



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:16 am GMT

PDB ID : 1EET  
Title : HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH THE INHIBITOR MSC204  
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Deposited on : 2000-02-03  
Resolution : 2.73 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

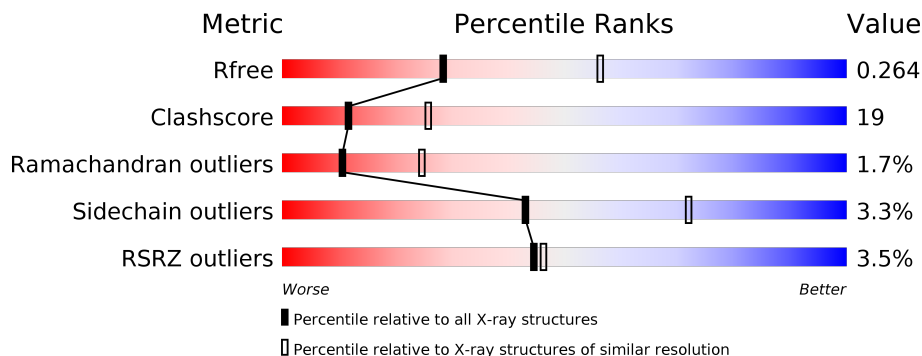
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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	3342 (2.78-2.70)
Clashscore	112137	3731 (2.78-2.70)
Ramachandran outliers	110173	3670 (2.78-2.70)
Sidechain outliers	110143	3671 (2.78-2.70)
RSRZ outliers	101464	3362 (2.78-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	557	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>• •</div> </div> </div>
2	B	427	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>32%</div> <div>• 7%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7764 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 HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	542	Total	C	N	O	S	0	0	0
			4405	2856	733	808	8			

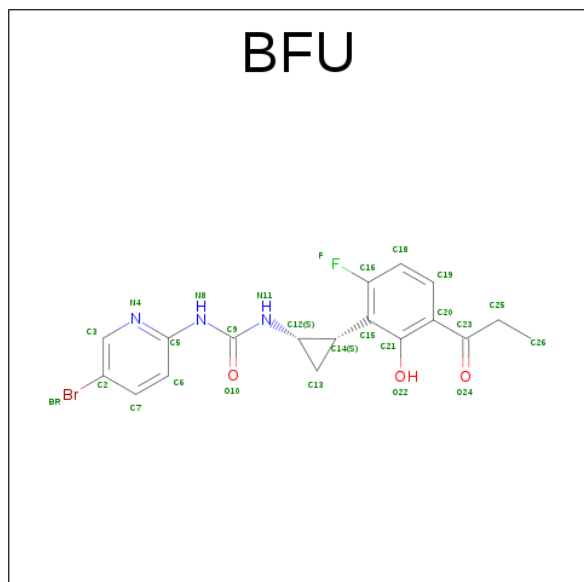
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	478	GLN	GLU	ENGINEERED	UNP P03366

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	399	Total	C	N	O	S	30	0	0
			3299	2152	538	602	7			

- Molecule 3 is 1-(5-BROMO-PYRIDIN-2-YL)-3-[2-(6-FLUORO-2-HYDROXY-3-PROPIONYL-PHENYL)-CYCLOPROPYL]-UREA (three-letter code: BFU) (formula: C<sub>18</sub>H<sub>17</sub>BrFN<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	Br	C	F	N	O	0	0
			26	1	18	1	3	3		

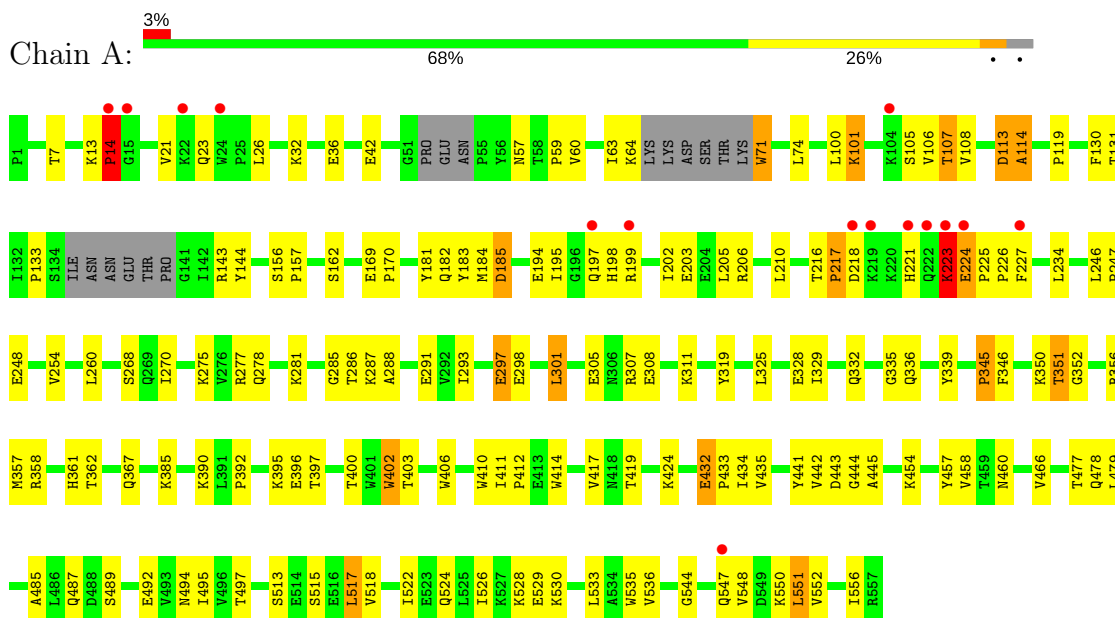
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	18	Total	O	0	0
			18	18		

