



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 07:33 AM EDT

PDB ID : 2ZEC  
Title : Potent, Nonpeptide Inhibitors of Human Mast Cell Tryptase  
Authors : Spurlino, J.C.; Lewandowski, F.; Milligan, C.  
Deposited on : unknown  
Resolution : 2.06 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

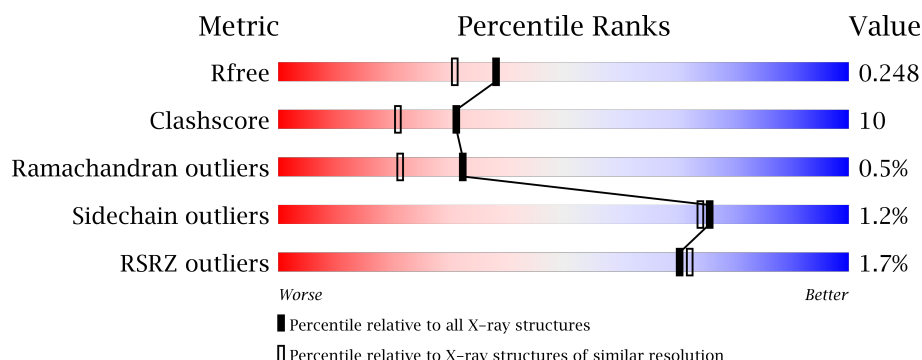
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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))
$R_{free}$	100719	2028 (2.08-2.04)
Clashscore	112137	2143 (2.08-2.04)
Ramachandran outliers	110173	2126 (2.08-2.04)
Sidechain outliers	110143	2126 (2.08-2.04)
RSRZ outliers	101464	2035 (2.08-2.04)

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. 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	243	 2% 82% 16%
1	B	243	 % 78% 21%
1	C	243	 3% 80% 19%
1	D	243	 % 82% 17%

## 2 Entry composition [i](#)

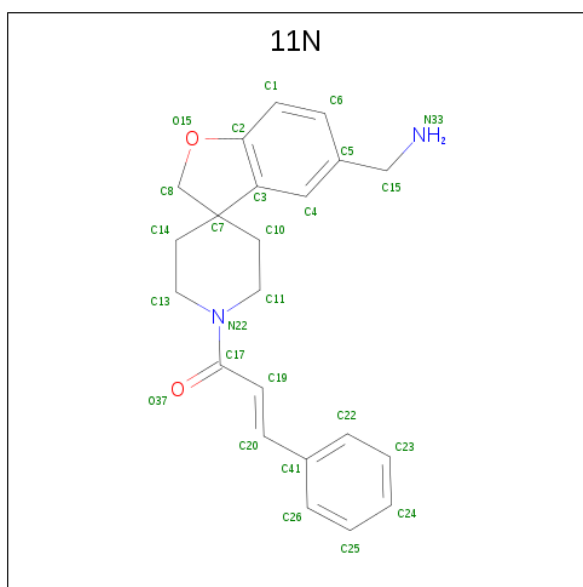
There are 3 unique types of molecules in this entry. The entry contains 8313 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tryptase beta 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	1
			1912	1224	337	339	12			
1	B	243	Total	C	N	O	S	0	0	1
			1912	1224	337	339	12			
1	C	243	Total	C	N	O	S	0	0	1
			1912	1224	337	339	12			
1	D	243	Total	C	N	O	S	0	0	1
			1912	1224	337	339	12			

- Molecule 2 is 1-[1'-(3-phenylacryloyl)spiro[1-benzofuran-3,4'-piperidin]-5-yl]methanamine (three-letter code: 11N) (formula: C<sub>22</sub>H<sub>24</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	22	2	2		
2	B	1	Total	C	N	O	0	0
			26	22	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			26	22	2	2		
2	D	1	Total	C	N	O	0	0
			26	22	2	2		

