



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:15 am GMT

PDB ID : 1IO4  
Title : CRYSTAL STRUCTURE OF RUNX-1/AML1/CBFALPHA RUNT DOMAIN-CBFBETA CORE DOMAIN HETERODIMER AND C/EBPBETA BZIP HOMODIMER BOUND TO A DNA FRAGMENT FROM THE CSF-1R PROMOTER  
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Deposited on : 2001-01-10  
Resolution : 3.00 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](mailto: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.

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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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

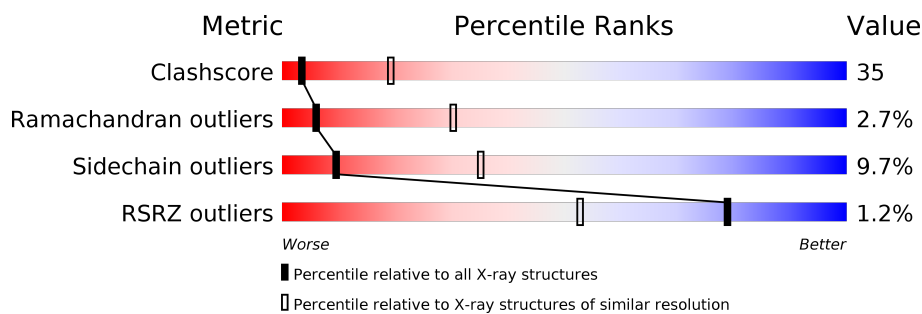
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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. 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	E	26	<div> <div>12%</div> <div>88%</div> </div>
2	F	26	<div> <div>15%</div> <div>73%</div> <div>12%</div> </div>
3	A	78	<div> <div>3%</div> <div>42%</div> <div>35%</div> <div>19%</div> </div>
3	B	78	<div> <div>56%</div> <div>29%</div> <div>10%</div> </div>
4	C	123	<div> <div>44%</div> <div>48%</div> <div>5%</div> </div>
5	D	141	<div> <div>3%</div> <div>34%</div> <div>48%</div> <div>9%</div> <div>9%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4197 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 DNA chain called CSF-1R PROMOTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	26	Total	C	N	O	P	0	0	0
			532	255	96	156	25			

- Molecule 2 is a DNA chain called CSF-1R PROMOTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	26	Total	C	N	O	P	0	0	0
			528	253	98	152	25			

- Molecule 3 is a protein called CAAT/ENHANCER BINDING PROTEIN BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	63	Total	C	N	O	S	0	0	0
			538	328	110	99	1			
3	B	70	Total	C	N	O	S	0	0	0
			595	364	120	110	1			

- Molecule 4 is a protein called RUNT-RELATED TRANSCRIPTION FACTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	120	Total	C	N	O	S	0	0	0
			934	586	175	169	4			

- Molecule 5 is a protein called CORE-BINDING FACTOR, BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	128	Total	C	N	O	S	0	0	0
			1059	663	193	197	6			

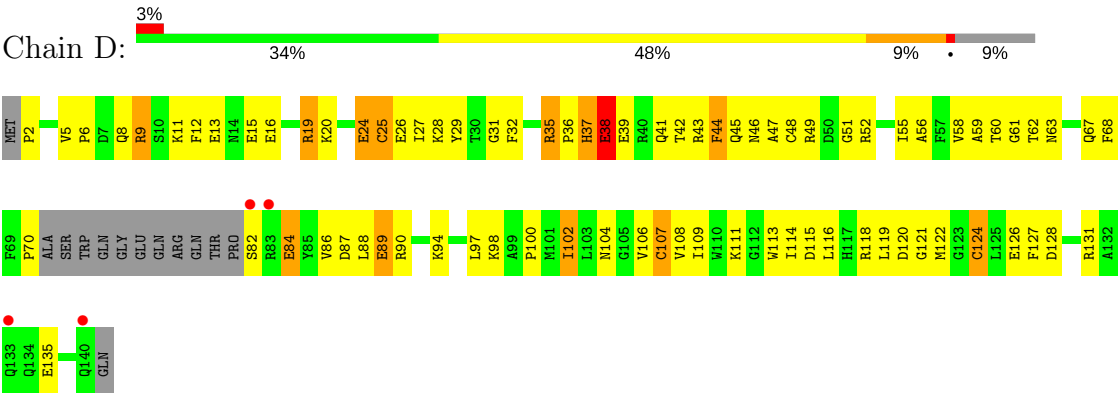
- Molecule 6 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total 2	Au 2	0	0
6	C	1	Total 1	Au 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 1	O 1	0	0
7	E	5	Total 5	O 5	0	0
7	F	2	Total 2	O 2	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.11Å 163.60Å 109.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 3.00 19.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.8 (19.95-3.00) 94.1 (19.94-2.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	6.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.29 (at 2.88Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.247 , 0.299 0.238 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	59.4	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4197	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
AU

