



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:56 AM UTC

PDB ID : 1X9T / pdb_00001x9t
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

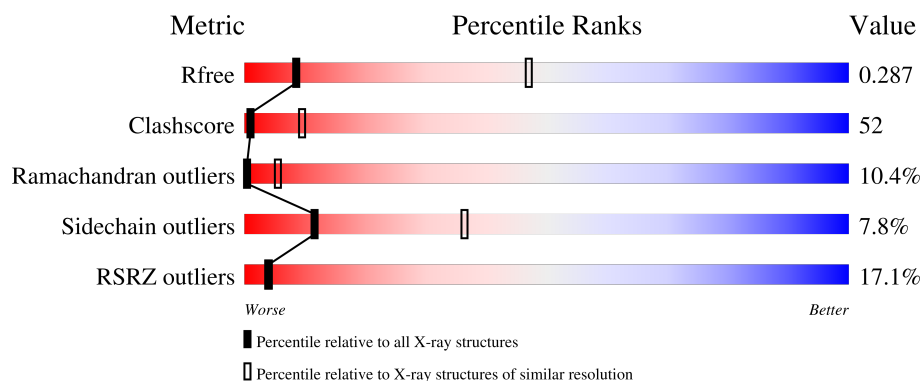
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	523	14% 29% 40% 13% • 16%
2	B	21	10% 10% 38% 52%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3645 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.

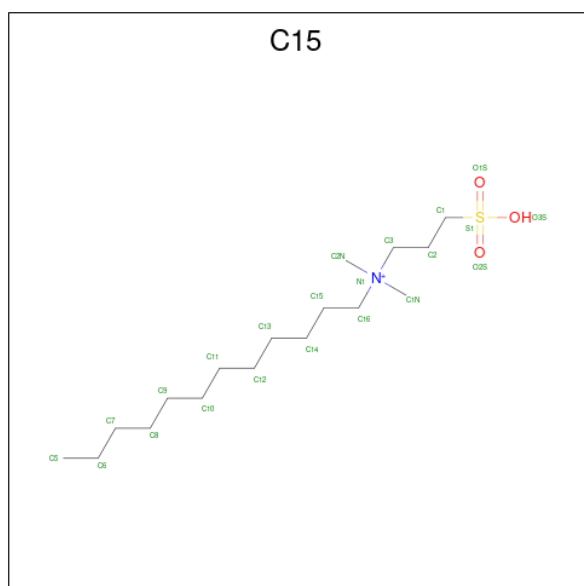
- Molecule 1 is a protein called Penton protein.

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 (CCD ID: 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		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	438.37Å 299.82Å 419.58Å 90.00° 103.22° 90.00°	Depositor
Resolution (Å)	29.98 – 3.50 29.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	53.6 (29.98-3.50) 53.6 (29.98-3.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.306 , 0.303 0.283 , 0.287	Depositor DCC
R_{free} test set	17745 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.14	EDS
Total number of atoms	3645	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.78	4/3602 (0.1%)	1.25	38/4904 (0.8%)
2	B	0.66	0/90	1.06	0/125
All	All	0.78	4/3692 (0.1%)	1.24	38/5029 (0.8%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	MET	SD-CE	5.51	1.93	1.79
1	A	379	ILE	CA-CB	5.46	1.61	1.54
1	A	482	TYR	C-O	5.31	1.30	1.23
1	A	450	THR	CA-CB	-5.29	1.44	1.53

