



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:01 PM GMT

PDB ID : 4IMY
Title : The AFF4 scaffold binds human P-TEFb adjacent to HIV Tat
Authors : Alber, T.; Schulze-Gahmen, U.
Deposited on : 2013-01-03
Resolution : 2.94 Å(reported)

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

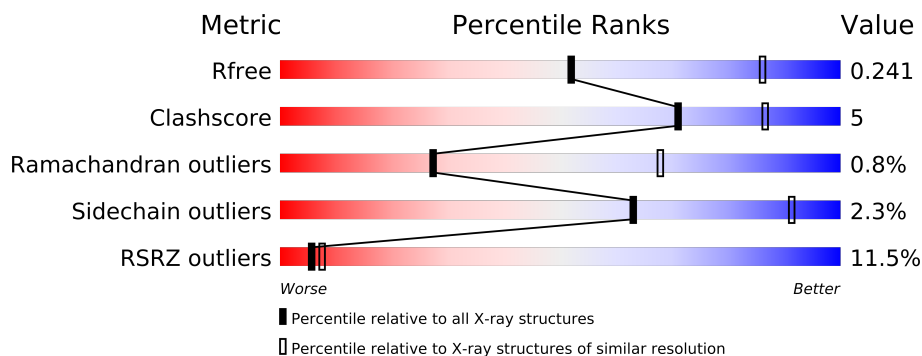
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
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) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.94 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	1424 (2.98-2.90)
Clashscore	79885	1761 (2.98-2.90)
Ramachandran outliers	78287	1708 (2.98-2.90)
Sidechain outliers	78261	1710 (2.98-2.90)
RSRZ outliers	66119	1425 (2.98-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	332	
1	C	332	
1	E	332	
2	B	264	
2	D	264	
2	F	264	
3	G	75	
3	H	75	
3	I	75	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	AMP	A	401	-	X
4	AMP	C	401	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29134 atoms, of which 14526 are hydrogens 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 Cyclin-dependent kinase 9.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	315	Total	C	H	N	O	P	S	0	0	0
			5120	1625	2585	435	459	1	15			
1	C	311	Total	C	H	N	O	P	S	0	0	0
			5079	1608	2569	433	453	1	15			
1	E	314	Total	C	H	N	O	P	S	0	0	0
			5128	1626	2593	435	458	1	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P50750
A	0	HIS	-	EXPRESSION TAG	UNP P50750
C	-1	GLY	-	EXPRESSION TAG	UNP P50750
C	0	HIS	-	EXPRESSION TAG	UNP P50750
E	-1	GLY	-	EXPRESSION TAG	UNP P50750
E	0	HIS	-	EXPRESSION TAG	UNP P50750

- Molecule 2 is a protein called Cyclin-T1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	250	Total	C	H	N	O	S	0	0	0
			3974	1282	1971	342	370	9			
2	D	251	Total	C	H	N	O	S	0	0	0
			4020	1292	1996	348	375	9			
2	F	249	Total	C	H	N	O	S	0	0	0
			3974	1280	1973	342	370	9			

- Molecule 3 is a protein called AF4/FMR2 family member 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	33	Total	C	H	N	O	S	0	0	0
			470	160	222	36	50	2			

Continued on next page...

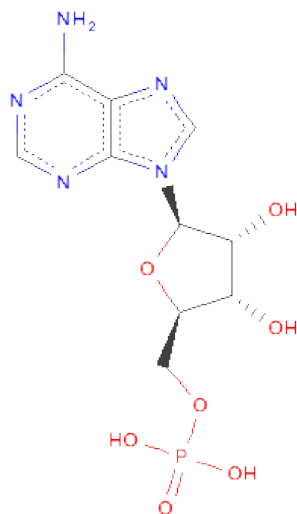
Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	53	Total	C	H	N	O	S	0	3	0
			783	254	362	83	80	4			
3	I	33	Total	C	H	N	O	S	0	0	0
			462	153	219	41	47	2			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	SER	-	EXPRESSION TAG	UNP Q9UHB7
G	0	ASN	-	EXPRESSION TAG	UNP Q9UHB7
G	1	ALA	-	EXPRESSION TAG	UNP Q9UHB7
H	-1	SER	-	EXPRESSION TAG	UNP Q9UHB7
H	0	ASN	-	EXPRESSION TAG	UNP Q9UHB7
H	1	ALA	-	EXPRESSION TAG	UNP Q9UHB7
I	-1	SER	-	EXPRESSION TAG	UNP Q9UHB7
I	0	ASN	-	EXPRESSION TAG	UNP Q9UHB7
I	1	ALA	-	EXPRESSION TAG	UNP Q9UHB7

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		
4	C	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	H	N	O	P	
			35	10	12	5	7	1	
								0	0

- Molecule 5 is water.

