



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:56 AM UTC

PDB ID : 2OPS / pdb\_00002ops  
Title : Crystal Structure of Y188C Mutant HIV-1 Reverse Transcriptase in Complex with GW420867X.  
Authors : Ren, J.; Nichols, C.E.; Chamberlain, P.P.; Weaver, K.L.; Short, S.A.; Chan, J.H.; Kleim, J.; Stammers, D.K.  
Deposited on : 2007-01-30  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

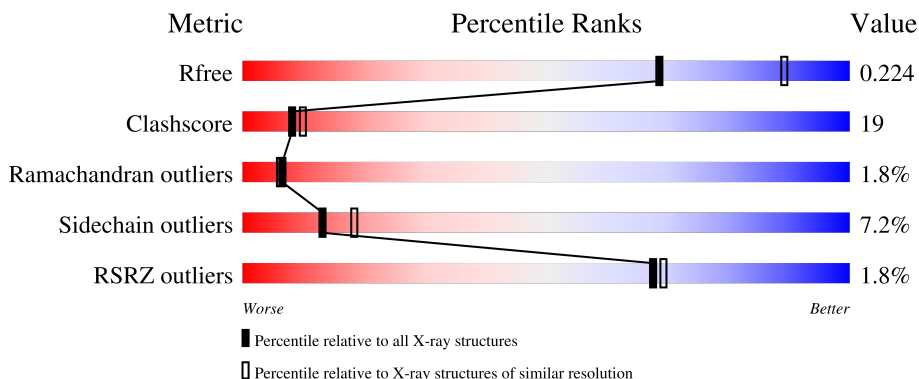
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	542	 2% 61% 32% 6%
2	B	435	 2% 55% 34% 6%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7928 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	536	4374	2829	729	807	9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	CYS	TYR	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	409	3373	2190	561	614	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

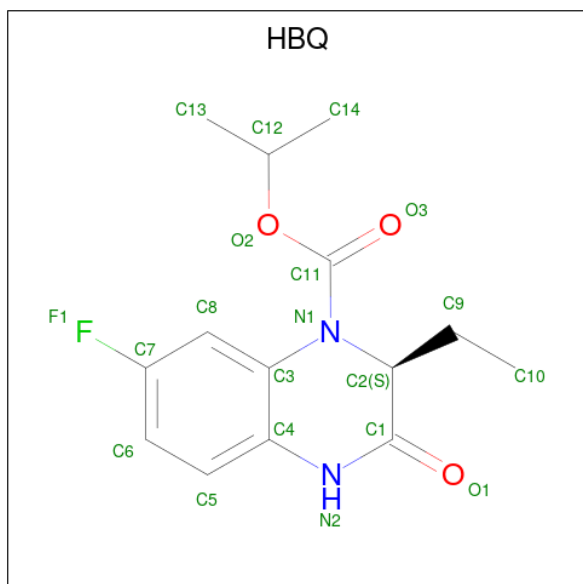
Chain	Residue	Modelled	Actual	Comment	Reference
B	188	CYS	TYR	engineered mutation	UNP P04585

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is ISOPROPYL (2S)-2-ETHYL-7-FLUORO-3-OXO-3,4-DIHYDROQUINOXALINE-1(2H)-CARBOXYLATE (CCD ID: HBQ) (formula: C<sub>14</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N O 20 14 1 2 3	0	0

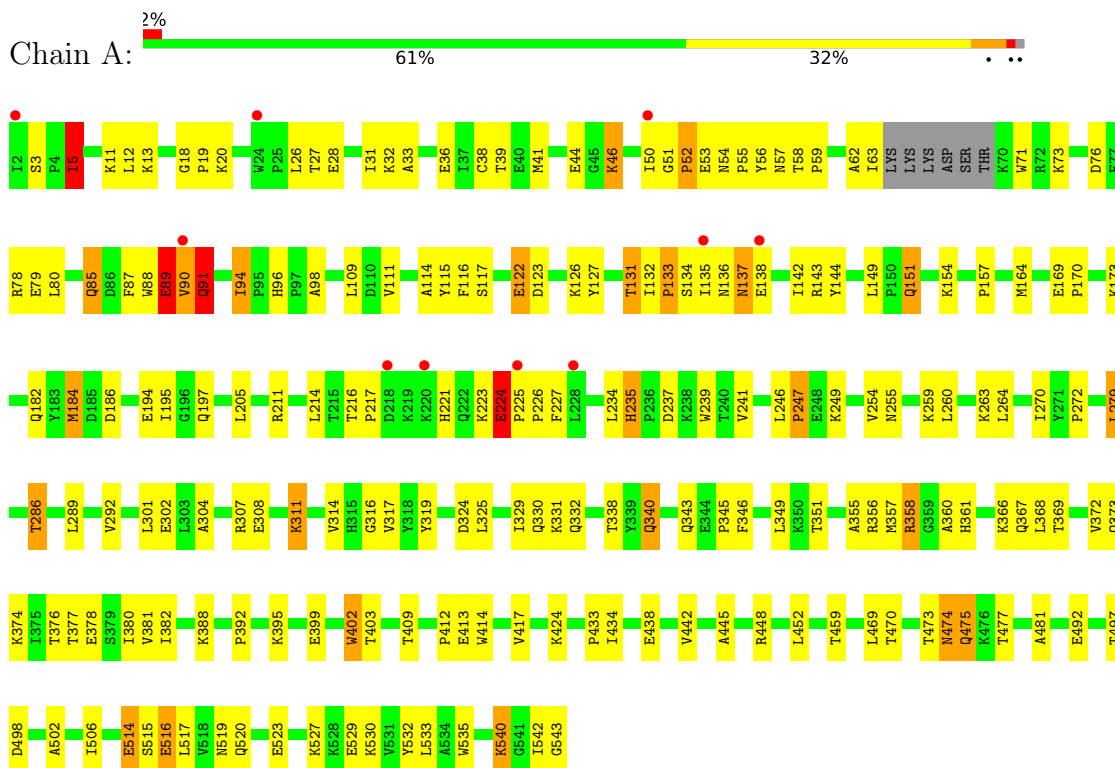
- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	93	Total 93	O 93	0	0
5	B	58	Total 58	O 58	0	0

