



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 01:55 AM EDT

PDB ID : 3N5N  
Title : Crystal structure analysis of the catalytic domain and interdomain connector of human MutY homologue  
Authors : Toth, E.A.; Luncsford, P.J.  
Deposited on : 2010-05-25  
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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

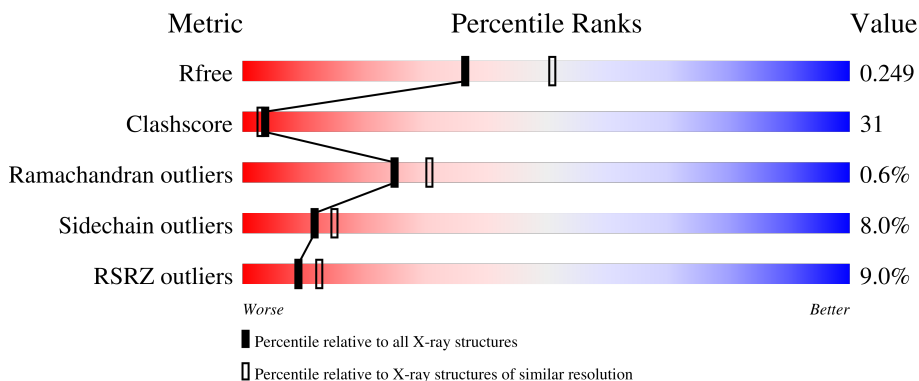
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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  $\geq 3$ , 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	X	287	
1	Y	287	

## 2 Entry composition [i](#)

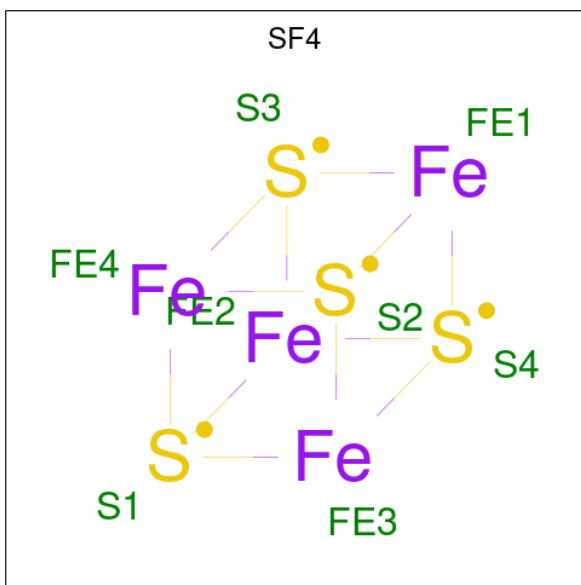
There are 4 unique types of molecules in this entry. The entry contains 4111 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 A/G-specific adenine DNA glycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	271	Total 2017	C 1261	N 362	O 382	S 12	0	0	0
1	Y	272	Total 2020	C 1262	N 360	O 385	S 13	0	0	0

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	X	1	Total 8	Fe 4	S 4	0	0
2	Y	1	Total 8	Fe 4	S 4	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Y	1	Total C O 3 2 1	0	0

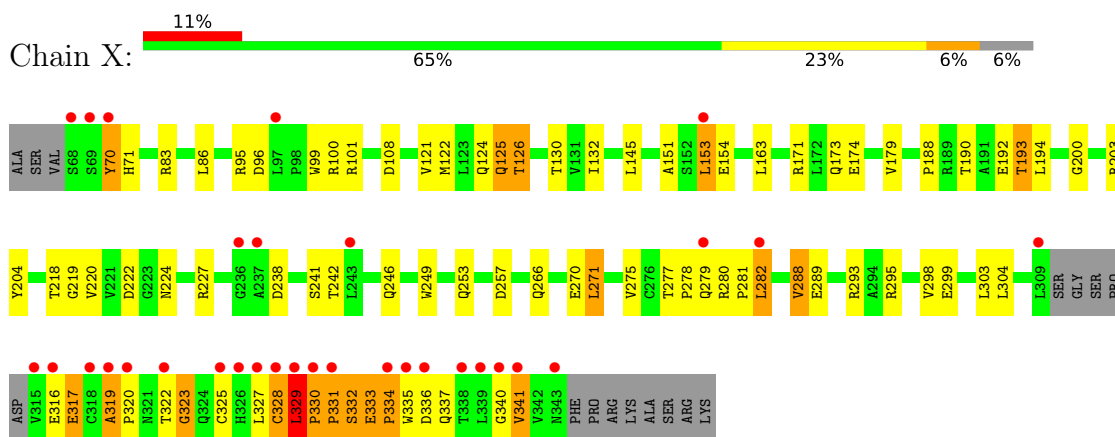
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	X	23	Total O 23 23	0	0
4	Y	32	Total O 32 32	0	0