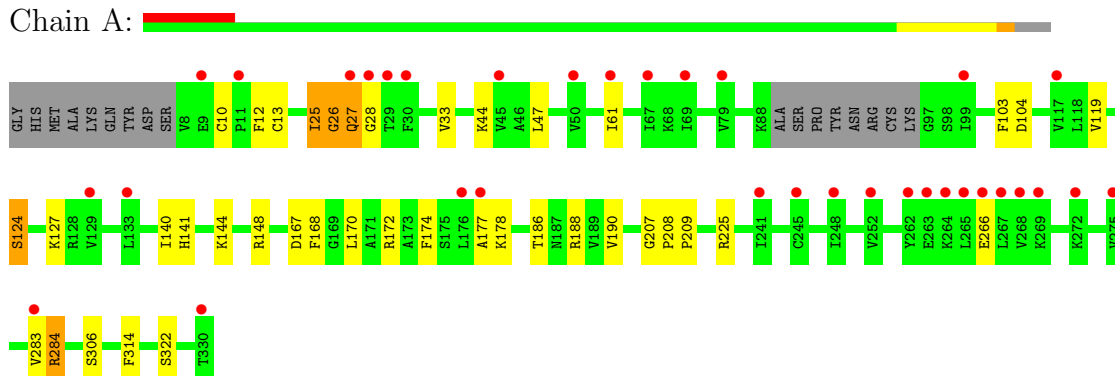
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O		
			3	3	0	0
5	B	2	Total	O		
			2	2	0	0
5	C	5	Total	O		
			5	5	0	0
5	D	3	Total	O		
			3	3	0	0
5	E	5	Total	O		
			5	5	0	0
5	F	1	Total	O		
			1	1	0	0

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.

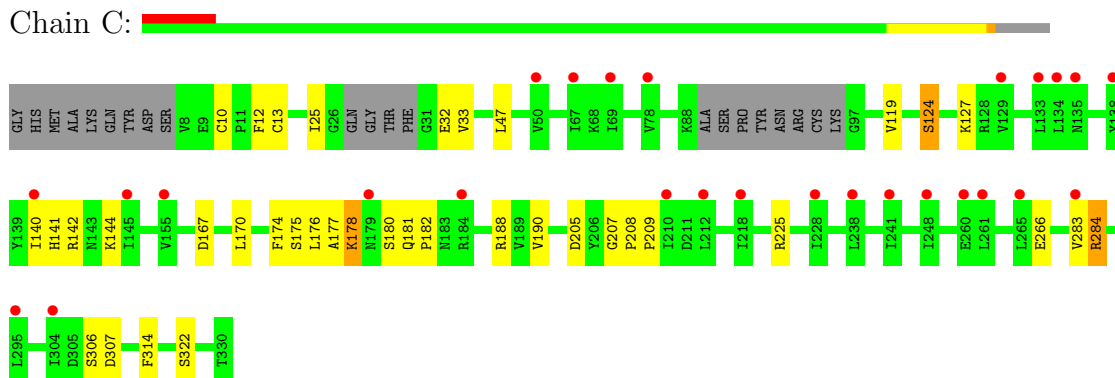
• Molecule 1: Cyclin-dependent kinase 9

Chain A:



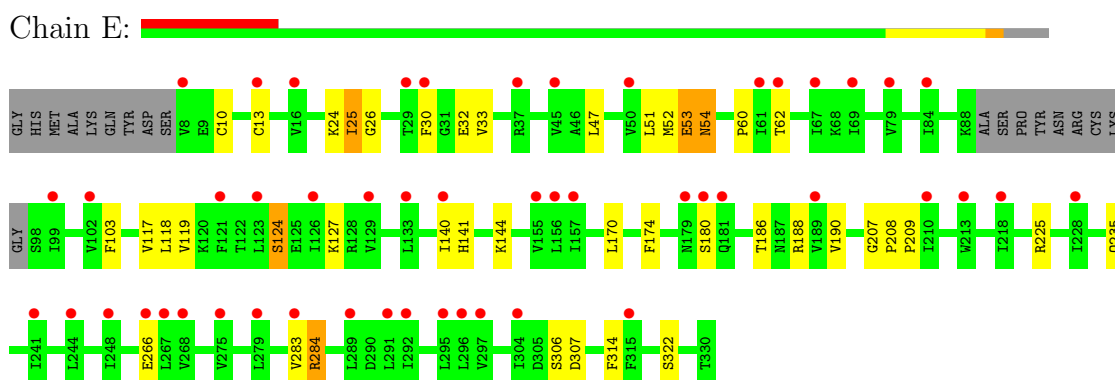
• Molecule 1: Cyclin-dependent kinase 9

Chain C:



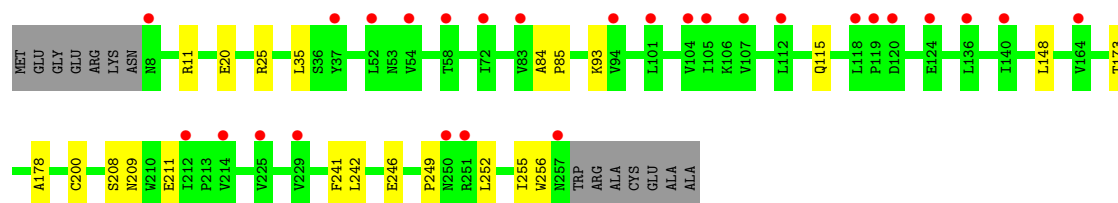
• Molecule 1: Cyclin-dependent kinase 9

Chain E:



