	2:D:356:PRO:HD2	2.34	0.43
2:D:365:THR:HG23	2:D:368:GLU:HB3	2.01	0.43
2:B:141:ALA:HB3	2:B:370:LEU:HD12	2.01	0.43
1:H:2:C:H5	2:C:110:TYR:HH	1.63	0.43
2:B:161:VAL:HG22	2:B:399:LEU:HD12	2.00	0.43
2:B:31:LYS:HG2	2:B:35:ILE:HD11	2.01	0.43
2:D:253:LEU:HB2	2:D:260:VAL:HG21	1.99	0.43
2:B:130:LYS:H	2:B:130:LYS:HD2	1.84	0.43
2:D:294:LEU:O	2:D:298:LYS:HG2	2.19	0.43
2:F:178:ALA:HA	2:F:179:PRO:HD3	1.89	0.43
2:A:173:ARG:N	2:A:340:ASN:HD21	2.13	0.43
2:E:353:ARG:HD2	2:E:353:ARG:HA	1.79	0.43
2:F:137:THR:HB	2:F:140:HIS:CE1	2.54	0.42
2:E:266:SER:H	2:E:318:THR:HG1	1.66	0.42
2:F:343:LEU:HD11	2:F:358:ILE:HG12	2.01	0.42
2:D:194:SER:O	2:D:198:ASN:HB2	2.18	0.42
2:D:356:PRO:HA	6:D:4705:HOH:O	2.19	0.42
4:E:6600:AGS:N7	2:F:186:MET:HB2	2.35	0.42
2:A:173:ARG:HH21	2:B:212:ARG:HB3	1.79	0.42
2:C:230:SER:HB2	2:C:242:VAL:HG21	2.01	0.42
2:C:261:ILE:HG12	2:C:314:THR:HG23	2.01	0.42
2:A:236:ALA:HA	2:A:239:HIS:HD2	1.83	0.42
2:C:341:MET:HG2	2:C:365:THR:CG2	2.43	0.42
2:D:167:PRO:HG2	2:D:365:THR:HG21	2.01	0.42
2:C:160:ARG:NH2	2:C:403:LEU:HB3	2.35	0.42
2:F:26:LEU:CD2	2:F:29:MET:HE1	2.49	0.42
2:E:14:LEU:HD13	2:E:35:ILE:HD11	2.01	0.42
2:A:9:THR:HA	2:A:10:PRO:HD3	1.92	0.42
2:A:65:LEU:HB2	2:A:79:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:210:ASP:OD1	2:A:232:PHE:HA	2.19	0.42
2:B:366:ARG:CD	4:C:3600:AGS:S1G	3.03	0.42
2:D:366:ARG:CD	4:E:5600:AGS:S1G	3.05	0.42
2:E:141:ALA:O	2:E:371:LEU:HG	2.20	0.42
2:F:65:LEU:HB2	2:F:79:ILE:HB	2.01	0.42
2:D:207:LEU:HD13	2:D:246:VAL:HG21	2.02	0.42
2:C:143:SER:OG	2:C:170:ARG:HD2	2.20	0.42
2:D:86:ILE:HA	2:D:91:LEU:HD12	2.02	0.42
2:E:366:ARG:NH1	2:E:366:ARG:HB2	2.35	0.42
2:D:131:ILE:HG21	2:D:133:PHE:HD2	1.84	0.42
2:B:161:VAL:HG21	2:B:396:MET:HE1	2.01	0.42
2:E:161:VAL:HG13	2:E:399:LEU:HD13	2.01	0.42
2:B:19:GLU:C	2:B:21:MET:H	2.22	0.42
2:E:160:ARG:HH22	2:E:403:LEU:HB3	1.85	0.42
2:F:356:PRO:C	2:F:358:ILE:N	2.73	0.42
2:A:132:LEU:HD22	2:A:251:LYS:HG2	2.01	0.42
2:C:254:VAL:HG21	2:C:313:LEU:HB2	2.02	0.42
2:C:50:PHE:CE1	2:C:100:LYS:HG2	2.55	0.42
2:A:172:GLN:H	2:A:314:THR:HB	1.84	0.42
2:E:230:SER:HB3	2:E:242:VAL:HG21	2.02	0.42
2:E:123:LYS:HA	2:E:124:PRO:HD3	1.87	0.42
5:E:5701:FPD:O4	5:E:5701:FPD:H121	2.20	0.42
2:A:86:ILE:HG23	2:A:91:LEU:HB2	2.02	0.42
2:E:342:GLU:HB3	2:E:344:HIS:CE1	2.54	0.42
2:E:357:ALA:O	2:E:358:ILE:O	2.37	0.41
2:F:195:ILE:HG21	2:F:204:LEU:HD13	2.01	0.41
