Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:53 PM GMT

PDB ID	:	1YVP
Title	:	Ro autoantigen complexed with RNAs
Authors	:	Stein, A.J.; Fuchs, G.; Fu, C.; Wolin, S.L.; Reinisch, K.M.
Deposited on	:	2005-02-16
Resolution	:	2.20 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
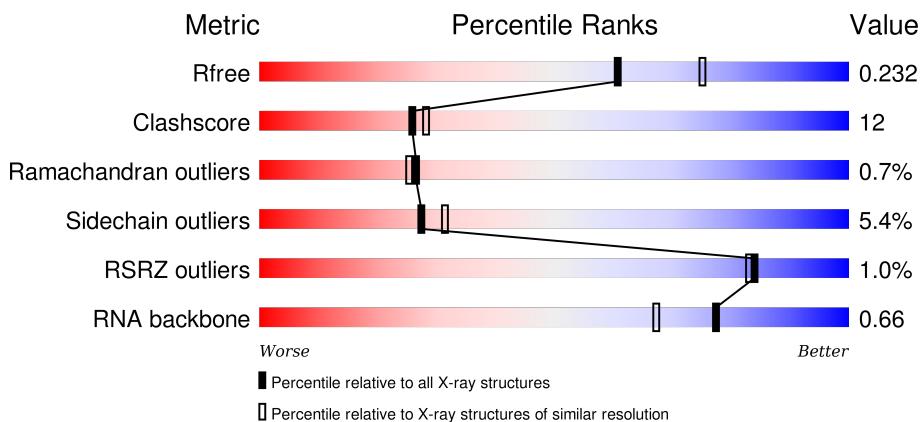
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)
RNA backbone	2183	1062 (2.80-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	C	10	80% 20%
1	E	10	80% 20%
1	G	10	30% 20% 50%
1	H	10	40% 10% 20% 30%

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Mol	Chain	Length	Quality of chain
2	D	10	60% ▬▬▬▬▬▬ 40%
2	F	10	50% ▬▬▬▬▬ 50%
3	A	538	% 72% 23%
3	B	538	% 75% 21%
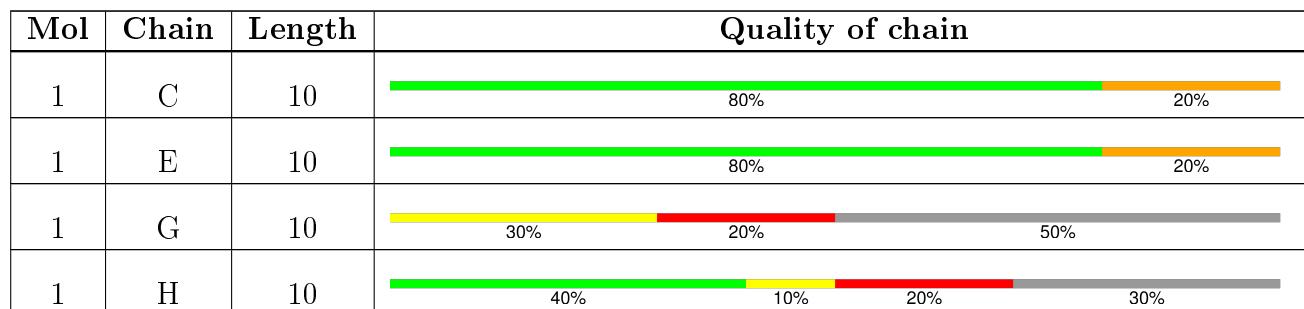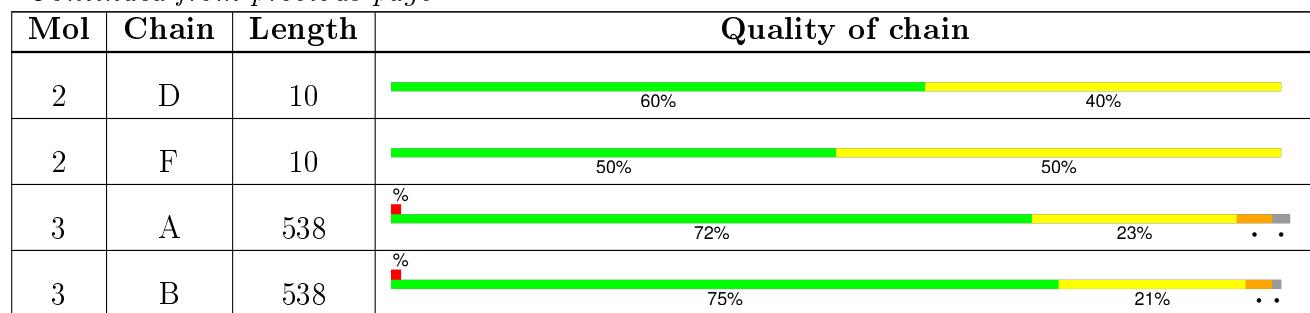
2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9890 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called Y RNA sequence, first strand.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	10	Total 212	C 95	I 1	N 38	O 69	P 9	0	0	0
1	E	10	Total 212	C 95	I 1	N 38	O 69	P 9	0	0	0
1	G	5	Total 102	C 47	N 18	O 33	P 4		0	0	0
1	H	7	Total 148	C 67	N 28	O 47	P 6		0	0	0

- Molecule 2 is a RNA chain called Y RNA sequence, second strand.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	10	Total 210	C 94	I 3	N 35	O 69	P 9	0	0	0
2	F	10	Total 210	C 94	I 3	N 35	O 69	P 9	0	0	0

