



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:09 PM GMT

PDB ID : 4AQH  
Title : Plasminogen activator inhibitor type-1 in complex with the inhibitor AZ3976  
Authors : Fjellstrom, O.; Deinum, J.; Sjogren, T.; Johansson, C.; Geschwindner, S.;  
Nerme, V.; Legnehed, A.; Mcpheat, J.; Olsson, K.; Bodin, C.; Gustafsson, D.  
Deposited on : 2012-04-17  
Resolution : 2.40 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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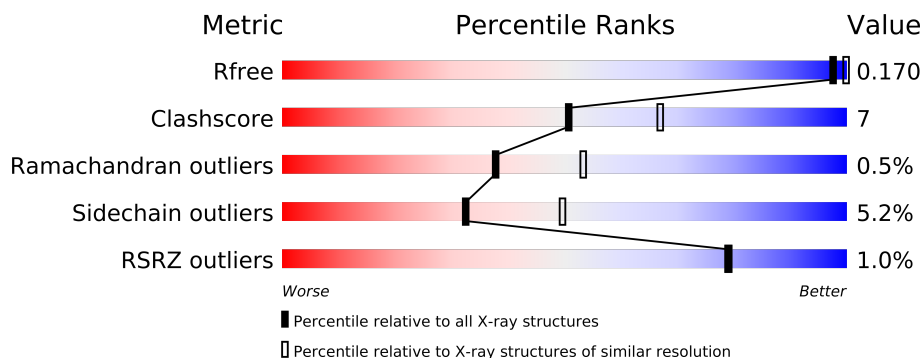
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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	383	
1	B	383	
1	C	383	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9428 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.

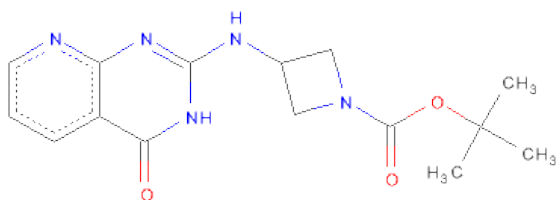
- Molecule 1 is a protein called PLASMINOGEN ACTIVATOR INHIBITOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			3037	1944	521	555	17			
1	B	383	Total	C	N	O	S	0	0	0
			3041	1946	522	556	17			
1	C	382	Total	C	N	O	S	0	0	0
			3037	1944	521	555	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P05121
A	-2	SER	-	EXPRESSION TAG	UNP P05121
A	-1	HIS	-	EXPRESSION TAG	UNP P05121
A	0	MET	-	EXPRESSION TAG	UNP P05121
B	-3	GLY	-	EXPRESSION TAG	UNP P05121
B	-2	SER	-	EXPRESSION TAG	UNP P05121
B	-1	HIS	-	EXPRESSION TAG	UNP P05121
B	0	MET	-	EXPRESSION TAG	UNP P05121
C	-3	GLY	-	EXPRESSION TAG	UNP P05121
C	-2	SER	-	EXPRESSION TAG	UNP P05121
C	-1	HIS	-	EXPRESSION TAG	UNP P05121
C	0	MET	-	EXPRESSION TAG	UNP P05121

- Molecule 2 is TERT-BUTYL 3-[(4-OXO-3H-PYRIDO[2,3-D]PYRIMIDIN-2-YL)AMINO]AZETIDINE-1-CARBOXYLATE (three-letter code: TB7) (formula: C<sub>15</sub>H<sub>19</sub>N<sub>5</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	15	5	3		
2	B	1	Total	C	N	O	0	0
			23	15	5	3		
2	C	1	Total	C	N	O	0	0
			23	15	5	3		

- Molecule 3 is water.