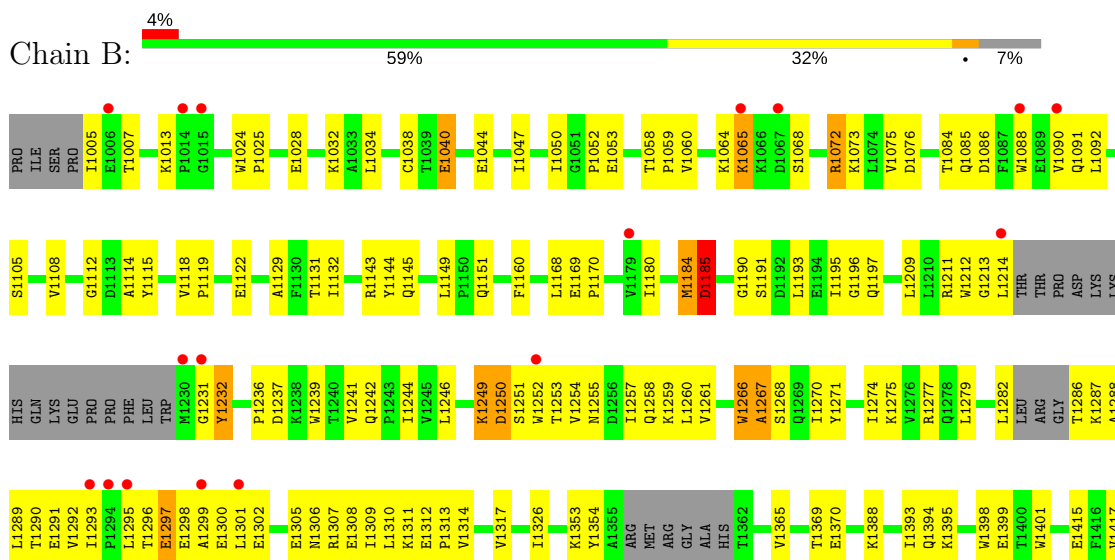
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: HIV-1 REVERSE TRANSCRIPTASE



#### • Molecule 2: HIV-1 REVERSE TRANSCRIPTASE



M1418
T1419
P1420
F1421
L1422
V1423
K1424
L1425
W1426
Y1427

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.57Å 156.45Å 156.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.50 – 2.73 47.50 – 2.73	Depositor EDS
% Data completeness (in resolution range)	94.1 (47.50-2.73) 94.2 (47.50-2.73)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.73Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.213 , 0.271 0.210 , 0.264	Depositor DCC
$R_{free}$ test set	1866 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.2	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7764	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.39	0/4518	0.62	0/6131
2	B	0.38	0/3391	0.65	0/4605
All	All	0.39	0/7909	0.64	0/10736

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4405	0	4460	161	0
2	B	3299	0	3326	148	0
3	A	26	0	17	3	0
4	A	16	0	0	0	0
4	B	18	0	0	0	0
All	All	7764	0	7803	300	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 19.

