



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 04:06 am GMT

PDB ID : 2IU0  
Title : crystal structures of transition state analogue inhibitors of inosine monophosphate cyclohydrolase  
Authors : Xu, L.; Chong, Y.; Hwang, I.; Onofrio, A.D.; Amore, K.; Beardsley, G.P.; Li, C.; Olson, A.J.; Boger, D.L.; Wilson, I.A.  
Deposited on : 2006-05-26  
Resolution : 2.53 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

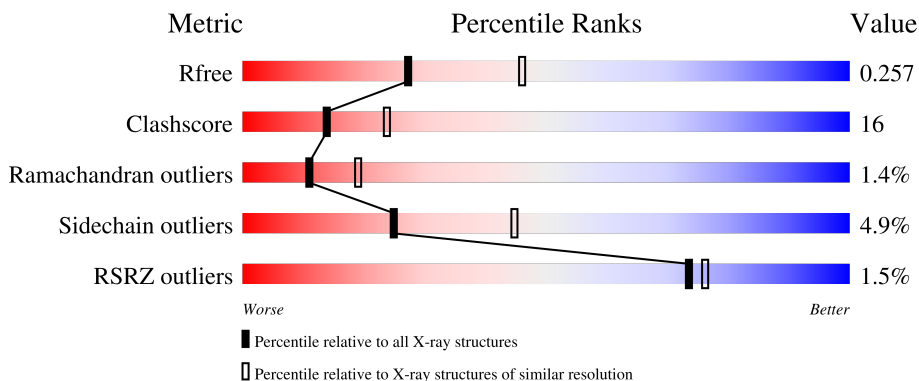
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	593	 2% (red), 66% (green), 31% (yellow), .. (grey)
1	B	593	 % (red), 66% (green), 32% (yellow), .. (grey)

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9289 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.

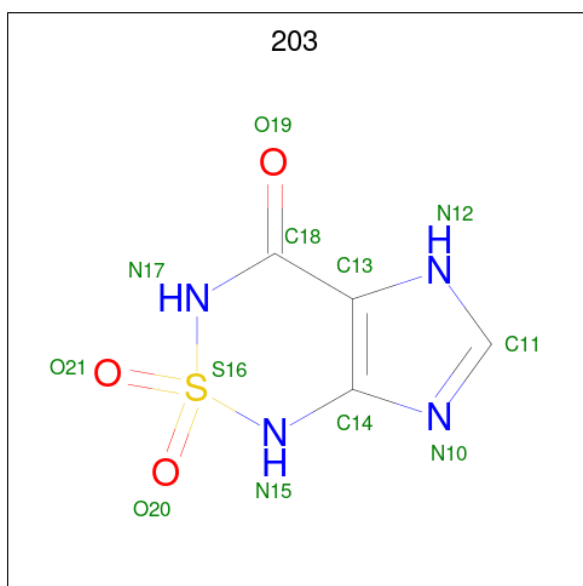
- Molecule 1 is a protein called BIFUNCTIONAL PURINE BIOSYNTHESIS PROTEIN PURH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	590	Total 4511	C 2843	N 800	O 849	S 19	0	0	0
1	B	590	Total 4511	C 2843	N 800	O 849	S 19	0	0	0

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total 1 K 1	0	0
2	B	1	Total 1 K 1	0	0

- Molecule 3 is 1,5-DIHYDROIMIDAZO[4,5-C][1,2,6]THIADIAZIN-4(3H)-ONE 2,2-DIOXIDE (three-letter code: 203) (formula: C<sub>4</sub>H<sub>4</sub>N<sub>4</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	B	1	12	4	4	3	1	0	0