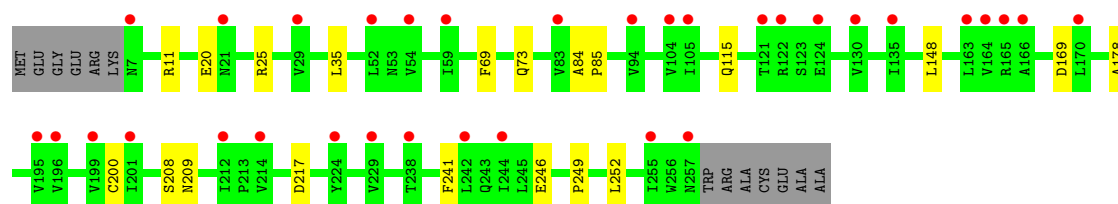
- Molecule 2: Cyclin-T1

Chain B:



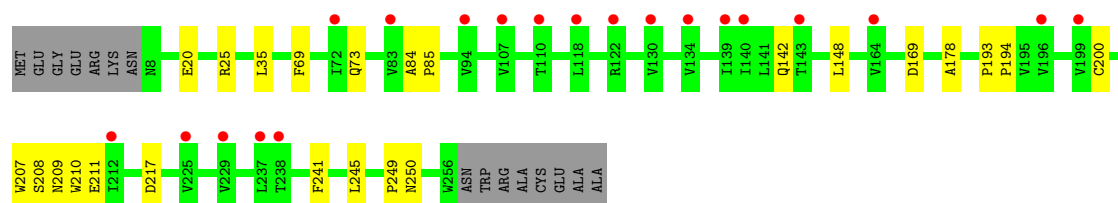
- Molecule 2: Cyclin-T1

Chain D:



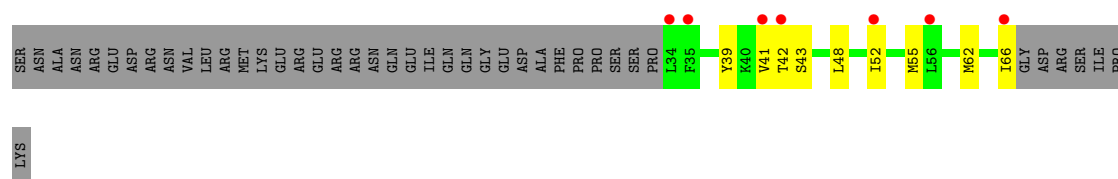
- Molecule 2: Cyclin-T1

Chain F:



- Molecule 3: AF4/FMR2 family member 4

Chain G:



- Molecule 3: AF4/FMR2 family member 4

Chain H:



- Molecule 3: AF4/FMR2 family member 4

Chain I:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.69Å 126.30Å 195.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 2.94 48.76 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.76-2.94) 94.7 (48.76-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.96Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8-1069)	Depositor
R, R_{free}	0.207 , 0.245 0.208 , 0.241	Depositor DCC
R_{free} test set	1886 reflections (3.67%)	DCC
Wilson B-factor (Å ²)	84.4	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 75.1	EDS
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 54129 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	29134	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: TPO, AMP

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	0.23	0/2574	0.40	0/3475
1	C	0.23	0/2547	0.40	0/3436
1	E	0.23	0/2574	0.40	0/3474
2	B	0.25	0/2053	0.39	0/2801
2	D	0.32	2/2074 (0.1%)	0.39	0/2828
2	F	0.25	0/2051	0.38	0/2798
3	G	0.24	0/252	0.36	0/340
3	H	0.22	0/424	0.38	0/566
3	I	0.23	0/246	0.37	0/330
All	All	0.25	2/14795 (0.0%)	0.39	0/20048

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	115	GLN	CD-NE2	-7.70	1.13	1.32
2	D	115	GLN	CD-OE1	-6.63	1.09	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2535	2585	0	27	1
1	C	2510	2569	0	30	0
1	E	2535	2593	0	33	1
2	B	2003	1971	0	17	0
2	D	2024	1996	0	10	0
2	F	2001	1973	0	13	0
3	G	248	222	0	10	0
3	H	421	362	0	13	0
3	I	243	219	0	7	0
4	A	23	12	0	7	0
4	C	23	12	0	1	0
4	E	23	12	0	1	0
5	A	3	0	0	0	0
5	B	2	0	0	1	0
5	C	5	0	0	0	0
5	D	3	0	0	0	0
5	E	5	0	0	0	0
5	F	1	0	0	0	0
All	All	14608	14526	0	131	1

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 5.

