



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:52 AM GMT

PDB ID : 1X9T  
Title : The crystal structure of human adenovirus 2 penton base in complex with an ad2 N-terminal fibre peptide  
Authors : Zubieta, C.; Schoehn, G.; Chroboczek, J.; Cusack, S.  
Deposited on : 2004-08-24  
Resolution : 3.50 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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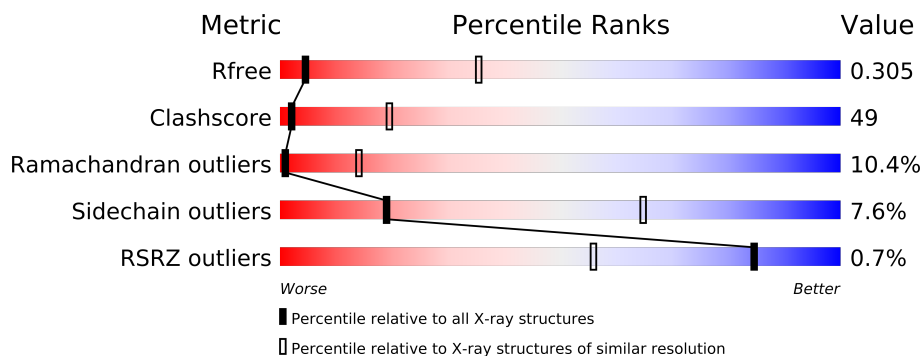
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 3.50 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))
$R_{free}$	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	523	
2	B	21	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	C15	A	1014	-	X
3	C15	A	2000	-	X

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3645 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

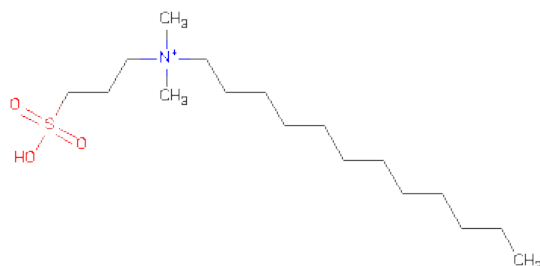
- Molecule 1 is a protein called Penton protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3519	2227	608	672	12			

- Molecule 2 is a protein called N-terminal peptide of Fiber protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	0	0	0
			86	58	11	17			

- Molecule 3 is N-DODECYL-N,N-DIMETHYL-3-AMMONIO-1-PROPANESULFONATE (three-letter code: C15) (formula:  $C_{17}H_{38}NO_3S$ ).



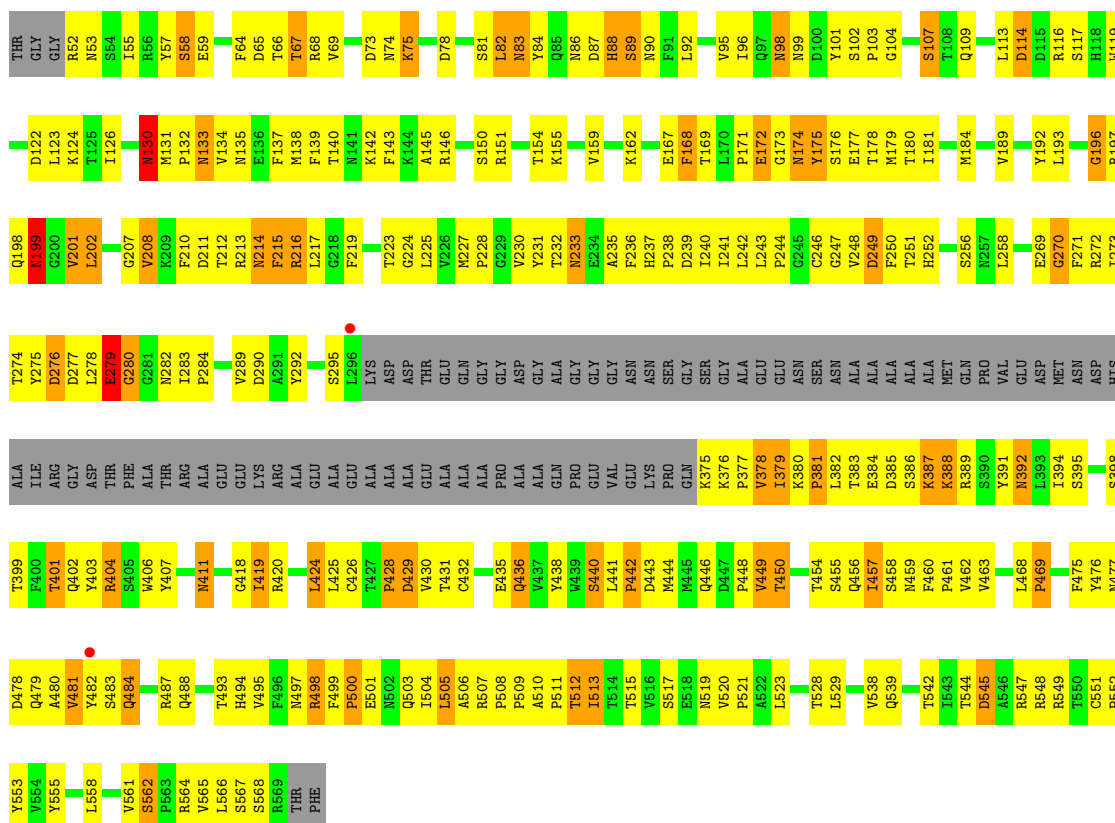
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			20	15	1	3	1		
3	A	1	Total	C	N	O	S	0	0
			20	15	1	3	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Penton protein