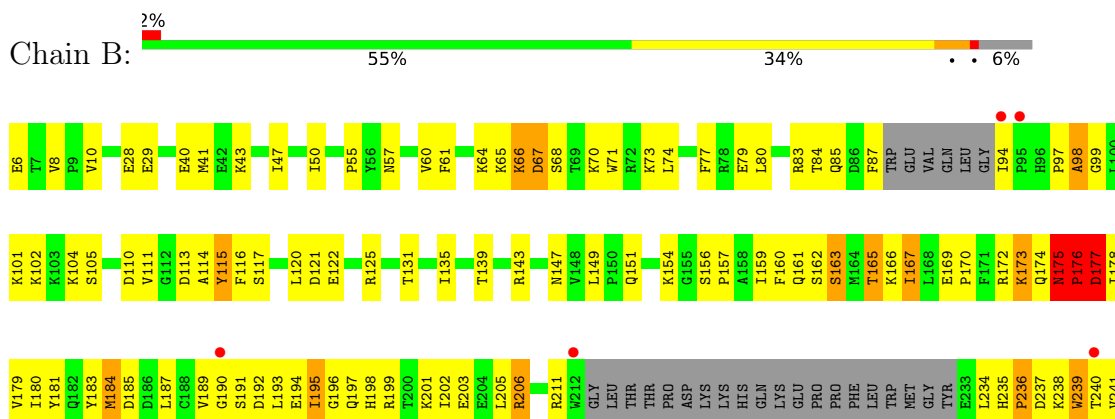
### 3 Residue-property plots

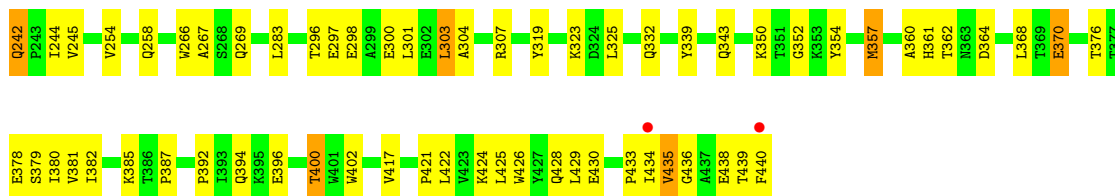
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 2: p51 RT





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.50Å 110.30Å 72.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.45 – 2.30 24.45 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (24.45-2.30) 98.6 (24.45-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.31Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.218 , 0.301 0.204 , 0.224	Depositor DCC
$R_{free}$ test set	2472 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.3	Xtrriage
Anisotropy	0.409	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 62.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7928	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: HBQ, CSD, PO4

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	0/4480	1.07	22/6089 (0.4%)
2	B	0.62	1/3465 (0.0%)	1.08	22/4703 (0.5%)
All	All	0.61	1/7945 (0.0%)	1.07	44/10792 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	357	MET	SD-CE	5.17	1.92	1.79

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLU	N-CA-C	9.78	123.89	109.42
2	B	177	ASP	N-CA-C	-8.03	101.05	113.02
2	B	195	ILE	N-CA-C	7.52	118.05	110.23
2	B	115	TYR	N-CA-C	7.38	119.32	111.28
1	A	235	HIS	N-CA-C	-7.36	99.21	110.32
1	A	388	LYS	N-CA-C	-7.27	97.75	109.96
1	A	54	ASN	CA-C-N	7.20	126.70	118.85
1	A	54	ASN	C-N-CA	7.20	126.70	118.85
1	A	3	SER	CA-C-N	7.19	127.19	119.28
1	A	3	SER	C-N-CA	7.19	127.19	119.28
1	A	5	ILE	N-CA-C	7.12	118.29	108.89
1	A	349	LEU	N-CA-C	-6.88	104.52	113.12
2	B	435	VAL	N-CA-C	-6.86	106.35	111.90
1	A	39	THR	N-CA-C	-6.69	102.41	112.04
1	A	224	GLU	CA-C-N	6.67	127.25	120.38
1	A	224	GLU	C-N-CA	6.67	127.25	120.38
2	B	241	VAL	N-CA-C	-6.65	98.80	108.71
2	B	382	ILE	N-CA-C	6.59	117.93	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	LYS	N-CA-C	6.44	119.58	110.50
2	B	43	LYS	N-CA-C	-6.38	104.01	110.97
1	A	131	THR	N-CA-C	6.35	119.92	108.69
1	A	195	ILE	N-CA-C	6.33	117.83	110.62
1	A	135	ILE	N-CA-C	-6.07	104.72	110.42
2	B	147	ASN	N-CA-C	-6.04	106.44	113.88
2	B	428	GLN	N-CA-C	-5.93	105.31	112.54
2	B	402	TRP	N-CA-C	5.90	117.72	111.28
2	B	242	GLN	CA-C-N	5.90	126.79	120.13
2	B	242	GLN	C-N-CA	5.90	126.79	120.13
2	B	343	GLN	N-CA-C	-5.84	106.80	114.04
1	A	154	LYS	N-CA-C	5.63	117.87	111.11
2	B	269	GLN	N-CA-C	-5.63	106.36	113.18
2	B	417	VAL	N-CA-C	5.60	116.97	108.80
2	B	360	ALA	N-CA-C	-5.57	104.72	113.02
2	B	131	THR	N-CA-C	5.55	117.47	108.26
2	B	50	ILE	N-CA-C	5.49	118.00	108.95
2	B	438	GLU	N-CA-C	5.27	117.09	110.24
2	B	175	ASN	CA-C-N	5.18	126.31	119.84
2	B	175	ASN	C-N-CA	5.18	126.31	119.84
1	A	184	MET	CB-CA-C	-5.17	110.59	116.54
2	B	352	GLY	N-CA-C	5.07	117.97	110.42
1	A	311	LYS	N-CA-C	-5.05	105.86	111.36
1	A	319	TYR	N-CA-C	5.05	117.84	109.46
1	A	514	GLU	N-CA-C	-5.04	105.26	111.40
1	A	331	LYS	N-CA-C	-5.03	99.60	108.20

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	4374	0	4414	178	1
2	B	3373	0	3408	130	1
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
4	A	20	0	17	0	0
5	A	93	0	0	6	0
5	B	58	0	0	3	0
All	All	7928	0	7839	303	1

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 19.