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	E	0.53	0/596	0.80	0/919
2	F	0.55	0/592	0.80	0/911
3	A	0.32	0/541	0.49	0/717
3	B	0.35	0/598	0.50	0/793
4	C	0.47	0/954	0.78	0/1297
5	D	0.36	0/1080	0.65	0/1448
All	All	0.43	0/4361	0.70	0/6085

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	F	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	18	DG	Sidechain
2	F	6	DA	Sidechain
2	F	7	DC	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	532	0	296	28	0
2	F	528	0	294	49	0
3	A	538	0	564	38	0
3	B	595	0	629	34	0
4	C	934	0	939	63	0
5	D	1059	0	1019	93	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
7	B	1	0	0	0	0
7	E	5	0	0	0	0
7	F	2	0	0	1	0
All	All	4197	0	3741	279	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 35.

All (279) 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:F:20:DA:H2''	2:F:21:DA:H5'	1.31	1.13
2:F:11:DA:H2''	2:F:12:DG:H5'	1.16	1.08
2:F:20:DA:H2''	2:F:21:DA:C5'	1.84	1.06
4:C:158:GLN:HG2	5:D:102:ILE:HD12	1.47	0.96
2:F:22:DA:H2''	2:F:23:DT:C5'	1.96	0.95
4:C:139:ARG:HD3	4:C:170:VAL:HG23	1.53	0.91
2:F:11:DA:C2'	2:F:12:DG:H5'	2.01	0.90
4:C:91:VAL:HB	4:C:129:ALA:HB3	1.53	0.90
2:F:9:DA:H1'	2:F:10:DC:H5'	1.53	0.89
2:F:22:DA:H2''	2:F:23:DT:H5''	1.56	0.87
1:E:22:DT:H2''	1:E:23:DT:H5''	1.55	0.86
3:B:280:ARG:HA	3:B:283:ILE:HD12	1.58	0.86
5:D:60:THR:HG23	5:D:62:THR:H	1.41	0.84
5:D:88:LEU:O	5:D:89:GLU:HB2	1.77	0.83
2:F:11:DA:H2''	2:F:12:DG:C5'	2.06	0.82
2:F:6:DA:H2''	2:F:7:DC:H5'	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:95:GLY:O	4:C:127:GLN:NE2	2.12	0.82
2:F:22:DA:H2''	2:F:23:DT:H5'	1.62	0.81
4:C:87:ILE:O	4:C:87:ILE:HD12	1.80	0.80
5:D:55:ILE:HG22	5:D:56:ALA:H	1.48	0.78
4:C:105:VAL:HG22	4:C:120:ALA:HB1	1.65	0.78
3:A:327:LEU:O	3:A:327:LEU:HD13	1.84	0.77
5:D:115:ASP:OD2	5:D:118:ARG:HG3	1.84	0.77
5:D:51:GLY:HA2	5:D:68:PHE:HD2	1.49	0.77
2:F:12:DG:H2''	2:F:13:DA:OP2	1.84	0.77
2:F:20:DA:H2''	2:F:21:DA:H5''	1.66	0.76
5:D:28:LYS:HG3	5:D:58:VAL:HG21	1.66	0.76
5:D:109:ILE:HG13	5:D:128:ASP:HB2	1.68	0.75
5:D:38:GLU:O	5:D:41:GLN:HG2	1.86	0.75
1:E:22:DT:H2''	1:E:23:DT:C5'	2.17	0.73
2:F:22:DA:C2'	2:F:23:DT:H5''	2.18	0.73
1:E:23:DT:H2''	1:E:24:DG:C8	2.23	0.73