Chain A: 



#### • Molecule 2: N-terminal peptide of Fiber protein

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	438.37Å 299.82Å 419.58Å 90.00° 103.22° 90.00°	Depositor
Resolution (Å)	29.98 – 3.50 39.81 – 3.50	Depositor EDS
% Data completeness (in resolution range)	53.6 (29.98-3.50) 53.7 (39.81-3.50)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	0.19	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 3.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.306 , 0.303 0.305 , 0.305	Depositor DCC
$R_{free}$ test set	17745 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.5	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 30.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	5 of 354797 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	3645	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C15

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	0.61	0/3602	0.81	1/4904 (0.0%)
2	B	0.66	0/90	0.69	0/125
All	All	0.61	0/3692	0.81	1/5029 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	482	TYR	N-CA-C	-7.26	91.39	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3519	0	3452	335	0
2	B	86	0	73	16	0
3	A	40	0	64	13	0
All	All	3645	0	3589	355	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 49.

All (355) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:68:ARG:NH1	1:A:562:SER:HB3	1.68	1.09
1:A:479:GLN:O	1:A:483:SER:HB2	1.59	1.03
1:A:468:LEU:HD12	1:A:469:PRO:HD2	1.41	1.01
1:A:197:ARG:HE	1:A:198:GLN:NE2	1.59	0.99
1:A:483:SER:O	1:A:487:ARG:N	1.95	0.98
1:A:479:GLN:O	1:A:483:SER:CB	2.13	0.97
1:A:68:ARG:HG2	1:A:68:ARG:HH11	1.26	0.95
1:A:197:ARG:HE	1:A:198:GLN:HE21	1.05	0.92
1:A:230:VAL:HG13	1:A:503:GLN:NE2	1.83	0.92
1:A:132:PRO:HA	1:A:175:TYR:OH	1.67	0.92
1:A:274:THR:HG22	1:A:276:ASP:H	1.37	0.89
1:A:275:TYR:CE1	1:A:404:ARG:HD3	2.09	0.88
1:A:83:ASN:HA	1:A:86:ASN:HD22	1.38	0.87
3:A:1014:C15:H7C1	3:A:2000:C15:H112	1.57	0.87
1:A:68:ARG:HH12	1:A:562:SER:HB3	1.36	0.85
1:A:475:PHE:O	1:A:513:ILE:HA	1.77	0.85
1:A:379:ILE:O	1:A:381:PRO:HD3	1.75	0.85
1:A:217:LEU:HB2	1:A:232:THR:HG21	1.57	0.84
1:A:528:THR:HG21	1:A:564:ARG:HH21	1.42	0.83
1:A:197:ARG:NE	1:A:198:GLN:HE21	1.80	0.80
1:A:444:MET:HE3	1:A:561:VAL:HG21	1.63	0.80
1:A:544:THR:CG2	1:A:548:ARG:HA	2.10	0.80
1:A:230:VAL:HG13	1:A:503:GLN:HE22	1.47	0.79
1:A:468:LEU:HD12	1:A:469:PRO:CD	2.12	0.79
1:A:68:ARG:NH1	1:A:68:ARG:HG2	1.97	0.78
1:A:403:TYR:CD1	1:A:504:ILE:HG12	2.19	0.78
1:A:104:GLY:O	1:A:107:SER:HB3	1.83	0.77
1:A:217:LEU:HB2	1:A:232:THR:CG2	2.14	0.76
1:A:145:ALA:HB3	1:A:168:PHE:HE1	1.50	0.76
1:A:135:ASN:HA	1:A:172:GLU:HG2	1.68	0.76
1:A:96:ILE:HG22	1:A:98:ASN:H	1.51	0.76
1:A:146:ARG:O	1:A:246:CYS:HB2	1.87	0.75
3:A:1014:C15:H9C1	3:A:2000:C15:H132	1.69	0.74
1:A:378:VAL:HG23	1:A:379:ILE:N	2.01	0.74
1:A:512:THR:O	1:A:513:ILE:HB	1.88	0.74
1:A:277:ASP:HB3	1:A:419:ILE:HD11	1.70	0.74
1:A:134:VAL:HG13	1:A:140:THR:O	1.87	0.74
1:A:528:THR:HG21	1:A:564:ARG:NH2	2.02	0.73
1:A:544:THR:HG22	1:A:548:ARG:HA	1.69	0.73
1:A:193:LEU:HD11	1:A:498:ARG:HH12	1.54	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:214:ASN:HD22	1:A:214:ASN:C	1.93	0.73
1:A:146:ARG:NH1	3:A:2000:C15:H1C2	2.04	0.73
2:B:10:THR:HG22	2:B:10:THR:O	1.89	0.73
1:A:215:PHE:O	1:A:216:ARG:HB2	1.89	0.72
1:A:275:TYR:CZ	1:A:404:ARG:HD3	2.26	0.71
1:A:154:THR:HG22	1:A:155:LYS:HG3	1.72	0.70