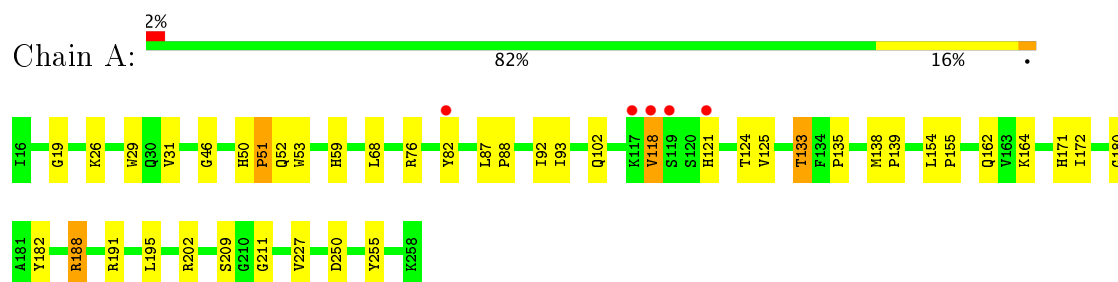
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total	O	0	0
			121	121		
3	B	138	Total	O	0	0
			138	138		
3	C	163	Total	O	0	0
			163	163		
3	D	139	Total	O	0	0
			139	139		

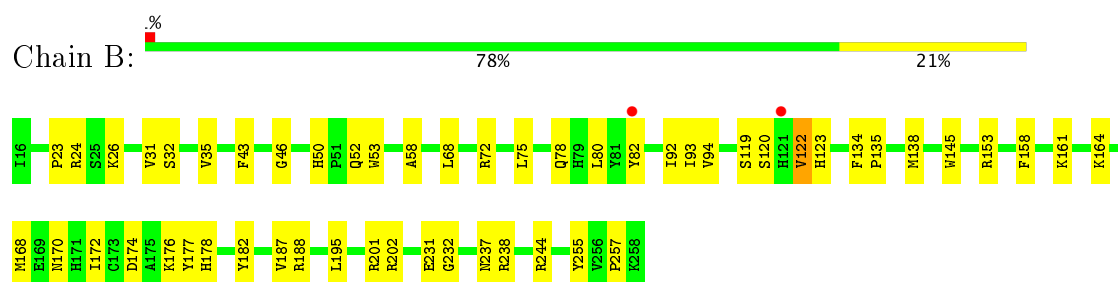
### 3 Residue-property plots

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

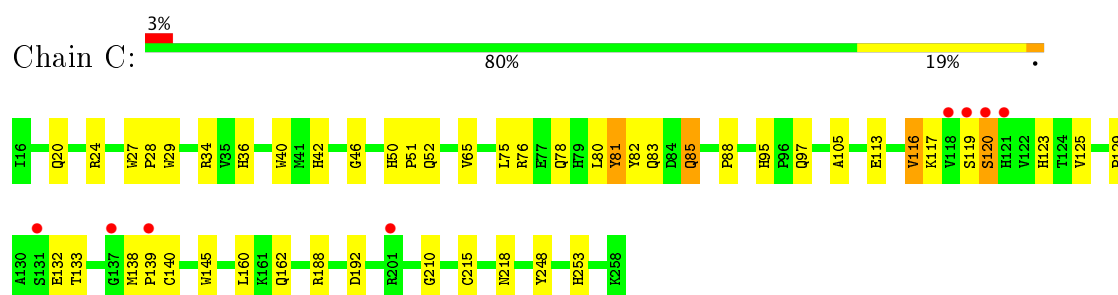
#### • Molecule 1: Trypsin beta 2



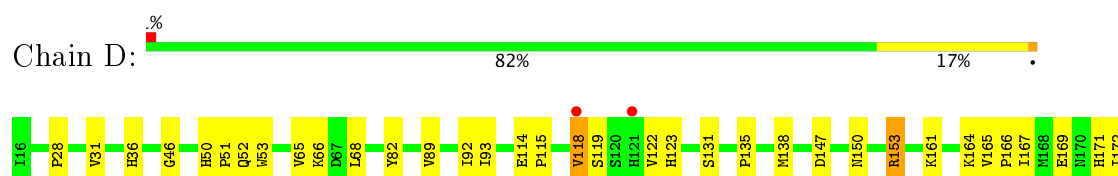
#### • Molecule 1: Trypsin beta 2



#### • Molecule 1: Trypsin beta 2



#### • Molecule 1: Trypsin beta 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.26 Å 82.26 Å 170.65 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.13 – 2.06 41.13 – 2.06	Depositor EDS
% Data completeness (in resolution range)	91.3 (41.13-2.06) 91.4 (41.13-2.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.60 (at 2.06 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.207 , 0.256 0.201 , 0.248	Depositor DCC
$R_{free}$ test set	3189 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.058 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8313	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: 11N

