



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:41 PM UTC

PDB ID : 3N5N / pdb_00003n5n
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

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

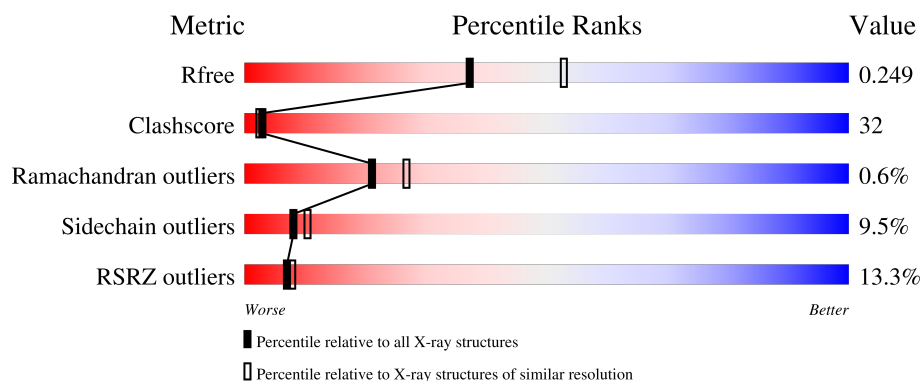
1 Overall quality at a glance

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	X	287	13% 63% 23% 7% 6%
1	Y	287	12% 62% 24% 8% 5%

2 Entry composition [i](#)

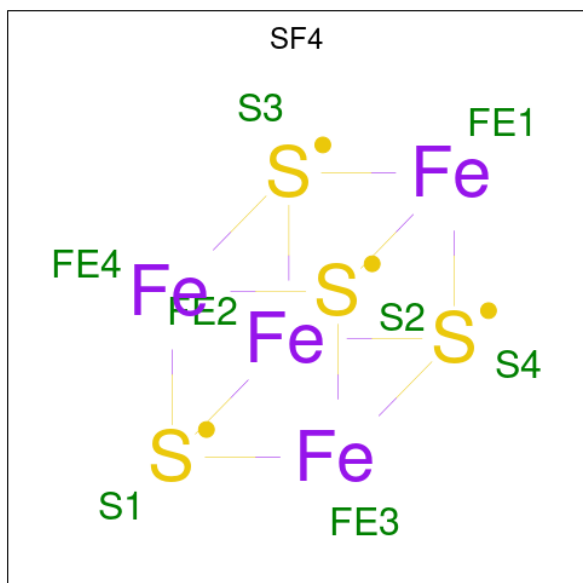
There are 4 unique types of molecules in this entry. The entry contains 4111 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

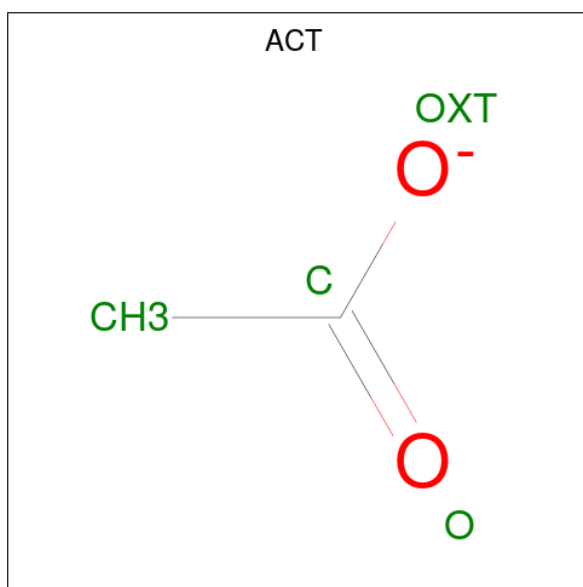
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	271	Total	C	N	O	S	0	0	0
			2017	1261	362	382	12			
1	Y	272	Total	C	N	O	S	0	0	0
			2020	1262	360	385	13			