- Molecule 3 is a protein called 60-kDa SS-A/Ro ribonucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	529	Total 4177	C 2649	N 716	O 778	S 34	0	0	0
3	B	532	Total 4201	C 2663	N 721	O 783	S 34	0	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
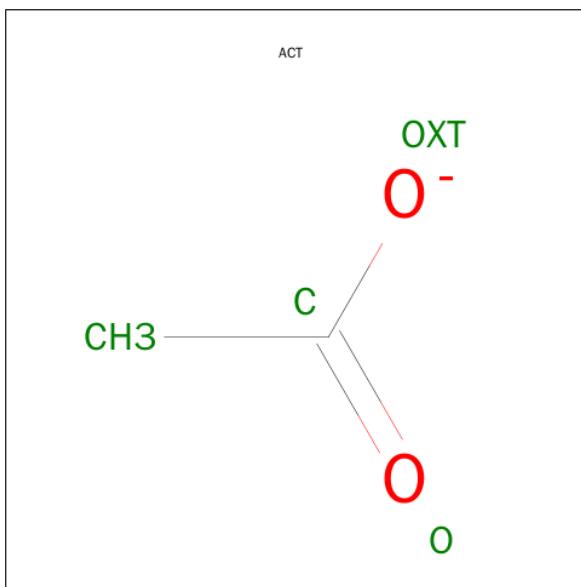
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Mg 1	0	0
5	A	1	Total 1	Mg 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	167	Total 167	O 167	0	0
6	B	169	Total 169	O 169	0	0
6	C	19	Total 19	O 19	0	0
6	D	3	Total 3	O 3	0	0
6	E	14	Total 14	O 14	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	6	Total 6	O 6	0	0
6	G	9	Total 9	O 9	0	0
6	H	21	Total 21	O 21	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: Y RNA sequence, first strand
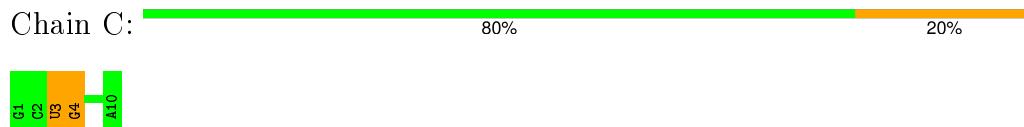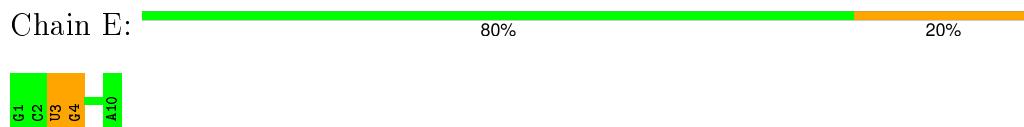
Chain C:

- Molecule 1: Y RNA sequence, first strand

Chain E:

- Molecule 1: Y RNA sequence, first strand

Chain G:

- Molecule 1: Y RNA sequence, first strand

Chain H:
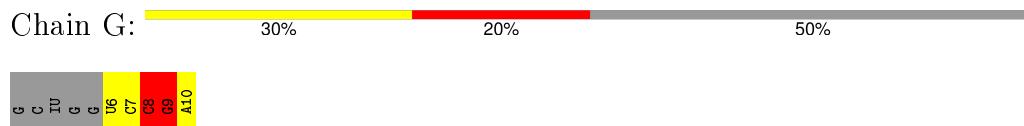
- Molecule 2: Y RNA sequence, second strand

Chain D:

- Molecule 2: Y RNA sequence, second strand

Chain F:
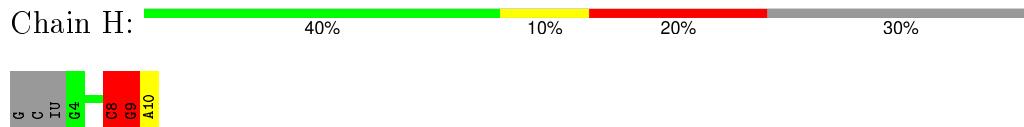
• Molecule 3: 60-kDa SS-A/Ro ribonucleoprotein

