



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:35 PM GMT

PDB ID : 3U6F  
Title : Mouse TREX1 D200N mutant  
Authors : Bailey, S.L.; Harvey, S.; Perrino, F.W.; Hollis, T.  
Deposited on : 2011-10-12  
Resolution : 2.30 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 (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

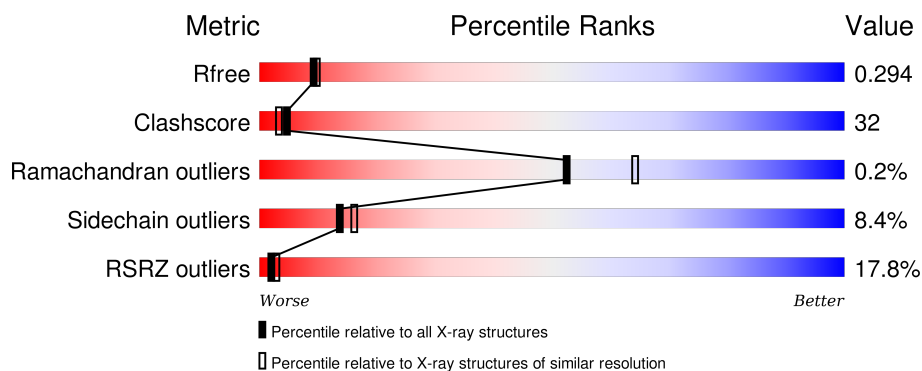
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	314	<div> <div>9%</div> <div>48%</div> <div>18%</div> <div>•</div> <div>31%</div> </div>
1	B	314	<div> <div>17%</div> <div>37%</div> <div>27%</div> <div>5%</div> <div>31%</div> </div>
2	C	4	<div> <div>100%</div> </div>
2	D	4	<div> <div>50%</div> <div>50%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BU1	B	315	-	-	X	X
4	MG	D	5	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7069 atoms, of which 3368 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 Three prime repair exonuclease 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	218	Total	C	H	N	O	S	11	0	0
			3359	1065	1681	296	308	9			
1	A	217	Total	C	H	N	O	S	0	0	0
			3338	1060	1667	295	307	9			

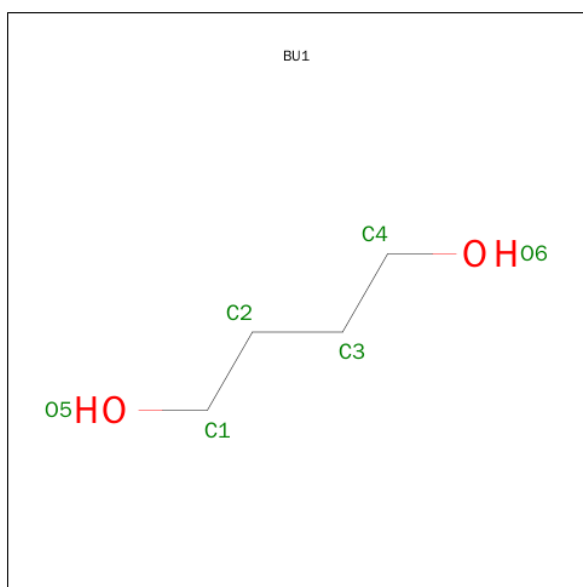
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	200	ASN	ASP	ENGINEERED MUTATION	UNP Q91XB0
A	200	ASN	ASP	ENGINEERED MUTATION	UNP Q91XB0

- Molecule 2 is a DNA chain called 5'-D(\*GP\*AP\*CP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	P	0	0	0
			81	39	18	21	3			
2	D	4	Total	C	N	O	P	0	0	0
			81	39	18	21	3			

- Molecule 3 is 1,4-BUTANEDIOL (three-letter code: BU1) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			16	4	10	2		
3	A	1	Total	C	H	O	0	0
			16	4	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	76	Total	O	0	0
			76	76		
5	A	83	Total	O	0	0
			83	83		
5	C	7	Total	O	0	0
			7	7		
5	D	10	Total	O	0	0
			10	10		



Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: 5'-D(\*GP\*AP\*CP\*G)-3'

