



# Full wwPDB X-ray Structure Validation Report

Oct 14, 2014 – 08:37 PM EDT

PDB ID : 4L18  
Title : Crystal structure of Runx1 and Ets1 bound to TCR alpha promoter (crystal form 3)  
Authors : Tahirov, T.H.  
Deposited on : 2013-06-02  
Resolution : 2.30 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>

---

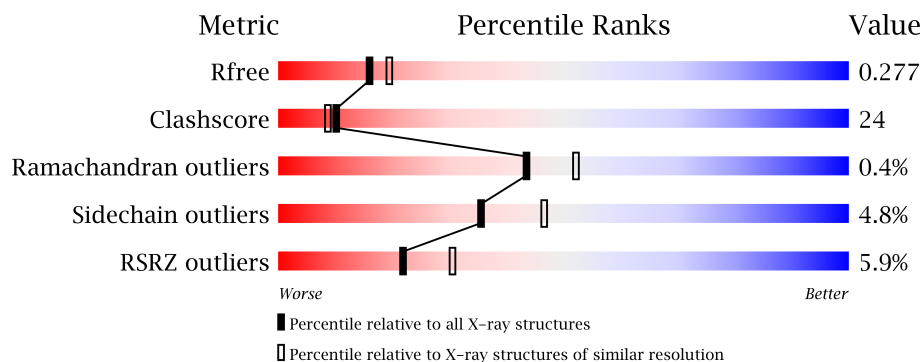
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23828  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23828

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	A	167	
1	E	167	
2	B	146	
2	F	146	
3	C	16	
3	G	16	
4	D	16	
4	H	16	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5431 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 protein called Runt-related transcription factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1103	692	201	206	4			
1	E	141	Total	C	N	O	S	0	0	0
			1092	686	197	205	4			

- Molecule 2 is a protein called Protein C-ets-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	107	Total	C	N	O	S	0	0	0
			897	580	154	159	4			
2	F	106	Total	C	N	O	S	0	0	0
			890	576	153	157	4			

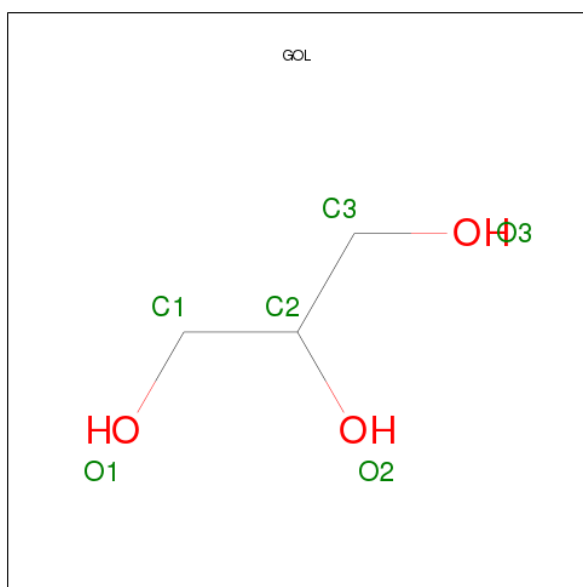
- Molecule 3 is a DNA chain called 5'-D(\*GP\*GP\*AP\*AP\*GP\*CP\*CP\*AP\*CP\*AP\*TP\*C P\*CP\*TP\*CP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	16	Total	C	N	O	P	0	0	0
			321	154	59	93	15			
3	G	16	Total	C	N	O	P	0	0	0
			321	154	59	93	15			

- Molecule 4 is a DNA chain called 5'-D(\*CP\*AP\*GP\*AP\*GP\*GP\*AP\*TP\*GP\*TP\*GP\*G P\*CP\*TP\*TP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	16	Total	C	N	O	P	0	0	0
			329	157	62	95	15			
4	H	16	Total	C	N	O	P	0	0	0
			329	157	62	95	15			

