



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 12:24 AM EDT

PDB ID : 3NYD  
Title : Crystal Structure of Kemp Eliminase HG-2 Complexed with Transition State Analog 5-Nitro Benzotriazole  
Authors : Lee, T.M.; Privett, H.K.; Kaiser, J.T.; Mayo, S.L.  
Deposited on : 2010-07-14  
Resolution : 1.23 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

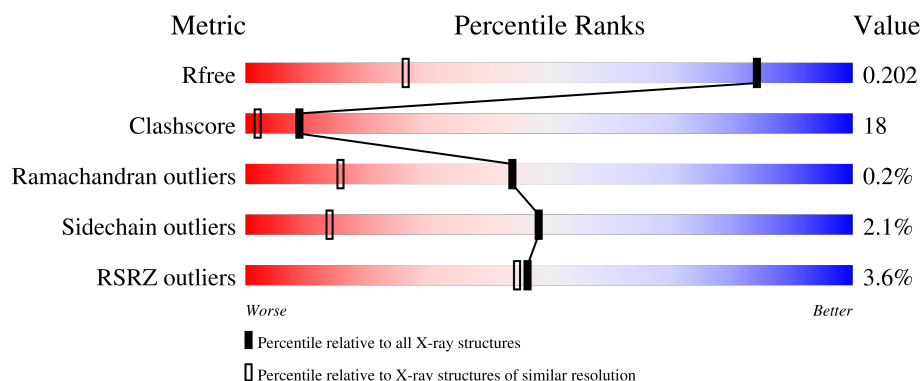
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.23 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))
$R_{free}$	164625	1389 (1.26-1.22)
Clashscore	180529	1509 (1.26-1.22)
Ramachandran outliers	177936	1478 (1.26-1.22)
Sidechain outliers	177891	1476 (1.26-1.22)
RSRZ outliers	164620	1389 (1.26-1.22)

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	A	316	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>82%</span> <span>13%</span> <span>• •</span> </div> </div>
1	B	316	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>6%</span> <span>59%</span> <span>33%</span> <span>• • 5%</span> </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3NY	A	317[B]	-	-	X	-
3	ACT	B	318	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6443 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 Endo-1,4-beta-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	23	1
			2427	1543	412	462	10			
1	B	301	Total	C	N	O	S	10	136	1
			3238	2043	552	628	15			

There are 52 discrepancies between the modelled and reference sequences:

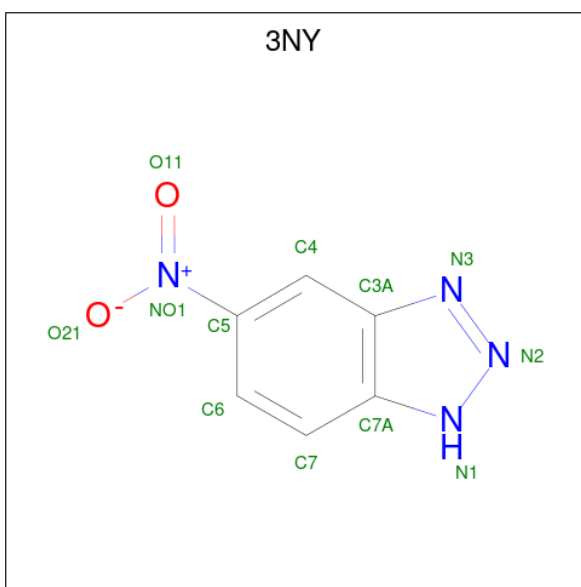
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	GLN	engineered mutation	UNP P23360
A	42	MET	GLN	engineered mutation	UNP P23360
A	44	TRP	THR	engineered mutation	UNP P23360
A	81	GLY	ARG	engineered mutation	UNP P23360
A	83	GLY	HIS	engineered mutation	UNP P23360
A	84	MET	THR	engineered mutation	UNP P23360
A	130	GLY	ASN	engineered mutation	UNP P23360
A	172	MET	ASN	engineered mutation	UNP P23360
A	234	SER	ALA	engineered mutation	UNP P23360
A	236	LEU	THR	engineered mutation	UNP P23360
A	237	MET	GLU	engineered mutation	UNP P23360
A	265	SER	THR	engineered mutation	UNP P23360
A	267	PHE	TRP	engineered mutation	UNP P23360
A	304	GLY	-	expression tag	UNP P23360
A	305	SER	-	expression tag	UNP P23360
A	306	ILE	-	expression tag	UNP P23360
A	307	GLU	-	expression tag	UNP P23360
A	308	GLY	-	expression tag	UNP P23360
A	309	ARG	-	expression tag	UNP P23360
A	310	GLY	-	expression tag	UNP P23360
A	311	HIS	-	expression tag	UNP P23360
A	312	HIS	-	expression tag	UNP P23360
A	313	HIS	-	expression tag	UNP P23360
A	314	HIS	-	expression tag	UNP P23360
A	315	HIS	-	expression tag	UNP P23360