All (131) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:26:GLY:O	1:A:28:GLY:N	2.06	0.88
1:E:186:TPO:HG22	1:E:186:TPO:O2P	1.79	0.82
1:C:307:ASP:OD1	3:H:17:ARG:NH2	2.14	0.81
1:C:178:LYS:NZ	1:C:180:SER:OG	2.14	0.81
1:C:177:ALA:HB1	1:C:178:LYS:HG3	1.64	0.80
1:C:177:ALA:HB1	1:C:178:LYS:CG	2.14	0.77
1:A:167:ASP:N	4:A:401:AMP:O1P	2.19	0.76
2:F:169:ASP:OD1	3:I:59:TYR:OH	2.11	0.69
1:C:181:GLN:OE1	1:C:181:GLN:N	2.26	0.69
1:C:180:SER:OG	1:C:181:GLN:OE1	2.13	0.66
1:E:32:GLU:N	1:E:32:GLU:OE1	2.31	0.64
1:A:103:PHE:CZ	4:A:401:AMP:O3P	2.51	0.64
1:E:10:CYS:SG	2:F:142:GLN:HB3	2.41	0.61
1:E:30:PHE:O	1:E:51:LEU:N	2.36	0.59
1:A:283:VAL:O	1:A:284:ARG:HB2	2.03	0.59
1:E:53:GLU:N	1:E:54:ASN:HA	2.18	0.59
1:E:283:VAL:O	1:E:284:ARG:HB2	2.04	0.58
1:C:283:VAL:O	1:C:284:ARG:HB2	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:61:ILE:HB	2:B:93:LYS:HD3	1.87	0.56
2:B:115:GLN:OE1	1:E:235:GLN:OE1	2.24	0.55
2:D:246:GLU:HG2	3:H:55:MET:SD	2.46	0.55
2:B:211:GLU:HB2	3:G:41:VAL:CG2	2.36	0.55
2:F:211:GLU:HB2	3:I:41:VAL:CG2	2.36	0.55
1:E:25:ILE:O	1:E:33:VAL:HB	2.07	0.54
2:F:207:TRP:HB2	3:I:52:ILE:HG21	1.89	0.54
1:E:117:VAL:HG12	3:H:65:PHE:CD2	2.42	0.54
1:A:103:PHE:CE2	4:A:401:AMP:O3P	2.62	0.53
2:D:20:GLU:O	2:D:25:ARG:NH1	2.42	0.53
2:D:252:LEU:CB	1:E:118:LEU:HD11	2.39	0.53
1:E:127:LYS:HG2	1:E:314:PHE:CZ	2.45	0.52
1:A:127:LYS:HG2	1:A:314:PHE:CZ	2.44	0.52
1:E:186:TPO:O2P	1:E:186:TPO:CG2	2.55	0.52
1:E:117:VAL:CG1	3:H:65:PHE:CD2	2.92	0.52
1:C:177:ALA:CB	1:C:178:LYS:HG3	2.36	0.52
2:F:20:GLU:O	2:F:25:ARG:NH1	2.43	0.51
1:E:207:GLY:C	1:E:209:PRO:HD2	2.31	0.51
2:B:246:GLU:HA	3:G:55:MET:HE1	1.92	0.51
1:A:119:VAL:O	1:A:225:ARG:NH2	2.44	0.51
1:C:207:GLY:C	1:C:209:PRO:HD2	2.31	0.51
1:E:103:PHE:CZ	4:E:401:AMP:O3P	2.62	0.51
1:A:207:GLY:C	1:A:209:PRO:HD2	2.31	0.51
2:B:84:ALA:HB3	2:B:85:PRO:HD3	1.92	0.51
3:H:6:ARG:O	3:H:10[B]:ARG:N	2.44	0.51
1:C:127:LYS:HG2	1:C:314:PHE:CZ	2.46	0.51
2:F:84:ALA:HB3	2:F:85:PRO:HD3	1.92	0.51
1:C:142:ARG:NH1	3:H:18:ASN:O	2.44	0.51
2:B:20:GLU:O	2:B:25:ARG:NH1	2.43	0.51
1:C:177:ALA:CB	1:C:178:LYS:CG	2.87	0.50
2:D:84:ALA:HB3	2:D:85:PRO:HD3	1.92	0.50
1:C:182:PRO:HB3	1:C:205:ASP:OD2	2.12	0.50
1:E:117:VAL:HG12	3:H:65:PHE:CE2	2.46	0.50
1:A:168:PHE:N	4:A:401:AMP:O2P	2.43	0.49
1:C:119:VAL:O	1:C:225:ARG:NH2	2.44	0.49
1:E:52:MET:SD	1:E:52:MET:N	2.86	0.49
1:E:119:VAL:O	1:E:225:ARG:NH2	2.44	0.49
2:B:115:GLN:NE2	1:E:235:GLN:NE2	2.61	0.49
1:C:182:PRO:CB	1:C:205:ASP:CG	2.82	0.48
1:A:124:SER:OG	1:A:322:SER:OG	2.31	0.48
1:E:124:SER:OG	1:E:322:SER:OG	2.31	0.47
1:A:25:ILE:O	1:A:26:GLY:O	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:177:ALA:HB1	1:C:178:LYS:HG2	1.95	0.47
2:F:211:GLU:HB2	3:I:41:VAL:HG21	1.97	0.47
2:B:173:THR:HA	3:G:66:ILE:HG21	1.95	0.47
1:E:52:MET:C	1:E:54:ASN:HA	2.36	0.47
2:B:115:GLN:HE22	1:E:235:GLN:NE2	2.13	0.47