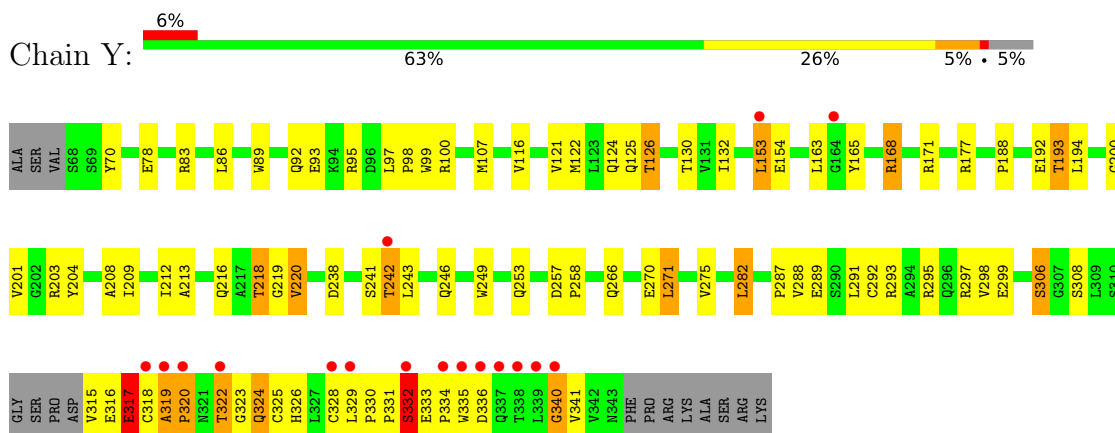
### 3 Residue-property plots [i](#)

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: A/G-specific adenine DNA glycosylase



- Molecule 1: A/G-specific adenine DNA glycosylase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.31Å 82.17Å 63.46Å 90.00° 100.90° 90.00°	Depositor
Resolution (Å)	62.31 – 2.30 39.37 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.7 (62.31-2.30) 95.7 (39.37-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.21 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.206 , 0.251 0.211 , 0.249	Depositor DCC
$R_{free}$ test set	1302 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtrriage
Anisotropy	0.195	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 61.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.029 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4111	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	X	0.79	0/2058	0.96	18/2808 (0.6%)
1	Y	0.82	0/2061	0.83	6/2813 (0.2%)
All	All	0.80	0/4119	0.90	24/5621 (0.4%)

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	X	0	1
1	Y	0	2
All	All	0	3

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	Y	332	SER	C-N-CA	15.84	161.30	121.70
1	X	341	VAL	CB-CA-C	-12.86	86.96	111.40
1	X	330	PRO	O-C-N	10.69	141.41	121.10
1	X	323	GLY	N-CA-C	-10.58	86.65	113.10
1	X	330	PRO	C-N-CD	9.96	149.32	128.40
1	X	328	CYS	CB-CA-C	-9.59	91.22	110.40
1	Y	317	GLU	CB-CA-C	-9.12	92.16	110.40
1	X	319	ALA	CB-CA-C	-8.96	96.66	110.10
1	X	333	GLU	C-N-CD	-8.07	102.84	120.60
1	Y	332	SER	N-CA-C	-7.64	90.38	111.00
1	X	336	ASP	C-N-CA	7.28	139.89	121.70
1	X	334	PRO	N-CA-C	-7.07	93.72	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	330	PRO	CA-C-N	-6.67	98.42	117.10
1	X	327	LEU	CB-CA-C	-6.34	98.15	110.20
1	Y	319	ALA	CB-CA-C	-6.27	100.69	110.10
1	X	319	ALA	N-CA-C	6.24	127.84	111.00
1	X	337	GLN	CB-CA-C	-5.88	98.63	110.40
1	X	316	GLU	CB-CA-C	-5.77	98.86	110.40
1	X	329	LEU	N-CA-C	-5.59	95.91	111.00
1	Y	306	SER	N-CA-C	-5.58	95.93	111.00
1	X	330	PRO	C-N-CA	-5.54	98.73	122.00
1	X	337	GLN	N-CA-C	-5.52	96.09	111.00
1	X	341	VAL	N-CA-C	5.33	125.40	111.00
1	Y	324	GLN	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	332	SER	Peptide
1	Y	332	SER	Peptide
1	Y	340	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	X	2017	0	1902	120	1
1	Y	2020	0	1898	130	1
2	X	8	0	0	0	0
2	Y	8	0	0	0	0
3	Y	3	0	3	0	0
4	X	23	0	0	0	0
4	Y	32	0	0	5	1
All	All	4111	0	3803	245	2

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 31.