• Molecule 3: 60-kDa SS-A/Ro ribonucleoprotein
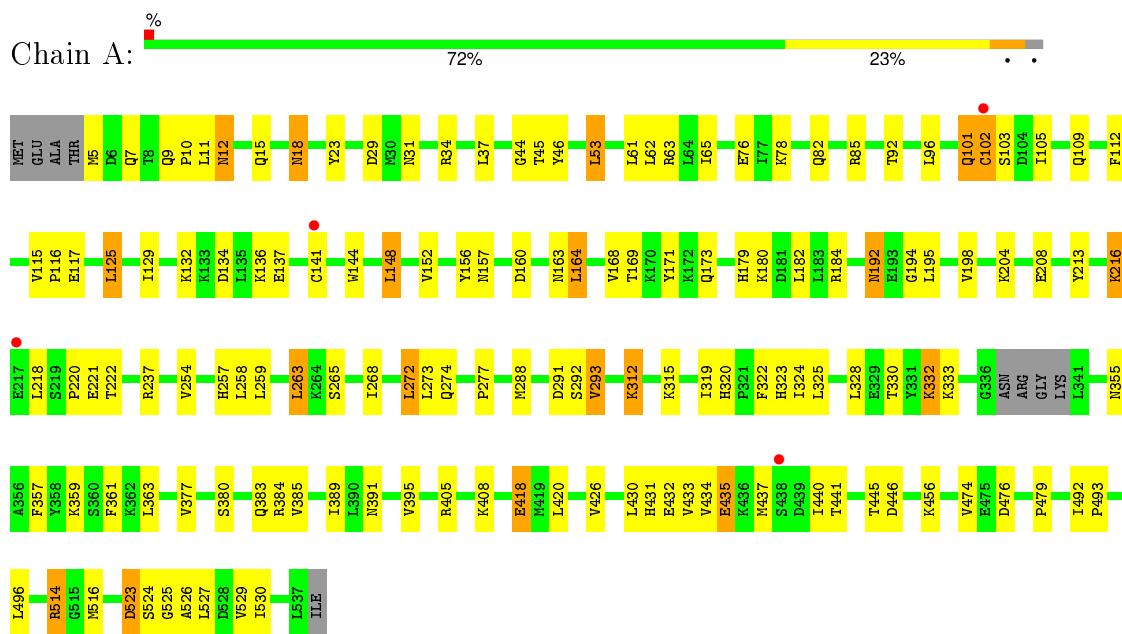
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.30Å 153.65Å 80.56Å 90.00° 92.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 41.54 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.20) 94.9 (41.54-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.37 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.238 0.198 , 0.232	Depositor DCC
R_{free} test set	7374 reflections (11.68%)	DCC
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.0	EDS
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Outliers	0 of 72908 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9890	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, IU, ACT

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	C	0.32	0/213	0.60	0/331
1	E	0.28	0/213	0.62	0/331
1	G	0.67	0/113	1.66	4/174 (2.3%)
1	H	0.58	0/165	1.35	2/256 (0.8%)
2	D	0.27	0/168	0.73	0/262
2	F	0.29	0/168	0.63	0/262
3	A	0.34	0/4251	0.59	1/5734 (0.0%)
3	B	0.33	0/4275	0.58	1/5766 (0.0%)
All	All	0.34	0/9566	0.64	8/13116 (0.1%)

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
1	G	1	0

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	6	U	N1-C1'-C2'	8.01	124.41	114.00
1	G	9	G	N9-C1'-C2'	6.39	122.31	114.00
3	A	523	ASP	N-CA-C	-6.33	93.91	111.00
1	H	9	G	N9-C1'-C2'	6.28	122.17	114.00
3	B	523	ASP	N-CA-C	-6.28	94.03	111.00
1	G	8	C	O4'-C1'-N1	5.78	112.83	108.20
1	H	8	C	O4'-C1'-N1	5.13	112.31	108.20
1	G	8	C	N1-C1'-C2'	5.10	120.63	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	6	U	C1'

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	212	0	109	2	0
1	E	212	0	109	1	0
1	G	102	0	56	3	0
1	H	148	0	78	6	0
2	D	210	0	105	2	0
2	F	210	0	105	4	0
3	A	4177	0	4247	122	0
3	B	4201	0	4273	99	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	167	0	0	7	0
6	B	169	0	0	4	0
6	C	19	0	0	1	0
6	D	3	0	0	0	0
6	E	14	0	0	0	0
6	F	6	0	0	0	0
6	G	9	0	0	0	0
6	H	21	0	0	0	0
All	All	9890	0	9088	231	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 12.