All (300) 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:131:THR:HG22	1:A:143:ARG:HG2	1.42	1.00
1:A:107:THR:HB	1:A:223:LYS:HG3	1.44	0.96
2:B:1297:GLU:HG3	2:B:1298:GLU:H	1.34	0.93
1:A:107:THR:HG22	1:A:198:HIS:HE1	1.37	0.89
1:A:485:ALA:O	1:A:489:SER:HB2	1.74	0.86
2:B:1191:SER:HB2	2:B:1193:LEU:HD13	1.59	0.85
2:B:1059:PRO:HG2	2:B:1076:ASP:HB3	1.59	0.85
1:A:268:SER:O	1:A:351:THR:HG22	1.78	0.83
1:A:107:THR:HG22	1:A:198:HIS:CE1	2.14	0.82
1:A:287:LYS:HG3	1:A:291:GLU:OE2	1.80	0.82
1:A:223:LYS:HG2	1:A:224:GLU:N	1.94	0.81
2:B:1326:ILE:HG22	2:B:1388:LYS:HB3	1.64	0.79
2:B:1309:ILE:HG22	2:B:1310:LEU:H	1.45	0.79
1:A:357:MET:HG3	1:A:358:ARG:H	1.48	0.79
2:B:1425:LEU:HD21	2:B:1427:TYR:CE1	2.19	0.78
1:A:221:HIS:HB3	1:A:223:LYS:HB3	1.67	0.76
2:B:1425:LEU:HD11	2:B:1427:TYR:CE2	2.20	0.76
1:A:406:TRP:CH2	2:B:1418:ASN:HA	2.23	0.73
2:B:1184:MET:O	2:B:1185:ASP:HB2	1.87	0.73
2:B:1254:VAL:O	2:B:1258:GLN:HG3	1.87	0.73
1:A:101:LYS:N	1:A:101:LYS:HE3	2.03	0.73
1:A:107:THR:HB	1:A:223:LYS:CG	2.17	0.73
2:B:1314:VAL:O	2:B:1317:VAL:HG22	1.89	0.72
2:B:1028:GLU:HG2	2:B:1032:LYS:HE2	1.71	0.72
1:A:194:GLU:HB2	1:A:197:GLN:OE1	1.90	0.71
2:B:1013:LYS:HG2	2:B:1086:ASP:OD1	1.91	0.70
1:A:221:HIS:C	1:A:223:LYS:H	1.94	0.70
1:A:458:VAL:HG21	1:A:547:GLN:OE1	1.92	0.70
1:A:223:LYS:HG2	1:A:224:GLU:H	1.55	0.69
2:B:1007:THR:HG22	2:B:1119:PRO:HG2	1.73	0.69
2:B:1169:GLU:HB3	2:B:1170:PRO:HD3	1.75	0.69
2:B:1266:TRP:CE2	2:B:1425:LEU:HD22	2.27	0.69
1:A:60:VAL:HG11	1:A:130:PHE:CD2	2.27	0.69
2:B:1309:ILE:C	2:B:1311:LYS:H	1.94	0.69
2:B:1160:PHE:HZ	2:B:1214:LEU:HD13	1.57	0.69
2:B:1254:VAL:HG23	2:B:1291:GLU:O	1.91	0.68
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.76	0.68
2:B:1231:GLY:O	2:B:1232:TYR:HB3	1.94	0.68
1:A:195:ILE:HD11	1:A:199:ARG:NH2	2.09	0.67
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.76	0.67
2:B:1253:THR:O	2:B:1257:ILE:HG22	1.95	0.67
2:B:1246:LEU:HD12	2:B:1307:ARG:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:TYR:HB2	3:A:2000:BFU:H14	1.78	0.65
1:A:325:LEU:HD22	1:A:385:LYS:HE3	1.79	0.65
1:A:223:LYS:CG	1:A:224:GLU:N	2.59	0.65
1:A:106:VAL:HG11	3:A:2000:BFU:BR	2.50	0.65
1:A:203:GLU:OE2	1:A:206:ARG:HD3	1.97	0.65
1:A:396:GLU:O	1:A:400:THR:HG22	1.96	0.65
1:A:106:VAL:HG22	1:A:227:PHE:HE2	1.62	0.64
1:A:57:ASN:OD1	1:A:131:THR:HG23	1.98	0.64
1:A:206:ARG:HE	1:A:216:THR:HG23	1.63	0.64
2:B:1193:LEU:HD23	2:B:1197:GLN:HB3	1.80	0.64
2:B:1271:TYR:O	2:B:1274:ILE:HG12	1.98	0.64
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.63	0.63
2:B:1279:LEU:HA	2:B:1282:LEU:HD13	1.80	0.63
1:A:223:LYS:HD3	1:A:224:GLU:HB2	1.78	0.63
2:B:1425:LEU:HD21	2:B:1427:TYR:CZ	2.33	0.63
1:A:131:THR:CG2	1:A:143:ARG:NH1	2.62	0.63
2:B:1266:TRP:HB3	2:B:1427:TYR:OH	1.98	0.63
2:B:1425:LEU:O	2:B:1426:TRP:HB2	1.99	0.63
2:B:1275:LYS:HE3	2:B:1277:ARG:HB2	1.80	0.62
1:A:26:LEU:HD23	1:A:133:PRO:HG3	1.81	0.62
1:A:361:HIS:HD2	1:A:513:SER:OG	1.82	0.62
2:B:1086:ASP:HA	2:B:1090:VAL:HG13	1.82	0.62
1:A:131:THR:CG2	1:A:143:ARG:HG2	2.25	0.62
2:B:1209:LEU:O	2:B:1211:ARG:O	2.17	0.61
1:A:106:VAL:HG13	1:A:225:PRO:HD3	1.81	0.61
1:A:221:HIS:C	1:A:223:LYS:N	2.52	0.61
1:A:458:VAL:HB	1:A:548:VAL:HG22	1.83	0.61
2:B:1365:VAL:O	2:B:1369:THR:HG23	1.99	0.61
1:A:402:TRP:CE3	1:A:403:THR:HG23	2.35	0.61
1:A:479:LEU:HB3	1:A:517:LEU:HD13	1.83	0.61
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.16	0.60
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.82	0.60
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.83	0.60