All (245) 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:X:322:THR:CG2	1:X:323:GLY:H	1.22	1.40
1:X:332:SER:CA	1:X:335:TRP:HD1	1.41	1.33
1:Y:188:PRO:HB3	1:Y:193:THR:CG2	1.69	1.21
1:X:332:SER:CA	1:X:335:TRP:CD1	2.22	1.20
1:X:335:TRP:CZ3	1:X:340:GLY:HA3	1.79	1.16
1:X:329:LEU:N	1:X:329:LEU:HD12	1.51	1.15
1:X:95:ARG:HB3	1:Y:107:MET:CG	1.77	1.15
1:X:322:THR:HG22	1:X:323:GLY:N	1.31	1.15
1:X:329:LEU:CD1	1:X:329:LEU:H	1.57	1.14
1:Y:322:THR:HG23	1:Y:323:GLY:H	0.99	1.13
1:X:329:LEU:N	1:X:329:LEU:CD1	2.08	1.12
1:X:95:ARG:HB3	1:Y:107:MET:HG2	1.33	1.09
1:Y:188:PRO:HB3	1:Y:193:THR:HG23	1.23	1.08
1:Y:340:GLY:HA3	1:Y:341:VAL:CB	1.83	1.05
1:X:332:SER:C	1:X:335:TRP:HD1	1.61	1.02
1:X:100:ARG:HD3	1:X:266:GLN:NE2	1.74	1.01
1:Y:188:PRO:CB	1:Y:193:THR:CG2	2.38	1.00
1:Y:332:SER:C	1:Y:335:TRP:HD1	1.63	1.00
1:Y:334:PRO:HB3	1:Y:335:TRP:O	1.63	0.99
1:X:334:PRO:HA	1:X:335:TRP:HB2	1.43	0.98
1:Y:322:THR:CG2	1:Y:323:GLY:H	1.72	0.98
1:X:335:TRP:CH2	1:X:341:VAL:HA	1.98	0.97
1:Y:332:SER:HA	1:Y:335:TRP:CD1	2.00	0.96
1:X:329:LEU:H	1:X:329:LEU:HD13	1.28	0.96
1:Y:322:THR:HG23	1:Y:323:GLY:N	1.77	0.95
1:X:317:GLU:OE1	1:X:317:GLU:HA	1.66	0.95
1:X:322:THR:CG2	1:X:323:GLY:N	1.97	0.95
1:Y:332:SER:CA	1:Y:335:TRP:CD1	2.48	0.95
1:Y:328:CYS:HA	1:Y:329:LEU:C	1.87	0.94
1:Y:334:PRO:HA	1:Y:335:TRP:HB2	1.45	0.94
1:Y:322:THR:CG2	1:Y:323:GLY:N	2.26	0.94
1:X:188:PRO:HB3	1:X:193:THR:CG2	1.98	0.93
1:X:95:ARG:CB	1:Y:107:MET:HG2	2.00	0.92
1:X:153:LEU:HD22	1:X:154:GLU:N	1.84	0.92
1:Y:332:SER:OG	1:Y:333:GLU:HB2	1.71	0.91
1:X:322:THR:HG22	1:X:323:GLY:H	0.78	0.90
1:Y:332:SER:CA	1:Y:335:TRP:HD1	1.85	0.90
1:X:322:THR:HG23	1:X:323:GLY:H	1.33	0.89
1:X:70:TYR:CE1	1:X:293:ARG:HD3	2.06	0.88
1:Y:335:TRP:CH2	1:Y:340:GLY:O	2.26	0.88
1:X:332:SER:O	1:X:333:GLU:HB2	1.71	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:317:GLU:HA	1:Y:317:GLU:OE1	1.76	0.86
1:X:333:GLU:H	1:X:335:TRP:HB2	1.39	0.85
1:X:335:TRP:HH2	1:X:341:VAL:HA	1.34	0.84
1:Y:332:SER:C	1:Y:335:TRP:CD1	2.50	0.84
1:Y:188:PRO:CB	1:Y:193:THR:HG23	2.02	0.84
1:X:188:PRO:CB	1:X:193:THR:CG2	2.55	0.84
1:Y:317:GLU:OE1	1:Y:317:GLU:CA	2.25	0.84
1:Y:324:GLN:NE2	1:Y:326:HIS:HE1	1.75	0.84
1:Y:153:LEU:HD22	1:Y:154:GLU:N	1.94	0.83
1:Y:324:GLN:NE2	1:Y:326:HIS:CE1	2.48	0.82
1:X:317:GLU:OE1	1:X:317:GLU:CA	2.22	0.82
1:Y:125:GLN:CB	1:Y:168:ARG:CZ	2.57	0.82
1:X:335:TRP:CZ3	1:X:340:GLY:CA	2.63	0.81
1:X:70:TYR:CD1	1:X:293:ARG:HD3	2.15	0.81
1:Y:317:GLU:HG3	1:Y:317:GLU:O	1.77	0.81
1:X:333:GLU:N	1:X:335:TRP:CD1	2.50	0.80
1:X:95:ARG:HB3	1:Y:107:MET:HG3	1.63	0.80
1:Y:332:SER:OG	1:Y:333:GLU:CB	2.30	0.80
1:Y:188:PRO:HB3	1:Y:193:THR:HG21	1.64	0.79
1:X:188:PRO:HB3	1:X:193:THR:HG23	1.63	0.79
