



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:15 PM GMT

PDB ID : 1XPR  
Title : Structural mechanism of inhibition of the Rho transcription termination factor  
by the antibiotic 5a-formylbicyclomycin(FB)  
Authors : Skordalakes, E.; Brogan, A.P.; Park, B.S.; Kohn, H.; Berger, J.M.  
Deposited on : 2004-10-09  
Resolution : 3.15 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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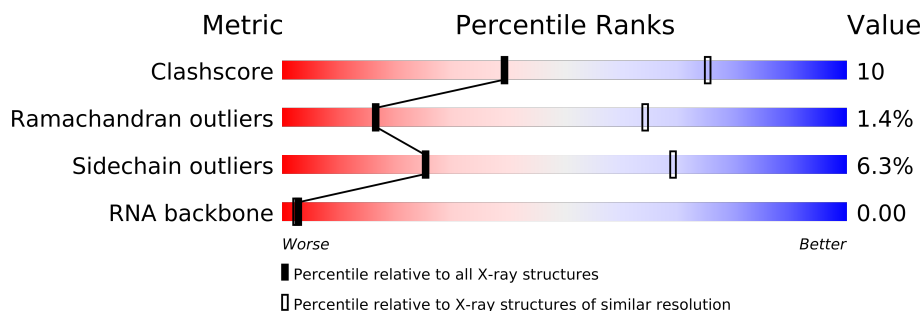
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **FAILED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.15 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))
Clashscore	79885	1681 (3.22-3.10)
Ramachandran outliers	78287	1639 (3.22-3.10)
Sidechain outliers	78261	1638 (3.22-3.10)
RNA backbone	1838	1000 (3.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

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

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19814 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			39	17	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			

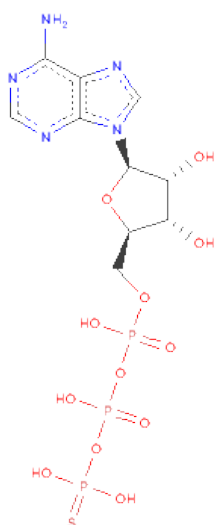
- Molecule 2 is a protein called Rho transcription termination factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	408	Total	C	N	O	S	0	0	0
			3210	2027	564	602	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 PHOSPHOTHIOPHOSPHORICACID-ADENYLATE ESTER (three-letter code: AGS) (formula:  $C_{10}H_{16}N_5O_{12}P_3S$ ).



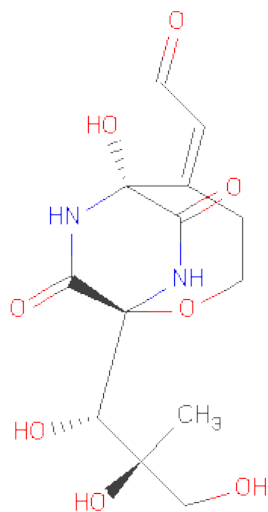
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

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

- Molecule 5 is 5A-FORMYLBICYCLOMYCIN (three-letter code: FB) (formula:  $C_{13}H_{18}N_2O_8$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			23	13	2	8		
5	C	1	Total	C	N	O	0	0
			23	13	2	8		
5	D	1	Total	C	N	O	0	0
			23	13	2	8		
5	E	1	Total	C	N	O	0	0
			23	13	2	8		
5	F	1	Total	C	N	O	0	0
			23	13	2	8		

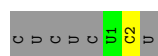
### 3 Residue-property plots

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

Note EDS failed to run properly.

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

Chain G: 



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

Chain M: 



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

Chain H: 



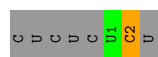
- Molecule 1: 5'-R(\*CP\*UP\*CP\*UP\*CP\*UP\*CP\*U)-3'

Chain J: 



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

Chain K: 



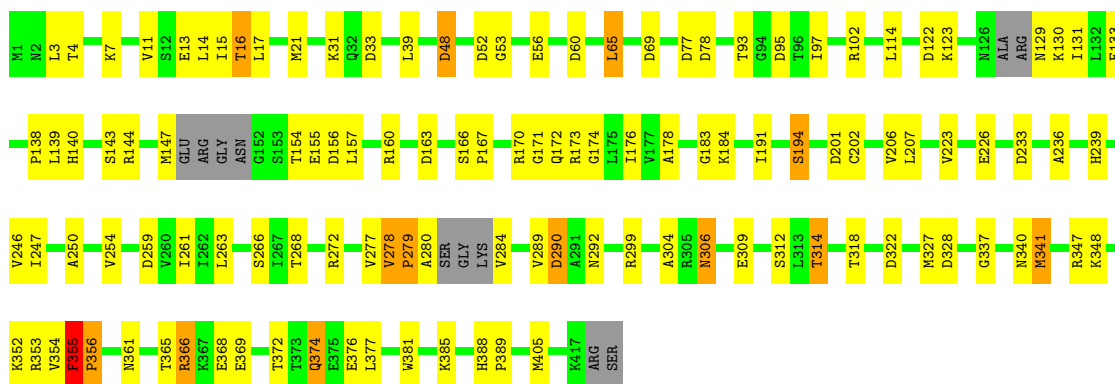
- Molecule 1: 5'-R(\*CP\*UP\*CP\*UP\*CP\*UP\*CP\*U)-3'

Chain L: 



- Molecule 2: Rho transcription termination factor

Chain A: 



• Molecule 2: Rho transcription termination factor

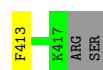
Chain B:

• Molecule 2: Rho transcription termination factor

Chain C:

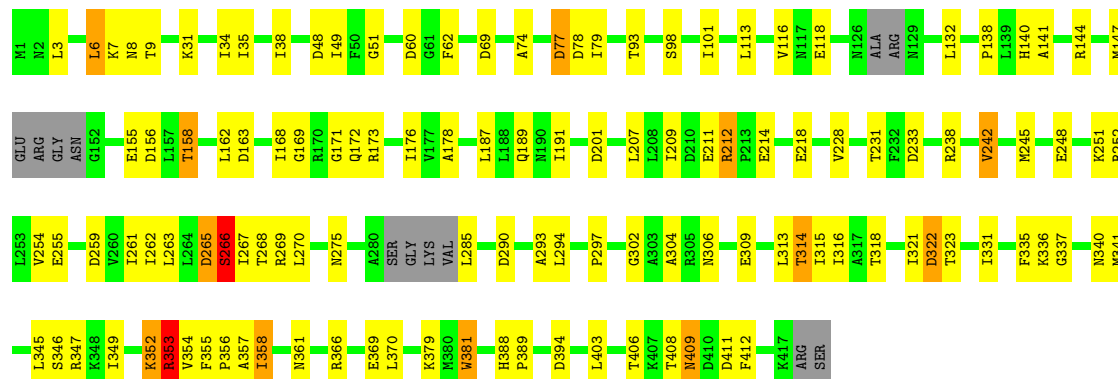
• Molecule 2: Rho transcription termination factor

Chain D:



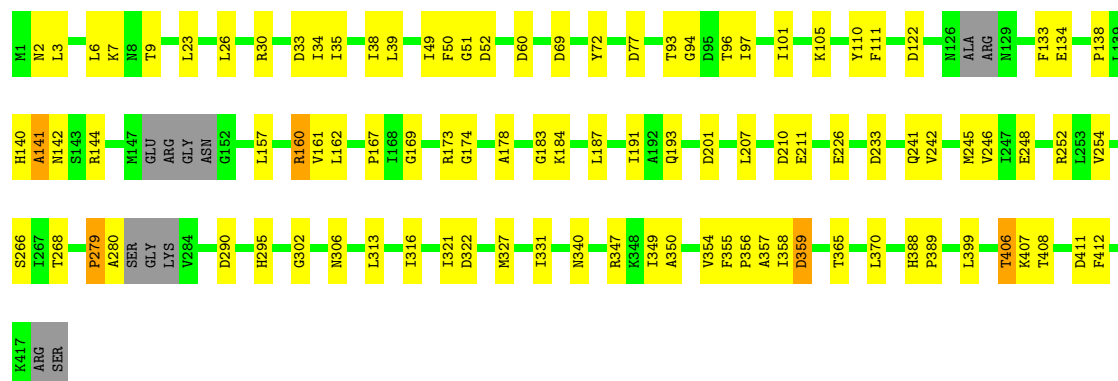
• Molecule 2: Rho transcription termination factor

Chain E:



• Molecule 2: Rho transcription termination factor

Chain F:





## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.53Å 109.68Å 160.05Å 90.00° 108.16° 90.00°	Depositor
Resolution (Å)	20.00 – 3.15	Depositor
% Data completeness (in resolution range)	86.5 (20.00-3.15)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.274 , 0.296	Depositor
Wilson B-factor (Å <sup>2</sup> )	100.9	Xtriage
Anisotropy	0.123	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 54063 reflections	Xtriage
Total number of atoms	19814	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FB, AGS, 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	G	0.73	0/43	1.04	0/64
1	H	0.79	0/43	1.15	0/64
1	J	0.70	0/43	1.02	0/64
1	K	0.72	0/43	0.94	0/64
1	L	0.79	0/43	1.52	0/64
1	M	0.75	0/41	1.12	0/60
2	A	0.31	0/3256	0.65	14/4383 (0.3%)
2	B	0.31	0/3259	0.65	10/4387 (0.2%)
2	C	0.30	0/3259	0.63	12/4387 (0.3%)
2	D	0.30	0/3259	0.64	14/4387 (0.3%)
2	E	0.30	0/3252	0.63	11/4377 (0.3%)
2	F	0.30	0/3259	0.64	10/4387 (0.2%)
All	All	0.31	0/19800	0.65	71/26688 (0.3%)

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	B	0	1
All	All	0	2

There are no bond length outliers.