1:A:101:LYS:HE3	1:A:101:LYS:H	1.66	0.59
2:B:1266:TRP:CE3	2:B:1425:LEU:HD13	2.38	0.59
1:A:524:GLN:HA	1:A:524:GLN:NE2	2.18	0.58
2:B:1266:TRP:CD2	2:B:1425:LEU:HD22	2.39	0.58
2:B:1275:LYS:HE3	2:B:1277:ARG:CB	2.33	0.58
1:A:298:GLU:CD	1:A:298:GLU:H	2.07	0.58
2:B:1114:ALA:CB	2:B:1214:LEU:HB3	2.33	0.58
1:A:356:ARG:NH1	1:A:358:ARG:HA	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1212:TRP:O	2:B:1214:LEU:HG	2.04	0.57
1:A:515:SER:HB3	1:A:518:VAL:HB	1.86	0.57
2:B:1244:ILE:CG1	2:B:1427:TYR:HD2	2.18	0.57
2:B:1267:ALA:HB1	2:B:1310:LEU:HD21	1.87	0.57
2:B:1417:VAL:HG12	2:B:1418:ASN:N	2.19	0.57
1:A:131:THR:HG21	1:A:143:ARG:HH11	1.69	0.57
2:B:1114:ALA:HB1	2:B:1214:LEU:HB3	1.86	0.57
2:B:1211:ARG:C	2:B:1213:GLY:H	2.07	0.57
2:B:1252:TRP:CZ3	2:B:1260:LEU:HD12	2.40	0.57
2:B:1060:VAL:HG12	2:B:1075:VAL:HG22	1.87	0.56
2:B:1267:ALA:O	2:B:1274:ILE:HG13	2.05	0.56
2:B:1425:LEU:HD11	2:B:1427:TYR:CZ	2.39	0.56
2:B:1005:ILE:HD11	2:B:1118:VAL:HG13	1.87	0.56
1:A:23:GLN:NE2	1:A:26:LEU:HD21	2.20	0.56
1:A:278:GLN:HA	1:A:278:GLN:NE2	2.19	0.56
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.87	0.56
1:A:308:GLU:O	1:A:311:LYS:HG2	2.05	0.56
2:B:1244:ILE:HG13	2:B:1427:TYR:HD2	1.71	0.56
1:A:332:GLN:O	1:A:336:GLN:HB2	2.06	0.56
1:A:536:VAL:HG11	2:B:1258:GLN:OE1	2.06	0.55
2:B:1369:THR:HG22	2:B:1398:TRP:CH2	2.42	0.55
1:A:32:LYS:O	1:A:36:GLU:HG2	2.07	0.55
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.87	0.55
1:A:234:LEU:HD12	1:A:234:LEU:N	2.22	0.55
1:A:131:THR:CG2	1:A:143:ARG:HH11	2.19	0.54
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.42	0.54
1:A:270:ILE:HA	1:A:351:THR:HB	1.90	0.54
1:A:412:PRO:HG3	2:B:1401:TRP:CZ2	2.42	0.54
2:B:1090:VAL:HG22	2:B:1091:GLN:N	2.23	0.54
1:A:26:LEU:CD2	1:A:133:PRO:HG3	2.37	0.54
1:A:432:GLU:OE1	1:A:432:GLU:HA	2.06	0.54
2:B:1297:GLU:HG3	2:B:1298:GLU:N	2.14	0.54
1:A:441:TYR:CE2	1:A:544:GLY:HA3	2.42	0.54
2:B:1311:LYS:HG2	2:B:1312:GLU:HG3	1.89	0.54
1:A:105:SER:HB3	1:A:198:HIS:ND1	2.23	0.54
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.43	0.54
2:B:1422:LEU:O	2:B:1422:LEU:HG	2.08	0.54
2:B:1309:ILE:C	2:B:1311:LYS:N	2.60	0.53
2:B:1427:TYR:OXT	2:B:1427:TYR:HD1	1.91	0.53
1:A:356:ARG:HH12	1:A:358:ARG:HA	1.73	0.53
2:B:1249:LYS:O	2:B:1250:ASP:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1266:TRP:C	2:B:1268:SER:H	2.12	0.53
1:A:494:ASN:HB3	2:B:1289:LEU:HD12	1.89	0.53
2:B:1424:LYS:HD3	2:B:1424:LYS:N	2.23	0.53
1:A:108:VAL:HG12	1:A:223:LYS:HA	1.89	0.53
1:A:107:THR:CB	1:A:223:LYS:HB2	2.39	0.53
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.23	0.53
2:B:1296:THR:HB	2:B:1299:ALA:CB	2.39	0.52
1:A:305:GLU:O	1:A:308:GLU:HB3	2.09	0.52
2:B:1417:VAL:CG1	2:B:1418:ASN:N	2.72	0.52
1:A:357:MET:HG3	1:A:358:ARG:N	2.20	0.52
2:B:1040:GLU:O	2:B:1044:GLU:HG3	2.10	0.52
2:B:1244:ILE:HG12	2:B:1427:TYR:CD2	2.44	0.52
1:A:223:LYS:NZ	1:A:224:GLU:HB2	2.25	0.52
1:A:42:GLU:HG3	1:A:144:TYR:HE1	1.75	0.52
2:B:1072:ARG:HG3	2:B:1072:ARG:HH11	1.76	0.51
2:B:1309:ILE:HG22	2:B:1310:LEU:N	2.19	0.51
1:A:346:PHE:N	1:A:346:PHE:CD2	2.75	0.51
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.11	0.51
1:A:454:LYS:O	1:A:552:VAL:HG13	2.10	0.51
2:B:1195:ILE:HG23	2:B:1196:GLY:N	2.25	0.51
1:A:443:ASP:OD1	1:A:444:GLY:N	2.40	0.51
1:A:441:TYR:O	1:A:548:VAL:HG21	2.11	0.50
1:A:497:THR:O	1:A:535:TRP:HA	2.12	0.50
2:B:1091:GLN:C	2:B:1092:LEU:HD12	2.32	0.50
2:B:1115:TYR:HB3	2:B:1149:LEU:HB2	1.92	0.50
2:B:1091:GLN:HG2	2:B:1092:LEU:HD12	1.94	0.50