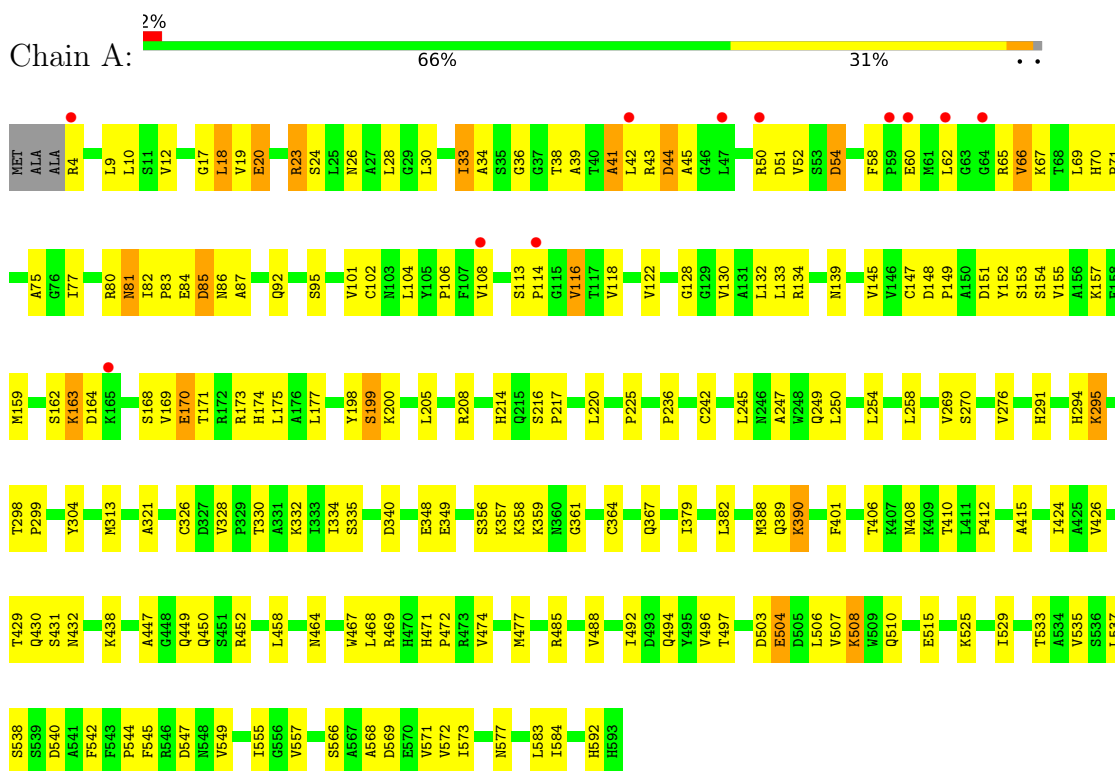
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	138	Total 138	O 138	0	0
4	B	115	Total 115	O 115	0	0

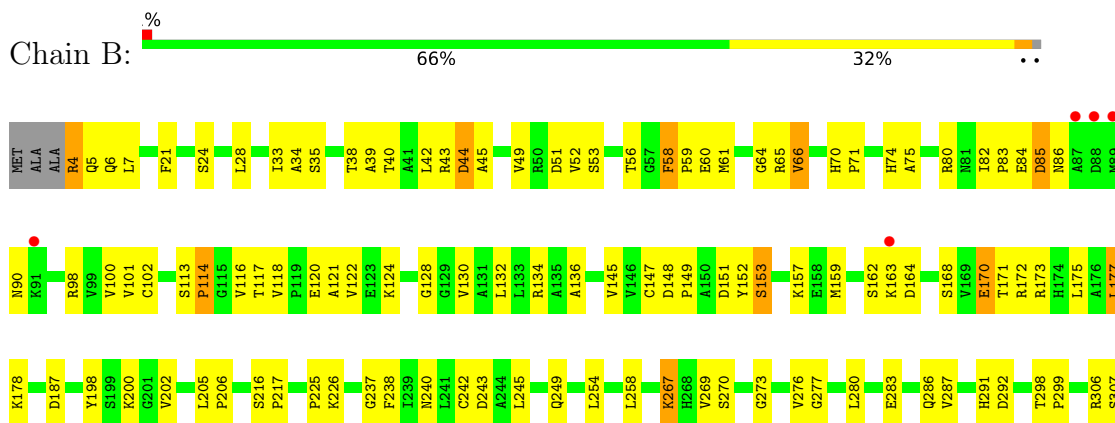
### 3 Residue-property plots [i](#)

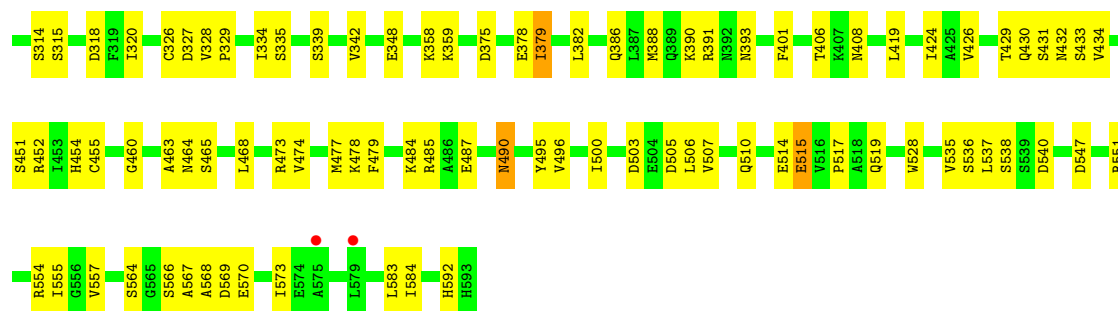
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: BIFUNCTIONAL PURINE BIOSYNTHESIS PROTEIN PURH



- Molecule 1: BIFUNCTIONAL PURINE BIOSYNTHESIS PROTEIN PURH





## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	387.00Å 57.00Å 62.10Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	38.23 – 2.53 38.23 – 2.43	Depositor EDS
% Data completeness (in resolution range)	93.5 (38.23-2.53) 90.5 (38.23-2.43)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.42Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.209 , 0.261 0.207 , 0.257	Depositor DCC
$R_{free}$ test set	1840 reflections (3.70%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.5	Xtrriage
Anisotropy	0.483	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.026 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9289	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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: 203, K

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	0.45	0/4595	0.67	0/6230
1	B	0.46	0/4595	0.66	0/6230
All	All	0.46	0/9190	0.66	0/12460

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	304	TYR	Sidechain

### 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	A	4511	0	4560	165	0
1	B	4511	0	4560	144	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	12	0	4	0	0
4	A	138	0	0	3	0
4	B	115	0	0	3	0
All	All	9289	0	9124	287	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 16.