All (303) 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)
2:B:172:ARG:O	2:B:176:PRO:HD3	1.56	1.06
1:A:96:HIS:HD2	1:A:98:ALA:H	1.14	0.94
1:A:51:GLY:H	1:A:52:PRO:HD2	1.36	0.91
1:A:225:PRO:HG3	1:A:227:PHE:CZ	2.05	0.91
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.53	0.90
2:B:195:ILE:HD11	2:B:199:ARG:NH2	1.90	0.87
2:B:163:SER:O	2:B:167:ILE:HG23	1.76	0.85
2:B:175:ASN:O	2:B:177:ASP:N	2.11	0.84
2:B:169:GLU:HA	2:B:173:LYS:HZ3	1.42	0.83
1:A:96:HIS:CD2	1:A:98:ALA:H	1.97	0.82
2:B:296:THR:HG22	2:B:298:GLU:H	1.43	0.82
1:A:357:MET:HB2	1:A:367:GLN:NE2	1.95	0.81
1:A:109:LEU:HG	1:A:216:THR:HG21	1.61	0.81
1:A:94:ILE:HD13	1:A:94:ILE:H	1.45	0.81
2:B:161:GLN:O	2:B:165:THR:HG22	1.82	0.79
1:A:57:ASN:HD22	1:A:143:ARG:NH2	1.80	0.79
1:A:136:ASN:ND2	1:A:138:GLU:HB3	1.98	0.79
2:B:180:ILE:HG12	2:B:189:VAL:HG12	1.65	0.78
1:A:50:ILE:HG13	1:A:51:GLY:H	1.50	0.77
1:A:32:LYS:HA	1:A:32:LYS:HE2	1.67	0.76
2:B:433:PRO:HB2	2:B:436:GLY:HA2	1.69	0.73
1:A:90:VAL:HG21	1:A:157:PRO:HB2	1.68	0.73
1:A:136:ASN:O	1:A:138:GLU:N	2.21	0.73
1:A:57:ASN:HD21	1:A:131:THR:HG22	1.53	0.73
1:A:182:GLN:HB2	5:A:1015:HOH:O	1.87	0.72
1:A:226:PRO:HG3	1:A:235:HIS:ND1	2.06	0.71
2:B:332:GLN:NE2	2:B:424:LYS:HE2	2.05	0.70
1:A:225:PRO:HG3	1:A:227:PHE:HZ	1.56	0.70
1:A:516:GLU:O	1:A:520:GLN:HG3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ILE:HB	1:A:142:ILE:HB	1.74	0.70
1:A:378:GLU:O	1:A:382:ILE:HG12	1.91	0.69
2:B:379:SER:OG	2:B:387:PRO:HD3	1.91	0.69
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.75	0.69
1:A:226:PRO:HA	1:A:234:LEU:O	1.93	0.69
1:A:514:GLU:HG3	1:A:515:SER:H	1.58	0.69
1:A:270:ILE:CG2	1:A:314:VAL:HG11	2.23	0.68
1:A:332:GLN:HG3	5:A:1030:HOH:O	1.92	0.68
1:A:217:PRO:HB3	1:A:221:HIS:HB2	1.74	0.68
2:B:350:LYS:HE2	2:B:378:GLU:OE2	1.94	0.68
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.29	0.67
1:A:41:MET:HG2	1:A:46:LYS:HE3	1.76	0.67
2:B:396:GLU:O	2:B:400:THR:HG23	1.94	0.67
1:A:122:GLU:H	1:A:122:GLU:CD	2.02	0.67
1:A:51:GLY:N	1:A:52:PRO:HD2	2.09	0.67
1:A:51:GLY:H	1:A:52:PRO:CD	2.08	0.66
2:B:254:VAL:O	2:B:258:GLN:HG3	1.96	0.66
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.31	0.66
1:A:360:ALA:HA	1:A:514:GLU:HG2	1.78	0.66
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.31	0.65
1:A:308:GLU:OE1	1:A:311:LYS:HE2	1.96	0.65
2:B:193:LEU:HD13	2:B:201:LYS:HE3	1.79	0.65
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.63	0.64
1:A:57:ASN:HD21	1:A:131:THR:CG2	2.09	0.64
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.27	0.64
2:B:194:GLU:OE1	2:B:197:GLN:HG3	1.98	0.64
1:A:357:MET:HE2	1:A:374:LYS:HE3	1.78	0.64
2:B:172:ARG:C	2:B:174:GLN:H	2.05	0.64
2:B:193:LEU:HD13	2:B:201:LYS:CE	2.28	0.64
2:B:421:PRO:O	2:B:425:LEU:HD13	1.98	0.64
2:B:29:GLU:CD	2:B:71:TRP:HZ2	2.06	0.63
2:B:193:LEU:HD13	2:B:201:LYS:CD	2.29	0.63
2:B:239:TRP:O	2:B:240:THR:HG23	1.98	0.63
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.81	0.63
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.34	0.63
1:A:57:ASN:HD22	1:A:143:ARG:HH21	1.44	0.63
1:A:96:HIS:HD2	1:A:98:ALA:N	1.93	0.63
2:B:79:GLU:O	2:B:83:ARG:HG3	1.99	0.63
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.80	0.62
1:A:51:GLY:N	1:A:52:PRO:CD	2.61	0.62
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:TRP:CD1	2:B:239:TRP:N	2.67	0.61
1:A:542:ILE:HG22	1:A:543:GLY:N	2.15	0.61
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.61	0.61
