Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2017 – 03:37 PM EDT

PDB ID	:	5G52
Title	:	Crystallographic structure of full particle of Deformed Wing Virus
Authors	:	Skubnik, K.; Novacek, J.; Fuzik, T.; Pridal, A.; Paxton, R.; Plevka, P.
Deposited on	:	2016-05-18
Resolution	:	3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

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 3.80 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.
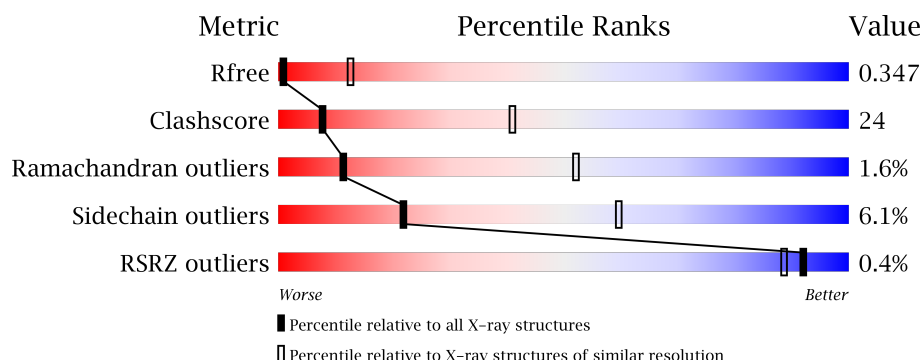
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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	A	243	·% 47% 48% 5%
2	B	250	54% 40% 6%
3	C	397	52% 43% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7045 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 protein called VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1910	1217	326	357	10			

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	250	Total	C	N	O	S	0	0	0
			1973	1253	335	378	7			

- Molecule 3 is a protein called VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	397	Total	C	N	O	S	0	0	0
			3142	2015	541	574	12			

- Molecule 4 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U5P) (formula: $C_9H_{13}N_2O_9P$).
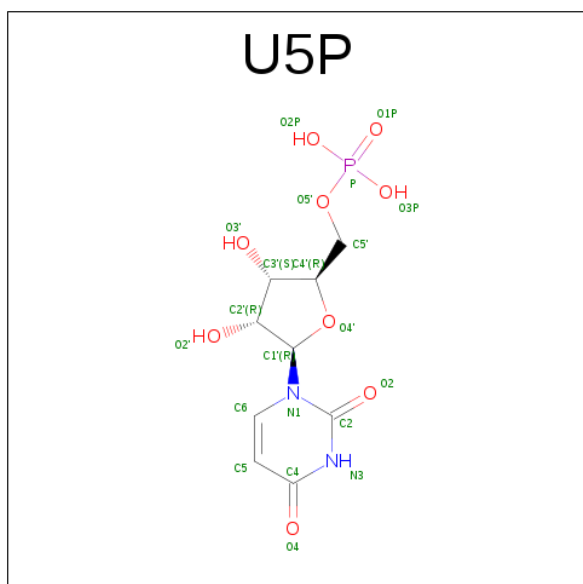
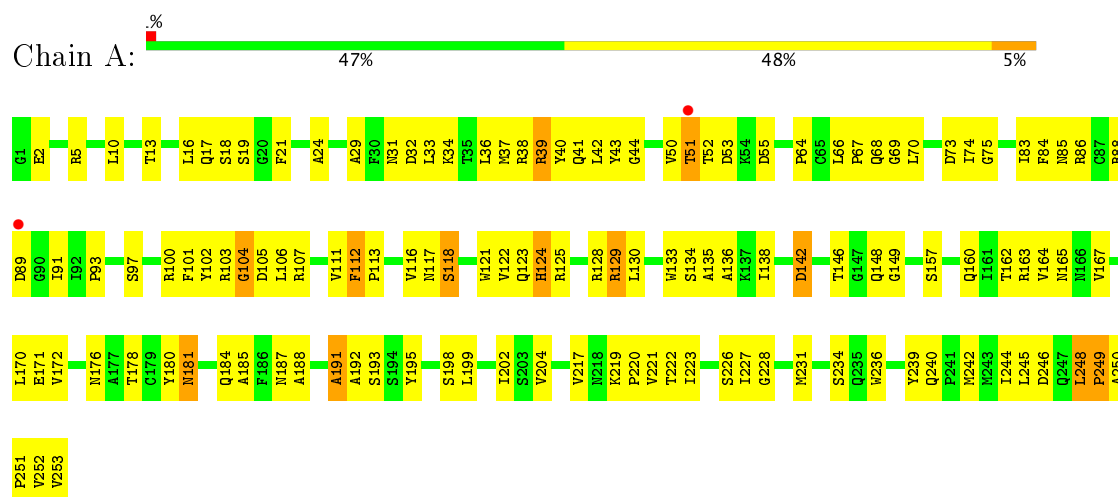| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	C	1	20	9	2	8	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: VP1

