



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:08 AM GMT

PDB ID : 3H8B  
Title : A combined crystallographic and molecular dynamics study of cathepsin-L retro-binding inhibitors(compound 9)  
Authors : Tulsidas, S.R.; Chowdhury, S.F.; Kumar, S.; Joseph, L.; Purisima, E.O.; Sivaraman, J.  
Deposited on : 2009-04-29  
Resolution : 1.80 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

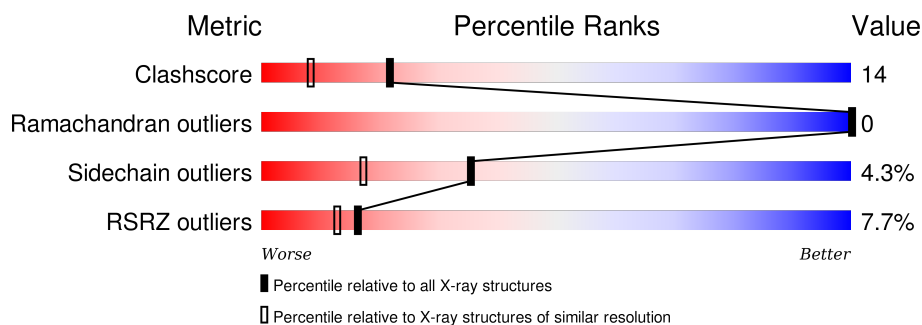
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	220	<div> <div>4%</div> <div>80%17%..</div> </div>
1	B	220	<div> <div>6%</div> <div>79%18%..</div> </div>
1	C	220	<div> <div>7%</div> <div>74%23%. </div> </div>
1	D	220	<div> <div>5%</div> <div>79%18%. </div> </div>
1	E	220	<div> <div>10%</div> <div>73%24%..</div> </div>
1	F	220	<div> <div>14%</div> <div>75%22%. </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NSY	A	300	-	-	-	X
2	NSY	B	400	-	-	-	X
2	NSY	C	500	-	-	-	X
2	NSY	D	600	-	-	-	X
2	NSY	E	700	-	-	-	X
2	NSY	F	800	-	-	-	X

## 2 Entry composition [i](#)

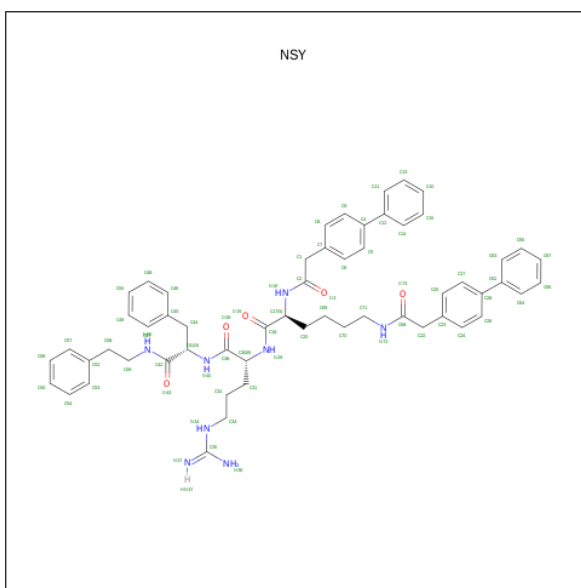
There are 3 unique types of molecules in this entry. The entry contains 10935 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cathepsin L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1659	1041	275	330	13			
1	B	215	Total	C	N	O	S	0	0	0
			1659	1041	275	330	13			
1	C	215	Total	C	N	O	S	0	0	0
			1659	1041	275	330	13			
1	D	215	Total	C	N	O	S	0	0	0
			1659	1041	275	330	13			
1	E	215	Total	C	N	O	S	0	0	0
			1659	1041	275	330	13			
1	F	215	Total	C	N	O	S	0	0	0
			1658	1041	275	329	13			

- Molecule 2 is N 2 ,N 6 -BIS(BIPHENYL-4-YLACETYL)-L-LYSYL-D-ARGINYL-N -(2-PHENYLETHYL)-L-PHENYLALANINAMIDE (three-letter code: NSY) (formula: C<sub>57</sub>H<sub>64</sub>N<sub>8</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			70	57	8	5		
2	B	1	Total	C	N	O	0	0
			70	57	8	5		
2	C	1	Total	C	N	O	0	0
			70	57	8	5		
2	D	1	Total	C	N	O	0	0
			70	57	8	5		
2	E	1	Total	C	N	O	0	0
			70	57	8	5		
2	F	1	Total	C	N	O	0	0
			70	57	8	5		

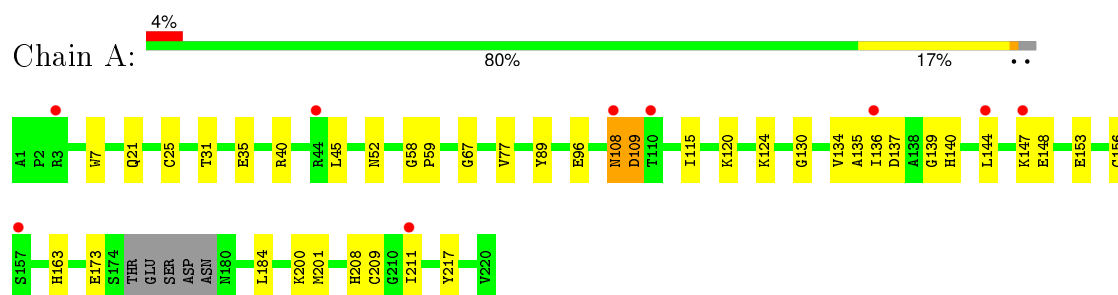
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	111	Total	O	0	0
			111	111		
3	B	124	Total	O	0	0
			124	124		
3	C	93	Total	O	0	0
			93	93		
3	D	88	Total	O	0	0
			88	88		
3	E	75	Total	O	0	0
			75	75		
3	F	71	Total	O	0	0
			71	71		

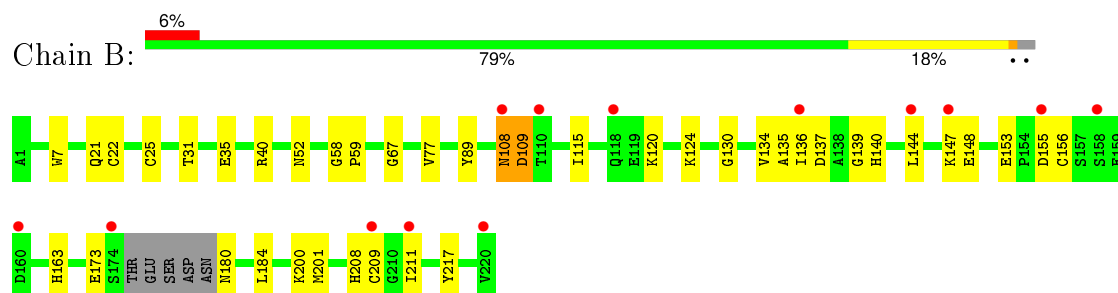
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