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	482	TYR	N-CA-C	-17.64	91.39	113.97
1	A	265	GLN	CA-C-N	8.87	130.92	119.84
1	A	265	GLN	C-N-CA	8.87	130.92	119.84
1	A	468	LEU	CA-C-N	8.72	130.74	119.84
1	A	468	LEU	C-N-CA	8.72	130.74	119.84
1	A	441	LEU	CA-C-N	8.66	130.67	119.84
1	A	441	LEU	C-N-CA	8.66	130.67	119.84
1	A	106	ALA	N-CA-C	-7.72	102.81	111.14
1	A	96	ILE	N-CA-C	7.35	117.88	110.23
1	A	447	ASP	CA-C-N	7.25	128.90	119.84
1	A	447	ASP	C-N-CA	7.25	128.90	119.84
1	A	478	ASP	N-CA-C	-7.10	104.35	112.87
1	A	450	THR	N-CA-C	7.09	122.11	113.17
1	A	512	THR	N-CA-C	-6.61	100.50	110.28
1	A	203	GLU	N-CA-C	-6.50	104.28	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	ASN	N-CA-C	-6.28	99.46	109.76
1	A	237	HIS	CA-C-N	-6.22	113.57	119.85
1	A	237	HIS	C-N-CA	-6.22	113.57	119.85
1	A	154	THR	N-CA-C	6.18	119.10	109.52
1	A	74	ASN	N-CA-C	6.12	121.47	111.37
1	A	105	GLU	N-CA-C	-6.08	104.97	112.38
1	A	275	TYR	N-CA-C	-6.03	104.62	111.07
1	A	131	MET	CA-C-N	6.02	125.78	119.76
1	A	131	MET	C-N-CA	6.02	125.78	119.76
1	A	224	GLY	N-CA-C	-5.90	106.00	115.08
1	A	491	SER	N-CA-C	-5.52	100.80	109.25
1	A	493	THR	N-CA-C	5.51	117.77	109.23
1	A	152	SER	N-CA-C	5.48	118.02	109.52
1	A	267	PHE	N-CA-C	5.43	119.39	112.87
1	A	77	THR	N-CA-C	5.39	116.85	110.97
1	A	84	TYR	N-CA-C	-5.38	99.35	110.80
1	A	553	TYR	N-CA-C	5.35	119.37	113.21
1	A	551	CYS	CA-C-N	5.28	125.60	119.47
1	A	551	CYS	C-N-CA	5.28	125.60	119.47
1	A	494	HIS	N-CA-C	-5.21	105.63	112.72
1	A	542	THR	N-CA-C	5.21	117.09	108.13
1	A	495	VAL	CB-CA-C	-5.18	105.25	112.04
1	A	398	SER	N-CA-C	5.14	117.55	110.35

There are no chirality outliers.

There are no planarity outliers.

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	3519	0	3452	356	0
2	B	86	0	73	16	0
3	A	40	0	64	13	0
All	All	3645	0	3589	377	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 52.