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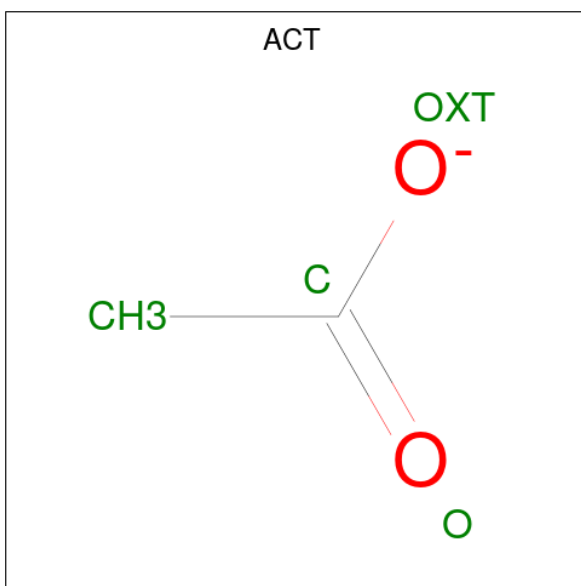
Chain	Residue	Modelled	Actual	Comment	Reference
A	316	HIS	-	expression tag	UNP P23360
B	1	GLU	GLN	engineered mutation	UNP P23360
B	42	MET	GLN	engineered mutation	UNP P23360
B	44	TRP	THR	engineered mutation	UNP P23360
B	81	GLY	ARG	engineered mutation	UNP P23360
B	83	GLY	HIS	engineered mutation	UNP P23360
B	84	MET	THR	engineered mutation	UNP P23360
B	130	GLY	ASN	engineered mutation	UNP P23360
B	172	MET	ASN	engineered mutation	UNP P23360
B	234	SER	ALA	engineered mutation	UNP P23360
B	236	LEU	THR	engineered mutation	UNP P23360
B	237	MET	GLU	engineered mutation	UNP P23360
B	265	SER	THR	engineered mutation	UNP P23360
B	267	PHE	TRP	engineered mutation	UNP P23360
B	304	GLY	-	expression tag	UNP P23360
B	305	SER	-	expression tag	UNP P23360
B	306	ILE	-	expression tag	UNP P23360
B	307	GLU	-	expression tag	UNP P23360
B	308	GLY	-	expression tag	UNP P23360
B	309	ARG	-	expression tag	UNP P23360
B	310	GLY	-	expression tag	UNP P23360
B	311	HIS	-	expression tag	UNP P23360
B	312	HIS	-	expression tag	UNP P23360
B	313	HIS	-	expression tag	UNP P23360
B	314	HIS	-	expression tag	UNP P23360
B	315	HIS	-	expression tag	UNP P23360
B	316	HIS	-	expression tag	UNP P23360

- Molecule 2 is 5-nitro-1H-benzotriazole (three-letter code: 3NY) (formula: C<sub>6</sub>H<sub>4</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			24	12	8	4		
2	B	1	Total	C	N	O	0	1
			12	6	4	2		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).




Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	401	Total	O	0	20
			421	421		
5	B	269	Total	O	0	25
			295	295		

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.

- Chain A:  82% 13% 5%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.77Å 78.05Å 98.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.08 – 1.23 34.08 – 1.23	Depositor EDS
% Data completeness (in resolution range)	98.6 (34.08-1.23) 98.6 (34.08-1.23)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 1.23Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.157 , 0.196 0.159 , 0.202	Depositor DCC
$R_{free}$ test set	8337 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.0	Xtriage
Anisotropy	1.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6443	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: 3NY, ACT, SO4

