



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:03 PM UTC

PDB ID : 3U6F / pdb_00003u6f
Title : Mouse TREX1 D200N mutant
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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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

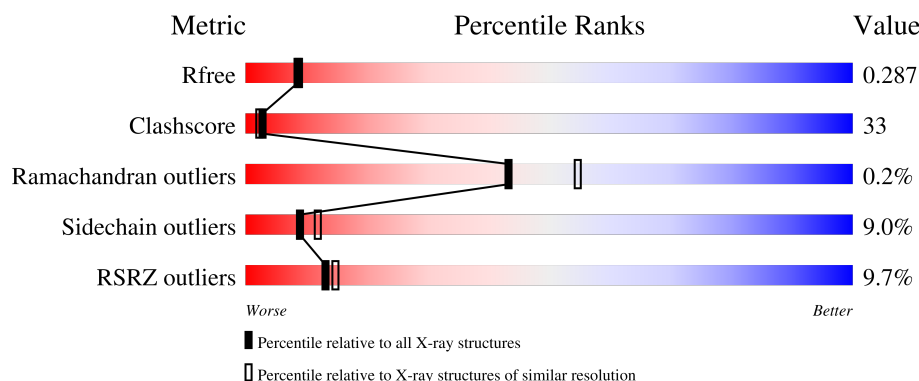
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	4% 48% 18% •• 31%
1	B	314	10% 35% 28% 6% 31%
2	C	4	100%
2	D	4	75% 25%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BU1	B	315	-	-	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			

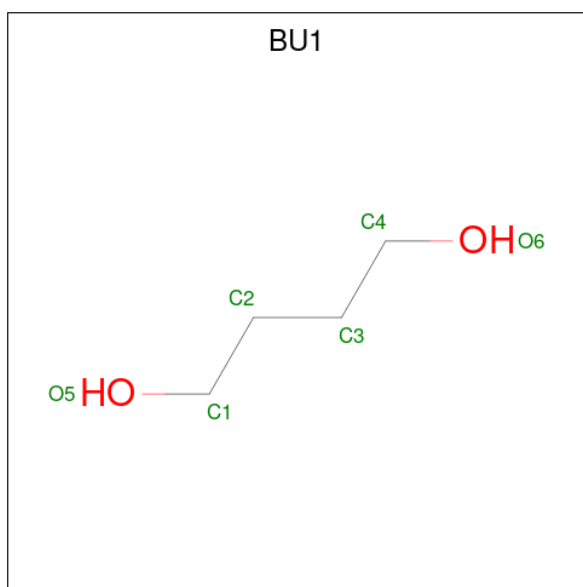
There are 2 discrepancies between the modelled and reference sequences:

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 (CCD ID: BU1) (formula: C₄H₁₀O₂).



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 (CCD ID: MG) (formula: Mg).