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	60	ASP	CB-CG-OD2	6.32	123.98	118.30
2	D	77	ASP	CB-CG-OD2	6.20	123.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	77	ASP	CB-CG-OD2	5.99	123.69	118.30
2	B	77	ASP	CB-CG-OD2	5.97	123.67	118.30
2	E	163	ASP	CB-CG-OD2	5.91	123.62	118.30
2	A	48	ASP	CB-CG-OD2	5.89	123.60	118.30
2	E	233	ASP	CB-CG-OD2	5.88	123.59	118.30
2	C	52	ASP	CB-CG-OD2	5.84	123.56	118.30
2	A	322	ASP	CB-CG-OD2	5.84	123.55	118.30
2	D	210	ASP	CB-CG-OD2	5.82	123.54	118.30
2	D	410	ASP	CB-CG-OD2	5.79	123.51	118.30
2	F	33	ASP	CB-CG-OD2	5.77	123.49	118.30
2	E	48	ASP	CB-CG-OD2	5.75	123.47	118.30
2	B	233	ASP	CB-CG-OD2	5.74	123.46	118.30
2	E	78	ASP	CB-CG-OD2	5.74	123.46	118.30
2	A	33	ASP	CB-CG-OD2	5.72	123.45	118.30
2	A	77	ASP	CB-CG-OD2	5.71	123.44	118.30
2	F	233	ASP	CB-CG-OD2	5.71	123.44	118.30
2	E	156	ASP	CB-CG-OD2	5.69	123.42	118.30
2	A	78	ASP	CB-CG-OD2	5.67	123.40	118.30
2	E	77	ASP	CB-CG-OD2	5.66	123.39	118.30
2	F	52	ASP	CB-CG-OD2	5.63	123.36	118.30
2	A	60	ASP	CB-CG-OD2	5.56	123.30	118.30
2	F	69	ASP	CB-CG-OD2	5.51	123.26	118.30
2	F	77	ASP	CB-CG-OD2	5.50	123.25	118.30
2	C	69	ASP	CB-CG-OD2	5.42	123.18	118.30
2	E	69	ASP	CB-CG-OD2	5.36	123.12	118.30
2	A	69	ASP	CB-CG-OD2	5.31	123.08	118.30
2	E	265	ASP	CB-CG-OD2	5.31	123.08	118.30
2	D	95	ASP	CB-CG-OD2	5.26	123.03	118.30
2	A	233	ASP	CB-CG-OD2	5.26	123.03	118.30
2	B	95	ASP	CB-CG-OD2	5.25	123.03	118.30
2	C	210	ASP	CB-CG-OD2	5.23	123.01	118.30
2	D	78	ASP	CB-CG-OD2	5.19	122.97	118.30
2	D	48	ASP	CB-CG-OD2	5.18	122.96	118.30
2	A	290	ASP	CB-CG-OD2	5.18	122.96	118.30
2	B	210	ASP	CB-CG-OD2	5.17	122.95	118.30
2	B	69	ASP	CB-CG-OD2	5.17	122.95	118.30
2	C	60	ASP	CB-CG-OD2	5.16	122.94	118.30
2	A	163	ASP	CB-CG-OD2	5.16	122.94	118.30
2	C	328	ASP	CB-CG-OD2	5.14	122.92	118.30
2	C	201	ASP	CB-CG-OD2	5.12	122.91	118.30
2	A	201	ASP	CB-CG-OD2	5.11	122.90	118.30
2	A	95	ASP	CB-CG-OD2	5.11	122.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	ASP	CB-CG-OD2	5.11	122.90	118.30
2	A	328	ASP	CB-CG-OD2	5.10	122.89	118.30
2	D	290	ASP	CB-CG-OD2	5.09	122.89	118.30
2	D	163	ASP	CB-CG-OD2	5.09	122.88	118.30
2	D	33	ASP	CB-CG-OD2	5.09	122.88	118.30
2	B	163	ASP	CB-CG-OD2	5.08	122.87	118.30
2	E	394	ASP	CB-CG-OD2	5.08	122.87	118.30
2	F	201	ASP	CB-CG-OD2	5.08	122.87	118.30
2	F	210	ASP	CB-CG-OD2	5.07	122.87	118.30
2	C	259	ASP	CB-CG-OD2	5.06	122.86	118.30
2	B	328	ASP	CB-CG-OD2	5.06	122.85	118.30
2	C	359	ASP	CB-CG-OD2	5.06	122.85	118.30
2	D	201	ASP	CB-CG-OD2	5.05	122.85	118.30
2	B	156	ASP	CB-CG-OD2	5.05	122.84	118.30
2	A	122	ASP	CB-CG-OD2	5.05	122.84	118.30
2	E	259	ASP	CB-CG-OD2	5.04	122.83	118.30
2	C	411	ASP	CB-CG-OD2	5.03	122.83	118.30
2	F	411	ASP	CB-CG-OD2	5.03	122.83	118.30
2	D	328	ASP	CB-CG-OD2	5.03	122.83	118.30
2	C	48	ASP	CB-CG-OD2	5.02	122.82	118.30
2	B	201	ASP	CB-CG-OD2	5.02	122.82	118.30
2	B	290	ASP	CB-CG-OD2	5.02	122.82	118.30
2	F	290	ASP	CB-CG-OD2	5.02	122.82	118.30
2	D	52	ASP	CB-CG-OD2	5.02	122.81	118.30
2	D	411	ASP	CB-CG-OD2	5.01	122.81	118.30
2	C	156	ASP	CB-CG-OD2	5.00	122.80	118.30
2	D	233	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	355	PHE	Peptide
2	B	355	PHE	Peptide