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	1.37	10/2551 (0.4%)	1.24	12/3478 (0.3%)
1	B	1.22	7/3365 (0.2%)	1.15	18/4594 (0.4%)
All	All	1.29	17/5916 (0.3%)	1.19	30/8072 (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	B	0	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	276	ARG	CB-CG	-8.21	1.30	1.52
1	A	248	TYR	CE1-CZ	-6.93	1.29	1.38
1	B	63	PHE	CD2-CE2	6.42	1.52	1.39
1	A	124	ARG	CZ-NH1	6.38	1.41	1.33
1	A	192	LYS	CB-CG	-6.16	1.35	1.52
1	A	158	GLN	CG-CD	5.92	1.64	1.51
1	A	183	LYS	CD-CE	-5.90	1.36	1.51
1	A	276	ARG	CB-CG	-5.78	1.36	1.52
1	A	83	GLY	C-O	5.73	1.32	1.23
1	B	110	ASN	CB-CG	5.55	1.63	1.51
1	A	166	ASN	CG-OD1	5.45	1.35	1.24
1	B	44	TRP	CB-CG	5.45	1.60	1.50
1	B	101	LYS	CB-CG	-5.22	1.38	1.52
1	B	3	ALA	C-O	5.19	1.33	1.23
1	A	59	GLY	N-CA	-5.16	1.38	1.46
1	A	26	ARG	CG-CD	-5.10	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	GLY	C-O	5.06	1.31	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	A	236[A]	LEU	CB-CG-CD1	8.86	126.06	111.00
1	A	236[B]	LEU	CB-CG-CD1	8.86	126.06	111.00
1	B	170[A]	TYR	CB-CA-C	-8.60	93.20	110.40
1	B	170[B]	TYR	CB-CA-C	-8.60	93.20	110.40
1	B	161	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	A	170	TYR	CB-CG-CD1	7.33	125.40	121.00
1	B	164	ASP	CB-CG-OD1	6.85	124.46	118.30
1	A	52	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	A	118	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	124	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	161	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	52[A]	ASP	CB-CG-OD2	6.06	123.75	118.30
1	B	52[B]	ASP	CB-CG-OD2	6.06	123.75	118.30
1	B	271	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	A	170	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	A	4	GLN	CA-CB-CG	5.61	125.75	113.40
1	A	151	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	136[A]	ASP	CB-CG-OD2	5.44	123.19	118.30
1	B	136[B]	ASP	CB-CG-OD2	5.44	123.19	118.30
1	B	206	SER	O-C-N	5.41	131.36	122.70
1	B	136[A]	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	B	136[B]	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	B	150[A]	GLU	CB-CA-C	-5.34	99.72	110.40
1	B	150[B]	GLU	CB-CA-C	-5.34	99.72	110.40
1	A	124	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	170[A]	TYR	N-CA-C	5.14	124.89	111.00
1	B	170[B]	TYR	N-CA-C	5.14	124.89	111.00
1	B	276	ARG	CA-CB-CG	5.05	124.51	113.40
1	A	276	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	111	HIS	Mainchain
1	B	170[B]	TYR	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	A	2427	0	2369	46	0
1	B	3238	0	3143	160	0
2	A	24	0	8	5	0
2	B	12	0	4	3	0
3	A	12	0	9	2	0
3	B	4	0	3	4	0
4	A	10	0	0	0	0
5	A	421	0	0	14	0
5	B	295	0	0	31	0
All	All	6443	0	5536	207	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 18.