All (287) 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:408:ASN:HB2	4:B:2078:HOH:O	1.75	0.85
1:B:254:LEU:HD23	1:B:424:ILE:HD12	1.61	0.81
1:B:569:ASP:O	1:B:573:ILE:HG13	1.81	0.79
1:A:379:ILE:HG12	1:A:388:MET:HG3	1.66	0.78
1:A:367:GLN:HG2	4:A:2067:HOH:O	1.83	0.77
1:A:154:SER:HA	1:A:157:LYS:HE2	1.67	0.77
1:A:4:ARG:HE	1:A:95:SER:HA	1.50	0.76
1:A:408:ASN:HD21	1:A:577:ASN:HA	1.50	0.76
1:B:153:SER:O	1:B:157:LYS:HD3	1.86	0.74
1:A:525:LYS:O	1:A:529:ILE:HG12	1.87	0.74
1:A:34:ALA:O	1:A:51:ASP:HA	1.88	0.74
1:A:464:ASN:ND2	1:A:555:ILE:HD13	2.04	0.71
1:A:464:ASN:HD22	1:A:555:ILE:HD13	1.55	0.70
1:B:432:ASN:HB2	1:B:452:ARG:NH2	2.07	0.70
1:B:53:SER:HB2	1:B:60:GLU:OE2	1.92	0.69
1:B:6:GLN:OE1	1:B:98:ARG:HB2	1.93	0.69
1:B:170:GLU:CD	1:B:170:GLU:H	1.95	0.68
1:B:503:ASP:O	1:B:507:VAL:HG23	1.93	0.68
1:B:464:ASN:ND2	1:B:555:ILE:HD13	2.08	0.67
1:A:198:TYR:CD1	1:B:173:ARG:HD3	2.29	0.67
1:A:450:GLN:HB2	1:B:314:SER:HB2	1.76	0.67
1:A:537:LEU:HD23	1:A:538:SER:N	2.08	0.67
1:A:92:GLN:NE2	1:B:59:PRO:HG3	2.10	0.66
1:B:468:LEU:HD23	1:B:528:TRP:CD1	2.31	0.66
1:B:298:THR:HG23	1:B:329:PRO:HG3	1.76	0.66
1:B:43:ARG:HB3	1:B:49:VAL:CG1	2.25	0.65
1:A:12:VAL:HG21	1:A:18:LEU:HD22	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:SER:O	1:A:28:LEU:HB2	1.96	0.65
1:A:401:PHE:HB3	1:A:584:ILE:HD13	1.79	0.65
1:A:198:TYR:CE1	1:B:173:ARG:HD3	2.31	0.65
1:A:468:LEU:HG	1:A:529:ILE:HD11	1.78	0.65
1:B:40:THR:O	1:B:44:ASP:HB2	1.97	0.64
1:A:438:LYS:HE2	1:A:533:THR:O	1.97	0.64
1:A:20:GLU:O	1:A:23:ARG:HB2	1.98	0.63
1:B:490:ASN:N	1:B:490:ASN:HD22	1.94	0.63
1:B:431:SER:HB3	1:B:432:ASN:HA	1.81	0.62
1:B:495:TYR:CE1	1:B:519:GLN:HA	2.34	0.62
1:A:170:GLU:H	1:A:170:GLU:CD	2.03	0.62
1:A:254:LEU:HD23	1:A:424:ILE:HD12	1.80	0.62
1:A:65:ARG:NH1	1:B:80:ARG:CZ	2.62	0.62
1:B:506:LEU:O	1:B:510:GLN:HG3	1.99	0.62
1:B:120:GLU:O	1:B:124:LYS:HG2	2.00	0.62
1:A:168:SER:HB2	1:A:170:GLU:OE1	2.00	0.61
1:A:406:THR:HG23	1:A:583:LEU:HB3	1.82	0.61
1:B:280:LEU:HD21	1:B:306:ARG:HG3	1.82	0.61
1:A:569:ASP:O	1:A:573:ILE:HG13	2.00	0.61
1:A:26:ASN:HA	1:A:30:LEU:O	2.01	0.61
1:B:118:VAL:O	1:B:122:VAL:HG23	2.01	0.61
1:A:171:THR:O	1:A:175:LEU:HD23	2.02	0.60
1:B:327:ASP:OD1	1:B:329:PRO:HG2	2.02	0.60
1:B:566:SER:C	1:B:568:ALA:H	2.04	0.60
1:A:65:ARG:HH12	1:B:80:ARG:CZ	2.14	0.60
1:A:154:SER:HA	1:A:157:LYS:CE	2.31	0.60
1:B:245:LEU:O	1:B:249:GLN:HG3	2.02	0.60
1:B:24:SER:O	1:B:28:LEU:HG	2.02	0.59
1:B:318:ASP:OD1	1:B:339:SER:HB3	2.01	0.59
1:B:391:ARG:HH11	1:B:393:ASN:ND2	2.01	0.59
1:A:102:CYS:O	1:A:147:CYS:HA	2.02	0.59
1:B:474:VAL:HA	1:B:477:MET:HG3	1.83	0.59
1:A:4:ARG:NE	1:A:95:SER:HA	2.16	0.59
1:A:245:LEU:O	1:A:249:GLN:HG3	2.03	0.59
1:A:295:LYS:HE3	1:A:295:LYS:H	1.68	0.59
1:A:506:LEU:O	1:A:510:GLN:HG3	2.03	0.59
1:A:43:ARG:HG3	1:A:44:ASP:OD1	2.03	0.59
1:B:145:VAL:O	1:B:175:LEU:HD12	2.03	0.58
1:A:432:ASN:OD1	1:A:449:GLN:HB2	2.03	0.58
1:B:537:LEU:HD23	1:B:538:SER:N	2.18	0.58
1:B:320:ILE:O	1:B:342:VAL:HA	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:SER:O	1:A:361:GLY:HA2	2.04	0.58
1:A:379:ILE:CG1	1:A:388:MET:HG3	2.34	0.57
1:A:545:PHE:HB2	1:A:547:ASP:OD1	2.05	0.57
1:A:118:VAL:O	1:A:122:VAL:HG23	2.04	0.57