2:A:133:PHE:HB3	2:B:30:ARG:NH2	2.35	0.41
2:F:349:ILE:H	2:F:349:ILE:HG12	1.60	0.41
2:F:359:ASP:OD2	2:F:362:ARG:HB2	2.19	0.41
2:B:342:GLU:OE1	2:B:344:HIS:HE1	2.03	0.41
2:A:137:THR:HG22	2:A:305:ARG:HD3	2.01	0.41
2:E:41:GLN:C	2:E:43:ALA:H	2.23	0.41
2:B:349:ILE:HD11	2:B:392:GLU:HB3	2.02	0.41
2:A:296:ARG:N	2:A:297:PRO:CD	2.83	0.41
2:E:236:ALA:HA	2:E:239:HIS:CD2	2.55	0.41
2:F:254:VAL:HG21	2:F:313:LEU:HB2	2.03	0.41
2:F:175:LEU:HA	2:F:317:ALA:O	2.19	0.41
2:E:46:GLY:C	2:E:48:ASP:H	2.23	0.41
2:A:167:PRO:HD2	2:A:365:THR:HG22	2.03	0.41
2:C:366:ARG:NH2	5:D:4701:FPD:H81	2.35	0.41
2:A:135:ASN:HB3	2:A:307:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:211:GLU:O	2:F:231:THR:HA	2.20	0.41
2:D:181:LYS:HG2	4:D:4600:AGS:S1G	2.60	0.41
2:A:173:ARG:HD3	2:A:304:ALA:HB3	2.03	0.41
2:D:119:VAL:HB	2:D:124:PRO:HA	2.02	0.41
2:B:268:THR:HA	2:B:331:ILE:HG21	2.02	0.41
2:F:160:ARG:HD2	2:F:408:THR:HB	2.02	0.41
2:A:147:MET:HB3	2:A:194:SER:CB	2.48	0.41
2:A:407:LYS:NZ	2:A:407:LYS:HA	2.35	0.41
2:D:2:ASN:OD1	2:D:5:GLU:HB2	2.20	0.41
2:D:294:LEU:HD13	2:D:334:GLU:HG3	2.03	0.41
2:A:132:LEU:HD13	2:A:251:LYS:HA	2.03	0.41
2:A:133:PHE:HB3	2:B:30:ARG:HH22	1.84	0.41
2:B:143:SER:HB3	2:B:170:ARG:HD2	2.02	0.41
2:D:178:ALA:HA	2:D:179:PRO:HD3	1.88	0.41
2:D:355:PHE:HB2	2:D:356:PRO:HD3	2.02	0.41
2:D:11:VAL:HG22	2:D:31:LYS:HG3	2.02	0.41
2:E:26:LEU:HD22	2:E:34:ILE:HG23	2.02	0.41
2:A:160:ARG:CD	2:A:403:LEU:HD22	2.50	0.41
2:A:144:ARG:HG2	2:A:145:LEU:H	1.84	0.41
2:D:188:LEU:HD22	2:D:263:LEU:HB3	2.03	0.41
2:E:212:ARG:NH1	5:E:5701:FPD:H72	2.36	0.41
2:A:208:LEU:HD11	2:A:219:MET:HG2	2.03	0.41
2:A:113:LEU:HD21	2:A:116:VAL:HG22	2.04	0.41
2:D:344:HIS:CD2	2:D:362:ARG:HD2	2.55	0.41
2:D:52:ASP:HB3	2:D:98:SER:HA	2.03	0.40
2:D:195:ILE:HG21	2:D:204:LEU:HD13	2.03	0.40
2:A:4:THR:HG22	2:A:7:LYS:HE2	2.03	0.40
2:B:388:HIS:HB3	2:B:389:PRO:HD3	2.03	0.40
2:C:183:GLY:CA	4:C:3600:AGS:H8	2.44	0.40
2:E:208:LEU:HD23	2:E:265:ASP:HB2	2.03	0.40
2:A:209:ILE:HG22	2:A:269:ARG:HB3	2.02	0.40
2:E:187:LEU:O	2:E:191:ILE:HG12	2.21	0.40
2:D:342:GLU:OE2	5:E:5701:FPD:H52	2.20	0.40
2:D:275:ASN:ND2	2:D:290:ASP:H	2.19	0.40
2:E:294:LEU:C	2:E:297:PRO:HD2	2.42	0.40
2:E:2:ASN:HB3	2:E:5:GLU:HB2	2.03	0.40
2:B:414:GLU:O	2:B:414:GLU:HG3	2.22	0.40
4:E:6600:AGS:H8	4:E:6600:AGS:H5'1	2.04	0.40
2:B:320:LEU:HD11	5:B:2701:FPD:H4	2.03	0.40
2:E:102:ARG:HA	2:E:103:PRO:HD3	1.88	0.40