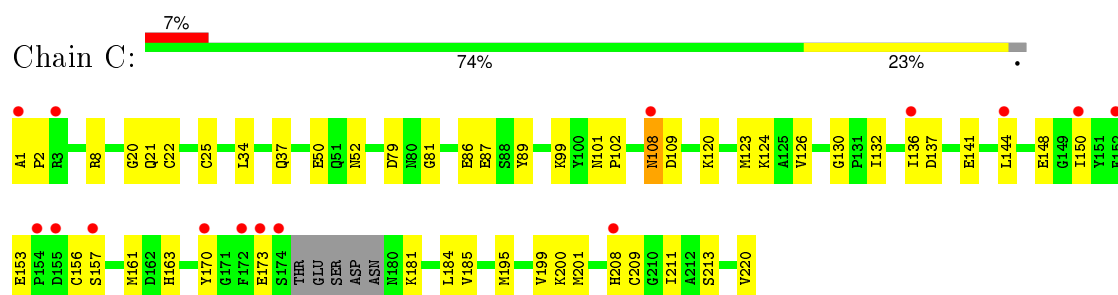
#### • Molecule 1: Cathepsin L1



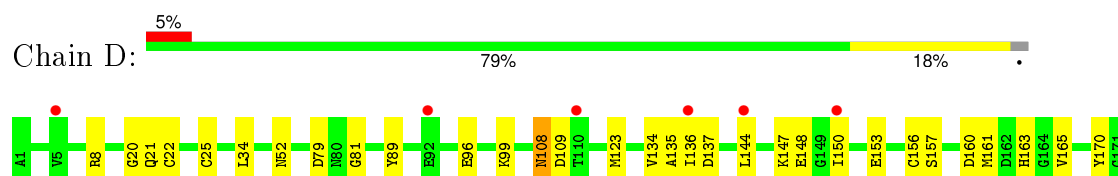
#### • Molecule 1: Cathepsin L1



#### • Molecule 1: Cathepsin L1

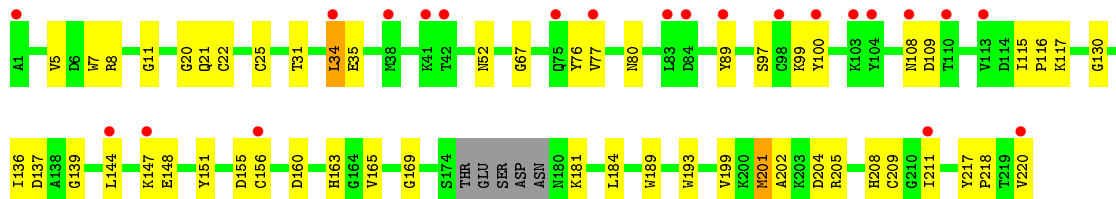


#### • Molecule 1: Cathepsin L1

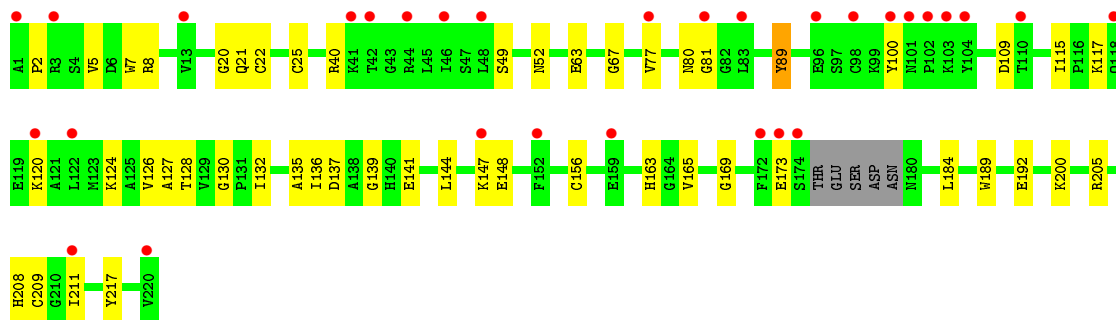
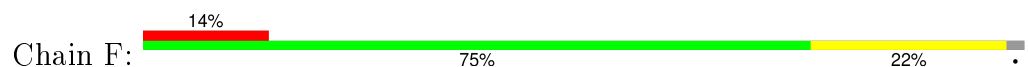




● Molecule 1: Cathepsin L1



● Molecule 1: Cathepsin L1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.99Å 99.23Å 206.46Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	45.00 – 1.80 48.24 – 1.79	Depositor EDS
% Data completeness (in resolution range)	94.2 (45.00-1.80) 97.2 (48.24-1.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.39 (at 1.79Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.216 , 0.250 0.229 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 25.1	EDS
Estimated twinning fraction	0.479 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 116974 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10935	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NSY

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	0.60	0/1700	0.66	0/2296
1	B	0.60	0/1700	0.65	0/2296
1	C	0.55	0/1700	0.67	0/2296
1	D	0.55	0/1700	0.67	0/2296
1	E	0.54	1/1700 (0.1%)	0.64	1/2296 (0.0%)
1	F	0.52	0/1699	0.64	0/2296
All	All	0.56	1/10199 (0.0%)	0.65	1/13776 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	201	MET	CG-SD	-6.24	1.65	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	201	MET	CA-CB-CG	-5.60	103.78	113.30

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	1659	0	1542	41	0
1	B	1659	0	1542	41	0
1	C	1659	0	1542	59	0
1	D	1659	0	1542	44	0
1	E	1659	0	1542	58	0
1	F	1658	0	1542	57	0
2	A	70	0	58	6	0
2	B	70	0	60	9	0
2	C	70	0	58	10	0
2	D	70	0	58	6	0
2	E	70	0	60	14	0
2	F	70	0	58	13	0
3	A	111	0	0	5	0
3	B	124	0	0	4	0
3	C	93	0	0	7	0
3	D	88	0	0	6	0
3	E	75	0	0	6	0
3	F	71	0	0	12	0
All	All	10935	0	9604	280	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 14.