Chain D:  50% 50%

G1	G2	G3	G4
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.89Å 56.64Å 68.14Å 90.00° 107.97° 90.00°	Depositor
Resolution (Å)	33.22 – 2.30 33.22 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.22-2.30) 99.8 (33.22-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.54 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.219 , 0.288 0.229 , 0.294	Depositor DCC
$R_{free}$ test set	1082 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 57.9	EDS
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 21095 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7069	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, BU1

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	0.43	0/1712	0.65	2/2333 (0.1%)
1	B	0.44	0/1720	0.68	1/2345 (0.0%)
2	C	0.73	0/91	1.12	0/139
2	D	0.87	0/91	1.19	1/139 (0.7%)
All	All	0.46	0/3614	0.70	4/4956 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	TYR	N-CA-C	5.72	126.46	111.00
1	A	129	TYR	N-CA-C	5.72	126.46	111.00
2	D	3	DC	O4'-C4'-C3'	-5.58	102.27	104.50
1	A	228	THR	CB-CA-C	-5.24	97.44	111.60

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	1671	1667	1665	84	0
1	B	1678	1681	1678	152	0
2	C	81	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	81	0	46	1	0
3	A	6	10	10	0	0
3	B	6	10	10	4	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	83	0	0	2	0
5	B	76	0	0	5	0
5	C	7	0	0	0	0
5	D	10	0	0	0	0
All	All	3701	3368	3455	222	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 32.