All (207) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236[B]:LEU:HD21	2:A:317[B]:3NY:N3	1.26	1.41
1:A:236[B]:LEU:CD2	2:A:317[B]:3NY:N3	1.93	1.31
1:B:179[B]:ALA:HA	1:B:224[B]:LEU:CD2	1.67	1.25
1:B:204[B]:ILE:HG13	1:B:230[B]:THR:HG21	1.24	1.15
1:A:236[B]:LEU:HD22	2:A:317[B]:3NY:N2	1.64	1.09
1:B:179[B]:ALA:HB1	1:B:224[B]:LEU:HD22	1.37	1.05
1:B:179[B]:ALA:HA	1:B:224[B]:LEU:HD23	1.06	1.05
1:B:179[B]:ALA:CA	1:B:224[B]:LEU:CD2	2.35	1.05
1:B:179[B]:ALA:CB	1:B:224[B]:LEU:HD22	1.87	1.04
1:B:188[A]:VAL:HG12	1:B:225[A]:LEU:HD23	1.41	1.03
1:B:212[B]:ALA:HB2	5:B:728[B]:HOH:O	1.59	0.99
1:B:220[B]:GLN:OE1	5:B:355:HOH:O	1.79	0.99
1:B:106[B]:ASN:O	5:B:341:HOH:O	1.81	0.98
1:B:110:ASN:HB2	5:B:341:HOH:O	1.63	0.96
1:B:214[A]:GLN:O	5:B:352[A]:HOH:O	1.82	0.95
1:B:195[A]:ARG:HD2	1:B:230[A]:THR:HG22	1.49	0.95
1:A:69[B]:LEU:CD2	1:A:80[B]:ILE:CD1	2.47	0.93
1:B:177[B]:ASP:OD1	5:B:350[B]:HOH:O	1.87	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69[B]:LEU:HD21	1:A:80[B]:ILE:CD1	2.02	0.89
1:A:236[B]:LEU:CD2	2:A:317[B]:3NY:N2	2.28	0.89
1:B:179[B]:ALA:CA	1:B:224[B]:LEU:HD22	1.98	0.88
1:B:177[A]:ASP:CG	1:B:210[A]:LEU:CD2	2.43	0.87
1:B:155[B]:ILE:HD13	1:B:158[B]:GLN:NE2	1.91	0.86
1:B:184[B]:THR:O	1:B:188[B]:VAL:HG12	1.76	0.86
1:A:91[B]:LEU:N	5:A:459:HOH:O	2.10	0.83
1:B:195[A]:ARG:HD2	1:B:230[A]:THR:CG2	2.10	0.81
1:A:90[B]:GLN:HA	5:A:857:HOH:O	1.80	0.81
1:A:69[B]:LEU:CD2	1:A:80[B]:ILE:HD11	2.11	0.80
1:B:177[A]:ASP:CG	1:B:210[A]:LEU:HD21	2.03	0.79
1:B:188[B]:VAL:HG23	1:B:228[B]:ALA:HA	1.65	0.78
1:B:211[B]:SER:HB3	5:B:592:HOH:O	1.82	0.78
1:B:176[B]:LEU:HB3	1:B:225[B]:LEU:HD21	1.65	0.78
1:B:155[B]:ILE:HD13	1:B:158[B]:GLN:HE21	1.47	0.77
1:B:201[A]:ILE:O	1:B:230[A]:THR:HG22	1.84	0.77
1:B:177[A]:ASP:OD1	1:B:210[A]:LEU:HD21	1.84	0.76
1:B:177[B]:ASP:O	1:B:221[B]:ALA:HB2	1.86	0.75
1:B:203[A]:GLY:HA2	1:B:232[A]:GLU:O	1.86	0.75
1:A:3:ALA:CB	1:A:302[B]:GLN:NE2	2.50	0.75
1:B:231[B]:PRO:O	1:B:260[B]:SER:HB2	1.88	0.74
1:B:188[B]:VAL:HB	1:B:228[B]:ALA:HB2	1.68	0.74
1:B:116[B]:MET:CE	1:B:164:ASP:HB3	2.18	0.73
1:B:148:ILE:HG21	1:B:152[B]:TYR:HB3	1.68	0.73
1:B:204[B]:ILE:HG13	1:B:230[B]:THR:CG2	2.13	0.73
1:B:52[B]:ASP:OD2	5:B:504:HOH:O	2.05	0.73
1:A:3:ALA:CB	1:A:302[B]:GLN:HE21	2.02	0.72
1:B:188[A]:VAL:HG11	1:B:224[A]:LEU:HG	1.69	0.72
1:B:195[A]:ARG:CZ	1:B:230[A]:THR:HA	2.19	0.72
1:A:69[B]:LEU:HD23	1:A:80[B]:ILE:HD13	1.71	0.72
1:A:90[B]:GLN:CA	5:A:857:HOH:O	2.37	0.71
1:B:177[B]:ASP:O	1:B:221[B]:ALA:CB	2.40	0.70
1:B:212[B]:ALA:HA	5:B:444[B]:HOH:O	1.91	0.69
1:A:3:ALA:HB1	1:A:302[B]:GLN:NE2	2.06	0.69
1:A:236[B]:LEU:CD1	1:A:237:MET:HG3	2.22	0.69
1:B:230[B]:THR:O	5:B:450:HOH:O	2.09	0.69
1:A:21:ALA:HB3	1:A:267[B]:PHE:O	1.93	0.68
1:A:236[B]:LEU:HD13	1:A:237:MET:HG3	1.76	0.68
1:A:69[B]:LEU:CD2	1:A:80[B]:ILE:HD13	2.20	0.68
1:B:194[A]:TRP:CD1	5:B:543:HOH:O	2.46	0.67
1:B:185[B]:GLN:HA	1:B:188[B]:VAL:HG13	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232[B]:GLU:HA	1:B:260[B]:SER:O	1.94	0.67
1:B:184[B]:THR:HG23	1:B:225[B]:LEU:CD2	2.25	0.66
1:B:184[B]:THR:O	1:B:188[B]:VAL:CG1	2.44	0.66
1:B:204[A]:ILE:HG21	1:B:225[A]:LEU:HD13	1.77	0.66
1:B:174[A]:TYR:HA	1:B:207[A]:GLN:O	1.95	0.66
1:B:155[B]:ILE:CD1	1:B:158[B]:GLN:NE2	2.59	0.65
1:A:110[A]:ASN:OD1	5:A:560:HOH:O	2.14	0.65
1:B:177[A]:ASP:CG	1:B:210[A]:LEU:HD23	2.18	0.64
1:B:204[A]:ILE:CG2	1:B:225[A]:LEU:HD13	2.27	0.64