All (280) 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:F:144:LEU:HD22	2:F:800:NSY:H26	1.22	1.14
1:E:144:LEU:HD22	2:E:700:NSY:H26	1.20	1.10
1:D:144:LEU:HD22	2:D:600:NSY:H26	1.30	1.10
1:C:126:VAL:HG22	1:C:132:ILE:HD13	1.40	1.03
1:C:144:LEU:HD22	2:C:500:NSY:H26	1.42	1.01
1:C:144:LEU:HD21	1:F:144:LEU:HD21	1.46	0.98
1:D:144:LEU:HD21	1:E:144:LEU:HD21	1.53	0.89
1:F:2:PRO:HD2	3:F:472:HOH:O	1.75	0.86
1:E:144:LEU:CD2	2:E:700:NSY:H26	2.07	0.84
1:D:163:HIS:HA	3:D:221:HOH:O	1.78	0.83
1:B:135:ALA:C	1:B:136:ILE:HD12	2.00	0.82
1:E:181:LYS:NZ	1:E:204:ASP:HB2	1.94	0.82
1:E:144:LEU:HD22	2:E:700:NSY:C26	2.08	0.82
1:C:99:LYS:HE2	1:D:99:LYS:HE2	1.63	0.80
1:A:135:ALA:C	1:A:136:ILE:HD12	2.02	0.80
1:C:144:LEU:HD21	1:F:144:LEU:CD2	2.12	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:HIS:HA	3:C:222:HOH:O	1.84	0.77
1:C:200:LYS:HE2	3:C:347:HOH:O	1.85	0.77
2:C:500:NSY:H27	1:F:21:GLN:HG2	1.66	0.76
1:E:163:HIS:HA	3:E:238:HOH:O	1.84	0.76
1:B:108:ASN:OD1	1:D:81:GLY:N	2.18	0.75
2:D:600:NSY:H27	1:E:21:GLN:HG2	1.68	0.75
1:A:108:ASN:OD1	1:C:81:GLY:N	2.19	0.74
1:F:163:HIS:HA	3:F:247:HOH:O	1.85	0.74
1:F:144:LEU:CD2	2:F:800:NSY:H26	2.12	0.74
1:F:144:LEU:HD22	2:F:800:NSY:C26	2.10	0.73
1:B:163:HIS:HA	3:B:221:HOH:O	1.88	0.73
1:E:25:CYS:SG	3:E:238:HOH:O	2.46	0.73
1:E:208:HIS:O	1:E:211:ILE:HG13	1.90	0.72
1:C:20:GLY:HA2	1:F:141:GLU:OE1	1.90	0.71
1:E:144:LEU:HD23	2:E:700:NSY:H63	1.74	0.70
1:D:144:LEU:HD21	1:E:144:LEU:CD2	2.22	0.70
1:C:120:LYS:HD3	1:C:124:LYS:HE3	1.74	0.70
1:E:181:LYS:HZ1	1:E:204:ASP:HB2	1.55	0.69
1:F:115:ILE:HD11	1:F:217:TYR:HE1	1.57	0.69
1:F:136:ILE:HG23	1:F:209:CYS:HB3	1.74	0.69
1:C:144:LEU:HD11	1:F:144:LEU:HD23	1.75	0.69
1:C:126:VAL:HA	1:C:132:ILE:HD11	1.74	0.68
1:A:115:ILE:HD11	1:A:217:TYR:HE1	1.57	0.68
1:A:163:HIS:HA	3:A:221:HOH:O	1.94	0.68
1:B:115:ILE:HD11	1:B:217:TYR:HE1	1.57	0.68
1:F:208:HIS:O	1:F:211:ILE:HG13	1.94	0.68
1:F:25:CYS:SG	3:F:247:HOH:O	2.52	0.67
1:F:135:ALA:C	1:F:136:ILE:HD12	2.15	0.67
1:B:136:ILE:HG23	1:B:209:CYS:HB3	1.77	0.66
1:E:25:CYS:SG	3:E:221:HOH:O	2.36	0.65
1:C:195:MET:SD	3:C:347:HOH:O	2.53	0.65
1:C:144:LEU:HD21	1:F:144:LEU:CG	2.28	0.64
1:C:144:LEU:CD2	2:C:500:NSY:H26	2.24	0.64
1:A:136:ILE:HG23	1:A:209:CYS:HB3	1.78	0.64
1:A:115:ILE:HD11	1:A:217:TYR:CE1	2.32	0.64
1:B:115:ILE:HD11	1:B:217:TYR:CE1	2.32	0.64
1:F:136:ILE:HG22	1:F:137:ASP:N	2.11	0.64
1:F:115:ILE:HD11	1:F:217:TYR:CE1	2.33	0.63
1:C:130:GLY:O	1:C:132:ILE:HD12	1.99	0.62
1:A:21:GLN:HA	2:A:300:NSY:H6	1.80	0.62
1:D:108:ASN:HD22	1:D:109:ASP:H	1.48	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ILE:HD12	1:C:150:ILE:N	2.14	0.62
1:C:126:VAL:CG2	1:C:132:ILE:HD13	2.25	0.62
1:A:136:ILE:HG22	1:A:137:ASP:N	2.15	0.61
1:C:120:LYS:HD2	1:C:120:LYS:C	2.20	0.61
1:F:136:ILE:HG23	1:F:209:CYS:CB	2.30	0.61
1:D:135:ALA:C	1:D:136:ILE:HD12	2.21	0.60
1:C:144:LEU:HD11	1:F:144:LEU:CD2	2.30	0.60
1:B:136:ILE:HG22	1:B:137:ASP:N	2.17	0.60
1:F:144:LEU:HD23	2:F:800:NSY:H63	1.84	0.60
1:C:132:ILE:N	1:C:132:ILE:HD12	2.17	0.60
1:C:144:LEU:HD23	2:C:500:NSY:H63	1.83	0.60
1:E:8:ARG:NH1	3:E:369:HOH:O	2.24	0.60
1:D:8:ARG:HA	3:D:402:HOH:O	2.02	0.59
1:D:96:GLU:HG3	3:D:408:HOH:O	2.01	0.59
1:C:123:MET:HG3	1:C:170:TYR:CE2	2.38	0.59
1:C:108:ASN:HD22	1:C:109:ASP:H	1.51	0.59
1:D:123:MET:HG3	1:D:170:TYR:CE2	2.38	0.58
1:E:136:ILE:HG22	1:E:137:ASP:N	2.19	0.58
1:B:208:HIS:O	1:B:211:ILE:HG13	2.03	0.58
1:B:108:ASN:ND2	1:B:109:ASP:H	2.01	0.58
1:E:151:TYR:HB3	1:E:201:MET:HG3	1.84	0.58
1:D:136:ILE:HG23	1:D:209:CYS:HB3	1.86	0.57
1:E:144:LEU:CD2	2:E:700:NSY:H63	2.34	0.57
1:D:147:LYS:HG2	1:E:147:LYS:NZ	2.19	0.57
1:A:108:ASN:ND2	1:A:109:ASP:H	2.03	0.56
1:E:108:ASN:ND2	1:E:109:ASP:H	2.03	0.56
1:A:208:HIS:O	1:A:211:ILE:HG13	2.05	0.56
1:F:136:ILE:CG2	1:F:137:ASP:N	2.67	0.56
1:C:150:ILE:HD11	1:C:173:GLU:CD	2.25	0.56
1:D:136:ILE:HD11	1:D:211:ILE:HG23	1.86	0.56
1:A:120:LYS:HD3	1:A:124:LYS:HE3	1.87	0.56
1:B:120:LYS:HD3	1:B:124:LYS:HE3	1.87	0.56
1:D:161:MET:CE	1:D:213:SER:HB2	2.36	0.56
1:D:144:LEU:HD21	1:E:144:LEU:CG	2.36	0.56
1:B:139:GLY:HA2	2:B:400:NSY:H22A	1.88	0.56
3:A:563:HOH:O	1:E:117:LYS:HE2	2.05	0.55
1:D:96:GLU:HG3	3:D:223:HOH:O	2.07	0.55
1:C:25:CYS:SG	3:C:222:HOH:O	2.38	0.55
1:B:21:GLN:HA	2:B:400:NSY:H6	1.87	0.55
1:F:8:ARG:NH1	3:F:242:HOH:O	2.28	0.55