All (377) 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: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:444:MET:HE1	1:A:561:VAL:HG21	1.39	1.02
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:HH11	1:A:68:ARG:HG2	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:179:MET:HE2	1:A:487:ARG:NH2	1.95	0.81
1:A:197:ARG:NE	1:A:198:GLN:HE21	1.80	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:214:ASN:HD22	1:A:214:ASN:C	1.93	0.77
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
1:A:378:VAL:HG23	1:A:379:ILE:N	2.01	0.74
3:A:1014:C15:H9C1	3:A:2000:C15:H132	1.69	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:130:ASN:HA	1:A:519:ASN:CG	2.16	0.71
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:440:SER:C	1:A:442:PRO:HD3	2.17	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:98:ASN:HD22	1:A:99:ASN:N	1.90	0.69
1:A:274:THR:HG22	1:A:276:ASP:N	2.06	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: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:179:MET:HE2	1:A:487:ARG:HH22	1.60	0.66
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:224:GLY:O	1:A:225:LEU:HD23	1.97	0.65
1:A:440:SER:HB3	1:A:461:PRO:O	1.97	0.65
1:A:145:ALA:HB3	1:A:168:PHE:CE1	2.31	0.65
1:A:57:TYR:O	1:A:58:SER:C	2.40	0.65
2:B:18:ASP:OD1	2:B:18:ASP:O	2.15	0.65
1:A:477:ASN:C	1:A:479:GLN:H	2.03	0.64
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:HG22	1:A:513:ILE:O	1.97	0.64
1:A:445:MET:HE3	1:A:529:LEU:HB2	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:171:PRO:O	1:A:174:ASN:ND2	2.32	0.63
1:A:134:VAL:HA	1:A:140:THR:OG1	1.98	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:436:GLN:NE2	1:A:438:TYR:HE2	1.96	0.63
1:A:477:ASN:C	1:A:479:GLN:N	2.53	0.63
1:A:98:ASN:HD22	1:A:98:ASN:C	2.06	0.62
1:A:498:ARG:C	1:A:499:PHE:HD2	2.08	0.61
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:385:ASP:OD1	1:A:389:ARG:HD2	2.00	0.61
1:A:481:VAL:HG12	1:A:481:VAL:O	2.00	0.61
1:A:498:ARG:C	1:A:499:PHE:CD2	2.78	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:52:ARG:N	1:A:116:ARG:HH12	2.00	0.60
1:A:378:VAL:CG2	1:A:379:ILE:H	2.14	0.60
1:A:210:PHE:CD2	1:A:240:ILE:HG22	2.37	0.59
1:A:378:VAL:CG2	1:A:379:ILE:N	2.65	0.59
1:A:159:VAL:HG23	1:A:159:VAL:O	2.00	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:493:THR:HB	1:A:495:VAL:HG23	1.84	0.59
2:B:18:ASP:O	2:B:18:ASP:CG	2.44	0.59
1:A:237:HIS:CD2	1:A:238:PRO:O	2.56	0.59
1:A:497:ASN:O	1:A:499:PHE:N	2.34	0.59
1:A:208:VAL:HG22	1:A:242:LEU:CD2	2.33	0.59
1:A:233:ASN:OD1	1:A:509:PRO:HG3	2.02	0.59
1:A:499:PHE:CD2	1:A:499:PHE:N	2.69	0.59
1:A:211:ASP:OD1	1:A:212:THR:N	2.31	0.59
1:A:389:ARG:HG2	1:A:389:ARG:HH11	1.67	0.59
1:A:435:GLU:OE1	1:A:435:GLU:HA	2.03	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:TYR:CD1	1:A:175:TYR:N	2.72	0.58
1:A:479:GLN:O	1:A:483:SER:N	2.36	0.58
2:B:15:TYR:HD2	2:B:16:PRO:N	2.02	0.58
1:A:279:GLU:O	1:A:280:GLY:C	2.45	0.58
1:A:538:VAL:HG23	1:A:538:VAL:O	2.02	0.57
1:A:273:ILE:O	1:A:273:ILE:HG23	2.02	0.57
1:A:175:TYR:HD1	1:A:175:TYR:H	1.52	0.57
1:A:295:SER:OG	1:A:377:PRO:HD3	2.03	0.57
1:A:411:ASN:OD1	1:A:411:ASN:N	2.36	0.57
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
1:A:558:LEU:C	1:A:558:LEU:HD12	2.30	0.56
1:A:378:VAL:C	1:A:380:LYS:N	2.62	0.56
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: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:130:ASN:HA	1:A:519:ASN:ND2	2.21	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
1:A:235:ALA:C	1:A:236:PHE:HD1	2.15	0.55
1:A:429:ASP:C	1:A:429:ASP:OD1	2.49	0.55
1:A:446:GLN:O	1:A:448:PRO:HD3	2.07	0.55
1:A:88:HIS:ND1	1:A:555:TYR:O	2.38	0.55
1:A:130:ASN:HD22	1:A:130:ASN:C	2.14	0.55
1:A:132:PRO:HD2	1:A:553:TYR:CE2	2.41	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:150:SER:HB3	1:A:199:ASN:HD22	1.71	0.55
1:A:197:ARG:HG3	1:A:198:GLN:HG3	1.89	0.55
1:A:113:LEU:O	1:A:114:ASP:C	2.47	0.54
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:98:ASN:C	1:A:98:ASN:ND2	2.66	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:O	1:A:216:ARG:N	2.41	0.54