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

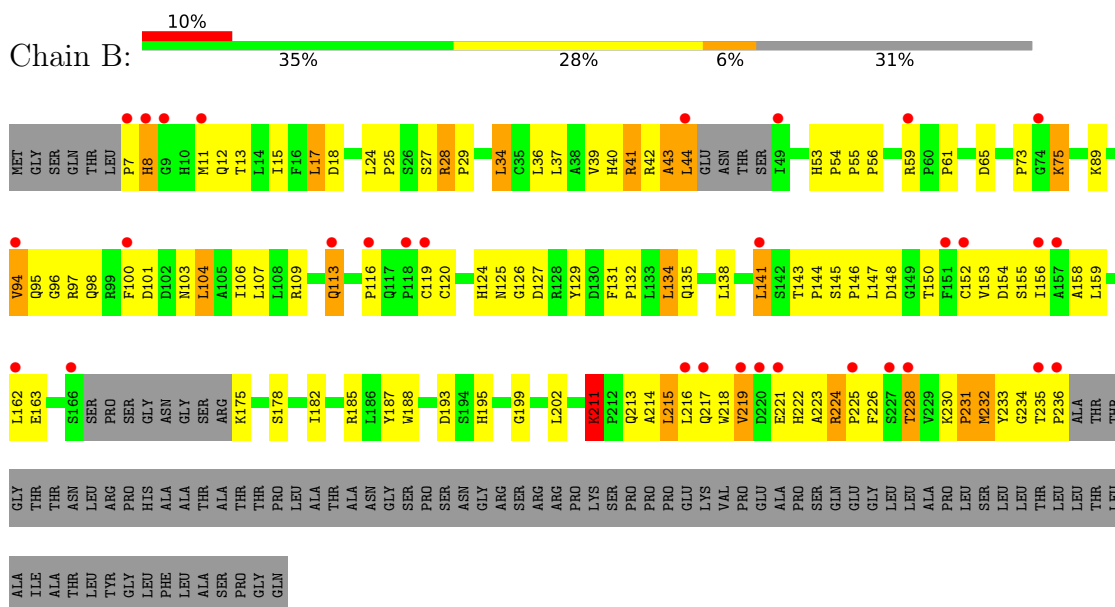
- Molecule 5 is water.

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		

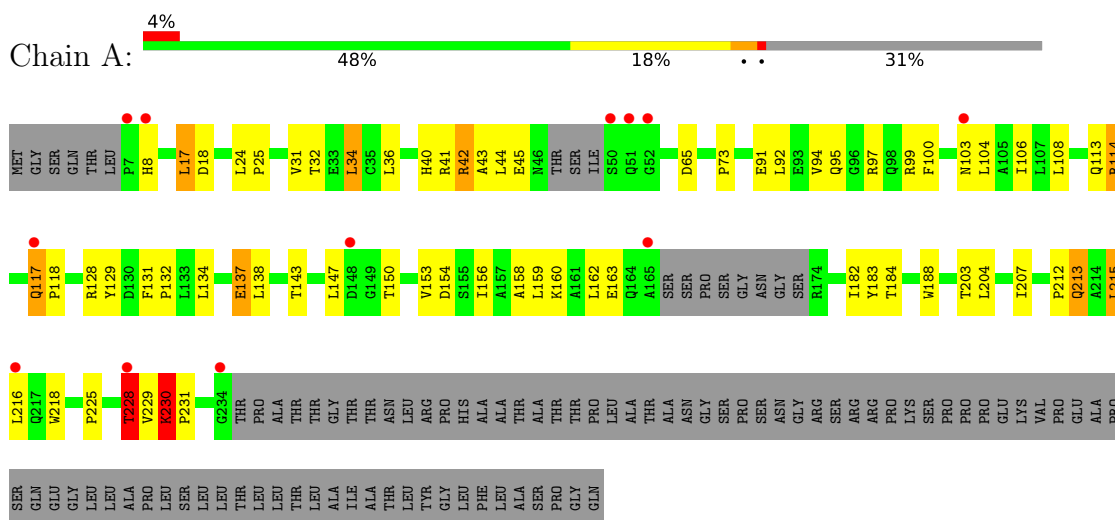
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Three prime repair exonuclease 1



- Molecule 1: Three prime repair exonuclease 1



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

Chain C:  100%

There are no outlier residues recorded for this chain.

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

Chain D:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.219 , 0.288 0.223 , 0.287	Depositor DCC
R_{free} test set	1083 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7069	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: BU1, MG