1:A:324:ASP:O	1:A:343:GLN:HG2	2.00	0.61
1:A:50:ILE:HG13	1:A:51:GLY:N	2.14	0.60
1:A:136:ASN:C	1:A:138:GLU:N	2.59	0.60
2:B:396:GLU:O	2:B:400:THR:CG2	2.50	0.60
1:A:217:PRO:CB	1:A:221:HIS:HB2	2.32	0.60
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.84	0.59
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.01	0.59
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.67	0.59
2:B:105:SER:O	2:B:190:GLY:HA2	2.02	0.59
1:A:62:ALA:C	1:A:63:ILE:HD12	2.27	0.59
1:A:211:ARG:HG2	1:A:211:ARG:NH1	2.16	0.59
2:B:170:PRO:O	2:B:174:GLN:HB2	2.03	0.59
1:A:57:ASN:ND2	1:A:143:ARG:HH21	2.01	0.58
1:A:117:SER:HB2	1:A:214:LEU:HD23	1.85	0.58
1:A:123:ASP:O	1:A:126:LYS:HE3	2.02	0.58
1:A:357:MET:HB2	1:A:367:GLN:HE22	1.67	0.58
1:A:346:PHE:N	1:A:346:PHE:CD2	2.70	0.58
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.68	0.58
2:B:169:GLU:HA	2:B:173:LYS:NZ	2.15	0.58
1:A:33:ALA:HB1	1:A:71:TRP:HB2	1.84	0.57
1:A:19:PRO:O	1:A:56:TYR:HA	2.04	0.57
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.39	0.57
1:A:540:LYS:HB3	1:A:542:ILE:HG13	1.87	0.57
1:A:301:LEU:C	1:A:301:LEU:HD23	2.29	0.57
2:B:6:GLU:HG2	2:B:6:GLU:O	2.05	0.57
1:A:44:GLU:OE1	1:A:46:LYS:HE2	2.06	0.56
1:A:57:ASN:ND2	1:A:131:THR:HG22	2.21	0.56
2:B:169:GLU:HG2	2:B:173:LYS:NZ	2.20	0.56
2:B:197:GLN:HB3	2:B:201:LYS:HE2	1.87	0.56
1:A:32:LYS:HE2	1:A:32:LYS:CA	2.35	0.56
1:A:11:LYS:O	1:A:85:GLN:HB3	2.06	0.56
1:A:194:GLU:HB2	1:A:197:GLN:HE21	1.71	0.56
1:A:409:THR:O	2:B:364:ASP:HB2	2.07	0.55
2:B:339:TYR:OH	2:B:350:LYS:HE3	2.07	0.55
1:A:357:MET:HE2	1:A:374:LYS:CE	2.37	0.55
1:A:542:ILE:HG22	1:A:543:GLY:H	1.72	0.55
1:A:358:ARG:HG2	1:A:358:ARG:NH1	2.22	0.55
2:B:172:ARG:O	2:B:174:GLN:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PHE:CZ	1:A:151:GLN:HB2	2.42	0.54
2:B:60:VAL:HG21	2:B:73:LYS:HZ2	1.72	0.54
2:B:84:THR:HB	2:B:154:LYS:HE2	1.89	0.54
1:A:301:LEU:HD23	1:A:302:GLU:N	2.23	0.54
1:A:28:GLU:O	1:A:32:LYS:HG2	2.07	0.54
2:B:376:THR:O	2:B:380:ILE:HG13	2.08	0.54
2:B:122:GLU:HA	2:B:122:GLU:OE2	2.07	0.53
1:A:402:TRP:CD1	1:A:402:TRP:C	2.87	0.53
2:B:169:GLU:HG2	2:B:173:LYS:HZ1	1.72	0.53
2:B:195:ILE:O	2:B:199:ARG:HG3	2.09	0.53
2:B:193:LEU:HD22	2:B:201:LYS:HE3	1.90	0.52
1:A:58:THR:HG23	1:A:76:ASP:O	2.09	0.52
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.91	0.52
2:B:97:PRO:O	2:B:99:GLY:N	2.43	0.52
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.92	0.52
1:A:116:PHE:HZ	1:A:151:GLN:HB2	1.74	0.52
1:A:20:LYS:HE3	1:A:55:PRO:CB	2.40	0.52
1:A:402:TRP:CH2	2:B:362:THR:HA	2.45	0.52
1:A:376:THR:O	1:A:380:ILE:HG12	2.09	0.51
2:B:175:ASN:N	2:B:176:PRO:CD	2.72	0.51
1:A:63:ILE:HD12	1:A:63:ILE:N	2.25	0.51
2:B:354:TYR:OH	2:B:370:GLU:HB3	2.11	0.51
1:A:473:THR:HB	5:A:1072:HOH:O	2.10	0.51
1:A:117:SER:CB	1:A:214:LEU:HD23	2.41	0.51
1:A:279:LEU:HD23	1:A:302:GLU:OE1	2.10	0.51
1:A:301:LEU:O	1:A:304:ALA:HB3	2.10	0.51
1:A:502:ALA:O	1:A:506:ILE:HG13	2.11	0.51
1:A:514:GLU:HG3	1:A:515:SER:N	2.24	0.51
1:A:12:LEU:O	1:A:13:LYS:C	2.54	0.51
1:A:225:PRO:CG	1:A:227:PHE:CZ	2.89	0.51
1:A:519:ASN:O	1:A:523:GLU:HG2	2.11	0.51
2:B:195:ILE:HG23	2:B:196:GLY:H	1.74	0.51
1:A:237:ASP:OD2	1:A:237:ASP:N	2.43	0.51
1:A:246:LEU:O	1:A:307:ARG:NH1	2.44	0.50
1:A:114:ALA:HB1	1:A:214:LEU:HD22	1.93	0.50
2:B:424:LYS:HD2	2:B:425:LEU:HD12	1.94	0.50
1:A:19:PRO:HG2	1:A:80:LEU:HB2	1.94	0.50
1:A:217:PRO:HB3	1:A:221:HIS:CB	2.42	0.50
1:A:270:ILE:HG22	1:A:314:VAL:HG11	1.94	0.50