1:E:21:DG:H1'	1:E:22:DT:H5''	1.71	0.72
3:A:324:LEU:O	3:A:328:ARG:HG3	1.88	0.72
3:A:324:LEU:HD12	3:B:324:LEU:HD13	1.71	0.72
3:B:287:LYS:HD3	3:B:288:SER:N	2.04	0.71
5:D:19:ARG:HG3	5:D:20:LYS:N	2.06	0.71
1:E:22:DT:C2'	1:E:23:DT:H5''	2.19	0.71
5:D:55:ILE:HG22	5:D:56:ALA:N	2.06	0.69
5:D:111:LYS:HD2	5:D:126:GLU:OE2	1.92	0.69
5:D:28:LYS:HG3	5:D:58:VAL:CG2	2.22	0.69
3:A:327:LEU:HD12	3:B:327:LEU:CD2	2.24	0.68
3:A:327:LEU:HG	3:B:328:ARG:HE	1.59	0.68
5:D:42:THR:O	5:D:46:ASN:HB2	1.94	0.67
4:C:130:ARG:HG3	4:C:130:ARG:HH11	1.59	0.67
4:C:76:PRO:O	4:C:166:ILE:HG13	1.94	0.67
4:C:108:GLY:HA3	5:D:61:GLY:O	1.94	0.67
4:C:116:GLU:C	4:C:117:LEU:HD23	2.15	0.66
5:D:35:ARG:HG3	5:D:39:GLU:OE2	1.96	0.66
1:E:9:DC:H1'	1:E:10:DC:H5''	1.77	0.66
3:A:324:LEU:CG	3:B:324:LEU:HD13	2.25	0.66
4:C:109:ASN:ND2	4:C:145:SER:O	2.30	0.65
5:D:107:CYS:SG	5:D:131:ARG:HB3	2.37	0.65
1:E:6:DT:H1'	1:E:7:DT:H5'	1.79	0.65
3:A:276:ILE:HD13	3:A:277:ARG:N	2.11	0.65
4:C:109:ASN:HB3	4:C:112:ASN:H	1.62	0.65
4:C:63:VAL:HG22	4:C:64:ARG:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:108:VAL:HG12	5:D:109:ILE:N	2.12	0.65
5:D:8:GLN:OE1	5:D:8:GLN:N	2.28	0.64
4:C:118:ARG:HB2	4:C:135:ARG:HB2	1.80	0.64
2:F:20:DA:C2'	2:F:21:DA:H5'	2.20	0.64
1:E:9:DC:H2''	1:E:10:DC:H5''	1.78	0.64
5:D:118:ARG:HB3	5:D:118:ARG:NH1	2.12	0.64
5:D:70:PRO:CD	5:D:84:GLU:HG3	2.28	0.64
3:A:292:ALA:HA	3:A:295:ARG:NH1	2.13	0.63
2:F:20:DA:C2'	2:F:21:DA:C5'	2.71	0.63
5:D:113:TRP:O	5:D:121:GLY:HA3	1.99	0.63
5:D:118:ARG:HH11	5:D:120:ASP:HB3	1.64	0.62
2:F:14:DG:H1'	2:F:15:DT:H5''	1.79	0.62
1:E:9:DC:H2''	1:E:10:DC:C5'	2.30	0.62
3:B:328:ARG:HG3	3:B:328:ARG:HH11	1.65	0.61
2:F:7:DC:H6	2:F:7:DC:H5'	1.65	0.61
3:B:267:VAL:HG12	3:B:268:ASP:N	2.16	0.61
2:F:15:DT:H1'	2:F:16:DT:H5'	1.82	0.60
2:F:23:DT:H1'	2:F:24:DC:H5'	1.81	0.60
3:A:269:LYS:N	3:A:269:LYS:HD2	2.16	0.60
5:D:70:PRO:HD2	5:D:84:GLU:HG3	1.82	0.60
3:A:324:LEU:CD1	3:B:324:LEU:HD13	2.31	0.60
5:D:118:ARG:NH1	5:D:120:ASP:HB3	2.17	0.60
1:E:14:DC:C6	1:E:15:DT:H72	2.37	0.60
5:D:19:ARG:HG3	5:D:20:LYS:H	1.67	0.59
5:D:8:GLN:HB3	5:D:106:VAL:HG13	1.82	0.59
5:D:109:ILE:HD11	5:D:128:ASP:OD2	2.03	0.59