1:A:223:LYS:HA	1:A:227:PHE:HZ	1.76	0.50
1:A:287:LYS:CG	1:A:291:GLU:OE2	2.57	0.50
1:A:529:GLU:O	1:A:530:LYS:HG3	2.11	0.50
2:B:1353:LYS:HB3	2:B:1353:LYS:NZ	2.26	0.50
1:A:107:THR:HG21	1:A:202:ILE:HG13	1.94	0.50
1:A:247:PRO:O	1:A:248:GLU:HB3	2.12	0.50
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.92	0.50
1:A:223:LYS:O	1:A:224:GLU:HB3	2.12	0.50
2:B:1090:VAL:CG2	2:B:1091:GLN:N	2.74	0.49
2:B:1296:THR:O	2:B:1300:GLU:HG2	2.12	0.49
2:B:1244:ILE:CG1	2:B:1427:TYR:CD2	2.95	0.49
1:A:495:ILE:HB	1:A:533:LEU:HD23	1.95	0.49
1:A:297:GLU:O	1:A:301:LEU:HD13	2.13	0.49
2:B:1065:LYS:HA	2:B:1065:LYS:HE3	1.94	0.49
2:B:1244:ILE:HD12	2:B:1244:ILE:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1302:GLU:HG2	2:B:1306:ASN:ND2	2.28	0.49
1:A:202:ILE:O	1:A:205:LEU:HB3	2.12	0.48
2:B:1271:TYR:CE2	2:B:1310:LEU:HA	2.48	0.48
1:A:489:SER:HB3	1:A:528:LYS:NZ	2.28	0.48
1:A:107:THR:CG2	1:A:198:HIS:CE1	2.91	0.48
1:A:466:VAL:CG2	1:A:551:LEU:HD13	2.44	0.48
2:B:1309:ILE:O	2:B:1311:LYS:N	2.47	0.48
1:A:113:ASP:O	1:A:114:ALA:C	2.52	0.48
2:B:1302:GLU:HG2	2:B:1306:ASN:HD21	1.79	0.48
1:A:435:VAL:HG13	2:B:1290:THR:HG21	1.96	0.48
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.48	0.48
2:B:1050:ILE:CG2	2:B:1145:GLN:HG2	2.44	0.48
1:A:457:TYR:C	1:A:457:TYR:CD1	2.87	0.48
2:B:1058:THR:HG23	2:B:1076:ASP:O	2.14	0.48
2:B:1047:ILE:HD12	2:B:1144:TYR:CD1	2.49	0.47
1:A:445:ALA:O	1:A:477:THR:HG21	2.13	0.47
1:A:108:VAL:HG12	1:A:227:PHE:CZ	2.48	0.47
1:A:361:HIS:HD2	1:A:513:SER:HG	1.62	0.47
2:B:1279:LEU:O	2:B:1282:LEU:HD13	2.15	0.47
1:A:217:PRO:HB2	1:A:221:HIS:HD2	1.79	0.47
1:A:107:THR:CA	1:A:223:LYS:HB2	2.44	0.47
1:A:356:ARG:NH1	1:A:358:ARG:CA	2.77	0.47
1:A:26:LEU:HD23	1:A:133:PRO:CG	2.44	0.47
2:B:1112:GLY:HA3	2:B:1151:GLN:HE21	1.79	0.47
2:B:1211:ARG:O	2:B:1212:TRP:HB2	2.13	0.47
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.43	0.47
2:B:1257:ILE:O	2:B:1261:VAL:HG23	2.15	0.47
2:B:1354:TYR:OH	2:B:1370:GLU:HB3	2.15	0.47
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.96	0.47
1:A:492:GLU:OE2	1:A:530:LYS:HD2	2.15	0.47
2:B:1084:THR:HG22	2:B:1084:THR:O	2.15	0.46
1:A:247:PRO:O	1:A:248:GLU:CB	2.63	0.46
2:B:1072:ARG:HD3	2:B:1073:LYS:O	2.15	0.46
2:B:1425:LEU:CD1	2:B:1427:TYR:CE2	2.97	0.46
1:A:223:LYS:CD	1:A:224:GLU:HB2	2.44	0.46
2:B:1053:GLU:OE1	2:B:1053:GLU:N	2.42	0.46
1:A:195:ILE:HD11	1:A:199:ARG:CZ	2.45	0.46
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.15	0.46
2:B:1129:ALA:HA	2:B:1144:TYR:O	2.15	0.46
2:B:1420:PRO:C	2:B:1422:LEU:H	2.19	0.46
1:A:223:LYS:HA	1:A:227:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LYS:HD2	1:A:288:ALA:H	1.80	0.46
1:A:246:LEU:HD12	1:A:307:ARG:HG2	1.98	0.46
1:A:362:THR:HG21	1:A:367:GLN:HE21	1.81	0.46
1:A:458:VAL:CG2	1:A:548:VAL:HG22	2.45	0.46
2:B:1072:ARG:HG3	2:B:1072:ARG:NH1	2.31	0.46
1:A:458:VAL:CB	1:A:548:VAL:HG22	2.45	0.46
2:B:1024:TRP:CG	2:B:1025:PRO:HD2	2.51	0.46
2:B:1038:CYS:SG	2:B:1132:ILE:HD11	2.56	0.46
2:B:1266:TRP:O	2:B:1268:SER:N	2.49	0.46
1:A:518:VAL:O	1:A:522:ILE:HG13	2.16	0.45
2:B:1231:GLY:O	2:B:1232:TYR:CB	2.64	0.45
1:A:466:VAL:HG22	1:A:551:LEU:HD13	1.99	0.45
2:B:1122:GLU:H	2:B:1122:GLU:CD	2.20	0.45
2:B:1427:TYR:OXT	2:B:1427:TYR:CD1	2.68	0.45
1:A:411:ILE:HG23	1:A:411:ILE:O	2.17	0.45
1:A:487:GLN:C	1:A:489:SER:H	2.20	0.45
1:A:402:TRP:CZ3	1:A:403:THR:HG23	2.51	0.45
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.98	0.45
1:A:356:ARG:HG2	1:A:356:ARG:NH1	2.31	0.45
2:B:1085:GLN:HA	2:B:1088:TRP:CE2	2.52	0.45