1:A:171:PRO:HG2	1:A:174:ASN:ND2	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:CG	1:A:178:THR:N	2.71	0.54
1:A:444:MET:HB2	1:A:539:GLN:OE1	2.08	0.54
1:A:122:ASP:OD1	1:A:528:THR:CG2	2.56	0.53
1:A:497:ASN:O	1:A:500:PRO:HD3	2.08	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: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:391:TYR:O	1:A:392:ASN:C	2.51	0.53
1:A:406:TRP:HE1	1:A:419:ILE:HG21	1.73	0.53
1:A:249:ASP:C	1:A:249:ASP:OD1	2.51	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
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:151:ARG:HB3	1:A:201:VAL:N	2.24	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:74:ASN:O	1:A:75:LYS:C	2.52	0.52
1:A:394:ILE:HA	1:A:402:GLN:HE21	1.74	0.52
1:A:479:GLN:O	1:A:483:SER:HB3	2.07	0.52
1:A:57:TYR:OH	1:A:109:GLN:NE2	2.42	0.52
1:A:227:MET:HB2	1:A:228:PRO:HD3	1.92	0.52
1:A:420:ARG:HG2	1:A:420:ARG:O	2.10	0.52
1:A:243:LEU:HG	1:A:403:TYR:CE2	2.44	0.51
1:A:476:TYR:CD1	1:A:513:ILE:HD11	2.45	0.51
1:A:102:SER:O	1:A:103:PRO:C	2.52	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:178:THR:OG1	1:A:511:PRO:HD2	2.10	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:487:ARG:NH1	1:A:507:ARG:HH22	2.07	0.51
1:A:214:ASN:ND2	1:A:216:ARG:HB3	2.24	0.51
1:A:385:ASP:C	1:A:386:SER:O	2.52	0.51
1:A:378:VAL:C	1:A:380:LYS:H	2.19	0.50
3:A:1014:C15:H7C1	3:A:2000:C15:H9C1	1.94	0.50
2:B:15:TYR:HD2	2:B:16:PRO:HD2	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:THR:CG2	1:A:155:LYS:HG3	2.41	0.50
1:A:214:ASN:C	1:A:214:ASN:ND2	2.58	0.50
1:A:270:GLY:O	3:A:1014:C15:O1S	2.29	0.50
1:A:504:ILE:C	1:A:506:ALA:H	2.20	0.50
1:A:544:THR:HG22	1:A:545:ASP:N	2.27	0.50
1:A:389:ARG:HG2	1:A:389:ARG:NH1	2.26	0.49
1:A:135:ASN:H	1:A:140:THR:HG1	1.61	0.49
1:A:375:LYS:O	1:A:376:LYS:HG3	2.12	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:378:VAL:O	1:A:379:ILE:C	2.55	0.49
1:A:68:ARG:NH1	1:A:68:ARG:CG	2.67	0.49
1:A:151:ARG:CB	1:A:201:VAL:H	2.25	0.49
1:A:292:TYR:HD1	1:A:378:VAL:HG12	1.75	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
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: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: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:240:ILE:HD11	1:A:273:ILE:HG21	1.94	0.48
1:A:135:ASN:OD1	1:A:135:ASN:C	2.55	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:493:THR:HG22	1:A:494:HIS:N	2.27	0.48
1:A:130:ASN:HD22	1:A:130:ASN:N	2.10	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:244:PRO:HA	1:A:275:TYR:CD2	2.49	0.48
1:A:542:THR:HG22	1:A:542:THR:O	2.13	0.48
1:A:130:ASN:N	1:A:130:ASN:ND2	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:142:LYS:O	1:A:143:PHE:HB3	2.14	0.47
1:A:180:THR:HG21	1:A:258:LEU:CD2	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ASP:HB3	1:A:407:TYR:HB2	1.96	0.47
2:B:15:TYR:C	2:B:15:TYR:CD2	2.92	0.47
1:A:142:LYS:HG2	1:A:169:THR:HG22	1.97	0.47
1:A:456:GLN:O	1:A:458:SER:N	2.47	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:277:ASP:O	1:A:279:GLU:N	2.46	0.47
1:A:476:TYR:HD1	1:A:513:ILE:HD11	1.80	0.47
1:A:75:LYS:O	1:A:78:ASP:OD1	2.32	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:493:THR:HG22	1:A:495:VAL:N	2.29	0.47
1:A:215:PHE:CE1	1:A:241:ILE:HD11	2.49	0.46
1:A:544:THR:CG2	1:A:549:ARG:H	2.28	0.46
2:B:15:TYR:CD2	2:B:16:PRO:HD2	2.51	0.46
1:A:463:VAL:HB	1:A:529:LEU:CD1	2.44	0.46
3:A:1014:C15:H9C1	3:A:2000:C15:C13	2.41	0.46
1:A:289:VAL:HG13	1:A:290:ASP:N	2.30	0.46
1:A:449:VAL:HG12	1:A:450:THR:HG23	1.97	0.46
1:A:78:ASP:HB2	1:A:82:LEU:HD12	1.97	0.46
1:A:242:LEU:HD22	1:A:247:GLY:HA2	1.98	0.46
1:A:171:PRO:O	1:A:172:GLU:C	2.59	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: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:479:GLN:OE1	1:A:479:GLN:HA	2.16	0.45
1:A:243:LEU:HD21	1:A:403:TYR:CE2	2.51	0.45
1:A:487:ARG:CZ	1:A:507:ARG:HH22	2.29	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:123:LEU:HD13	1:A:561:VAL:HG22	1.98	0.45