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	27	Total	O	0	0
			27	27		
6	B	25	Total	O	0	0
			25	25		
6	C	13	Total	O	0	0
			13	13		
6	D	18	Total	O	0	0
			18	18		
6	E	32	Total	O	0	0
			32	32		
6	F	14	Total	O	0	0
			14	14		
6	G	8	Total	O	0	0
			8	8		
6	H	6	Total	O	0	0
			6	6		



- Molecule 3: 5'-D(\*GP\*GP\*AP\*AP\*GP\*CP\*CP\*AP\*CP\*AP\*TP\*CP\*CP\*TP\*CP\*T)-3'

Chain C: 



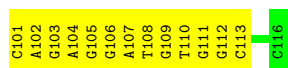
- Molecule 3: 5'-D(\*GP\*GP\*AP\*AP\*GP\*CP\*CP\*AP\*CP\*AP\*TP\*CP\*CP\*TP\*CP\*T)-3'

Chain G: 



- Molecule 4: 5'-D(\*CP\*AP\*GP\*AP\*GP\*GP\*AP\*TP\*GP\*TP\*GP\*GP\*CP\*TP\*TP\*C)-3',

Chain D: 



- Molecule 4: 5'-D(\*CP\*AP\*GP\*AP\*GP\*GP\*AP\*TP\*GP\*TP\*GP\*GP\*CP\*TP\*TP\*C)-3',

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.15Å 100.03Å 72.06Å 90.00° 110.23° 90.00°	Depositor
Resolution (Å)	29.64 – 2.30 29.64 – 2.31	Depositor EDS
% Data completeness (in resolution range)	87.5 (29.64-2.30) 87.6 (29.64-2.31)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.10 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.231 , 0.280 0.232 , 0.277	Depositor DCC
$R_{free}$ test set	1665 reflections (5.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.0	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 35366 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5431	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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: GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.44	0/1125	0.73	0/1527
1	E	0.46	0/1113	0.75	1/1512 (0.1%)
2	B	0.43	0/922	0.61	0/1243
2	F	0.37	0/915	0.58	0/1233
3	C	0.68	0/359	0.87	0/551
3	G	0.48	0/359	0.78	0/551
4	D	0.57	0/369	0.85	0/569
4	H	0.49	0/369	0.83	0/569
All	All	0.47	0/5531	0.73	1/7755 (0.0%)

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
3	C	0	2
3	G	0	1
4	D	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	55	LEU	N-CA-C	-6.91	92.36	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
3	C	13	DC	Sidechain
3	C	5	DG	Sidechain
4	D	103	DG	Sidechain
3	G	205	DG	Sidechain

## 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	A	1103	0	1104	51	0
1	E	1092	0	1092	49	0
2	B	897	0	889	29	0
2	F	890	0	885	41	0
3	C	321	0	181	15	0
3	G	321	0	181	24	0
4	D	329	0	182	17	0
4	H	329	0	182	27	0
5	D	6	0	8	0	0
6	A	27	0	0	5	0
6	B	25	0	0	1	0
6	C	13	0	0	1	0
6	D	18	0	0	0	0
6	E	32	0	0	5	0
6	F	14	0	0	0	0
6	G	8	0	0	1	0
6	H	6	0	0	1	0
All	All	5431	0	4704	236	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 24.

All (236) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:304:DA:H2''	4:H:305:DG:H5''	1.25	1.10
4:H:307:DA:H2''	4:H:308:DT:H5'	1.34	1.07
4:H:315:DT:H2''	4:H:316:DC:H5''	1.46	0.95