1:A:90[B]:GLN:N	5:A:857:HOH:O	2.30	0.63
1:B:109[B]:LYS:HB3	5:B:617:HOH:O	1.99	0.63
3:A:320:ACT:CH3	5:A:379:HOH:O	2.48	0.62
1:B:84:MET:HE1	1:B:172[A]:MET:CE	2.30	0.62
1:B:135[B]:GLU:HB3	1:B:181[B]:TYR:OH	1.99	0.62
1:A:236[B]:LEU:HD13	1:A:236[B]:LEU:C	2.20	0.62
1:B:172[A]:MET:CE	1:B:207[A]:GLN:NE2	2.63	0.62
1:A:87:TRP:CE2	1:A:89[B]:SER:HB2	2.36	0.60
1:B:116[B]:MET:HE2	1:B:164:ASP:HB3	1.82	0.60
1:A:4:GLN:HB2	5:A:869:HOH:O	2.01	0.60
1:B:116[B]:MET:O	1:B:120:LYS:N	2.34	0.60
1:A:74:GLN:HE22	1:A:122:LYS:HD3	1.65	0.60
1:A:4:GLN:CG	5:A:709:HOH:O	2.49	0.60
1:B:184[B]:THR:HG23	1:B:225[B]:LEU:HD21	1.83	0.59
1:B:148:ILE:CG2	1:B:152[B]:TYR:HB3	2.31	0.59
1:A:50:LYS:NZ	1:A:90[A]:GLN:HE22	1.99	0.59
1:B:195[A]:ARG:NH2	1:B:229[A]:GLY:O	2.36	0.59
1:B:179[B]:ALA:CB	1:B:224[B]:LEU:CD2	2.69	0.59
1:B:240[B]:VAL:HG12	5:B:444[B]:HOH:O	2.03	0.58
1:B:191[A]:VAL:HG12	1:B:228[A]:ALA:HB1	1.87	0.57
1:B:155[B]:ILE:CD1	1:B:158[B]:GLN:HE21	2.14	0.57
1:B:84:MET:CE	1:B:172[B]:MET:SD	2.93	0.57
1:B:175[A]:ASN:N	5:B:349[A]:HOH:O	2.10	0.57
1:B:252[A]:VAL:HA	1:B:264[A]:ILE:HD11	1.85	0.56
1:B:116[B]:MET:HE1	1:B:164:ASP:HB3	1.86	0.56
1:B:85:LEU:HD12	1:B:128[B]:VAL:HA	1.87	0.56
1:B:44:TRP:HH2	3:B:318:ACT:H3	1.71	0.56
1:B:44:TRP:CH2	3:B:318:ACT:H3	2.40	0.56
1:B:209[B]:HIS:CD2	1:B:275:TRP:HZ2	2.24	0.56
1:B:108[B]:MET:C	1:B:110:ASN:N	2.48	0.55
1:A:69[B]:LEU:HD23	1:A:80[B]:ILE:CD1	2.28	0.55
1:B:52[B]:ASP:CG	5:B:504:HOH:O	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211[B]:SER:CB	5:B:592:HOH:O	2.48	0.55
1:B:84:MET:HE1	1:B:172[A]:MET:HE2	1.89	0.54
1:B:204[A]:ILE:HD13	1:B:225[A]:LEU:HD22	1.89	0.54
1:A:4:GLN:HG3	5:A:709:HOH:O	2.06	0.54
1:B:252[A]:VAL:HG22	1:B:264[A]:ILE:HD13	1.90	0.54
1:B:107[B]:VAL:HG13	5:B:392:HOH:O	2.09	0.53
1:B:107[B]:VAL:O	1:B:110:ASN:HB3	2.09	0.53
1:B:128[B]:VAL:HG21	1:B:169:LEU:HD22	1.89	0.53
1:B:184[B]:THR:HG23	1:B:225[B]:LEU:HD23	1.91	0.53
1:B:87:TRP:HE1	1:B:131[B]:GLU:CD	2.12	0.53
1:B:108[B]:MET:O	1:B:109[B]:LYS:C	2.43	0.53
1:B:248[B]:TYR:CD1	1:B:283:LEU:HD21	2.44	0.53
1:B:236[B]:LEU:HD12	1:B:237[B]:MET:HG3	1.89	0.53
1:B:280[B]:THR:O	1:B:291:LYS:NZ	2.42	0.53
1:B:87:TRP:CZ2	1:B:89:SER:HB2	2.44	0.52
1:B:185[B]:GLN:HA	1:B:188[B]:VAL:CG1	2.40	0.52
1:A:90[B]:GLN:OE1	5:A:833:HOH:O	2.19	0.51
1:B:21:ALA:HB3	1:B:267[B]:PHE:O	2.10	0.51
1:B:107[B]:VAL:HG22	5:B:369:HOH:O	2.11	0.51
1:B:172[A]:MET:C	1:B:172[A]:MET:SD	2.89	0.51
1:B:4:GLN:OE1	1:B:302:GLN:NE2	2.44	0.50
1:B:179[B]:ALA:O	1:B:224[B]:LEU:CD2	2.59	0.50
1:B:153[B]:ILE:HB	1:B:154[B]:PRO:HD3	1.92	0.50
1:B:159[B]:THR:O	1:B:163:ALA:N	2.44	0.50
1:B:201[A]:ILE:O	1:B:230[A]:THR:CG2	2.56	0.50
1:B:87:TRP:CE2	1:B:89:SER:HB2	2.47	0.50
1:A:127:ASP:OD2	2:A:317[A]:3NY:N3	2.44	0.49
1:A:236[B]:LEU:HD11	1:A:237:MET:HG3	1.92	0.49
1:B:225[B]:LEU:HD12	5:B:438:HOH:O	2.10	0.49
1:B:185[B]:GLN:CA	1:B:188[B]:VAL:HG13	2.40	0.49
1:B:248[B]:TYR:CE1	1:B:283:LEU:HD21	2.47	0.49
1:A:90[B]:GLN:CA	5:A:459:HOH:O	2.60	0.49
1:B:177[B]:ASP:C	1:B:221[B]:ALA:CB	2.81	0.49
1:B:236[A]:LEU:HD11	2:B:317[A]:3NY:H4	1.95	0.49
1:B:177[A]:ASP:HB2	5:B:531:HOH:O	2.13	0.49
1:B:177[A]:ASP:CB	1:B:210[A]:LEU:CD2	2.90	0.48
1:B:212[B]:ALA:CB	5:B:728[B]:HOH:O	2.36	0.48
1:A:90[B]:GLN:N	5:A:459:HOH:O	2.46	0.48
1:B:140[B]:ARG:HG2	1:B:142:THR:HG23	1.95	0.48
1:B:173[A]:ASP:O	1:B:207[A]:GLN:N	2.47	0.48
1:B:172[A]:MET:HE1	1:B:207[A]:GLN:NE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ASP:OD1	3:B:318:ACT:OXT	2.32	0.48