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

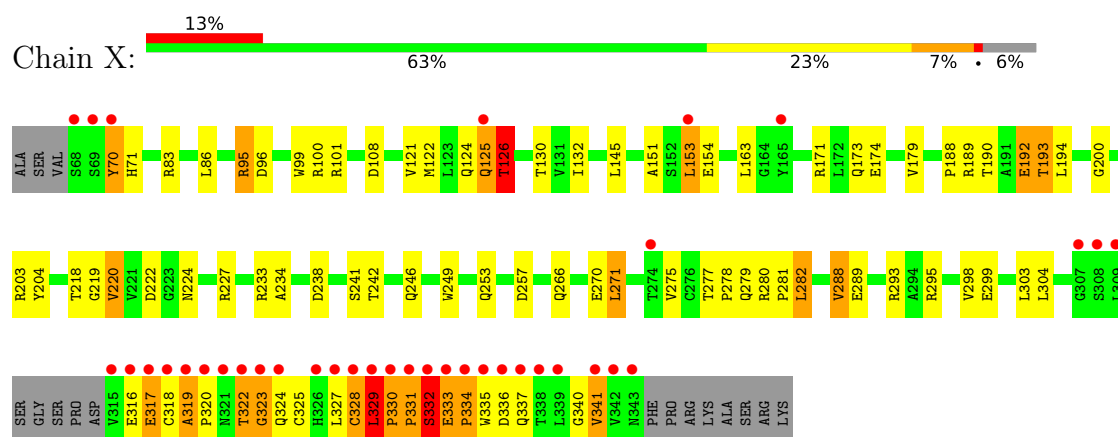
- Molecule 4 is water.

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

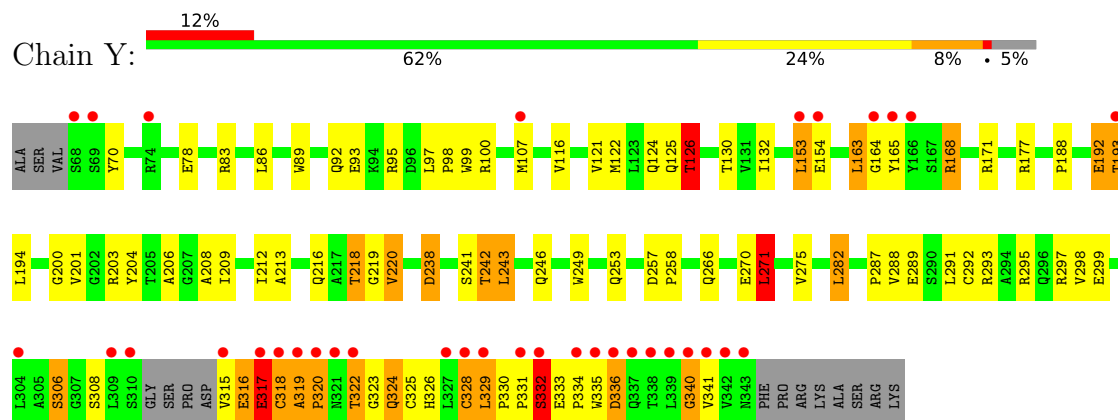
3 Residue-property plots [i](#)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.31Å 82.17Å 63.46Å 90.00° 100.90° 90.00°	Depositor
Resolution (Å)	62.31 – 2.30 62.31 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.7 (62.31-2.30) 95.7 (62.31-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.21 (at 2.29Å)	Xtriage
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 ²)	43.1	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4111	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage'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.*

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: 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	1.02	1/2058 (0.0%)	1.39	33/2808 (1.2%)
1	Y	1.04	1/2061 (0.0%)	1.26	19/2813 (0.7%)
All	All	1.03	2/4119 (0.0%)	1.33	52/5621 (0.9%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	332	SER	C-N	-5.31	1.22	1.33
1	Y	206	ALA	CA-CB	5.10	1.61	1.53