1:A:330:THR:O	1:A:334:ILE:HG13	2.04	0.57
1:A:474:VAL:O	1:A:477:MET:HG3	2.04	0.57
1:B:426:VAL:CG1	1:B:540:ASP:HB3	2.35	0.57
1:B:171:THR:HG22	1:B:175:LEU:HD23	1.86	0.57
1:A:535:VAL:HB	1:A:557:VAL:HA	1.85	0.57
1:A:10:LEU:HD12	1:A:10:LEU:O	2.04	0.57
1:A:33:ILE:HD11	1:A:52:VAL:HA	1.87	0.57
1:A:168:SER:OG	1:A:170:GLU:HG2	2.05	0.56
1:B:390:LYS:HD3	1:B:391:ARG:O	2.05	0.56
1:A:145:VAL:O	1:A:175:LEU:HD12	2.04	0.56
1:B:66:VAL:HG12	1:B:66:VAL:O	2.04	0.56
1:B:485:ARG:HG3	1:B:485:ARG:HH11	1.70	0.56
1:A:66:VAL:HG12	1:A:66:VAL:O	2.06	0.56
1:A:113:SER:O	1:A:116:VAL:HG12	2.06	0.56
1:A:485:ARG:C	1:A:488:VAL:HG12	2.26	0.56
1:B:35:SER:HB2	1:B:52:VAL:HG23	1.88	0.56
1:A:39:ALA:O	1:A:41:ALA:N	2.39	0.55
1:A:10:LEU:HD11	1:A:42:LEU:HD11	1.89	0.55
1:A:225:PRO:HG3	1:B:178:LYS:HE3	1.88	0.55
1:A:326:CYS:O	1:A:348:GLU:HG3	2.07	0.55
1:B:473:ARG:HD2	1:B:495:TYR:OH	2.07	0.55
1:A:149:PRO:HA	1:A:152:TYR:CE2	2.41	0.55
1:A:62:LEU:HD22	1:B:85:ASP:CG	2.27	0.55
1:A:555:ILE:HG13	1:A:555:ILE:O	2.07	0.55
1:A:485:ARG:HA	1:A:488:VAL:HG12	1.88	0.54
1:B:168:SER:HB2	1:B:170:GLU:OE1	2.07	0.54
1:A:130:VAL:O	1:A:134:ARG:HG3	2.08	0.54
1:A:163:LYS:H	1:A:163:LYS:HD3	1.72	0.54
1:A:335:SER:HA	1:A:358:LYS:HD2	1.89	0.54
1:A:389:GLN:HB3	1:B:238:PHE:CE2	2.42	0.54
1:A:382:LEU:HD21	1:B:242:CYS:HA	1.88	0.54
1:B:102:CYS:O	1:B:147:CYS:HA	2.08	0.54
1:B:515:GLU:HG3	1:B:515:GLU:O	2.07	0.54
1:B:335:SER:HA	1:B:358:LYS:HD2	1.90	0.54
1:B:555:ILE:O	1:B:555:ILE:HG13	2.07	0.53
1:A:12:VAL:HG22	1:A:38:THR:HG23	1.89	0.53
1:A:426:VAL:CG1	1:A:540:ASP:HB3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:SER:O	1:B:116:VAL:HG12	2.08	0.53
1:B:149:PRO:HA	1:B:152:TYR:CE2	2.43	0.53
1:A:408:ASN:ND2	1:A:577:ASN:HA	2.20	0.53
1:B:258:LEU:HD12	1:B:276:VAL:HG11	1.90	0.53
1:B:334:ILE:O	1:B:358:LYS:HE2	2.09	0.53
1:B:159:MET:O	1:B:162:SER:HB3	2.09	0.52
1:B:468:LEU:HD23	1:B:528:TRP:HD1	1.73	0.52
1:B:359:LYS:O	1:B:359:LYS:HG2	2.09	0.52
1:A:450:GLN:O	1:B:267:LYS:HE2	2.10	0.52
1:A:20:GLU:OE2	1:A:23:ARG:HG3	2.09	0.52
1:B:429:THR:O	1:B:592:HIS:HB3	2.10	0.52
1:A:43:ARG:C	1:A:45:ALA:H	2.13	0.52
1:A:503:ASP:O	1:A:507:VAL:HG23	2.09	0.52
1:A:199:SER:HB2	1:B:177:LEU:CD1	2.40	0.52
1:A:568:ALA:HB1	1:A:571:VAL:HG22	1.92	0.51
1:B:43:ARG:HG3	1:B:44:ASP:OD1	2.09	0.51
1:A:92:GLN:HE22	1:B:59:PRO:HG3	1.76	0.51
1:A:431:SER:HB3	1:A:432:ASN:HA	1.93	0.51
1:A:65:ARG:O	1:A:67:LYS:N	2.43	0.51
1:A:568:ALA:O	1:A:572:VAL:HG23	2.10	0.51
1:A:429:THR:HG22	1:A:430:GLN:N	2.25	0.51
1:A:328:VAL:CG1	1:A:332:LYS:HE3	2.41	0.51
1:A:359:LYS:O	1:A:359:LYS:HG2	2.11	0.51
1:A:10:LEU:HB3	1:A:101:VAL:HB	1.93	0.50
1:A:12:VAL:CG2	1:A:18:LEU:HD22	2.42	0.50
1:B:406:THR:HG23	1:B:583:LEU:HB3	1.93	0.50
1:A:154:SER:CA	1:A:157:LYS:HE2	2.37	0.50
1:A:485:ARG:O	1:A:488:VAL:HG12	2.10	0.50
1:B:484:LYS:HG3	1:B:487:GLU:OE2	2.10	0.50
1:A:432:ASN:HB2	1:A:452:ARG:NH2	2.26	0.50
1:B:434:VAL:HG13	1:B:537:LEU:HD21	1.94	0.50
1:A:148:ASP:HB3	1:A:151:ASP:OD2	2.12	0.50
1:A:488:VAL:O	1:A:492:ILE:HG13	2.12	0.50
1:A:50:ARG:HB3	1:A:54:ASP:OD2	2.11	0.50
1:A:242:CYS:HA	1:B:382:LEU:CD2	2.42	0.50
1:B:171:THR:O	1:B:175:LEU:HD23	2.12	0.49