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	0.28	0/1977	0.50	0/2711
1	B	0.31	0/1977	0.49	0/2711
1	C	0.31	0/1977	0.50	0/2711
1	D	0.30	0/1977	0.50	0/2711
All	All	0.30	0/7908	0.50	0/10844

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1912	0	1842	34	0
1	B	1912	0	1842	50	0
1	C	1912	0	1842	46	0
1	D	1912	0	1842	30	0
2	A	26	0	24	0	0
2	B	26	0	24	0	0
2	C	26	0	24	0	0
2	D	26	0	24	1	0
3	A	121	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	138	0	0	7	0
3	C	163	0	0	11	0
3	D	139	0	0	5	0
All	All	8313	0	7464	156	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 10.

All (156) 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:C:27:TRP:HE1	1:C:162:GLN:HE21	1.11	0.98
1:C:129:PRO:HG2	1:C:132:GLU:HG2	1.46	0.95
1:B:161:LYS:HE2	3:B:319:HOH:O	1.70	0.91
1:A:50:HIS:HD2	1:A:52:GLN:H	1.28	0.81
1:C:50:HIS:HD2	1:C:52:GLN:H	1.31	0.76
1:C:113:GLU:HB3	3:C:482:HOH:O	1.84	0.76
3:B:276:HOH:O	1:D:66:LYS:HB2	1.86	0.75
1:A:50:HIS:CD2	1:A:52:GLN:H	2.05	0.74
1:C:140:CYS:HA	3:C:493:HOH:O	1.87	0.72
1:D:150:ASN:HD21	1:D:233:CYS:H	1.34	0.71
1:C:215:CYS:HA	3:C:493:HOH:O	1.90	0.71
1:B:35:VAL:HG13	1:B:43:PHE:CD1	2.25	0.71
1:C:28:PRO:HB2	1:C:123:HIS:H	1.56	0.70
1:C:27:TRP:HE1	1:C:162:GLN:NE2	1.86	0.70
1:B:23:PRO:HD2	1:B:26:LYS:HE2	1.72	0.70
1:C:188:ARG:HD2	3:C:473:HOH:O	1.92	0.69
1:B:168:MET:HE1	1:B:176:LYS:HE2	1.74	0.68
1:C:188:ARG:HH12	1:C:192:ASP:CG	1.97	0.68
1:B:201:ARG:NH2	1:B:202:ARG:HE	1.93	0.67
1:C:50:HIS:CD2	1:C:52:GLN:H	2.13	0.67
1:D:52:GLN:NE2	1:D:115:PRO:HG3	2.11	0.66
1:B:168:MET:CE	1:B:176:LYS:HE2	2.26	0.65
1:B:50:HIS:CE1	1:B:257:PRO:HG2	2.31	0.65
1:C:50:HIS:HE1	3:C:479:HOH:O	1.81	0.64
1:B:201:ARG:HG3	1:B:202:ARG:HG3	1.80	0.63
1:B:75:LEU:HD13	1:B:122:VAL:HG21	1.81	0.62
1:B:164:LYS:O	1:B:202:ARG:HD3	1.99	0.62
1:C:95:HIS:HD2	1:C:97:GLN:H	1.47	0.62
1:C:24:ARG:HG2	1:C:78:GLN:HG3	1.80	0.62
1:C:75:LEU:HD11	1:C:116:VAL:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ARG:HG2	1:C:78:GLN:CG	2.30	0.61
1:B:170:ASN:HD21	1:B:244:ARG:HH21	1.49	0.60
1:B:174:ASP:O	1:B:178:HIS:HD2	1.85	0.60
1:C:119:SER:HB2	3:C:492:HOH:O	2.01	0.60
1:B:153:ARG:HD2	3:B:382:HOH:O	2.00	0.60
1:B:50:HIS:CD2	1:B:52:GLN:H	2.20	0.60
1:B:201:ARG:CG	1:B:202:ARG:HG3	2.33	0.59
1:B:50:HIS:HD2	1:B:52:GLN:H	1.51	0.59
1:D:68:LEU:HD23	3:D:412:HOH:O	2.03	0.59
1:C:120:SER:HA	1:C:123:HIS:NE2	2.18	0.58
1:D:114:GLU:HG3	1:D:115:PRO:HD2	1.87	0.57
1:B:35:VAL:HG13	1:B:43:PHE:CE1	2.39	0.56
1:A:182:TYR:CE2	1:C:65:VAL:HA	2.40	0.56
1:C:132:GLU:HA	1:C:132:GLU:OE1	2.06	0.56
1:C:95:HIS:CD2	1:C:97:GLN:H	2.24	0.56