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	332	SER	CA-C-N	17.87	161.30	122.17
1	Y	332	SER	C-N-CA	17.87	161.30	122.17
1	X	330	PRO	O-C-N	16.90	141.41	121.46
1	X	330	PRO	CA-C-N	-16.89	98.73	119.84
1	X	330	PRO	C-N-CA	-16.89	98.73	119.84
1	X	341	VAL	CB-CA-C	-12.86	86.96	111.40
1	Y	318	CYS	N-CA-C	-11.21	99.31	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	323	GLY	N-CA-C	-11.20	86.65	113.18
1	X	328	CYS	CB-CA-C	-10.91	91.22	109.55
1	X	319	ALA	N-CA-C	10.36	127.84	113.45
1	Y	332	SER	N-CA-C	-9.59	90.38	110.80
1	X	336	ASP	CA-C-N	9.48	139.89	123.01
1	X	336	ASP	C-N-CA	9.48	139.89	123.01
1	X	337	GLN	N-CA-C	-9.22	96.09	109.18
1	Y	317	GLU	CB-CA-C	-9.18	92.16	110.42
1	X	329	LEU	CA-C-N	8.70	129.34	120.38
1	X	329	LEU	C-N-CA	8.70	129.34	120.38
1	Y	306	SER	N-CA-C	-8.43	95.93	109.76
1	X	336	ASP	N-CA-C	8.32	123.56	113.41
1	X	333	GLU	C-N-CD	-8.07	102.84	120.60
1	Y	324	GLN	N-CA-C	-8.01	97.31	109.96
1	Y	329	LEU	CA-C-N	7.83	125.30	119.66
1	Y	329	LEU	C-N-CA	7.83	125.30	119.66
1	X	316	GLU	CB-CA-C	-7.81	98.86	109.71
1	X	319	ALA	CB-CA-C	-7.28	96.66	111.80
1	Y	319	ALA	N-CA-C	7.13	123.29	113.16
1	X	334	PRO	N-CA-C	-7.07	93.72	112.10
1	X	329	LEU	N-CA-C	-6.81	95.91	109.60
1	X	324	GLN	N-CA-C	-6.63	100.02	109.96
1	X	316	GLU	N-CA-C	6.54	119.98	110.42
1	X	317	GLU	N-CA-C	6.28	121.07	113.41
1	X	322	THR	CB-CA-C	-6.22	99.20	112.63
1	X	336	ASP	CB-CA-C	6.10	119.91	109.24
1	X	327	LEU	N-CA-C	5.96	118.25	110.43
1	Y	319	ALA	CB-CA-C	-5.95	100.69	112.05
1	X	337	GLN	CB-CA-C	-5.94	98.63	111.11
1	X	330	PRO	C-N-CD	5.93	149.32	125.00
1	Y	238	ASP	CA-C-N	5.89	125.75	119.28
1	Y	238	ASP	C-N-CA	5.89	125.75	119.28
1	Y	271	LEU	N-CA-C	-5.79	104.89	111.14
1	Y	328	CYS	CB-CA-C	-5.72	102.33	110.34
1	X	318	CYS	CB-CA-C	-5.62	101.30	110.85
1	X	328	CYS	N-CA-C	5.56	120.94	113.72
1	X	327	LEU	CB-CA-C	-5.56	98.15	109.65
1	Y	316	GLU	CB-CA-C	-5.54	109.70	117.23
1	X	333	GLU	N-CA-C	-5.28	98.13	109.81
1	X	189	ARG	N-CA-C	5.19	119.60	113.16
1	X	341	VAL	N-CA-C	5.14	125.40	111.00
1	Y	316	GLU	N-CA-C	5.12	117.21	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	126	THR	N-CA-C	5.11	116.83	108.76
1	Y	126	THR	N-CA-C	5.05	116.86	109.24
1	Y	164	GLY	N-CA-C	5.04	125.12	113.18

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

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	126	1
1	Y	2020	0	1898	131	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	252	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 32.