All (231) 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)
3:B:254:VAL:H	3:B:257:HIS:HD2	1.18	0.89
3:A:431:HIS:O	3:A:435:GLU:HG2	1.72	0.88
3:A:254:VAL:H	3:A:257:HIS:HD2	1.22	0.87
3:B:45:THR:HG22	3:B:48:ILE:H	1.41	0.86
3:A:385:VAL:HG21	3:A:395:VAL:HG21	1.64	0.76
3:A:85:ARG:HD2	3:A:523:ASP:OD2	1.86	0.76
3:A:92:THR:HG23	6:A:2002:HOH:O	1.85	0.75
3:B:164:LEU:HD13	3:B:198:VAL:HG11	1.67	0.74
3:A:164:LEU:HD13	3:A:198:VAL:HG11	1.69	0.74
1:G:8:C:H5"	3:A:171:TYR:OH	1.89	0.72
3:A:44:GLY:HA2	3:A:53:LEU:HD12	1.71	0.72
3:A:192:ASN:ND2	3:A:195:LEU:H	1.88	0.71
3:A:46:TYR:H	3:A:383:GLN:NE2	1.88	0.71
3:B:288:MET:HB3	3:B:293:VAL:HG22	1.73	0.71
3:B:102:CYS:SG	3:B:141:CYS:HB3	2.31	0.70
3:B:197:MET:HE1	3:B:222:THR:O	1.91	0.70
3:B:384:ARG:HH11	3:B:391:ASN:HB3	1.56	0.70
3:B:384:ARG:NH1	3:B:391:ASN:HB3	2.08	0.68
3:A:437:MET:O	3:A:440:ILE:HG22	1.92	0.68
3:A:288:MET:HB3	3:A:293:VAL:HG22	1.75	0.68
1:H:8:C:H5"	3:B:171:TYR:OH	1.93	0.67
3:B:46:TYR:H	3:B:383:GLN:HE21	1.42	0.67
3:B:46:TYR:H	3:B:383:GLN:NE2	1.91	0.67
3:A:216:LYS:NZ	3:A:216:LYS:HB2	2.10	0.67
3:A:312:LYS:HA	3:A:312:LYS:HE3	1.76	0.67
3:A:355:ASN:HD21	3:A:359:LYS:HZ1	1.43	0.67
3:B:45:THR:HG22	3:B:47:TYR:H	1.60	0.66
3:A:37:LEU:HD22	3:A:92:THR:HG22	1.78	0.65
3:B:77:ILE:HG23	3:B:92:THR:HG23	1.79	0.64
3:B:45:THR:CG2	3:B:47:TYR:H	2.11	0.63
3:B:320:HIS:HD2	3:B:322:PHE:H	1.47	0.63
3:A:430:LEU:O	3:A:433:VAL:HG22	1.99	0.63
3:A:46:TYR:H	3:A:383:GLN:HE21	1.46	0.63
3:B:18:ASN:HD22	3:B:18:ASN:C	2.01	0.63
3:B:481:THR:HA	3:B:484:LYS:HE3	1.80	0.62
3:A:389:ILE:HG13	6:A:2069:HOH:O	1.99	0.62
3:B:310:ASN:HD22	3:B:310:ASN:C	2.02	0.62
3:A:10:PRO:HB3	3:A:23:TYR:CD2	2.35	0.62
3:B:425:THR:HG22	3:B:427:ASN:H	1.63	0.62
3:B:288:MET:HB3	3:B:293:VAL:CG2	2.29	0.62
3:A:355:ASN:HD21	3:A:359:LYS:NZ	1.99	0.61
3:A:479:PRO:HG2	6:A:2034:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:11:LEU:H	3:A:15:GLN:NE2	1.98	0.61
3:A:12:ASN:C	3:A:12:ASN:HD22	2.04	0.61
3:A:216:LYS:HZ3	3:A:216:LYS:HB2	1.66	0.60
3:B:45:THR:HG21	6:B:2004:HOH:O	2.02	0.60
3:A:204:LYS:HB2	3:A:208:GLU:HG2	1.84	0.60
3:B:87:ALA:O	3:B:323:HIS:HE1	1.85	0.59
3:B:171:TYR:O	3:B:179:HIS:HE1	1.86	0.59
3:A:105:ILE:O	3:A:109:GLN:HG3	2.02	0.59
3:A:156:TYR:OH	3:A:179:HIS:HD2	1.85	0.58
3:A:102:CYS:SG	3:A:141:CYS:HB3	2.43	0.58
3:A:85:ARG:HA	3:A:524:SER:OG	2.04	0.58
3:A:85:ARG:HD3	3:A:525:GLY:HA3	1.84	0.58
3:A:446:ASP:CG	3:A:474:VAL:HG21	2.24	0.58
3:A:144:TRP:CZ3	3:A:148:LEU:HD13	2.38	0.58
3:A:137:GLU:CD	3:A:137:GLU:N	2.57	0.58
2:F:6:IU:H2'	2:F:7:A:C8	2.39	0.57
3:B:45:THR:HG23	3:B:46:TYR:N	2.20	0.57
3:B:200:LYS:HG2	3:B:208:GLU:OE2	2.04	0.57
3:A:18:ASN:C	3:A:18:ASN:HD22	2.05	0.57
3:A:432:GLU:HA	3:A:435:GLU:HG3	1.86	0.57
1:C:3:IU:O2'	1:C:4:G:O5'	2.23	0.57
3:B:216:LYS:O	3:B:218:LEU:HG	2.05	0.57
3:B:332:LYS:HE3	3:B:431:HIS:CD2	2.39	0.56
3:A:330:THR:O	3:A:333:LYS:HB2	2.05	0.56
3:B:218:LEU:HB3	3:B:222:THR:HG23	1.88	0.56
3:B:320:HIS:CD2	3:B:322:PHE:H	2.24	0.56
3:A:445:THR:O	3:A:474:VAL:HG13	2.05	0.56
3:B:254:VAL:H	3:B:257:HIS:CD2	2.11	0.55
3:A:101:GLN:HG2	3:A:141:CYS:SG	2.46	0.55
3:B:105:ILE:O	3:B:109:GLN:HG3	2.06	0.55
3:B:20:GLU:HG3	6:B:2048:HOH:O	2.07	0.55
3:B:201:TYR:HB2	3:B:209:VAL:HG21	1.88	0.55
3:A:220:PRO:HG2	3:A:221:GLU:OE2	2.07	0.55
3:B:355:ASN:HD21	3:B:359:LYS:HE3	1.73	0.55
3:A:526:ALA:O	3:A:529:VAL:HG22	2.07	0.54
3:B:192:ASN:C	3:B:192:ASN:HD22	2.11	0.54
3:A:171:TYR:O	3:A:179:HIS:HE1	1.91	0.54
3:A:357:PHE:CG	3:A:430:LEU:HD11	2.42	0.54