- Molecule 2: VP2

- Molecule 3: VP3

M153 D154 Y155 M156 K157 L158 K159 S160 Y163 V164 V165 F166 D167 L168 N172 S173 F174 V178 P179 Y180 Y183 R184 P185 W186 W187 V188 R189 K190 Y191 G192 G193 N194 Y195 L196 P197 T200 P203 S204 T205 L206 F207 M208 Y209 V210 Q211 V212 P213 L214 V220 S221 D222 T223 I224

D225 I226 N227 V228 Y229 V230 R231 G232 G233 F236 E237 V238 C239 V240 Q243 P244 S245 L246 G247 L248 N249 W250 D253 F254 I255 L256 R257 N258 D259 E260 E261 Y262 R263 A264 A269 P270 Y271 Y272 A273 G274 V275 W276 H277 S278 S284 L285 S303 E308 L309 L312 R313

V322 G323 T324 T329 M330 W333 P334 S335 Y339 N340 I341 A348 E349 R350 A355 Q356 H357 L364 A369 L372 F373 Q378 Q379 K383 N388 P389 V390 W391 E392 V393 M394 R395 A396 P397 L398

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	360.13Å 360.13Å 360.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 3.80 29.80 – 3.80	Depositor EDS
% Data completeness (in resolution range)	75.0 (29.80-3.80) 75.0 (29.80-3.80)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.34 (at 3.75Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.283 , 0.322 0.331 , 0.347	Depositor DCC
R_{free} test set	2844 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	53.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	3.36 , 1.1	EDS
L-test for twinning[2]	$<\|L\|>$ = 0.41, $<L^2>$ = 0.23	Xtriage
Estimated twinning fraction	0.048 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.66	EDS
Total number of atoms	7045	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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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: U5P

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	0.32	0/1957	0.71	1/2660 (0.0%)
2	B	0.31	0/2024	0.64	3/2763 (0.1%)
3	C	0.28	0/3238	0.53	1/4418 (0.0%)
All	All	0.30	0/7219	0.61	5/9841 (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	A	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	86	PRO	C-N-CA	5.97	136.62	121.70
2	B	86	PRO	CA-C-N	5.57	129.45	117.20
1	A	191	ALA	C-N-CA	5.38	135.15	121.70
2	B	171	SER	C-N-CA	5.35	135.08	121.70
3	C	168	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	GLY	Peptide

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	A	1910	0	1851	126	0
2	B	1973	0	1928	95	0
3	C	3142	0	3051	162	0
4	C	20	0	11	0	0
All	All	7045	0	6841	336	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 24.