All (252) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:X:332:SER:C	1:X:335:TRP:HD1	1.61	1.07
1:Y:340:GLY:HA3	1:Y:341:VAL:CB	1.83	1.05
1:Y:332:SER:C	1:Y:335:TRP:HD1	1.63	1.05
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:328:CYS:HA	1:Y:329:LEU:C	1.87	0.99
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: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:Y:332:SER:C	1:Y:335:TRP:CD1	2.50	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
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:332:SER:C	1:X:335:TRP:CD1	2.49	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:335:TRP:HH2	1:X:341:VAL:HA	1.34	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: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
1:Y:334:PRO:CB	1:Y:335:TRP:C	2.63	0.71
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:C	1:X:329:LEU:HD12	2.16	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Y:334:PRO:HB3	1:Y:335:TRP:C	2.18	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: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:333:GLU:H	1:X:335:TRP:CD1	2.12	0.67
1:X:100:ARG:HG2	1:X:266:GLN:HE22	1.59	0.66
1:Y:315:VAL:HG12	1:Y:315:VAL:O	1.94	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:122:MET:O	1:X:126:THR:HG23	1.96	0.65
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:330:PRO:C	1:X:331:PRO:O	2.42	0.62
1:X:188:PRO:HB2	1:X:193:THR:CG2	2.28	0.62
1:X:322:THR:HG22	1:X:323:GLY:C	2.24	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: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
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:Y:328:CYS:CA	1:Y:329:LEU:C	2.70	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:333:GLU:H	1:X:335:TRP:CG	2.22	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:X:322:THR:CG2	1:X:323:GLY:C	2.76	0.57
1:Y:95:ARG:NH1	1:Y:270:GLU:OE1	2.33	0.57
1:X:108:ASP:OD2	1:X:108:ASP:C	2.48	0.56
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:X:330:PRO:O	1:X:331:PRO:C	2.44	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:X:334:PRO:CA	1:X:335:TRP:HB2	2.27	0.54
1:Y:306:SER:O	1:Y:308:SER:N	2.40	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:331:PRO:O	1:Y:332:SER:C	2.51	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: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: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
1:Y:208:ALA:O	1:Y:212:ILE:HB	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:317:GLU:OE1	1:Y:317:GLU:C	2.53	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:X:281:PRO:C	1:X:282:LEU:HD12	2.37	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:X:95:ARG:HD2	1:X:270:GLU:OE2	2.12	0.48
1:X:317:GLU:OE1	1:X:317:GLU:C	2.56	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:125:GLN:C	1:X:126:THR:HG22	2.39	0.47
1:X:279:GLN:O	1:X:280:ARG:C	2.56	0.47
1:X:298:VAL:HG23	1:X:299:GLU:N	2.30	0.47
1:Y:316:GLU:CD	1:Y:319:ALA:CB	2.87	0.47
1:Y:271:LEU:HD22	1:Y:275:VAL:HB	1.96	0.47
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:Y:325:CYS:C	1:Y:326:HIS:CG	2.95	0.45
1:X:204:TYR:CE1	1:X:222:ASP:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:Y:95:ARG:CD	1:Y:270:GLU:OE2	2.63	0.45
1:Y:153:LEU:HD22	1:Y:153:LEU:C	2.42	0.45
1:Y:209:ILE:O	1:Y:213:ALA:HB3	2.17	0.45
1:X:204:TYR:CD2	1:X:204:TYR:C	2.95	0.44
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: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:243:LEU:HD12	1:Y:243:LEU:C	2.42	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:X:233:ARG:O	1:X:234:ALA:C	2.61	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:332:SER:CA	1:X:334:PRO:O	2.67	0.42
1:X:222:ASP:OD1	1:X:222:ASP:C	2.61	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:X:332:SER:CA	1:X:334:PRO:C	2.92	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:335:TRP:HH2	1:Y:340:GLY:C	2.27	0.41
1:Y:116:VAL:CG2	1:Y:212:ILE:CG2	2.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 symmetry 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%)	30	38
1	Y	268/287 (93%)	247 (92%)	19 (7%)	2 (1%)	18	23
All	All	535/574 (93%)	498 (93%)	34 (6%)	3 (1%)	21	27

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%)	182 (92%)	17 (8%)	10	13
1	Y	200/236 (85%)	179 (90%)	21 (10%)	6	8
All	All	399/472 (84%)	361 (90%)	38 (10%)	8	10

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	70	TYR
1	X	86	LEU
1	X	95	ARG
1	X	125	GLN
1	X	126	THR
1	X	130	THR
1	X	153	LEU
1	X	163	LEU
1	X	192	GLU
1	X	193	THR
1	X	218	THR
1	X	220	VAL
1	X	271	LEU
1	X	282	LEU
1	X	288	VAL
1	X	304	LEU
1	X	329	LEU
1	Y	86	LEU
1	Y	126	THR
1	Y	130	THR
1	Y	153	LEU
1	Y	163	LEU
1	Y	168	ARG
1	Y	192	GLU
1	Y	193	THR
1	Y	218	THR
1	Y	220	VAL
1	Y	242	THR
1	Y	243	LEU
1	Y	271	LEU
1	Y	282	LEU
1	Y	288	VAL
1	Y	297	ARG