1:B:225:PRO:O	1:B:226:LYS:HG3	2.12	0.49
1:A:401:PHE:HA	1:A:584:ILE:HG21	1.93	0.49
1:B:7:LEU:HD13	1:B:33:ILE:HG13	1.94	0.49
1:B:570:GLU:OE1	1:B:570:GLU:HA	2.13	0.49
1:A:20:GLU:HA	1:A:23:ARG:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:SER:CB	1:B:432:ASN:HA	2.40	0.49
1:A:62:LEU:HD22	1:B:85:ASP:OD2	2.13	0.49
1:B:71:PRO:O	1:B:75:ALA:CB	2.61	0.49
1:B:283:GLU:O	1:B:287:VAL:HG23	2.13	0.48
1:A:298:THR:HB	1:A:299:PRO:HD2	1.94	0.48
1:A:458:LEU:O	1:A:458:LEU:HD23	2.13	0.48
1:B:495:TYR:HE1	1:B:519:GLN:HA	1.76	0.48
1:B:43:ARG:C	1:B:45:ALA:H	2.17	0.48
1:A:70:HIS:CE1	1:A:71:PRO:HG2	2.49	0.48
1:A:295:LYS:H	1:A:295:LYS:CE	2.27	0.48
1:A:568:ALA:O	1:A:571:VAL:HG22	2.13	0.48
1:B:270:SER:OG	1:B:430:GLN:HG2	2.14	0.48
1:A:82:ILE:C	1:A:86:ASN:ND2	2.67	0.48
1:A:467:TRP:CD1	1:A:529:ILE:HA	2.49	0.48
1:B:535:VAL:HB	1:B:557:VAL:HA	1.96	0.47
1:A:537:LEU:HD23	1:A:537:LEU:C	2.33	0.47
1:B:83:PRO:HG2	1:B:84:GLU:OE1	2.14	0.47
1:B:38:THR:O	1:B:42:LEU:HG	2.14	0.47
1:B:326:CYS:O	1:B:348:GLU:HG3	2.15	0.47
1:A:214:HIS:CD2	1:A:214:HIS:H	2.32	0.47
1:A:429:THR:O	1:A:592:HIS:HB3	2.14	0.47
1:A:549:VAL:HG21	1:A:572:VAL:HG13	1.97	0.47
1:B:401:PHE:HB3	1:B:584:ILE:HD13	1.97	0.47
1:A:485:ARG:CA	1:A:488:VAL:HG12	2.44	0.47
1:B:298:THR:HB	1:B:299:PRO:CD	2.45	0.46
1:A:173:ARG:HD3	1:B:198:TYR:CE1	2.50	0.46
1:A:542:PHE:CD1	1:A:566:SER:HB2	2.51	0.46
1:B:202:VAL:CG1	1:B:226:LYS:HG2	2.45	0.46
1:A:242:CYS:HA	1:B:382:LEU:HD21	1.96	0.46
1:B:151:ASP:O	1:B:152:TYR:C	2.54	0.46
1:A:295:LYS:HD3	1:A:295:LYS:N	2.31	0.46
1:A:169:VAL:HG23	1:A:170:GLU:N	2.31	0.46
1:A:412:PRO:HD2	1:A:415:ALA:CB	2.46	0.46
1:A:485:ARG:HA	1:A:488:VAL:CG1	2.45	0.46
1:B:477:MET:HE2	1:B:517:PRO:HG3	1.97	0.46
1:B:121:ALA:O	1:B:124:LYS:HB2	2.15	0.46
1:A:33:ILE:HA	1:A:50:ARG:O	2.16	0.46
1:A:247:ALA:HB1	1:A:321:ALA:HB2	1.97	0.46
1:A:547:ASP:OD1	1:A:547:ASP:N	2.49	0.46
1:B:216:SER:OG	1:B:217:PRO:HA	2.16	0.46
1:A:171:THR:HG22	1:A:175:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:GLU:O	1:A:508:LYS:HG2	2.15	0.46
1:B:375:ASP:HB3	4:B:2070:HOH:O	2.16	0.46
1:A:128:GLY:O	1:A:132:LEU:HG	2.16	0.45
1:A:154:SER:HA	1:A:157:LYS:CD	2.46	0.45
1:B:4:ARG:HD3	1:B:4:ARG:N	2.32	0.45
1:B:173:ARG:NH1	4:B:2020:HOH:O	2.49	0.45
1:B:566:SER:C	1:B:568:ALA:N	2.69	0.45
1:A:65:ARG:C	1:A:67:LYS:H	2.20	0.45
1:B:286:GLN:HG2	1:B:291:HIS:HB2	1.98	0.45
1:A:359:LYS:HB2	1:A:359:LYS:NZ	2.32	0.45
1:B:56:THR:C	1:B:58:PHE:N	2.70	0.45
1:A:80:ARG:O	1:A:85:ASP:HB2	2.17	0.45
1:B:65:ARG:C	1:B:66:VAL:HG23	2.37	0.45
1:B:433:SER:HA	1:B:455:CYS:SG	2.57	0.45
1:B:273:GLY:HA3	1:B:307:SER:O	2.17	0.44
1:A:173:ARG:HD3	1:B:198:TYR:CD1	2.52	0.44
1:A:250:LEU:C	1:A:250:LEU:HD23	2.36	0.44
1:A:81:ASN:C	1:A:81:ASN:HD22	2.20	0.44
1:A:151:ASP:O	1:A:152:TYR:C	2.56	0.44
1:B:172:ARG:HG3	1:B:172:ARG:HH11	1.81	0.44
1:B:490:ASN:N	1:B:490:ASN:ND2	2.65	0.44
1:A:294:HIS:HB3	1:A:295:LYS:HE2	1.99	0.44
1:A:469:ARG:HG3	1:A:496:VAL:HG11	1.99	0.44
1:B:177:LEU:HD23	1:B:177:LEU:C	2.38	0.44
1:A:69:LEU:HD13	1:B:74:HIS:CG	2.53	0.44
1:A:159:MET:O	1:A:162:SER:HB3	2.18	0.44
1:B:551:ARG:HD2	1:B:554:ARG:NH1	2.33	0.44
1:A:104:LEU:HD11	1:A:133:LEU:HD12	1.99	0.44
1:A:200:LYS:HD2	4:A:2018:HOH:O	2.17	0.43