All (336) 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)
1:A:191:ALA:H	1:A:192:ALA:HB3	1.33	0.92
1:A:133:TRP:HB2	2:B:147:LEU:HD11	1.54	0.89
2:B:55:TYR:HH	2:B:112:HIS:HE2	1.19	0.88
1:A:192:ALA:HB2	2:B:194:ASP:HB3	1.55	0.88
1:A:38:ARG:HB3	1:A:39:ARG:HA	1.60	0.84
3:C:111:SER:HB2	3:C:114:PHE:HB2	1.57	0.83
1:A:118:SER:HB3	1:A:162:THR:HG22	1.59	0.83
1:A:37:MET:HG3	1:A:227:ILE:HG13	1.61	0.82
3:C:118:ARG:HB2	3:C:186:TRP:HA	1.61	0.81
1:A:42:LEU:HD22	1:A:83:ILE:HD13	1.63	0.80
2:B:120:GLU:HB3	2:B:230:LYS:HB3	1.64	0.80
1:A:88:ARG:NH2	3:C:253:ASP:O	2.16	0.79
2:B:87:ARG:NH1	2:B:199:ILE:O	2.17	0.77
1:A:123:GLN:HB3	1:A:157:SER:HB3	1.68	0.76
3:C:322:VAL:HB	3:C:383:LYS:HB2	1.68	0.76
1:A:42:LEU:HD11	1:A:222:THR:HB	1.67	0.75
3:C:258:ASN:H	3:C:260:GLU:H	1.32	0.75
3:C:258:ASN:N	3:C:260:GLU:H	1.83	0.74
1:A:146:THR:HB	1:A:148:GLN:H	1.52	0.74
2:B:70:TRP:HB3	2:B:223:CYS:HB3	1.70	0.74
3:C:271:TYR:HH	3:C:391:TRP:HE1	1.34	0.73
2:B:55:TYR:OH	2:B:112:HIS:NE2	2.21	0.73
1:A:251:PRO:O	3:C:395:ARG:NH2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:TYR:HE1	1:A:70:LEU:HD13	1.54	0.72
2:B:107:ILE:HG13	2:B:108:PRO:HD3	1.70	0.72
3:C:151:LEU:HD12	3:C:152:GLN:HG3	1.70	0.72
1:A:148:GLN:N	1:A:149:GLY:HA3	2.04	0.72
3:C:118:ARG:HG2	3:C:118:ARG:O	1.89	0.71
1:A:227:ILE:HD12	1:A:231:MET:HG2	1.73	0.70
3:C:116:GLN:HB3	3:C:186:TRP:HB3	1.73	0.70
3:C:115:MET:HB3	3:C:240:VAL:HG13	1.72	0.70
2:B:171:SER:HA	2:B:172:ASN:CB	2.22	0.69
3:C:119:GLY:HA3	3:C:236:PHE:HA	1.74	0.68
3:C:183:TYR:OH	3:C:184:ARG:NH2	2.26	0.68
2:B:136:GLN:OE1	2:B:208:ARG:NH2	2.27	0.67
3:C:145:LEU:HD12	3:C:150:GLN:HA	1.76	0.67
2:B:40:VAL:O	2:B:116:ARG:NH1	2.29	0.66
3:C:70:TRP:HZ3	3:C:168:LEU:HD21	1.61	0.66
1:A:129:ARG:NH2	1:A:191:ALA:O	2.24	0.65
1:A:97:SER:O	1:A:184:GLN:NE2	2.29	0.65
2:B:171:SER:HA	2:B:172:ASN:HB2	1.77	0.65
2:B:182:HIS:CE1	2:B:195:TRP:HH2	2.14	0.65
1:A:122:VAL:HG12	1:A:204:VAL:HG22	1.78	0.65
1:A:103:ARG:NH2	3:C:47:CYS:SG	2.69	0.65
1:A:191:ALA:N	1:A:192:ALA:HB3	2.09	0.65
1:A:100:ARG:NE	2:B:142:SER:OG	2.29	0.65
2:B:138:THR:HG21	2:B:158:PHE:HB3	1.78	0.64
3:C:313:ARG:HG2	3:C:329:THR:HG22	1.79	0.64
3:C:143:PRO:HA	3:C:204:SER:HB2	1.78	0.64
1:A:198:SER:CB	1:A:199:LEU:HA	2.27	0.64
3:C:152:GLN:O	3:C:157:LYS:NZ	2.22	0.64
1:A:133:TRP:O	1:A:136:ALA:N	2.31	0.64
1:A:16:LEU:N	1:A:17:GLN:HB2	2.12	0.64
1:A:116:VAL:HG22	1:A:118:SER:HA	1.80	0.64
3:C:257:ARG:HB2	3:C:258:ASN:HB2	1.80	0.63
3:C:92:ARG:NH2	3:C:100:SER:OG	2.30	0.63
1:A:187:ASN:OD1	1:A:188:ALA:N	2.30	0.63
3:C:115:MET:HG2	3:C:116:GLN:HG3	1.79	0.63
1:A:198:SER:HB3	1:A:199:LEU:HA	1.81	0.62
2:B:32:THR:HG22	2:B:175:LYS:HD3	1.80	0.62
3:C:261:GLU:HB3	3:C:390:VAL:HG13	1.80	0.62
1:A:21:PHE:HE2	3:C:238:VAL:HG23	1.66	0.61
1:A:176:ASN:HB3	1:A:178:THR:HG23	1.83	0.60
3:C:93:ILE:HD12	3:C:103:TRP:HE1	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:TYR:O	2:B:59:THR:HG22	2.01	0.60
2:B:155:VAL:HA	2:B:208:ARG:HH21	1.67	0.60
2:B:138:THR:HG23	2:B:163:HIS:HB3	1.84	0.60
2:B:79:GLU:HB3	2:B:208:ARG:HG2	1.84	0.60
2:B:187:LEU:HD11	2:B:202:MET:HB2	1.83	0.60
1:A:125:ARG:NH1	1:A:148:GLN:O	2.34	0.59
2:B:245:TYR:CG	2:B:246:ALA:N	2.70	0.59
1:A:253:VAL:HA	3:C:303:SER:HB3	1.84	0.59
3:C:117:TRP:HE3	3:C:119:GLY:H	1.51	0.59
1:A:122:VAL:HG21	1:A:170:LEU:HD11	1.85	0.58
2:B:86:PRO:HB2	2:B:87:ARG:HB2	1.85	0.58
3:C:159:LYS:HE2	3:C:211:GLN:HE22	1.69	0.58
2:B:133:GLY:H	2:B:168:ALA:HB3	1.68	0.58
2:B:214:ARG:NH1	3:C:223:THR:OG1	2.36	0.58
3:C:51:GLU:OE2	3:C:61:ARG:NH2	2.37	0.58
2:B:22:VAL:HG11	2:B:62:TRP:H	1.69	0.57
2:B:215:MET:SD	2:B:221:THR:HA	2.44	0.57
2:B:39:SER:OG	2:B:180:PHE:O	2.20	0.57
3:C:309:LEU:HD23	3:C:398:LEU:HB2	1.86	0.57
2:B:152:LYS:NZ	2:B:157:GLY:O	2.37	0.57