1:F:136:ILE:HD11	1:F:211:ILE:HG23	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:VAL:HG21	3:F:472:HOH:O	2.07	0.54
1:C:130:GLY:O	1:C:132:ILE:CD1	2.55	0.54
1:D:136:ILE:CG2	1:D:137:ASP:N	2.70	0.54
1:B:136:ILE:N	1:B:136:ILE:HD12	2.23	0.54
1:F:7:TRP:CE2	1:F:130:GLY:HA2	2.42	0.54
1:A:25:CYS:SG	3:A:271:HOH:O	2.59	0.54
1:C:144:LEU:HD22	2:C:500:NSY:C26	2.29	0.53
1:D:21:GLN:HG2	2:E:700:NSY:H27	1.88	0.53
1:F:205:ARG:NH1	3:F:266:HOH:O	2.39	0.53
1:A:96:GLU:HG3	3:A:403:HOH:O	2.06	0.53
1:E:7:TRP:CE2	1:E:130:GLY:HA2	2.42	0.53
1:A:136:ILE:CG2	1:A:137:ASP:N	2.71	0.53
1:C:136:ILE:HG22	1:C:137:ASP:N	2.22	0.53
1:F:144:LEU:CD2	2:F:800:NSY:H63	2.39	0.52
1:B:136:ILE:CG2	1:B:137:ASP:N	2.72	0.52
1:E:80:ASN:ND2	1:E:100:TYR:CD2	2.77	0.52
1:A:40:ARG:HG3	1:A:40:ARG:HH11	1.74	0.52
1:B:40:ARG:HH11	1:B:40:ARG:HG3	1.74	0.52
1:E:151:TYR:HB3	1:E:201:MET:CG	2.39	0.52
1:D:25:CYS:SG	3:D:221:HOH:O	2.37	0.52
1:E:181:LYS:HZ1	1:E:204:ASP:CB	2.22	0.52
1:C:120:LYS:O	1:C:120:LYS:HD2	2.10	0.51
1:C:136:ILE:HD11	1:C:211:ILE:HG23	1.92	0.51
1:A:108:ASN:OD1	1:C:79:ASP:C	2.48	0.51
1:D:20:GLY:O	2:E:700:NSY:H66	2.09	0.51
1:C:150:ILE:HD11	1:C:173:GLU:OE1	2.10	0.51
1:F:127:ALA:HB2	3:F:472:HOH:O	2.10	0.51
1:D:136:ILE:HG22	1:D:137:ASP:N	2.24	0.51
1:D:208:HIS:O	1:D:211:ILE:HG13	2.10	0.51
1:F:126:VAL:HG22	1:F:132:ILE:HG12	1.93	0.51
1:A:136:ILE:N	1:A:136:ILE:HD12	2.26	0.51
1:E:202:ALA:HB1	1:E:205:ARG:HG3	1.93	0.51
1:B:180:ASN:N	3:B:288:HOH:O	2.44	0.51
1:F:77:VAL:HB	1:F:109:ASP:OD2	2.11	0.50
1:E:136:ILE:HD12	1:E:165:VAL:HG21	1.94	0.50
1:E:136:ILE:HG23	1:E:209:CYS:CB	2.41	0.50
1:B:58:GLY:N	1:B:59:PRO:CD	2.74	0.50
1:B:21:GLN:HA	2:B:400:NSY:C6	2.41	0.50
1:F:81:GLY:HA2	3:F:464:HOH:O	2.10	0.50
1:E:115:ILE:HD11	1:E:217:TYR:CD1	2.46	0.50
1:C:185:VAL:HB	1:C:199:VAL:HG13	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:GLN:HG2	2:F:800:NSY:H27	1.93	0.50
1:A:136:ILE:HG21	1:A:201:MET:CE	2.42	0.50
1:B:108:ASN:OD1	1:D:79:ASP:C	2.50	0.50
1:B:136:ILE:HD11	1:B:211:ILE:HG23	1.92	0.49
1:F:117:LYS:NZ	3:F:238:HOH:O	2.45	0.49
1:A:40:ARG:NH1	1:A:40:ARG:HG3	2.27	0.49
1:B:40:ARG:HG3	1:B:40:ARG:NH1	2.27	0.49
1:D:185:VAL:HB	1:D:199:VAL:HG13	1.95	0.49
1:F:22:CYS:N	2:F:800:NSY:H6	2.28	0.49
1:A:58:GLY:N	1:A:59:PRO:CD	2.76	0.49
1:E:136:ILE:HD11	1:E:211:ILE:HG23	1.94	0.49
2:D:600:NSY:H66	1:E:20:GLY:O	2.13	0.49
1:E:136:ILE:CG2	1:E:137:ASP:N	2.75	0.49
1:F:67:GLY:HA2	2:F:800:NSY:O39	2.13	0.48
1:D:25:CYS:SG	3:D:299:HOH:O	2.60	0.48
1:F:136:ILE:CG2	1:F:209:CYS:HB3	2.41	0.48
1:B:136:ILE:HG21	1:B:201:MET:CE	2.44	0.48
1:B:134:VAL:HG23	1:B:136:ILE:CD1	2.44	0.48
1:C:8:ARG:HA	3:C:455:HOH:O	2.14	0.48
1:B:155:ASP:HB2	3:B:565:HOH:O	2.13	0.48
1:F:136:ILE:N	1:F:136:ILE:HD12	2.29	0.48
1:B:22:CYS:N	2:B:400:NSY:H6	2.29	0.48
1:A:136:ILE:HD11	1:A:211:ILE:HG23	1.94	0.48
1:E:22:CYS:N	2:E:700:NSY:H6	2.29	0.47
1:E:136:ILE:HG23	1:E:209:CYS:HB3	1.95	0.47
1:C:208:HIS:O	1:C:211:ILE:HG13	2.13	0.47
1:B:153:GLU:O	1:B:208:HIS:HE1	1.96	0.47
1:B:77:VAL:HB	1:B:109:ASP:OD2	2.15	0.47
1:E:136:ILE:HG12	1:E:211:ILE:HG12	1.97	0.47
1:F:80:ASN:ND2	1:F:100:TYR:CD2	2.78	0.47
1:C:20:GLY:O	2:F:800:NSY:H66	2.15	0.47
1:F:5:VAL:CG2	3:F:472:HOH:O	2.62	0.47
1:C:87:GLU:HG2	3:C:305:HOH:O	2.14	0.47
1:C:22:CYS:N	2:C:500:NSY:H6	2.30	0.47
1:A:77:VAL:HB	1:A:109:ASP:OD2	2.15	0.47
1:E:115:ILE:HG23	1:E:116:PRO:HD2	1.96	0.47
1:A:120:LYS:CD	1:A:124:LYS:HE3	2.45	0.46
1:C:161:MET:CE	1:C:213:SER:HB2	2.45	0.46
1:D:157:SER:HB3	1:D:160:ASP:OD1	2.16	0.46
1:A:136:ILE:HG21	1:A:201:MET:HE1	1.97	0.46
1:F:80:ASN:ND2	1:F:100:TYR:CE2	2.83	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ILE:HD12	1:D:150:ILE:N	2.31	0.46
1:A:21:GLN:HA	2:A:300:NSY:C6	2.45	0.46
1:A:139:GLY:HA2	2:A:300:NSY:C22	2.45	0.46
1:A:31:THR:O	1:A:35:GLU:HG3	2.16	0.46
1:B:173:GLU:OE2	1:B:200:LYS:NZ	2.48	0.46
1:F:49:SER:OG	1:F:89:TYR:HB3	2.16	0.46
1:B:135:ALA:O	1:B:136:ILE:HD12	2.16	0.45
1:A:136:ILE:HG23	1:A:209:CYS:CB	2.46	0.45
1:C:150:ILE:N	1:C:150:ILE:CD1	2.79	0.45
1:D:144:LEU:HD21	1:E:144:LEU:HD11	1.96	0.45
1:E:31:THR:O	1:E:35:GLU:HG3	2.17	0.45
1:E:34:LEU:HG	1:E:218:PRO:HG3	1.97	0.45
1:F:173:GLU:OE2	1:F:200:LYS:NZ	2.50	0.45
1:A:173:GLU:OE2	1:A:200:LYS:NZ	2.48	0.45
1:E:181:LYS:HB2	1:E:181:LYS:HZ2	1.80	0.45
1:B:120:LYS:CD	1:B:124:LYS:HE3	2.45	0.45
2:C:500:NSY:H67	1:F:189:TRP:CD1	2.51	0.45
1:C:157:SER:HB2	3:C:551:HOH:O	2.17	0.45