3:B:192:ASN:ND2	3:B:195:LEU:HB2	2.23	0.54
1:H:8:C:H3'	1:H:9:G:H5'	1.90	0.54
3:B:101:GLN:O	3:B:102:CYS:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:259:LEU:O	3:A:263:LEU:HD22	2.08	0.54
3:B:45:THR:HG22	3:B:47:TYR:N	2.23	0.53
3:A:312:LYS:HE3	3:A:312:LYS:CA	2.38	0.53
3:A:65:ILE:HD13	3:A:103:SER:OG	2.07	0.53
3:A:132:LYS:HE2	3:A:148:LEU:HG	1.90	0.53
3:A:15:GLN:NE2	3:A:23:TYR:HB3	2.24	0.53
6:C:320:HOH:O	3:A:136:LYS:HE3	2.08	0.53
3:B:169:THR:OG1	3:B:257:HIS:HE1	1.91	0.53
3:A:319:ILE:HG21	3:A:324:ILE:HD11	1.91	0.53
3:A:496:LEU:HB3	3:A:516:MET:HG2	1.91	0.53
3:A:332:LYS:HE2	3:A:431:HIS:CD2	2.44	0.53
3:A:157:ASN:OD1	3:A:195:LEU:HD13	2.10	0.52
1:H:9:G:H4'	3:B:277:PRO:HB3	1.92	0.52
3:A:148:LEU:HD22	3:A:152:VAL:HG23	1.90	0.52
3:A:514:ARG:HD2	3:A:514:ARG:C	2.29	0.52
3:B:192:ASN:ND2	3:B:195:LEU:H	2.07	0.52
3:B:389:ILE:HD12	3:B:390:LEU:HG	1.92	0.52
3:A:160:ASP:HB3	3:A:163:ASN:HD22	1.74	0.52
3:A:101:GLN:HE21	3:A:132:LYS:NZ	2.08	0.51
3:A:169:THR:OG1	3:A:257:HIS:HE1	1.94	0.51
3:A:46:TYR:CD2	3:A:380:SER:HA	2.46	0.51
3:B:85:ARG:O	3:B:320:HIS:HE1	1.94	0.51
3:A:82:GLN:NE2	3:A:117:GLU:OE1	2.44	0.51
3:B:282:LEU:HD22	3:B:327:ALA:CB	2.40	0.50
3:B:45:THR:CG2	3:B:46:TYR:N	2.73	0.50
3:B:148:LEU:HD22	3:B:152:VAL:HG23	1.93	0.50
3:A:273:LEU:HB2	3:A:288:MET:HE1	1.92	0.50
3:B:320:HIS:H	3:B:323:HIS:CD2	2.30	0.50
3:B:51:LYS:O	3:B:55:GLN:HG3	2.10	0.50
3:A:137:GLU:CD	3:A:137:GLU:H	2.13	0.50
3:A:526:ALA:O	3:A:530:ILE:HG13	2.12	0.50
3:A:7:GLN:HG3	3:A:476:ASP:O	2.11	0.50
3:A:408:LYS:HG3	6:A:2142:HOH:O	2.11	0.50
3:B:259:LEU:H	3:B:262:HIS:CD2	2.30	0.49
3:A:5:MET:HE3	3:A:11:LEU:HA	1.93	0.49
3:B:44:GLY:HA2	3:B:53:LEU:HD12	1.94	0.49
3:A:78:LYS:HE3	3:A:117:GLU:CD	2.32	0.49
3:A:432:GLU:HA	3:A:435:GLU:CG	2.42	0.49
3:B:355:ASN:ND2	3:B:359:LYS:HE3	2.28	0.49
3:B:219:SER:C	3:B:221:GLU:H	2.16	0.49
3:B:188:ILE:HG12	3:B:189:LYS:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:216:LYS:O	3:B:218:LEU:N	2.46	0.49
3:A:180:LYS:HD3	3:A:184:ARG:NH1	2.28	0.49
3:B:237:ARG:HH11	3:B:237:ARG:HG3	1.78	0.49
3:B:102:CYS:SG	3:B:141:CYS:CB	3.01	0.49
1:G:8:C:H3'	1:G:9:G:H5'	1.95	0.48
3:A:218:LEU:HD22	3:A:222:THR:HG21	1.94	0.48
3:B:479:PRO:HG2	6:B:2006:HOH:O	2.13	0.48
3:A:288:MET:HE3	3:A:293:VAL:HG21	1.95	0.48
3:A:213:TYR:HD2	3:A:218:LEU:HD21	1.79	0.48
3:A:29:ASP:OD2	3:A:63:ARG:HD2	2.14	0.48
3:B:116:PRO:HG2	3:B:117:GLU:OE2	2.14	0.48
3:A:102:CYS:SG	3:A:141:CYS:SG	3.10	0.47
3:B:168:VAL:HG11	3:B:202:VAL:HG22	1.95	0.47
3:B:291:ASP:O	3:B:292:SER:HB2	2.14	0.47
3:A:361:PHE:O	3:A:363:LEU:HD13	2.14	0.47
3:A:192:ASN:HD22	3:A:194:GLY:N	2.12	0.47
1:H:8:C:OP1	3:B:170:LYS:NZ	2.38	0.47
3:B:213:TYR:O	3:B:215:GLU:N	2.48	0.47
3:A:265:SER:OG	3:A:268:ILE:HG12	2.15	0.47
3:A:164:LEU:HD22	3:A:168:VAL:HG13	1.96	0.47
2:F:6:IU:H2'	2:F:7:A:H8	1.78	0.47
3:B:209:VAL:O	3:B:213:TYR:HD1	1.98	0.47
3:B:190:PRO:HB3	3:B:195:LEU:HB3	1.98	0.46
3:A:288:MET:HB3	3:A:293:VAL:CG2	2.45	0.46
3:B:205:GLY:O	3:B:209:VAL:HG23	2.13	0.46
3:A:377:VAL:O	3:A:441:THR:HA	2.15	0.46
3:A:315:LYS:HE3	3:A:359:LYS:O	2.15	0.46
3:A:527:LEU:HB2	6:A:2040:HOH:O	2.15	0.46
3:B:405:ARG:HG2	3:B:426:VAL:CG1	2.46	0.46
3:A:288:MET:CE	3:A:293:VAL:HG21	2.46	0.46
3:A:115:VAL:N	3:A:116:PRO:HD2	2.31	0.46
3:B:171:TYR:O	3:B:179:HIS:CE1	2.68	0.46
3:B:357:PHE:CG	3:B:430:LEU:HD11	2.51	0.46
2:D:8:G:O2'	2:D:9:C:H5'	2.17	0.45
1:H:8:C:H4'	3:B:121:ILE:HG21	1.98	0.45
3:A:320:HIS:CD2	3:A:322:PHE:H	2.34	0.45