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	40	0	22	0	0
1	H	40	0	22	0	0
1	J	40	0	22	1	0
1	K	40	0	22	1	0
1	L	40	0	22	2	0
1	M	39	0	19	0	0
2	A	3210	0	3287	77	0
2	B	3213	0	3288	75	0
2	C	3213	0	3289	56	0
2	D	3213	0	3288	44	0
2	E	3206	0	3280	76	0
2	F	3213	0	3289	51	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	6	0
4	B	31	0	12	9	0
4	C	31	0	12	6	0
4	D	31	0	12	9	0
4	E	31	0	12	4	0
4	F	31	0	12	7	0
5	B	23	0	16	4	0
5	C	23	0	16	8	0
5	D	23	0	16	5	0
5	E	23	0	16	8	0
5	F	23	0	16	6	0
All	All	19814	0	20002	383	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (383) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:366:ARG:NE	4:C:3600:AGS:S1G	2.12	1.21
2:A:355:PHE:CE1	4:A:1600:AGS:H1'	1.82	1.12
2:C:366:ARG:HD2	4:D:4600:AGS:S1G	1.95	1.04
2:B:355:PHE:CZ	4:B:2600:AGS:H1'	1.94	1.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:140:HIS:HB3	2:C:306:ASN:HB3	1.38	1.03
2:C:355:PHE:HB3	2:C:356:PRO:HD2	1.39	1.00
2:A:167:PRO:CD	2:A:365:THR:HG21	1.91	0.99
2:A:167:PRO:HD2	2:A:365:THR:CG2	1.94	0.98
2:B:385:LYS:HA	2:B:388:HIS:CD2	1.98	0.98
2:A:167:PRO:HD2	2:A:365:THR:HG21	0.97	0.93
2:D:355:PHE:CD1	4:D:4600:AGS:H1'	2.05	0.91
2:A:355:PHE:CE1	4:A:1600:AGS:C1'	2.54	0.90
2:C:355:PHE:CB	2:C:356:PRO:HD2	2.04	0.86
2:C:183:GLY:HA2	4:C:3600:AGS:H8	1.58	0.84
2:F:183:GLY:HA2	4:F:6600:AGS:H8	1.62	0.81
2:F:183:GLY:CA	4:F:6600:AGS:H8	2.11	0.80
2:E:336:LYS:NZ	5:F:6701:FB:O12	2.13	0.80
2:F:141:ALA:HB1	2:F:370:LEU:HB2	1.64	0.80
2:A:139:LEU:O	2:A:306:ASN:ND2	2.15	0.79
2:A:355:PHE:CZ	4:A:1600:AGS:H1'	2.16	0.79
2:E:346:SER:HB3	2:E:349:ILE:HG22	1.66	0.78
2:D:355:PHE:HD1	4:D:4600:AGS:H1'	1.46	0.78
2:C:366:ARG:CD	4:D:4600:AGS:S1G	2.71	0.77
2:B:132:LEU:HD22	2:B:251:LYS:HD2	1.66	0.77
2:A:289:VAL:HG22	2:A:327:MET:HG3	1.67	0.77
2:E:340:ASN:HA	2:E:366:ARG:HD2	1.65	0.76
2:A:340:ASN:HA	2:A:366:ARG:HD2	1.68	0.76
2:F:349:ILE:HG22	2:F:354:VAL:HB	1.67	0.75
2:B:355:PHE:CZ	4:B:2600:AGS:C1'	2.71	0.74
2:B:355:PHE:CE1	4:B:2600:AGS:C1'	2.70	0.74
2:C:184:LYS:HD2	2:C:318:THR:HG21	1.72	0.72
2:D:341:MET:HG2	2:D:365:THR:HG22	1.70	0.72
2:A:172:GLN:H	2:A:314:THR:HB	1.55	0.71
2:A:365:THR:HG23	2:A:368:GLU:HG2	1.71	0.71
2:D:340:ASN:HA	2:D:366:ARG:HD2	1.71	0.71
2:B:385:LYS:HA	2:B:388:HIS:HD2	1.52	0.70
2:E:366:ARG:NE	4:F:6600:AGS:S1G	2.64	0.70
2:D:336:LYS:NZ	5:E:5701:FB:O12	2.22	0.70
2:F:140:HIS:O	2:F:141:ALA:HB2	1.90	0.69
2:B:185:THR:O	2:B:189:GLN:HB2	1.93	0.68
2:B:355:PHE:CE1	4:B:2600:AGS:O4'	2.48	0.67
2:A:289:VAL:CG2	2:A:327:MET:HG3	2.24	0.67
2:A:277:VAL:O	2:A:278:VAL:HG23	1.95	0.67
2:C:266:SER:H	2:C:318:THR:HB	1.61	0.66
2:F:141:ALA:CB	2:F:370:LEU:HB2	2.24	0.66
2:E:212:ARG:H	2:E:212:ARG:HD2	1.59	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:126:ASN:HB3	2:B:129:ASN:HD21	1.61	0.66
2:B:343:LEU:HD21	2:B:358:ILE:HG12	1.78	0.66
2:C:181:LYS:HG2	4:C:3600:AGS:S1G	2.37	0.65
2:E:7:LYS:HG2	2:E:35:ILE:HD13	1.78	0.65
2:D:138:PRO:HD2	2:D:306:ASN:O	1.97	0.64
2:E:355:PHE:CZ	4:E:5600:AGS:H1'	2.32	0.64
1:L:1:U:O2	1:L:1:U:H2'	1.98	0.63
2:E:169:GLY:H	2:E:172:GLN:HG3	1.63	0.63
2:C:355:PHE:HB3	2:C:356:PRO:CD	2.24	0.63
2:C:355:PHE:CB	2:C:356:PRO:CD	2.77	0.63
2:A:183:GLY:HA2	4:A:1600:AGS:H8	1.79	0.63
2:E:211:GLU:HA	5:E:5701:FB:C2B	2.29	0.62
2:B:2:ASN:ND2	2:B:50:PHE:HB2	2.14	0.62
2:B:355:PHE:CE1	4:B:2600:AGS:H1'	2.32	0.62
2:B:355:PHE:CE2	4:B:2600:AGS:H1'	2.35	0.61
2:D:211:GLU:HA	5:D:4701:FB:C2B	2.30	0.61
2:C:130:LYS:HE3	2:D:11:VAL:HB	1.82	0.61
2:E:187:LEU:O	2:E:191:ILE:HG12	2.01	0.61
2:B:388:HIS:HB2	2:B:389:PRO:HD3	1.82	0.61
2:F:23:LEU:HD22	2:F:26:LEU:HD23	1.82	0.61
2:E:238:ARG:HH12	2:E:242:VAL:HG13	1.66	0.60
2:F:211:GLU:HA	5:F:6701:FB:C2B	2.31	0.60
2:A:102:ARG:HB3	2:A:114:LEU:HD12	1.84	0.60
2:A:236:ALA:HA	2:A:239:HIS:HD2	1.66	0.60
2:B:154:THR:HA	2:B:157:LEU:HB2	1.83	0.60
2:A:166:SER:HA	2:A:365:THR:CG2	2.33	0.59
2:F:7:LYS:HG2	2:F:35:ILE:HD13	1.85	0.59
2:C:387:ILE:HG23	2:C:395:ALA:HB1	1.85	0.59
2:E:140:HIS:HA	2:E:306:ASN:HB2	1.84	0.58
2:E:178:ALA:HB2	2:E:345:LEU:HD12	1.84	0.58
2:F:140:HIS:O	2:F:141:ALA:CB	2.50	0.58
2:A:277:VAL:HG12	2:A:277:VAL:O	2.02	0.58
2:F:321:ILE:HG13	2:F:322:ASP:H	1.69	0.58
2:D:174:GLY:HA2	2:D:341:MET:HB3	1.86	0.57
2:D:355:PHE:CE1	4:D:4600:AGS:H1'	2.39	0.57
2:F:355:PHE:CD1	4:F:6600:AGS:N3	2.72	0.57
2:F:268:THR:HA	2:F:331:ILE:HG21	1.85	0.57
2:C:140:HIS:CD2	2:C:305:ARG:HB2	2.38	0.57
2:D:183:GLY:HA2	4:D:4600:AGS:H8	1.86	0.57
2:D:366:ARG:NE	4:E:5600:AGS:S1G	2.75	0.57
2:C:183:GLY:CA	4:C:3600:AGS:H8	2.34	0.57
2:E:297:PRO:HB2	2:E:335:PHE:HZ	1.70	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:337:GLY:HA3	5:C:3701:FB:H32	1.87	0.57
2:B:365:THR:HG23	2:B:368:GLU:HB3	1.86	0.56
2:C:388:HIS:HB3	2:C:389:PRO:HD3	1.86	0.56
2:D:183:GLY:CA	4:D:4600:AGS:H8	2.36	0.56
5:C:3701:FB:H32	5:C:3701:FB:C7	2.36	0.56
2:E:49:ILE:HG22	2:E:101:ILE:HG13	1.86	0.56
2:C:275:ASN:HD21	2:C:290:ASP:H	1.54	0.56
2:F:183:GLY:HA3	4:F:6600:AGS:H8	1.85	0.56
2:B:34:ILE:O	2:B:38:ILE:HG12	2.05	0.56
2:A:156:ASP:O	2:A:160:ARG:HB2	2.06	0.56
5:B:2701:FB:C7	5:B:2701:FB:H32	2.35	0.56
5:F:6701:FB:C7	5:F:6701:FB:H32	2.35	0.56
2:F:51:GLY:HA3	2:F:101:ILE:HD11	1.87	0.55
2:B:341:MET:HG2	2:B:365:THR:HB	1.89	0.55
2:C:379:LYS:HE2	2:C:412:PHE:HB2	1.87	0.55
2:D:49:ILE:H	2:D:49:ILE:HD13	1.71	0.55
2:A:372:THR:HB	2:A:376:GLU:HB3	1.88	0.55
2:E:337:GLY:O	5:F:6701:FB:H31	2.06	0.54
2:A:166:SER:HA	2:A:365:THR:HG21	1.88	0.54
2:A:355:PHE:HE1	4:A:1600:AGS:C1'	2.19	0.54
2:B:3:LEU:HD21	2:B:39:LEU:HD11	1.88	0.54
2:A:154:THR:HA	2:A:157:LEU:HD13	1.89	0.54
2:B:366:ARG:CZ	4:C:3600:AGS:S1G	2.94	0.54
2:C:406:THR:HB	2:C:410:ASP:HB2	1.90	0.54
2:A:369:GLU:HA	2:A:377:LEU:HD22	1.90	0.54
2:B:137:THR:HG22	2:B:305:ARG:HD3	1.90	0.54
2:A:130:LYS:HZ1	2:A:309:GLU:HG2	1.73	0.54
2:E:211:GLU:CD	5:E:5701:FB:HB1	2.29	0.54
2:E:141:ALA:HB1	2:E:370:LEU:HB2	1.90	0.53
2:B:209:ILE:HG13	2:B:270:LEU:HB2	1.90	0.53
2:A:280:ALA:C	2:A:284:VAL:N	2.62	0.53
2:C:290:ASP:HB3	2:C:293:ALA:HB2	1.91	0.53
2:D:275:ASN:HA	2:D:293:ALA:HB1	1.90	0.53
2:A:279:PRO:HA	2:A:290:ASP:OD2	2.08	0.53
2:E:403:LEU:HA	2:E:411:ASP:OD2	2.08	0.53
2:B:2:ASN:ND2	2:B:50:PHE:HD2	2.07	0.53
2:F:358:ILE:O	2:F:359:ASP:CB	2.57	0.53
2:F:355:PHE:HB2	2:F:356:PRO:HD3	1.91	0.52
2:D:132:LEU:HD13	2:D:251:LYS:HA	1.91	0.52
2:F:248:GLU:O	2:F:252:ARG:HG2	2.08	0.52
2:B:299:ARG:HA	2:C:233:ASP:HB2	1.92	0.52
2:E:176:ILE:HB	2:E:318:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:5701:FB:H32	5:E:5701:FB:C7	2.39	0.52
5:D:4701:FB:C7	5:D:4701:FB:H32	2.37	0.52
2:C:387:ILE:HD11	2:C:399:LEU:HD13	1.91	0.52
2:B:143:SER:HB2	2:B:170:ARG:HD3	1.90	0.52
2:E:337:GLY:HA3	5:F:6701:FB:C3	2.40	0.52
2:D:269:ARG:HD3	2:D:272:ARG:HD2	1.90	0.52
2:F:347:ARG:HA	2:F:350:ALA:HB3	1.92	0.52
5:B:2701:FB:C3	5:B:2701:FB:C7	2.88	0.52
2:A:279:PRO:O	2:A:280:ALA:CB	2.57	0.52
2:B:332:TYR:O	2:B:336:LYS:HG3	2.10	0.52
2:C:174:GLY:HA2	2:C:341:MET:HB3	1.92	0.52
2:E:265:ASP:OD1	5:E:5701:FB:HA2	2.09	0.52
2:E:352:LYS:O	2:E:354:VAL:N	2.42	0.52
2:B:145:LEU:HG	2:B:170:ARG:HD2	1.92	0.51
2:D:139:LEU:HD22	2:D:367:LYS:HG3	1.91	0.51
5:C:3701:FB:C3	5:C:3701:FB:C7	2.87	0.51
2:F:327:MET:O	2:F:331:ILE:HG12	2.10	0.51
2:E:147:MET:HG3	2:E:162:LEU:HD23	1.92	0.51
2:D:132:LEU:HD22	2:D:251:LYS:HG2	1.92	0.51
2:A:131:ILE:HD12	2:A:133:PHE:HD2	1.76	0.50
2:C:144:ARG:NH2	2:C:167:PRO:HB3	2.26	0.50
2:D:268:THR:HG21	2:D:320:LEU:H	1.75	0.50
2:A:56:GLU:HA	2:A:93:THR:HG23	1.93	0.50
2:F:388:HIS:HB3	2:F:389:PRO:HD3	1.94	0.50
2:E:98:SER:HB2	2:E:118:GLU:HB2	1.93	0.50
2:D:284:VAL:HG23	2:D:285:LEU:HD12	1.94	0.50
2:F:160:ARG:HG3	2:F:408:THR:HB	1.92	0.50
2:C:140:HIS:CG	2:C:306:ASN:H	2.29	0.50
2:C:348:LYS:HG2	2:C:393:ILE:HD11	1.92	0.50
2:F:355:PHE:CD1	4:F:6600:AGS:H1'	2.47	0.50
2:B:3:LEU:HD13	2:B:79:ILE:HD11	1.93	0.50
2:A:65:LEU:HD11	2:A:97:ILE:HB	1.94	0.50
2:A:140:HIS:ND1	2:A:340:ASN:ND2	2.59	0.49
2:A:279:PRO:O	2:A:280:ALA:HB2	2.12	0.49
2:E:140:HIS:HB3	2:E:306:ASN:HB2	1.94	0.49
2:B:65:LEU:HB2	2:B:79:ILE:HB	1.93	0.49
2:E:31:LYS:HA	2:E:34:ILE:HD12	1.95	0.49
5:D:4701:FB:C3	5:D:4701:FB:C7	2.89	0.49
2:E:140:HIS:CA	2:E:306:ASN:HB2	2.42	0.49
2:B:52:ASP:OD1	2:B:53:GLY:N	2.46	0.49
2:C:183:GLY:HA2	4:C:3600:AGS:C8	2.36	0.49
2:A:13:GLU:O	2:A:16:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:211:GLU:HA	5:C:3701:FB:C2B	2.43	0.49
2:B:30:ARG:O	2:B:34:ILE:HG12	2.12	0.49
2:C:294:LEU:HD21	2:C:331:ILE:HG12	1.95	0.49
2:C:160:ARG:HD2	2:C:403:LEU:HD12	1.93	0.49
2:E:140:HIS:CB	2:E:306:ASN:HB2	2.43	0.48
2:D:147:MET:HE1	2:D:191:ILE:HG12	1.94	0.48
2:A:355:PHE:CB	2:A:356:PRO:CD	2.90	0.48
2:C:184:LYS:HD2	2:C:318:THR:CG2	2.40	0.48
2:B:386:ILE:HG23	2:B:387:ILE:HD12	1.94	0.48
2:B:236:ALA:HA	2:B:239:HIS:HD2	1.77	0.48
2:D:140:HIS:O	2:D:140:HIS:ND1	2.46	0.48
2:A:289:VAL:HG22	2:A:327:MET:CG	2.42	0.48
2:B:2:ASN:ND2	2:B:50:PHE:CD2	2.82	0.48
2:A:268:THR:O	2:A:272:ARG:HG3	2.13	0.48
2:E:144:ARG:HA	2:E:169:GLY:HA2	1.95	0.48
2:F:2:ASN:HA	2:F:50:PHE:HB2	1.95	0.48