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	0.56	0/1712	0.97	7/2333 (0.3%)
1	B	0.60	0/1720	1.01	7/2345 (0.3%)
2	C	0.27	0/91	0.73	0/139
2	D	0.30	0/91	0.65	0/139
All	All	0.57	0/3614	0.97	14/4956 (0.3%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	TYR	N-CA-C	10.70	126.46	112.12
1	A	129	TYR	N-CA-C	10.28	126.46	111.96
1	A	228	THR	CB-CA-C	-7.89	97.44	110.85
1	B	211	LYS	CA-C-N	7.31	127.16	119.05
1	B	211	LYS	C-N-CA	7.31	127.16	119.05
1	A	230	LYS	CA-C-N	7.30	127.33	119.89
1	A	230	LYS	C-N-CA	7.30	127.33	119.89
1	B	156	ILE	CB-CA-C	-6.95	103.13	111.81
1	A	143	THR	CA-C-N	6.26	126.03	119.76
1	A	143	THR	C-N-CA	6.26	126.03	119.76
1	B	231	PRO	CB-CA-C	-5.85	104.21	111.64
1	A	128	ARG	N-CA-C	-5.40	105.50	112.68
1	B	145	SER	CA-C-N	5.05	125.12	119.87
1	B	145	SER	C-N-CA	5.05	125.12	119.87

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	87	0
1	B	1678	1681	1678	157	0
2	C	81	0	46	0	0
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	229	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 33.