2:B:357:MET:HE2	2:B:370:GLU:CD	2.36	0.50
1:A:279:LEU:CD2	1:A:302:GLU:OE1	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:HIS:C	2:B:237:ASP:H	2.20	0.49
2:B:245:VAL:HG22	2:B:429:LEU:O	2.12	0.49
2:B:361:HIS:HB3	5:B:1153:HOH:O	2.11	0.49
2:B:193:LEU:HD13	2:B:201:LYS:HD3	1.94	0.49
1:A:19:PRO:HG3	1:A:80:LEU:HA	1.94	0.49
1:A:88:TRP:O	1:A:89:GLU:CB	2.60	0.49
1:A:136:ASN:C	1:A:138:GLU:H	2.19	0.49
1:A:164:MET:HB3	1:A:182:GLN:NE2	2.28	0.49
1:A:260:LEU:O	1:A:264:LEU:HD23	2.13	0.49
1:A:368:LEU:O	1:A:372:VAL:HG23	2.12	0.49
2:B:97:PRO:HG3	2:B:181:TYR:HB2	1.94	0.49
2:B:111:VAL:HG23	2:B:111:VAL:O	2.12	0.49
1:A:498:ASP:C	1:A:498:ASP:OD1	2.55	0.49
1:A:329:ILE:O	1:A:392:PRO:HD3	2.12	0.49
1:A:492:GLU:HA	1:A:530:LYS:O	2.14	0.48
1:A:452:LEU:HD23	1:A:470:THR:HG22	1.94	0.48
2:B:120:LEU:O	2:B:121:ASP:C	2.56	0.48
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.95	0.48
2:B:301:LEU:O	2:B:304:ALA:HB3	2.13	0.48
1:A:50:ILE:O	1:A:143:ARG:HB2	2.14	0.48
2:B:97:PRO:HB2	2:B:179:VAL:HG11	1.96	0.48
2:B:198:HIS:O	2:B:202:ILE:HG12	2.13	0.48
1:A:226:PRO:CG	1:A:235:HIS:ND1	2.76	0.48
2:B:297:GLU:O	2:B:300:GLU:HB3	2.13	0.48
2:B:235:HIS:O	2:B:237:ASP:N	2.47	0.47
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.37	0.47
2:B:183:TYR:O	2:B:184:MET:C	2.57	0.47
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.44	0.47
1:A:5:ILE:H	1:A:5:ILE:HG12	1.41	0.47
1:A:211:ARG:HH11	1:A:211:ARG:CG	2.28	0.47
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.95	0.47
2:B:172:ARG:C	2:B:174:GLN:N	2.72	0.47
1:A:90:VAL:O	1:A:91:GLN:C	2.58	0.47
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.49	0.47
2:B:94:ILE:O	2:B:94:ILE:HG13	2.15	0.47
1:A:51:GLY:HA2	1:A:143:ARG:HD3	1.96	0.47
1:A:117:SER:HB2	1:A:214:LEU:CD2	2.45	0.47
1:A:366:LYS:NZ	2:B:394:GLN:NE2	2.62	0.46
2:B:98:ALA:O	2:B:101:LYS:HG2	2.14	0.46
2:B:175:ASN:C	2:B:177:ASP:H	2.21	0.46
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:H	1:A:94:ILE:CD1	2.24	0.46
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.15	0.46
2:B:433:PRO:HB2	2:B:436:GLY:CA	2.43	0.46
2:B:159:ILE:HG22	2:B:159:ILE:O	2.14	0.46
1:A:523:GLU:O	1:A:527:LYS:HG3	2.15	0.46
1:A:373:GLN:HG2	5:A:1038:HOH:O	2.16	0.46
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.34	0.46
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.51	0.46
1:A:330:GLN:HB2	1:A:338:THR:OG1	2.15	0.46
2:B:41:MET:HE2	2:B:47:ILE:HG23	1.96	0.46
2:B:242:GLN:HB2	2:B:430:GLU:CD	2.41	0.46
1:A:136:ASN:O	1:A:137:ASN:C	2.58	0.46
2:B:28:GLU:HA	2:B:135:ILE:HD11	1.97	0.46
2:B:206:ARG:HG3	2:B:206:ARG:HH11	1.81	0.46
1:A:239:TRP:CH2	1:A:316:GLY:HA3	2.51	0.45
2:B:434:ILE:HD12	2:B:434:ILE:N	2.31	0.45
2:B:161:GLN:HB3	5:B:1142:HOH:O	2.15	0.45
1:A:412:PRO:O	1:A:413:GLU:C	2.60	0.45
1:A:109:LEU:CG	1:A:216:THR:HG21	2.40	0.45
1:A:346:PHE:N	1:A:346:PHE:HD2	2.14	0.45
1:A:58:THR:CG2	1:A:76:ASP:O	2.63	0.45
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.31	0.45
1:A:109:LEU:HG	1:A:216:THR:CG2	2.40	0.45
2:B:376:THR:O	2:B:379:SER:HB3	2.17	0.44
1:A:260:LEU:HG	1:A:264:LEU:CD2	2.47	0.44
1:A:239:TRP:CD2	1:A:316:GLY:HA3	2.53	0.44
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.52	0.44
2:B:65:LYS:NZ	2:B:110:ASP:OD1	2.51	0.44
1:A:241:VAL:HG23	1:A:314:VAL:O	2.17	0.44
2:B:64:LYS:HE2	2:B:71:TRP:CE2	2.53	0.44
2:B:303:LEU:O	2:B:307:ARG:HG3	2.18	0.44
2:B:325:LEU:HB2	2:B:385:LYS:HE3	2.00	0.44
2:B:439:THR:HG22	2:B:439:THR:O	2.17	0.44