1:A:146:ARG:HH12	3:A:2000:C15:H1C2	1.57	0.70
1:A:424:LEU:HD23	1:A:425:LEU:N	2.06	0.69
1:A:378:VAL:O	1:A:380:LYS:N	2.25	0.69
1:A:274:THR:HG22	1:A:276:ASP:N	2.06	0.69
1:A:98:ASN:HD22	1:A:99:ASN:N	1.90	0.69
1:A:504:ILE:HG22	1:A:505:LEU:N	2.06	0.69
1:A:211:ASP:OD1	1:A:213:ARG:HG2	1.94	0.68
1:A:378:VAL:HG23	1:A:379:ILE:H	1.57	0.68
1:A:283:ILE:O	1:A:401:THR:HG23	1.93	0.68
1:A:499:PHE:HD1	1:A:505:LEU:HB3	1.59	0.68
1:A:428:PRO:O	1:A:429:ASP:HB3	1.93	0.68
1:A:217:LEU:CB	1:A:232:THR:HG21	2.25	0.67
1:A:274:THR:HG22	1:A:275:TYR:N	2.10	0.67
1:A:83:ASN:HA	1:A:86:ASN:ND2	2.09	0.67
1:A:457:ILE:HD12	1:A:458:SER:H	1.58	0.67
1:A:130:ASN:HA	1:A:519:ASN:CG	2.16	0.66
1:A:214:ASN:HD21	1:A:216:ARG:HB3	1.60	0.66
1:A:487:ARG:NH1	1:A:507:ARG:NH2	2.44	0.66
1:A:440:SER:C	1:A:442:PRO:HD3	2.17	0.65
1:A:215:PHE:HB3	1:A:283:ILE:HG23	1.77	0.65
1:A:133:ASN:HB2	1:A:175:TYR:CD2	2.32	0.65
1:A:440:SER:HB3	1:A:461:PRO:O	1.97	0.65
1:A:224:GLY:O	1:A:225:LEU:HD23	1.97	0.65
1:A:145:ALA:HB3	1:A:168:PHE:CE1	2.31	0.65
2:B:18:ASP:OD1	2:B:18:ASP:O	2.15	0.65
1:A:498:ARG:HD3	2:B:14:VAL:HG12	1.80	0.64
3:A:1014:C15:H122	3:A:2000:C15:H121	1.78	0.64
1:A:513:ILE:O	1:A:513:ILE:HG22	1.97	0.64
1:A:468:LEU:CD1	1:A:469:PRO:HD2	2.24	0.64
1:A:210:PHE:HD2	1:A:240:ILE:HG22	1.63	0.63
1:A:444:MET:CE	1:A:561:VAL:HG21	2.28	0.63
1:A:171:PRO:O	1:A:174:ASN:ND2	2.32	0.63
1:A:138:MET:O	1:A:139:PHE:HB2	1.99	0.63
1:A:207:GLY:O	1:A:208:VAL:HB	1.97	0.63
1:A:544:THR:HG21	1:A:548:ARG:HA	1.80	0.63
1:A:134:VAL:HA	1:A:140:THR:OG1	1.98	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:436:GLN:NE2	1:A:438:TYR:HE2	1.96	0.63
1:A:477:ASN:C	1:A:479:GLN:N	2.53	0.62
1:A:177:GLU:HG3	1:A:178:THR:N	2.15	0.61
1:A:154:THR:HG22	1:A:155:LYS:N	2.14	0.61
1:A:481:VAL:HA	1:A:484:GLN:HB3	1.83	0.61
1:A:481:VAL:HG12	1:A:481:VAL:O	2.00	0.61
1:A:385:ASP:OD1	1:A:389:ARG:HD2	2.00	0.61
1:A:477:ASN:C	1:A:479:GLN:H	2.03	0.61
1:A:292:TYR:CD1	1:A:378:VAL:HG12	2.35	0.60
1:A:430:VAL:HG21	1:A:517:SER:N	2.16	0.60
1:A:378:VAL:CG2	1:A:379:ILE:H	2.14	0.60
1:A:57:TYR:O	1:A:58:SER:C	2.40	0.60
1:A:52:ARG:N	1:A:116:ARG:HH12	2.00	0.60
1:A:378:VAL:CG2	1:A:379:ILE:N	2.65	0.59
1:A:210:PHE:CD2	1:A:240:ILE:HG22	2.37	0.59
1:A:493:THR:HB	1:A:495:VAL:HG23	1.84	0.59
1:A:278:LEU:HD22	1:A:406:TRP:HA	1.84	0.59
1:A:480:ALA:HB1	1:A:510:ALA:HB3	1.83	0.59
1:A:159:VAL:O	1:A:159:VAL:HG23	2.00	0.59
1:A:435:GLU:OE1	1:A:435:GLU:HA	2.03	0.59
1:A:497:ASN:O	1:A:499:PHE:N	2.34	0.59
1:A:237:HIS:CD2	1:A:238:PRO:O	2.56	0.59
1:A:208:VAL:HG22	1:A:242:LEU:CD2	2.33	0.59
1:A:499:PHE:N	1:A:499:PHE:CD2	2.69	0.59
1:A:233:ASN:OD1	1:A:509:PRO:HG3	2.02	0.59
1:A:211:ASP:OD1	1:A:212:THR:N	2.31	0.59
1:A:389:ARG:HH11	1:A:389:ARG:HG2	1.67	0.59
1:A:122:ASP:OD1	1:A:528:THR:HG22	2.03	0.58
1:A:173:GLY:O	1:A:175:TYR:CD1	2.55	0.58
1:A:274:THR:CG2	1:A:275:TYR:N	2.67	0.58
1:A:498:ARG:O	2:B:16:PRO:HD3	2.03	0.58
1:A:504:ILE:O	1:A:506:ALA:N	2.37	0.58
1:A:98:ASN:C	1:A:98:ASN:HD22	2.06	0.58
1:A:479:GLN:O	1:A:483:SER:N	2.36	0.58
1:A:175:TYR:CD1	1:A:175:TYR:N	2.72	0.58
2:B:15:TYR:HD2	2:B:16:PRO:N	2.02	0.58
1:A:538:VAL:HG23	1:A:538:VAL:O	2.02	0.57
1:A:273:ILE:HG23	1:A:273:ILE:O	2.02	0.57
1:A:498:ARG:C	1:A:499:PHE:HD2	2.08	0.57
1:A:175:TYR:H	1:A:175:TYR:HD1	1.52	0.57
1:A:295:SER:OG	1:A:377:PRO:HD3	2.03	0.57
1:A:411:ASN:N	1:A:411:ASN:OD1	2.36	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:500:PRO:HG2	1:A:501:GLU:OE2	2.04	0.57