3:C:138:ILE:HG12	3:C:211:GLN:HB2	1.84	0.57
3:C:51:GLU:HA	3:C:52:ASP:HB3	1.85	0.57
3:C:54:THR:HB	3:C:57:SER:H	1.69	0.57
1:A:250:ALA:HB3	3:C:395:ARG:HG3	1.87	0.57
1:A:100:ARG:HD3	2:B:140:TYR:HE1	1.70	0.56
2:B:94:GLU:OE2	2:B:245:TYR:OH	2.14	0.56
1:A:21:PHE:CG	1:A:31:ASN:HB2	2.40	0.56
1:A:227:ILE:HG23	1:A:231:MET:HB3	1.86	0.56
3:C:68:VAL:HG11	3:C:80:LEU:HB3	1.87	0.56
1:A:36:LEU:C	1:A:38:ARG:H	2.08	0.56
3:C:70:TRP:HH2	3:C:135:GLY:HA3	1.71	0.56
1:A:2:GLU:HG3	2:B:165:LEU:H	1.71	0.56
2:B:18:LYS:HB3	2:B:23:VAL:HG13	1.88	0.56
3:C:118:ARG:HA	3:C:180:TYR:CZ	2.41	0.56
3:C:121:LEU:HA	3:C:233:GLY:H	1.71	0.56
3:C:142:VAL:O	3:C:204:SER:OG	2.21	0.56
2:B:223:CYS:SG	2:B:224:ASN:N	2.78	0.55
1:A:111:VAL:HG12	1:A:167:VAL:HG13	1.89	0.55
3:C:357:HIS:ND1	3:C:369:ALA:HB2	2.22	0.55
1:A:33:LEU:HD12	1:A:36:LEU:HB3	1.88	0.55
3:C:121:LEU:O	3:C:178:VAL:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:SER:OG	1:A:19:SER:N	2.38	0.54
1:A:165:ASN:ND2	3:C:16:GLY:O	2.40	0.54
2:B:70:TRP:CG	2:B:213:LEU:HD11	2.42	0.54
3:C:172:ASN:N	3:C:172:ASN:OD1	2.29	0.54
3:C:83:LEU:HD13	3:C:89:VAL:HG21	1.88	0.54
1:A:38:ARG:HB3	1:A:39:ARG:HD2	1.88	0.54
1:A:117:ASN:HA	1:A:118:SER:HB2	1.90	0.54
1:A:217:VAL:N	1:A:219:LYS:HE2	2.23	0.54
1:A:41:GLN:OE1	1:A:91:ILE:N	2.38	0.54
2:B:50:ASP:HB3	2:B:237:THR:HG23	1.90	0.54
1:A:104:GLY:HA2	1:A:231:MET:HB2	1.90	0.54
3:C:183:TYR:HE1	3:C:184:ARG:HE	1.55	0.53
1:A:111:VAL:HG23	1:A:112:PHE:HD1	1.74	0.53
1:A:84:PHE:O	1:A:88:ARG:NH1	2.41	0.53
2:B:55:TYR:HB3	2:B:58:ILE:HD13	1.90	0.53
2:B:124:GLN:HG2	2:B:173:GLU:HG3	1.89	0.53
2:B:192:VAL:HG13	2:B:193:PRO:HD2	1.91	0.53
1:A:13:THR:HG22	3:C:179:PRO:HB3	1.91	0.53
2:B:125:ILE:O	2:B:171:SER:OG	2.27	0.53
3:C:142:VAL:O	3:C:145:LEU:HD23	2.09	0.53
1:A:39:ARG:HB3	3:C:20:LEU:O	2.09	0.53
2:B:132:VAL:HG12	3:C:128:ILE:HG22	1.91	0.52
3:C:189:ARG:NH2	3:C:243:GLN:O	2.42	0.52
1:A:146:THR:HB	1:A:148:GLN:N	2.23	0.52
1:A:185:ALA:HB1	2:B:147:LEU:HD12	1.90	0.52
3:C:104:PHE:CE2	3:C:246:LEU:HD21	2.44	0.52
2:B:136:GLN:HB3	2:B:210:ILE:HD11	1.91	0.52
3:C:92:ARG:HA	3:C:102:TYR:HD1	1.73	0.52
1:A:107:ARG:HB2	1:A:226:SER:HB3	1.92	0.52
1:A:86:ARG:HH22	1:A:250:ALA:HA	1.74	0.52
3:C:159:LYS:HG2	3:C:163:TYR:CE2	2.44	0.52
3:C:309:LEU:HB2	3:C:355:ALA:HB1	1.92	0.52
3:C:153:MET:HG2	3:C:207:PHE:CE2	2.45	0.52
3:C:88:PHE:HE2	3:C:189:ARG:HA	1.74	0.52
2:B:39:SER:HB3	2:B:116:ARG:HH12	1.74	0.51
1:A:121:TRP:HZ3	1:A:123:GLN:HG2	1.75	0.51
2:B:206:ASN:N	2:B:206:ASN:OD1	2.43	0.51
3:C:81:LEU:HD21	3:C:228:VAL:HG21	1.93	0.51
2:B:140:TYR:HE2	2:B:152:LYS:HG2	1.76	0.51
1:A:239:TYR:CD1	3:C:109:VAL:HG21	2.45	0.51
1:A:75:GLY:O	3:C:255:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:ASN:ND2	3:C:25:ASN:O	2.44	0.51
1:A:165:ASN:ND2	1:A:167:VAL:HB	2.25	0.51
1:A:124:HIS:HB3	3:C:33:LEU:HD13	1.92	0.51
1:A:113:PRO:HD3	1:A:221:VAL:HG22	1.93	0.50
1:A:162:THR:OG1	1:A:163:ARG:N	2.44	0.50
1:A:244:ILE:HG22	1:A:246:ASP:H	1.76	0.50
2:B:156:TYR:OH	3:C:91:GLN:NE2	2.32	0.50
3:C:335:SER:N	3:C:339:TYR:O	2.40	0.50
3:C:324:THR:OG1	3:C:378:GLN:OE1	2.19	0.50
3:C:36:ASP:OD1	3:C:37:ALA:N	2.45	0.50
3:C:70:TRP:CH2	3:C:135:GLY:HA3	2.47	0.50
1:A:101:PHE:HB2	1:A:234:SER:HB2	1.92	0.50
3:C:312:LEU:HB2	3:C:330:MET:HG2	1.93	0.50
1:A:105:ASP:HB3	1:A:228:GLY:HA3	1.94	0.49
1:A:239:TYR:CG	3:C:109:VAL:HG21	2.46	0.49
1:A:32:ASP:OD1	1:A:33:LEU:N	2.44	0.49
1:A:40:TYR:HB2	3:C:20:LEU:HA	1.94	0.49
1:A:100:ARG:NE	2:B:142:SER:HG	2.10	0.49
1:A:89:ASP:CG	3:C:248:LEU:HG	2.33	0.49
1:A:103:ARG:HH21	3:C:47:CYS:CB	2.25	0.49
2:B:190:ARG:HG3	2:B:244:PHE:O	2.12	0.49
3:C:312:LEU:HD11	3:C:393:VAL:HG22	1.94	0.49
1:A:178:THR:HG22	2:B:184:TYR:HE1	1.77	0.49
1:A:103:ARG:HG2	3:C:43:HIS:CD2	2.48	0.49