5:D:19:ARG:HH11	5:D:19:ARG:HB2	1.68	0.59
4:C:139:ARG:H	4:C:139:ARG:HE	1.48	0.59
2:F:18:DG:H2''	2:F:19:DG:OP2	2.03	0.59
2:F:21:DA:H2''	2:F:22:DA:OP2	2.03	0.58
1:E:9:DC:C2'	1:E:10:DC:H5''	2.33	0.58
4:C:118:ARG:HH12	4:C:135:ARG:NH1	2.01	0.58
4:C:90:LYS:HA	4:C:129:ALA:O	2.04	0.58
4:C:91:VAL:HB	4:C:129:ALA:CB	2.31	0.58
4:C:70:PHE:CZ	4:C:152:VAL:HG21	2.38	0.58
5:D:108:VAL:CG1	5:D:109:ILE:N	2.67	0.58
2:F:12:DG:H1'	2:F:13:DA:C8	2.39	0.57
4:C:139:ARG:N	4:C:139:ARG:HE	2.01	0.57
3:A:327:LEU:HD12	3:B:327:LEU:HD23	1.84	0.57
2:F:9:DA:C1'	2:F:10:DC:H5'	2.30	0.57
2:F:7:DC:H1'	2:F:8:DC:H5'	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:51:GLY:HA2	5:D:68:PHE:CD2	2.37	0.57
5:D:46:ASN:O	5:D:49:ARG:HB3	2.05	0.57
4:C:154:THR:O	4:C:156:PRO:C	2.44	0.57
1:E:16:DC:H1'	1:E:17:DT:H5'	1.87	0.56
5:D:29:TYR:CE1	5:D:31:GLY:HA3	2.41	0.56
4:C:67:SER:HB2	5:D:104:ASN:HA	1.86	0.56
3:A:318:GLU:O	3:A:322:ARG:HG2	2.06	0.56
5:D:24:GLU:HG2	5:D:124:CYS:SG	2.46	0.56
4:C:104:THR:HA	4:C:120:ALA:O	2.06	0.56
2:F:20:DA:C2'	2:F:21:DA:H5''	2.36	0.56
4:C:64:ARG:HA	4:C:71:LEU:CD2	2.36	0.55
5:D:82:SER:CB	5:D:111:LYS:NZ	2.70	0.54
1:E:8:DT:H1'	1:E:9:DC:H5'	1.90	0.54
4:C:114:SER:HA	5:D:63:ASN:HD21	1.73	0.54
1:E:4:DG:H2''	1:E:5:DA:OP2	2.08	0.54
3:B:278:ARG:NH2	3:B:281:ASN:HB3	2.23	0.53
5:D:28:LYS:O	5:D:55:ILE:HG23	2.08	0.53
2:F:24:DC:H2''	2:F:25:DT:OP2	2.08	0.53
3:A:313:LEU:O	3:A:317:VAL:HG23	2.08	0.53
4:C:157:PRO:O	5:D:102:ILE:HG13	2.09	0.53
5:D:9:ARG:O	5:D:13:GLU:HG3	2.09	0.53
2:F:8:DC:H2''	2:F:9:DA:H5'	1.91	0.53
5:D:26:GLU:HA	5:D:122:MET:HG2	1.90	0.53
4:C:64:ARG:HA	4:C:71:LEU:HD23	1.91	0.53
1:E:24:DG:H1'	1:E:25:DC:H5'	1.91	0.52
3:A:310:ASN:HB2	3:B:310:ASN:HD21	1.73	0.52
4:C:163:HIS:O	4:C:164:ARG:C	2.47	0.52
3:A:277:ARG:O	3:A:280:ARG:HB3	2.10	0.52
4:C:116:GLU:O	4:C:117:LEU:HD23	2.09	0.52
2:F:9:DA:H2''	2:F:10:DC:O5'	2.09	0.52
5:D:82:SER:HB2	5:D:111:LYS:NZ	2.25	0.52
2:F:14:DG:H2''	2:F:15:DT:H5'	1.92	0.52
5:D:118:ARG:O	5:D:119:LEU:HB2	2.09	0.52
3:A:324:LEU:CB	3:B:324:LEU:HD13	2.40	0.51
3:A:326:THR:O	3:A:330:LEU:HG	2.10	0.51
5:D:25:CYS:O	5:D:27:ILE:HG23	2.10	0.51
4:C:63:VAL:CG2	4:C:64:ARG:N	2.73	0.51