1:B:378:GLU:HG3	1:B:391:ARG:HB3	2.01	0.43
1:B:177:LEU:C	1:B:177:LEU:CD2	2.87	0.43
1:A:220:LEU:HD12	1:B:386:GLN:O	2.19	0.43
1:A:568:ALA:HB1	1:A:571:VAL:CG2	2.48	0.43
1:B:117:THR:OG1	1:B:120:GLU:HG3	2.18	0.43
1:A:9:LEU:HA	1:A:33:ILE:HG23	1.99	0.43
1:A:412:PRO:HD2	1:A:415:ALA:HB2	2.01	0.43
1:A:485:ARG:O	1:A:488:VAL:CG1	2.67	0.43
1:B:479:PHE:O	1:B:514:GLU:HG2	2.19	0.43
1:A:65:ARG:NH1	1:B:80:ARG:NH2	2.66	0.43
1:A:106:PRO:HB3	1:A:108:VAL:HG12	2.01	0.43
1:A:429:THR:CG2	1:A:447:ALA:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:ILE:HG21	1:B:506:LEU:HD12	2.00	0.43
1:B:130:VAL:O	1:B:134:ARG:HG3	2.19	0.42
1:B:465:SER:HA	1:B:496:VAL:HG11	2.01	0.42
1:A:236:PRO:HB3	1:A:364:CYS:SG	2.58	0.42
1:B:64:GLY:O	1:B:65:ARG:C	2.57	0.42
1:A:39:ALA:HA	1:A:42:LEU:HD12	2.00	0.42
1:A:452:ARG:HG2	1:A:544:PRO:HD3	2.01	0.42
1:B:21:PHE:HE2	1:B:101:VAL:HG22	1.83	0.42
1:A:71:PRO:O	1:A:75:ALA:CB	2.67	0.42
1:B:59:PRO:O	1:B:61:MET:N	2.44	0.42
1:A:12:VAL:HG22	1:A:38:THR:CG2	2.50	0.42
1:B:547:ASP:OD1	1:B:547:ASP:N	2.52	0.42
1:A:471:HIS:ND1	1:A:472:PRO:HD2	2.35	0.42
1:B:451:SER:HB3	1:B:454:HIS:HB2	2.01	0.42
1:A:295:LYS:N	1:A:295:LYS:CD	2.83	0.42
1:B:379:ILE:HB	1:B:388:MET:CE	2.50	0.42
1:A:216:SER:OG	1:A:217:PRO:HA	2.20	0.42
1:A:426:VAL:HG13	1:A:540:ASP:HB3	2.01	0.42
1:B:172:ARG:HG3	1:B:172:ARG:NH1	2.35	0.42
1:A:349:GLU:HG3	4:A:2062:HOH:O	2.19	0.42
1:B:177:LEU:HD23	1:B:177:LEU:O	2.20	0.42
1:B:205:LEU:HA	1:B:206:PRO:HD3	1.86	0.41
1:A:450:GLN:CB	1:B:314:SER:HB2	2.46	0.41
1:B:128:GLY:O	1:B:132:LEU:HG	2.20	0.41
1:B:148:ASP:HB3	1:B:151:ASP:OD2	2.21	0.41
1:B:237:GLY:O	1:B:240:ASN:HB2	2.20	0.41
1:A:62:LEU:HB2	1:A:65:ARG:HD3	2.01	0.41
1:A:151:ASP:O	1:A:155:VAL:HG23	2.21	0.41
1:B:100:VAL:HG21	1:B:136:ALA:HB2	2.01	0.41
1:A:20:GLU:HA	1:A:23:ARG:CG	2.49	0.41
1:A:258:LEU:HD12	1:A:276:VAL:HG11	2.02	0.41
1:A:149:PRO:HA	1:A:152:TYR:CD2	2.55	0.41
1:A:208:ARG:HE	1:A:208:ARG:HB2	1.69	0.41
1:B:243:ASP:OD1	1:B:269:VAL:N	2.48	0.41
1:A:406:THR:CG2	1:A:583:LEU:HB3	2.50	0.41
1:B:460:GLY:O	1:B:463:ALA:HB3	2.21	0.41
1:A:496:VAL:HG23	1:A:497:THR:HG23	2.03	0.41
1:B:90:ASN:HD22	1:B:90:ASN:HA	1.63	0.41
1:B:426:VAL:HG13	1:B:540:ASP:HB3	2.02	0.41
1:B:464:ASN:HD22	1:B:555:ILE:HD13	1.80	0.41
1:A:77:ILE:O	1:A:139:ASN:ND2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:HG12	1:A:332:LYS:HE3	2.02	0.41
1:B:419:LEU:HD23	1:B:536:SER:HB3	2.03	0.41
1:A:43:ARG:C	1:A:45:ALA:N	2.75	0.40
1:A:84:GLU:O	1:A:87:ALA:HB3	2.21	0.40
1:A:549:VAL:CG2	1:A:572:VAL:HG13	2.51	0.40
1:B:83:PRO:HA	1:B:86:ASN:HD22	1.87	0.40
1:B:432:ASN:HB2	1:B:452:ARG:HH22	1.86	0.40
1:A:270:SER:OG	1:A:430:GLN:HG2	2.21	0.40
1:B:34:ALA:O	1:B:51:ASP:HA	2.22	0.40
1:B:39:ALA:O	1:B:42:LEU:N	2.54	0.40
1:A:389:GLN:HG3	1:A:390:LYS:O	2.21	0.40
1:B:70:HIS:CE1	1:B:71:PRO:HG2	2.56	0.40
1:B:200:LYS:HE2	1:B:206:PRO:HG2	2.04	0.40
1:B:328:VAL:N	1:B:329:PRO:HD2	2.36	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	588/593 (99%)	532 (90%)	45 (8%)	11 (2%)	<b>8</b> <b>12</b>
1	B	588/593 (99%)	538 (92%)	44 (8%)	6 (1%)	<b>15</b> <b>27</b>
All	All	1176/1186 (99%)	1070 (91%)	89 (8%)	17 (1%)	<b>11</b> <b>19</b>