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Mol	Chain	Res	Type
1	Y	317	GLU
1	Y	318	CYS
1	Y	322	THR
1	Y	332	SER
1	Y	336	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	71	HIS
1	X	92	GLN
1	X	124	GLN
1	X	247	GLN
1	X	253	GLN
1	X	254	GLN
1	X	266	GLN
1	X	279	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	279	GLN
1	Y	324	GLN
1	Y	326	HIS

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 oligosaccharides 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	X	400	1	0,12,12	-	-	-		
2	SF4	Y	400	1	0,12,12	-	-	-		
3	ACT	Y	2	-	1,2,3	1.46	0	0,1,3	-	-

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	X	400	1	-	-	0/6/5/5
2	SF4	Y	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, 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	X	271/287 (94%)	0.78	37 (13%) 6 7	38, 61, 146, 189	0
1	Y	272/287 (94%)	0.65	35 (12%) 7 8	36, 61, 97, 131	0
All	All	543/574 (94%)	0.72	72 (13%) 7 8	36, 61, 126, 189	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	329	LEU	6.2
1	X	315	VAL	5.7
1	X	318	CYS	5.6
1	X	68	SER	5.6
1	Y	319	ALA	5.4
1	X	319	ALA	5.1
1	X	338	THR	4.9
1	Y	164	GLY	4.8
1	X	309	LEU	4.7
1	X	327	LEU	4.4
1	X	335	TRP	4.4
1	Y	315	VAL	4.4
1	X	334	PRO	4.2
1	Y	153	LEU	4.1
1	X	320	PRO	3.8
1	Y	322	THR	3.8
1	X	336	ASP	3.8
1	Y	335	TRP	3.8
1	Y	318	CYS	3.8
1	Y	327	LEU	3.7
1	Y	304	LEU	3.7
1	Y	334	PRO	3.6
1	X	324	GLN	3.6
1	Y	339	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	Y	343	ASN	3.5
1	Y	68	SER	3.5
1	X	343	ASN	3.5
1	X	308	SER	3.5
1	X	321	ASN	3.5
1	X	339	LEU	3.5
1	X	326	HIS	3.4
1	X	317	GLU	3.4
1	X	333	GLU	3.4
1	Y	340	GLY	3.4
1	Y	320	PRO	3.3
1	X	331	PRO	3.3
1	Y	332	SER	3.3
1	Y	329	LEU	3.3
1	X	69	SER	3.3
1	X	341	VAL	3.3
1	Y	309	LEU	3.2
1	X	322	THR	3.2
1	X	328	CYS	3.1
1	Y	317	GLU	3.1
1	X	342	VAL	3.1
1	X	316	GLU	2.9
1	Y	337	GLN	2.9
1	Y	338	THR	2.9
1	Y	310	SER	2.9
1	Y	321	ASN	2.8
1	X	330	PRO	2.8
1	X	70	TYR	2.8
1	Y	328	CYS	2.7
1	X	332	SER	2.7
1	X	153	LEU	2.7
1	Y	69	SER	2.6
1	X	337	GLN	2.6
1	Y	336	ASP	2.5
1	X	323	GLY	2.5
1	X	125	GLN	2.4
1	Y	342	VAL	2.4
1	Y	331	PRO	2.3
1	Y	107	MET	2.3
1	X	274	THR	2.3
1	Y	341	VAL	2.2
1	Y	154	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	Y	193	THR	2.2
1	X	165	TYR	2.2
1	X	307	GLY	2.2
1	Y	74	ARG	2.1
1	Y	165	TYR	2.1
1	Y	166	TYR	2.1

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($\text{\AA}^2$)	Q<0.9
3	ACT	Y	2	3/4	0.80	0.25	81,81,82,83	0
2	SF4	X	400	8/8	0.98	0.05	56,60,63,65	0
2	SF4	Y	400	8/8	0.99	0.04	54,59,61,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.