1:A:441:LEU:N	1:A:442:PRO:HD3	2.19	0.57
1:A:258:LEU:CD1	1:A:430:VAL:HA	2.35	0.57
2:B:15:TYR:HD2	2:B:16:PRO:CD	2.18	0.56
1:A:69:VAL:CG2	1:A:561:VAL:HB	2.36	0.56
1:A:130:ASN:HA	1:A:519:ASN:ND2	2.21	0.56
1:A:498:ARG:C	1:A:499:PHE:CD2	2.78	0.56
1:A:520:VAL:HG23	1:A:521:PRO:HD2	1.87	0.56
1:A:86:ASN:HB3	1:A:90:ASN:O	2.06	0.56
1:A:431:THR:O	1:A:432:CYS:HB2	2.05	0.56
1:A:463:VAL:HB	1:A:529:LEU:HD13	1.87	0.56
1:A:243:LEU:HG	1:A:403:TYR:HE2	1.71	0.56
1:A:279:GLU:O	1:A:280:GLY:O	2.24	0.55
2:B:18:ASP:O	2:B:18:ASP:CG	2.44	0.55
1:A:446:GLN:O	1:A:448:PRO:HD3	2.07	0.55
1:A:132:PRO:HD2	1:A:553:TYR:CE2	2.41	0.55
1:A:88:HIS:ND1	1:A:555:TYR:O	2.38	0.55
1:A:151:ARG:HB3	1:A:201:VAL:H	1.70	0.55
1:A:154:THR:CG2	1:A:155:LYS:N	2.69	0.55
1:A:197:ARG:HG3	1:A:198:GLN:HG3	1.89	0.55
1:A:150:SER:HB3	1:A:199:ASN:HD22	1.71	0.55
1:A:544:THR:CG2	1:A:549:ARG:N	2.70	0.54
1:A:565:VAL:HG12	1:A:566:LEU:N	2.23	0.54
1:A:377:PRO:O	1:A:379:ILE:N	2.40	0.54
1:A:67:THR:OG1	1:A:68:ARG:N	2.39	0.54
1:A:214:ASN:ND2	1:A:214:ASN:C	2.58	0.54
1:A:214:ASN:O	1:A:216:ARG:N	2.41	0.54
1:A:171:PRO:HG2	1:A:174:ASN:ND2	2.23	0.54
1:A:444:MET:HB2	1:A:539:GLN:OE1	2.08	0.54
1:A:177:GLU:CG	1:A:178:THR:N	2.71	0.54
1:A:497:ASN:O	1:A:500:PRO:HD3	2.08	0.53
1:A:122:ASP:OD1	1:A:528:THR:CG2	2.56	0.53
1:A:403:TYR:HD1	1:A:504:ILE:HG12	1.69	0.53
1:A:406:TRP:NE1	1:A:419:ILE:HG21	2.22	0.53
1:A:430:VAL:CG1	1:A:515:THR:HB	2.38	0.53
1:A:52:ARG:N	1:A:116:ARG:NH1	2.56	0.53
1:A:65:ASP:O	1:A:66:THR:HB	2.06	0.53
1:A:279:GLU:O	1:A:280:GLY:C	2.45	0.53
1:A:406:TRP:HE1	1:A:419:ILE:HG21	1.73	0.53
1:A:544:THR:HG22	1:A:545:ASP:H	1.74	0.53
1:A:126:ILE:HG12	1:A:523:LEU:HD23	1.91	0.53
1:A:223:THR:HG21	1:A:227:MET:SD	2.49	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:488:GLN:HE22	1:A:497:ASN:ND2	2.07	0.52
1:A:493:THR:HG23	2:B:15:TYR:CE1	2.45	0.52
1:A:457:ILE:HD12	1:A:458:SER:N	2.25	0.52
1:A:457:ILE:HA	1:A:460:PHE:CE2	2.45	0.52
1:A:151:ARG:HB3	1:A:201:VAL:N	2.24	0.52
1:A:479:GLN:O	1:A:483:SER:HB3	2.07	0.52
1:A:394:ILE:HA	1:A:402:GLN:HE21	1.74	0.52
1:A:57:TYR:OH	1:A:109:GLN:NE2	2.42	0.52
1:A:558:LEU:HD12	1:A:558:LEU:C	2.30	0.52
1:A:227:MET:HB2	1:A:228:PRO:HD3	1.92	0.52
1:A:420:ARG:O	1:A:420:ARG:HG2	2.10	0.52
1:A:243:LEU:HG	1:A:403:TYR:CE2	2.44	0.51
1:A:378:VAL:C	1:A:380:LYS:N	2.62	0.51
1:A:476:TYR:CD1	1:A:513:ILE:HD11	2.45	0.51
1:A:513:ILE:N	1:A:513:ILE:HD12	2.25	0.51
1:A:277:ASP:O	1:A:419:ILE:HD13	2.10	0.51
1:A:132:PRO:HA	1:A:175:TYR:CZ	2.45	0.51
1:A:487:ARG:NH1	1:A:507:ARG:HH22	2.07	0.51
1:A:231:TYR:HD1	1:A:503:GLN:HB3	1.75	0.51
1:A:237:HIS:CD2	1:A:425:LEU:HD11	2.46	0.51
1:A:178:THR:OG1	1:A:511:PRO:HD2	2.10	0.51
1:A:214:ASN:ND2	1:A:216:ARG:HB3	2.24	0.51
1:A:429:ASP:C	1:A:429:ASP:OD1	2.49	0.50
2:B:15:TYR:HD2	2:B:16:PRO:HD2	1.77	0.50
3:A:1014:C15:H7C1	3:A:2000:C15:H9C1	1.94	0.50
1:A:130:ASN:C	1:A:130:ASN:HD22	2.14	0.50
1:A:235:ALA:C	1:A:236:PHE:HD1	2.15	0.50
1:A:270:GLY:O	3:A:1014:C15:O1S	2.29	0.50
1:A:544:THR:HG22	1:A:545:ASP:N	2.27	0.50
1:A:154:THR:CG2	1:A:155:LYS:HG3	2.41	0.50
1:A:389:ARG:NH1	1:A:389:ARG:HG2	2.26	0.49
1:A:113:LEU:O	1:A:114:ASP:C	2.47	0.49
1:A:375:LYS:O	1:A:376:LYS:HG3	2.12	0.49
1:A:98:ASN:C	1:A:98:ASN:ND2	2.66	0.49
1:A:386:SER:O	1:A:388:LYS:N	2.45	0.49
1:A:394:ILE:HD11	1:A:398:SER:OG	2.13	0.49
1:A:493:THR:HG22	1:A:494:HIS:N	2.27	0.49