1:A:410:TRP:CG	1:A:411:ILE:N	2.85	0.44
1:A:361:HIS:CD2	1:A:513:SER:OG	2.67	0.44
2:B:1287:LYS:HD3	2:B:1291:GLU:OE2	2.17	0.44
2:B:1255:ASN:O	2:B:1259:LYS:HG3	2.16	0.44
1:A:71:TRP:HA	1:A:71:TRP:CE3	2.52	0.44
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.99	0.44
2:B:1034:LEU:CD2	2:B:1073:LYS:HG3	2.47	0.44
2:B:1305:GLU:O	2:B:1308:GLU:HB3	2.18	0.44
1:A:478:GLN:OE1	1:A:478:GLN:HA	2.18	0.44
2:B:1064:LYS:O	2:B:1065:LYS:O	2.35	0.44
2:B:1258:GLN:HE22	2:B:1289:LEU:CD2	2.31	0.44
1:A:108:VAL:H	1:A:223:LYS:HB2	1.82	0.43
2:B:1267:ALA:O	2:B:1270:ILE:O	2.36	0.43
2:B:1211:ARG:O	2:B:1212:TRP:CB	2.65	0.43
2:B:1298:GLU:O	2:B:1301:LEU:HB3	2.18	0.43
1:A:60:VAL:O	1:A:60:VAL:HG23	2.18	0.43
2:B:1193:LEU:HD12	2:B:1193:LEU:N	2.33	0.43
1:A:225:PRO:HA	1:A:226:PRO:C	2.39	0.43
2:B:1422:LEU:CG	2:B:1422:LEU:O	2.67	0.43
1:A:184:MET:HB3	1:A:185:ASP:H	1.46	0.43
1:A:162:SER:OG	2:B:1052:PRO:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1105:SER:O	2:B:1190:GLY:HA2	2.19	0.43
2:B:1241:VAL:HG12	2:B:1242:GLN:N	2.33	0.43
2:B:1296:THR:HB	2:B:1299:ALA:HB2	2.00	0.43
1:A:329:ILE:O	1:A:392:PRO:HD3	2.19	0.43
1:A:350:LYS:HG2	1:A:351:THR:N	2.33	0.43
1:A:63:ILE:HG12	1:A:64:LYS:N	2.34	0.43
1:A:325:LEU:CD2	1:A:385:LYS:HE3	2.47	0.43
2:B:1024:TRP:CD1	2:B:1025:PRO:HD2	2.54	0.43
2:B:1168:LEU:HD13	2:B:1180:ILE:HG21	2.01	0.43
1:A:397:THR:HG21	1:A:424:LYS:HA	2.01	0.43
2:B:1064:LYS:O	2:B:1065:LYS:C	2.57	0.42
1:A:275:LYS:HB2	1:A:275:LYS:HE3	1.70	0.42
2:B:1251:SER:O	2:B:1252:TRP:HB2	2.19	0.42
1:A:524:GLN:HA	1:A:524:GLN:HE21	1.84	0.42
2:B:1184:MET:O	2:B:1184:MET:HG2	2.19	0.42
2:B:1286:THR:HG22	2:B:1286:THR:O	2.18	0.42
1:A:131:THR:HG21	1:A:143:ARG:NH1	2.32	0.42
2:B:1279:LEU:HB2	2:B:1302:GLU:OE1	2.20	0.42
2:B:1236:PRO:HA	2:B:1239:TRP:CD2	2.55	0.42
1:A:410:TRP:CE3	1:A:410:TRP:HA	2.54	0.42
2:B:1193:LEU:HB3	2:B:1197:GLN:HB2	2.00	0.42
2:B:1297:GLU:CG	2:B:1298:GLU:N	2.81	0.42
1:A:100:LEU:HD22	3:A:2000:BFU:H131	2.01	0.42
1:A:285:GLY:O	1:A:286:THR:C	2.57	0.41
1:A:550:LYS:HA	1:A:550:LYS:HD2	1.88	0.41
2:B:1211:ARG:C	2:B:1213:GLY:N	2.72	0.41
1:A:221:HIS:O	1:A:223:LYS:N	2.52	0.41
1:A:60:VAL:HG11	1:A:130:PHE:HD2	1.80	0.41
2:B:1108:VAL:HB	2:B:1232:TYR:CD2	2.55	0.41
2:B:1393:ILE:HG12	2:B:1394:GLN:N	2.35	0.41
2:B:1395:LYS:HG2	2:B:1399:GLU:OE1	2.20	0.41
1:A:287:LYS:HA	1:A:287:LYS:HD2	1.68	0.41
2:B:1252:TRP:HD1	2:B:1295:LEU:HD22	1.86	0.41
1:A:246:LEU:HA	1:A:247:PRO:HD3	1.86	0.41
1:A:433:PRO:CG	2:B:1255:ASN:OD1	2.69	0.41
2:B:1195:ILE:CG2	2:B:1196:GLY:N	2.84	0.41
1:A:460:ASN:ND2	2:B:1288:ALA:HB2	2.35	0.41
1:A:278:GLN:NE2	1:A:281:LYS:HD3	2.35	0.41
2:B:1266:TRP:CD2	2:B:1425:LEU:HD13	2.55	0.41
1:A:417:VAL:O	1:A:417:VAL:HG13	2.20	0.41
2:B:1108:VAL:HB	2:B:1232:TYR:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLN:HA	1:A:278:GLN:HE21	1.87	0.41
2:B:1213:GLY:O	2:B:1214:LEU:C	2.59	0.41
2:B:1275:LYS:HZ1	2:B:1277:ARG:HD3	1.85	0.41
1:A:460:ASN:HD22	2:B:1288:ALA:HB2	1.86	0.40
2:B:1131:THR:OG1	2:B:1143:ARG:HD2	2.21	0.40
1:A:522:ILE:O	1:A:526:ILE:HG13	2.22	0.40
2:B:1065:LYS:HB3	2:B:1068:SER:OG	2.21	0.40
2:B:1388:LYS:HE2	2:B:1415:GLU:OE2	2.22	0.40
1:A:7:THR:HG22	1:A:119:PRO:HG2	2.04	0.40
2:B:1271:TYR:CG	2:B:1310:LEU:HD23	2.57	0.40
2:B:1249:LYS:O	2:B:1250:ASP:CB	2.70	0.40
2:B:1296:THR:CG2	2:B:1297:GLU:N	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	534/557 (96%)	474 (89%)	53 (10%)	7 (1%)	14	32
2	B	391/427 (92%)	348 (89%)	34 (9%)	9 (2%)	7	17
All	All	925/984 (94%)	822 (89%)	87 (9%)	16 (2%)	11	25