All (222) 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:B:224:ARG:CG	1:B:225:PRO:HD2	1.85	1.06
1:B:224:ARG:HG2	1:B:225:PRO:CD	1.90	1.01
1:B:224:ARG:HG2	1:B:225:PRO:HD2	0.95	0.94
1:B:40:HIS:CE1	1:B:42:ARG:HG2	2.07	0.88
1:B:232:MET:HG2	1:B:233:TYR:CD2	2.14	0.83
1:A:225:PRO:O	1:A:228:THR:HG23	1.81	0.81
1:B:153:VAL:HG23	1:B:223:ALA:HA	1.62	0.80
1:A:41:ARG:CZ	1:A:216:LEU:HD21	2.12	0.79
1:A:91:GLU:O	1:A:94:VAL:HG12	1.84	0.78
1:B:44:LEU:HD23	1:B:44:LEU:N	1.98	0.77
2:D:1:DG:N3	2:D:1:DG:O5'	2.17	0.76
1:B:218:TRP:CE2	1:B:222:HIS:CD2	2.74	0.76
1:B:95:GLN:OE1	1:A:43:ALA:HB2	1.86	0.75
1:B:218:TRP:O	1:B:222:HIS:CD2	2.40	0.75
1:B:41:ARG:HH22	1:B:216:LEU:HD21	1.55	0.72
1:B:94:VAL:HG12	1:B:95:GLN:N	2.04	0.71
1:A:131:PHE:HB2	1:A:132:PRO:HD3	1.73	0.70
1:B:225:PRO:HG2	1:B:228:THR:CG2	2.22	0.69
1:B:216:LEU:HA	1:B:219:VAL:HG13	1.72	0.69
1:B:41:ARG:NH2	1:B:216:LEU:HD21	2.06	0.69
1:B:218:TRP:CD2	1:B:222:HIS:HD2	2.09	0.69
1:A:94:VAL:HG13	1:A:95:GLN:N	2.08	0.69
1:B:37:LEU:HD23	1:B:39:VAL:HG23	1.73	0.68
1:B:7:PRO:O	1:B:8:HIS:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ALA:C	1:B:44:LEU:HD23	2.14	0.68
1:B:199:GLY:HA2	3:B:315:BU1:H21	1.76	0.68
1:B:113:GLN:HB2	1:A:103:ASN:HD21	1.57	0.67
1:B:13:THR:HG22	1:B:15:ILE:HG13	1.76	0.67
1:A:42:ARG:HA	1:A:45:GLU:OE2	1.95	0.67
1:B:109:ARG:O	1:B:113:GLN:HG3	1.93	0.67
1:B:11:MET:SD	1:B:120:CYS:HB2	2.35	0.66
1:A:44:LEU:CD2	1:A:212:PRO:HB3	2.25	0.66
1:A:41:ARG:NH1	1:A:216:LEU:HD21	2.11	0.66
1:B:11:MET:HG2	1:B:120:CYS:CB	2.25	0.66
1:B:162:LEU:HD23	1:B:211:LYS:CG	2.27	0.65
1:B:98:GLN:HB2	1:A:114:ARG:NH1	2.10	0.65
1:B:215:LEU:CD1	1:B:219:VAL:HG11	2.27	0.64
1:A:104:LEU:O	1:A:108:LEU:HG	1.97	0.64
1:A:138:LEU:HD11	1:A:147:LEU:HD12	1.78	0.64
1:A:44:LEU:HD23	1:A:212:PRO:HB3	1.80	0.63
1:B:103:ASN:HB3	5:B:378:HOH:O	1.99	0.62
1:B:218:TRP:CD2	1:B:222:HIS:CD2	2.87	0.62
1:B:37:LEU:CD2	1:B:39:VAL:HG23	2.28	0.62
1:A:94:VAL:CG1	1:A:95:GLN:N	2.63	0.61
1:B:103:ASN:HD21	1:A:113:GLN:HB3	1.65	0.61
1:B:214:ALA:O	1:B:215:LEU:C	2.37	0.61
1:B:100:PHE:HA	1:B:104:LEU:HD23	1.83	0.61
1:B:94:VAL:HG12	1:B:95:GLN:HG2	1.83	0.61
1:B:153:VAL:CG2	1:B:223:ALA:HA	2.31	0.61
1:A:103:ASN:O	1:A:106:ILE:N	2.33	0.61
1:B:215:LEU:O	1:B:219:VAL:HG12	2.01	0.60
1:A:215:LEU:HG	1:A:215:LEU:O	2.00	0.60
1:A:44:LEU:HD23	1:A:44:LEU:O	2.02	0.60
1:B:11:MET:SD	1:B:119:CYS:C	2.80	0.60
1:B:215:LEU:HD12	1:B:219:VAL:HG11	1.83	0.60
1:A:91:GLU:HA	1:A:94:VAL:HG12	1.82	0.60