1:A:483:SER:O	1:A:484:GLN:C	2.59	0.45
1:A:177:GLU:CG	1:A:178:THR:H	2.30	0.45
1:A:278:LEU:C	1:A:279:GLU:O	2.60	0.45
1:A:476:TYR:CD1	1:A:513:ILE:CD1	3.00	0.45
1:A:87:ASP:O	1:A:89:SER:N	2.46	0.44
1:A:132:PRO:CA	1:A:175:TYR:OH	2.53	0.44
1:A:171:PRO:O	1:A:172:GLU:O	2.35	0.44
1:A:202:LEU:N	1:A:202:LEU:HD23	2.33	0.44
1:A:231:TYR:H	1:A:503:GLN:HE21	1.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:THR:O	2:B:10:THR:CG2	2.60	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:250:PHE:O	1:A:251:THR:C	2.60	0.44
1:A:272:ARG:HH12	3:A:2000:C15:H1C1	1.83	0.44
1:A:381:PRO:O	1:A:382:LEU:C	2.61	0.44
1:A:460:PHE:O	1:A:548:ARG:NH2	2.50	0.44
1:A:448:PRO:HG2	1:A:462:VAL:O	2.17	0.44
1:A:237:HIS:HE1	1:A:426:CYS:O	2.00	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:189:VAL:O	1:A:192:TYR:N	2.51	0.44
1:A:386:SER:C	1:A:388:LYS:N	2.76	0.44
1:A:441:LEU:N	1:A:442:PRO:CD	2.79	0.44
3:A:1014:C15:H102	3:A:2000:C15:H9C1	2.00	0.44
1:A:130:ASN:C	1:A:130:ASN:ND2	2.76	0.44
1:A:207:GLY:HA3	1:A:246:CYS:SG	2.58	0.44
1:A:243:LEU:O	1:A:244:PRO:C	2.59	0.44
1:A:69:VAL:HG22	1:A:561:VAL:HB	2.00	0.44
1:A:113:LEU:HB3	1:A:119:TRP:CE2	2.53	0.44
1:A:383:THR:HG22	1:A:384:GLU:HG3	1.99	0.44
1:A:64:PHE:O	1:A:65:ASP:HB2	2.17	0.43
1:A:430:VAL:HG13	1:A:515:THR:HB	2.00	0.43
1:A:255:LEU:O	1:A:256:SER:C	2.61	0.43
1:A:384:GLU:HA	1:A:389:ARG:O	2.17	0.43
1:A:394:ILE:HG13	1:A:395:SER:N	2.32	0.43
1:A:508:PRO:HA	1:A:509:PRO:HD3	1.81	0.43
1:A:69:VAL:O	1:A:69:VAL:HG23	2.18	0.43
1:A:138:MET:HE3	1:A:254:ARG:NH1	2.33	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:99:ASN:OD1	1:A:99:ASN:C	2.62	0.43
1:A:181:ILE:O	1:A:184:MET:HB2	2.19	0.43
1:A:75:LYS:HE2	1:A:75:LYS:HB3	1.88	0.43
1:A:192:TYR:CD1	1:A:196:GLY:HA3	2.54	0.43
1:A:499:PHE:CD1	1:A:505:LEU:HB3	2.44	0.43
3:A:1014:C15:H102	3:A:2000:C15:C9	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:HG3	1:A:178:THR:H	1.82	0.43
1:A:268:GLN:O	1:A:269:GLU:C	2.62	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:430:VAL:C	1:A:432:CYS:N	2.76	0.42
1:A:95:VAL:HG12	1:A:95:VAL:O	2.19	0.42
1:A:109:GLN:C	1:A:110:THR:HG23	2.45	0.42
1:A:177:GLU:O	1:A:178:THR:C	2.63	0.42
2:B:15:TYR:HD2	2:B:15:TYR:C	2.28	0.42
1:A:419:ILE:C	1:A:421:SER:N	2.76	0.42
1:A:117:SER:HA	1:A:568:SER:HA	2.02	0.42
1:A:243:LEU:HD23	1:A:244:PRO:HD3	2.01	0.42
1:A:481:VAL:O	1:A:481:VAL:CG1	2.66	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:424:LEU:CD2	1:A:425:LEU:N	2.80	0.42
1:A:126:ILE:HG12	1:A:523:LEU:CD2	2.49	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:525:ASP:OD1	1:A:525:ASP:C	2.63	0.42
1:A:197:ARG:C	1:A:199:ASN:H	2.28	0.42
1:A:549:ARG:O	1:A:550:THR:C	2.63	0.42
1:A:73:ASP:OD1	1:A:73:ASP:N	2.53	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
1:A:200:GLY:O	1:A:201:VAL:C	2.62	0.41
1:A:444:MET:CE	1:A:561:VAL:HG21	2.28	0.41
3:A:1014:C15:H111	3:A:2000:C15:H141	2.01	0.41
1:A:476:TYR:CE2	1:A:478:ASP:CG	2.99	0.41
2:B:12:ASN:HA	2:B:13:PRO:HD3	1.90	0.41
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:CE	1:A:487:ARG:NH2	2.77	0.41
1:A:63:LEU:C	1:A:64:PHE:CD2	2.99	0.41
1:A:154:THR:CG2	1:A:155:LYS:H	2.34	0.41
1:A:403:TYR:CE1	1:A:504:ILE:HG12	2.56	0.41
1:A:419:ILE:C	1:A:421:SER:H	2.29	0.41
1:A:83:ASN:OD1	1:A:92:LEU:N	2.38	0.41
1:A:114:ASP:OD2	1:A:116:ARG:NH1	2.54	0.41
1:A:544:THR:HG21	1:A:548:ARG:HD2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:CYS:HA	1:A:552:PRO:HD3	1.89	0.41
3:A:1014:C15:H161	3:A:1014:C15:H2C1	1.72	0.41
1:A:196:GLY:O	1:A:201:VAL:HG12	2.21	0.40
1:A:565:VAL:CG1	1:A:566:LEU:N	2.84	0.40
2:B:18:ASP:O	2:B:19:THR:HB	2.21	0.40
1:A:53:ASN:O	1:A:53:ASN:ND2	2.55	0.40
1:A:211:ASP:C	1:A:212:THR:CG2	2.94	0.40
1:A:375:LYS:O	1:A:376:LYS:CG	2.70	0.40
1:A:441:LEU:O	1:A:443:ASP:N	2.54	0.40
1:A:150:SER:OG	1:A:162:LYS:HB2	2.21	0.40
1:A:283:ILE:HG22	1:A:284:PRO:O	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	436/523 (83%)	321 (74%)	69 (16%)	46 (11%)	0	5
2	B	8/21 (38%)	5 (62%)	3 (38%)	0	100	100
All	All	444/544 (82%)	326 (73%)	72 (16%)	46 (10%)	0	5