1:A:68:ARG:NH1	1:A:68:ARG:CG	2.67	0.49
1:A:292:TYR:HD1	1:A:378:VAL:HG12	1.75	0.49
1:A:151:ARG:CB	1:A:201:VAL:H	2.25	0.49
1:A:197:ARG:HG3	1:A:198:GLN:N	2.27	0.49
1:A:295:SER:CB	1:A:377:PRO:CG	2.90	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:545:ASP:OD1	1:A:549:ARG:HG2	2.12	0.49
1:A:497:ASN:ND2	1:A:500:PRO:HB3	2.28	0.49
1:A:503:GLN:HA	1:A:503:GLN:OE1	2.12	0.49
1:A:243:LEU:CD2	1:A:244:PRO:HD3	2.42	0.49
1:A:499:PHE:O	1:A:501:GLU:N	2.45	0.49
1:A:131:MET:HA	1:A:553:TYR:CD2	2.47	0.49
1:A:173:GLY:O	1:A:175:TYR:CE1	2.65	0.49
1:A:240:ILE:HD11	1:A:273:ILE:HG21	1.94	0.48
1:A:391:TYR:O	1:A:392:ASN:C	2.51	0.48
1:A:179:MET:CE	1:A:487:ARG:NH2	2.77	0.48
1:A:243:LEU:CG	1:A:403:TYR:HE2	2.25	0.48
1:A:520:VAL:CG2	1:A:521:PRO:HD2	2.43	0.48
1:A:201:VAL:O	1:A:201:VAL:HG13	2.12	0.48
1:A:424:LEU:HD23	1:A:425:LEU:H	1.76	0.48
1:A:130:ASN:HD22	1:A:130:ASN:N	2.10	0.48
1:A:249:ASP:OD1	1:A:249:ASP:C	2.51	0.48
1:A:244:PRO:HA	1:A:275:TYR:CD2	2.49	0.48
1:A:145:ALA:HA	1:A:248:VAL:HA	1.96	0.48
1:A:211:ASP:HA	1:A:508:PRO:CG	2.44	0.48
1:A:542:THR:HG22	1:A:542:THR:O	2.13	0.48
1:A:130:ASN:ND2	1:A:130:ASN:N	2.61	0.48
1:A:142:LYS:HD3	1:A:167:GLU:OE2	2.14	0.48
1:A:237:HIS:HD2	1:A:238:PRO:O	1.96	0.47
1:A:269:GLU:HG3	1:A:269:GLU:O	2.14	0.47
1:A:180:THR:HG21	1:A:258:LEU:CD2	2.44	0.47
1:A:142:LYS:O	1:A:143:PHE:HB3	2.14	0.47
1:A:239:ASP:HB3	1:A:407:TYR:HB2	1.96	0.47
1:A:74:ASN:O	1:A:75:LYS:C	2.52	0.47
1:A:179:MET:HE3	1:A:487:ARG:HH22	1.78	0.47
1:A:456:GLN:O	1:A:458:SER:N	2.47	0.47
1:A:142:LYS:HG2	1:A:169:THR:HG22	1.97	0.47
1:A:193:LEU:HD22	1:A:197:ARG:NH1	2.29	0.47
1:A:499:PHE:HD1	1:A:505:LEU:CB	2.25	0.47
1:A:476:TYR:HD1	1:A:513:ILE:HD11	1.80	0.47
1:A:277:ASP:O	1:A:279:GLU:N	2.46	0.47
1:A:131:MET:SD	1:A:138:MET:HG3	2.55	0.47
1:A:544:THR:HG22	1:A:549:ARG:H	1.79	0.47
1:A:75:LYS:O	1:A:78:ASP:OD1	2.32	0.47
1:A:493:THR:HG22	1:A:495:VAL:N	2.29	0.47
1:A:102:SER:O	1:A:103:PRO:C	2.52	0.46
1:A:215:PHE:CE1	1:A:241:ILE:HD11	2.49	0.46
2:B:15:TYR:CD2	2:B:16:PRO:HD2	2.51	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:544:THR:CG2	1:A:549:ARG:H	2.28	0.46
3:A:1014:C15:H9C1	3:A:2000:C15:C13	2.41	0.46
1:A:385:ASP:C	1:A:386:SER:O	2.52	0.46
1:A:463:VAL:HB	1:A:529:LEU:CD1	2.44	0.46
1:A:378:VAL:C	1:A:380:LYS:H	2.19	0.46
1:A:449:VAL:HG12	1:A:450:THR:HG23	1.97	0.46
1:A:289:VAL:HG13	1:A:290:ASP:N	2.30	0.46
1:A:242:LEU:HD22	1:A:247:GLY:HA2	1.98	0.46
1:A:78:ASP:HB2	1:A:82:LEU:HD12	1.97	0.46
1:A:250:PHE:O	1:A:252:HIS:N	2.49	0.46
1:A:454:THR:OG1	1:A:455:SER:N	2.49	0.46
1:A:479:GLN:OE1	1:A:479:GLN:HA	2.16	0.45
1:A:295:SER:CB	1:A:377:PRO:HG2	2.46	0.45
1:A:295:SER:HB3	1:A:377:PRO:HG2	1.98	0.45
1:A:487:ARG:CZ	1:A:507:ARG:HH22	2.29	0.45
1:A:243:LEU:HD21	1:A:403:TYR:CE2	2.51	0.45
1:A:225:LEU:CD2	1:A:399:THR:HB	2.47	0.45
1:A:436:GLN:NE2	1:A:438:TYR:CE2	2.81	0.45
1:A:504:ILE:C	1:A:506:ALA:H	2.20	0.45
1:A:123:LEU:HD13	1:A:561:VAL:HG22	1.98	0.45
1:A:476:TYR:CD1	1:A:513:ILE:CD1	3.00	0.45
1:A:177:GLU:CG	1:A:178:THR:H	2.30	0.45
1:A:132:PRO:CA	1:A:175:TYR:OH	2.53	0.44
1:A:378:VAL:O	1:A:379:ILE:C	2.55	0.44
1:A:87:ASP:O	1:A:89:SER:N	2.46	0.44
1:A:231:TYR:H	1:A:503:GLN:HE21	1.65	0.44
1:A:171:PRO:O	1:A:172:GLU:O	2.35	0.44
2:B:10:THR:CG2	2:B:10:THR:O	2.60	0.44
1:A:202:LEU:HD23	1:A:202:LEU:N	2.33	0.44
1:A:231:TYR:CD1	1:A:503:GLN:HB3	2.51	0.44
1:A:131:MET:HA	1:A:132:PRO:HD3	1.80	0.44