1:L:1:U:H1'	2:F:110:TYR:HE2	1.79	0.48
2:D:294:LEU:HD21	2:D:331:ILE:HG12	1.96	0.48
2:E:408:THR:O	2:E:409:ASN:HB2	2.14	0.48
2:E:352:LYS:HE2	2:E:353:ARG:N	2.29	0.48
2:D:345:LEU:HA	2:D:357:ALA:O	2.13	0.48
2:B:2:ASN:HD22	2:B:50:PHE:HD2	1.59	0.48
2:E:238:ARG:NH1	2:E:242:VAL:HG13	2.28	0.48
2:A:176:ILE:HB	2:A:318:THR:HG22	1.96	0.48
2:C:31:LYS:O	2:C:35:ILE:HG12	2.14	0.48
2:F:30:ARG:O	2:F:34:ILE:HG12	2.14	0.48
2:D:212:ARG:NH2	4:D:4600:AGS:S1G	2.87	0.48
2:B:356:PRO:C	2:B:358:ILE:H	2.17	0.48
2:C:337:GLY:O	5:D:4701:FB:H31	2.14	0.48
2:B:337:GLY:HA3	5:C:3701:FB:C3	2.43	0.48
2:A:3:LEU:HD23	2:A:39:LEU:HD23	1.96	0.48
2:D:296:ARG:HB2	2:D:297:PRO:HD3	1.96	0.48
2:C:144:ARG:HD2	2:C:371:LEU:O	2.14	0.47
2:E:209:ILE:HD13	2:E:270:LEU:HD13	1.96	0.47
2:F:3:LEU:HA	2:F:6:LEU:HD12	1.96	0.47
2:E:381:TRP:CE3	2:E:381:TRP:HA	2.49	0.47
2:E:323:THR:HG23	5:E:5701:FB:O12	2.13	0.47
2:E:34:ILE:O	2:E:38:ILE:HG12	2.14	0.47
5:F:6701:FB:C7	5:F:6701:FB:C3	2.87	0.47
2:F:72:TYR:HB3	2:F:245:MET:HE3	1.96	0.47
5:E:5701:FB:C7	5:E:5701:FB:C3	2.91	0.47
2:E:321:ILE:HG13	2:E:322:ASP:H	1.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:18:GLY:HA3	2:C:26:LEU:CD1	2.45	0.47
2:A:250:ALA:O	2:A:254:VAL:HG23	2.15	0.47
1:J:1:U:H1'	2:D:110:TYR:CE2	2.49	0.46
2:D:396:MET:O	2:D:400:ILE:HG12	2.15	0.46
2:B:296:ARG:HB2	2:B:297:PRO:HD3	1.97	0.46
2:D:349:ILE:HD11	2:D:392:GLU:HG2	1.96	0.46
2:E:138:PRO:HD2	2:E:306:ASN:O	2.15	0.46
2:A:144:ARG:HH12	2:A:372:THR:HG22	1.81	0.46
2:B:156:ASP:O	2:B:160:ARG:HG2	2.15	0.46
2:E:254:VAL:HG21	2:E:313:LEU:HB2	1.96	0.46
2:E:275:ASN:HA	2:E:293:ALA:HB1	1.97	0.46
2:A:4:THR:HG22	2:A:7:LYS:HD3	1.97	0.46
2:E:158:THR:HG21	4:E:5600:AGS:HN62	1.80	0.46
2:F:157:LEU:O	2:F:161:VAL:HG23	2.15	0.46
2:A:178:ALA:HB3	2:A:184:LYS:HD3	1.98	0.46
2:B:384:ARG:HB3	2:B:388:HIS:CE1	2.51	0.46
2:B:211:GLU:HA	5:B:2701:FB:C2B	2.46	0.46
2:F:207:LEU:HD13	2:F:246:VAL:HG21	1.98	0.46
2:B:340:ASN:HA	2:B:366:ARG:NH1	2.31	0.46
2:B:137:THR:O	2:C:214:GLU:HA	2.16	0.46
2:B:57:ILE:H	2:B:93:THR:HB	1.81	0.46
2:C:306:ASN:O	2:C:306:ASN:CG	2.54	0.46
2:A:53:GLY:HA3	2:A:65:LEU:HB3	1.98	0.46
2:F:207:LEU:HD11	2:F:242:VAL:HG12	1.97	0.46
2:B:175:LEU:O	2:B:342:GLU:HA	2.15	0.45
2:B:177:VAL:HG13	2:B:321:ILE:HG13	1.98	0.45
2:E:172:GLN:H	2:E:314:THR:HB	1.82	0.45
2:D:268:THR:HA	2:D:331:ILE:HG21	1.98	0.45
2:D:173:ARG:NH2	2:E:214:GLU:OE1	2.49	0.45
2:F:34:ILE:O	2:F:38:ILE:HG12	2.16	0.45
2:F:279:PRO:HB2	2:F:280:ALA:H	1.60	0.45
2:B:183:GLY:HA2	4:B:2600:AGS:H8	1.98	0.45
2:A:261:ILE:HG12	2:A:314:THR:HG23	1.97	0.45
2:D:240:VAL:HG21	2:D:277:VAL:HG11	1.97	0.45
2:F:174:GLY:HA3	2:F:316:ILE:HG13	1.98	0.45
2:A:143:SER:HB2	2:A:170:ARG:HE	1.81	0.45
2:F:183:GLY:HA3	4:F:6600:AGS:C8	2.46	0.45
2:E:211:GLU:OE1	5:E:5701:FB:HB1	2.17	0.45
2:A:278:VAL:HA	2:A:279:PRO:HD3	1.58	0.45
2:E:261:ILE:HG12	2:E:314:THR:HG23	1.99	0.45
2:F:173:ARG:HD3	2:F:302:GLY:HA2	1.99	0.45
2:E:211:GLU:O	2:E:231:THR:HA	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:211:GLU:O	2:C:231:THR:HA	2.16	0.45
2:F:187:LEU:O	2:F:191:ILE:HG12	2.17	0.45
2:F:39:LEU:HB3	2:F:111:PHE:CZ	2.52	0.44
2:B:254:VAL:HG21	2:B:313:LEU:HB2	1.99	0.44
2:A:166:SER:HB2	2:A:365:THR:HB	1.98	0.44
2:A:174:GLY:HA2	2:A:341:MET:HB3	1.99	0.44
2:A:352:LYS:O	2:A:354:VAL:HG23	2.18	0.44
2:B:355:PHE:CG	4:B:2600:AGS:C4	3.01	0.44
2:A:183:GLY:CA	4:A:1600:AGS:H8	2.45	0.44
2:E:251:LYS:O	2:E:255:GLU:HG3	2.18	0.44
2:B:1:MET:O	2:B:49:ILE:HA	2.17	0.44
2:C:207:LEU:HD13	2:C:246:VAL:HG21	1.98	0.44
2:A:17:LEU:HB3	2:A:21:MET:HG3	2.00	0.44
2:C:178:ALA:HB2	2:C:345:LEU:HD12	1.99	0.44
2:A:355:PHE:HB3	2:A:356:PRO:CD	2.47	0.44
2:A:355:PHE:CB	2:A:356:PRO:HD2	2.48	0.44
2:F:349:ILE:HB	2:F:357:ALA:HB1	1.99	0.44
2:B:336:LYS:NZ	5:C:3701:FB:O12	2.50	0.44
2:E:132:LEU:HD13	2:E:251:LYS:HA	2.00	0.44
2:A:173:ARG:HG3	2:A:304:ALA:HB3	2.00	0.44
2:C:138:PRO:HD2	2:C:140:HIS:CE1	2.53	0.43
2:F:138:PRO:HD2	2:F:306:ASN:O	2.18	0.43
2:B:131:ILE:HD12	2:B:133:PHE:HB2	2.00	0.43
2:C:269:ARG:NH2	5:C:3701:FB:O7	2.49	0.43
2:F:167:PRO:HD2	2:F:365:THR:HG22	2.00	0.43
2:B:171:GLY:H	2:B:314:THR:HB	1.84	0.43
2:B:54:VAL:HG22	2:B:96:THR:HG22	2.00	0.43
2:E:158:THR:HA	2:E:356:PRO:HG3	1.99	0.43
2:E:173:ARG:HG3	2:E:304:ALA:HB3	2.01	0.43
2:B:169:GLY:H	2:B:172:GLN:HG3	1.83	0.43
2:A:171:GLY:HA3	2:A:312:SER:HB2	2.00	0.43
2:A:207:LEU:HD13	2:A:246:VAL:HG21	2.00	0.43
2:B:268:THR:HG21	2:B:320:LEU:HB2	1.99	0.43
2:A:11:VAL:HG22	2:A:31:LYS:HE3	2.01	0.43
2:E:349:ILE:HG23	2:E:357:ALA:HB1	2.01	0.43
2:F:321:ILE:HG13	2:F:322:ASP:N	2.32	0.43
2:B:3:LEU:HD22	2:B:7:LYS:HZ2	1.83	0.43
2:E:113:LEU:HD21	2:E:116:VAL:HG22	2.00	0.43
2:D:355:PHE:HB2	2:D:356:PRO:HD3	2.01	0.43
2:B:268:THR:HA	2:B:331:ILE:HG21	2.01	0.43
2:A:388:HIS:N	2:A:389:PRO:HD2	2.34	0.43
2:A:355:PHE:HB2	2:A:356:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:206:VAL:HG21	2:A:223:VAL:HG11	2.00	0.43
2:A:355:PHE:O	2:A:356:PRO:C	2.56	0.43
2:B:207:LEU:O	2:B:264:LEU:HA	2.19	0.43
2:E:6:LEU:HD22	2:E:35:ILE:HG23	2.01	0.43
2:D:355:PHE:HD1	4:D:4600:AGS:C1'	2.24	0.42
2:B:170:ARG:HB3	2:B:312:SER:OG	2.18	0.42
2:E:266:SER:HB3	2:E:269:ARG:HB2	2.01	0.42
2:D:406:THR:HB	2:D:407:LYS:H	1.68	0.42
2:A:129:ASN:HD22	2:A:129:ASN:HA	1.63	0.42
2:E:262:ILE:HB	2:E:315:ILE:HG12	2.00	0.42
2:C:137:THR:O	2:D:214:GLU:HA	2.20	0.42
2:D:290:ASP:HB3	2:D:293:ALA:HB2	2.01	0.42
2:E:309:GLU:H	2:E:309:GLU:HG2	1.62	0.42
2:C:137:THR:HA	2:C:140:HIS:CE1	2.54	0.42
2:E:357:ALA:O	2:E:358:ILE:C	2.57	0.42
2:E:355:PHE:CZ	4:E:5600:AGS:C1'	3.01	0.42
2:D:268:THR:HG21	2:D:320:LEU:HB2	2.00	0.42
2:E:207:LEU:HA	2:E:228:VAL:O	2.19	0.42
2:B:138:PRO:HD2	2:B:306:ASN:O	2.19	0.42
2:E:388:HIS:HB3	2:E:389:PRO:HD3	2.02	0.42
2:A:166:SER:CB	2:A:365:THR:HB	2.50	0.42
2:F:349:ILE:HB	2:F:357:ALA:CB	2.50	0.42
2:B:349:ILE:HG12	2:B:393:ILE:HG13	2.01	0.42
2:F:406:THR:HB	2:F:407:LYS:H	1.57	0.42
2:F:144:ARG:HA	2:F:169:GLY:HA2	2.01	0.42
2:A:261:ILE:HG12	2:A:314:THR:CG2	2.50	0.42
2:F:39:LEU:HD11	2:F:49:ILE:HG21	2.02	0.42
1:K:2:C:H42	2:E:74:ALA:HB1	1.83	0.42
2:B:355:PHE:CD2	4:B:2600:AGS:N3	2.87	0.42
2:A:202:CYS:HB3	2:A:259:ASP:HB2	2.02	0.42
2:B:257:LYS:HG2	2:B:310:GLY:HA3	2.02	0.42
2:B:207:LEU:HD13	2:B:246:VAL:HG21	2.02	0.42
2:B:162:LEU:HD11	2:B:187:LEU:HD21	2.02	0.42
2:B:266:SER:HB3	2:B:269:ARG:HB2	2.01	0.42
2:F:72:TYR:CG	2:F:245:MET:HG2	2.55	0.42
2:C:257:LYS:HG2	2:C:310:GLY:HA3	2.02	0.42
2:C:138:PRO:HD2	2:C:140:HIS:HE1	1.84	0.41
2:F:358:ILE:O	2:F:359:ASP:HB2	2.19	0.41
2:E:263:LEU:HD23	2:E:316:ILE:HB	2.01	0.41
2:E:3:LEU:HB3	2:E:51:GLY:HA2	2.02	0.41
2:A:140:HIS:CE1	2:A:340:ASN:OD1	2.73	0.41
2:A:337:GLY:O	5:B:2701:FB:H31	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:309:GLU:HG2	2:B:309:GLU:H	1.63	0.41
2:E:189:GLN:HE22	2:E:218:GLU:HG2	1.85	0.41
2:C:337:GLY:HA3	5:D:4701:FB:C3	2.50	0.41
2:D:160:ARG:HB3	2:D:408:THR:HG21	2.01	0.41
2:E:60:ASP:HB2	2:E:62:PHE:HE2	1.85	0.41
2:D:207:LEU:HD13	2:D:246:VAL:HG21	2.03	0.41
2:B:3:LEU:CD1	2:B:79:ILE:HD11	2.50	0.41
2:E:3:LEU:HD22	2:E:79:ILE:HD11	2.02	0.41
2:C:47:GLU:HB3	2:C:48:ASP:H	1.65	0.41
2:C:32:GLN:HB3	2:C:76:PRO:HD2	2.02	0.41
2:C:173:ARG:HD2	2:C:301:PHE:O	2.20	0.41
2:A:17:LEU:HB3	2:A:21:MET:CG	2.51	0.41
2:B:349:ILE:HG22	2:B:349:ILE:O	2.21	0.41
2:E:141:ALA:CB	2:E:370:LEU:HB2	2.51	0.41
2:E:381:TRP:HA	2:E:381:TRP:HE3	1.85	0.41
2:B:102:ARG:HA	2:B:103:PRO:HD3	1.93	0.41
2:A:365:THR:O	2:A:366:ARG:O	2.39	0.41
2:C:31:LYS:HA	2:C:34:ILE:HD12	2.03	0.41
2:C:382:ILE:O	2:C:386:ILE:HG12	2.20	0.41
2:A:147:MET:HE2	2:A:194:SER:HB3	2.03	0.41
2:A:277:VAL:O	2:A:277:VAL:CG1	2.69	0.41
2:E:294:LEU:C	2:E:297:PRO:HD2	2.42	0.41
2:B:337:GLY:O	5:C:3701:FB:H31	2.21	0.41
2:C:169:GLY:H	2:C:172:GLN:CG	2.34	0.41
2:E:248:GLU:O	2:E:252:ARG:HG2	2.21	0.40
2:E:168:ILE:HD11	2:E:341:MET:HE3	2.03	0.40
2:E:171:GLY:H	2:E:314:THR:HB	1.86	0.40
2:C:268:THR:HA	2:C:331:ILE:HG21	2.02	0.40
2:A:352:LYS:HE3	2:F:295:HIS:HE1	1.86	0.40
2:E:173:ARG:HD3	2:E:302:GLY:HA2	2.03	0.40
2:E:379:LYS:HG3	2:E:412:PHE:CG	2.56	0.40
2:F:178:ALA:HB3	2:F:184:LYS:HD3	2.02	0.40
2:D:387:ILE:O	2:D:390:MET:HG2	2.21	0.40
2:C:158:THR:HG23	2:C:356:PRO:HB3	2.02	0.40
2:D:176:ILE:HB	2:D:318:THR:HG22	2.02	0.40
2:A:352:LYS:O	2:A:354:VAL:N	2.54	0.40
2:D:144:ARG:HG3	2:D:146:ARG:H	1.85	0.40
2:C:169:GLY:O	2:C:172:GLN:HG2	2.21	0.40
2:A:385:LYS:NZ	2:B:353:ARG:HH21	2.20	0.40
2:A:191:ILE:HG21	2:A:263:LEU:HD21	2.03	0.40
2:A:374:GLN:HE21	2:A:374:GLN:H	1.69	0.40
2:E:268:THR:HA	2:E:331:ILE:HG21	2.04	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:254:VAL:HG21	2:F:313:LEU:HB2	2.03	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	
2	A	400/419 (96%)	356 (89%)	35 (9%)	9 (2%)	10	50
2	B	400/419 (96%)	362 (90%)	35 (9%)	3 (1%)	27	77
2	C	400/419 (96%)	372 (93%)	23 (6%)	5 (1%)	18	66
2	D	400/419 (96%)	374 (94%)	20 (5%)	6 (2%)	15	63
2	E	399/419 (95%)	367 (92%)	28 (7%)	4 (1%)	22	73
2	F	400/419 (96%)	368 (92%)	26 (6%)	6 (2%)	15	63
All	All	2399/2514 (95%)	2199 (92%)	167 (7%)	33 (1%)	16	64