All (229) 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:N	1:B:44:LEU:HD23	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:43:ALA:C	1:B:44:LEU:HD23	2.14	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:216:LEU:HA	1:B:219:VAL:HG13	1.72	0.69
1:B:225:PRO:HG2	1:B:228:THR:CG2	2.22	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
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:B:214:ALA:O	1:B:215:LEU:C	2.37	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:98:GLN:HB2	1:A:114:ARG:NH1	2.10	0.65
1:B:162:LEU:HD23	1:B:211:LYS:CG	2.27	0.65
1:B:11:MET:SD	1:B:119:CYS:C	2.80	0.65
1:A:44:LEU:HD23	1:A:44:LEU:C	2.21	0.64
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: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:44:LEU:HD23	1:A:44:LEU:O	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:THR:HG22	1:B:144:PRO:O	2.02	0.60
1:A:91:GLU:OE1	1:A:94:VAL:HG11	2.02	0.60
1:B:11:MET:HG2	1:B:120:CYS:HB3	1.84	0.59
1:B:103:ASN:HB2	1:A:113:GLN:NE2	2.16	0.59
1:B:215:LEU:O	1:B:219:VAL:CG1	2.49	0.59
1:B:59:ARG:HG3	1:B:59:ARG:HH11	1.66	0.59
1:B:216:LEU:C	1:B:216:LEU:HD23	2.27	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
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:HG2	1:B:28:ARG:HH11	1.68	0.58
1:A:159:LEU:CD2	1:A:182:ILE:HG21	2.33	0.58
1:B:17:LEU:HD23	1:B:36:LEU:HD23	1.86	0.58
1:B:218:TRP:O	1:B:221:GLU:HG2	2.04	0.58
1:B:37:LEU:HD23	1:B:37:LEU:C	2.28	0.58
1:A:215:LEU:HG	1:A:215:LEU:O	2.00	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:42:ARG:C	1:B:44:LEU:H	2.12	0.56
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:233:TYR:CD1	1:B:233:TYR:C	2.83	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:B:215:LEU:C	1:B:215:LEU:CD1	2.78	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:44:LEU:CD2	1:A:44:LEU:C	2.81	0.53
1:A:147:LEU:HD23	1:A:150:THR:HG21	1.89	0.53
1:B:53:HIS:HA	1:B:54:PRO:C	2.33	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:A:91:GLU:C	1:A:94:VAL:HG12	2.33	0.53
1:B:162:LEU:HB3	1:B:211:LYS:HD2	1.90	0.53
1:B:17:LEU:HD23	1:B:36:LEU:CD2	2.40	0.52
1:B:225:PRO:CG	1:B:228:THR:HB	2.40	0.52
1:B:97:ARG:NH1	1:A:65:ASP:OD2	2.43	0.51
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: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:75:LYS:C	1:B:89:LYS:HD3	2.36	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:B:103:ASN:CG	1:A:113:GLN:CD	2.79	0.51
1:B:17:LEU:HD22	1:B:18:ASP:N	2.26	0.50
1:A:94:VAL:HG13	1:A:95:GLN:HG3	1.93	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:SER:O	1:B:75:LYS:NZ	2.46	0.49
1:B:34:LEU:C	1:B:34:LEU:HD23	2.37	0.49
1:A:91:GLU:HA	1:A:94:VAL:CG1	2.41	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:A:228:THR:O	1:A:229:VAL:C	2.57	0.47
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:42:ARG:C	1:B:44:LEU:N	2.72	0.47
1:B:233:TYR:HD1	1:B:234:GLY:HA3	1.79	0.47
1:B:178:SER:O	1:B:182:ILE:HD12	2.14	0.47
1:A:138:LEU:CD1	1:A:147:LEU:HD12	2.44	0.47
1:B:147:LEU:CA	1:B:150:THR:OG1	2.63	0.47
1:B:193:ASP:OD2	3:B:315:BU1:H32	2.14	0.47
1:B:218:TRP:CE3	1:B:222:HIS:HD2	2.33	0.47
1:B:230:LYS:HG3	1:B:231:PRO:HD2	1.97	0.47
1:A:104:LEU:O	1:A:104:LEU:HD12	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:224:ARG:CD	1:B:228:THR:HG21	2.45	0.46
1:A:24:LEU:HB3	1:A:25:PRO:CD	2.45	0.46
1:A:31:VAL:HG23	1:A:137:GLU:OE1	2.16	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:100:PHE:CE2	1:B:138:LEU:HD23	2.51	0.45
1:B:158:ALA:O	1:B:162:LEU:HD13	2.15	0.45
1:B:103:ASN:CG	1:A:113:GLN:NE2	2.75	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:B:231:PRO:O	1:B:232:MET:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:94:VAL:C	1:B:96:GLY:H	2.24	0.44
1:A:159:LEU:HD22	1:A:207:ILE:HD12	2.00	0.44
1:B:195:HIS:CD2	5:B:377:HOH:O	2.71	0.44
1:A:34:LEU:C	1:A:34:LEU:HD23	2.43	0.44
1:A:212:PRO:HD2	1:A:213:GLN:NE2	2.32	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:215:LEU:C	1:B:215:LEU:HD13	2.43	0.43
1:B:34:LEU:HD23	1:B:34:LEU:O	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:215:LEU:HD12	1:B:219:VAL:CG1	2.47	0.42
1:B:233:TYR:HD1	1:B:234:GLY:N	2.17	0.42
1:B:28:ARG:HG2	1:B:28:ARG:NH1	2.31	0.42
1:B:109:ARG:HH21	1:B:146:PRO:HA	1.84	0.42
1:B:124:HIS:O	1:B:125:ASN:CB	2.66	0.42
1:B:59:ARG:HG3	1:B:59:ARG:NH1	2.34	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:B:55:PRO:HA	1:B:56:PRO:HD3	1.98	0.41
1:B:65:ASP:OD2	1:A:97:ARG:NH1	2.54	0.41
1:A:204:LEU:O	1:A:207:ILE:HG12	2.20	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:187:TYR:O	1:B:188:TRP:HB2	2.20	0.41
1:B:73:PRO:HG2	1:B:89:LYS:HG3	2.03	0.41
1:B:109:ARG:CZ	5:B:326:HOH:O	2.68	0.41
1:B:152:CYS:O	1:B:153:VAL:HG23	2.21	0.41
1:A:32:THR:HG22	1:A:73:PRO:HG3	2.02	0.41
1:A:100:PHE:CG	1:A:137:GLU:HG2	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:216:LEU:O	1:B:217:GLN:C	2.63	0.40
1:B:42:ARG:HG3	1:B:42:ARG:HH11	1.85	0.40
1:A:230:LYS:HA	1:A:231:PRO:HD3	1.86	0.40
1:B:95:GLN:CD	1:A:43:ALA:HB2	2.44	0.40
1:A:92:LEU:O	1:A:97:ARG:HB2	2.21	0.40
1:A:159:LEU:O	1:A:163:GLU:HB2	2.21	0.40
1:A:17:LEU:C	1:A:17:LEU:HD13	2.47	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%)	24	31
All	All	423/628 (67%)	399 (94%)	23 (5%)	1 (0%)	43	55