3:B:12:ASN:OD1	3:B:14:LYS:N	2.39	0.45
3:B:85:ARG:HA	3:B:524:SER:OG	2.17	0.45
1:E:3:IU:O2'	1:E:4:G:O5'	2.34	0.45
1:C:3:IU:HO2'	1:C:4:G:P	2.39	0.45
3:A:184:ARG:HG3	6:A:2129:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:125:LEU:HD22	3:A:129:ILE:HD12	1.99	0.45
3:A:5:MET:HA	3:A:9:GLN:NE2	2.31	0.44
3:A:192:ASN:HD21	3:A:195:LEU:H	1.65	0.44
3:B:445:THR:O	3:B:474:VAL:HG23	2.18	0.44
3:A:101:GLN:NE2	3:A:132:LYS:NZ	2.65	0.44
3:A:192:ASN:ND2	3:A:195:LEU:HG	2.33	0.44
3:A:101:GLN:NE2	3:A:132:LYS:HZ1	2.15	0.44
3:A:237:ARG:HH21	3:A:237:ARG:HG2	1.83	0.44
3:B:18:ASN:ND2	3:B:20:GLU:H	2.16	0.44
3:A:319:ILE:CG2	3:A:324:ILE:HD11	2.47	0.43
3:A:213:TYR:CD2	3:A:218:LEU:HD21	2.53	0.43
3:A:272:LEU:HD12	3:A:272:LEU:HA	1.92	0.43
3:A:192:ASN:HD21	3:A:195:LEU:HG	1.82	0.43
3:A:102:CYS:SG	3:A:141:CYS:CB	3.06	0.43
3:A:291:ASP:O	3:A:292:SER:HB2	2.19	0.43
3:B:377:VAL:O	3:B:441:THR:HA	2.18	0.43
3:B:207:LYS:HG2	3:B:207:LYS:H	1.57	0.43
3:A:391:ASN:O	3:A:395:VAL:HG23	2.17	0.43
3:A:112:PHE:HA	3:A:115:VAL:HG23	2.00	0.43
3:A:125:LEU:HD22	3:A:129:ILE:CD1	2.49	0.43
3:A:216:LYS:NZ	3:A:216:LYS:CB	2.81	0.43
3:B:115:VAL:N	3:B:116:PRO:HD2	2.34	0.43
3:A:405:ARG:NH1	3:A:426:VAL:O	2.40	0.43
3:B:389:ILE:HD12	3:B:390:LEU:N	2.34	0.43
3:A:31:ASN:HD22	3:A:34:ARG:HH11	1.67	0.42
3:A:273:LEU:HB2	3:A:288:MET:CE	2.48	0.42
3:A:430:LEU:O	3:A:434:VAL:HG23	2.19	0.42
3:A:101:GLN:CG	3:A:141:CYS:SG	3.07	0.42
3:B:342:ARG:HH11	3:B:342:ARG:HG3	1.83	0.42
3:B:46:TYR:N	3:B:383:GLN:HE21	2.12	0.42
2:D:7:A:H2'	2:D:8:G:O4'	2.19	0.42
3:B:104:ASP:OD2	3:B:106:LYS:HB2	2.19	0.42
2:F:1:IU:I5	3:B:204:LYS:NZ	3.06	0.42
3:B:168:VAL:HG11	3:B:202:VAL:CG2	2.50	0.42
3:B:144:TRP:CZ3	3:B:148:LEU:HD13	2.55	0.42
3:B:189:LYS:HD2	3:B:189:LYS:HA	1.93	0.42
3:B:418:GLU:O	3:B:420:LEU:HD22	2.19	0.42
3:A:328:LEU:HD21	3:A:431:HIS:HB3	2.02	0.42
3:A:171:TYR:O	3:A:179:HIS:CE1	2.70	0.42
3:B:407:GLU:HB3	6:B:2016:HOH:O	2.20	0.42
3:B:45:THR:HG22	3:B:48:ILE:N	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:134:ASP:O	3:A:137:GLU:OE1	2.38	0.41
3:A:492:ILE:HA	3:A:493:PRO:HD3	1.86	0.41
3:A:76:GLU:OE2	3:A:76:GLU:HA	2.20	0.41
1:H:8:C:H5"	3:B:171:TYR:HH	1.83	0.41
3:B:102:CYS:HG	3:B:141:CYS:CB	2.33	0.41
3:B:455:GLN:NE2	3:B:489:LYS:HG2	2.34	0.41
3:B:53:LEU:HA	3:B:53:LEU:HD23	1.94	0.41
3:B:234:ARG:O	3:B:238:THR:HG22	2.21	0.41
3:A:92:THR:CG2	6:A:2002:HOH:O	2.57	0.41
3:B:342:ARG:HH11	3:B:342:ARG:CG	2.34	0.41
1:G:9:G:H4'	3:A:277:PRO:HB3	2.03	0.41
3:A:45:THR:HB	3:A:383:GLN:NE2	2.36	0.41
3:B:197:MET:HE2	3:B:222:THR:OG1	2.20	0.41
3:A:31:ASN:ND2	3:A:34:ARG:HH11	2.19	0.41
3:B:193:GLU:OE1	3:B:193:GLU:HA	2.20	0.41
3:A:355:ASN:HD21	3:A:359:LYS:CE	2.34	0.41
3:B:382:ASN:HD22	3:B:391:ASN:HD22	1.69	0.41
3:B:325:LEU:HD13	3:B:390:LEU:HD13	2.03	0.41
2:F:5:C:H2'	2:F:6:IU:O4'	2.21	0.40
3:A:129:ILE:HD13	3:A:182:LEU:CD2	2.51	0.40
3:B:402:LEU:HD13	3:B:527:LEU:HD11	2.03	0.40
3:B:77:ILE:CG2	3:B:92:THR:HG23	2.47	0.40
3:A:254:VAL:H	3:A:257:HIS:CD2	2.14	0.40
3:A:320:HIS:HB3	3:A:323:HIS:CD2	2.56	0.40
3:A:418:GLU:O	3:A:420:LEU:HD22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	525/538 (98%)	501 (95%)	23 (4%)	1 (0%)	52	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	528/538 (98%)	502 (95%)	20 (4%)	6 (1%)	17	14
All	All	1053/1076 (98%)	1003 (95%)	43 (4%)	7 (1%)	26	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	214	LYS
3	B	217	GLU
3	A	102	CYS
3	B	137	GLU
3	B	140	LYS
3	B	215	GLU
3	B	220	PRO