1:X:332:SER:O	1:X:333:GLU:CB	2.30	0.79
1:Y:317:GLU:O	1:Y:317:GLU:CG	2.28	0.78
1:X:332:SER:C	1:X:335:TRP:CD1	2.49	0.78
1:Y:335:TRP:HH2	1:Y:340:GLY:O	1.67	0.77
1:X:100:ARG:CD	1:X:266:GLN:NE2	2.47	0.77
1:Y:332:SER:HA	1:Y:335:TRP:NE1	1.98	0.76
1:X:282:LEU:N	1:X:282:LEU:HD12	2.00	0.75
1:X:335:TRP:CH2	1:X:340:GLY:CA	2.70	0.75
1:X:188:PRO:HB2	1:X:193:THR:HG22	1.69	0.74
1:X:282:LEU:N	1:X:282:LEU:CD1	2.50	0.74
1:X:333:GLU:N	1:X:335:TRP:HD1	1.85	0.74
1:X:322:THR:HG21	1:X:325:CYS:SG	2.28	0.73
1:X:335:TRP:CH2	1:X:340:GLY:HA3	2.23	0.73
1:Y:116:VAL:HG21	1:Y:212:ILE:HG22	1.69	0.73
1:Y:125:GLN:CB	1:Y:168:ARG:NH1	2.51	0.73
1:X:289:GLU:HG3	1:X:295:ARG:HG2	1.69	0.73
1:Y:204:TYR:CE1	1:Y:220:VAL:CG1	2.72	0.73
1:Y:324:GLN:HE22	1:Y:326:HIS:HE1	1.33	0.72
1:Y:171:ARG:HD2	1:Y:200:GLY:HA3	1.70	0.72
1:Y:92:GLN:HG3	1:Y:93:GLU:HG2	1.72	0.71
1:X:334:PRO:HA	1:X:335:TRP:CB	2.18	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:203:ARG:HD2	4:Y:350:HOH:O	1.90	0.71
1:Y:204:TYR:CE1	1:Y:220:VAL:HG13	2.26	0.70
1:X:328:CYS:O	1:X:328:CYS:SG	2.50	0.70
1:Y:243:LEU:HD12	1:Y:243:LEU:O	1.91	0.69
1:X:192:GLU:HG3	1:X:193:THR:N	2.06	0.69
1:Y:316:GLU:O	1:Y:317:GLU:CB	2.39	0.69
1:X:333:GLU:H	1:X:335:TRP:CB	2.05	0.68
1:Y:204:TYR:CD1	1:Y:220:VAL:HG13	2.28	0.68
1:Y:98:PRO:HD3	4:Y:48:HOH:O	1.94	0.68
1:X:100:ARG:CD	1:X:266:GLN:HE22	2.06	0.68
1:X:322:THR:CG2	1:X:323:GLY:O	2.42	0.68
1:Y:315:VAL:HG12	1:Y:315:VAL:O	1.94	0.68
1:X:190:THR:OG1	1:X:193:THR:HB	1.94	0.68
1:Y:282:LEU:HD12	1:Y:282:LEU:N	2.08	0.68
1:X:100:ARG:HG2	1:X:266:GLN:HE22	1.59	0.66
1:Y:334:PRO:CB	1:Y:335:TRP:C	2.63	0.66
1:X:335:TRP:CH2	1:X:340:GLY:HA2	2.31	0.66
1:Y:100:ARG:HD3	1:Y:266:GLN:NE2	2.10	0.66
1:Y:332:SER:OG	1:Y:333:GLU:N	2.29	0.66
1:X:328:CYS:C	1:X:329:LEU:HD12	2.16	0.65
1:X:122:MET:O	1:X:126:THR:HG23	1.96	0.65
1:Y:334:PRO:HB3	1:Y:335:TRP:C	2.18	0.64
1:X:319:ALA:HB3	1:X:320:PRO:CD	2.27	0.64
1:Y:116:VAL:HG21	1:Y:212:ILE:CG2	2.28	0.63
1:Y:70:TYR:CE1	1:Y:293:ARG:HD3	2.33	0.63
1:X:188:PRO:HB2	1:X:193:THR:CG2	2.28	0.62
1:X:100:ARG:HD3	1:X:266:GLN:HE22	1.61	0.61
1:Y:99:TRP:CZ3	1:Y:132:ILE:HD13	2.36	0.61
1:X:335:TRP:HH2	1:X:341:VAL:CA	2.10	0.61
1:X:224:ASN:OD1	1:X:227:ARG:NH2	2.33	0.61
1:Y:219:GLY:H	1:Y:253:GLN:NE2	1.98	0.61
1:X:322:THR:HG22	1:X:323:GLY:CA	2.25	0.60
1:Y:95:ARG:HD3	1:Y:270:GLU:OE2	2.00	0.60
1:X:335:TRP:CZ3	1:X:341:VAL:HA	2.35	0.60
1:X:100:ARG:CG	1:X:266:GLN:HE22	2.14	0.60
1:X:334:PRO:CA	1:X:335:TRP:HB2	2.27	0.60
1:Y:334:PRO:CB	1:Y:335:TRP:O	2.46	0.60
1:X:246:GLN:OE1	1:X:246:GLN:HA	2.02	0.59
1:X:271:LEU:HD22	1:X:275:VAL:HB	1.84	0.59
1:Y:126:THR:HG21	1:Y:163:LEU:HD12	1.85	0.59
1:X:219:GLY:H	1:X:253:GLN:HE22	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:319:ALA:HB3	1:Y:320:PRO:CD	2.32	0.59