5:D:32:PHE:CE2	5:D:43:ARG:HD2	2.45	0.51
3:A:279:GLU:HA	3:A:282:ASN:HD22	1.76	0.51
2:F:22:DA:C2'	2:F:23:DT:C5'	2.78	0.51
4:C:142:ARG:C	4:C:144:LYS:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:70:PHE:CE2	4:C:152:VAL:HG21	2.46	0.51
3:B:278:ARG:NH1	3:B:282:ASN:OD1	2.37	0.51
5:D:56:ALA:HB2	5:D:63:ASN:HA	1.92	0.51
1:E:17:DT:H2''	1:E:18:DG:OP2	2.11	0.51
4:C:78:HIS:CD2	4:C:167:LYS:HE3	2.46	0.51
5:D:70:PRO:HG2	5:D:84:GLU:CD	2.32	0.50
3:B:314:GLN:HA	3:B:314:GLN:OE1	2.10	0.50
3:B:328:ARG:HG3	3:B:328:ARG:NH1	2.24	0.50
5:D:39:GLU:O	5:D:43:ARG:HG2	2.11	0.50
4:C:118:ARG:NH1	4:C:135:ARG:NH1	2.59	0.50
5:D:45:GLN:O	5:D:48:CYS:HB3	2.11	0.50
4:C:118:ARG:NH1	4:C:135:ARG:HH11	2.10	0.50
1:E:9:DC:C1'	1:E:10:DC:H5''	2.41	0.50
2:F:5:DA:H1'	2:F:6:DA:H5''	1.94	0.49
3:A:324:LEU:HB2	3:B:324:LEU:HD22	1.93	0.49
3:B:267:VAL:HG12	3:B:268:ASP:H	1.74	0.49
1:E:20:DG:O6	4:C:174:ARG:NH1	2.39	0.49
2:F:14:DG:H2''	2:F:15:DT:OP2	2.11	0.49
5:D:87:ASP:OD2	5:D:90:ARG:HB2	2.12	0.49
3:B:316:LYS:NZ	3:B:316:LYS:HA	2.27	0.49
3:B:324:LEU:O	3:B:328:ARG:HG2	2.13	0.49
5:D:44:PHE:CD2	5:D:44:PHE:C	2.84	0.49
5:D:47:ALA:HB1	5:D:52:ARG:O	2.12	0.49
5:D:56:ALA:CB	5:D:63:ASN:HA	2.42	0.48
3:A:327:LEU:HG	3:B:328:ARG:NE	2.26	0.48
4:C:151:THR:HG23	4:C:159:VAL:CG2	2.44	0.48
2:F:7:DC:H2''	2:F:8:DC:H5'	1.95	0.48
5:D:51:GLY:CA	5:D:68:PHE:HD2	2.22	0.48
3:A:322:ARG:HA	3:A:325:SER:HB3	1.96	0.48
4:C:105:VAL:HG23	4:C:117:LEU:HD12	1.95	0.48
5:D:82:SER:HB3	5:D:111:LYS:NZ	2.28	0.48
4:C:69:ASN:HB2	5:D:2:PRO:O	2.14	0.48
5:D:88:LEU:O	5:D:89:GLU:CB	2.56	0.48
2:F:13:DA:H2''	2:F:14:DG:H5'	1.94	0.48
5:D:16:GLU:HA	5:D:19:ARG:HG2	1.95	0.48
4:C:117:LEU:N	4:C:117:LEU:HD23	2.27	0.48
5:D:86:VAL:HG23	5:D:97:LEU:CD2	2.44	0.48
5:D:86:VAL:HG23	5:D:97:LEU:HD23	1.95	0.48
2:F:14:DG:H1'	2:F:15:DT:C5'	2.44	0.48
2:F:8:DC:H1'	2:F:9:DA:H5''	1.96	0.48
3:A:327:LEU:CG	3:B:328:ARG:HE	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:273:GLU:O	3:A:276:ILE:HG23	2.14	0.47
5:D:94:LYS:HB2	5:D:114:ILE:O	2.14	0.47
5:D:127:PHE:H	5:D:127:PHE:HD1	1.62	0.47
4:C:109:ASN:N	4:C:112:ASN:O	2.46	0.47
5:D:82:SER:HB2	5:D:111:LYS:HZ1	1.79	0.47
1:E:15:DT:H1'	1:E:16:DC:H5'	1.95	0.47