5.3.2 Protein sidechains (i)

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	460/467 (98%)	434 (94%)	26 (6%)	25	29
3	B	463/467 (99%)	439 (95%)	24 (5%)	29	33
All	All	923/934 (99%)	873 (95%)	50 (5%)	27	31

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	18	ASN
3	A	53	LEU
3	A	61	LEU
3	A	62	LEU
3	A	96	LEU
3	A	101	GLN
3	A	125	LEU
3	A	148	LEU

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Mol	Chain	Res	Type
3	A	164	LEU
3	A	173	GLN
3	A	192	ASN
3	A	216	LYS
3	A	258	LEU
3	A	263	LEU
3	A	272	LEU
3	A	274	GLN
3	A	293	VAL
3	A	312	LYS
3	A	325	LEU
3	A	332	LYS
3	A	384	ARG
3	A	418	GLU
3	A	435	GLU
3	A	456	LYS
3	A	514	ARG
3	B	13	GLU
3	B	18	ASN
3	B	45	THR
3	B	49	GLU
3	B	53	LEU
3	B	104	ASP
3	B	148	LEU
3	B	160	ASP
3	B	164	LEU
3	B	175	ASN
3	B	192	ASN
3	B	193	GLU
3	B	195	LEU
3	B	207	LYS
3	B	263	LEU
3	B	282	LEU
3	B	294	LEU
3	B	300	GLU
3	B	310	ASN
3	B	316	LYS
3	B	325	LEU
3	B	385	VAL
3	B	402	LEU
3	B	528	ASP

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

sidechains are listed below:

Mol	Chain	Res	Type
3	A	7	GLN
3	A	9	GLN
3	A	12	ASN
3	A	15	GLN
3	A	18	ASN
3	A	31	ASN
3	A	57	ASN
3	A	101	GLN
3	A	163	ASN
3	A	173	GLN
3	A	179	HIS
3	A	192	ASN
3	A	257	HIS
3	A	320	HIS
3	A	323	HIS
3	A	355	ASN
3	A	382	ASN
3	A	383	GLN
3	A	431	HIS
3	A	485	GLN
3	B	7	GLN
3	B	18	ASN
3	B	57	ASN
3	B	75	GLN
3	B	173	GLN
3	B	179	HIS
3	B	192	ASN
3	B	210	GLN
3	B	257	HIS
3	B	262	HIS
3	B	310	ASN
3	B	320	HIS
3	B	323	HIS
3	B	355	ASN
3	B	382	ASN
3	B	383	GLN
3	B	431	HIS
3	B	455	GLN
3	B	485	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	9/10 (90%)	2 (22%)	0
1	E	9/10 (90%)	2 (22%)	0
1	G	4/10 (40%)	3 (75%)	3 (75%)
1	H	6/10 (60%)	3 (50%)	2 (33%)
2	D	9/10 (90%)	1 (11%)	0
2	F	9/10 (90%)	1 (11%)	0
All	All	46/60 (76%)	12 (26%)	5 (10%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	3	IU
1	C	4	G
2	D	3	G
1	E	3	IU
1	E	4	G
2	F	3	G
1	G	8	C
1	G	9	G
1	G	10	A
1	H	8	C
1	H	9	G
1	H	10	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	G	7	C
1	G	8	C
1	G	9	G
1	H	8	C
1	H	9	G