1:A:44:GLU:HB2	1:A:46:LYS:HD3	2.00	0.44
1:A:417:VAL:O	1:A:417:VAL:HG13	2.18	0.44
2:B:66:LYS:O	2:B:67:ASP:O	2.36	0.43
2:B:175:ASN:N	2:B:176:PRO:HD3	2.33	0.43
1:A:366:LYS:NZ	2:B:394:GLN:HE21	2.15	0.43
1:A:445:ALA:HA	1:A:474:ASN:HD21	1.84	0.43
1:A:41:MET:SD	1:A:73:LYS:HE3	2.58	0.43
1:A:50:ILE:HG13	1:A:52:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:VAL:HB	1:A:289:LEU:O	2.18	0.43
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.16	0.43
2:B:113:ASP:O	2:B:116:PHE:CD2	2.71	0.43
2:B:65:LYS:O	2:B:66:LYS:C	2.60	0.43
2:B:77:PHE:CD2	2:B:80:LEU:HD23	2.54	0.43
2:B:195:ILE:HG23	2:B:196:GLY:N	2.33	0.43
1:A:434:ILE:HG23	5:A:1062:HOH:O	2.19	0.43
1:A:26:LEU:CD1	1:A:133:PRO:HG2	2.48	0.43
1:A:254:VAL:HG22	1:A:286:THR:HG21	2.00	0.43
2:B:245:VAL:O	2:B:245:VAL:HG23	2.19	0.43
1:A:26:LEU:HD12	1:A:133:PRO:HG2	2.00	0.43
2:B:68:SER:C	2:B:70:LYS:H	2.27	0.43
1:A:366:LYS:HZ2	2:B:394:GLN:NE2	2.16	0.43
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.84	0.42
1:A:434:ILE:HD11	1:A:530:LYS:HB3	1.98	0.42
2:B:154:LYS:O	2:B:157:PRO:HD2	2.18	0.42
1:A:88:TRP:O	1:A:89:GLU:HB3	2.19	0.42
1:A:90:VAL:O	1:A:91:GLN:O	2.38	0.42
2:B:379:SER:CB	2:B:387:PRO:HD3	2.49	0.42
1:A:87:PHE:O	1:A:88:TRP:C	2.60	0.42
2:B:85:GLN:NE2	2:B:87:PHE:CE1	2.88	0.42
2:B:98:ALA:O	2:B:101:LYS:HE3	2.19	0.42
1:A:224:GLU:HA	1:A:225:PRO:HD3	1.62	0.42
2:B:162:SER:N	5:B:1142:HOH:O	2.31	0.42
2:B:197:GLN:HB3	2:B:201:LYS:CE	2.49	0.42
1:A:111:VAL:O	1:A:114:ALA:HB3	2.19	0.42
2:B:195:ILE:CD1	2:B:199:ARG:HH21	2.31	0.42
1:A:377:THR:O	1:A:381:VAL:HG23	2.19	0.42
2:B:156:SER:N	2:B:157:PRO:HD2	2.34	0.42
1:A:540:LYS:C	1:A:542:ILE:H	2.27	0.42
2:B:6:GLU:O	2:B:6:GLU:CG	2.67	0.42
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.54	0.42
1:A:38:CYS:HB3	1:A:144:TYR:CE1	2.55	0.41
1:A:255:ASN:O	1:A:259:LYS:HG2	2.19	0.41
1:A:272:PRO:HA	5:A:1020:HOH:O	2.20	0.41
1:A:314:VAL:O	1:A:314:VAL:HG12	2.19	0.41
2:B:85:GLN:NE2	2:B:87:PHE:HE1	2.18	0.41
2:B:239:TRP:O	2:B:240:THR:CG2	2.68	0.41
2:B:240:THR:O	2:B:350:LYS:HG3	2.20	0.41
2:B:332:GLN:HE21	2:B:424:LYS:HE2	1.81	0.41
1:A:438:GLU:OE1	1:A:459:THR:OG1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:ASP:O	2:B:116:PHE:HD2	2.03	0.41
2:B:101:LYS:O	2:B:236:PRO:HB3	2.20	0.41
1:A:53:GLU:O	1:A:55:PRO:HD3	2.20	0.41
2:B:97:PRO:O	2:B:98:ALA:C	2.64	0.41
2:B:242:GLN:HA	2:B:242:GLN:OE1	2.19	0.41
1:A:63:ILE:C	1:A:71:TRP:CE3	2.99	0.41
1:A:497:THR:O	1:A:535:TRP:HA	2.21	0.41
2:B:120:LEU:HD23	2:B:125:ARG:HG2	2.02	0.41
2:B:165:THR:HG23	2:B:166:LYS:H	1.85	0.41
2:B:169:GLU:O	2:B:170:PRO:C	2.64	0.41
2:B:180:ILE:HG12	2:B:189:VAL:CG1	2.44	0.41
1:A:27:THR:O	1:A:31:ILE:HG13	2.21	0.41
1:A:247:PRO:O	1:A:307:ARG:NH1	2.49	0.41
1:A:115:TYR:CE1	1:A:151:GLN:NE2	2.88	0.41
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.03	0.41
2:B:101:LYS:HG3	2:B:102:LYS:HG3	2.03	0.41
2:B:267:ALA:HB2	2:B:426:TRP:CH2	2.56	0.41
2:B:211:ARG:HE	2:B:211:ARG:HB3	1.65	0.41
1:A:399:GLU:O	1:A:403:THR:HB	2.20	0.40
2:B:116:PHE:CD1	2:B:116:PHE:C	2.98	0.40
2:B:197:GLN:O	2:B:201:LYS:HG3	2.21	0.40
1:A:169:GLU:O	1:A:173:LYS:HD3	2.20	0.40
2:B:440:PHE:CD2	2:B:440:PHE:C	2.99	0.40
1:A:355:ALA:O	1:A:356:ARG:C	2.64	0.40
1:A:475:GLN:HE21	1:A:475:GLN:HB3	1.57	0.40
2:B:115:TYR:C	2:B:117:SER:H	2.29	0.40
1:A:78:ARG:CG	1:A:79:GLU:N	2.85	0.40
2:B:234:LEU:CD1	2:B:381:VAL:HG21	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ALA:N	2:B:297:GLU:OE1[2_555]	2.17	0.03