3:B:300:GLN:O	3:B:303:VAL:HB	2.13	0.47
3:B:316:LYS:HZ2	3:B:316:LYS:HA	1.79	0.47
2:F:14:DG:H3'	3:B:287:LYS:HE3	1.97	0.47
4:C:120:ALA:HA	4:C:134:LEU:HD13	1.96	0.47
4:C:151:THR:HG23	4:C:159:VAL:HG22	1.96	0.47
1:E:19:DT:H1'	1:E:20:DG:H5''	1.97	0.47
1:E:12:DA:H2''	1:E:13:DA:OP2	2.15	0.47
5:D:111:LYS:HD2	5:D:126:GLU:CD	2.36	0.46
5:D:118:ARG:HB3	5:D:118:ARG:HH11	1.78	0.46
5:D:16:GLU:O	5:D:19:ARG:HG2	2.15	0.46
4:C:142:ARG:O	4:C:144:LYS:N	2.49	0.46
5:D:5:VAL:HB	5:D:6:PRO:CD	2.45	0.46
3:A:326:THR:HA	3:A:329:ASN:HD22	1.80	0.46
5:D:89:GLU:O	5:D:90:ARG:C	2.52	0.46
5:D:106:VAL:O	5:D:108:VAL:HG23	2.16	0.46
1:E:25:DC:H2''	1:E:26:DG:O5'	2.15	0.46
2:F:25:DT:H71	7:F:27:HOH:O	2.15	0.46
2:F:7:DC:H5'	2:F:7:DC:C6	2.49	0.46
3:A:322:ARG:HH11	3:A:322:ARG:HG3	1.80	0.46
5:D:12:PHE:C	5:D:12:PHE:CD1	2.89	0.46
5:D:55:ILE:CG2	5:D:56:ALA:N	2.77	0.46
3:A:276:ILE:HG23	3:A:277:ARG:H	1.81	0.45
1:E:21:DG:H2''	1:E:22:DT:C5'	2.45	0.45
4:C:116:GLU:CD	4:C:137:VAL:HG11	2.37	0.45
5:D:108:VAL:CG1	5:D:109:ILE:H	2.29	0.45
4:C:75:LEU:HD11	4:C:148:LEU:HD21	1.98	0.44
5:D:70:PRO:HG2	5:D:84:GLU:CG	2.48	0.44
5:D:37:HIS:CE1	5:D:119:LEU:HD12	2.52	0.44
5:D:55:ILE:CG2	5:D:56:ALA:H	2.25	0.44
2:F:8:DC:H2''	2:F:9:DA:C5'	2.48	0.44
4:C:68:PRO:HG3	5:D:5:VAL:CG1	2.48	0.44
5:D:82:SER:CB	5:D:111:LYS:HZ3	2.30	0.44
5:D:8:GLN:HG3	5:D:106:VAL:HA	2.00	0.44
5:D:19:ARG:CB	5:D:19:ARG:NH1	2.81	0.44
2:F:24:DC:H1'	2:F:25:DT:H5''	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:276:ILE:HD11	3:A:280:ARG:HE	1.83	0.44
5:D:98:LYS:HG2	5:D:111:LYS:HG2	1.99	0.44
4:C:130:ARG:NH1	4:C:130:ARG:HG3	2.28	0.43
3:B:276:ILE:O	3:B:280:ARG:HG3	2.18	0.43
4:C:67:SER:CB	5:D:104:ASN:HA	2.48	0.43
5:D:67:GLN:O	5:D:100:PRO:HD2	2.17	0.43
2:F:7:DC:OP1	4:C:139:ARG:HG2	2.18	0.43
4:C:87:ILE:C	4:C:87:ILE:HD12	2.38	0.43
3:A:292:ALA:CB	3:A:295:ARG:NH1	2.81	0.43
3:A:324:LEU:HG	3:B:324:LEU:HD13	1.99	0.43
3:A:304:LEU:HA	3:A:304:LEU:HD12	1.90	0.43
5:D:70:PRO:HD3	5:D:84:GLU:HB2	2.01	0.43
3:B:281:ASN:O	3:B:285:VAL:HG23	2.19	0.43
5:D:19:ARG:HH11	5:D:19:ARG:CB	2.29	0.43
2:F:5:DA:C6	2:F:6:DA:C6	3.07	0.43
4:C:136:PHE:HB3	4:C:168:ILE:HG13	2.01	0.43
2:F:10:DC:H1'	2:F:11:DA:C8	2.54	0.43