2:B:242:LEU:HD11	3:G:52:ILE:CG1	2.45	0.47
1:C:144:LYS:HA	1:C:174:PHE:CE1	2.51	0.46
2:B:115:GLN:OE1	1:E:235:GLN:CD	2.54	0.46
3:H:6:ARG:O	3:H:9:LEU:N	2.47	0.46
1:C:182:PRO:HB3	1:C:205:ASP:CG	2.35	0.46
1:A:177:ALA:HB1	1:A:178:LYS:HA	1.98	0.46
1:A:27:GLN:OE1	1:A:27:GLN:HA	2.16	0.46
1:A:144:LYS:HA	1:A:174:PHE:CE1	2.51	0.46
1:A:283:VAL:O	1:A:284:ARG:CB	2.64	0.46
2:F:245:LEU:CB	3:I:55:MET:HE2	2.45	0.46
2:D:178:ALA:HA	2:D:200:CYS:SG	2.56	0.46
1:A:186:TPO:HG21	1:A:186:TPO:O1P	2.16	0.46
1:C:124:SER:OG	1:C:322:SER:OG	2.33	0.45
1:E:208:PRO:N	1:E:209:PRO:CD	2.79	0.45
1:C:167:ASP:HA	4:C:401:AMP:O2P	2.16	0.45
1:A:208:PRO:N	1:A:209:PRO:CD	2.80	0.45
1:E:144:LYS:HA	1:E:174:PHE:CE1	2.52	0.45
5:B:301:HOH:O	3:G:48:LEU:CD1	2.64	0.45
1:C:208:PRO:N	1:C:209:PRO:CD	2.79	0.45
3:H:6:ARG:O	3:H:10[A]:ARG:N	2.44	0.45
1:A:186:TPO:HG22	1:A:186:TPO:O2P	2.16	0.45
1:A:33:VAL:HA	1:A:47:LEU:O	2.17	0.44
1:C:33:VAL:HA	1:C:47:LEU:O	2.17	0.44
1:E:10:CYS:SG	1:E:13:CYS:HB3	2.58	0.44
1:E:283:VAL:O	1:E:284:ARG:CB	2.65	0.43
2:F:210:TRP:CZ2	3:I:40:LYS:HE2	2.52	0.43
1:A:104:ASP:O	4:A:401:AMP:N6	2.51	0.43
1:E:24:LYS:HE3	1:E:32:GLU:HB2	2.00	0.43
1:E:33:VAL:HA	1:E:47:LEU:O	2.18	0.43
1:A:10:CYS:SG	1:A:13:CYS:HB3	2.58	0.43
1:C:283:VAL:O	1:C:284:ARG:CB	2.65	0.43
1:E:140:ILE:HG13	1:E:141:HIS:N	2.33	0.43
2:F:178:ALA:HA	2:F:200:CYS:SG	2.58	0.43
1:C:10:CYS:SG	1:C:13:CYS:HB3	2.58	0.43
1:A:167:ASP:HA	4:A:401:AMP:P	2.58	0.43
2:D:208:SER:O	2:D:209:ASN:HB2	2.19	0.43
3:H:39:TYR:CD1	3:H:39:TYR:N	2.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:193:PRO:N	2:F:194:PRO:CD	2.82	0.42
2:D:169:ASP:OD1	3:H:59:TYR:OH	2.36	0.42
1:C:12:PHE:CD1	2:D:11:ARG:CZ	3.03	0.42
2:B:208:SER:O	2:B:209:ASN:HB2	2.19	0.42
1:A:140:ILE:HG13	1:A:141:HIS:N	2.34	0.42
1:C:177:ALA:CA	1:C:178:LYS:CG	2.97	0.42
1:C:140:ILE:HG13	1:C:141:HIS:N	2.33	0.42
2:B:178:ALA:HA	2:B:200:CYS:SG	2.59	0.42
1:C:175:SER:OG	1:C:177:ALA:HB2	2.20	0.42
2:B:211:GLU:HB2	3:G:41:VAL:HG21	2.00	0.42
2:F:208:SER:O	2:F:209:ASN:HB2	2.19	0.42
2:D:246:GLU:HA	3:H:55:MET:HE1	2.01	0.42
2:B:252:LEU:O	2:B:256:TRP:CB	2.68	0.42
1:A:12:PHE:CD1	2:B:11:ARG:CZ	3.02	0.42
1:C:177:ALA:C	1:C:178:LYS:HG3	2.40	0.41
1:E:30:PHE:CE2	1:E:62:THR:HG23	2.54	0.41
3:I:41:VAL:HG12	3:I:42:THR:N	2.35	0.41
1:A:148:ARG:NH1	1:A:172:ARG:CD	2.83	0.41
1:E:30:PHE:CZ	1:E:60:PRO:HB3	2.56	0.41
1:C:177:ALA:CA	1:C:178:LYS:HG3	2.50	0.41
1:A:167:ASP:H	4:A:401:AMP:P	2.43	0.41
2:D:69:PHE:CZ	2:D:73:GLN:HG3	2.56	0.41
3:G:39:TYR:N	3:G:39:TYR:CD1	2.89	0.41
1:E:24:LYS:HE3	1:E:32:GLU:CB	2.52	0.41
3:G:42:THR:O	3:G:43:SER:C	2.60	0.41
3:G:41:VAL:HG12	3:G:42:THR:N	2.36	0.40
2:F:69:PHE:CZ	2:F:73:GLN:HG3	2.57	0.40
2:B:255:ILE:HG21	3:G:62:MET:HE2	2.02	0.40
3:H:49:SER:O	3:H:53:GLN:HG2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:44:LYS:NZ	1:E:307:ASP:OD2[2_554]	2.02	0.18