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:348:LYS:HA	2:B:351:GLN:HE21	1.34	0.92
1:A:147:THR:HG23	1:A:163:HIS:HA	1.51	0.91
1:E:56:ALA:HB1	1:E:61:GLU:HG2	1.55	0.89
4:D:104:DA:H2''	4:D:105:DG:H5'	1.56	0.86
1:E:56:ALA:HB2	1:E:62:LEU:HG	1.59	0.83
2:F:419:GLN:NE2	2:F:425:THR:HG22	1.94	0.83
1:E:116:GLU:HG2	1:E:137:VAL:HB	1.61	0.83
2:F:348:LYS:HA	2:F:351:GLN:HE21	1.48	0.79
3:C:12:DC:H1'	3:C:13:DC:H5'	1.64	0.79
1:A:56:ALA:HB1	1:A:61:GLU:HG2	1.64	0.79
4:H:307:DA:H2''	4:H:308:DT:C5'	2.12	0.79
2:B:361:TRP:HZ3	2:B:429:LEU:HD23	1.47	0.78
3:C:2:DG:H2''	3:C:3:DA:N7	2.00	0.77
3:G:206:DC:H2''	3:G:207:DC:H5'	1.66	0.77
3:C:2:DG:H2''	3:C:3:DA:C8	2.20	0.76
1:A:192:LEU:HD23	1:A:192:LEU:H	1.50	0.76
3:G:212:DC:H1'	3:G:213:DC:H5'	1.67	0.76
4:H:313:DC:C6	4:H:314:DT:H72	2.20	0.75
2:B:348:LYS:HG3	2:B:351:GLN:NE2	2.02	0.75
1:E:138:GLY:HA3	6:E:332:HOH:O	1.86	0.75
2:F:425:THR:OG1	2:F:428:GLU:HG3	1.88	0.73
1:A:58:HIS:CE1	1:A:61:GLU:HB2	2.24	0.72
4:H:302:DA:H1'	4:H:303:DG:H5'	1.71	0.71
3:G:210:DA:H1'	3:G:211:DT:H5''	1.72	0.70
3:C:6:DC:H1'	3:C:7:DC:H5'	1.72	0.70
1:E:52:VAL:HG22	1:E:55:LEU:HG	1.75	0.68
2:F:405:THR:HG21	2:F:408:LYS:HE2	1.76	0.68
4:H:314:DT:H1'	4:H:315:DT:H5''	1.75	0.68
1:A:56:ALA:HB2	1:A:62:LEU:HG	1.75	0.68
2:F:348:LYS:HA	2:F:351:GLN:NE2	2.10	0.67
3:G:205:DG:H2''	3:G:206:DC:H5'	1.77	0.66
4:H:304:DA:C2'	4:H:305:DG:H5''	2.15	0.66
1:E:192:LEU:H	1:E:192:LEU:HD23	1.61	0.66
1:E:56:ALA:CB	1:E:62:LEU:HG	2.25	0.66
4:D:104:DA:H2''	4:D:105:DG:C5'	2.25	0.65
3:C:11:DT:H1'	3:C:12:DC:H5'	1.79	0.64
1:A:68:PRO:O	1:A:94:LEU:HD12	1.98	0.64
2:F:419:GLN:HE21	2:F:425:THR:HG22	1.61	0.64
1:A:126:ASN:HD22	1:A:126:ASN:N	1.94	0.64
1:A:176:PRO:HB3	6:A:323:HOH:O	1.97	0.63
1:A:99:ASP:O	1:E:192:LEU:HD23	1.99	0.63
2:B:336:GLN:HG3	2:B:339:GLN:OE1	1.99	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:69:ASN:HB3	6:A:325:HOH:O	1.99	0.62
1:A:56:ALA:CB	1:A:61:GLU:HG2	2.31	0.60
2:B:362:GLU:OE1	2:B:411:VAL:HG11	2.02	0.60
1:A:194:PHE:CZ	2:B:429:LEU:HD13	2.37	0.60
1:A:87:ILE:HD12	1:A:87:ILE:O	2.02	0.59
2:F:389:LEU:HD23	2:F:389:LEU:C	2.22	0.59
3:G:212:DC:H1'	3:G:213:DC:C5'	2.31	0.59