2:C:178:ALA:HA	2:C:179:PRO:HD3	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:341:MET:HA	2:D:365:THR:HA	2.04	0.40
2:B:181:LYS:HE3	5:B:2701:FPD:C13	2.52	0.40
2:F:102:ARG:HA	2:F:103:PRO:HD3	1.92	0.40
2:B:24:GLU:HB3	2:B:25:ASN:H	1.63	0.40
2:D:296:ARG:HB2	2:D:297:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	400/419 (96%)	368 (92%)	25 (6%)	7 (2%)	11	39
2	B	400/419 (96%)	366 (92%)	32 (8%)	2 (0%)	34	70
2	C	400/419 (96%)	364 (91%)	29 (7%)	7 (2%)	11	39
2	D	400/419 (96%)	358 (90%)	37 (9%)	5 (1%)	15	48
2	E	399/419 (95%)	368 (92%)	25 (6%)	6 (2%)	13	44
2	F	400/419 (96%)	366 (92%)	28 (7%)	6 (2%)	13	44
All	All	2399/2514 (95%)	2190 (91%)	176 (7%)	33 (1%)	14	46

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	47	GLU
2	C	140	HIS
2	E	356	PRO
2	E	358	ILE
2	F	355	PHE
2	F	356	PRO
2	A	356	PRO

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Mol	Chain	Res	Type
2	C	106	GLU
2	C	141	ALA
2	E	47	GLU
2	F	49	ILE
2	F	142	ASN
2	F	357	ALA
2	A	42	HIS
2	A	45	SER
2	A	153	SER
2	A	357	ALA
2	B	266	SER
2	C	358	ILE
2	D	50	PHE
2	D	359	ASP
2	D	407	LYS
2	E	140	HIS
2	B	90	ASN
2	C	266	SER
2	D	124	PRO
2	E	139	LEU
2	E	266	SER
2	F	266	SER
2	A	404	ALA
2	C	124	PRO
2	D	139	LEU
2	A	355	PHE

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	
2	A	351/359 (98%)	331 (94%)	20 (6%)	25	60
2	B	351/359 (98%)	331 (94%)	20 (6%)	25	60
2	C	351/359 (98%)	327 (93%)	24 (7%)	20	53
2	D	351/359 (98%)	329 (94%)	22 (6%)	22	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	350/359 (98%)	325 (93%)	25 (7%)	18	52
2	F	351/359 (98%)	333 (95%)	18 (5%)	29	65
All	All	2105/2154 (98%)	1976 (94%)	129 (6%)	23	57

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	14	LEU
2	A	60	ASP
2	A	90	ASN
2	A	118	GLU
2	A	129	ASN
2	A	130	LYS
2	A	140	HIS
2	A	198	ASN
2	A	221	ARG
2	A	266	SER
2	A	284	VAL
2	A	299	ARG
2	A	314	THR
2	A	340	ASN
2	A	341	MET
2	A	353	ARG
2	A	379	LYS
2	A	406	THR
2	A	407	LYS
2	A	411	ASP
2	B	58	LEU
2	B	59	GLN
2	B	90	ASN
2	B	110	TYR
2	B	130	LYS
2	B	147	MET
2	B	184	LYS
2	B	193	GLN
2	B	210	ASP
2	B	244	GLU
2	B	252	ARG
2	B	299	ARG
2	B	314	THR
2	B	349	ILE

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Mol	Chain	Res	Type
2	B	352	LYS
2	B	378	GLN
2	B	379	LYS
2	B	384	ARG
2	B	399	LEU
2	B	408	THR
2	C	1	MET
2	C	14	LEU
2	C	41	GLN
2	C	48	ASP
2	C	49	ILE
2	C	58	LEU
2	C	69	ASP
2	C	93	THR