1:Y:282:LEU:N	1:Y:282:LEU:CD1	2.66	0.59
1:X:330:PRO:C	1:X:331:PRO:O	2.42	0.58
1:Y:78:GLU:HG3	1:Y:291:LEU:HD22	1.86	0.58
1:Y:192:GLU:HG3	1:Y:193:THR:N	2.19	0.57
1:Y:332:SER:HA	1:Y:335:TRP:HE1	1.68	0.57
1:Y:188:PRO:HB2	1:Y:193:THR:CG2	2.31	0.57
1:Y:325:CYS:O	1:Y:326:HIS:ND1	2.37	0.57
1:Y:95:ARG:NH1	1:Y:270:GLU:OE1	2.33	0.57
1:X:322:THR:HG22	1:X:323:GLY:C	2.24	0.57
1:X:219:GLY:H	1:X:253:GLN:NE2	2.03	0.56
1:X:121:VAL:O	1:X:124:GLN:HG2	2.05	0.56
1:Y:322:THR:HG22	1:Y:323:GLY:N	2.20	0.56
1:X:204:TYR:CE1	1:X:220:VAL:CG1	2.89	0.56
1:Y:289:GLU:HG3	1:Y:295:ARG:HG2	1.88	0.56
1:X:319:ALA:HB3	1:X:320:PRO:HD3	1.86	0.55
1:X:171:ARG:HD2	1:X:200:GLY:HA3	1.87	0.55
1:Y:271:LEU:CD2	1:Y:275:VAL:HB	2.36	0.55
1:X:95:ARG:CD	1:X:270:GLU:OE2	2.55	0.55
1:Y:177:ARG:HB2	4:Y:61:HOH:O	2.07	0.55
1:Y:306:SER:O	1:Y:308:SER:N	2.40	0.54
1:Y:328:CYS:CA	1:Y:329:LEU:C	2.70	0.54
1:X:204:TYR:CD1	1:X:220:VAL:HG13	2.43	0.54
1:Y:328:CYS:HA	1:Y:329:LEU:O	2.06	0.54
1:Y:336:ASP:OD2	1:Y:336:ASP:N	2.40	0.54
1:X:188:PRO:CB	1:X:193:THR:HG23	2.33	0.54
1:Y:188:PRO:HB2	1:Y:194:LEU:HD23	1.90	0.54
1:Y:219:GLY:H	1:Y:253:GLN:HE22	1.56	0.54
1:Y:316:GLU:O	1:Y:317:GLU:HB3	2.08	0.54
1:Y:188:PRO:O	1:Y:194:LEU:HD21	2.08	0.53
1:Y:126:THR:HG22	1:Y:168:ARG:HH22	1.72	0.53
1:X:188:PRO:O	1:X:194:LEU:HD21	2.08	0.53
1:X:203:ARG:HG2	1:X:249:TRP:CH2	2.44	0.53
1:X:322:THR:CG2	1:X:323:GLY:C	2.76	0.53
1:X:288:VAL:O	1:X:288:VAL:CG1	2.57	0.52
1:X:188:PRO:HD2	1:X:194:LEU:HD23	1.90	0.52
1:X:317:GLU:OE1	1:X:317:GLU:O	2.26	0.52
1:X:204:TYR:CE1	1:X:220:VAL:HG13	2.44	0.52
1:X:108:ASP:OD2	1:X:108:ASP:C	2.48	0.52
1:X:322:THR:HG22	1:X:323:GLY:O	2.07	0.52
1:X:153:LEU:HD22	1:X:154:GLU:CG	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:330:PRO:O	1:X:331:PRO:C	2.44	0.52
1:Y:208:ALA:O	1:Y:212:ILE:HB	2.10	0.51
1:X:95:ARG:CB	1:Y:107:MET:CG	2.64	0.51
1:Y:193:THR:HG22	1:Y:194:LEU:N	2.25	0.51
1:Y:324:GLN:HE21	1:Y:326:HIS:CE1	2.29	0.51
1:Y:122:MET:O	1:Y:126:THR:HG23	2.11	0.51
1:Y:201:VAL:HG12	1:Y:201:VAL:O	2.11	0.51
1:Y:97:LEU:HA	4:Y:48:HOH:O	2.10	0.51
1:X:333:GLU:N	1:X:334:PRO:CA	2.74	0.50
1:X:299:GLU:O	1:X:303:LEU:HG	2.11	0.50
1:Y:83:ARG:HD3	1:Y:257:ASP:OD2	2.11	0.50
1:Y:203:ARG:HG2	1:Y:249:TRP:CH2	2.47	0.50
1:X:288:VAL:O	1:X:288:VAL:HG13	2.12	0.50
1:Y:121:VAL:O	1:Y:124:GLN:HG2	2.11	0.50
1:Y:333:GLU:HA	1:Y:335:TRP:HB2	1.94	0.50
1:X:238:ASP:O	1:X:241:SER:HB3	2.12	0.49
1:X:153:LEU:HD13	1:X:153:LEU:H	1.78	0.49
1:Y:171:ARG:HD2	1:Y:200:GLY:CA	2.40	0.49
1:Y:331:PRO:O	1:Y:332:SER:C	2.51	0.49
1:X:95:ARG:HD2	1:X:270:GLU:OE2	2.12	0.48
1:Y:165:TYR:O	1:Y:168:ARG:HG2	2.14	0.48
1:X:100:ARG:HD3	1:X:266:GLN:HE21	1.71	0.48