1:A:68:GLN:HG2	1:A:184:GLN:O	2.13	0.49
3:C:195:TYR:CD1	3:C:197:PRO:HD2	2.47	0.49
1:A:134:SER:HA	1:A:136:ALA:H	1.77	0.49
2:B:113:ALA:N	2:B:238:GLY:O	2.40	0.48
2:B:94:GLU:OE1	2:B:248:GLN:N	2.45	0.48
3:C:139:VAL:HA	3:C:207:PHE:O	2.13	0.48
2:B:100:ILE:O	2:B:106:THR:OG1	2.30	0.48
1:A:172:VAL:HG21	1:A:202:ILE:HD11	1.94	0.48
1:A:37:MET:O	1:A:227:ILE:HB	2.13	0.48
2:B:76:PHE:O	2:B:209:VAL:HB	2.13	0.48
3:C:204:SER:OG	3:C:205:THR:N	2.45	0.48
3:C:189:ARG:NH2	3:C:245:SER:HB2	2.29	0.48
3:C:155:TYR:HB3	3:C:209:TYR:CD2	2.49	0.48
1:A:67:PRO:C	1:A:69:GLY:H	2.16	0.48
1:A:121:TRP:CZ3	1:A:123:GLN:HG2	2.49	0.48
2:B:149:ILE:O	2:B:153:ARG:N	2.46	0.48
3:C:128:ILE:HD12	3:C:128:ILE:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:127:ILE:HG12	3:C:226:ILE:HD12	1.96	0.48
2:B:158:PHE:HB2	2:B:208:ARG:NH2	2.28	0.48
3:C:118:ARG:NH1	3:C:237:GLU:HG3	2.29	0.48
1:A:100:ARG:HA	1:A:100:ARG:HD2	1.73	0.47
2:B:79:GLU:OE2	2:B:82:ARG:HD2	2.14	0.47
3:C:116:GLN:HA	3:C:187:TRP:O	2.15	0.47
3:C:79:LEU:HB3	3:C:209:TYR:CE2	2.49	0.47
2:B:100:ILE:HA	2:B:100:ILE:HD13	1.64	0.47
1:A:50:VAL:CG2	1:A:217:VAL:HG13	2.44	0.47
3:C:62:TYR:CD1	3:C:231:ARG:HB3	2.49	0.47
1:A:55:ASP:N	1:A:55:ASP:OD1	2.46	0.47
3:C:274:GLY:O	3:C:285:LEU:HA	2.15	0.47
2:B:125:ILE:HG22	2:B:225:VAL:HA	1.95	0.47
1:A:5:ARG:O	3:C:124:ARG:NH1	2.44	0.47
3:C:44:PRO:HD2	3:C:47:CYS:HB2	1.95	0.47
2:B:156:TYR:CD1	3:C:64:LEU:HB3	2.49	0.47
1:A:66:LEU:HD11	1:A:130:LEU:HD21	1.96	0.46
1:A:240:GLN:O	1:A:242:MET:HG3	2.15	0.46
3:C:190:LYS:HA	3:C:200:THR:O	2.14	0.46
3:C:269:ALA:HB2	3:C:388:ASN:HB2	1.96	0.46
2:B:125:ILE:HG13	2:B:171:SER:OG	2.16	0.46
2:B:79:GLU:HA	2:B:208:ARG:HA	1.97	0.46
3:C:68:VAL:O	3:C:226:ILE:N	2.37	0.46
3:C:196:LEU:HD12	3:C:308:GLU:HG2	1.97	0.46
3:C:335:SER:HB3	3:C:341:ILE:HG23	1.98	0.46
3:C:271:TYR:OH	3:C:391:TRP:NE1	2.30	0.46
2:B:22:VAL:HG13	2:B:62:TRP:HD1	1.80	0.46
1:A:125:ARG:HB3	1:A:128:ARG:HD3	1.98	0.46
3:C:350:ARG:HD2	3:C:372:LEU:CD2	2.46	0.46
3:C:92:ARG:HA	3:C:102:TYR:CD1	2.50	0.46
2:B:130:PHE:HD2	3:C:220:VAL:HG22	1.81	0.46
3:C:88:PHE:HD2	3:C:190:LYS:HB3	1.80	0.46
3:C:333:TRP:CD1	3:C:364:LEU:HD11	2.50	0.45
2:B:2:ASP:O	2:B:4:PRO:HD3	2.15	0.45
1:A:18:SER:HA	3:C:118:ARG:HH22	1.81	0.45
1:A:2:GLU:HG3	2:B:165:LEU:N	2.31	0.45
3:C:276:TRP:CE2	3:C:278:SER:HB2	2.51	0.45
3:C:66:ARG:HG3	3:C:83:LEU:HD22	1.99	0.45
3:C:136:ARG:HA	3:C:166:PHE:O	2.17	0.45
1:A:160:GLN:NE2	1:A:167:VAL:O	2.47	0.45
3:C:189:ARG:HE	3:C:192:GLY:HA2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:79:LEU:HD23	3:C:79:LEU:H	1.80	0.45
1:A:245:LEU:HA	1:A:248:LEU:HD22	1.98	0.45
1:A:85:ASN:HA	1:A:88:ARG:HH12	1.82	0.45
1:A:184:GLN:HA	3:C:250:TRP:HZ2	1.82	0.45
2:B:214:ARG:HD3	3:C:223:THR:O	2.16	0.45
1:A:111:VAL:HG12	1:A:167:VAL:HG22	1.99	0.45
1:A:42:LEU:HD23	1:A:84:PHE:CE1	2.51	0.45
2:B:155:VAL:HG11	2:B:210:ILE:HG23	1.99	0.45
1:A:102:TYR:CE1	1:A:181:ASN:HB2	2.52	0.44
1:A:10:LEU:HD12	3:C:174:PHE:CD2	2.52	0.44
1:A:73:ASP:HB3	1:A:84:PHE:HD2	1.82	0.44
1:A:240:GLN:HB3	3:C:249:ASN:OD1	2.17	0.44
2:B:87:ARG:HD3	2:B:200:LEU:O	2.17	0.44
1:A:10:LEU:HD13	3:C:164:VAL:HG11	1.99	0.44
3:C:17:MET:HG2	3:C:18:HIS:N	2.32	0.44
3:C:19:SER:HB2	3:C:21:ALA:O	2.18	0.44
3:C:187:TRP:NE1	3:C:203:PRO:HD3	2.33	0.44
3:C:261:GLU:HB2	3:C:263:ARG:NH1	2.32	0.44
3:C:34:ARG:HD3	3:C:39:GLY:HA3	1.98	0.44
1:A:248:LEU:N	1:A:249:PRO:HA	2.33	0.44
1:A:39:ARG:HD2	1:A:39:ARG:HA	1.71	0.44
3:C:284:SER:HB3	3:C:373:PHE:HB3	1.99	0.44
2:B:142:SER:HB2	2:B:145:GLU:HG3	1.99	0.44
1:A:103:ARG:O	1:A:231:MET:HA	2.18	0.43
2:B:15:GLU:HG3	2:B:26:THR:HG23	1.99	0.43
2:B:131:GLN:NE2	2:B:213:LEU:HD23	2.34	0.43
3:C:138:ILE:O	3:C:208:MET:HA	2.18	0.43
1:A:40:TYR:HD2	3:C:20:LEU:HA	1.84	0.43