## 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	531/542 (98%)	494 (93%)	29 (6%)	8 (2%)	8	8
2	B	403/435 (93%)	365 (91%)	29 (7%)	9 (2%)	5	4
All	All	934/977 (96%)	859 (92%)	58 (6%)	17 (2%)	6	6

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	91	GLN
1	A	137	ASN
2	B	67	ASP
2	B	173	LYS
2	B	176	PRO
1	A	52	PRO
1	A	85	GLN
2	B	66	LYS
2	B	98	ALA
1	A	133	PRO
1	A	247	PRO
1	A	361	HIS
2	B	236	PRO
2	B	238	LYS
2	B	184	MET
2	B	175	ASN

### 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	478/484 (99%)	442 (92%)	36 (8%)	12	17
2	B	372/395 (94%)	347 (93%)	25 (7%)	15	21
All	All	850/879 (97%)	789 (93%)	61 (7%)	13	18

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	36	GLU
1	A	46	LYS
1	A	89	GLU
1	A	90	VAL
1	A	91	GLN
1	A	94	ILE
1	A	122	GLU
1	A	134	SER
1	A	149	LEU
1	A	151	GLN
1	A	184	MET
1	A	186	ASP
1	A	205	LEU
1	A	224	GLU
1	A	249	LYS
1	A	263	LYS
1	A	279	LEU
1	A	286	THR
1	A	292	VAL
1	A	317	VAL
1	A	325	LEU
1	A	340	GLN
1	A	345	PRO
1	A	358	ARG
1	A	369	THR
1	A	402	TRP
1	A	424	LYS
1	A	448	ARG
1	A	474	ASN
1	A	475	GLN
1	A	516	GLU
1	A	517	LEU
1	A	529	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	533	LEU
1	A	540	LYS
2	B	8	VAL
2	B	10	VAL
2	B	40	GLU
2	B	55	PRO
2	B	139	THR
2	B	163	SER
2	B	165	THR
2	B	167	ILE
2	B	176	PRO
2	B	177	ASP
2	B	187	LEU
2	B	203	GLU
2	B	205	LEU
2	B	206	ARG
2	B	239	TRP
2	B	244	ILE
2	B	283	LEU
2	B	303	LEU
2	B	323	LYS
2	B	368	LEU
2	B	370	GLU
2	B	392	PRO
2	B	400	THR
2	B	422	LEU
2	B	435	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	57	ASN
1	A	96	HIS
1	A	136	ASN
1	A	174	GLN
1	A	197	GLN
1	A	207	GLN
1	A	208	HIS
1	A	221	HIS
1	A	222	GLN
1	A	242	GLN
1	A	265	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	269	GLN
1	A	278	GLN
1	A	334	GLN
1	A	363	ASN
1	A	474	ASN
1	A	475	GLN
1	A	512	GLN
2	B	57	ASN
2	B	147	ASN
2	B	182	GLN
2	B	197	GLN
2	B	255	ASN
2	B	265	ASN
2	B	332	GLN
2	B	394	GLN
2	B	418	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	CSD	A	280	1	4,7,8	1.25	0	1,8,10	0.10	0

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	280	1	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	HBQ	A	999	-	21,21,21	1.68	6 (28%)	28,30,30	1.07	3 (10%)
3	PO4	B	1302	-	4,4,4	1.73	1 (25%)	6,6,6	0.46	0
3	PO4	A	1301	-	4,4,4	1.68	0	6,6,6	0.48	0

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
4	HBQ	A	999	-	-	1/10/26/26	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	HBQ	C11-N1	3.83	1.43	1.37
4	A	999	HBQ	C4-C3	3.17	1.44	1.40
4	A	999	HBQ	C2-N1	2.96	1.51	1.47
4	A	999	HBQ	C3-N1	2.85	1.46	1.42
4	A	999	HBQ	C6-C5	2.32	1.42	1.38
4	A	999	HBQ	O3-C11	2.05	1.24	1.21
3	B	1302	PO4	P-O4	-2.03	1.48	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	HBQ	O3-C11-N1	-2.36	120.13	123.99
4	A	999	HBQ	O2-C12-C13	-2.24	101.17	107.13
4	A	999	HBQ	O2-C11-N1	2.03	113.62	110.93

There are no chirality outliers.

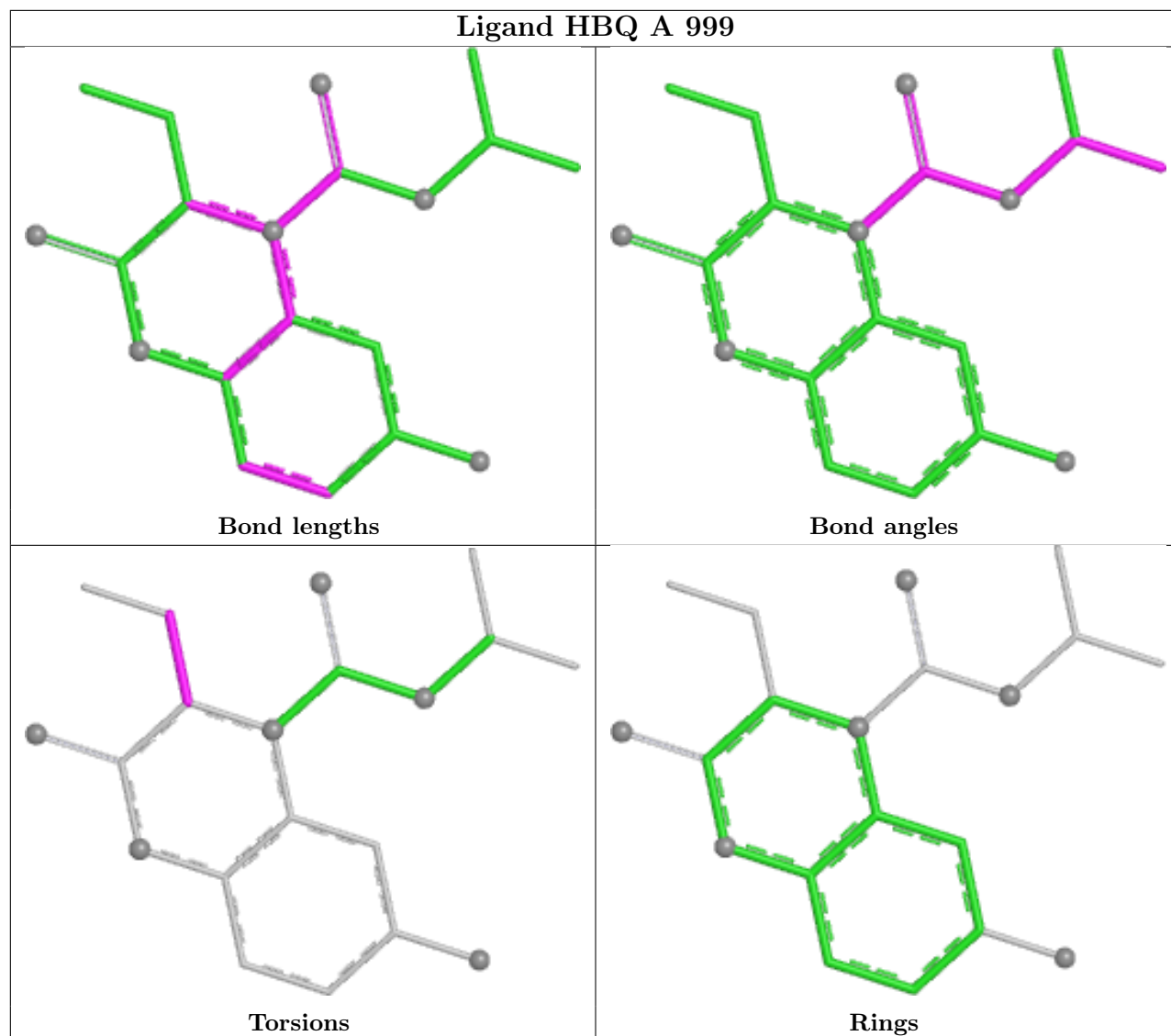
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	999	HBQ	C1-C2-C9-C10