1:F:127:ALA:CB	3:F:472:HOH:O	2.63	0.45
1:F:211:ILE:H	1:F:211:ILE:HG13	1.55	0.45
1:E:77:VAL:HG12	1:E:108:ASN:HD22	1.82	0.45
1:F:5:VAL:O	1:F:169:GLY:HA3	2.17	0.45
1:B:136:ILE:HG21	1:B:201:MET:HE1	1.99	0.45
1:C:144:LEU:CD2	2:C:500:NSY:H63	2.45	0.44
1:E:139:GLY:HA2	2:E:700:NSY:C22	2.47	0.44
1:D:144:LEU:CD2	1:E:144:LEU:HG	2.47	0.44
1:B:7:TRP:CE2	1:B:130:GLY:HA2	2.52	0.44
1:D:144:LEU:CD2	2:D:600:NSY:H63	2.47	0.44
1:E:193:TRP:CH2	1:E:199:VAL:HB	2.53	0.44
1:C:126:VAL:HA	1:C:132:ILE:CD1	2.43	0.44
1:B:144:LEU:HD23	2:B:400:NSY:H26	1.98	0.44
1:D:181:LYS:HZ3	1:D:181:LYS:HB2	1.83	0.44
2:C:500:NSY:H66	1:F:20:GLY:O	2.18	0.44
1:A:135:ALA:O	1:A:136:ILE:HD12	2.18	0.44
1:A:153:GLU:O	1:A:208:HIS:HE1	1.99	0.44
1:A:7:TRP:CE2	1:A:130:GLY:HA2	2.52	0.44
1:C:144:LEU:CD2	1:F:144:LEU:HD21	2.32	0.44
1:F:124:LYS:O	1:F:128:THR:HG23	2.18	0.44
1:F:120:LYS:HD3	1:F:124:LYS:HE3	1.99	0.44
1:D:144:LEU:CD2	1:E:144:LEU:CG	2.96	0.44
1:A:25:CYS:SG	3:A:221:HOH:O	2.43	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASP:OD2	1:B:140:HIS:HE1	2.01	0.43
1:A:137:ASP:OD2	1:A:140:HIS:HE1	2.01	0.43
1:D:147:LYS:HG2	1:E:147:LYS:HZ2	1.82	0.43
1:D:153:GLU:O	1:D:208:HIS:HE1	2.01	0.43
1:E:139:GLY:HA2	2:E:700:NSY:H22A	2.01	0.43
1:E:67:GLY:HA2	2:E:700:NSY:O39	2.19	0.43
1:A:67:GLY:HA2	2:A:300:NSY:O39	2.18	0.43
1:E:11:GLY:N	3:E:247:HOH:O	2.51	0.43
1:D:161:MET:HE3	1:D:213:SER:HB2	2.00	0.43
1:C:37:GLN:HB3	1:C:220:VAL:CG2	2.49	0.43
1:F:63:GLU:HG2	2:F:800:NSY:H55	2.00	0.42
1:D:22:CYS:N	2:D:600:NSY:H6	2.34	0.42
1:F:136:ILE:HD13	1:F:165:VAL:CG2	2.50	0.42
1:D:150:ILE:HD11	1:D:173:GLU:CD	2.39	0.42
2:D:600:NSY:H67	1:E:189:TRP:CD1	2.54	0.42
1:B:31:THR:O	1:B:35:GLU:HG3	2.20	0.42
1:A:134:VAL:HG23	1:A:136:ILE:CD1	2.49	0.42
1:A:144:LEU:HD23	2:A:300:NSY:H26	2.00	0.42
1:C:136:ILE:CG2	1:C:137:ASP:N	2.83	0.42
1:C:136:ILE:HG23	1:C:209:CYS:CB	2.49	0.42
1:D:193:TRP:CH2	1:D:199:VAL:HB	2.54	0.42
1:B:25:CYS:SG	3:B:245:HOH:O	2.62	0.42
1:F:40:ARG:HG3	1:F:40:ARG:HH11	1.84	0.42
1:F:139:GLY:HA2	2:F:800:NSY:C22	2.50	0.42
1:B:136:ILE:HG23	1:B:209:CYS:CB	2.46	0.42
1:C:1:ALA:HA	1:C:2:PRO:HD3	1.88	0.42
1:E:220:VAL:HG23	1:E:220:VAL:OXT	2.19	0.42
1:E:21:GLN:HA	2:E:700:NSY:C6	2.50	0.42
1:E:211:ILE:H	1:E:211:ILE:HG13	1.58	0.42
1:C:120:LYS:CD	1:C:120:LYS:C	2.88	0.42
1:D:181:LYS:HB2	1:D:181:LYS:NZ	2.35	0.41
1:D:134:VAL:HG23	1:D:136:ILE:CD1	2.49	0.41
1:D:136:ILE:HG23	1:D:209:CYS:CB	2.50	0.41
1:B:144:LEU:HA	1:B:144:LEU:HD12	1.93	0.41
2:E:700:NSY:H17	3:E:238:HOH:O	2.21	0.41
1:D:136:ILE:HD13	1:D:165:VAL:CG2	2.50	0.41
1:B:67:GLY:HA2	2:B:400:NSY:O39	2.19	0.41
1:C:153:GLU:O	1:C:208:HIS:HE1	2.03	0.41
1:B:144:LEU:CD2	2:B:400:NSY:H26	2.51	0.41
1:E:21:GLN:HA	2:E:700:NSY:H6	2.02	0.41
1:E:5:VAL:O	1:E:169:GLY:HA3	2.20	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ASN:HD22	1:C:109:ASP:N	2.17	0.41
1:E:76:TYR:CE1	1:E:80:ASN:HB2	2.56	0.41
1:E:97:SER:O	1:E:99:LYS:HG3	2.21	0.41
1:F:192:GLU:OE2	1:F:192:GLU:HA	2.21	0.41
1:B:139:GLY:HA2	2:B:400:NSY:C22	2.50	0.41
1:A:45:LEU:HB3	1:E:160:ASP:HB3	2.02	0.41
1:C:181:LYS:HB2	1:C:181:LYS:NZ	2.36	0.41
1:C:144:LEU:HG	1:F:144:LEU:HG	2.03	0.40
1:A:108:ASN:OD1	1:C:79:ASP:O	2.39	0.40
2:B:400:NSY:H5	2:B:400:NSY:H14	1.87	0.40
1:A:144:LEU:CD2	2:A:300:NSY:H26	2.51	0.40
1:A:144:LEU:HD12	1:A:144:LEU:HA	1.90	0.40
1:F:21:GLN:HA	2:F:800:NSY:C6	2.51	0.40
2:F:800:NSY:H17	3:F:247:HOH:O	2.21	0.40
1:C:99:LYS:NZ	1:D:99:LYS:NZ	2.70	0.40
2:C:500:NSY:H5	2:C:500:NSY:H14	1.89	0.40
1:C:101:ASN:HA	1:C:102:PRO:HD3	1.96	0.40
1:C:50:GLU:OE1	1:C:86:GLU:OE1	2.40	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	211/220 (96%)	207 (98%)	4 (2%)	0	100	100
1	B	211/220 (96%)	208 (99%)	3 (1%)	0	100	100
1	C	211/220 (96%)	204 (97%)	7 (3%)	0	100	100
1	D	211/220 (96%)	206 (98%)	5 (2%)	0	100	100
1	E	211/220 (96%)	200 (95%)	11 (5%)	0	100	100
1	F	211/220 (96%)	204 (97%)	7 (3%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1266/1320 (96%)	1229 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	174/179 (97%)	166 (95%)	8 (5%)	33	15
1	B	174/179 (97%)	166 (95%)	8 (5%)	33	15
1	C	174/179 (97%)	165 (95%)	9 (5%)	29	12
1	D	174/179 (97%)	167 (96%)	7 (4%)	38	20
1	E	174/179 (97%)	167 (96%)	7 (4%)	38	20
1	F	174/179 (97%)	168 (97%)	6 (3%)	44	26
All	All	1044/1074 (97%)	999 (96%)	45 (4%)	35	17