1:A:55:LEU:HG	1:A:55:LEU:O	2.02	0.59
2:B:373:ARG:HH21	2:B:373:ARG:HG2	1.67	0.58
2:B:361:TRP:CZ3	2:B:429:LEU:HD23	2.34	0.58
4:D:112:DG:H2''	4:D:113:DC:H5'	1.85	0.58
3:G:204:DA:N7	6:G:303:HOH:O	2.31	0.58
4:H:308:DT:H2''	4:H:309:DG:OP2	2.03	0.58
4:H:307:DA:C2'	4:H:308:DT:H5'	2.22	0.58
3:C:10:DA:H2''	3:C:11:DT:H5'	1.85	0.58
1:A:174:ARG:NH2	4:D:111:DG:N7	2.49	0.58
2:F:419:GLN:NE2	2:F:425:THR:HA	2.19	0.58
4:H:311:DG:H2''	4:H:312:DG:OP2	2.04	0.58
2:F:403:HIS:CG	2:F:415:VAL:HG11	2.39	0.58
2:F:436:LYS:O	2:F:436:LYS:HD2	2.04	0.57
1:E:139:ARG:HD3	1:E:139:ARG:H	1.70	0.57
4:D:108:DT:H2''	4:D:109:DG:C8	2.39	0.57
3:G:201:DG:H2''	3:G:202:DG:C8	2.40	0.57
1:A:139:ARG:HB2	1:A:139:ARG:HH11	1.68	0.57
2:F:405:THR:HG22	2:F:408:LYS:HG3	1.85	0.56
1:E:144:LYS:O	1:E:167:LYS:HG3	2.04	0.56
4:H:312:DG:H2''	4:H:313:DC:H5''	1.87	0.56
1:E:53:GLU:CD	1:E:64:ARG:HG3	2.25	0.56
1:A:79:TRP:CZ2	1:A:86:PRO:HD3	2.40	0.56
1:A:192:LEU:HD23	1:A:192:LEU:N	2.20	0.56
1:E:193:SER:O	1:E:197:ARG:HG3	2.05	0.56
3:G:206:DC:C2'	3:G:207:DC:H5'	2.35	0.56
3:G:211:DT:H2''	3:G:212:DC:H5'	1.88	0.56
1:A:139:ARG:HD2	6:A:307:HOH:O	2.06	0.56
1:E:52:VAL:HG13	1:E:52:VAL:O	2.06	0.55
2:F:427:GLU:H	2:F:427:GLU:CD	2.03	0.55
1:A:139:ARG:CD	6:A:307:HOH:O	2.54	0.55
1:A:199:SER:O	1:A:203:GLN:HG3	2.07	0.55
1:E:87:ILE:O	1:E:87:ILE:HD12	2.07	0.55
2:F:388:LYS:NZ	3:G:211:DT:OP2	2.37	0.55
4:H:302:DA:N3	6:H:401:HOH:O	2.33	0.55
1:A:63:VAL:HG22	1:A:64:ARG:N	2.23	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:58:HIS:CE1	1:E:61:GLU:HB2	2.42	0.54
2:F:348:LYS:HG3	2:F:351:GLN:NE2	2.22	0.54
2:F:409:ARG:HG2	2:F:410:TYR:CD2	2.42	0.54
1:A:203:GLN:O	1:A:204:LEU:C	2.46	0.54
2:F:348:LYS:HG3	2:F:351:GLN:HE22	1.73	0.53
2:B:404:LYS:HG2	4:D:104:DA:OP1	2.08	0.53
4:H:304:DA:H2''	4:H:305:DG:C5'	2.18	0.53
2:B:337:LEU:HD13	2:B:375:TRP:CE2	2.44	0.53
3:C:5:DG:H2''	3:C:6:DC:H5'	1.91	0.53
3:C:10:DA:H1'	3:C:11:DT:H5''	1.91	0.52
2:F:389:LEU:HD23	2:F:389:LEU:O	2.09	0.52
1:A:139:ARG:H	1:A:139:ARG:HD3	1.74	0.52
3:G:210:DA:C2	4:H:309:DG:C2	2.98	0.52
4:H:313:DC:H2'	4:H:314:DT:H72	1.91	0.52
1:A:192:LEU:CD2	1:E:98:PRO:HB2	2.40	0.52