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	310/332 (93%)	291 (94%)	15 (5%)	4 (1%)	18	54
1	C	304/332 (92%)	288 (95%)	14 (5%)	2 (1%)	30	72
1	E	309/332 (93%)	289 (94%)	16 (5%)	4 (1%)	18	54
2	B	248/264 (94%)	237 (96%)	10 (4%)	1 (0%)	43	82
2	D	249/264 (94%)	237 (95%)	11 (4%)	1 (0%)	43	82
2	F	247/264 (94%)	236 (96%)	10 (4%)	1 (0%)	43	82
3	G	31/75 (41%)	30 (97%)	1 (3%)	0	100	100
3	H	52/75 (69%)	49 (94%)	2 (4%)	1 (2%)	12	42
3	I	31/75 (41%)	30 (97%)	1 (3%)	0	100	100
All	All	1781/2013 (88%)	1687 (95%)	80 (4%)	14 (1%)	27	68

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	26	GLY
1	A	190	VAL
2	B	249	PRO
1	C	190	VAL
2	D	249	PRO
1	E	26	GLY
1	E	190	VAL
1	A	284	ARG
1	C	284	ARG
1	E	180	SER
1	E	284	ARG
2	F	249	PRO
3	H	66	ILE

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	276/292 (94%)	270 (98%)	6 (2%)	64	91
1	C	274/292 (94%)	265 (97%)	9 (3%)	50	86
1	E	277/292 (95%)	269 (97%)	8 (3%)	55	88
2	B	221/239 (92%)	218 (99%)	3 (1%)	78	95
2	D	225/239 (94%)	221 (98%)	4 (2%)	71	93
2	F	222/239 (93%)	217 (98%)	5 (2%)	63	91
3	G	25/69 (36%)	25 (100%)	0	100	100
3	H	36/69 (52%)	33 (92%)	3 (8%)	16	43
3	I	23/69 (33%)	23 (100%)	0	100	100
All	All	1579/1800 (88%)	1541 (98%)	38 (2%)	63	91

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	124	SER
1	A	170	LEU
1	A	188	ARG
1	A	266	GLU
1	A	306	SER
2	B	35	LEU
2	B	148	LEU
2	B	241	PHE
1	C	25	ILE
1	C	32	GLU
1	C	124	SER
1	C	170	LEU
1	C	176	LEU
1	C	178	LYS
1	C	188	ARG
1	C	266	GLU
1	C	306	SER
2	D	35	LEU
2	D	148	LEU
2	D	217	ASP
2	D	241	PHE
1	E	25	ILE
1	E	53	GLU
1	E	54	ASN
1	E	124	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	170	LEU
1	E	188	ARG
1	E	266	GLU
1	E	306	SER
2	F	35	LEU
2	F	148	LEU
2	F	217	ASP
2	F	241	PHE
2	F	250	ASN
3	H	11[A]	MET
3	H	11[B]	MET
3	H	35	PHE

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

Mol	Chain	Res	Type
1	A	71	GLN
1	A	80	ASN
1	A	143	ASN
1	A	154	ASN
1	A	187	ASN
1	A	230	GLN
1	A	302	GLN
1	A	311	ASN
2	B	46	GLN
2	B	53	ASN
2	B	56	GLN
2	B	180	ASN
1	C	80	ASN
1	C	143	ASN
1	C	187	ASN
1	C	230	GLN
1	C	302	GLN
2	D	46	GLN
2	D	53	ASN
2	D	56	GLN
2	D	180	ASN
1	E	80	ASN
1	E	143	ASN
1	E	154	ASN
1	E	187	ASN
1	E	230	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	302	GLN
1	E	311	ASN
2	F	46	GLN
2	F	53	ASN
2	F	56	GLN
2	F	115	GLN
2	F	180	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	A	186	1	10,10,11	5.65	2 (20%)	12,14,16	1.20	2 (16%)
1	TPO	C	186	1	10,10,11	5.79	2 (20%)	12,14,16	0.98	1 (8%)
1	TPO	E	186	1	10,10,11	5.73	2 (20%)	12,14,16	1.60	3 (25%)

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
1	TPO	A	186	1	-	0/9/11/13	0/0/0/0
1	TPO	C	186	1	-	0/9/11/13	0/0/0/0
1	TPO	E	186	1	-	0/9/11/13	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	186	TPO	O-C	17.82	1.23	1.11
1	E	186	TPO	O-C	17.75	1.23	1.11
1	A	186	TPO	O-C	17.44	1.23	1.11
1	C	186	TPO	CA-C	2.84	1.53	1.48
1	A	186	TPO	CA-C	2.51	1.53	1.48
1	E	186	TPO	CA-C	2.06	1.52	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	186	TPO	OG1-CB-CG2	3.51	115.99	110.13
1	E	186	TPO	O2P-P-OG1	2.68	114.81	107.09
1	E	186	TPO	C-CA-N	-2.51	107.86	111.94
1	A	186	TPO	OG1-CB-CG2	2.17	113.75	110.13
1	C	186	TPO	P-OG1-CB	-2.12	110.82	120.17
1	A	186	TPO	CG2-CB-CA	-2.04	109.01	113.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	AMP	A	401	-	25,25,25	0.99	2 (8%)	38,38,38	1.91	6 (15%)
4	AMP	C	401	-	25,25,25	1.01	2 (8%)	38,38,38	2.01	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AMP	E	401	-	25,25,25	0.98	2 (8%)	38,38,38	1.92	6 (15%)