1:A:91:GLU:OE1	1:A:94:VAL:HG11	2.02	0.60
1:A:44:LEU:HD23	1:A:44:LEU:C	2.21	0.60
1:B:143:THR:HG22	1:B:144:PRO:O	2.02	0.60
1:B:11:MET:HG2	1:B:120:CYS:HB3	1.84	0.59
1:B:215:LEU:O	1:B:219:VAL:CG1	2.49	0.59
1:B:103:ASN:HB2	1:A:113:GLN:NE2	2.16	0.59
1:B:59:ARG:HH11	1:B:59:ARG:HG3	1.66	0.59
1:B:218:TRP:O	1:B:222:HIS:HD2	1.83	0.59
1:B:211:LYS:O	1:B:211:LYS:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:VAL:HG11	1:B:218:TRP:HZ3	1.67	0.59
1:B:233:TYR:HD1	1:B:234:GLY:CA	2.16	0.59
1:B:29:PRO:HD2	1:B:232:MET:SD	2.43	0.59
1:A:147:LEU:CD2	1:A:150:THR:HG21	2.33	0.58
1:B:28:ARG:HH11	1:B:28:ARG:HG2	1.68	0.58
1:A:159:LEU:CD2	1:A:182:ILE:HG21	2.33	0.58
1:B:218:TRP:O	1:B:221:GLU:HG2	2.04	0.58
1:B:17:LEU:HD23	1:B:36:LEU:HD23	1.86	0.58
1:A:17:LEU:HD23	1:A:36:LEU:HD23	1.85	0.57
1:B:216:LEU:HD23	1:B:216:LEU:O	2.04	0.57
1:B:40:HIS:ND1	1:B:42:ARG:HG2	2.19	0.57
1:A:100:PHE:HE2	1:A:138:LEU:HD23	1.69	0.57
1:A:147:LEU:O	1:A:150:THR:HG22	2.05	0.57
1:B:155:SER:O	1:B:159:LEU:HD23	2.04	0.57
1:B:158:ALA:HB2	1:B:218:TRP:CZ3	2.40	0.56
1:A:156:ILE:O	1:A:160:LYS:HG3	2.05	0.56
1:B:225:PRO:HG2	1:B:228:THR:HB	1.88	0.55
1:B:11:MET:SD	1:B:120:CYS:N	2.79	0.55
1:B:37:LEU:CD2	1:B:39:VAL:CG2	2.84	0.55
1:A:100:PHE:CE2	1:A:138:LEU:HD23	2.40	0.55
1:B:106:ILE:O	1:B:109:ARG:HB3	2.06	0.55
1:B:158:ALA:HA	1:B:218:TRP:CE2	2.42	0.55
1:B:109:ARG:O	1:B:113:GLN:CG	2.54	0.55
1:B:216:LEU:HD23	1:B:216:LEU:C	2.27	0.55
1:A:153:VAL:CG2	1:A:218:TRP:HZ3	2.20	0.55
1:B:232:MET:CG	1:B:233:TYR:CD2	2.90	0.54
1:B:162:LEU:HD23	1:B:211:LYS:HG2	1.89	0.54
1:A:225:PRO:O	1:A:228:THR:CG2	2.52	0.54
1:A:17:LEU:HD22	1:A:18:ASP:N	2.22	0.54
1:B:94:VAL:HG12	1:B:95:GLN:CG	2.37	0.54
1:B:28:ARG:O	1:B:75:LYS:NZ	2.35	0.54
1:B:232:MET:CG	1:B:233:TYR:HD2	2.20	0.53
1:B:37:LEU:HD23	1:B:37:LEU:C	2.28	0.53
1:A:147:LEU:HD23	1:A:150:THR:HG21	1.89	0.53
1:B:215:LEU:CD1	1:B:219:VAL:CG1	2.87	0.53
1:B:225:PRO:HG2	1:B:228:THR:HG21	1.91	0.53
1:B:162:LEU:HB3	1:B:211:LYS:HD2	1.90	0.53
1:B:42:ARG:C	1:B:44:LEU:H	2.12	0.52
1:B:225:PRO:CG	1:B:228:THR:HB	2.40	0.52
1:B:17:LEU:HD23	1:B:36:LEU:CD2	2.40	0.52
1:B:97:ARG:NH1	1:A:65:ASP:OD2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:HD13	1:B:147:LEU:CD1	2.39	0.51
1:B:42:ARG:NH1	1:A:94:VAL:CG2	2.73	0.51
1:B:215:LEU:C	1:B:215:LEU:CD1	2.78	0.51
1:B:221:GLU:HG3	1:B:222:HIS:CD2	2.45	0.51
1:A:40:HIS:ND1	1:A:42:ARG:HB2	2.25	0.51
1:A:159:LEU:HD21	1:A:207:ILE:HB	1.91	0.51
1:B:233:TYR:C	1:B:233:TYR:CD1	2.83	0.51