4:H:307:DA:C2'	4:H:308:DT:C5'	2.85	0.52
3:C:9:DC:H2''	3:C:10:DA:C8	2.45	0.52
1:A:70:PHE:CE2	1:A:152:VAL:HG21	2.46	0.51
3:G:209:DC:H2''	3:G:210:DA:C8	2.45	0.51
1:A:192:LEU:HD23	1:E:99:ASP:O	2.10	0.51
4:D:101:DC:H2''	4:D:102:DA:C8	2.45	0.51
4:D:107:DA:H1'	4:D:108:DT:H5''	1.93	0.51
1:A:192:LEU:HD22	1:E:98:PRO:HB2	1.92	0.51
1:E:98:PRO:HG2	1:E:101:THR:OG1	2.10	0.51
1:E:56:ALA:HB2	1:E:62:LEU:CG	2.34	0.50
1:E:68:PRO:O	1:E:94:LEU:HD12	2.12	0.50
2:F:425:THR:OG1	2:F:427:GLU:HG2	2.11	0.50
1:E:147:THR:HG23	1:E:163:HIS:HA	1.93	0.50
1:E:198:LEU:CD1	2:F:343:GLU:HA	2.42	0.50
2:F:436:LYS:C	2:F:436:LYS:HD2	2.32	0.50
1:A:75:LEU:HD11	1:A:148:LEU:HD11	1.94	0.49
3:G:210:DA:H2''	3:G:211:DT:H5'	1.94	0.49
2:B:425:THR:OG1	2:B:428:GLU:HG3	2.11	0.49
4:H:312:DG:H2''	4:H:313:DC:C5'	2.42	0.49
4:H:305:DG:H2''	4:H:306:DG:H8	1.76	0.49
2:B:357:THR:O	2:B:438:ASP:HB2	2.12	0.49
1:A:56:ALA:CB	1:A:62:LEU:HG	2.43	0.49
1:E:132:ASN:C	1:E:132:ASN:ND2	2.65	0.49
2:F:436:LYS:HD2	2:F:437:PRO:O	2.13	0.49
3:C:11:DT:H2''	3:C:12:DC:H5'	1.94	0.49
2:B:353:PHE:HB2	2:B:367:ASP:HB3	1.95	0.48
1:E:132:ASN:HD22	1:E:132:ASN:C	2.15	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:61:GLU:HG3	1:E:62:LEU:HD23	1.95	0.48
2:F:409:ARG:HG2	2:F:410:TYR:CE2	2.48	0.48
2:F:404:LYS:NZ	4:H:303:DG:OP1	2.45	0.48
1:A:91:VAL:HG22	1:A:150:ILE:HD13	1.95	0.48
2:F:408:LYS:HE3	2:F:411:VAL:HG11	1.96	0.48
2:F:362:GLU:HB2	2:F:413:ARG:NH1	2.29	0.48
1:A:139:ARG:HD3	1:A:139:ARG:N	2.28	0.48
2:B:426:PRO:HG2	2:B:427:GLU:OE2	2.14	0.47
4:D:104:DA:C8	4:D:104:DA:H5'	2.49	0.47
4:D:104:DA:H1'	4:D:105:DG:H5''	1.96	0.47
1:E:177:ARG:NH1	6:E:327:HOH:O	2.41	0.47
3:G:215:DC:H2''	3:G:216:DT:O5'	2.14	0.47
2:F:362:GLU:HB2	2:F:413:ARG:CZ	2.45	0.47
4:D:111:DG:H1'	4:D:112:DG:C8	2.50	0.47
1:A:75:LEU:CD1	1:A:148:LEU:HD11	2.44	0.47
2:F:404:LYS:HE3	4:H:303:DG:OP1	2.15	0.47
2:B:405:THR:HG21	2:B:408:LYS:HD2	1.97	0.47
2:F:342:LEU:O	2:F:346:THR:HG23	2.14	0.47
3:G:210:DA:H2''	3:G:211:DT:C5'	2.45	0.47
2:B:428:GLU:O	2:B:432:MET:HG3	2.15	0.47
4:H:312:DG:C2'	4:H:313:DC:H5''	2.44	0.47
1:A:126:ASN:ND2	1:A:126:ASN:N	2.63	0.47
1:A:136:PHE:HB2	1:A:168:ILE:HD12	1.96	0.47