2	C	106	GLU
2	C	129	ASN
2	C	142	ASN
2	C	210	ASP
2	C	214	GLU
2	C	272	ARG
2	C	286	THR
2	C	299	ARG
2	C	314	THR
2	C	321	ILE
2	C	352	LYS
2	C	379	LYS
2	C	383	LEU
2	C	408	THR
2	C	413	PHE
2	C	415	MET
2	D	2	ASN
2	D	5	GLU
2	D	26	LEU
2	D	41	GLN
2	D	58	LEU
2	D	62	PHE
2	D	69	ASP
2	D	132	LEU
2	D	140	HIS
2	D	144	ARG
2	D	146	ARG
2	D	187	LEU

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Mol	Chain	Res	Type
2	D	197	TYR
2	D	198	ASN
2	D	257	LYS
2	D	272	ARG
2	D	278	VAL
2	D	299	ARG
2	D	314	THR
2	D	341	MET
2	D	349	ILE
2	D	383	LEU
2	E	5	GLU
2	E	41	GLN
2	E	47	GLU
2	E	69	ASP
2	E	109	ARG
2	E	132	LEU
2	E	154	THR
2	E	162	LEU
2	E	170	ARG
2	E	201	ASP
2	E	257	LYS
2	E	268	THR
2	E	292	ASN
2	E	309	GLU
2	E	314	THR
2	E	321	ILE
2	E	326	LYS
2	E	349	ILE
2	E	365	THR
2	E	371	LEU
2	E	399	LEU
2	E	400	ILE
2	E	408	THR
2	E	415	MET
2	E	416	MET
2	F	9	THR
2	F	19	GLU
2	F	32	GLN
2	F	41	GLN
2	F	93	THR
2	F	134	GLU
2	F	162	LEU

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Mol	Chain	Res	Type
2	F	184	LYS
2	F	210	ASP
2	F	244	GLU
2	F	277	VAL
2	F	299	ARG
2	F	314	THR
2	F	340	ASN
2	F	349	ILE
2	F	403	LEU
2	F	410	ASP
2	F	413	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	42	HIS
2	A	90	ASN
2	A	172	GLN
2	A	198	ASN
2	A	256	HIS
2	A	340	ASN
2	A	344	HIS
2	B	41	GLN
2	B	90	ASN
2	B	193	GLN
2	B	198	ASN
2	B	220	GLN
2	B	241	GLN
2	B	344	HIS
2	B	378	GLN
2	C	41	GLN
2	C	117	ASN
2	C	142	ASN
2	C	172	GLN
2	C	193	GLN
2	C	256	HIS
2	C	275	ASN
2	C	409	ASN
2	D	41	GLN
2	D	90	ASN
2	D	126	ASN
2	D	129	ASN

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Mol	Chain	Res	Type
2	D	172	GLN
2	D	189	GLN
2	D	239	HIS
2	D	275	ASN
2	D	306	ASN
2	D	344	HIS
2	E	41	GLN
2	E	292	ASN
2	E	344	HIS
2	E	374	GLN
2	F	199	HIS
2	F	340	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	G	2/8 (25%)	1 (50%)	1 (50%)
1	H	2/8 (25%)	1 (50%)	1 (50%)
1	J	1/8 (12%)	1 (100%)	0
1	K	2/8 (25%)	1 (50%)	1 (50%)
1	L	1/8 (12%)	1 (100%)	0
1	M	1/8 (12%)	0	0
All	All	9/48 (18%)	5 (55%)	3 (33%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	G	2	C
1	H	2	C
1	J	2	C
1	K	2	C
1	L	2	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	G	1	U
1	H	1	U
1	K	1	U

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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$
4	AGS	A	1600	3	24,33,33	2.20	5 (20%)	28,52,52	2.03	6 (21%)
4	AGS	B	2600	3	24,33,33	2.08	5 (20%)	28,52,52	2.00	5 (17%)