1:X:151:ALA:O	1:X:173:GLN:NE2	2.46	0.48
1:Y:246:GLN:HA	1:Y:246:GLN:OE1	2.14	0.48
1:Y:292:CYS:HB3	1:Y:295:ARG:HB3	1.95	0.48
1:X:298:VAL:HG23	1:X:299:GLU:N	2.30	0.47
1:Y:271:LEU:HD22	1:Y:275:VAL:HB	1.96	0.47
1:Y:317:GLU:OE1	1:Y:317:GLU:C	2.53	0.46
1:X:145:LEU:HD13	1:X:179:VAL:HG11	1.96	0.46
1:Y:153:LEU:HD22	1:Y:154:GLU:CA	2.45	0.46
1:Y:340:GLY:CA	1:Y:341:VAL:CB	2.70	0.46
1:X:153:LEU:H	1:X:153:LEU:CD1	2.28	0.46
1:Y:242:THR:HG22	1:Y:243:LEU:N	2.29	0.46
1:X:277:THR:HB	1:X:278:PRO:HD2	1.97	0.46
1:Y:188:PRO:HB2	1:Y:193:THR:HG22	1.98	0.46
1:Y:188:PRO:CB	1:Y:193:THR:HG21	2.30	0.45
1:X:99:TRP:CZ3	1:X:132:ILE:HD13	2.52	0.45
1:X:281:PRO:C	1:X:282:LEU:HD12	2.37	0.45
1:X:204:TYR:CE1	1:X:222:ASP:HB3	2.52	0.45
1:X:153:LEU:HD13	1:X:153:LEU:N	2.31	0.45
1:X:153:LEU:HD22	1:X:154:GLU:CA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:95:ARG:CD	1:Y:270:GLU:OE2	2.63	0.45
1:Y:209:ILE:O	1:Y:213:ALA:HB3	2.17	0.45
1:X:153:LEU:CD2	1:X:154:GLU:CG	2.95	0.44
1:X:242:THR:O	1:X:246:GLN:HG2	2.17	0.44
1:Y:99:TRP:CH2	1:Y:132:ILE:HD13	2.52	0.44
1:X:317:GLU:OE1	1:X:317:GLU:C	2.56	0.44
1:Y:238:ASP:O	1:Y:241:SER:HB3	2.18	0.44
1:Y:257:ASP:HA	1:Y:258:PRO:HD3	1.79	0.43
1:Y:218:THR:HA	1:Y:253:GLN:HE22	1.82	0.43
1:Y:319:ALA:CB	1:Y:320:PRO:CD	2.96	0.43
1:Y:70:TYR:CD1	1:Y:293:ARG:HD3	2.53	0.43
1:Y:333:GLU:N	1:Y:335:TRP:HD1	2.12	0.43
1:Y:335:TRP:CZ3	1:Y:340:GLY:O	2.68	0.43
1:X:171:ARG:HA	1:X:174:GLU:HG2	2.00	0.43
1:Y:316:GLU:O	1:Y:317:GLU:HB2	2.15	0.43
1:X:83:ARG:HD3	1:X:257:ASP:OD2	2.19	0.43
1:X:329:LEU:HA	1:X:330:PRO:HD2	1.80	0.42
1:X:125:GLN:C	1:X:126:THR:HG22	2.39	0.42
1:X:332:SER:CA	1:X:334:PRO:O	2.67	0.42
1:X:279:GLN:O	1:X:280:ARG:C	2.56	0.42
1:Y:316:GLU:CD	1:Y:319:ALA:CB	2.87	0.42
1:X:295:ARG:O	1:X:298:VAL:HG22	2.19	0.42
1:Y:89:TRP:CG	1:Y:287:PRO:HG3	2.55	0.42
1:Y:329:LEU:HA	1:Y:330:PRO:HD3	1.83	0.42
1:X:96:ASP:OD2	1:X:101:ARG:NH2	2.52	0.41
1:Y:289:GLU:CG	1:Y:295:ARG:HG2	2.49	0.41
1:Y:319:ALA:HB3	1:Y:320:PRO:HD2	2.01	0.41
1:Y:216:GLN:HG2	1:Y:218:THR:HG22	2.02	0.41
1:Y:334:PRO:HA	1:Y:335:TRP:CB	2.24	0.41
1:X:333:GLU:N	1:X:335:TRP:HB2	2.20	0.41
1:Y:116:VAL:CG2	1:Y:212:ILE:CG2	2.96	0.41
1:Y:193:THR:CG2	1:Y:194:LEU:N	2.81	0.41
1:X:275:VAL:HG13	1:X:282:LEU:HB2	2.02	0.41
1:Y:203:ARG:HG3	4:Y:345:HOH:O	2.21	0.41
1:Y:325:CYS:C	1:Y:326:HIS:CG	2.95	0.41
1:Y:333:GLU:HA	1:Y:334:PRO:HA	1.64	0.41
1:Y:298:VAL:HG23	1:Y:299:GLU:N	2.36	0.40
1:Y:153:LEU:HD13	1:Y:154:GLU:H	1.86	0.40
1:X:188:PRO:CB	1:X:193:THR:HG22	2.29	0.40
1:Y:204:TYR:CE1	1:Y:220:VAL:HG11	2.52	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:316:GLU:O	4:Y:14:HOH:O[2_745]	1.56	0.64
1:X:71:HIS:CE1	1:X:335:TRP:CE2[2_544]	2.14	0.06