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	353	ARG
2	A	355	PHE
2	A	356	PRO
2	A	366	ARG
2	B	355	PHE
2	B	356	PRO
2	F	141	ALA
2	F	142	ASN
2	C	141	ALA
2	C	355	PHE
2	D	24	GLU
2	D	90	ASN
2	D	140	HIS
2	D	146	ARG

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Mol	Chain	Res	Type
2	E	353	ARG
2	F	279	PRO
2	F	359	ASP
2	A	138	PRO
2	A	279	PRO
2	C	106	GLU
2	C	266	SER
2	D	407	LYS
2	E	358	ILE
2	F	266	SER
2	D	124	PRO
2	A	15	ILE
2	A	266	SER
2	E	266	SER
2	E	409	ASN
2	F	94	GLY
2	A	278	VAL
2	B	209	ILE
2	C	307	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	
2	A	350/359 (98%)	329 (94%)	21 (6%)	27	71
2	B	351/359 (98%)	324 (92%)	27 (8%)	18	60
2	C	351/359 (98%)	334 (95%)	17 (5%)	35	79
2	D	351/359 (98%)	323 (92%)	28 (8%)	17	58
2	E	350/359 (98%)	327 (93%)	23 (7%)	24	67
2	F	351/359 (98%)	334 (95%)	17 (5%)	35	79
All	All	2104/2154 (98%)	1971 (94%)	133 (6%)	25	69