1:D:36:HIS:CD2	3:D:405:HOH:O	2.57	0.56
1:A:172:ILE:HG23	3:A:378:HOH:O	2.06	0.56
1:A:164:LYS:O	1:A:202:ARG:HD3	2.07	0.55
1:A:76:ARG:HD3	1:A:121:HIS:CE1	2.42	0.55
1:D:50:HIS:HB3	1:D:53:TRP:HB2	1.88	0.55
1:B:135:PRO:HD2	1:B:138:MET:HE2	1.88	0.55
1:B:50:HIS:CD2	1:B:53:TRP:HD1	2.26	0.54
1:D:169:GLU:OE1	1:D:171:HIS:HE1	1.90	0.53
1:A:102:GLN:O	1:A:191:ARG:NH2	2.41	0.53
1:D:118:VAL:HG23	3:D:354:HOH:O	2.08	0.53
1:B:201:ARG:CZ	1:B:202:ARG:HE	2.21	0.53
1:B:135:PRO:HD2	1:B:138:MET:CE	2.39	0.52
1:B:201:ARG:HH21	1:B:202:ARG:HE	1.58	0.52
1:B:237:ASN:O	1:B:238:ARG:HD3	2.09	0.52
1:C:88:PRO:HG2	3:C:482:HOH:O	2.10	0.52
1:A:138:MET:HG3	1:A:139:PRO:HD2	1.90	0.51
1:B:119:SER:OG	1:B:120:SER:N	2.42	0.51
1:C:20:GLN:HB2	3:C:486:HOH:O	2.10	0.51
1:D:147:ASP:OD1	1:D:153:ARG:HD3	2.10	0.51
1:C:218:ASN:HB2	3:C:480:HOH:O	2.10	0.51
1:A:180:GLY:O	1:C:65:VAL:HG22	2.11	0.50
1:C:82:TYR:O	1:C:83:GLN:HB2	2.12	0.50
1:A:82:TYR:HB2	1:D:82:TYR:CE1	2.47	0.49
1:D:50:HIS:CG	1:D:51:PRO:HD2	2.46	0.49
1:A:68:LEU:CD2	1:A:92:ILE:HG12	2.43	0.49
1:B:123:HIS:HB2	3:B:288:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:TYR:CE2	1:D:65:VAL:HA	2.48	0.49
1:C:253:HIS:HD2	3:C:372:HOH:O	1.97	0.48
1:A:171:HIS:HA	1:A:188:ARG:NH2	2.28	0.48
1:D:68:LEU:CD2	1:D:92:ILE:HG13	2.43	0.48
1:B:134:PHE:HA	1:B:138:MET:HE2	1.96	0.48
1:B:80:LEU:HB2	1:B:158:PHE:HB2	1.94	0.48
1:B:93:ILE:HD13	1:B:255:TYR:CD1	2.49	0.48
1:A:209:SER:HA	1:A:227:VAL:CG1	2.44	0.48
1:D:164:LYS:O	1:D:202:ARG:HD3	2.14	0.48
1:D:150:ASN:HD21	1:D:233:CYS:N	2.08	0.47
1:B:170:ASN:ND2	1:B:244:ARG:HH21	2.12	0.47
1:A:29:TRP:CG	1:A:125:VAL:HB	2.49	0.47
1:C:46:GLY:HA2	1:C:210:GLY:O	2.14	0.47
1:A:188:ARG:NH1	3:A:344:HOH:O	2.48	0.47
1:B:168:MET:CE	1:B:172:ILE:HG22	2.45	0.47
1:B:58:ALA:HB1	1:B:94:VAL:HG13	1.95	0.47
1:B:178:HIS:HE1	1:B:187:VAL:O	1.96	0.47
1:B:68:LEU:HD21	1:B:92:ILE:HG13	1.97	0.47
1:A:211:GLY:HA3	3:A:275:HOH:O	2.14	0.46
1:A:82:TYR:HE1	3:A:307:HOH:O	1.98	0.46
1:B:195:LEU:C	1:B:195:LEU:HD23	2.36	0.46
1:B:232:GLY:HA2	3:B:338:HOH:O	2.15	0.46
1:B:32:SER:HB2	1:B:145:TRP:CZ3	2.51	0.46
1:C:105:ALA:HA	1:C:248:TYR:OH	2.16	0.46
1:A:51:PRO:HD3	1:A:124:THR:HG21	1.98	0.46
1:D:131:SER:HB2	3:D:355:HOH:O	2.15	0.45
1:B:178:HIS:CE1	1:B:187:VAL:O	2.69	0.45
1:B:24:ARG:HE	1:B:78:GLN:HG2	1.81	0.45
1:B:174:ASP:OD2	1:B:188:ARG:HD2	2.17	0.45
1:C:80:LEU:HG	1:C:145:TRP:CD1	2.52	0.45
1:C:95:HIS:CD2	1:C:97:GLN:HB2	2.52	0.45
1:A:26:LYS:HE2	3:A:311:HOH:O	2.15	0.45
1:D:135:PRO:O	1:D:138:MET:HG3	2.16	0.45
1:A:195:LEU:HD23	1:A:195:LEU:C	2.37	0.45
1:B:23:PRO:HB2	1:B:26:LYS:HG3	1.99	0.45