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	114	ALA
1	A	223	LYS
2	B	1065	LYS
2	B	1250	ASP
2	B	1267	ALA

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Mol	Chain	Res	Type
2	B	1297	GLU
2	B	1184	MET
2	B	1249	LYS
2	B	1313	PRO
1	A	345	PRO
2	B	1185	ASP
2	B	1232	TYR
1	A	224	GLU
1	A	217	PRO
1	A	556	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	480/497 (97%)	461 (96%)	19 (4%)	36	65
2	B	364/389 (94%)	355 (98%)	9 (2%)	53	80
All	All	844/886 (95%)	816 (97%)	28 (3%)	43	72

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	71	TRP
1	A	74	LEU
1	A	101	LYS
1	A	107	THR
1	A	113	ASP
1	A	182	GLN
1	A	185	ASP
1	A	210	LEU
1	A	223	LYS
1	A	260	LEU
1	A	297	GLU
1	A	301	LEU

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Mol	Chain	Res	Type
1	A	345	PRO
1	A	351	THR
1	A	402	TRP
1	A	432	GLU
1	A	517	LEU
1	A	551	LEU
2	B	1040	GLU
2	B	1072	ARG
2	B	1185	ASP
2	B	1237	ASP
2	B	1266	TRP
2	B	1292	VAL
2	B	1293	ILE
2	B	1422	LEU
2	B	1423	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	161	GLN
1	A	182	GLN
1	A	198	HIS
1	A	221	HIS
1	A	278	GLN
1	A	334	GLN
1	A	336	GLN
1	A	361	HIS
1	A	407	GLN
1	A	428	GLN
1	A	509	GLN
1	A	524	GLN
2	B	1091	GLN
2	B	1161	GLN
2	B	1182	GLN
2	B	1407	GLN
2	B	1418	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
3	BFU	A	2000	-	26,28,28	1.94	8 (30%)	33,40,40	1.92	7 (21%)