1:A:272:ARG:HH12	3:A:2000:C15:H1C1	1.83	0.44
1:A:460:PHE:O	1:A:548:ARG:NH2	2.50	0.44
1:A:387:LYS:HZ2	2:B:16:PRO:HB3	1.82	0.44
1:A:448:PRO:HG2	1:A:462:VAL:O	2.17	0.44
1:A:244:PRO:HA	1:A:275:TYR:CE2	2.53	0.44
1:A:493:THR:HG23	2:B:15:TYR:CZ	2.52	0.44
1:A:547:ARG:O	1:A:548:ARG:HB2	2.16	0.44
1:A:237:HIS:HE1	1:A:426:CYS:O	2.00	0.44
1:A:394:ILE:HG13	1:A:395:SER:N	2.32	0.44
3:A:1014:C15:H102	3:A:2000:C15:H9C1	2.00	0.44
1:A:441:LEU:N	1:A:442:PRO:CD	2.79	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:189:VAL:O	1:A:192:TYR:N	2.51	0.44
1:A:207:GLY:HA3	1:A:246:CYS:SG	2.58	0.44
1:A:69:VAL:HG22	1:A:561:VAL:HB	2.00	0.44
1:A:135:ASN:C	1:A:135:ASN:OD1	2.55	0.44
1:A:383:THR:HG22	1:A:384:GLU:HG3	1.99	0.44
1:A:113:LEU:HB3	1:A:119:TRP:CE2	2.53	0.44
1:A:430:VAL:HG13	1:A:515:THR:HB	2.00	0.43
1:A:64:PHE:O	1:A:65:ASP:HB2	2.17	0.43
1:A:508:PRO:HA	1:A:509:PRO:HD3	1.81	0.43
1:A:384:GLU:HA	1:A:389:ARG:O	2.17	0.43
1:A:69:VAL:HG23	1:A:69:VAL:O	2.18	0.43
1:A:83:ASN:CA	1:A:86:ASN:HD22	2.21	0.43
1:A:207:GLY:O	1:A:208:VAL:CB	2.64	0.43
1:A:383:THR:O	1:A:383:THR:CG2	2.65	0.43
1:A:566:LEU:O	1:A:567:SER:HB3	2.19	0.43
1:A:223:THR:HG22	1:A:225:LEU:HB2	1.99	0.43
1:A:181:ILE:O	1:A:184:MET:HB2	2.19	0.43
1:A:499:PHE:CD1	1:A:505:LEU:HB3	2.44	0.43
1:A:192:TYR:CD1	1:A:196:GLY:HA3	2.54	0.43
1:A:75:LYS:HE2	1:A:75:LYS:HB3	1.88	0.43
3:A:1014:C15:H102	3:A:2000:C15:C9	2.49	0.43
1:A:177:GLU:HG3	1:A:178:THR:H	1.82	0.43
1:A:179:MET:HE3	1:A:487:ARG:NH2	2.34	0.42
1:A:544:THR:HG23	1:A:549:ARG:N	2.34	0.42
1:A:132:PRO:CD	1:A:553:TYR:CE2	3.02	0.42
1:A:223:THR:CG2	1:A:225:LEU:HB2	2.49	0.42
1:A:95:VAL:HG12	1:A:95:VAL:O	2.19	0.42
1:A:481:VAL:O	1:A:481:VAL:CG1	2.66	0.42
1:A:243:LEU:HD23	1:A:244:PRO:HD3	2.01	0.42
1:A:117:SER:HA	1:A:568:SER:HA	2.02	0.42
1:A:424:LEU:CD2	1:A:425:LEU:N	2.80	0.42
1:A:58:SER:OG	1:A:59:GLU:N	2.52	0.42
1:A:87:ASP:OD1	1:A:89:SER:HB3	2.19	0.42
1:A:243:LEU:CG	1:A:403:TYR:CE2	3.03	0.42
1:A:282:ASN:HA	1:A:404:ARG:HA	2.02	0.42
1:A:126:ILE:HG12	1:A:523:LEU:CD2	2.49	0.42
1:A:73:ASP:OD1	1:A:73:ASP:N	2.53	0.41
2:B:15:TYR:CD2	2:B:15:TYR:C	2.92	0.41
1:A:224:GLY:O	1:A:399:THR:HB	2.20	0.41
1:A:137:PHE:HE1	1:A:549:ARG:NE	2.18	0.41
3:A:1014:C15:H111	3:A:2000:C15:H141	2.01	0.41
2:B:12:ASN:HA	2:B:13:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:208:VAL:HG22	1:A:242:LEU:HD22	2.03	0.41
1:A:443:ASP:HB2	1:A:539:GLN:OE1	2.21	0.41
1:A:179:MET:HE2	1:A:487:ARG:NH2	2.35	0.41
1:A:171:PRO:O	1:A:172:GLU:C	2.59	0.41
1:A:403:TYR:CE1	1:A:504:ILE:HG12	2.56	0.41
1:A:154:THR:CG2	1:A:155:LYS:H	2.34	0.41
1:A:132:PRO:HA	1:A:175:TYR:HH	1.79	0.41
1:A:83:ASN:OD1	1:A:92:LEU:N	2.38	0.41
1:A:544:THR:HG21	1:A:548:ARG:HD2	2.02	0.41
1:A:114:ASP:OD2	1:A:116:ARG:NH1	2.54	0.41
1:A:551:CYS:HA	1:A:552:PRO:HD3	1.89	0.41
3:A:1014:C15:H2C1	3:A:1014:C15:H161	1.72	0.41
1:A:196:GLY:O	1:A:201:VAL:HG12	2.21	0.40
2:B:18:ASP:O	2:B:19:THR:HB	2.21	0.40
1:A:565:VAL:CG1	1:A:566:LEU:N	2.84	0.40
1:A:441:LEU:O	1:A:443:ASP:N	2.54	0.40
1:A:375:LYS:O	1:A:376:LYS:CG	2.70	0.40
1:A:53:ASN:O	1:A:53:ASN:ND2	2.55	0.40
1:A:483:SER:O	1:A:484:GLN:C	2.59	0.40
1:A:283:ILE:HG22	1:A:284:PRO:O	2.22	0.40
1:A:150:SER:OG	1:A:162:LYS:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	436/523 (83%)	321 (74%)	69 (16%)	46 (11%)	1	14
2	B	8/21 (38%)	5 (62%)	3 (38%)	0	100	100
All	All	444/544 (82%)	326 (73%)	72 (16%)	46 (10%)	1	14