1:B:106:ILE:HG23	5:B:372:HOH:O	2.10	0.51
1:B:24:LEU:HB3	1:B:25:PRO:CD	2.40	0.51
1:A:94:VAL:HG13	1:A:95:GLN:HG3	1.93	0.50
1:B:17:LEU:HD22	1:B:18:ASP:N	2.26	0.50
1:B:11:MET:HG2	1:B:120:CYS:HB2	1.94	0.50
1:B:101:ASP:O	1:B:104:LEU:HB3	2.12	0.50
1:B:100:PHE:HE2	1:B:138:LEU:HD23	1.76	0.50
1:A:117:GLN:HB3	1:A:118:PRO:HA	1.92	0.50
1:B:24:LEU:HB3	1:B:25:PRO:HD2	1.94	0.50
1:A:41:ARG:HB2	1:A:216:LEU:HD11	1.93	0.49
1:B:225:PRO:HG2	1:B:228:THR:CB	2.42	0.49
1:B:218:TRP:CZ2	1:B:222:HIS:CD2	3.00	0.49
1:A:41:ARG:O	1:A:45:GLU:OE1	2.30	0.49
1:A:159:LEU:HD23	1:A:182:ILE:HG21	1.92	0.49
1:B:127:ASP:OD2	1:B:154:ASP:HB2	2.11	0.49
1:B:42:ARG:O	1:B:44:LEU:N	2.46	0.49
1:A:44:LEU:CD2	1:A:44:LEU:C	2.81	0.49
1:B:147:LEU:O	1:B:150:THR:OG1	2.29	0.49
1:B:235:THR:N	1:B:236:PRO:HD3	2.27	0.49
1:B:53:HIS:HA	1:B:54:PRO:C	2.33	0.49
1:B:103:ASN:O	1:B:106:ILE:HB	2.13	0.49
1:A:158:ALA:HB2	1:A:218:TRP:CZ3	2.47	0.49
1:B:27:SER:O	1:B:75:LYS:NZ	2.46	0.49
1:A:91:GLU:HA	1:A:94:VAL:CG1	2.41	0.48
1:A:91:GLU:C	1:A:94:VAL:HG12	2.33	0.48
1:A:17:LEU:HD23	1:A:36:LEU:CD2	2.43	0.48
1:B:224:ARG:HD3	1:B:228:THR:HG21	1.96	0.48
1:A:8:HIS:HB2	5:A:392:HOH:O	2.12	0.48
1:B:11:MET:O	1:B:41:ARG:HD2	2.13	0.47
1:B:199:GLY:CA	3:B:315:BU1:H21	2.43	0.47
1:B:233:TYR:HD1	1:B:234:GLY:HA3	1.79	0.47
1:A:138:LEU:CD1	1:A:147:LEU:HD12	2.44	0.47
1:B:178:SER:O	1:B:182:ILE:HD12	2.14	0.47
1:B:218:TRP:CE3	1:B:222:HIS:HD2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ASP:OD2	3:B:315:BU1:H32	2.14	0.47
1:B:147:LEU:CA	1:B:150:THR:OG1	2.63	0.47
1:B:230:LYS:HG3	1:B:231:PRO:HD2	1.97	0.47
1:A:104:LEU:HD12	1:A:104:LEU:O	2.15	0.47
1:B:138:LEU:O	1:B:141:LEU:CD1	2.62	0.46
1:B:147:LEU:HA	1:B:150:THR:OG1	2.15	0.46
1:B:75:LYS:C	1:B:89:LYS:HD3	2.36	0.46
1:B:224:ARG:CD	1:B:228:THR:HG21	2.45	0.46
1:A:31:VAL:HG23	1:A:137:GLU:OE1	2.16	0.46
1:A:24:LEU:HB3	1:A:25:PRO:CD	2.45	0.46
1:B:42:ARG:NH1	1:A:94:VAL:HG22	2.31	0.46
1:A:153:VAL:HG21	1:A:218:TRP:HZ3	1.81	0.46
1:B:12:GLN:HB3	1:B:116:PRO:HB2	1.97	0.46
1:B:41:ARG:HB3	1:B:216:LEU:HD11	1.98	0.46
1:A:99:ARG:HD3	5:A:380:HOH:O	2.16	0.46
1:A:91:GLU:CA	1:A:94:VAL:HG12	2.46	0.46
1:B:158:ALA:O	1:B:162:LEU:HD13	2.15	0.45
1:B:100:PHE:CE2	1:B:138:LEU:HD23	2.51	0.45
1:B:109:ARG:NH2	1:B:146:PRO:HA	2.32	0.45
1:B:135:GLN:NE2	1:B:226:PHE:O	2.50	0.45
1:A:24:LEU:HB3	1:A:25:PRO:HD2	1.98	0.45
1:B:131:PHE:HB2	1:B:132:PRO:HD3	1.99	0.45
1:B:42:ARG:NH1	1:B:42:ARG:HG3	2.32	0.45
1:B:11:MET:CG	1:B:120:CYS:HB2	2.47	0.45