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	89	TYR
1	A	108	ASN
1	A	109	ASP
1	A	147	LYS
1	A	148	GLU
1	A	156	CYS
1	A	184	LEU
1	B	52	ASN
1	B	89	TYR
1	B	108	ASN
1	B	109	ASP
1	B	147	LYS
1	B	148	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	156	CYS
1	B	184	LEU
1	C	34	LEU
1	C	52	ASN
1	C	89	TYR
1	C	108	ASN
1	C	141	GLU
1	C	148	GLU
1	C	156	CYS
1	C	184	LEU
1	C	201	MET
1	D	34	LEU
1	D	52	ASN
1	D	89	TYR
1	D	108	ASN
1	D	148	GLU
1	D	156	CYS
1	D	184	LEU
1	E	34	LEU
1	E	52	ASN
1	E	89	TYR
1	E	148	GLU
1	E	155	ASP
1	E	156	CYS
1	E	184	LEU
1	F	52	ASN
1	F	89	TYR
1	F	147	LYS
1	F	148	GLU
1	F	156	CYS
1	F	184	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	118	GLN
1	C	108	ASN
1	D	108	ASN
1	E	108	ASN
1	F	75	GLN
1	F	78	GLN
1	F	108	ASN

### 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 ⓘ

6 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	NSY	A	300	-	72,75,75	5.75	55 (76%)	93,97,97	2.26	28 (30%)
2	NSY	B	400	-	72,75,75	5.74	55 (76%)	93,97,97	2.30	29 (31%)
2	NSY	C	500	-	72,75,75	5.84	57 (79%)	93,97,97	2.23	30 (32%)
2	NSY	D	600	-	72,75,75	5.84	56 (77%)	93,97,97	2.24	31 (33%)
2	NSY	E	700	-	72,75,75	5.77	55 (76%)	93,97,97	2.28	35 (37%)
2	NSY	F	800	-	72,75,75	5.77	55 (76%)	93,97,97	2.26	32 (34%)