1:A:82:ASN:OD1	1:A:118:ARG:NH1	2.47	0.47
4:D:108:DT:H2''	4:D:109:DG:H8	1.79	0.47
2:F:353:PHE:HB2	2:F:367:ASP:HB3	1.97	0.47
2:F:419:GLN:HE22	2:F:425:THR:HG22	1.76	0.46
1:E:171:ASP:HB3	1:E:174:ARG:HD2	1.95	0.46
1:E:70:PHE:CE2	1:E:152:VAL:HG21	2.51	0.46
1:A:75:LEU:HD21	1:A:89:PHE:CD2	2.51	0.46
4:D:111:DG:H2''	4:D:112:DG:OP2	2.16	0.46
1:E:54:VAL:HG12	6:E:321:HOH:O	2.15	0.46
2:F:425:THR:HG23	2:F:428:GLU:OE1	2.16	0.46
1:E:118:ARG:HG2	6:E:328:HOH:O	2.16	0.46
1:E:63:VAL:HG22	1:E:64:ARG:N	2.30	0.46
3:G:211:DT:H1'	3:G:212:DC:H5'	1.98	0.45
2:B:429:LEU:HD12	2:B:433:LEU:HD23	1.97	0.45
4:D:109:DG:H1'	4:D:110:DT:H5'	1.97	0.45
4:H:304:DA:H5'	4:H:304:DA:H8	1.81	0.45
1:A:63:VAL:CG2	1:A:64:ARG:N	2.79	0.45
1:A:84:THR:HG23	6:A:301:HOH:O	2.15	0.45
2:B:341:LEU:HD11	2:B:393:LEU:HD21	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:370:GLU:HA	2:B:370:GLU:OE1	2.17	0.45
1:E:92:VAL:HG13	1:E:128:VAL:HG22	1.98	0.45
4:D:107:DA:H2''	4:D:108:DT:H5'	1.98	0.45
2:F:375:TRP:CH2	2:F:379:LYS:HG3	2.52	0.45
1:A:56:ALA:HB2	1:A:62:LEU:CG	2.45	0.45
1:E:57:ASP:OD2	1:E:57:ASP:N	2.48	0.45
4:H:307:DA:H1'	4:H:308:DT:H5''	1.99	0.45
2:B:373:ARG:HG2	2:B:373:ARG:NH2	2.32	0.44
3:C:11:DT:C2'	3:C:12:DC:H5'	2.47	0.44
2:F:394:ARG:HA	2:F:397:TYR:CE2	2.51	0.44
1:A:78:HIS:NE2	1:A:172:GLY:HA2	2.33	0.44
1:A:193:SER:O	1:A:197:ARG:HG3	2.17	0.44
2:B:378:ARG:HG3	2:B:378:ARG:HH11	1.83	0.44
2:B:385:ASN:OD1	2:B:387:GLU:HB3	2.18	0.44
1:E:116:GLU:HG2	1:E:137:VAL:CB	2.40	0.44
2:F:385:ASN:ND2	2:F:388:LYS:HE2	2.33	0.44
2:B:430:HIS:HB3	2:B:435:VAL:HB	2.00	0.44
4:H:305:DG:H2''	4:H:306:DG:C8	2.53	0.44
3:G:206:DC:H1'	3:G:207:DC:H5'	1.99	0.44
1:A:58:HIS:O	1:A:61:GLU:HB3	2.18	0.43
3:G:212:DC:C1'	3:G:213:DC:H5'	2.43	0.43
1:E:171:ASP:HB3	1:E:174:ARG:CD	2.48	0.43
1:E:175:GLU:HA	1:E:175:GLU:OE2	2.17	0.43
1:E:78:HIS:NE2	1:E:172:GLY:HA2	2.33	0.43
3:G:211:DT:C2'	3:G:212:DC:H5'	2.47	0.43
2:B:361:TRP:HB3	2:B:414:PHE:HB2	2.00	0.43
3:G:206:DC:H1'	3:G:207:DC:C5'	2.49	0.43
1:E:79:TRP:HB2	1:E:166:ILE:HD11	2.01	0.43
2:F:408:LYS:HB2	2:F:411:VAL:HB	2.00	0.43
3:G:206:DC:H2''	3:G:207:DC:C5'	2.45	0.43