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
3	BFU	A	2000	-	-	0/18/23/23	0/2/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	BFU	BR-C2	-3.51	1.83	1.90
3	A	2000	BFU	C15-C14	2.05	1.55	1.52
3	A	2000	BFU	C20-C21	2.08	1.44	1.41
3	A	2000	BFU	C21-C15	2.40	1.44	1.40
3	A	2000	BFU	C13-C14	2.48	1.54	1.50
3	A	2000	BFU	C19-C20	2.50	1.43	1.39
3	A	2000	BFU	C20-C23	2.50	1.53	1.48
3	A	2000	BFU	C15-C16	5.00	1.43	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	BFU	C18-C16-C15	-3.61	120.72	124.07
3	A	2000	BFU	O10-C9-N8	-3.33	117.90	123.58
3	A	2000	BFU	C13-C14-C15	-2.43	117.44	122.26
3	A	2000	BFU	F-C16-C15	2.40	120.44	118.05
3	A	2000	BFU	C25-C23-C20	3.38	123.42	119.08
3	A	2000	BFU	C3-N4-C5	4.30	122.38	117.91
3	A	2000	BFU	N8-C9-N11	5.08	121.92	113.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2000	BFU	3	0

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	542/557 (97%)	0.10	15 (2%) 53 56	21, 48, 80, 102	0
2	B	399/427 (93%)	0.05	18 (4%) 34 34	21, 45, 101, 133	9 (2%)
All	All	941/984 (95%)	0.08	33 (3%) 44 46	21, 47, 93, 133	9 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1214	LEU	5.7
2	B	1067	ASP	4.7
2	B	1230	MET	4.0
1	A	24	TRP	3.8
2	B	1427	TYR	3.8
1	A	223	LYS	3.7
1	A	224	GLU	3.3
1	A	221	HIS	3.0
2	B	1252	TRP	3.0
1	A	222	GLN	3.0
1	A	104	LYS	2.9
2	B	1090	VAL	2.9
1	A	227	PHE	2.8
1	A	14	PRO	2.7
1	A	197	GLN	2.6
2	B	1294	PRO	2.6
2	B	1301	LEU	2.6
2	B	1088	TRP	2.4
1	A	547	GLN	2.4
2	B	1231	GLY	2.3
2	B	1299	ALA	2.3
2	B	1065	LYS	2.3
1	A	199	ARG	2.2
2	B	1014	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	22	LYS	2.2
1	A	219	LYS	2.2
2	B	1293	ILE	2.1
2	B	1295	LEU	2.1
2	B	1006	GLU	2.1
2	B	1015	GLY	2.1
1	A	218	ASP	2.1
1	A	15	GLY	2.0
2	B	1179	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	BFU	A	2000	26/26	0.98	0.17	-0.48	28,33,39,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.