All (133) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
2	A	14	LEU
2	A	16	THR
2	A	48	ASP
2	A	52	ASP
2	A	65	LEU
2	A	123	LYS
2	A	155	GLU
2	A	194	SER
2	A	226	GLU
2	A	247	ILE
2	A	292	ASN
2	A	299	ARG
2	A	306	ASN
2	A	314	THR
2	A	341	MET
2	A	347	ARG
2	A	348	LYS
2	A	361	ASN
2	A	374	GLN
2	A	381	TRP
2	A	405	MET
2	B	14	LEU
2	B	26	LEU
2	B	60	ASP
2	B	91	LEU
2	B	93	THR
2	B	100	LYS
2	B	108	GLU
2	B	122	ASP
2	B	130	LYS
2	B	132	LEU
2	B	139	LEU
2	B	157	LEU
2	B	172	GLN
2	B	187	LEU
2	B	218	GLU
2	B	244	GLU
2	B	252	ARG
2	B	268	THR
2	B	299	ARG
2	B	314	THR
2	B	331	ILE
2	B	333	GLU

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Mol	Chain	Res	Type
2	B	340	ASN
2	B	383	LEU
2	B	387	ILE
2	B	409	ASN
2	B	411	ASP
2	C	19	GLU
2	C	49	ILE
2	C	93	THR
2	C	125	GLU
2	C	137	THR
2	C	139	LEU
2	C	160	ARG
2	C	186	MET
2	C	187	LEU
2	C	188	LEU
2	C	193	GLN
2	C	284	VAL
2	C	306	ASN
2	C	314	THR
2	C	354	VAL
2	C	383	LEU
2	C	394	ASP
2	D	4	THR
2	D	14	LEU
2	D	49	ILE
2	D	69	ASP
2	D	89	PHE
2	D	100	LYS
2	D	110	TYR
2	D	115	LYS
2	D	129	ASN
2	D	130	LYS
2	D	136	LEU
2	D	139	LEU
2	D	170	ARG
2	D	184	LYS
2	D	190	ASN
2	D	212	ARG
2	D	222	LEU
2	D	244	GLU
2	D	252	ARG
2	D	286	THR

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Mol	Chain	Res	Type
2	D	309	GLU
2	D	314	THR
2	D	327	MET
2	D	362	ARG
2	D	378	GLN
2	D	399	LEU
2	D	403	LEU
2	D	413	PHE
2	E	6	LEU
2	E	8	ASN
2	E	9	THR
2	E	77	ASP
2	E	93	THR
2	E	155	GLU
2	E	158	THR
2	E	212	ARG
2	E	242	VAL
2	E	245	MET
2	E	266	SER
2	E	267	ILE
2	E	285	LEU
2	E	290	ASP
2	E	314	THR
2	E	322	ASP
2	E	347	ARG
2	E	352	LYS
2	E	353	ARG
2	E	361	ASN
2	E	369	GLU
2	E	381	TRP
2	E	406	THR
2	F	9	THR
2	F	93	THR
2	F	96	THR
2	F	97	ILE
2	F	105	LYS
2	F	122	ASP
2	F	133	PHE
2	F	134	GLU
2	F	160	ARG
2	F	162	LEU
2	F	193	GLN

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Mol	Chain	Res	Type
2	F	226	GLU
2	F	241	GLN
2	F	340	ASN
2	F	399	LEU
2	F	406	THR
2	F	412	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	59	GLN
2	A	129	ASN
2	A	135	ASN
2	A	193	GLN
2	A	256	HIS
2	A	275	ASN
2	A	374	GLN
2	B	126	ASN
2	B	129	ASN
2	B	172	GLN
2	B	256	HIS
2	B	275	ASN
2	B	306	ASN
2	B	388	HIS
2	C	20	ASN
2	C	41	GLN
2	C	90	ASN
2	C	117	ASN
2	C	120	ASN
2	C	275	ASN
2	D	90	ASN
2	D	198	ASN
2	D	275	ASN
2	D	292	ASN
2	D	306	ASN
2	E	41	GLN
2	E	189	GLN
2	E	361	ASN
2	F	90	ASN
2	F	189	GLN
2	F	241	GLN
2	F	295	HIS

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Mol	Chain	Res	Type
2	F	340	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	G	1/8 (12%)	1 (100%)	0
1	H	1/8 (12%)	1 (100%)	0
1	J	1/8 (12%)	1 (100%)	0
1	K	1/8 (12%)	1 (100%)	0
1	L	1/8 (12%)	1 (100%)	0
1	M	1/8 (12%)	0	1 (100%)
All	All	6/48 (12%)	5 (83%)	1 (16%)

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 (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	M	1	U