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	AMP	A	401	-	-	0/10/26/26	0/1/3/3
4	AMP	C	401	-	-	0/10/26/26	0/1/3/3
4	AMP	E	401	-	-	0/10/26/26	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	AMP	C5-C4	2.97	1.47	1.40
4	E	401	AMP	C5-C4	2.89	1.47	1.40
4	A	401	AMP	C5-C4	2.83	1.46	1.40
4	A	401	AMP	C4-N9	-2.44	1.34	1.37
4	C	401	AMP	C4-N9	-2.33	1.34	1.37
4	E	401	AMP	C4-N9	-2.33	1.34	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	AMP	N3-C2-N1	-6.88	122.96	128.71
4	E	401	AMP	N3-C2-N1	-6.88	122.96	128.71
4	A	401	AMP	N3-C2-N1	-6.81	123.01	128.71
4	C	401	AMP	N3-C4-N9	5.94	136.16	125.43
4	A	401	AMP	N3-C4-N9	5.86	136.00	125.43
4	E	401	AMP	N3-C4-N9	5.80	135.91	125.43
4	E	401	AMP	C5-C4-N3	-3.41	118.29	125.70
4	C	401	AMP	C5-C4-N3	-3.40	118.29	125.70
4	A	401	AMP	C5-C4-N3	-3.40	118.29	125.70
4	E	401	AMP	C4-C5-N7	-2.91	107.03	109.52
4	A	401	AMP	C4-C5-N7	-2.86	107.07	109.52
4	A	401	AMP	C8-N9-C4	2.84	109.06	106.90
4	E	401	AMP	C2-N3-C4	2.65	121.56	114.01
4	C	401	AMP	C4-C5-N7	-2.64	107.26	109.52
4	A	401	AMP	C2-N3-C4	2.62	121.47	114.01
4	C	401	AMP	C2-N3-C4	2.61	121.45	114.01
4	C	401	AMP	C8-N9-C4	2.58	108.87	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	401	AMP	C8-N9-C4	2.56	108.85	106.90
4	C	401	AMP	O2'-C2'-C3'	2.38	119.58	111.83