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	535/542 (98%)	-0.17	10 (1%) 66 68	25, 52, 104, 143	0
2	B	409/435 (94%)	-0.20	7 (1%) 69 70	27, 52, 107, 150	0
All	All	944/977 (96%)	-0.18	17 (1%) 67 69	25, 52, 106, 150	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	ILE	3.4
1	A	228	LEU	3.4
1	A	2	ILE	3.3
2	B	240	THR	3.1
2	B	94	ILE	2.7
1	A	90	VAL	2.7
1	A	218	ASP	2.5
1	A	24	TRP	2.4
1	A	50	ILE	2.4
2	B	190	GLY	2.3
2	B	440	PHE	2.2
2	B	434	ILE	2.2
1	A	225	PRO	2.2
1	A	138	GLU	2.1
2	B	212	TRP	2.1
2	B	95	PRO	2.1
1	A	220	LYS	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	A	280	8/9	0.94	0.08	44,52,75,76	0

### 6.3 Carbohydrates [i](#)

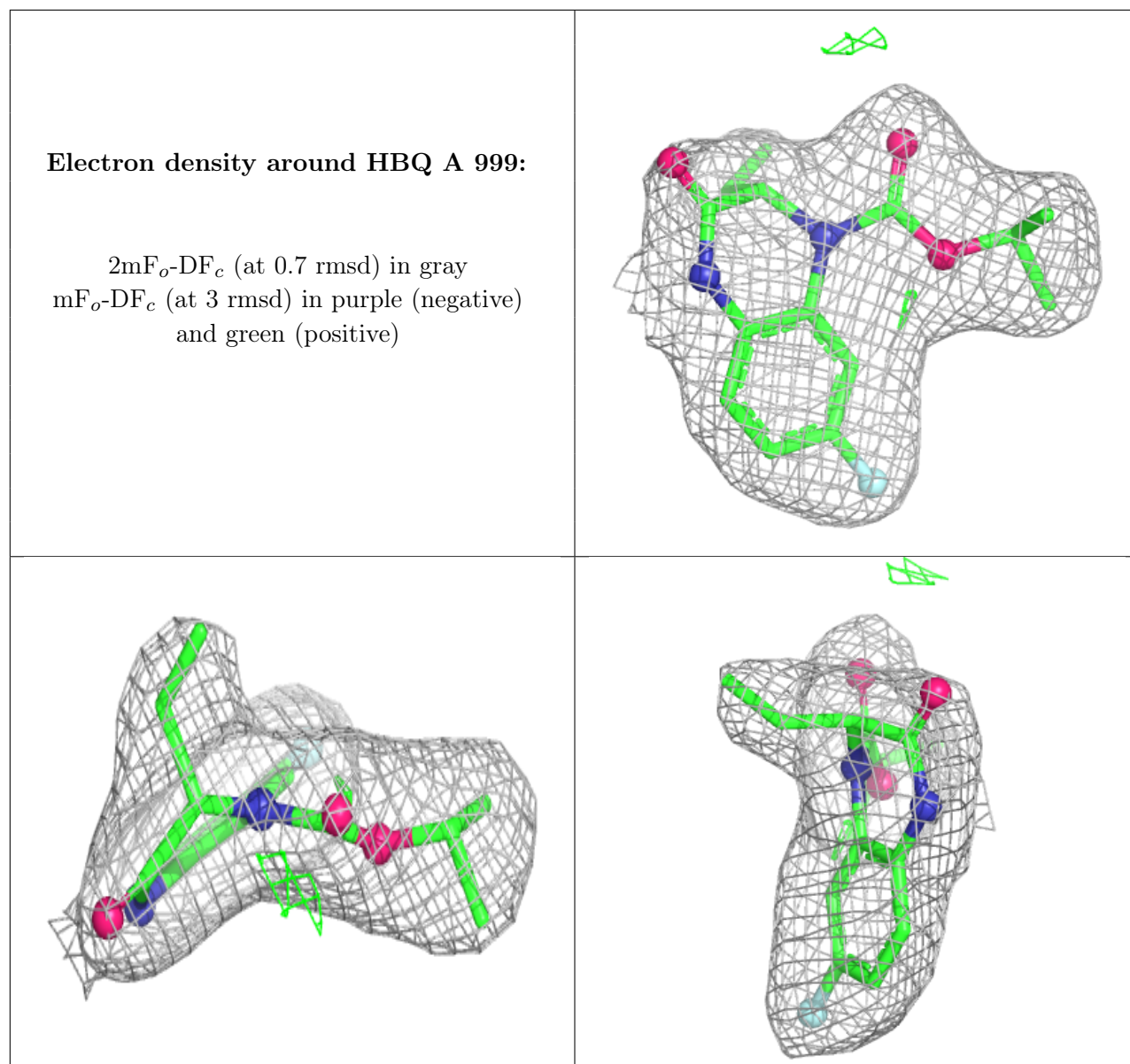
There are no oligosaccharides in this entry.

### 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, 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	PO4	B	1302	5/5	0.81	0.10	94,107,112,114	0
3	PO4	A	1301	5/5	0.85	0.13	90,127,129,137	0
4	HBQ	A	999	20/20	0.97	0.06	29,38,61,69	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.