1:A:176:ASN:ND2	1:A:195:TYR:O	2.48	0.43
2:B:211:ALA:HA	2:B:212:PRO:HD2	1.90	0.43
3:C:51:GLU:HA	3:C:52:ASP:CB	2.48	0.43
1:A:74:ILE:HB	3:C:255:ILE:HD13	1.99	0.43
2:B:152:LYS:O	2:B:154:SER:N	2.52	0.43
2:B:50:ASP:O	2:B:52:VAL:HG23	2.19	0.43
3:C:118:ARG:HH11	3:C:237:GLU:HG3	1.82	0.43
2:B:212:PRO:HD2	3:C:225:ASP:OD2	2.18	0.43
1:A:21:PHE:CE2	3:C:238:VAL:HG23	2.52	0.43
3:C:114:PHE:CG	3:C:238:VAL:HG12	2.53	0.43
3:C:141:TYR:CD2	3:C:179:PRO:HG2	2.53	0.43
1:A:39:ARG:NH2	1:A:107:ARG:HH11	2.16	0.43
3:C:166:PHE:CE2	3:C:168:LEU:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:LYS:HA	3:C:213:PRO:HD3	2.01	0.43
3:C:273:ALA:O	3:C:379:GLN:HG3	2.18	0.43
1:A:50:VAL:HG21	1:A:217:VAL:HG13	2.01	0.42
3:C:18:HIS:HB2	3:C:19:SER:HB3	2.01	0.42
1:A:32:ASP:OD1	1:A:34:LYS:N	2.48	0.42
1:A:52:THR:OG1	1:A:53:ASP:N	2.52	0.42
2:B:62:TRP:HH2	2:B:120:GLU:HG2	1.83	0.42
2:B:158:PHE:HB2	2:B:208:ARG:HH22	1.84	0.42
3:C:72:LYS:HG3	3:C:214:LEU:O	2.19	0.42
3:C:132:PHE:HB2	3:C:220:VAL:HG21	2.01	0.42
1:A:171:GLU:HG2	3:C:34:ARG:HH12	1.84	0.42
3:C:34:ARG:NE	3:C:39:GLY:O	2.53	0.42
2:B:191:ILE:HD12	2:B:191:ILE:H	1.84	0.42
3:C:334:PRO:HA	3:C:340:ASN:HA	2.02	0.42
3:C:309:LEU:HG	3:C:396:ALA:O	2.19	0.42
3:C:97:ASN:ND2	3:C:99:ILE:O	2.53	0.42
2:B:188:PRO:HG3	2:B:195:TRP:CG	2.55	0.42
1:A:40:TYR:HB3	3:C:20:LEU:HD23	2.01	0.42
1:A:101:PHE:HB3	1:A:180:TYR:HB3	2.01	0.42
1:A:44:GLY:H	1:A:223:ILE:HG23	1.85	0.42
3:C:158:LEU:HD12	3:C:207:PHE:HD2	1.85	0.42
3:C:57:SER:O	3:C:61:ARG:NH1	2.51	0.42
2:B:187:LEU:HA	2:B:188:PRO:HD3	1.89	0.41
3:C:64:LEU:HG	3:C:229:TYR:CE2	2.55	0.41
1:A:70:LEU:HD21	1:A:138:ILE:HG13	2.02	0.41
1:A:19:SER:O	1:A:24:ALA:HB2	2.20	0.41
1:A:36:LEU:HG	1:A:36:LEU:O	2.20	0.41
3:C:196:LEU:HA	3:C:196:LEU:HD22	1.91	0.41
1:A:64:PRO:HG3	1:A:135:ALA:O	2.20	0.41
2:B:35:PRO:HB3	2:B:162:ASP:OD2	2.19	0.41
3:C:66:ARG:HB2	3:C:228:VAL:HB	2.02	0.41
1:A:68:GLN:NE2	1:A:93:PRO:O	2.52	0.41
2:B:30:PRO:HB2	2:B:175:LYS:H	1.86	0.41
1:A:180:TYR:O	2:B:183:VAL:HG13	2.21	0.41
2:B:86:PRO:HG2	2:B:201:ASP:HA	2.01	0.41
2:B:108:PRO:HB2	2:B:236:PHE:CD2	2.55	0.41
3:C:5:TYR:HE1	3:C:7:GLN:HB3	1.85	0.41
1:A:106:LEU:O	1:A:171:GLU:HG3	2.20	0.41
1:A:227:ILE:HA	1:A:227:ILE:HD13	1.94	0.41
1:A:236:TRP:HE1	2:B:161:MET:HA	1.86	0.41
3:C:131:GLN:H	3:C:131:GLN:HG2	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:TYR:HD1	3:C:64:LEU:HB3	1.84	0.41
1:A:107:ARG:NE	1:A:228:GLY:HA2	2.35	0.41
3:C:110:VAL:HG12	3:C:111:SER:HA	2.03	0.41
3:C:134:THR:HA	3:C:168:LEU:O	2.20	0.41
3:C:133:HIS:NE2	3:C:221:SER:O	2.42	0.41
3:C:256:LEU:HA	3:C:256:LEU:HD22	1.94	0.41
3:C:51:GLU:HB3	3:C:52:ASP:C	2.41	0.41
1:A:51:THR:HG23	1:A:142:ASP:OD1	2.20	0.41
3:C:193:GLY:HA2	3:C:194:ASN:HA	1.64	0.41
3:C:71:LYS:HG3	3:C:223:THR:HG22	2.03	0.41
1:A:134:SER:HA	1:A:135:ALA:HA	1.73	0.40
2:B:119:MET:CE	2:B:229:ILE:HD11	2.51	0.40
2:B:64:GLN:HB2	2:B:228:PHE:HE1	1.86	0.40
3:C:159:LYS:HA	3:C:163:TYR:CD1	2.56	0.40
2:B:70:TRP:CD2	2:B:213:LEU:HD11	2.56	0.40
2:B:245:TYR:CD2	2:B:246:ALA:N	2.90	0.40
3:C:157:LYS:O	3:C:160:SER:HB3	2.21	0.40
3:C:264:ALA:N	3:C:388:ASN:HD21	2.18	0.40
2:B:86:PRO:CG	2:B:202:MET:H	2.35	0.40
3:C:123:TYR:CE2	3:C:230:VAL:HB	2.56	0.40
3:C:313:ARG:HD3	3:C:348:ALA:HB2	2.03	0.40
2:B:42:TRP:O	2:B:47:THR:HG22	2.20	0.40
3:C:116:GLN:HB3	3:C:186:TRP:CB	2.46	0.40
2:B:70:TRP:CE2	2:B:135:LEU:HD21	2.57	0.40
3:C:85:ALA:H	3:C:205:THR:HA	1.87	0.40
3:C:81:LEU:HD22	3:C:83:LEU:HD23	2.03	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	
1	A	239/243 (98%)	183 (77%)	49 (20%)	7 (3%)	5	41
2	B	248/250 (99%)	204 (82%)	40 (16%)	4 (2%)	11	52
3	C	395/397 (100%)	339 (86%)	53 (13%)	3 (1%)	22	65
All	All	882/890 (99%)	726 (82%)	142 (16%)	14 (2%)	11	52