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	NSY	A	300	-	-	0/63/65/65	0/6/6/6
2	NSY	B	400	-	-	0/63/65/65	0/6/6/6
2	NSY	C	500	-	-	0/63/65/65	0/6/6/6

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NSY	D	600	-	-	0/63/65/65	0/6/6/6
2	NSY	E	700	-	-	0/63/65/65	0/6/6/6
2	NSY	F	800	-	-	0/63/65/65	0/6/6/6

All (333) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	NSY	C22-C23	-12.63	1.29	1.51
2	B	400	NSY	C22-C23	-12.14	1.30	1.51
2	C	500	NSY	C22-C23	-11.97	1.30	1.51
2	D	600	NSY	C22-C23	-11.85	1.31	1.51
2	F	800	NSY	C22-C23	-11.64	1.31	1.51
2	E	700	NSY	C22-C23	-11.29	1.32	1.51
2	F	800	NSY	C1-C2	-7.84	1.32	1.51
2	E	700	NSY	C1-C2	-7.79	1.32	1.51
2	C	500	NSY	C1-C2	-7.65	1.32	1.51
2	A	300	NSY	C1-C2	-7.49	1.33	1.51
2	D	600	NSY	C1-C2	-7.40	1.33	1.51
2	B	400	NSY	C1-C2	-7.37	1.33	1.51
2	E	700	NSY	C22-C68	-5.50	1.38	1.51
2	F	800	NSY	C22-C68	-5.48	1.38	1.51
2	D	600	NSY	C22-C68	-5.48	1.38	1.51
2	C	500	NSY	C22-C68	-5.39	1.38	1.51
2	D	600	NSY	O73-C68	-4.53	1.13	1.23
2	C	500	NSY	O73-C68	-4.44	1.13	1.23
2	A	300	NSY	C22-C68	-4.34	1.41	1.51
2	A	300	NSY	C69-C70	-4.27	1.26	1.51
2	D	600	NSY	C69-C70	-4.25	1.27	1.51
2	F	800	NSY	O73-C68	-4.20	1.14	1.23
2	C	500	NSY	C69-C70	-4.18	1.27	1.51
2	E	700	NSY	O73-C68	-4.16	1.14	1.23
2	B	400	NSY	C22-C68	-4.15	1.41	1.51
2	B	400	NSY	C69-C70	-4.15	1.27	1.51
2	F	800	NSY	C69-C70	-3.94	1.28	1.51
2	E	700	NSY	C69-C70	-3.92	1.28	1.51
2	F	800	NSY	C58-C52	-3.91	1.40	1.51
2	A	300	NSY	C20-C17	-3.86	1.44	1.53
2	A	300	NSY	C58-C52	-3.70	1.41	1.51
2	B	400	NSY	C58-C52	-3.67	1.41	1.51
2	D	600	NSY	C58-C52	-3.63	1.41	1.51
2	E	700	NSY	C58-C52	-3.58	1.41	1.51
2	C	500	NSY	C58-C52	-3.57	1.41	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	NSY	C20-C17	-3.49	1.45	1.53
2	D	600	NSY	C20-C17	-3.39	1.45	1.53
2	C	500	NSY	C20-C17	-3.34	1.45	1.53
2	A	300	NSY	O73-C68	-3.32	1.16	1.23
2	B	400	NSY	O73-C68	-3.25	1.16	1.23
2	F	800	NSY	C20-C17	-3.21	1.46	1.53
2	E	700	NSY	C20-C17	-3.04	1.46	1.53
2	F	800	NSY	C68-N72	-2.92	1.26	1.33
2	D	600	NSY	C30-C38	-2.90	1.44	1.52
2	A	300	NSY	C28-C62	-2.90	1.41	1.49
2	E	700	NSY	C68-N72	-2.80	1.26	1.33
2	F	800	NSY	C30-C38	-2.79	1.45	1.52
2	B	400	NSY	C28-C62	-2.79	1.41	1.49
2	C	500	NSY	C68-N72	-2.76	1.26	1.33
2	D	600	NSY	C68-N72	-2.74	1.26	1.33
2	D	600	NSY	C28-C62	-2.64	1.42	1.49
2	E	700	NSY	C28-C62	-2.63	1.42	1.49
2	C	500	NSY	C28-C62	-2.58	1.42	1.49
2	B	400	NSY	C68-N72	-2.48	1.27	1.33
2	C	500	NSY	C30-C38	-2.47	1.45	1.52
2	D	600	NSY	C30-N29	-2.45	1.40	1.45
2	A	300	NSY	C68-N72	-2.43	1.27	1.33
2	E	700	NSY	C30-C38	-2.38	1.46	1.52
2	F	800	NSY	C28-C62	-2.35	1.42	1.49
2	B	400	NSY	C30-C38	-2.30	1.46	1.52
2	A	300	NSY	C30-C38	-2.23	1.46	1.52
2	C	500	NSY	C30-N29	-2.02	1.41	1.45
2	C	500	NSY	O3-C2	-2.01	1.19	1.23
2	A	300	NSY	C41-C42	2.05	1.58	1.52
2	B	400	NSY	C41-C42	2.23	1.58	1.52
2	C	500	NSY	C41-C42	2.35	1.59	1.52
2	B	400	NSY	C6-C5	2.37	1.43	1.38
2	D	600	NSY	C44-C45	2.52	1.57	1.51
2	D	600	NSY	C41-C42	2.57	1.59	1.52
2	C	500	NSY	C44-C45	2.62	1.57	1.51
2	F	800	NSY	C71-N72	2.75	1.52	1.46
2	E	700	NSY	C71-N72	2.81	1.52	1.46
2	E	700	NSY	C41-C42	2.81	1.60	1.52
2	B	400	NSY	C44-C45	2.86	1.58	1.51
2	F	800	NSY	C41-C42	2.87	1.60	1.52
2	A	300	NSY	C6-C5	2.88	1.43	1.38
2	E	700	NSY	C44-C45	2.91	1.58	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	NSY	C71-N72	2.95	1.53	1.46
2	D	600	NSY	C71-N72	2.96	1.53	1.46
2	A	300	NSY	C44-C45	2.97	1.58	1.51
2	F	800	NSY	C44-C45	3.04	1.58	1.51
2	E	700	NSY	C6-C5	3.08	1.44	1.38
2	F	800	NSY	C6-C5	3.10	1.44	1.38
2	A	300	NSY	C65-C67	3.22	1.46	1.38
2	F	800	NSY	C65-C67	3.32	1.46	1.38
2	E	700	NSY	C66-C67	3.46	1.46	1.38
2	B	400	NSY	C66-C64	3.48	1.46	1.38
2	E	700	NSY	C65-C67	3.49	1.47	1.38
2	B	400	NSY	C65-C67	3.55	1.47	1.38
2	D	600	NSY	C59-N60	3.56	1.54	1.46
2	A	300	NSY	C66-C64	3.56	1.46	1.38
2	D	600	NSY	C65-C67	3.59	1.47	1.38
2	C	500	NSY	C65-C67	3.60	1.47	1.38
2	A	300	NSY	C59-N60	3.61	1.54	1.46
2	B	400	NSY	C59-N60	3.63	1.54	1.46
2	D	600	NSY	C6-C5	3.69	1.45	1.38
2	C	500	NSY	C59-N60	3.72	1.54	1.46
2	F	800	NSY	C66-C67	3.76	1.47	1.38
2	C	500	NSY	C6-C5	3.85	1.45	1.38
2	A	300	NSY	O19-C18	3.87	1.31	1.23
2	B	400	NSY	C71-N72	3.95	1.55	1.46
2	B	400	NSY	O19-C18	3.95	1.31	1.23
2	A	300	NSY	C71-N72	3.98	1.55	1.46
2	F	800	NSY	O19-C18	4.04	1.31	1.23
2	D	600	NSY	C66-C67	4.14	1.48	1.38
2	D	600	NSY	O19-C18	4.15	1.31	1.23
2	E	700	NSY	C59-N60	4.16	1.55	1.46
2	C	500	NSY	O19-C18	4.18	1.31	1.23
2	C	500	NSY	C66-C67	4.19	1.48	1.38
2	C	500	NSY	C25-C23	4.21	1.47	1.38
2	E	700	NSY	O19-C18	4.25	1.31	1.23
2	B	400	NSY	C25-C23	4.26	1.47	1.38
2	D	600	NSY	C25-C23	4.28	1.47	1.38
2	D	600	NSY	C66-C64	4.28	1.47	1.38
2	D	600	NSY	C15-C14	4.32	1.47	1.38
2	C	500	NSY	C66-C64	4.37	1.47	1.38
2	F	800	NSY	C59-N60	4.38	1.56	1.46
2	A	300	NSY	C24-C26	4.39	1.46	1.38
2	B	400	NSY	C66-C67	4.40	1.49	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	NSY	C25-C23	4.42	1.48	1.38
2	C	500	NSY	C15-C14	4.44	1.48	1.38
2	C	500	NSY	C49-C47	4.46	1.48	1.38
2	A	300	NSY	C66-C67	4.50	1.49	1.38
2	F	800	NSY	C66-C64	4.52	1.48	1.38
2	D	600	NSY	C49-C47	4.54	1.48	1.38
2	B	400	NSY	C50-C49	4.70	1.50	1.38
2	C	500	NSY	C50-C49	4.73	1.50	1.38
2	E	700	NSY	C66-C64	4.74	1.48	1.38
2	F	800	NSY	C54-C55	4.75	1.50	1.38
2	E	700	NSY	C49-C47	4.75	1.48	1.38
2	F	800	NSY	C49-C47	4.76	1.48	1.38
2	F	800	NSY	C15-C14	4.78	1.48	1.38
2	A	300	NSY	C49-C47	4.79	1.48	1.38
2	B	400	NSY	C24-C26	4.80	1.47	1.38
2	E	700	NSY	C15-C14	4.83	1.48	1.38
2	A	300	NSY	C50-C49	4.83	1.50	1.38
2	D	600	NSY	C50-C49	4.85	1.50	1.38
2	D	600	NSY	C55-C56	4.88	1.50	1.38
2	B	400	NSY	C49-C47	4.89	1.49	1.38
2	E	700	NSY	C50-C49	4.90	1.50	1.38
2	D	600	NSY	C31-C30	4.92	1.64	1.53
2	E	700	NSY	C54-C55	4.96	1.50	1.38
2	E	700	NSY	C24-C23	4.99	1.49	1.38
2	C	500	NSY	C31-C30	5.00	1.65	1.53
2	A	300	NSY	C54-C55	5.04	1.50	1.38
2	D	600	NSY	C26-C28	5.05	1.50	1.39
2	B	400	NSY	C54-C55	5.09	1.51	1.38
2	B	400	NSY	C55-C56	5.13	1.51	1.38
2	E	700	NSY	C24-C26	5.14	1.48	1.38
2	A	300	NSY	C55-C56	5.14	1.51	1.38
2	C	500	NSY	C56-C57	5.15	1.49	1.38
2	F	800	NSY	C24-C23	5.15	1.49	1.38
2	C	500	NSY	C55-C56	5.15	1.51	1.38
2	A	300	NSY	C26-C28	5.17	1.50	1.39
2	B	400	NSY	C26-C28	5.17	1.50	1.39
2	F	800	NSY	C24-C26	5.17	1.48	1.38
2	E	700	NSY	C26-C28	5.22	1.50	1.39
2	F	800	NSY	C50-C49	5.22	1.51	1.38
2	D	600	NSY	C56-C57	5.25	1.49	1.38
2	D	600	NSY	C54-C55	5.27	1.51	1.38
2	C	500	NSY	C26-C28	5.30	1.50	1.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	NSY	C57-C52	5.32	1.50	1.38