1:A:193[A]:GLN:NE2	5:A:858[A]:HOH:O	2.46	0.48
1:B:52[B]:ASP:OD2	1:B:90:GLN:HA	2.14	0.48
1:B:148:ILE:HG21	1:B:152[B]:TYR:CB	2.40	0.47
1:B:179[B]:ALA:O	1:B:224[B]:LEU:HD21	2.14	0.47
1:B:204[B]:ILE:CG1	1:B:230[B]:THR:HG21	2.17	0.47
1:B:214[A]:GLN:HB3	5:B:352[A]:HOH:O	2.13	0.47
1:A:87:TRP:CZ2	1:A:89[B]:SER:HB2	2.50	0.47
1:A:257:ASN:ND2	5:A:796:HOH:O	2.48	0.47
1:B:214[A]:GLN:CA	5:B:352[A]:HOH:O	2.62	0.47
1:B:236[A]:LEU:HD13	3:B:318:ACT:C	2.45	0.47
1:B:176[A]:LEU:HB2	5:B:350[A]:HOH:O	2.15	0.46
1:B:252[B]:VAL:HG21	1:B:297:ILE:HG12	1.97	0.46
1:B:116[B]:MET:O	1:B:120:LYS:CA	2.63	0.46
1:B:127:ASP:OD2	2:B:317[A]:3NY:N3	2.48	0.46
1:B:172[A]:MET:SD	1:B:207[A]:GLN:NE2	2.88	0.46
1:A:74:GLN:NE2	1:A:122:LYS:HD3	2.31	0.46
1:B:135[B]:GLU:OE2	1:B:181[B]:TYR:OH	2.25	0.46
1:A:203:GLY:HA2	1:A:232:GLU:O	2.16	0.45
1:B:219[A]:LEU:HD23	1:B:254:ALA:HA	1.98	0.45
1:B:222[B]:LEU:HD23	1:B:254:ALA:C	2.37	0.45
1:B:83:GLY:HA3	2:B:317[A]:3NY:N2	2.32	0.44
1:A:236[B]:LEU:HD13	1:A:237:MET:N	2.32	0.44
1:B:179[B]:ALA:C	1:B:224[B]:LEU:CD2	2.86	0.44
1:B:177[A]:ASP:OD1	1:B:210[A]:LEU:CD2	2.58	0.44
1:B:177[A]:ASP:OD1	1:B:208[A]:THR:HG23	2.16	0.44
1:B:217[B]:GLY:N	5:B:533:HOH:O	2.48	0.44
1:B:280[B]:THR:N	1:B:281[B]:PRO:HD3	2.32	0.44
1:B:202[B]:ASP:O	1:B:231[B]:PRO:HD2	2.18	0.43
1:B:279[A]:THR:O	1:B:280[A]:THR:C	2.57	0.43
1:A:236[B]:LEU:HD13	1:A:237:MET:CG	2.47	0.43
1:B:195[A]:ARG:NH1	1:B:230[A]:THR:HA	2.32	0.43
1:B:244:SER:HB3	5:B:444[A]:HOH:O	2.18	0.43
1:B:252[A]:VAL:HA	1:B:264[A]:ILE:CD1	2.47	0.43
1:B:287[A]:ASN:ND2	5:B:375:HOH:O	2.52	0.43
1:B:155[B]:ILE:HD13	1:B:155[B]:ILE:HA	1.68	0.43
1:A:50:LYS:HZ3	1:A:90[A]:GLN:HE22	1.66	0.43
1:B:195[A]:ARG:HD2	1:B:230[A]:THR:HG23	1.99	0.43
1:A:3:ALA:HB2	1:A:302[B]:GLN:NE2	2.34	0.42
1:B:128[B]:VAL:CG2	1:B:169:LEU:HD22	2.50	0.42
1:B:248[B]:TYR:CD2	1:B:293:ALA:HB1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279[B]:THR:HA	5:B:443[B]:HOH:O	2.18	0.42
1:B:176[A]:LEU:CB	5:B:350[A]:HOH:O	2.67	0.42
1:B:226[B]:ALA:HB2	1:B:258:VAL:HG11	2.01	0.42
1:B:207[A]:GLN:HG3	1:B:237[A]:MET:SD	2.60	0.42
1:B:230[B]:THR:N	5:B:396:HOH:O	2.25	0.42
1:A:50:LYS:HZ2	1:A:90[A]:GLN:HE22	1.65	0.42
1:B:20:VAL:HG11	1:B:36:ILE:HG12	2.02	0.42
1:B:54:THR:O	1:B:61:PHE:HA	2.21	0.41
1:B:185[B]:GLN:O	1:B:188[B]:VAL:HG13	2.20	0.41
1:B:170[B]:TYR:HA	1:B:203[B]:GLY:O	2.20	0.41
1:B:117[B]:THR:HA	1:B:120:LYS:HB2	2.02	0.41
1:A:56:PRO:HB2	3:A:319:ACT:H3	2.02	0.41
1:B:151[A]:ASP:O	1:B:155[A]:ILE:HG12	2.20	0.41
1:B:140[B]:ARG:O	1:B:145:LEU:HD22	2.21	0.41
1:B:222[B]:LEU:HB3	1:B:254:ALA:HB1	2.03	0.41
1:B:239[A]:ASP:HB2	1:B:281[A]:PRO:HB2	2.03	0.41
1:A:44:TRP:CE3	1:A:81:GLY:HA3	2.56	0.40
1:B:177[A]:ASP:HB3	1:B:210[A]:LEU:CD2	2.51	0.40
1:B:240[B]:VAL:CG1	5:B:444[B]:HOH:O	2.67	0.40
1:A:54:THR:O	1:A:61:PHE:HA	2.22	0.40
1:B:173[A]:ASP:O	1:B:207[A]:GLN:HB3	2.22	0.40
1:B:202[A]:ASP:O	1:B:230[A]:THR:HB	2.22	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	325/316 (103%)	321 (99%)	4 (1%)	0	100	100
1	B	435/316 (138%)	430 (99%)	3 (1%)	2 (0%)	25	6
All	All	760/632 (120%)	751 (99%)	7 (1%)	2 (0%)	44	13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	281[A]	PRO
1	B	281[B]	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/254 (105%)	259 (97%)	7 (3%)	41	7
1	B	352/254 (139%)	344 (98%)	8 (2%)	45	11
All	All	618/508 (122%)	603 (98%)	15 (2%)	48	10