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ALA
1	B	66	VAL
1	B	114	PRO
1	A	19	VAL

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Mol	Chain	Res	Type
1	A	60	GLU
1	A	66	VAL
1	A	23	ARG
1	A	36	GLY
1	A	114	PRO
1	A	116	VAL
1	A	153	SER
1	B	164	ASP
1	A	18	LEU
1	B	153	SER
1	B	567	ALA
1	B	277	GLY
1	A	17	GLY

### 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	484/485 (100%)	457 (94%)	27 (6%)	21	38
1	B	484/485 (100%)	464 (96%)	20 (4%)	30	53
All	All	968/970 (100%)	921 (95%)	47 (5%)	25	45

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	33	ILE
1	A	44	ASP
1	A	54	ASP
1	A	58	PHE
1	A	81	ASN
1	A	83	PRO
1	A	85	ASP
1	A	163	LYS
1	A	164	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	170	GLU
1	A	174	HIS
1	A	177	LEU
1	A	199	SER
1	A	205	LEU
1	A	269	VAL
1	A	291	HIS
1	A	295	LYS
1	A	313	MET
1	A	340	ASP
1	A	357	LYS
1	A	390	LYS
1	A	410	THR
1	A	494	GLN
1	A	504	GLU
1	A	508	LYS
1	A	515	GLU
1	B	4	ARG
1	B	5	GLN
1	B	44	ASP
1	B	58	PHE
1	B	82	ILE
1	B	85	ASP
1	B	114	PRO
1	B	163	LYS
1	B	170	GLU
1	B	177	LEU
1	B	187	ASP
1	B	267	LYS
1	B	292	ASP
1	B	315	SER
1	B	379	ILE
1	B	478	LYS
1	B	490	ASN
1	B	505	ASP
1	B	515	GLU
1	B	564	SER