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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%)	367 (92%)	32 (8%)	11	35
2	B	10/20 (50%)	10 (100%)	0	100	100
All	All	409/471 (87%)	377 (92%)	32 (8%)	11	36

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

Mol	Chain	Res	Type
1	A	68	ARG
1	A	83	ASN
1	A	98	ASN
1	A	124	LYS
1	A	130	ASN
1	A	166	VAL
1	A	168	PHE
1	A	199	ASN
1	A	202	LEU
1	A	249	ASP
1	A	256	SER
1	A	276	ASP
1	A	279	GLU
1	A	401	THR
1	A	411	ASN
1	A	419	ILE
1	A	424	LEU
1	A	428	PRO
1	A	429	ASP
1	A	430	VAL
1	A	436	GLN
1	A	438	TYR
1	A	440	SER
1	A	450	THR
1	A	457	ILE
1	A	473	LYS
1	A	478	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	484	GLN
1	A	512	THR
1	A	542	THR
1	A	545	ASP
1	A	562	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) 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	268	GLN
1	A	402	GLN
1	A	436	GLN
1	A	459	ASN
1	A	471	HIS
1	A	488	GLN
1	A	503	GLN
1	A	526	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	2000	-	19,19,21	2.55	5 (26%)	21,21,26	2.23	7 (33%)
3	C15	A	1014	-	19,19,21	2.47	5 (26%)	21,21,26	1.68	6 (28%)

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	2000	-	-	9/17/17/21	-
3	C15	A	1014	-	-	8/17/17/21	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	C15	O3S-S1	8.07	1.77	1.47
3	A	1014	C15	O3S-S1	7.59	1.75	1.47
3	A	2000	C15	C1-S1	5.13	1.84	1.77
3	A	1014	C15	C1-S1	4.58	1.84	1.77
3	A	1014	C15	C10-C9	3.02	1.66	1.51
3	A	2000	C15	C15-C14	2.94	1.66	1.51
3	A	2000	C15	C14-C13	2.63	1.64	1.51
3	A	1014	C15	C12-C11	2.54	1.64	1.51
3	A	2000	C15	C15-C16	2.19	1.60	1.51
3	A	1014	C15	C9-C8	2.06	1.62	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	C15	C2-C1-S1	5.29	121.35	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	C15	O2S-S1-C1	5.15	114.51	106.73
3	A	1014	C15	O2S-S1-C1	4.64	113.75	106.73
3	A	2000	C15	C15-C16-N1	3.30	120.92	112.07
3	A	1014	C15	O3S-S1-C1	2.87	111.62	106.00
3	A	2000	C15	O3S-S1-O1S	-2.87	104.23	111.40
3	A	2000	C15	O3S-S1-C1	2.66	111.21	106.00
3	A	1014	C15	C2-C1-S1	2.52	117.11	113.25
3	A	2000	C15	O2S-S1-O1S	-2.48	105.77	113.82
3	A	1014	C15	O3S-S1-O1S	-2.44	105.30	111.40
3	A	2000	C15	C9-C8-C7	-2.20	103.23	114.37
3	A	1014	C15	C14-C13-C12	2.18	125.39	114.37
3	A	1014	C15	O2S-S1-O1S	-2.10	106.98	113.82

There are no chirality outliers.

All (17) torsion outliers are listed below:

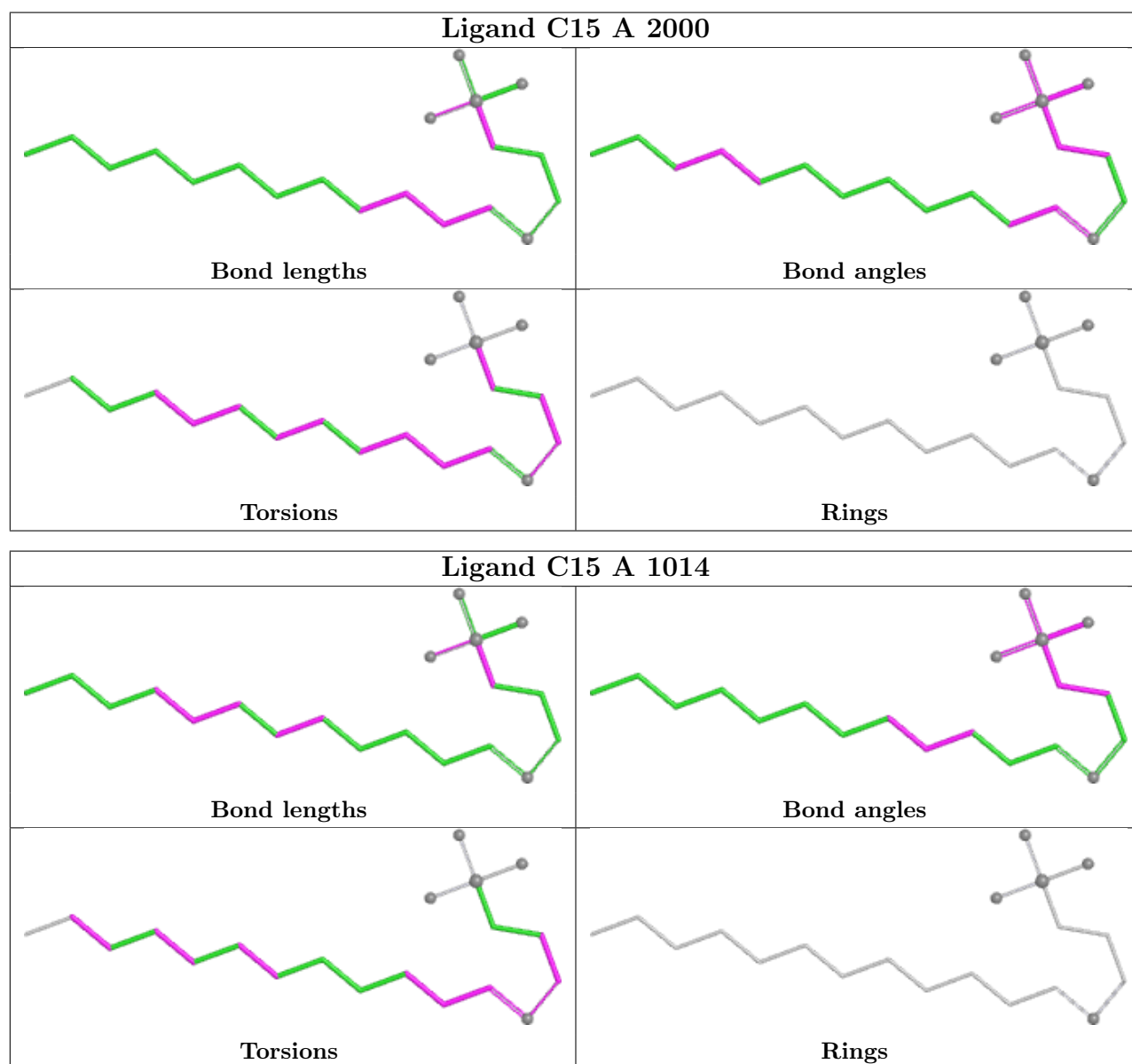
Mol	Chain	Res	Type	Atoms
3	A	1014	C15	C2-C3-N1-C16
3	A	2000	C15	C1-C2-C3-N1
3	A	2000	C15	C14-C15-C16-N1
3	A	1014	C15	C14-C15-C16-N1
3	A	1014	C15	C7-C8-C9-C10
3	A	1014	C15	C15-C16-N1-C3
3	A	1014	C15	C9-C10-C11-C12
3	A	2000	C15	C13-C14-C15-C16
3	A	2000	C15	C11-C10-C9-C8
3	A	1014	C15	C13-C14-C15-C16
3	A	2000	C15	C7-C8-C9-C10
3	A	2000	C15	C2-C3-N1-C16
3	A	2000	C15	C2-C1-S1-O3S
3	A	2000	C15	C12-C13-C14-C15
3	A	1014	C15	C1-C2-C3-N1
3	A	2000	C15	C10-C11-C12-C13
3	A	1014	C15	C5-C6-C7-C8