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
1	A	130	ASN
1	A	172	GLU
1	A	174	ASN
1	A	201	VAL
1	A	216	ARG
1	A	280	GLY
1	A	378	VAL
1	A	449	VAL
1	A	457	ILE
1	A	469	PRO
1	A	481	VAL
1	A	498	ARG
1	A	58	SER
1	A	84	TYR
1	A	175	TYR
1	A	196	GLY
1	A	215	PHE
1	A	219	PHE
1	A	251	THR
1	A	279	GLU
1	A	379	ILE
1	A	387	LYS
1	A	388	LYS
1	A	428	PRO
1	A	442	PRO
1	A	505	LEU
1	A	75	LYS
1	A	81	SER
1	A	88	HIS
1	A	89	SER
1	A	101	TYR
1	A	114	ASP
1	A	176	SER
1	A	199	ASN
1	A	233	ASN
1	A	270	GLY
1	A	500	PRO
1	A	513	ILE
1	A	55	ILE
1	A	67	THR
1	A	208	VAL
1	A	382	LEU

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Mol	Chain	Res	Type
1	A	392	ASN
1	A	381	PRO
1	A	418	GLY

### 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	399/451 (88%)	369 (92%)	30 (8%)	19	65
2	B	10/20 (50%)	9 (90%)	1 (10%)	11	49
All	All	409/471 (87%)	378 (92%)	31 (8%)	19	65