2:F:3:DG:H1'	2:F:4:DC:H5'	2.01	0.43
3:B:270:HIS:O	3:B:271:SER:O	2.37	0.42
4:C:62:LEU:HD23	4:C:73:SER:HA	2.01	0.42
5:D:35:ARG:HD3	5:D:39:GLU:OE1	2.19	0.42
4:C:63:VAL:CG2	4:C:64:ARG:H	2.33	0.42
2:F:3:DG:H2''	2:F:4:DC:OP2	2.18	0.42
3:A:292:ALA:CA	3:A:295:ARG:NH1	2.82	0.42
5:D:27:ILE:HG13	5:D:27:ILE:O	2.18	0.42
3:B:267:VAL:CG1	3:B:268:ASP:N	2.82	0.42
3:B:316:LYS:HZ3	3:B:316:LYS:HB2	1.84	0.42
4:C:66:ASP:OD2	4:C:163:HIS:CE1	2.72	0.42
4:C:63:VAL:HG22	4:C:64:ARG:H	1.82	0.42
1:E:23:DT:H6	1:E:23:DT:H5'	1.84	0.42
4:C:84:THR:HG23	4:C:133:ASP:OD1	2.20	0.42
5:D:68:PHE:CZ	5:D:97:LEU:HD13	2.56	0.41
3:A:272:ASP:O	3:A:276:ILE:HG22	2.20	0.41
3:A:279:GLU:HA	3:A:282:ASN:ND2	2.35	0.41
5:D:36:PRO:O	5:D:37:HIS:C	2.58	0.41
5:D:60:THR:HG23	5:D:61:GLY:N	2.36	0.41
1:E:11:DA:H2'	3:B:278:ARG:HD3	2.01	0.41
3:A:324:LEU:HA	3:B:324:LEU:HD11	2.03	0.41
2:F:7:DC:C1'	2:F:8:DC:H5'	2.51	0.41
4:C:116:GLU:O	4:C:137:VAL:HB	2.21	0.41
4:C:66:ASP:OD2	4:C:163:HIS:ND1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:82:SER:HB3	5:D:111:LYS:HZ3	1.84	0.41
1:E:5:DA:H1'	1:E:6:DT:H5'	2.03	0.41
3:A:320:LEU:HB2	3:B:320:LEU:HD23	2.03	0.41
4:C:93:ALA:HB2	4:C:124:MET:CE	2.51	0.41
4:C:155:ASN:HA	4:C:156:PRO:HA	1.81	0.41
4:C:171:ASP:C	4:C:172:GLY:O	2.59	0.41
3:A:269:LYS:N	3:A:269:LYS:CD	2.83	0.40
1:E:13:DA:H1'	1:E:14:DC:H5''	2.03	0.40
2:F:6:DA:H2''	2:F:7:DC:C5'	2.39	0.40
3:A:281:ASN:O	3:A:282:ASN:C	2.59	0.40
3:A:285:VAL:O	3:A:286:ARG:C	2.59	0.40
2:F:7:DC:H2''	2:F:8:DC:C5'	2.51	0.40
4:C:86:PRO:HG2	4:C:87:ILE:HG13	2.01	0.40
5:D:11:LYS:O	5:D:15:GLU:N	2.49	0.40
5:D:39:GLU:O	5:D:42:THR:HB	2.21	0.40
5:D:5:VAL:HB	5:D:6:PRO:HD2	2.03	0.40
1:E:21:DG:H2''	1:E:22:DT:H5'	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	
3	A	61/78 (78%)	51 (84%)	9 (15%)	1 (2%)	11	46
3	B	68/78 (87%)	63 (93%)	4 (6%)	1 (2%)	12	48
4	C	118/123 (96%)	108 (92%)	8 (7%)	2 (2%)	11	44
5	D	124/141 (88%)	102 (82%)	16 (13%)	6 (5%)	2	16
All	All	371/420 (88%)	324 (87%)	37 (10%)	10 (3%)	6	30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	271	SER
5	D	9	ARG
5	D	24	GLU
5	D	37	HIS
5	D	89	GLU
3	A	271	SER
4	C	109	ASN
4	C	143	GLY
5	D	38	GLU
5	D	59	ALA