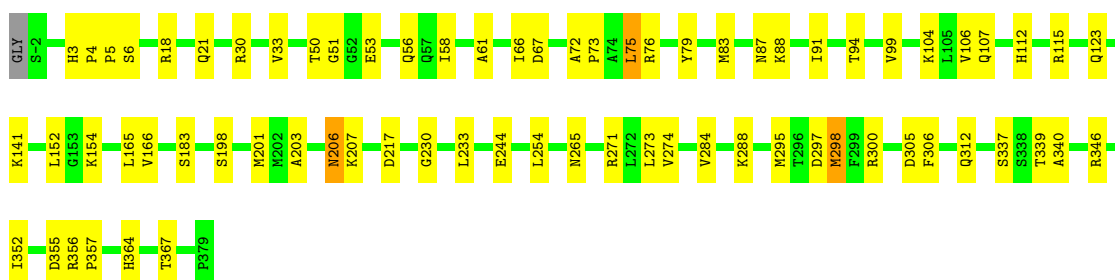
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total	O	0	0
			98	98		
3	B	78	Total	O	0	0
			78	78		
3	C	68	Total	O	0	0
			68	68		

### 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.

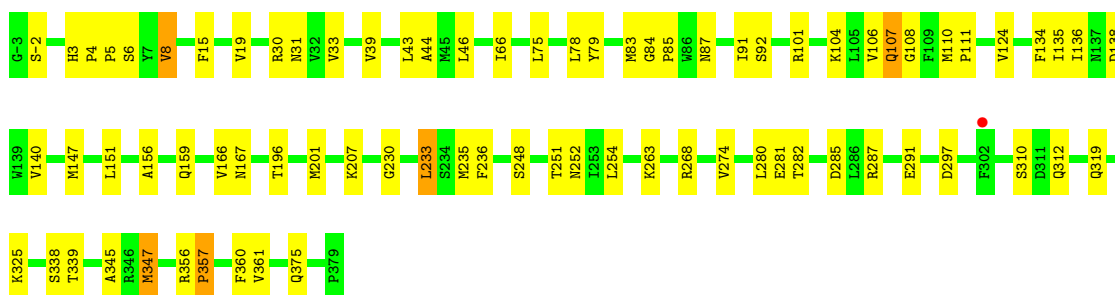
#### • Molecule 1: PLASMINOGEN ACTIVATOR INHIBITOR 1

Chain A:



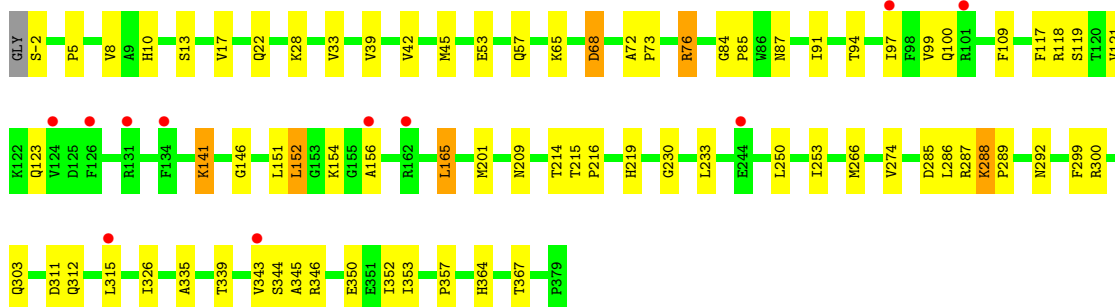
#### • Molecule 1: PLASMINOGEN ACTIVATOR INHIBITOR 1

Chain B:



#### • Molecule 1: PLASMINOGEN ACTIVATOR INHIBITOR 1

Chain C:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.40 Å   119.40 Å   99.69 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	60.01 – 2.40 45.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (60.01-2.40) 98.7 (45.90-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.157 , 0.181 0.158 , 0.170	Depositor DCC
$R_{free}$ test set	3111 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.7	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 17.0	EDS
Estimated twinning fraction	0.655 for H, K, L 0.345 for K, H, -L 0.099 for -h,-k,l 0.339 for h,-h-k,-l 0.098 for -k,-h,-l	Xtriage
Reported twinning fraction	0.655 for H, K, L 0.345 for K, H, -L	Depositor
L-test for twinning	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 62153 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: TB7

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	0.75	0/3112	0.74	0/4219
1	B	0.64	0/3116	0.70	0/4224
1	C	0.58	0/3112	0.65	0/4219
All	All	0.66	0/9340	0.70	0/12662

There are no bond length outliers.