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	98	ASN
1	A	107	SER
1	A	124	LYS
1	A	130	ASN
1	A	133	ASN
1	A	168	PHE
1	A	199	ASN
1	A	202	LEU
1	A	214	ASN
1	A	249	ASP
1	A	256	SER
1	A	271	PHE
1	A	276	ASP
1	A	279	GLU
1	A	401	THR
1	A	404	ARG
1	A	411	ASN
1	A	419	ILE
1	A	424	LEU
1	A	429	ASP
1	A	436	GLN

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Mol	Chain	Res	Type
1	A	440	SER
1	A	450	THR
1	A	459	ASN
1	A	478	ASP
1	A	484	GLN
1	A	512	THR
1	A	545	ASP
1	A	562	SER
2	B	15	TYR

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

Mol	Chain	Res	Type
1	A	53	ASN
1	A	74	ASN
1	A	86	ASN
1	A	98	ASN
1	A	109	GLN
1	A	130	ASN
1	A	174	ASN
1	A	198	GLN
1	A	199	ASN
1	A	214	ASN
1	A	237	HIS
1	A	402	GLN
1	A	436	GLN
1	A	459	ASN
1	A	471	HIS
1	A	497	ASN
1	A	503	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 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	$\# Z  > 2$
3	C15	A	1014	-	19,19,21	3.15	4 (21%)	21,21,26	2.56	6 (28%)
3	C15	A	2000	-	19,19,21	3.33	5 (26%)	21,21,26	4.19	9 (42%)

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	C15	A	1014	-	-	1/17/17/21	0/0/0/0
3	C15	A	2000	-	-	0/17/17/21	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	C15	O3S-S1	12.69	1.77	1.46
3	A	1014	C15	O3S-S1	11.97	1.75	1.46
3	A	2000	C15	C1-S1	4.80	1.84	1.77
3	A	1014	C15	C1-S1	4.29	1.84	1.77
3	A	1014	C15	C10-C9	2.52	1.66	1.51
3	A	2000	C15	C15-C14	2.46	1.66	1.51
3	A	2000	C15	C14-C13	2.21	1.64	1.51
3	A	1014	C15	C12-C11	2.13	1.64	1.51
3	A	2000	C15	C16-N1	2.04	1.49	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	C15	C15-C16-N1	13.13	120.92	111.63
3	A	2000	C15	O2S-S1-C1	8.98	114.51	106.81
3	A	1014	C15	O2S-S1-C1	8.10	113.75	106.81
3	A	2000	C15	C2-C1-S1	6.29	121.35	113.24
3	A	2000	C15	C16-N1-C3	4.78	121.27	113.00
3	A	1014	C15	O3S-S1-C1	4.50	111.62	105.93
3	A	2000	C15	O3S-S1-C1	4.17	111.21	105.93
3	A	1014	C15	C16-N1-C3	3.77	119.52	113.00
3	A	2000	C15	O3S-S1-O1S	-3.50	104.23	111.78
3	A	1014	C15	C2-C1-S1	3.00	117.11	113.24
3	A	1014	C15	O3S-S1-O1S	-3.00	105.30	111.78
3	A	2000	C15	O1S-S1-C1	-2.38	104.77	106.81
3	A	1014	C15	O1S-S1-C1	-2.15	104.97	106.81
3	A	2000	C15	C9-C8-C7	-2.10	103.23	114.61
3	A	2000	C15	O2S-S1-O1S	-2.10	105.77	113.26

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1014	C15	C2-C3-N1-C16

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	440/523 (84%)	-0.17	2 (0%) 88 64	50, 74, 113, 130	0
2	B	10/21 (47%)	0.49	0 100 100	104, 109, 126, 129	0
All	All	450/544 (82%)	-0.16	2 (0%) 84 71	50, 74, 114, 130	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	LEU	2.3
1	A	482	TYR	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	C15	A	2000	20/22	0.75	11.28	127,133,139,139	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	C15	A	1014	20/22	0.57	8.13	107,120,124,125	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.