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	18	PHE
1	A	172	MET
1	A	267[A]	PHE
1	A	267[B]	PHE
1	A	275[A]	TRP
1	A	275[B]	TRP
1	B	18	PHE
1	B	158[A]	GLN
1	B	158[B]	GLN
1	B	172[A]	MET
1	B	172[B]	MET
1	B	275	TRP
1	B	281[A]	PRO
1	B	281[B]	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	175	ASN
1	A	207	GLN
1	A	257	ASN
1	A	287	ASN
1	A	299	GLN
1	B	4	GLN
1	B	71	ASN
1	B	74	GLN
1	B	302	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](#)

9 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	$\# Z  > 2$
4	SO4	A	322	-	4,4,4	0.53	0	6,6,6	1.06	1 (16%)
4	SO4	A	321	-	4,4,4	0.46	0	6,6,6	0.65	0
3	ACT	B	318	-	3,3,3	0.93	0	3,3,3	0.80	0
3	ACT	A	318	-	3,3,3	0.82	0	3,3,3	1.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ACT	A	319	-	3,3,3	1.66	1 (33%)	3,3,3	0.80	0
2	3NY	A	317[B]	-	9,13,13	2.04	2 (22%)	10,18,18	4.27	4 (40%)
2	3NY	A	317[A]	-	9,13,13	1.33	1 (11%)	10,18,18	2.26	4 (40%)
3	ACT	A	320	-	3,3,3	0.66	0	3,3,3	3.46	2 (66%)
2	3NY	B	317[A]	-	9,13,13	1.58	1 (11%)	10,18,18	1.20	1 (10%)