5	FPD	B	2701	3	28,32,32	1.21	3 (10%)	21,49,49	0.99	1 (4%)
4	AGS	C	3600	-	24,33,33	2.14	4 (16%)	28,52,52	2.03	5 (17%)
5	FPD	C	3701	-	28,32,32	1.17	3 (10%)	21,49,49	1.02	1 (4%)
4	AGS	D	4600	3	24,33,33	2.08	4 (16%)	28,52,52	1.97	5 (17%)
5	FPD	D	4701	-	28,32,32	1.12	3 (10%)	21,49,49	1.02	1 (4%)
4	AGS	E	5600	-	24,33,33	2.05	5 (20%)	28,52,52	1.98	5 (17%)
5	FPD	E	5701	-	28,32,32	1.14	3 (10%)	21,49,49	0.93	1 (4%)
4	AGS	E	6600	3,2	24,33,33	2.20	5 (20%)	28,52,52	2.11	6 (21%)
5	FPD	F	6701	3	28,32,32	1.18	4 (14%)	21,49,49	0.90	1 (4%)

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
4	AGS	A	1600	3	-	0/15/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	B	2600	3	-	0/15/38/38	0/3/3/3
5	FPD	B	2701	3	-	0/13/57/57	0/1/3/3
4	AGS	C	3600	-	-	0/15/38/38	0/3/3/3
5	FPD	C	3701	-	-	0/13/57/57	0/1/3/3
4	AGS	D	4600	3	-	0/15/38/38	0/3/3/3
5	FPD	D	4701	-	-	0/13/57/57	0/1/3/3
4	AGS	E	5600	-	-	0/15/38/38	0/3/3/3
5	FPD	E	5701	-	-	0/13/57/57	0/1/3/3
4	AGS	E	6600	3,2	-	0/15/38/38	0/3/3/3
5	FPD	F	6701	3	-	0/13/57/57	0/1/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2701	FPD	C-S1	-3.57	1.69	1.76
5	F	6701	FPD	C-S1	-3.39	1.69	1.76
5	C	3701	FPD	C-S1	-3.35	1.69	1.76
5	E	5701	FPD	C-S1	-3.31	1.69	1.76
5	D	4701	FPD	C-S1	-3.21	1.70	1.76
5	E	5701	FPD	C10-C11	-2.55	1.50	1.53
5	F	6701	FPD	C10-C11	-2.54	1.50	1.53
5	D	4701	FPD	C10-C11	-2.34	1.51	1.53
5	B	2701	FPD	C10-C11	-2.27	1.51	1.53
5	C	3701	FPD	C10-C11	-2.11	1.51	1.53
5	C	3701	FPD	C12-S1	-2.10	1.76	1.81
5	E	5701	FPD	C12-S1	-2.08	1.76	1.81
5	D	4701	FPD	C12-S1	-2.07	1.76	1.81
5	F	6701	FPD	C12-S1	-2.01	1.77	1.81
4	E	5600	AGS	PB-O1B	2.00	1.58	1.51
4	B	2600	AGS	PB-O1B	2.02	1.58	1.51
5	B	2701	FPD	C8-C9	2.05	1.56	1.54
4	E	6600	AGS	PB-O1B	2.07	1.58	1.51
5	F	6701	FPD	C8-C9	2.08	1.56	1.54
4	A	1600	AGS	PB-O1B	2.19	1.59	1.51
4	E	6600	AGS	O4'-C1'	2.27	1.44	1.41
4	C	3600	AGS	O4'-C1'	2.32	1.44	1.41
4	E	6600	AGS	PA-O1A	2.35	1.59	1.51
4	B	2600	AGS	PA-O1A	2.35	1.59	1.51
4	A	1600	AGS	PA-O1A	2.38	1.59	1.51
4	E	5600	AGS	O4'-C1'	2.39	1.44	1.41
4	B	2600	AGS	O4'-C1'	2.39	1.44	1.41
4	D	4600	AGS	O4'-C1'	2.44	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1600	AGS	O4'-C1'	2.46	1.44	1.41
4	C	3600	AGS	PA-O1A	2.46	1.60	1.51
4	E	5600	AGS	PA-O1A	2.51	1.60	1.51
4	D	4600	AGS	PA-O1A	2.65	1.60	1.51
4	A	1600	AGS	C4-N3	5.72	1.44	1.35