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ALA
1	A	118	SER
1	A	193	SER
2	B	87	ARG
2	B	172	ASN
3	C	3	PRO
2	B	56	ALA
3	C	98	PRO
1	A	220	PRO
1	A	248	LEU
2	B	193	PRO
1	A	112	PHE
3	C	185	PRO
1	A	249	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	
1	A	207/207 (100%)	199 (96%)	8 (4%)	37	70
2	B	221/221 (100%)	204 (92%)	17 (8%)	15	52
3	C	338/338 (100%)	316 (94%)	22 (6%)	20	57
All	All	766/766 (100%)	719 (94%)	47 (6%)	22	60

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	51	THR
1	A	124	HIS
1	A	129	ARG
1	A	142	ASP
1	A	164	VAL
1	A	181	ASN
1	A	252	VAL
2	B	11	GLU
2	B	16	LEU
2	B	22	VAL
2	B	42	TRP
2	B	46	TRP
2	B	51	VAL
2	B	58	ILE
2	B	100	ILE
2	B	103	VAL
2	B	140	TYR
2	B	148	ASN
2	B	190	ARG
2	B	191	ILE
2	B	194	ASP
2	B	224	ASN
2	B	239	THR
2	B	249	ILE
3	C	11	HIS
3	C	17	MET
3	C	18	HIS
3	C	20	LEU
3	C	22	LEU
3	C	30	LEU
3	C	54	THR
3	C	62	TYR
3	C	86	ASP
3	C	110	VAL
3	C	138	ILE
3	C	155	TYR
3	C	172	ASN
3	C	195	TYR
3	C	196	LEU
3	C	220	VAL
3	C	231	ARG
3	C	238	VAL