2:B:397:TYR:HB2	6:B:523:HOH:O	2.18	0.43
2:F:357:THR:HG21	2:F:362:GLU:HG2	1.99	0.43
2:B:336:GLN:HE21	2:B:336:GLN:HB3	1.68	0.42
1:E:155:ASN:HA	1:E:156:PRO:HA	1.92	0.42
3:G:203:DA:C6	3:G:204:DA:C6	3.07	0.42
3:G:202:DG:H2''	3:G:203:DA:OP2	2.19	0.42
3:C:11:DT:C1'	3:C:12:DC:H5'	2.49	0.42
1:A:98:PRO:HB2	1:E:192:LEU:HD22	2.02	0.42
1:E:196:GLU:O	1:E:200:GLU:HG3	2.20	0.42
1:E:63:VAL:CG2	1:E:64:ARG:N	2.83	0.42
1:A:112:ASN:N	1:A:112:ASN:HD22	2.18	0.42
3:C:10:DA:H1'	3:C:11:DT:C5'	2.49	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:139:ARG:HB3	6:E:325:HOH:O	2.19	0.42
1:A:79:TRP:NE1	1:A:83:LYS:HG2	2.34	0.42
1:E:139:ARG:HD3	1:E:139:ARG:N	2.32	0.42
1:A:142:ARG:HH22	3:C:3:DA:H2	1.68	0.42
2:B:390:SER:O	2:B:394:ARG:HG3	2.19	0.42
2:F:357:THR:CG2	2:F:362:GLU:HG2	2.50	0.42
1:A:80:ARG:HG3	1:A:171:ASP:O	2.19	0.41
1:A:79:TRP:HB2	1:A:166:ILE:HD11	2.02	0.41
4:D:104:DA:C2'	4:D:105:DG:C5'	2.98	0.41
2:F:404:LYS:CE	4:H:303:DG:OP1	2.69	0.41
2:B:426:PRO:O	2:B:430:HIS:CG	2.73	0.41
1:A:112:ASN:O	1:A:113:TYR:C	2.58	0.41
1:E:139:ARG:N	1:E:139:ARG:CD	2.84	0.41
4:H:304:DA:C6	4:H:305:DG:C6	3.09	0.41
2:B:391:ARG:NH2	4:D:106:DG:N7	2.53	0.41
2:F:354:ILE:O	2:F:354:ILE:HG23	2.19	0.41
2:F:361:TRP:HZ3	2:F:429:LEU:HD22	1.85	0.41
2:F:388:LYS:HZ1	3:G:211:DT:P	2.40	0.41
1:A:131:PHE:N	1:A:131:PHE:CD2	2.88	0.40
3:C:13:DC:H2'	6:C:110:HOH:O	2.21	0.40
1:E:119:ASN:ND2	1:E:133:ASP:O	2.54	0.40
1:E:60:GLY:O	1:E:74:VAL:HG21	2.22	0.40
1:E:61:GLU:HG3	1:E:62:LEU:N	2.34	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	138/167 (83%)	131 (95%)	5 (4%)	2 (1%)	16	15
1	E	137/167 (82%)	131 (96%)	6 (4%)	0	100	100
2	B	105/146 (72%)	100 (95%)	5 (5%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	104/146 (71%)	101 (97%)	3 (3%)	0	100	100
All	All	484/626 (77%)	463 (96%)	19 (4%)	2 (0%)	43	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	LEU
1	A	190	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	122/146 (84%)	114 (93%)	8 (7%)	24	29
1	E	121/146 (83%)	112 (93%)	9 (7%)	20	24
2	B	96/127 (76%)	94 (98%)	2 (2%)	66	83
2	F	96/127 (76%)	94 (98%)	2 (2%)	66	83
All	All	435/546 (80%)	414 (95%)	21 (5%)	35	46