1:A:250:ASP:HB2	3:A:381:HOH:O	2.18	0.44
1:D:167:ILE:HD13	1:D:197:ALA:HB2	2.00	0.44
1:D:36:HIS:CG	3:D:405:HOH:O	2.70	0.44
1:B:23:PRO:CD	1:B:26:LYS:HE2	2.45	0.44
2:D:3:11N:H13A	2:D:3:11N:H19	1.90	0.44
1:C:29:TRP:CG	1:C:125:VAL:HB	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:GLN:HE21	1:C:85:GLN:HB2	1.54	0.44
1:D:161:LYS:HB3	1:D:161:LYS:HE2	1.84	0.43
1:C:36:HIS:HD2	1:C:40:TRP:CZ2	2.36	0.43
1:D:31:VAL:HG22	1:D:46:GLY:C	2.39	0.43
1:A:133:THR:HG22	1:A:135:PRO:HD3	1.99	0.43
1:C:50:HIS:CG	1:C:51:PRO:HD2	2.54	0.43
1:A:93:ILE:HD13	1:A:255:TYR:CD1	2.53	0.43
1:C:188:ARG:NH1	1:C:192:ASP:OD1	2.52	0.43
1:C:34:ARG:HD3	1:C:42:HIS:HA	2.01	0.43
1:C:80:LEU:O	1:C:81:TYR:HB2	2.19	0.43
1:C:119:SER:O	1:C:120:SER:HB2	2.19	0.42
1:D:138:MET:CE	1:D:217:VAL:HG22	2.49	0.42
1:A:29:TRP:CD2	1:A:125:VAL:HB	2.54	0.42
1:C:138:MET:HA	1:C:139:PRO:HD3	1.70	0.42
1:C:34:ARG:HD2	1:C:40:TRP:O	2.20	0.42
1:B:170:ASN:ND2	3:B:301:HOH:O	2.51	0.42
1:B:82:TYR:HB2	1:C:82:TYR:CE2	2.54	0.42
1:C:50:HIS:CD2	1:C:51:PRO:HD2	2.55	0.42
1:D:227:VAL:HG22	1:D:242:TYR:CE2	2.55	0.42
1:C:117:LYS:HB3	3:C:469:HOH:O	2.19	0.42
1:A:87:LEU:HA	1:A:88:PRO:HD2	1.90	0.41
1:D:165:VAL:HA	1:D:166:PRO:HD2	1.77	0.41
1:A:19:GLY:HA3	1:A:162:GLN:O	2.20	0.41
1:B:72:ARG:NH2	3:B:352:HOH:O	2.54	0.41
1:C:76:ARG:NH2	1:C:160:LEU:HD23	2.36	0.41
1:D:93:ILE:HD13	1:D:255:TYR:CD1	2.55	0.41
1:C:27:TRP:NE1	1:C:162:GLN:NE2	2.63	0.41
1:A:59:HIS:CE1	1:A:209:SER:HB3	2.56	0.41
1:A:68:LEU:HD23	1:A:92:ILE:HG12	2.03	0.41
1:B:176:LYS:HD3	1:B:237:ASN:HD22	1.85	0.41
1:B:177:TYR:HE2	1:B:231:GLU:HG3	1.86	0.41
1:D:171:HIS:CD2	1:D:172:ILE:HG13	2.55	0.41
1:A:50:HIS:CD2	1:A:53:TRP:HD1	2.39	0.41
1:A:50:HIS:HB3	1:A:53:TRP:HB2	2.02	0.41
1:A:191:ARG:HD3	3:A:316:HOH:O	2.20	0.41
1:A:31:VAL:HG22	1:A:46:GLY:C	2.42	0.40
1:D:119:SER:HB2	1:D:122:VAL:HB	2.03	0.40
1:A:154:LEU:HA	1:A:155:PRO:HD3	1.96	0.40
1:D:169:GLU:OE1	1:D:171:HIS:CE1	2.73	0.40
1:D:28:PRO:HB2	1:D:123:HIS:H	1.87	0.40
1:B:201:ARG:HG2	1:B:202:ARG:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:HIS:HB3	1:B:53:TRP:HB2	2.03	0.40
1:A:118:VAL:O	1:A:118:VAL:HG23	2.21	0.40
1:B:31:VAL:HG22	1:B:46:GLY:C	2.42	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	241/243 (99%)	230 (95%)	9 (4%)	2 (1%)	22	11
1	B	241/243 (99%)	229 (95%)	12 (5%)	0	100	100
1	C	241/243 (99%)	225 (93%)	14 (6%)	2 (1%)	22	11
1	D	241/243 (99%)	231 (96%)	9 (4%)	1 (0%)	38	27
All	All	964/972 (99%)	915 (95%)	44 (5%)	5 (0%)	32	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	VAL
1	C	120	SER
1	D	118	VAL
1	C	81	TYR
1	A	51	PRO