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Mol	Chain	Res	Type
3	C	240	VAL
3	C	250	TRP
3	C	256	LEU
3	C	257	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3　RNA (i)

There are no RNA molecules in this entry.

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

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

5.5　Carbohydrates (i)

There are no carbohydrates in this entry.

5.6　Ligand geometry (i)

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	#$|Z| > 2$
4	U5P	C	1399	-	14,21,22	1.14	1 (7%)	15,30,33	4.34	2 (13%)

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.

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	U5P	C	1399	-	-	0/3/25/26	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1399	U5P	C4-N3	2.87	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1399	U5P	C5-C4-N3	-3.80	114.05	123.12
4	C	1399	U5P	C4-N3-C2	16.15	128.00	114.13

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	206:PHE	C	217:VAL	N	14.19

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	A	243/243 (100%)	0.03	2 (0%)	86	79	23, 43, 77, 107	0
2	B	250/250 (100%)	-0.06	1 (0%)	92	88	22, 39, 58, 120	0
3	C	397/397 (100%)	0.03	1 (0%)	93	91	20, 43, 85, 98	0
All	All	890/890 (100%)	0.01	4 (0%)	92	88	20, 42, 80, 120	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	THR	2.7
2	B	1	MET	2.4
1	A	89	ASP	2.1
3	C	45	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	U5P	C	1399	20/21	0.89	0.29	-	41,98,100,101	0

6.5 Other polymers (i)

There are no such residues in this entry.