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 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	33,33,33	2.24	5 (15%)	52,52,52	2.54	14 (26%)
4	AGS	B	2600	3	33,33,33	2.21	5 (15%)	52,52,52	3.25	14 (26%)
5	FB	B	2701	-	24,24,24	3.11	6 (25%)	38,38,38	5.93	14 (36%)
4	AGS	C	3600	3	33,33,33	2.10	6 (18%)	52,52,52	3.64	12 (23%)
5	FB	C	3701	-	24,24,24	2.97	5 (20%)	38,38,38	6.57	14 (36%)
4	AGS	D	4600	3	33,33,33	2.13	6 (18%)	52,52,52	2.76	12 (23%)
5	FB	D	4701	-	24,24,24	3.07	5 (20%)	38,38,38	7.21	14 (36%)
4	AGS	E	5600	3	33,33,33	2.15	5 (15%)	52,52,52	2.63	13 (25%)
5	FB	E	5701	-	24,24,24	2.74	6 (25%)	38,38,38	5.26	15 (39%)
4	AGS	F	6600	3	33,33,33	2.12	6 (18%)	52,52,52	3.25	12 (23%)
5	FB	F	6701	-	24,24,24	2.86	5 (20%)	38,38,38	5.48	15 (39%)

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	-	0/21/38/38	0/1/3/3
4	AGS	B	2600	3	-	0/21/38/38	0/1/3/3
5	FB	B	2701	-	-	1/16/53/53	0/0/2/2
4	AGS	C	3600	3	-	0/21/38/38	0/1/3/3
5	FB	C	3701	-	-	1/16/53/53	0/0/2/2
4	AGS	D	4600	3	-	0/21/38/38	0/1/3/3
5	FB	D	4701	-	-	1/16/53/53	0/0/2/2
4	AGS	E	5600	3	-	0/21/38/38	0/1/3/3
5	FB	E	5701	-	-	1/16/53/53	0/0/2/2
4	AGS	F	6600	3	-	0/21/38/38	0/1/3/3
5	FB	F	6701	-	-	1/16/53/53	0/0/2/2

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2701	FB	C5A-C12	-12.40	1.24	1.44
5	D	4701	FB	C5A-C12	-12.18	1.25	1.44
5	C	3701	FB	C5A-C12	-11.54	1.26	1.44
5	F	6701	FB	C5A-C12	-10.87	1.27	1.44
5	E	5701	FB	C5A-C12	-10.28	1.28	1.44
4	A	1600	AGS	PG-S1G	9.04	2.07	1.90
4	B	2600	AGS	PG-S1G	8.81	2.07	1.90
4	E	5600	AGS	PG-S1G	8.47	2.06	1.90
4	D	4600	AGS	PG-S1G	8.42	2.06	1.90
4	F	6600	AGS	PG-S1G	8.39	2.06	1.90
4	C	3600	AGS	PG-S1G	8.09	2.05	1.90
4	A	1600	AGS	C4-N3	6.07	1.44	1.35
4	B	2600	AGS	C4-N3	6.00	1.44	1.35
4	E	5600	AGS	C4-N3	5.95	1.44	1.35
4	D	4600	AGS	C4-N3	5.91	1.44	1.35
4	F	6600	AGS	C4-N3	5.89	1.44	1.35
4	C	3600	AGS	C4-N3	5.86	1.44	1.35
5	B	2701	FB	C5A-C5	-5.40	1.26	1.33
5	E	5701	FB	C5A-C5	-4.93	1.26	1.33
5	F	6701	FB	C5A-C5	-4.91	1.26	1.33
5	C	3701	FB	C5A-C5	-4.84	1.27	1.33
5	D	4701	FB	C5A-C5	-4.74	1.27	1.33
5	C	3701	FB	O6-C6	4.19	1.44	1.40
5	F	6701	FB	O6-C6	4.06	1.44	1.40
5	D	4701	FB	C4-C5	4.06	1.54	1.51
5	C	3701	FB	C4-C5	3.83	1.54	1.51
5	E	5701	FB	C4-C5	3.67	1.54	1.51
5	F	6701	FB	C4-C5	3.67	1.54	1.51
5	D	4701	FB	O6-C6	3.59	1.44	1.40
5	B	2701	FB	C4-C5	3.51	1.54	1.51
5	B	2701	FB	O6-C6	3.39	1.44	1.40
5	E	5701	FB	O6-C6	3.31	1.43	1.40
4	C	3600	AGS	C4-N9	-3.28	1.33	1.37
4	E	5600	AGS	C4-N9	-3.27	1.33	1.37
4	A	1600	AGS	C4-N9	-3.24	1.33	1.37
4	B	2600	AGS	C4-N9	-3.20	1.33	1.37
4	D	4600	AGS	C4-N9	-3.15	1.33	1.37
4	F	6600	AGS	C4-N9	-3.07	1.33	1.37
5	F	6701	FB	C6-C7	-2.50	1.50	1.54
5	D	4701	FB	C6-C7	-2.47	1.51	1.54
5	C	3701	FB	C6-C7	-2.42	1.51	1.54
5	B	2701	FB	C6-C7	-2.28	1.51	1.54
4	E	5600	AGS	PA-O1A	2.24	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1600	AGS	PA-O1A	2.23	1.59	1.51
4	D	4600	AGS	PA-O1A	2.23	1.59	1.51
4	F	6600	AGS	PA-O1A	2.22	1.59	1.51
4	C	3600	AGS	PA-O1A	2.21	1.59	1.51
4	B	2600	AGS	PA-O1A	2.20	1.59	1.51
5	E	5701	FB	O2-C1	2.20	1.44	1.42
5	E	5701	FB	C6-C7	-2.14	1.51	1.54
4	B	2600	AGS	PB-O1B	2.11	1.59	1.51
5	B	2701	FB	O2-C1	2.11	1.44	1.42
4	A	1600	AGS	PB-O1B	2.10	1.59	1.51
4	F	6600	AGS	PB-O1B	2.09	1.59	1.51
4	E	5600	AGS	PB-O1B	2.08	1.59	1.51
4	C	3600	AGS	C5-C4	2.07	1.45	1.40
4	D	4600	AGS	PB-O1B	2.05	1.59	1.51
4	C	3600	AGS	PB-O1B	2.02	1.59	1.51
4	D	4600	AGS	C5-C4	2.02	1.45	1.40
4	F	6600	AGS	C5-C4	2.01	1.45	1.40