There are no bond angle outliers.

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	3037	0	3028	49	0
1	B	3041	0	3031	44	0
1	C	3037	0	3028	43	0
2	A	23	0	19	0	0
2	B	23	0	19	1	0
2	C	23	0	19	2	0
3	A	98	0	0	2	0
3	B	78	0	0	2	0
3	C	68	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9428	0	9144	135	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 7.

All (135) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:201:MET:CE	1:A:274:VAL:HG12	1.76	1.14
1:A:206:ASN:HD22	1:A:207:LYS:H	1.11	0.92
1:B:201:MET:CE	1:B:274:VAL:HG12	1.98	0.92
1:A:201:MET:HE2	1:A:274:VAL:HG12	1.58	0.85
1:B:151:LEU:HD22	1:B:338:SER:OG	1.77	0.84
1:A:104:LYS:H	1:A:312:GLN:NE2	1.76	0.83
1:A:201:MET:HE3	1:A:274:VAL:HG12	1.59	0.82
1:A:206:ASN:HD22	1:A:207:LYS:N	1.80	0.80
1:A:72:ALA:HB3	1:A:73:PRO:HD3	1.67	0.76
1:B:201:MET:HE2	1:B:274:VAL:HG12	1.71	0.73
1:A:61:ALA:HB3	1:A:295:MET:CE	2.23	0.69
1:B:3:HIS:HD2	1:B:6:SER:OG	1.76	0.69
1:A:61:ALA:HB3	1:A:295:MET:HE3	1.77	0.67
1:A:3:HIS:HE1	3:A:2003:HOH:O	1.77	0.67
1:A:3:HIS:HD2	1:A:6:SER:OG	1.78	0.66
1:A:206:ASN:ND2	1:A:207:LYS:H	1.88	0.66
1:A:295:MET:HB3	1:A:298:MET:CE	2.26	0.65
1:B:281:GLU:HG2	1:B:325:LYS:HG2	1.78	0.65
1:A:123:GLN:HE21	1:B:107:GLN:HE21	1.44	0.64
1:A:201:MET:CE	1:A:274:VAL:CG1	2.65	0.64
1:B:5:PRO:O	1:B:8:VAL:HG22	1.98	0.63
1:B:44:ALA:HB1	1:B:66:ILE:HD12	1.78	0.63
1:C:151:LEU:HG	1:C:152:LEU:HD13	1.81	0.62
1:C:287:ARG:HG3	1:C:299:PHE:CE1	2.34	0.61
1:C:76:ARG:NH2	2:C:1380:TB7:N21	2.48	0.61
1:B:104:LYS:HB2	1:B:312:GLN:NE2	2.16	0.61
2:C:1380:TB7:H43C	2:C:1380:TB7:O7	2.01	0.60
1:B:108:GLY:O	1:B:111:PRO:HD2	2.02	0.60
1:A:58:ILE:HG23	1:A:295:MET:HE2	1.83	0.60
1:C:250:LEU:O	1:C:253:ILE:HG13	2.01	0.60
1:B:91:ILE:HD11	1:B:233:LEU:HD11	1.83	0.59
1:B:4:PRO:HB2	1:B:5:PRO:HD3	1.84	0.59
1:C:53:GLU:O	1:C:57:GLN:HG3	2.03	0.59
1:A:18:ARG:HA	1:A:21:GLN:HE21	1.67	0.58
1:A:364:HIS:HD2	1:A:367:THR:OG1	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:201:MET:HE2	1:B:274:VAL:CG1	2.33	0.58
1:A:295:MET:HB3	1:A:298:MET:HE2	1.84	0.58
1:A:201:MET:HE2	1:A:274:VAL:CG1	2.29	0.57
1:B:43:LEU:HD13	1:B:46:LEU:HD23	1.86	0.57
1:B:201:MET:HE1	1:B:274:VAL:HG12	1.82	0.57