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	3NY	A	317[A]	-	-	0/2/4/4	0/2/2/2
2	3NY	B	317[A]	-	-	0/2/4/4	0/2/2/2
2	3NY	A	317[B]	-	-	0/2/4/4	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	317[B]	3NY	C5-NO1	-4.47	1.34	1.45
2	B	317[A]	3NY	C5-NO1	-3.16	1.37	1.45
2	A	317[B]	3NY	C4-C3A	-3.15	1.37	1.41
2	A	317[A]	3NY	C4-C3A	-2.27	1.38	1.41
3	A	319	ACT	O-C	2.15	1.31	1.22

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	317[B]	3NY	C4-C5-NO1	-10.71	109.51	118.74
2	A	317[B]	3NY	C6-C5-NO1	6.98	125.44	119.34
3	A	320	ACT	OXT-C-CH3	4.61	134.37	115.05
2	A	317[A]	3NY	C4-C5-NO1	3.85	122.05	118.74
3	A	320	ACT	O-C-CH3	-3.69	107.39	122.53
2	A	317[A]	3NY	N3-N2-N1	-3.51	106.70	111.25
2	B	317[A]	3NY	C6-C7-C7A	-3.23	116.94	120.80
2	A	317[A]	3NY	C5-C4-C3A	3.20	121.72	118.21
2	A	317[A]	3NY	C7-C7A-N1	3.19	135.38	130.19
2	A	317[B]	3NY	C6-C5-C4	2.91	125.05	120.53
2	A	317[B]	3NY	C7-C6-C5	-2.29	116.53	120.02
4	A	322	SO4	O4-S-O2	2.20	121.08	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	318	ACT	4	0
3	A	319	ACT	1	0
2	A	317[B]	3NY	4	0
2	A	317[A]	3NY	1	0
3	A	320	ACT	1	0
2	B	317[A]	3NY	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	304/316 (96%)	-0.19	3 (0%) 79 78	6, 13, 21, 32	25 (8%)
1	B	301/316 (95%)	0.41	19 (6%) 27 25	5, 12, 27, 31	141 (46%)
All	All	605/632 (95%)	0.11	22 (3%) 46 45	5, 13, 24, 32	166 (27%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	4.9
1	A	304	GLY	4.2
1	B	83	GLY	4.0
1	B	149[A]	GLY	3.9
1	B	181[A]	TYR	3.6
1	B	150[A]	GLU	3.6
1	A	3	ALA	3.4
1	B	89	SER	3.2
1	B	145	LEU	3.1
1	B	148	ILE	3.0
1	B	275	TRP	3.0
1	B	166	ASN	2.8
1	B	197[A]	ALA	2.5
1	B	101	LYS	2.5
1	B	102	ASN	2.4
1	B	3	ALA	2.4
1	B	179[A]	ALA	2.4
1	B	87	TRP	2.3
1	B	199[A]	VAL	2.3
1	B	91	LEU	2.2
1	B	141	GLN	2.2
1	B	98	ILE	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 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
2	3NY	A	317[A]	12/12	0.91	0.10	16,21,25,26	12
2	3NY	A	317[B]	12/12	0.91	0.10	18,20,25,27	12
2	3NY	B	317[A]	12/12	0.91	0.09	22,24,29,29	12
3	ACT	A	320	4/4	0.91	0.12	25,29,31,33	2
3	ACT	A	319	4/4	0.92	0.08	23,27,28,28	0
4	SO4	A	322	5/5	0.95	0.09	29,29,35,35	2
4	SO4	A	321	5/5	0.96	0.08	26,30,36,40	3
3	ACT	B	318	4/4	0.96	0.07	25,25,26,26	0
3	ACT	A	318	4/4	0.98	0.08	15,15,16,19	2

## 6.5 Other polymers [i](#)

There are no such residues in this entry.