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	4701	FB	O12-C12-C5A	34.96	161.64	123.42
5	C	3701	FB	O12-C12-C5A	31.09	157.41	123.42
5	B	2701	FB	O12-C12-C5A	24.09	149.76	123.42
4	C	3600	AGS	O3B-PG-S1G	-22.72	104.45	114.53
5	F	6701	FB	O12-C12-C5A	22.20	147.69	123.42
5	D	4701	FB	C12-C5A-C5	21.54	163.06	125.74
5	B	2701	FB	C12-C5A-C5	21.25	162.56	125.74
5	E	5701	FB	O12-C12-C5A	20.57	145.91	123.42
5	C	3701	FB	C12-C5A-C5	19.44	159.43	125.74
4	B	2600	AGS	O3B-PG-S1G	-19.35	105.95	114.53
4	F	6600	AGS	O3B-PG-S1G	-19.22	106.00	114.53
5	E	5701	FB	C12-C5A-C5	18.28	157.41	125.74
5	F	6701	FB	C12-C5A-C5	18.10	157.11	125.74
4	D	4600	AGS	O3B-PG-S1G	-14.45	108.12	114.53
4	E	5600	AGS	O3B-PG-S1G	-13.47	108.55	114.53
4	A	1600	AGS	O3B-PG-S1G	-12.74	108.87	114.53
5	B	2701	FB	O2-C1-N8	-9.47	101.38	112.53
5	F	6701	FB	O2-C1-N8	-9.40	101.46	112.53
5	C	3701	FB	O2-C1-N8	-9.32	101.55	112.53
5	E	5701	FB	O2-C1-N8	-9.14	101.76	112.53
5	D	4701	FB	O2-C1-N8	-9.04	101.88	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	6600	AGS	N3-C2-N1	-7.21	122.68	128.71
4	D	4600	AGS	N3-C2-N1	-7.19	122.70	128.71
4	A	1600	AGS	N3-C2-N1	-7.17	122.72	128.71
4	E	5600	AGS	N3-C2-N1	-7.13	122.75	128.71
4	B	2600	AGS	N3-C2-N1	-7.13	122.75	128.71
4	C	3600	AGS	N3-C2-N1	-6.79	123.03	128.71
5	F	6701	FB	C5-C6-C7	-6.33	96.52	108.59
5	E	5701	FB	C5-C6-C7	-6.31	96.55	108.59
5	C	3701	FB	C5-C6-C7	-5.96	97.23	108.59
5	D	4701	FB	C5-C6-C7	-5.86	97.41	108.59
5	B	2701	FB	C5-C6-C7	-5.85	97.44	108.59
5	B	2701	FB	C5-C6-N10	-5.76	102.34	111.02
5	F	6701	FB	C7-C6-N10	5.70	118.50	110.40
5	D	4701	FB	C5-C6-N10	-5.59	102.59	111.02
5	E	5701	FB	C7-C6-N10	5.57	118.32	110.40
5	B	2701	FB	C7-C6-N10	5.47	118.17	110.40
5	E	5701	FB	C5-C6-N10	-5.47	102.78	111.02
5	D	4701	FB	C7-C6-N10	5.44	118.12	110.40
5	C	3701	FB	C7-C6-N10	5.42	118.09	110.40
5	C	3701	FB	C5-C6-N10	-5.23	103.14	111.02
5	F	6701	FB	C6-C5-C5A	-5.13	114.30	120.10
5	F	6701	FB	C5-C6-N10	-5.07	103.38	111.02
5	C	3701	FB	O2-C1-C9	-4.80	99.74	107.81
5	D	4701	FB	O2-C1-C9	-4.75	99.82	107.81
5	B	2701	FB	O2-C1-C9	-4.69	99.93	107.81
5	F	6701	FB	O2-C1-C9	-4.68	99.94	107.81
5	E	5701	FB	O2-C1-C9	-4.48	100.27	107.81
4	D	4600	AGS	O2G-PG-S1G	-4.21	108.29	112.73
5	D	4701	FB	C9-C1-N8	4.21	117.29	111.43
5	E	5701	FB	C9-C1-N8	4.18	117.25	111.43
5	F	6701	FB	C9-C1-N8	4.17	117.24	111.43
5	B	2701	FB	C9-C1-N8	4.10	117.14	111.43
4	B	2600	AGS	C4-C5-N7	-4.05	106.05	109.52
4	C	3600	AGS	C4-C5-N7	-4.02	106.08	109.52
4	F	6600	AGS	C4-C5-N7	-4.01	106.09	109.52
5	C	3701	FB	C9-C1-N8	4.00	117.01	111.43
4	E	5600	AGS	O2G-PG-S1G	-4.00	108.51	112.73
4	B	2600	AGS	O2G-PG-S1G	-3.97	108.54	112.73
4	D	4600	AGS	C4-C5-N7	-3.95	106.14	109.52
5	F	6701	FB	O2-C1-C1A	3.94	114.25	106.47
4	E	5600	AGS	C4-C5-N7	-3.87	106.21	109.52
5	C	3701	FB	C6-C5-C5A	-3.87	115.72	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1600	AGS	C4-C5-N7	-3.85	106.22	109.52
5	B	2701	FB	C6-C5-C5A	-3.85	115.74	120.10
4	C	3600	AGS	O3G-PG-S1G	-3.82	108.70	112.73
5	D	4701	FB	O2-C1-C1A	3.76	113.89	106.47
4	F	6600	AGS	C8-N9-C4	-3.75	104.03	106.90
5	C	3701	FB	O2-C1-C1A	3.73	113.83	106.47
5	D	4701	FB	C6-C5-C5A	-3.60	116.03	120.10
5	B	2701	FB	O2-C1-C1A	3.58	113.53	106.47
4	C	3600	AGS	C8-N9-C4	-3.44	104.27	106.90
4	E	5600	AGS	O3G-PG-S1G	-3.44	109.10	112.73
4	A	1600	AGS	O2G-PG-S1G	-3.43	109.11	112.73
4	C	3600	AGS	C3'-C2'-C1'	3.43	106.27	100.91
4	F	6600	AGS	O3G-PG-S1G	-3.41	109.14	112.73
4	D	4600	AGS	C8-N9-C4	-3.36	104.34	106.90
5	E	5701	FB	C6-C5-C5A	-3.32	116.35	120.10
4	F	6600	AGS	C3'-C2'-C1'	3.21	105.94	100.91
4	D	4600	AGS	O3G-PG-S1G	-3.20	109.36	112.73
4	D	4600	AGS	PB-O3B-PG	-3.15	121.03	131.81
5	E	5701	FB	O2-C1-C1A	3.13	112.65	106.47
4	D	4600	AGS	C3'-C2'-C1'	3.12	105.80	100.91
4	E	5600	AGS	C3'-C2'-C1'	3.12	105.78	100.91
5	E	5701	FB	O2A-C2A-C1A	3.11	112.56	107.50
4	E	5600	AGS	PB-O3B-PG	-3.06	121.37	131.81
4	A	1600	AGS	O3G-PG-S1G	-3.03	109.53	112.73
5	F	6701	FB	O2A-C2A-C1A	3.02	112.42	107.50
5	D	4701	FB	O2A-C2A-C1A	3.02	112.41	107.50
4	A	1600	AGS	PB-O3B-PG	-3.01	121.52	131.81
4	B	2600	AGS	C8-N9-C4	-2.98	104.62	106.90
4	E	5600	AGS	C8-N9-C4	-2.94	104.66	106.90
4	A	1600	AGS	C8-N9-C4	-2.93	104.66	106.90
5	B	2701	FB	O2A-C2A-C1A	2.92	112.26	107.50
4	F	6600	AGS	PB-O3B-PG	-2.90	121.89	131.81
5	C	3701	FB	O2A-C2A-C1A	2.80	112.06	107.50
4	C	3600	AGS	PB-O3B-PG	-2.79	122.27	131.81
5	F	6701	FB	O6-C6-N10	2.78	113.51	107.23
4	A	1600	AGS	C3'-C2'-C1'	2.71	105.15	100.91
5	B	2701	FB	O6-C6-N10	2.69	113.31	107.23
5	E	5701	FB	O6-C6-N10	2.67	113.25	107.23
4	B	2600	AGS	C3'-C2'-C1'	2.63	105.02	100.91
4	D	4600	AGS	O3A-PB-O3B	2.57	106.89	101.66
5	C	3701	FB	O6-C6-N10	2.53	112.93	107.23
4	F	6600	AGS	O2G-PG-S1G	-2.52	110.07	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2600	AGS	O3G-PG-S1G	-2.50	110.09	112.73
5	C	3701	FB	C1A-C1-C9	2.45	118.16	109.66
4	E	5600	AGS	C2-N1-C6	2.42	123.14	118.77
4	A	1600	AGS	C2-N1-C6	2.42	123.13	118.77
4	F	6600	AGS	C5-C4-N9	2.42	110.65	107.16
5	D	4701	FB	C3-O2-C1	-2.41	115.13	118.62
4	C	3600	AGS	O2G-PG-S1G	-2.41	110.19	112.73
4	D	4600	AGS	C2-N1-C6	2.40	123.10	118.77
5	F	6701	FB	C3-O2-C1	-2.39	115.16	118.62
4	B	2600	AGS	C2-N1-C6	2.39	123.08	118.77
4	C	3600	AGS	C2-N1-C6	2.38	123.07	118.77
4	B	2600	AGS	PB-O3B-PG	-2.38	123.68	131.81
4	A	1600	AGS	O3A-PB-O3B	2.37	106.48	101.66
4	F	6600	AGS	C2-N1-C6	2.36	123.03	118.77
4	C	3600	AGS	C5-C4-N9	2.31	110.50	107.16
5	B	2701	FB	C3-O2-C1	-2.29	115.30	118.62
5	E	5701	FB	C1A-C1-C9	2.29	117.60	109.66
4	D	4600	AGS	C5-C4-N9	2.26	110.43	107.16
5	D	4701	FB	C1A-C1-C9	2.26	117.50	109.66
5	F	6701	FB	C1A-C1-C9	2.24	117.44	109.66
5	B	2701	FB	C1A-C1-C9	2.22	117.36	109.66
4	B	2600	AGS	C2'-C3'-C4'	2.21	107.06	102.65
4	B	2600	AGS	PA-O3A-PB	-2.20	125.23	131.68
4	B	2600	AGS	C5-C4-N9	2.20	110.34	107.16
4	E	5600	AGS	C5-C4-N9	2.19	110.33	107.16
4	A	1600	AGS	C5-C4-N9	2.16	110.28	107.16
4	F	6600	AGS	C5-C4-N3	-2.13	121.06	125.70
4	E	5600	AGS	O3A-PB-O3B	2.11	105.95	101.66
5	C	3701	FB	C3-O2-C1	-2.10	115.57	118.62
4	A	1600	AGS	C2'-C3'-C4'	2.09	106.82	102.65
4	F	6600	AGS	PA-O3A-PB	-2.09	125.56	131.68
4	E	5600	AGS	PA-O3A-PB	-2.06	125.65	131.68
5	D	4701	FB	O6-C6-N10	2.05	111.86	107.23
4	C	3600	AGS	C4'-O4'-C1'	2.04	111.96	109.75
4	B	2600	AGS	C5-C4-N3	-2.04	121.26	125.70
4	A	1600	AGS	PA-O3A-PB	-2.03	125.72	131.68
4	A	1600	AGS	C6-C5-N7	2.03	139.10	131.34
5	F	6701	FB	O9-C9-N10	-2.02	119.94	123.32
4	B	2600	AGS	C6-C5-N7	2.02	139.05	131.34
5	E	5701	FB	O6-C6-C7	2.02	112.33	107.43
4	D	4600	AGS	C5-C4-N3	-2.02	121.31	125.70
4	C	3600	AGS	PA-O3A-PB	-2.01	125.78	131.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	5701	FB	C3-O2-C1	-2.01	115.70	118.62
4	E	5600	AGS	C6-C5-N7	2.01	139.03	131.34

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	3701	FB	C2A-C1A-C1-N8
5	F	6701	FB	C2A-C1A-C1-N8
5	D	4701	FB	C2A-C1A-C1-N8
5	E	5701	FB	C2A-C1A-C1-N8
5	B	2701	FB	C2A-C1A-C1-N8

There are no ring outliers.

## 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 ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.