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	315/332 (94%)	0.66	34 (10%) 6 9	75, 100, 196, 269	0
1	C	311/332 (93%)	0.48	27 (8%) 10 13	78, 107, 185, 227	0
1	E	314/332 (94%)	0.75	50 (15%) 3 4	70, 114, 191, 246	0
2	B	250/264 (94%)	0.77	27 (10%) 6 9	80, 113, 192, 228	0
2	D	251/264 (95%)	0.64	33 (13%) 4 6	70, 118, 186, 241	0
2	F	249/264 (94%)	0.52	20 (8%) 12 15	79, 113, 171, 214	0
3	G	33/75 (44%)	0.85	7 (21%) 1 2	98, 161, 215, 237	0
3	H	53/75 (70%)	0.67	9 (16%) 2 3	115, 164, 213, 250	0
3	I	33/75 (44%)	-0.02	1 (3%) 48 58	116, 159, 206, 208	0
All	All	1809/2013 (89%)	0.63	208 (11%) 5 7	70, 112, 194, 269	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	248	ILE	9.4
1	A	330	THR	9.1
1	A	29	THR	7.8
1	E	248	ILE	6.6
1	E	275	VAL	6.5
2	B	119	PRO	6.1
1	E	8	VAL	6.0
2	B	104	VAL	5.8
3	H	20	GLU	5.6
1	A	248	ILE	5.6
1	E	228	ILE	4.9
2	D	164	VAL	4.9
2	B	124	GLU	4.6
1	A	176	LEU	4.6
3	G	52	ILE	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	263	GLU	4.6
2	B	164	VAL	4.4
1	C	179	ASN	4.4
3	H	17	ARG	4.4
2	B	72	ILE	4.3
1	A	177	ALA	4.2
1	A	30	PHE	4.2
1	A	28	GLY	4.2
1	E	283	VAL	4.2
1	A	264	LYS	4.1
2	D	104	VAL	4.1
2	B	250	ASN	4.1
3	G	41	VAL	4.0
2	B	105	ILE	4.0
1	C	260	GLU	4.0
1	E	279	LEU	4.0
1	E	126	ILE	3.9
2	D	229	VAL	3.9
1	A	117	VAL	3.9
2	B	118	LEU	3.9
3	H	19	GLN	3.9
2	B	83	VAL	3.8
3	G	56	LEU	3.8
1	A	269	LYS	3.7
2	B	212	ILE	3.6
1	E	99	ILE	3.6
2	F	72	ILE	3.6
2	D	165	ARG	3.6
2	F	212	ILE	3.6
1	E	292	ILE	3.5
2	D	83	VAL	3.5
1	E	13	CYS	3.4
1	E	297	VAL	3.4
1	E	181	GLN	3.4
1	E	180	SER	3.4
1	A	27	GLN	3.4
2	F	130	VAL	3.4
1	A	50	VAL	3.4
1	E	157	ILE	3.4
2	D	199	VAL	3.3
1	A	265	LEU	3.3
1	A	283	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	129	VAL	3.3
2	F	164	VAL	3.3
2	D	163	LEU	3.3
2	D	29	VAL	3.3
3	H	52	ILE	3.3
1	E	189	VAL	3.3
3	G	42	THR	3.3
1	A	245	CYS	3.2
1	E	267	LEU	3.2
2	F	139	ILE	3.2
1	C	241	ILE	3.2
2	B	107	VAL	3.1
1	E	179	ASN	3.1
2	D	130	VAL	3.1
1	E	121	PHE	3.1
1	C	133	LEU	3.1
1	C	228	ILE	3.1
1	E	155	VAL	3.1
2	B	225	VAL	3.1
1	E	84	ILE	3.1
2	B	140	ILE	3.1
2	D	105	ILE	3.1
1	A	267	LEU	3.1
2	B	112	LEU	3.1
3	H	41	VAL	3.0
1	E	67	ILE	3.0
2	D	54	VAL	3.0
2	D	196	VAL	3.0
1	C	238	LEU	3.0
1	E	16	VAL	3.0
1	E	50	VAL	3.0
1	E	102	VAL	3.0
1	C	140	ILE	2.9
1	C	129	VAL	2.9
1	E	244	LEU	2.9
1	E	295	LEU	2.9
2	D	195	VAL	2.9
1	C	134	LEU	2.9
2	D	214	VAL	2.8
2	D	166	ALA	2.8
1	C	218	ILE	2.8
2	D	224	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	34	LEU	2.8
1	A	252	VAL	2.7
2	F	143	THR	2.7
1	E	268	VAL	2.7
2	B	52	LEU	2.7
2	F	110	THR	2.7
2	D	170	LEU	2.7
3	H	16	ARG	2.7
1	A	61	ILE	2.7
1	C	155	VAL	2.7
3	G	66	ILE	2.7
1	E	79	VAL	2.6
2	B	54	VAL	2.6
1	C	212	LEU	2.6
1	C	295	LEU	2.6
1	A	99	ILE	2.6
1	A	129	VAL	2.6
1	A	11	PRO	2.6
2	D	212	ILE	2.6
1	E	296	LEU	2.6
1	A	275	VAL	2.6
2	F	225	VAL	2.6
1	E	266	GLU	2.6
1	E	156	LEU	2.5
1	E	315	PHE	2.5
1	E	241	ILE	2.5
1	C	184	ARG	2.5
1	C	265	LEU	2.5
1	C	78	VAL	2.5
1	E	45	VAL	2.5
1	E	289	LEU	2.5
3	G	34	LEU	2.5
2	B	214	VAL	2.5
1	A	79	VAL	2.5
1	E	123	LEU	2.5
2	F	237	LEU	2.5
2	B	229	VAL	2.4
2	F	238	THR	2.4
2	D	124	GLU	2.4
1	A	9	GLU	2.4
2	D	255	ILE	2.4
1	C	283	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	257	ASN	2.4
1	A	266	GLU	2.4
2	F	118	LEU	2.4
1	E	61	ILE	2.4
2	B	37	TYR	2.4
2	D	242	LEU	2.4
1	E	218	ILE	2.4
3	I	48	LEU	2.3
2	D	94	VAL	2.3
1	A	241	ILE	2.3
2	F	140	ILE	2.3
2	F	94	VAL	2.3
2	F	196	VAL	2.3
2	B	94	VAL	2.3
1	C	135	ASN	2.3
2	B	251	ARG	2.3
1	A	45	VAL	2.3
1	E	29	THR	2.3
2	B	8	ASN	2.3
1	A	69	ILE	2.3
2	D	21	ASN	2.2
1	E	69	ILE	2.2
2	D	238	THR	2.2
2	D	257	ASN	2.2
2	F	134	VAL	2.2
3	H	42	THR	2.2
1	E	210	ILE	2.2
2	D	122	ARG	2.2
2	F	122	ARG	2.2
3	G	35	PHE	2.2
1	C	50	VAL	2.2
2	D	121	THR	2.2
2	F	107	VAL	2.2
1	C	145	ILE	2.2
2	B	58	THR	2.2
2	F	199	VAL	2.1
2	F	229	VAL	2.1
1	E	140	ILE	2.1
2	D	201	ILE	2.1
1	C	69	ILE	2.1
2	D	135	ILE	2.1
2	D	244	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	133	LEU	2.1
2	B	101	LEU	2.1
1	C	304	ILE	2.1
1	E	304	ILE	2.1
1	A	67	ILE	2.1
1	C	67	ILE	2.1
1	A	268	VAL	2.1
2	F	83	VAL	2.1
1	C	210	ILE	2.1
2	D	7	ASN	2.1
1	E	30	PHE	2.1
1	C	261	LEU	2.1
1	A	262	TYR	2.1
1	A	272	LYS	2.1
1	A	133	LEU	2.1
2	B	120	ASP	2.0
1	C	138	TYR	2.0
1	E	291	LEU	2.0
2	B	136	LEU	2.0
1	E	62	THR	2.0
1	E	213	TRP	2.0
1	E	37	ARG	2.0
2	D	59	ILE	2.0
2	D	52	LEU	2.0
3	H	67	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	TPO	E	186	11/12	0.23	-0.32	110,124,152,177	0
1	TPO	C	186	11/12	0.20	-0.45	92,106,125,130	0
1	TPO	A	186	11/12	0.17	-0.68	106,118,141,146	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	AMP	A	401	23/23	0.46	4.04	111,153,371,371	0
4	AMP	C	401	23/23	0.34	2.52	112,157,206,211	0
4	AMP	E	401	23/23	0.38	1.73	124,160,241,245	0

6.5 Other polymers ⓘ

There are no such residues in this entry.