1:B:156:ALA:O	1:B:345:ALA:HB3	2.04	0.57
1:B:134:PHE:O	1:B:138:ASP:HB2	2.04	0.57
1:A:30:ARG:HG3	1:A:352:ILE:HG23	1.88	0.56
1:B:15:PHE:O	1:B:19:VAL:HG23	2.06	0.56
1:B:156:ALA:O	1:B:345:ALA:CB	2.53	0.56
1:A:203:ALA:HA	1:A:273:LEU:O	2.06	0.55
1:C:13:SER:O	1:C:17:VAL:HG23	2.07	0.54
1:C:326:ILE:HG13	1:C:335:ALA:HB2	1.88	0.54
1:C:99:VAL:HG22	1:C:100:GLN:H	1.71	0.54
1:A:87:ASN:OD1	1:A:364:HIS:HE1	1.92	0.53
1:C:364:HIS:HD2	1:C:367:THR:OG1	1.92	0.53
1:B:33:VAL:HG13	1:B:360:PHE:HZ	1.72	0.52
1:A:58:ILE:HA	1:A:295:MET:HE3	1.91	0.52
1:C:65:LYS:O	1:C:68:ASP:HB2	2.09	0.52
1:C:288:LYS:HD3	1:C:292:ASN:HD21	1.74	0.52
1:A:76:ARG:CZ	1:A:76:ARG:HA	2.39	0.52
1:B:3:HIS:CD2	1:B:6:SER:OG	2.60	0.51
1:C:97:ILE:HG12	1:C:165:LEU:HD23	1.92	0.51
1:A:88:LYS:HD2	1:A:230:GLY:HA2	1.93	0.51
1:C:5:PRO:O	1:C:8:VAL:HG22	2.11	0.51
1:B:79:TYR:O	1:B:83:MET:HG2	2.12	0.50
1:C:201:MET:CE	1:C:274:VAL:HG12	2.41	0.50
1:C:76:ARG:HA	1:C:76:ARG:NE	2.27	0.49
1:A:201:MET:HE3	1:A:274:VAL:CG1	2.34	0.49
1:A:295:MET:HB3	1:A:298:MET:HE3	1.93	0.49
1:C:117:PHE:C	1:C:119:SER:H	2.14	0.49
1:C:288:LYS:HD3	1:C:292:ASN:ND2	2.28	0.49
1:C:99:VAL:HG22	1:C:100:GLN:N	2.28	0.48
1:C:91:ILE:HD11	1:C:233:LEU:HD21	1.95	0.48
1:C:22:GLN:HB2	1:C:289:PRO:HB3	1.96	0.48
1:A:112:HIS:CD2	1:A:115:ARG:HH22	2.32	0.48
1:B:207:LYS:HD2	1:B:268:ARG:HG2	1.96	0.48
1:A:58:ILE:HA	1:A:295:MET:CE	2.44	0.47
1:A:61:ALA:HB3	1:A:295:MET:HE1	1.93	0.47
1:C:287:ARG:HG3	1:C:299:PHE:CD1	2.50	0.47
1:B:78:LEU:HD23	2:B:1380:TB7:O7	2.15	0.47
1:A:355:ASP:O	1:A:356:ARG:C	2.52	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:79:TYR:CE2	1:B:83:MET:HG3	2.50	0.46
1:C:352:ILE:HG22	1:C:353:ILE:N	2.30	0.46
1:A:297:ASP:OD1	1:A:300:ARG:NH2	2.49	0.46
1:B:251:THR:HG21	1:B:375:GLN:OE1	2.15	0.46
1:B:106:VAL:HG13	1:B:310:SER:HA	1.96	0.46
1:A:76:ARG:NE	1:A:76:ARG:HA	2.30	0.46
1:B:356:ARG:HG3	3:B:2077:HOH:O	2.16	0.46
1:B:87:ASN:O	1:B:230:GLY:HA3	2.16	0.46
1:C:156:ALA:O	1:C:345:ALA:HB3	2.15	0.45
1:C:209:ASN:HB3	1:C:266:MET:SD	2.56	0.45
1:B:287:ARG:O	1:B:291:GLU:HG3	2.16	0.45
1:C:343:VAL:O	1:C:344:SER:HB2	2.16	0.45
1:B:84:GLY:HA2	1:B:85:PRO:HD3	1.65	0.45
1:C:10:HIS:HE1	3:C:2065:HOH:O	2.00	0.45
1:A:166:VAL:HA	1:A:339:THR:O	2.17	0.44