### 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	207/208 (100%)	205 (99%)	2 (1%)	80	79
1	B	207/208 (100%)	206 (100%)	1 (0%)	91	91
1	C	207/208 (100%)	204 (99%)	3 (1%)	71	69
1	D	207/208 (100%)	203 (98%)	4 (2%)	62	58
All	All	828/832 (100%)	818 (99%)	10 (1%)	75	74

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	THR
1	A	188	ARG
1	B	122	VAL
1	C	85	GLN
1	C	116	VAL
1	C	133	THR
1	D	89	VAL
1	D	153	ARG
1	D	186	ASP
1	D	220	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	36	HIS
1	A	50	HIS
1	A	52	GLN
1	A	171	HIS
1	A	223	GLN
1	B	20	GLN
1	B	36	HIS
1	B	50	HIS
1	B	52	GLN
1	B	97	GLN
1	B	170	ASN
1	B	178	HIS
1	B	237	ASN
1	B	254	HIS

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Mol	Chain	Res	Type
1	C	20	GLN
1	C	30	GLN
1	C	36	HIS
1	C	50	HIS
1	C	85	GLN
1	C	95	HIS
1	C	97	GLN
1	C	162	GLN
1	C	223	GLN
1	C	253	HIS
1	C	254	HIS
1	D	30	GLN
1	D	36	HIS
1	D	52	GLN
1	D	85	GLN
1	D	150	ASN
1	D	171	HIS
1	D	237	ASN
1	D	253	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 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	11N	A	1	-	28,29,29	2.50	10 (35%)	35,41,41	2.49	10 (28%)
2	11N	B	4	-	28,29,29	2.48	12 (42%)	35,41,41	2.50	10 (28%)
2	11N	C	2	-	28,29,29	2.46	9 (32%)	35,41,41	2.43	11 (31%)
2	11N	D	3	-	28,29,29	2.43	12 (42%)	35,41,41	2.35	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	11N	A	1	-	-	0/11/35/35	0/4/4/4
2	11N	B	4	-	-	0/11/35/35	0/4/4/4
2	11N	C	2	-	-	0/11/35/35	0/4/4/4
2	11N	D	3	-	-	0/11/35/35	0/4/4/4

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	11N	O37-C17	-2.27	1.18	1.23
2	B	4	11N	C7-C3	-2.23	1.50	1.52
2	C	2	11N	O37-C17	-2.12	1.18	1.23
2	D	3	11N	O37-C17	-2.05	1.19	1.23
2	A	1	11N	O37-C17	-2.04	1.19	1.23
2	D	3	11N	C4-C5	2.00	1.42	1.39
2	B	4	11N	C23-C22	2.00	1.42	1.38
2	A	1	11N	C22-C41	2.04	1.43	1.39
2	D	3	11N	C22-C41	2.05	1.43	1.39
2	C	2	11N	C25-C26	2.06	1.42	1.38
2	B	4	11N	C25-C24	2.14	1.43	1.38
2	B	4	11N	C41-C20	2.14	1.54	1.47
2	D	3	11N	C25-C24	2.16	1.43	1.38
2	A	1	11N	C25-C26	2.17	1.43	1.38
2	A	1	11N	C41-C20	2.18	1.54	1.47
2	D	3	11N	C41-C20	2.18	1.54	1.47
2	C	2	11N	C41-C20	2.20	1.54	1.47
2	D	3	11N	C25-C26	2.27	1.43	1.38
2	B	4	11N	C25-C26	2.29	1.43	1.38
2	B	4	11N	C1-C6	2.58	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	11N	C1-C6	2.89	1.43	1.38
2	C	2	11N	C1-C6	2.98	1.44	1.38
2	D	3	11N	C1-C6	3.00	1.44	1.38
2	C	2	11N	C19-C17	3.23	1.53	1.48
2	D	3	11N	C19-C17	3.24	1.53	1.48