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%)	17	25
1	B	185/263 (70%)	163 (88%)	22 (12%)	5	6
All	All	368/526 (70%)	335 (91%)	33 (9%)	9	12

All (33) 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
1	B	44	LEU
1	B	75	LYS
1	B	94	VAL
1	B	104	LEU
1	B	107	LEU
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	219	VAL
1	B	224	ARG
1	B	228	THR
1	B	232	MET
1	A	17	LEU
1	A	34	LEU
1	A	42	ARG
1	A	114	ARG
1	A	117	GLN
1	A	134	LEU
1	A	137	GLU
1	A	213	GLN
1	A	215	LEU
1	A	228	THR
1	A	230	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	12	GLN
1	B	209	GLN
1	B	222	HIS
1	A	103	ASN
1	A	113	GLN
1	A	195	HIS
1	A	209	GLN

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 oligosaccharides 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	$\# Z > 2$
3	BU1	B	315	-	5,5,5	0.37	0	4,4,4	0.29	0
3	BU1	A	315	-	5,5,5	0.37	0	4,4,4	0.27	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	B	315	-	-	1/3/3/3	-
3	BU1	A	315	-	-	3/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	315	BU1	C2-C3-C4-O6
3	A	315	BU1	C1-C2-C3-C4
3	B	315	BU1	C1-C2-C3-C4
3	A	315	BU1	O5-C1-C2-C3

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, 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	217/314 (69%)	0.38	12 (5%) 30 32	27, 50, 80, 121	0
1	B	218/314 (69%)	0.75	31 (14%) 6 7	26, 58, 106, 146	1 (0%)
2	C	4/4 (100%)	-0.55	0 100 100	27, 39, 42, 48	0
2	D	4/4 (100%)	-0.85	0 100 100	25, 32, 32, 41	0
All	All	443/636 (69%)	0.54	43 (9%) 13 15	25, 53, 99, 146	1 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	MET	5.5
1	A	148	ASP	4.6
1	B	227	SER	4.5
1	B	9	GLY	4.0
1	B	225	PRO	3.9
1	B	44	LEU	3.9
1	B	141	LEU	3.6
1	B	7	PRO	3.6
1	A	165	ALA	3.5
1	A	50	SER	3.5
1	A	216	LEU	3.4
1	B	236	PRO	3.3
1	B	216	LEU	3.3
1	B	94	VAL	3.2
1	A	52	GLY	3.2
1	B	166	SER	3.1
1	B	152	CYS	3.0
1	B	59	ARG	2.8
1	A	51	GLN	2.8
1	B	219	VAL	2.8
1	B	49	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	220	ASP	2.7
1	B	119	CYS	2.6
1	B	118	PRO	2.6
1	B	8	HIS	2.5
1	B	74	GLY	2.5
1	A	117	GLN	2.5
1	A	103	ASN	2.4
1	B	151	PHE	2.3
1	B	217	GLN	2.3
1	A	228	THR	2.3
1	B	157	ALA	2.3
1	A	234	GLY	2.2
1	B	235	THR	2.2
1	B	100	PHE	2.1
1	B	162	LEU	2.1
1	B	228	THR	2.0
1	B	221	GLU	2.0
1	B	156	ILE	2.0
1	B	116	PRO	2.0
1	A	7	PRO	2.0
1	B	113	GLN	2.0
1	A	8	HIS	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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
3	BU1	B	315	6/6	0.77	0.14	19,42,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BU1	A	315	6/6	0.83	0.14	42,65,78,81	0
4	MG	D	5	1/1	0.92	0.10	45,45,45,45	0
4	MG	C	5	1/1	0.96	0.04	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.