1:A:147:LEU:HD22	1:A:150:THR:HG21	1.99	0.44
1:B:103:ASN:HB2	1:A:113:GLN:HE22	1.82	0.44
5:B:378:HOH:O	1:A:114:ARG:HD2	2.16	0.44
1:A:162:LEU:HD21	1:A:215:LEU:HB2	2.00	0.44
1:B:202:LEU:HD12	3:B:315:BU1:H22	2.00	0.44
1:B:34:LEU:C	1:B:34:LEU:HD23	2.37	0.44
1:A:159:LEU:HD22	1:A:207:ILE:HD12	2.00	0.44
1:A:212:PRO:HD2	1:A:213:GLN:NE2	2.32	0.44
1:B:195:HIS:CD2	5:B:377:HOH:O	2.71	0.44
1:B:7:PRO:O	1:B:8:HIS:CB	2.63	0.43
1:A:41:ARG:NH2	1:A:216:LEU:CD2	2.81	0.43
1:B:42:ARG:C	1:B:44:LEU:N	2.72	0.43
1:A:228:THR:O	1:A:229:VAL:C	2.57	0.43
1:B:34:LEU:O	1:B:34:LEU:HD23	2.18	0.43
1:B:163:GLU:OE1	1:B:185:ARG:NH2	2.41	0.43
1:B:113:GLN:HB2	1:A:103:ASN:ND2	2.30	0.42
1:B:233:TYR:HD1	1:B:234:GLY:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:LEU:HD12	1:B:219:VAL:CG1	2.47	0.42
1:B:109:ARG:HH21	1:B:146:PRO:HA	1.84	0.42
1:B:28:ARG:NH1	1:B:28:ARG:HG2	2.31	0.42
1:B:124:HIS:O	1:B:125:ASN:CB	2.66	0.42
1:B:59:ARG:NH1	1:B:59:ARG:HG3	2.34	0.42
1:B:187:TYR:O	1:B:188:TRP:HB2	2.20	0.42
1:B:42:ARG:HH12	1:A:94:VAL:CG2	2.32	0.42
1:B:233:TYR:CD1	1:B:234:GLY:HA3	2.55	0.42
1:B:126:GLY:O	1:B:132:PRO:HD3	2.20	0.42
1:A:153:VAL:HG22	1:A:154:ASP:N	2.35	0.42
1:B:109:ARG:HD3	1:B:113:GLN:OE1	2.20	0.41
1:A:204:LEU:O	1:A:207:ILE:HG12	2.20	0.41
1:B:65:ASP:OD2	1:A:97:ARG:NH1	2.54	0.41
1:B:55:PRO:HA	1:B:56:PRO:HD3	1.98	0.41
1:B:27:SER:O	1:B:28:ARG:HB2	2.20	0.41
1:A:153:VAL:CG2	1:A:218:TRP:CZ3	3.01	0.41
1:B:152:CYS:O	1:B:153:VAL:HG23	2.21	0.41
1:B:103:ASN:CG	1:A:113:GLN:CD	2.79	0.41
1:B:109:ARG:CZ	5:B:326:HOH:O	2.68	0.41
1:A:100:PHE:CG	1:A:137:GLU:HG2	2.55	0.41
1:B:73:PRO:HG2	1:B:89:LYS:HG3	2.03	0.41
1:A:32:THR:HG22	1:A:73:PRO:HG3	2.02	0.41
1:A:44:LEU:HD13	1:A:216:LEU:HD12	2.02	0.41
1:B:43:ALA:HB1	1:B:61:PRO:CB	2.50	0.41
1:B:103:ASN:CB	1:A:113:GLN:NE2	2.83	0.41
1:B:103:ASN:CG	1:A:113:GLN:NE2	2.75	0.41
1:B:37:LEU:HD21	1:B:39:VAL:CG2	2.50	0.40
1:A:153:VAL:HG21	1:A:218:TRP:CZ3	2.55	0.40
1:A:183:TYR:CD2	1:A:203:THR:HG23	2.56	0.40
1:A:184:THR:O	1:A:188:TRP:N	2.51	0.40
1:B:42:ARG:HH11	1:B:42:ARG:HG3	1.85	0.40
1:A:230:LYS:HA	1:A:231:PRO:HD3	1.86	0.40
1:A:159:LEU:O	1:A:163:GLU:HB2	2.21	0.40
1:A:92:LEU:O	1:A:97:ARG:HB2	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	
1	A	211/314 (67%)	204 (97%)	7 (3%)	0	100	100
1	B	212/314 (68%)	195 (92%)	16 (8%)	1 (0%)	34	41
All	All	423/628 (67%)	399 (94%)	23 (5%)	1 (0%)	52	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	43	ALA