### 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	
3	A	60/74 (81%)	55 (92%)	5 (8%)	13	44
3	B	67/74 (90%)	61 (91%)	6 (9%)	11	40
4	C	102/105 (97%)	91 (89%)	11 (11%)	7	29
5	D	112/123 (91%)	101 (90%)	11 (10%)	9	34
All	All	341/376 (91%)	308 (90%)	33 (10%)	9	35

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	269	LYS
3	A	276	ILE
3	A	294	MET
3	A	325	SER
3	A	331	PHE
3	B	272	ASP
3	B	287	LYS
3	B	309	GLU
3	B	316	LYS
3	B	332	LYS
3	B	334	LEU
4	C	96	ASP

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Mol	Chain	Res	Type
4	C	109	ASN
4	C	110	ASP
4	C	114	SER
4	C	119	ASN
4	C	130	ARG
4	C	139	ARG
4	C	148	LEU
4	C	151	THR
4	C	162	TYR
4	C	170	VAL
5	D	19	ARG
5	D	25	CYS
5	D	35	ARG
5	D	38	GLU
5	D	44	PHE
5	D	84	GLU
5	D	102	ILE
5	D	107	CYS
5	D	116	LEU
5	D	124	CYS
5	D	135	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	310	ASN
3	A	329	ASN
3	B	300	GLN
3	B	310	ASN
4	C	132	ASN
5	D	41	GLN
5	D	63	ASN
5	D	134	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	E	26/26 (100%)	-0.90	0	100 100	39, 60, 85, 93	0
2	F	26/26 (100%)	-0.90	0	100 100	34, 63, 83, 87	0
3	A	63/78 (80%)	-0.48	1 (1%)	72 44	52, 89, 144, 166	0
3	B	70/78 (89%)	-0.65	0	100 100	26, 89, 130, 148	0
4	C	120/123 (97%)	-0.57	0	100 100	21, 57, 109, 128	0
5	D	128/141 (90%)	-0.24	4 (3%)	49 22	60, 102, 149, 171	0
All	All	433/472 (91%)	-0.51	5 (1%)	79 53	21, 82, 138, 171	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	82	SER	3.1
5	D	140	GLN	2.7
3	A	330	LEU	2.5
5	D	133	GLN	2.4
5	D	83	ARG	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	AU	D	200	1/1	0.97	0.08	-2.42	145,145,145,145	1
6	AU	C	200	1/1	0.99	0.05	-	89,89,89,89	0
6	AU	D	201	1/1	0.92	0.13	-	136,136,136,136	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.