1:A:107:GLN:HE22	1:B:104:LYS:HA	1.83	0.44
1:A:79:TYR:CZ	1:A:83:MET:HG3	2.52	0.44
1:A:66:ILE:HD11	1:A:75:LEU:HD21	1.99	0.44
1:C:42:VAL:HA	1:C:45:MET:CE	2.48	0.43
1:A:154:LYS:HB3	1:A:154:LYS:HE3	1.83	0.43
1:B:166:VAL:HG12	1:B:167:ASN:N	2.34	0.43
1:B:156:ALA:O	1:B:319:GLN:NE2	2.51	0.43
1:C:288:LYS:N	1:C:289:PRO:CD	2.82	0.43
1:C:201:MET:HE2	1:C:274:VAL:HG12	1.99	0.43
1:B:248:SER:O	1:B:252:ASN:ND2	2.52	0.43
1:C:285:ASP:HB3	1:C:350:GLU:OE2	2.18	0.43
1:C:109:PHE:CD1	1:C:109:PHE:C	2.91	0.43
1:C:286:LEU:C	1:C:289:PRO:HD2	2.39	0.43
1:B:136:ILE:O	1:B:140:VAL:HG23	2.19	0.43
1:A:4:PRO:HB2	1:A:5:PRO:HD3	2.00	0.42
1:C:39:VAL:HA	1:C:339:THR:HG21	2.01	0.42
1:A:87:ASN:O	1:A:230:GLY:HA3	2.20	0.42
1:C:214:THR:HA	1:C:219:HIS:O	2.20	0.42
1:B:356:ARG:HA	1:B:357:PRO:HD3	1.93	0.42
1:C:84:GLY:HA2	1:C:85:PRO:HD3	1.96	0.42
1:C:123:GLN:HE21	1:C:123:GLN:HB2	1.71	0.42
1:A:265:ASN:HB3	3:A:2069:HOH:O	2.20	0.42
1:C:300:ARG:HB2	1:C:303:GLN:HB2	2.01	0.42
1:A:50:THR:HA	1:A:306:PHE:HA	2.01	0.42
1:A:112:HIS:CD2	1:A:115:ARG:NH2	2.87	0.41
1:C:141:LYS:HG2	1:C:146:GLY:HA2	2.02	0.41
1:B:235:MET:HA	1:B:361:VAL:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:165:LEU:O	1:A:340:ALA:HA	2.20	0.41
1:B:236:PHE:HZ	1:B:263:LYS:HD2	1.85	0.41
1:B:33:VAL:HG22	1:B:280:LEU:HD23	2.03	0.41
1:C:72:ALA:HB3	1:C:73:PRO:HD3	2.02	0.41
1:A:91:ILE:HD11	1:A:233:LEU:HD21	2.03	0.41
1:A:51:GLY:O	1:A:305:ASP:HB3	2.21	0.41
1:A:53:GLU:HA	1:A:56:GLN:HB3	2.03	0.41
1:B:39:VAL:HA	1:B:339:THR:HG21	2.02	0.41
1:C:352:ILE:O	1:C:353:ILE:HD13	2.21	0.40
1:C:117:PHE:O	1:C:119:SER:N	2.53	0.40
1:C:215:THR:HB	1:C:216:PRO:HD2	2.03	0.40
1:B:347:MET:SD	1:B:347:MET:N	2.95	0.40
1:A:30:ARG:NH2	1:A:284:VAL:HG12	2.36	0.40
1:B:30:ARG:NH2	3:B:2010:HOH:O	2.53	0.40
1:B:108:GLY:C	1:B:111:PRO:HD2	2.42	0.40
1:C:87:ASN:O	1:C:230:GLY:HA3	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	380/383 (99%)	369 (97%)	10 (3%)	1 (0%)	50	68
1	B	381/383 (100%)	370 (97%)	9 (2%)	2 (0%)	38	53
1	C	380/383 (99%)	358 (94%)	19 (5%)	3 (1%)	27	39
All	All	1141/1149 (99%)	1097 (96%)	38 (3%)	6 (0%)	38	53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	-2	SER
1	C	118	ARG
1	C	312	GLN