2	B	4	11N	C6-C5	3.28	1.45	1.38
2	C	2	11N	C6-C5	3.35	1.45	1.38
2	D	3	11N	C6-C5	3.37	1.45	1.38
2	A	1	11N	C19-C17	3.44	1.53	1.48
2	A	1	11N	C6-C5	3.49	1.46	1.38
2	B	4	11N	C19-C17	3.73	1.54	1.48
2	D	3	11N	C17-N22	4.62	1.46	1.35
2	B	4	11N	C17-N22	4.71	1.46	1.35
2	C	2	11N	C17-N22	4.74	1.46	1.35
2	A	1	11N	C17-N22	4.97	1.46	1.35
2	D	3	11N	C2-C3	5.75	1.48	1.38
2	B	4	11N	C2-C3	5.91	1.48	1.38
2	D	3	11N	O15-C2	6.11	1.46	1.38
2	C	2	11N	C2-C3	6.12	1.48	1.38
2	A	1	11N	C2-C3	6.14	1.48	1.38
2	B	4	11N	O15-C2	6.22	1.46	1.38
2	C	2	11N	O15-C2	6.39	1.46	1.38
2	A	1	11N	O15-C2	6.58	1.47	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	11N	O15-C2-C3	-7.72	107.35	113.03
2	D	3	11N	O15-C2-C3	-7.15	107.76	113.03
2	C	2	11N	O15-C2-C3	-6.89	107.95	113.03
2	B	4	11N	O15-C2-C3	-6.60	108.17	113.03
2	B	4	11N	C10-C7-C3	-6.08	101.16	111.88
2	C	2	11N	C10-C7-C3	-6.03	101.25	111.88
2	D	3	11N	C10-C7-C3	-5.32	102.50	111.88
2	A	1	11N	C10-C7-C3	-4.98	103.11	111.88
2	A	1	11N	C14-C7-C3	-3.11	106.40	111.88
2	A	1	11N	C20-C19-C17	-2.50	115.00	120.48
2	C	2	11N	C20-C19-C17	-2.27	115.50	120.48
2	B	4	11N	C1-C2-C3	-2.19	120.04	122.92
2	C	2	11N	C1-C2-C3	-2.18	120.05	122.92
2	D	3	11N	C20-C19-C17	-2.17	115.73	120.48
2	B	4	11N	C20-C19-C17	-2.15	115.78	120.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	11N	O37-C17-C19	-2.14	117.74	122.16
2	A	1	11N	C1-C2-C3	-2.14	120.10	122.92
2	D	3	11N	C1-C2-C3	-2.11	120.14	122.92
2	C	2	11N	C11-N22-C17	-2.02	116.13	123.08
2	C	2	11N	C41-C20-C19	-2.01	121.97	126.92
2	B	4	11N	C14-C7-C10	2.17	110.95	108.82
2	B	4	11N	O15-C2-C1	2.32	131.79	127.86
2	C	2	11N	O15-C2-C1	2.45	132.00	127.86
2	D	3	11N	O15-C2-C1	2.50	132.09	127.86
2	D	3	11N	C19-C17-N22	2.71	121.33	118.20
2	A	1	11N	O15-C2-C1	2.77	132.54	127.86
2	C	2	11N	C11-N22-C13	2.78	117.86	112.61
2	D	3	11N	C8-O15-C2	3.00	108.61	105.92
2	C	2	11N	C8-O15-C2	3.15	108.75	105.92
2	A	1	11N	C11-N22-C13	3.18	118.62	112.61
2	B	4	11N	C8-O15-C2	3.34	108.92	105.92
2	D	3	11N	C11-N22-C13	3.56	119.33	112.61
2	B	4	11N	C11-N22-C13	3.74	119.69	112.61
2	C	2	11N	C19-C17-N22	4.04	122.87	118.20
2	B	4	11N	C19-C17-N22	4.06	122.89	118.20
2	A	1	11N	C19-C17-N22	4.41	123.30	118.20
2	D	3	11N	C4-C3-C7	6.50	133.32	125.61
2	A	1	11N	C4-C3-C7	6.54	133.37	125.61
2	B	4	11N	C4-C3-C7	6.59	133.42	125.61
2	C	2	11N	C4-C3-C7	6.60	133.43	125.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	11N	1	0