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

8 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	IU	C	3	1,2	12,22,23	1.27	2 (16%)	12,32,35	3.82	1 (8%)
2	IU	D	1	2	13,19,23	1.13	2 (15%)	12,28,35	4.01	1 (8%)
2	IU	D	2	2	12,22,23	1.09	1 (8%)	12,32,35	3.95	1 (8%)
2	IU	D	6	1,2	12,22,23	1.29	2 (16%)	12,32,35	4.02	1 (8%)
1	IU	E	3	1,2	12,22,23	1.18	1 (8%)	12,32,35	4.03	2 (16%)
2	IU	F	1	2	13,19,23	1.07	1 (7%)	12,28,35	3.96	1 (8%)
2	IU	F	2	2	12,22,23	1.13	1 (8%)	12,32,35	3.90	1 (8%)
2	IU	F	6	1,2	12,22,23	1.17	2 (16%)	12,32,35	4.01	1 (8%)

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	IU	C	3	1,2	-	0/3/25/26	0/2/2/2
2	IU	D	1	2	-	0/2/22/26	0/2/2/2
2	IU	D	2	2	-	0/3/25/26	0/2/2/2
2	IU	D	6	1,2	-	0/3/25/26	0/2/2/2
1	IU	E	3	1,2	-	0/3/25/26	0/2/2/2
2	IU	F	1	2	-	0/2/22/26	0/2/2/2
2	IU	F	2	2	-	0/3/25/26	0/2/2/2
2	IU	F	6	1,2	-	0/3/25/26	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3	IU	C6-C5	-2.90	1.31	1.38
2	D	1	IU	C6-N1	2.34	1.38	1.35
2	F	6	IU	C6-N1	2.39	1.38	1.35
2	D	2	IU	C4-N3	2.63	1.38	1.33
2	F	6	IU	C4-N3	2.63	1.38	1.33
2	F	1	IU	C4-N3	2.64	1.38	1.33
2	F	2	IU	C4-N3	2.69	1.38	1.33
2	D	6	IU	C4-N3	2.71	1.38	1.33
1	C	3	IU	C4-N3	2.72	1.38	1.33
1	E	3	IU	C4-N3	2.73	1.38	1.33
2	D	1	IU	C4-N3	2.75	1.38	1.33
2	D	6	IU	C6-N1	2.88	1.39	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	3	IU	O3'-C3'-C4'	-2.34	104.03	111.05
1	C	3	IU	C4-N3-C2	12.80	126.31	115.25
2	F	2	IU	C4-N3-C2	13.45	126.87	115.25
2	D	2	IU	C4-N3-C2	13.49	126.91	115.25
1	E	3	IU	C4-N3-C2	13.51	126.93	115.25
2	F	1	IU	C4-N3-C2	13.67	127.06	115.25
2	F	6	IU	C4-N3-C2	13.80	127.18	115.25
2	D	6	IU	C4-N3-C2	13.84	127.21	115.25
2	D	1	IU	C4-N3-C2	13.86	127.23	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	3	IU	2	0
1	E	3	IU	1	0
2	F	1	IU	1	0
2	F	6	IU	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ACT	A	2001	5	1,3,3	4.04	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ACT	B	2002	5	1,3,3	3.06	1 (100%)	0,3,3	0.00	-

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	ACT	A	2001	5	-	0/0/0/0	0/0/0/0
4	ACT	B	2002	5	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2002	ACT	CH3-C	3.06	1.53	1.48
4	A	2001	ACT	CH3-C	4.04	1.54	1.48

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, 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	C	9/10 (90%)	-0.58	0	100	100	30, 34, 44, 46	0
1	E	9/10 (90%)	-0.48	0	100	100	36, 37, 44, 49	0
1	G	5/10 (50%)	0.56	0	100	100	30, 30, 61, 66	0
1	H	7/10 (70%)	-0.18	0	100	100	29, 37, 45, 56	0
2	D	7/10 (70%)	-0.47	0	100	100	39, 44, 55, 58	0
2	F	7/10 (70%)	-0.01	0	100	100	43, 46, 57, 59	0
3	A	529/538 (98%)	-0.27	4 (0%)	87	87	23, 36, 54, 70	0
3	B	532/538 (98%)	-0.23	7 (1%)	79	78	21, 35, 60, 90	0
All	All	1105/1136 (97%)	-0.25	11 (0%)	84	83	21, 36, 57, 90	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	218	LEU	3.9
3	B	217	GLU	3.9
3	B	102	CYS	3.1
3	A	141	CYS	2.6
3	A	217	GLU	2.6
3	A	102	CYS	2.6
3	B	537	LEU	2.6
3	B	336	GLY	2.5
3	B	4	THR	2.1
3	A	438	SER	2.1
3	B	212	ALA	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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	IU	F	6	21/22	0.93	0.12	-	51,57,66,83	0
2	IU	F	2	21/22	0.95	0.12	-	49,54,59,73	0
1	IU	E	3	21/22	0.92	0.14	-	43,51,60,72	0
1	IU	C	3	21/22	0.92	0.13	-	39,49,54,70	0
2	IU	D	6	21/22	0.92	0.10	-	49,51,56,75	0
2	IU	D	1	18/22	0.86	0.16	-	46,57,74,94	0
2	IU	F	1	18/22	0.93	0.11	-	51,57,68,85	0
2	IU	D	2	21/22	0.92	0.12	-	42,48,53,72	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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	ACT	B	2002	4/4	0.97	0.13	1.23	32,33,33,33	0
4	ACT	A	2001	4/4	0.95	0.12	0.62	27,28,29,30	0
5	MG	A	1001	1/1	0.58	0.09	-0.72	32,32,32,32	0
5	MG	B	1002	1/1	0.97	0.05	-2.30	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.