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	61	GLU
1	A	83	LYS
1	A	112	ASN
1	A	126	ASN
1	A	139	ARG
1	A	162	TYR
1	A	192	LEU
2	B	434	ASP
2	B	436	LYS
1	E	57	ASP
1	E	61	GLU
1	E	77	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	114	SER
1	E	130	ARG
1	E	132	ASN
1	E	139	ARG
1	E	162	TYR
1	E	192	LEU
2	F	398	ASP
2	F	436	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	112	ASN
1	A	126	ASN
2	B	336	GLN
2	B	351	GLN
2	B	380	ASN
1	E	58	HIS
1	E	112	ASN
1	E	132	ASN
2	F	351	GLN
2	F	419	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	GOL	D	201	-	5,5,5	0.49	0	5,5,5	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	D	201	-	-	0/4/4/4	0/0/0/0

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.

## 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, 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	A	142/167 (85%)	0.53	12 (8%) 11 17	18, 50, 82, 101	0
1	E	141/167 (84%)	0.48	10 (7%) 16 23	18, 47, 86, 111	0
2	B	107/146 (73%)	0.28	3 (2%) 50 60	28, 48, 74, 109	0
2	F	106/146 (72%)	0.56	8 (7%) 14 21	39, 59, 80, 111	0
3	C	16/16 (100%)	0.06	0 100 100	28, 39, 65, 71	0
3	G	16/16 (100%)	0.05	0 100 100	38, 55, 85, 88	0
4	D	16/16 (100%)	-0.36	0 100 100	34, 46, 56, 62	0
4	H	16/16 (100%)	-0.23	0 100 100	44, 57, 67, 73	0
All	All	560/690 (81%)	0.40	33 (5%) 22 30	18, 51, 82, 111	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	ALA	7.6
1	E	55	LEU	6.2
1	A	55	LEU	5.7
2	F	437	PRO	4.7
1	A	54	VAL	4.6
1	E	56	ALA	4.6
1	E	113	TYR	4.6
2	F	332	SER	4.5
1	A	96	ASP	3.4
1	E	175	GLU	3.4
1	A	177	ARG	3.3
1	A	113	TYR	3.3
1	E	190	GLY	3.3
1	E	57	ASP	3.2
2	B	439	ALA	3.2
1	A	57	ASP	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	110	ASP	2.9
1	A	175	GLU	2.7
1	E	53	GLU	2.7
2	F	398	ASP	2.7
1	E	111	GLU	2.5
2	B	349	SER	2.4
2	B	433	LEU	2.4
1	A	194	PHE	2.4
2	F	408	LYS	2.3
2	F	429	LEU	2.3
2	F	389	LEU	2.1
2	F	405	THR	2.1
1	E	156	PRO	2.1
2	F	407	GLY	2.1
1	A	60	GLY	2.0
1	A	64	ARG	2.0
1	A	102	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	D	201	6/6	0.13	-0.82	53,54,55,56	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.