## 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	243/243 (100%)	-0.10	5 (2%) 64 66	17, 28, 49, 69	0
1	B	243/243 (100%)	-0.25	2 (0%) 86 87	14, 24, 40, 68	0
1	C	243/243 (100%)	-0.15	8 (3%) 47 50	14, 25, 43, 65	0
1	D	243/243 (100%)	-0.23	2 (0%) 86 87	14, 24, 41, 59	0
All	All	972/972 (100%)	-0.18	17 (1%) 70 72	14, 25, 44, 69	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	TYR	4.3
1	A	117	LYS	4.1
1	C	120	SER	3.6
1	C	118	VAL	3.2
1	C	121	HIS	2.9
1	D	118	VAL	2.9
1	A	118	VAL	2.8
1	C	137	GLY	2.8
1	A	121	HIS	2.8
1	C	139	PRO	2.7
1	C	119	SER	2.7
1	D	121	HIS	2.6
1	A	119	SER	2.6
1	C	131	SER	2.3
1	C	201	ARG	2.2
1	B	121	HIS	2.2
1	B	82	TYR	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 [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	11N	B	4	26/26	0.93	0.14	1.77	16,22,27,34	0
2	11N	D	3	26/26	0.94	0.12	1.03	17,22,28,29	0
2	11N	A	1	26/26	0.95	0.10	0.12	17,23,30,31	0
2	11N	C	2	26/26	0.95	0.10	-0.11	18,23,32,34	0

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

There are no such residues in this entry.