### 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	183/263 (70%)	172 (94%)	11 (6%)	24	31
1	B	185/263 (70%)	165 (89%)	20 (11%)	8	9
All	All	368/526 (70%)	337 (92%)	31 (8%)	14	16

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	HIS
1	B	17	LEU
1	B	28	ARG
1	B	34	LEU
1	B	41	ARG

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Mol	Chain	Res	Type
1	B	75	LYS
1	B	94	VAL
1	B	104	LEU
1	B	107	LEU
1	B	109	ARG
1	B	113	GLN
1	B	134	LEU
1	B	141	LEU
1	B	148	ASP
1	B	175	LYS
1	B	211	LYS
1	B	213	GLN
1	B	215	LEU
1	B	228	THR
1	B	232	MET
1	A	17	LEU
1	A	34	LEU
1	A	42	ARG
1	A	117	GLN
1	A	134	LEU
1	A	137	GLU
1	A	213	GLN
1	A	215	LEU
1	A	224	ARG
1	A	228	THR
1	A	230	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	222	HIS
1	A	103	ASN
1	A	113	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
3	BU1	A	315	-	5,5,5	0.37	0	4,4,4	0.29	0
3	BU1	B	315	-	5,5,5	0.36	0	4,4,4	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BU1	A	315	-	-	0/3/3/3	0/0/0/0
3	BU1	B	315	-	-	0/3/3/3	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	315	BU1	4	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	217/314 (69%)	0.76	27 (12%) 5 8	25, 46, 73, 110	0
1	B	218/314 (69%)	1.27	52 (23%) 1 1	23, 54, 97, 132	1 (0%)
2	C	4/4 (100%)	-0.31	0 100 100	27, 39, 42, 48	0
2	D	4/4 (100%)	-0.66	0 100 100	25, 32, 32, 41	0
All	All	443/636 (69%)	0.99	79 (17%) 2 3	23, 49, 93, 132	1 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	LEU	5.2
1	B	9	GLY	5.1
1	B	141	LEU	4.9
1	B	11	MET	4.8
1	B	227	SER	4.5
1	B	235	THR	4.5
1	B	216	LEU	4.5
1	A	50	SER	4.4
1	B	44	LEU	4.2
1	B	221	GLU	4.1
1	B	220	ASP	4.1
1	B	67	LEU	4.1
1	B	118	PRO	4.1
1	B	236	PRO	4.0
1	B	218	TRP	4.0
1	A	148	ASP	4.0
1	B	69	LEU	4.0
1	B	217	GLN	3.9
1	B	157	ALA	3.9
1	A	188	TRP	3.9
1	B	225	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	214	ALA	3.8
1	A	67	LEU	3.7
1	B	68	SER	3.6
1	A	51	GLN	3.6
1	A	68	SER	3.6
1	A	216	LEU	3.4
1	A	64	VAL	3.4
1	A	214	ALA	3.3
1	B	59	ARG	3.2
1	B	142	SER	3.2
1	B	156	ILE	3.0
1	B	37	LEU	3.0
1	B	228	THR	3.0
1	A	45	GLU	2.9
1	B	177	TYR	2.9
1	B	234	GLY	2.8
1	A	117	GLN	2.8
1	B	74	GLY	2.7
1	B	119	CYS	2.7
1	A	35	CYS	2.7
1	A	52	GLY	2.7
1	A	217	GLN	2.7
1	B	111	PHE	2.7
1	B	8	HIS	2.7
1	B	35	CYS	2.6
1	B	109	ARG	2.6
1	B	222	HIS	2.6
1	A	69	LEU	2.6
1	A	9	GLY	2.5
1	B	36	LEU	2.5
1	B	211	LYS	2.5
1	A	165	ALA	2.4
1	A	142	SER	2.4
1	B	160	LYS	2.4
1	A	36	LEU	2.4
1	B	66	LYS	2.4
1	B	152	CYS	2.4
1	A	34	LEU	2.3
1	B	140	ARG	2.3
1	B	213	GLN	2.3
1	B	100	PHE	2.3
1	B	158	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	148	ASP	2.3
1	A	37	LEU	2.3
1	A	162	LEU	2.2
1	B	76	ALA	2.2
1	B	224	ARG	2.1
1	A	113	GLN	2.1
1	B	70	CYS	2.1
1	B	64	VAL	2.1
1	A	177	TYR	2.1
1	B	94	VAL	2.1
1	A	112	LEU	2.1
1	B	161	ALA	2.1
1	B	164	GLN	2.0
1	B	38	ALA	2.0
1	A	17	LEU	2.0
1	A	111	PHE	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
4	MG	D	5	1/1	0.94	0.22	3.73	45,45,45,45	0
3	BU1	B	315	6/6	0.72	0.32	2.47	19,42,57,58	0
3	BU1	A	315	6/6	0.78	0.31	0.98	42,65,78,81	0
4	MG	C	5	1/1	0.89	0.17	0.06	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.