4	E	5600	AGS	C4-N3	5.79	1.44	1.35
4	D	4600	AGS	C4-N3	5.85	1.44	1.35
4	B	2600	AGS	C4-N3	5.89	1.44	1.35
4	C	3600	AGS	C4-N3	5.94	1.44	1.35
4	E	6600	AGS	C4-N3	5.94	1.44	1.35
4	E	5600	AGS	PG-S1G	6.18	2.02	1.90
4	D	4600	AGS	PG-S1G	6.31	2.02	1.90
4	B	2600	AGS	PG-S1G	6.35	2.02	1.90
4	C	3600	AGS	PG-S1G	6.73	2.03	1.90
4	E	6600	AGS	PG-S1G	7.26	2.04	1.90
4	A	1600	AGS	PG-S1G	7.31	2.04	1.90

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3600	AGS	N3-C2-N1	-7.46	123.19	128.89
4	B	2600	AGS	N3-C2-N1	-7.38	123.25	128.89
4	E	6600	AGS	N3-C2-N1	-7.37	123.25	128.89
4	A	1600	AGS	N3-C2-N1	-7.24	123.35	128.89
4	E	5600	AGS	N3-C2-N1	-7.19	123.39	128.89
4	D	4600	AGS	N3-C2-N1	-6.96	123.57	128.89
4	E	6600	AGS	PB-O3B-PG	-4.39	117.94	132.67
4	C	3600	AGS	PB-O3B-PG	-3.32	121.53	132.67
4	A	1600	AGS	PB-O3B-PG	-3.18	122.01	132.67
5	D	4701	FPD	C12-S1-C	-3.01	98.64	104.00
4	E	5600	AGS	PB-O3B-PG	-2.86	123.08	132.67
4	B	2600	AGS	PB-O3B-PG	-2.85	123.12	132.67
4	A	1600	AGS	C4-C5-N7	-2.79	106.91	109.48
4	D	4600	AGS	C4-C5-N7	-2.76	106.94	109.48
4	E	6600	AGS	C4-C5-N7	-2.73	106.97	109.48
4	B	2600	AGS	C4-C5-N7	-2.72	106.98	109.48
4	E	5600	AGS	C4-C5-N7	-2.72	106.98	109.48
4	C	3600	AGS	C4-C5-N7	-2.71	106.99	109.48
4	D	4600	AGS	PB-O3B-PG	-2.70	123.60	132.67
5	B	2701	FPD	C12-S1-C	-2.54	99.47	104.00
5	E	5701	FPD	C12-S1-C	-2.43	99.67	104.00
5	C	3701	FPD	C12-S1-C	-2.21	100.07	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	6701	FPD	C12-S1-C	-2.09	100.27	104.00
4	A	1600	AGS	O3A-PA-O5'	-2.09	97.40	102.94
4	E	6600	AGS	O3A-PA-O5'	-2.01	97.62	102.94
4	D	4600	AGS	C2-N1-C6	2.27	122.83	118.77
4	A	1600	AGS	C2-N1-C6	2.30	122.88	118.77
4	E	5600	AGS	C2-N1-C6	2.34	122.94	118.77
4	E	6600	AGS	C2-N1-C6	2.34	122.95	118.77
4	B	2600	AGS	C2-N1-C6	2.34	122.96	118.77
4	C	3600	AGS	C2-N1-C6	2.39	123.03	118.77
4	E	5600	AGS	O5'-C5'-C4'	2.69	119.05	109.12
4	A	1600	AGS	O5'-C5'-C4'	2.71	119.12	109.12
4	B	2600	AGS	O5'-C5'-C4'	2.73	119.19	109.12
4	E	6600	AGS	O5'-C5'-C4'	2.76	119.30	109.12
4	D	4600	AGS	O5'-C5'-C4'	2.76	119.31	109.12
4	C	3600	AGS	O5'-C5'-C4'	2.81	119.48	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1600	AGS	4	0
4	B	2600	AGS	6	0
5	B	2701	FPD	6	0
4	C	3600	AGS	7	0
5	C	3701	FPD	9	0
4	D	4600	AGS	5	0
5	D	4701	FPD	8	0
4	E	5600	AGS	10	0
5	E	5701	FPD	11	0
4	E	6600	AGS	6	0