### 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	X	267/287 (93%)	251 (94%)	15 (6%)	1 (0%)	34	42
1	Y	268/287 (93%)	247 (92%)	19 (7%)	2 (1%)	22	26
All	All	535/574 (93%)	498 (93%)	34 (6%)	3 (1%)	25	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	317	GLU
1	X	331	PRO
1	Y	320	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	X	199/236 (84%)	184 (92%)	15 (8%)	13	17
1	Y	200/236 (85%)	183 (92%)	17 (8%)	10	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	399/472 (84%)	367 (92%)	32 (8%)	12	15

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	70	TYR
1	X	86	LEU
1	X	125	GLN
1	X	126	THR
1	X	130	THR
1	X	153	LEU
1	X	163	LEU
1	X	193	THR
1	X	218	THR
1	X	271	LEU
1	X	282	LEU
1	X	288	VAL
1	X	304	LEU
1	X	317	GLU
1	X	329	LEU
1	Y	86	LEU
1	Y	126	THR
1	Y	130	THR
1	Y	153	LEU
1	Y	168	ARG
1	Y	193	THR
1	Y	218	THR
1	Y	220	VAL
1	Y	242	THR
1	Y	271	LEU
1	Y	282	LEU
1	Y	288	VAL
1	Y	297	ARG
1	Y	317	GLU
1	Y	318	CYS
1	Y	322	THR
1	Y	332	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:



Mol	Chain	Res	Type
1	X	71	HIS
1	X	92	GLN
1	X	124	GLN
1	X	253	GLN
1	X	254	GLN
1	X	266	GLN
1	Y	71	HIS
1	Y	92	GLN
1	Y	124	GLN
1	Y	253	GLN
1	Y	254	GLN
1	Y	266	GLN
1	Y	324	GLN
1	Y	326	HIS

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SF4	Y	400	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ACT	Y	2	-	1,2,3	1.39	0	1,1,3	0.19	0
2	SF4	X	400	1	0,12,12	-	-	-		

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
2	SF4	Y	400	1	-	-	0/6/5/5
2	SF4	X	400	1	-	-	0/6/5/5

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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	X	271/287 (94%)	0.71	32 (11%) 4 6	38, 61, 146, 189	0
1	Y	272/287 (94%)	0.51	17 (6%) 20 25	36, 61, 97, 131	0
All	All	543/574 (94%)	0.61	49 (9%) 9 12	36, 61, 126, 189	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	334	PRO	6.4
1	Y	336	ASP	6.3
1	X	338	THR	6.2
1	X	315	VAL	6.2
1	X	339	LEU	6.2
1	X	330	PRO	6.0
1	X	320	PRO	5.1
1	Y	340	GLY	5.0
1	X	340	GLY	4.7
1	X	328	CYS	4.6
1	X	322	THR	4.6
1	X	319	ALA	4.5
1	Y	334	PRO	4.4
1	X	331	PRO	4.2
1	X	318	CYS	4.2
1	X	329	LEU	4.1
1	X	327	LEU	4.1
1	X	243	LEU	4.1
1	X	316	GLU	3.9
1	X	336	ASP	3.7
1	X	70	TYR	3.7
1	X	153	LEU	3.6
1	Y	339	LEU	3.6
1	X	341	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	Y	337	GLN	3.4
1	Y	322	THR	3.3
1	X	237	ALA	3.3
1	X	68	SER	3.1
1	Y	164	GLY	3.1
1	X	325	CYS	3.1
1	X	309	LEU	2.8
1	X	279	GLN	2.8
1	X	69	SER	2.7
1	X	335	TRP	2.7
1	Y	335	TRP	2.6
1	Y	338	THR	2.6
1	Y	242	THR	2.5
1	Y	332	SER	2.5
1	Y	153	LEU	2.5
1	Y	320	PRO	2.4
1	Y	319	ALA	2.3
1	X	282	LEU	2.2
1	Y	329	LEU	2.2
1	Y	318	CYS	2.2
1	Y	328	CYS	2.2
1	X	326	HIS	2.1
1	X	97	LEU	2.1
1	X	343	ASN	2.0
1	X	236	GLY	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 monosaccharides 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACT	Y	2	3/4	0.74	0.30	81,81,82,83	0
2	SF4	Y	400	8/8	0.98	0.06	54,59,61,62	0
2	SF4	X	400	8/8	0.99	0.06	56,60,63,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.