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	81	ASN

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Mol	Chain	Res	Type
1	A	86	ASN
1	A	90	ASN
1	A	92	GLN
1	A	185	GLN
1	A	214	HIS
1	A	294	HIS
1	A	408	ASN
1	A	464	ASN
1	B	5	GLN
1	B	86	ASN
1	B	90	ASN
1	B	185	GLN
1	B	393	ASN
1	B	464	ASN
1	B	490	ASN
1	B	494	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 monosaccharides in this entry.

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

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	203	B	1595	-	6,13,13	7.34	4 (66%)	5,20,20	7.73	4 (80%)

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	203	B	1595	-	-	-	0/1/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1595	203	O20-S16	14.55	1.64	1.43
3	B	1595	203	O21-S16	9.03	1.56	1.43
3	B	1595	203	C13-C18	4.64	1.56	1.47
3	B	1595	203	C14-N15	2.76	1.40	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1595	203	O21-S16-O20	-16.12	98.61	118.85
3	B	1595	203	C11-N12-C13	-4.84	93.78	102.99
3	B	1595	203	O19-C18-C13	-2.76	118.98	124.37
3	B	1595	203	O19-C18-N17	2.11	123.67	120.82

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	590/593 (99%)	-0.06	11 (1%) 66 70	19, 39, 78, 89	0
1	B	590/593 (99%)	0.05	7 (1%) 79 81	23, 45, 72, 84	0
All	All	1180/1186 (99%)	-0.01	18 (1%) 73 76	19, 42, 74, 89	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	64	GLY	7.7
1	B	91	LYS	4.5
1	A	50	ARG	3.6
1	B	89	MET	3.4
1	A	60	GLU	3.3
1	A	4	ARG	3.0
1	A	59	PRO	2.9
1	A	42	LEU	2.6
1	A	62	LEU	2.6
1	B	87	ALA	2.5
1	A	165	LYS	2.4
1	A	108	VAL	2.4
1	B	163	LYS	2.4
1	A	47	LEU	2.4
1	B	579	LEU	2.1
1	B	88	ASP	2.1
1	A	114	PRO	2.1
1	B	575	ALA	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	203	B	1595	12/12	0.80	0.24	76,77,79,81	0
2	K	A	1594	1/1	0.96	0.09	33,33,33,33	0
2	K	B	1594	1/1	0.97	0.15	37,37,37,37	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.