5	F	6701	FPD	3	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	G	2/8 (25%)	0.06	0 100 100	53, 53, 53, 53	0
1	H	2/8 (25%)	1.99	1 (50%) 0 0	53, 53, 53, 53	0
1	J	2/8 (25%)	3.51	2 (100%) 0 0	53, 53, 53, 53	0
1	K	2/8 (25%)	4.17	2 (100%) 0 0	55, 55, 55, 56	0
1	L	2/8 (25%)	3.28	2 (100%) 0 0	53, 53, 53, 53	0
1	M	2/8 (25%)	4.39	2 (100%) 0 0	53, 53, 53, 53	0
2	A	408/419 (97%)	-0.15	8 (1%) 68 44	53, 53, 53, 53	0
2	B	408/419 (97%)	0.04	6 (1%) 76 55	53, 53, 53, 53	0
2	C	408/419 (97%)	-0.19	6 (1%) 76 55	53, 53, 53, 53	0
2	D	408/419 (97%)	-0.02	1 (0%) 95 89	53, 53, 53, 53	0
2	E	407/419 (97%)	0.01	6 (1%) 76 55	53, 53, 53, 53	0
2	F	408/419 (97%)	0.00	7 (1%) 73 49	53, 53, 53, 53	0
All	All	2459/2562 (95%)	-0.04	43 (1%) 73 49	53, 53, 53, 56	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	140	HIS	5.8
1	K	2	C	5.3
1	M	2	C	5.0
1	J	2	C	4.8
2	B	51	GLY	4.5
2	A	140	HIS	4.4
2	A	412	PHE	4.4
2	A	45	SER	4.2
1	L	2	C	3.9
1	M	1	U	3.8
2	B	140	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
2	C	51	GLY	3.5
2	F	1	MET	3.4
2	F	25	ASN	3.3
1	H	2	C	3.3
2	E	60	ASP	3.3
2	C	416	MET	3.2
1	K	1	U	3.0
2	C	140	HIS	2.9
2	C	417	LYS	2.8
2	A	355	PHE	2.8
2	E	157	LEU	2.7
2	F	126	ASN	2.7
1	L	1	U	2.7
2	D	356	PRO	2.6
2	E	117	ASN	2.6
2	B	412	PHE	2.6
2	E	412	PHE	2.5
2	E	140	HIS	2.5
2	B	47	GLU	2.5
2	F	49	ILE	2.5
2	A	414	GLU	2.5
2	A	337	GLY	2.4
2	B	11	VAL	2.3
2	F	61	GLY	2.3
2	A	26	LEU	2.3
1	J	1	U	2.2
2	B	106	GLU	2.2
2	C	48	ASP	2.2
2	C	47	GLU	2.1
2	A	23	LEU	2.0
2	E	89	PHE	2.0
2	F	112	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	FPD	C	3701	30/30	0.33	0.76	11.88	53,53,53,53	0
3	MG	E	5601	1/1	0.84	0.73	8.50	53,53,53,53	0
5	FPD	F	6701	30/30	0.67	0.59	6.25	53,53,53,53	0
5	FPD	D	4701	30/30	0.61	0.52	5.41	53,53,53,53	0
5	FPD	E	5701	30/30	0.58	0.52	4.83	53,53,53,53	0
3	MG	D	4601	1/1	0.86	0.38	4.01	53,53,53,53	0
5	FPD	B	2701	30/30	0.67	0.47	2.69	53,53,53,53	0
4	AGS	B	2600	31/31	0.89	0.33	1.15	53,53,53,53	0
4	AGS	C	3600	31/31	0.81	0.26	0.99	53,53,53,53	0
4	AGS	A	1600	31/31	0.83	0.33	0.99	53,53,53,53	0
4	AGS	E	5600	31/31	0.87	0.25	0.47	53,53,53,53	0
4	AGS	E	6600	31/31	0.78	0.27	0.32	53,53,53,53	0
4	AGS	D	4600	31/31	0.89	0.25	0.05	53,53,53,53	0
3	MG	B	2601	1/1	0.76	0.33	-	54,54,54,54	0
3	MG	A	1601	1/1	0.96	0.22	-	54,54,54,54	0
3	MG	C	3601	1/1	0.71	0.43	-	53,53,53,53	0
3	MG	F	6601	1/1	0.76	0.34	-	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.