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Mol	Chain	Res	Type
1	C	357	PRO
1	A	357	PRO
1	B	357	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/336 (100%)	317 (94%)	19 (6%)	29	44
1	B	336/336 (100%)	318 (95%)	18 (5%)	31	47
1	C	336/336 (100%)	321 (96%)	15 (4%)	38	57
All	All	1008/1008 (100%)	956 (95%)	52 (5%)	32	49

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	67	ASP
1	A	75	LEU
1	A	94	THR
1	A	99	VAL
1	A	106	VAL
1	A	141	LYS
1	A	152	LEU
1	A	183	SER
1	A	198	SER
1	A	206	ASN
1	A	217	ASP
1	A	244	GLU
1	A	254	LEU
1	A	271	ARG
1	A	288	LYS
1	A	298	MET
1	A	337	SER
1	A	346	ARG
1	B	8	VAL

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Mol	Chain	Res	Type
1	B	31	ASN
1	B	75	LEU
1	B	92	SER
1	B	101	ARG
1	B	107	GLN
1	B	110	MET
1	B	124	VAL
1	B	135	ILE
1	B	147	MET
1	B	159	GLN
1	B	196	THR
1	B	233	LEU
1	B	254	LEU
1	B	282	THR
1	B	285	ASP
1	B	297	ASP
1	B	347	MET
1	C	-2	SER
1	C	28	LYS
1	C	33	VAL
1	C	68	ASP
1	C	76	ARG
1	C	94	THR
1	C	121	VAL
1	C	141	LYS
1	C	152	LEU
1	C	154	LYS
1	C	165	LEU
1	C	288	LYS
1	C	311	ASP
1	C	315	LEU
1	C	346	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	21	GLN
1	A	25	GLN
1	A	123	GLN
1	A	143	HIS
1	A	190	HIS

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Mol	Chain	Res	Type
1	A	206	ASN
1	A	312	GLN
1	A	364	HIS
1	B	3	HIS
1	B	25	GLN
1	B	31	ASN
1	B	143	HIS
1	B	364	HIS
1	C	3	HIS
1	C	21	GLN
1	C	25	GLN
1	C	100	GLN
1	C	123	GLN
1	C	292	ASN
1	C	303	GLN
1	C	364	HIS

### 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 ⓘ

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
2	TB7	A	1380	-	25,25,25	1.43	4 (16%)	35,37,37	1.72	8 (22%)
2	TB7	B	1380	-	25,25,25	1.22	2 (8%)	35,37,37	2.00	11 (31%)
2	TB7	C	1380	-	25,25,25	1.27	4 (16%)	35,37,37	2.19	9 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TB7	A	1380	-	-	0/13/21/21	0/0/3/3
2	TB7	B	1380	-	-	0/13/21/21	0/0/3/3
2	TB7	C	1380	-	-	0/13/21/21	0/0/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1380	TB7	C22-N23	2.60	1.41	1.36
2	C	1380	TB7	O5-C2	-2.48	1.43	1.48
2	C	1380	TB7	C22-N21	-2.42	1.33	1.37
2	A	1380	TB7	C13-N12	2.31	1.39	1.33
2	B	1380	TB7	C22-N23	2.29	1.41	1.36
2	A	1380	TB7	O5-C6	2.20	1.38	1.34
2	A	1380	TB7	C15-C17	2.19	1.47	1.39
2	C	1380	TB7	C13-N23	-2.09	1.28	1.33
2	C	1380	TB7	C18-C17	-2.07	1.37	1.42
2	B	1380	TB7	O5-C2	-2.04	1.44	1.48