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2000	C15	11	0
3	A	1014	C15	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	440/523 (84%)	1.18	75 (17%) 4 4	50, 74, 113, 130	0
2	B	10/21 (47%)	1.33	2 (20%) 3 3	104, 109, 126, 129	0
All	All	450/544 (82%)	1.18	77 (17%) 4 4	50, 74, 114, 130	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	LYS	6.6
1	A	147	VAL	4.3
1	A	481	VAL	4.3
1	A	506	ALA	4.1
1	A	520	VAL	4.0
2	B	19	THR	3.9
1	A	207	GLY	3.9
1	A	549	ARG	3.7
1	A	206	ILE	3.7
1	A	145	ALA	3.7
1	A	489	PHE	3.7
1	A	414	ASP	3.6
1	A	272	ARG	3.4
1	A	156	ASP	3.4
1	A	473	LYS	3.4
1	A	153	LEU	3.4
1	A	527	GLY	3.3
1	A	388	LYS	3.2
1	A	502	ASN	3.2
1	A	378	VAL	3.2
1	A	281	GLY	3.1
1	A	230	VAL	3.1
1	A	160	GLU	3.0
1	A	158	GLN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	379	ILE	3.0
1	A	289	VAL	3.0
1	A	533	ASN	2.9
1	A	469	PRO	2.9
1	A	149	VAL	2.9
1	A	545	ASP	2.8
1	A	484	GLN	2.8
1	A	166	VAL	2.8
2	B	10	THR	2.8
1	A	259	LEU	2.8
1	A	380	LYS	2.8
1	A	238	PRO	2.7
1	A	276	ASP	2.7
1	A	479	GLN	2.7
1	A	121	GLY	2.6
1	A	480	ALA	2.6
1	A	177	GLU	2.6
1	A	154	THR	2.6
1	A	152	SER	2.6
1	A	490	THR	2.5
1	A	249	ASP	2.5
1	A	408	LEU	2.5
1	A	433	GLY	2.5
1	A	244	PRO	2.4
1	A	161	LEU	2.4
1	A	406	TRP	2.4
1	A	277	ASP	2.4
1	A	270	GLY	2.3
1	A	563	PRO	2.3
1	A	492	LEU	2.3
1	A	398	SER	2.3
1	A	494	HIS	2.3
1	A	279	GLU	2.3
1	A	522	ALA	2.2
1	A	228	PRO	2.2
1	A	294	ALA	2.2
1	A	268	GLN	2.2
1	A	232	THR	2.2
1	A	443	ASP	2.2
1	A	180	THR	2.2
1	A	431	THR	2.2
1	A	251	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	275	TYR	2.1
1	A	137	PHE	2.1
1	A	155	LYS	2.1
1	A	375	LYS	2.1
1	A	226	VAL	2.1
1	A	192	TYR	2.1
1	A	65	ASP	2.1
1	A	140	THR	2.1
1	A	162	LYS	2.1
1	A	477	ASN	2.0
1	A	111	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

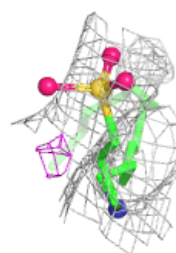
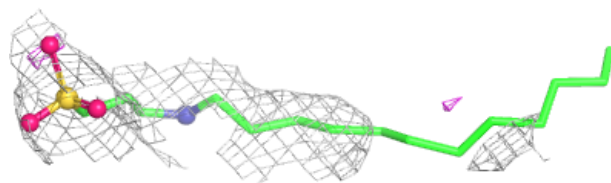
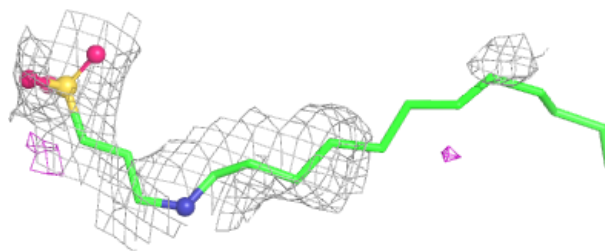
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	C15	A	1014	20/22	0.81	0.38	107,120,124,125	0
3	C15	A	2000	20/22	0.84	0.30	127,133,139,139	0

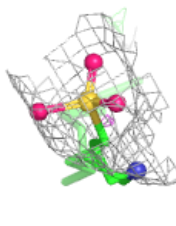
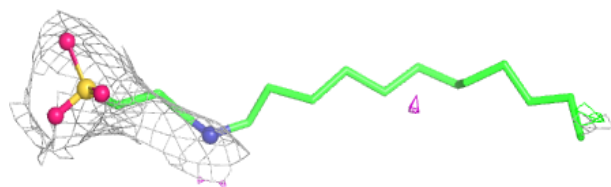
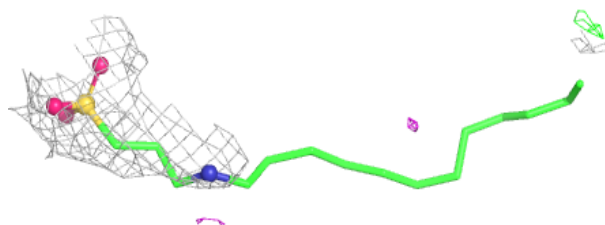
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around C15 A 1014:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around C15 A 2000:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.