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1380	TB7	C2-O5-C6	-7.40	112.35	121.06
2	B	1380	TB7	C13-N12-C10	-5.41	116.97	123.25
2	A	1380	TB7	C13-N12-C10	-4.30	118.26	123.25
2	C	1380	TB7	C17-C15-N14	-3.98	112.04	115.40
2	C	1380	TB7	C11-C10-N12	-3.93	104.82	116.18
2	A	1380	TB7	C15-N14-C13	3.57	126.03	119.87
2	B	1380	TB7	C19-C18-C17	-3.56	115.69	120.88
2	C	1380	TB7	C15-N14-C13	3.55	125.98	119.87
2	B	1380	TB7	C15-N14-C13	3.47	125.86	119.87
2	A	1380	TB7	C13-N23-C22	3.46	119.70	115.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1380	TB7	N12-C13-N14	-3.35	110.39	117.34
2	C	1380	TB7	C13-N12-C10	-3.29	119.44	123.25
2	C	1380	TB7	C19-C18-C17	-3.19	116.24	120.88
2	B	1380	TB7	C11-C10-N12	-2.90	107.80	116.18
2	B	1380	TB7	N12-C13-N14	-2.84	111.44	117.34
2	A	1380	TB7	N12-C13-N23	2.81	127.86	119.60
2	B	1380	TB7	C18-C17-C22	2.74	122.93	116.96
2	B	1380	TB7	C18-C17-C15	-2.73	117.64	122.83
2	B	1380	TB7	N12-C13-N23	2.71	127.56	119.60
2	A	1380	TB7	N12-C13-N14	-2.61	111.93	117.34
2	B	1380	TB7	C19-C20-N21	2.55	127.73	123.89
2	A	1380	TB7	C17-C15-N14	-2.49	113.30	115.40
2	C	1380	TB7	N12-C13-N23	2.46	126.82	119.60
2	B	1380	TB7	C20-N21-C22	-2.13	113.68	116.43
2	A	1380	TB7	C2-O5-C6	-2.12	118.56	121.06
2	B	1380	TB7	C13-N23-C22	2.11	117.88	115.03
2	A	1380	TB7	C3-C2-C1	-2.03	105.54	111.19
2	C	1380	TB7	C18-C17-C22	2.02	121.35	116.96

There are no chirality outliers.

There are no torsion outliers.

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	382/383 (99%)	-0.25	0 100 100	23, 36, 51, 62	0
1	B	383/383 (100%)	-0.15	1 (0%) 91 92	31, 44, 67, 75	0
1	C	382/383 (99%)	0.01	11 (2%) 49 47	29, 50, 82, 92	0
All	All	1147/1149 (99%)	-0.13	12 (1%) 79 79	23, 43, 72, 92	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	126	PHE	3.7
1	C	315	LEU	3.5
1	B	302	PHE	3.3
1	C	162	ARG	3.1
1	C	244	GLU	2.6
1	C	156	ALA	2.6
1	C	101	ARG	2.3
1	C	131	ARG	2.3
1	C	124	VAL	2.3
1	C	343	VAL	2.2
1	C	97	ILE	2.1
1	C	134	PHE	2.0

### 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
2	TB7	A	1380	23/23	0.14	0.23	21,30,33,34	0
2	TB7	C	1380	23/23	0.14	-0.15	36,41,45,45	0
2	TB7	B	1380	23/23	0.13	-0.60	29,33,36,37	0

## 6.5 Other polymers

There are no such residues in this entry.