2	C	500	NSY	C57-C52	5.37	1.50	1.38
2	F	800	NSY	C31-C30	5.39	1.66	1.53
2	F	800	NSY	C55-C56	5.40	1.51	1.38
2	E	700	NSY	C55-C56	5.41	1.51	1.38
2	C	500	NSY	C24-C23	5.42	1.50	1.38
2	D	600	NSY	C24-C23	5.47	1.50	1.38
2	E	700	NSY	C31-C30	5.51	1.66	1.53
2	F	800	NSY	C26-C28	5.53	1.51	1.39
2	C	500	NSY	C54-C55	5.54	1.52	1.38
2	F	800	NSY	C56-C57	5.56	1.50	1.38
2	E	700	NSY	C56-C57	5.67	1.50	1.38
2	F	800	NSY	C57-C52	5.75	1.51	1.38
2	D	600	NSY	C24-C26	5.81	1.49	1.38
2	A	300	NSY	C24-C23	5.81	1.51	1.38
2	F	800	NSY	C25-C23	5.82	1.51	1.38
2	E	700	NSY	C57-C52	5.83	1.51	1.38
2	A	300	NSY	C57-C52	5.84	1.51	1.38
2	B	400	NSY	C24-C23	5.84	1.51	1.38
2	B	400	NSY	C56-C57	5.84	1.50	1.38
2	C	500	NSY	C24-C26	5.87	1.49	1.38
2	E	700	NSY	C64-C62	5.96	1.52	1.39
2	B	400	NSY	C57-C52	5.98	1.51	1.38
2	B	400	NSY	C15-C14	6.01	1.51	1.38
2	C	500	NSY	C27-C28	6.02	1.52	1.39
2	A	300	NSY	C56-C57	6.02	1.51	1.38
2	E	700	NSY	C25-C23	6.06	1.51	1.38
2	A	300	NSY	C15-C14	6.07	1.51	1.38
2	B	400	NSY	C31-C30	6.09	1.67	1.53
2	F	800	NSY	C64-C62	6.12	1.52	1.39
2	D	600	NSY	C48-C46	6.17	1.51	1.38
2	A	300	NSY	C65-C63	6.22	1.51	1.38
2	A	300	NSY	C31-C30	6.25	1.68	1.53
2	A	300	NSY	C48-C46	6.30	1.51	1.38
2	B	400	NSY	C48-C46	6.30	1.51	1.38
2	B	400	NSY	C10-C13	6.34	1.54	1.38
2	D	600	NSY	C64-C62	6.39	1.53	1.39
2	B	400	NSY	C65-C63	6.41	1.52	1.38
2	D	600	NSY	C27-C28	6.41	1.53	1.39
2	D	600	NSY	C25-C27	6.42	1.50	1.38
2	C	500	NSY	C48-C46	6.43	1.52	1.38
2	C	500	NSY	C64-C62	6.51	1.53	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	NSY	C15-C10	6.55	1.54	1.38
2	D	600	NSY	C15-C10	6.59	1.54	1.38
2	A	300	NSY	C10-C13	6.61	1.55	1.38
2	B	400	NSY	C18-N29	6.62	1.49	1.34
2	F	800	NSY	C48-C46	6.63	1.52	1.38
2	D	600	NSY	C46-C45	6.65	1.53	1.38
2	A	300	NSY	C27-C28	6.66	1.53	1.39
2	F	800	NSY	C63-C62	6.69	1.53	1.39
2	A	300	NSY	C18-N29	6.69	1.49	1.34
2	A	300	NSY	C15-C10	6.69	1.55	1.38
2	A	300	NSY	C42-N60	6.71	1.47	1.33
2	A	300	NSY	C46-C45	6.76	1.53	1.38
2	A	300	NSY	C64-C62	6.76	1.53	1.39
2	D	600	NSY	C18-N29	6.78	1.49	1.34
2	B	400	NSY	C15-C10	6.79	1.55	1.38
2	B	400	NSY	C64-C62	6.79	1.53	1.39
2	B	400	NSY	C27-C28	6.81	1.54	1.39
2	C	500	NSY	C25-C27	6.83	1.51	1.38
2	F	800	NSY	C46-C45	6.84	1.53	1.38
2	B	400	NSY	C42-N60	6.85	1.47	1.33
2	E	700	NSY	C63-C62	6.85	1.54	1.39
2	F	800	NSY	C15-C10	6.88	1.55	1.38
2	E	700	NSY	C10-C13	6.88	1.55	1.38
2	E	700	NSY	C48-C46	6.89	1.53	1.38
2	C	500	NSY	C46-C45	6.92	1.53	1.38
2	B	400	NSY	C2-N16	6.92	1.48	1.34
2	F	800	NSY	C18-N29	6.93	1.50	1.34
2	E	700	NSY	C15-C10	6.94	1.55	1.38
2	C	500	NSY	C42-N60	6.94	1.48	1.33
2	C	500	NSY	C65-C63	6.96	1.53	1.38
2	F	800	NSY	C10-C13	6.96	1.55	1.38
2	B	400	NSY	C46-C45	6.97	1.53	1.38
2	E	700	NSY	C46-C45	6.97	1.53	1.38
2	B	400	NSY	C48-C50	6.98	1.55	1.38
2	F	800	NSY	C27-C28	7.02	1.54	1.39
2	D	600	NSY	C65-C63	7.02	1.53	1.38
2	F	800	NSY	C25-C27	7.03	1.51	1.38
2	A	300	NSY	C48-C50	7.03	1.56	1.38
2	E	700	NSY	C25-C27	7.07	1.51	1.38
2	D	600	NSY	C48-C50	7.07	1.56	1.38
2	C	500	NSY	C48-C50	7.09	1.56	1.38
2	A	300	NSY	C6-C7	7.10	1.53	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	NSY	C6-C7	7.14	1.54	1.38
2	A	300	NSY	C25-C27	7.15	1.51	1.38
2	D	600	NSY	C9-C4	7.15	1.54	1.39
2	F	800	NSY	C54-C53	7.15	1.53	1.38
2	E	700	NSY	C2-N16	7.21	1.48	1.34
2	A	300	NSY	C2-N16	7.21	1.48	1.34
2	C	500	NSY	C9-C4	7.22	1.54	1.39
2	F	800	NSY	C2-N16	7.24	1.48	1.34
2	C	500	NSY	C18-N29	7.26	1.50	1.34
2	C	500	NSY	C54-C53	7.27	1.53	1.38
2	D	600	NSY	C54-C53	7.33	1.54	1.38
2	E	700	NSY	C18-N29	7.34	1.51	1.34
2	F	800	NSY	C48-C50	7.34	1.56	1.38
2	D	600	NSY	C42-N60	7.35	1.49	1.33
2	E	700	NSY	C27-C28	7.35	1.55	1.39
2	C	500	NSY	C63-C62	7.35	1.55	1.39
2	E	700	NSY	C48-C50	7.39	1.57	1.38
2	F	800	NSY	C65-C63	7.40	1.54	1.38
2	B	400	NSY	C25-C27	7.42	1.52	1.38
2	B	400	NSY	C54-C53	7.43	1.54	1.38
2	F	800	NSY	C9-C4	7.44	1.55	1.39
2	C	500	NSY	C10-C13	7.44	1.57	1.38
2	D	600	NSY	C13-C11	7.45	1.54	1.38
2	F	800	NSY	C6-C7	7.47	1.54	1.38
2	E	700	NSY	C9-C4	7.50	1.55	1.39
2	E	700	NSY	C65-C63	7.51	1.54	1.38
2	A	300	NSY	C9-C4	7.51	1.55	1.39
2	D	600	NSY	C10-C13	7.55	1.57	1.38
2	E	700	NSY	C6-C7	7.59	1.54	1.38
2	E	700	NSY	C8-C9	7.60	1.52	1.38
2	C	500	NSY	C13-C11	7.61	1.54	1.38
2	B	400	NSY	C11-C12	7.66	1.55	1.39
2	A	300	NSY	C63-C62	7.66	1.55	1.39
2	E	700	NSY	C54-C53	7.66	1.54	1.38
2	A	300	NSY	C54-C53	7.69	1.54	1.38
2	D	600	NSY	C2-N16	7.75	1.49	1.34
2	D	600	NSY	C63-C62	7.76	1.56	1.39
2	F	800	NSY	C8-C9	7.78	1.52	1.38
2	C	500	NSY	C2-N16	7.84	1.49	1.34
2	A	300	NSY	C11-C12	7.85	1.56	1.39
2	D	600	NSY	C6-C7	7.87	1.55	1.38
2	B	400	NSY	C9-C4	7.87	1.56	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	NSY	C6-C7	7.88	1.55	1.38
2	E	700	NSY	C42-N60	7.90	1.50	1.33
2	A	300	NSY	C8-C9	7.92	1.53	1.38
2	F	800	NSY	C42-N60	7.92	1.50	1.33
2	F	800	NSY	C11-C12	8.02	1.56	1.39
2	B	400	NSY	C63-C62	8.02	1.56	1.39
2	C	500	NSY	C11-C12	8.05	1.56	1.39
2	D	600	NSY	C11-C12	8.06	1.56	1.39
2	B	400	NSY	C5-C4	8.09	1.56	1.39
2	E	700	NSY	C11-C12	8.10	1.56	1.39
2	B	400	NSY	C8-C9	8.34	1.53	1.38
2	E	700	NSY	C5-C4	8.47	1.57	1.39
2	F	800	NSY	C13-C11	8.47	1.56	1.38
2	F	800	NSY	C5-C4	8.48	1.57	1.39
2	E	700	NSY	C13-C11	8.51	1.56	1.38
2	A	300	NSY	C5-C4	8.70	1.58	1.39
2	C	500	NSY	C8-C9	8.88	1.54	1.38
2	D	600	NSY	C8-C9	9.02	1.55	1.38
2	A	300	NSY	C13-C11	9.48	1.58	1.38
2	C	500	NSY	C5-C4	9.50	1.59	1.39
2	D	600	NSY	C5-C4	9.53	1.59	1.39
2	B	400	NSY	C13-C11	9.77	1.59	1.38
2	E	700	NSY	C8-C7	10.54	1.61	1.38
2	E	700	NSY	C47-C45	10.56	1.61	1.38
2	A	300	NSY	C47-C45	10.62	1.61	1.38
2	B	400	NSY	C47-C45	10.71	1.61	1.38
2	F	800	NSY	C8-C7	10.77	1.61	1.38
2	F	800	NSY	C47-C45	10.77	1.61	1.38
2	C	500	NSY	C47-C45	10.86	1.61	1.38
2	D	600	NSY	C47-C45	11.06	1.62	1.38
2	A	300	NSY	C8-C7	11.07	1.62	1.38
2	D	600	NSY	C8-C7	11.09	1.62	1.38
2	C	500	NSY	C8-C7	11.10	1.62	1.38
2	B	400	NSY	C8-C7	11.10	1.62	1.38
2	B	400	NSY	C53-C52	11.19	1.62	1.38
2	F	800	NSY	C53-C52	11.23	1.62	1.38
2	A	300	NSY	C53-C52	11.37	1.63	1.38
2	E	700	NSY	C53-C52	11.48	1.63	1.38
2	C	500	NSY	C53-C52	11.69	1.63	1.38
2	D	600	NSY	C53-C52	11.79	1.63	1.38
2	B	400	NSY	C14-C12	13.16	1.67	1.39
2	A	300	NSY	C14-C12	13.21	1.67	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	700	NSY	C14-C12	13.58	1.68	1.39
2	F	800	NSY	C14-C12	13.73	1.68	1.39
2	C	500	NSY	C14-C12	15.03	1.71	1.39
2	D	600	NSY	C14-C12	15.23	1.72	1.39

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	NSY	C1-C7-C6	-7.21	110.04	120.86
2	C	500	NSY	C1-C7-C6	-7.00	110.35	120.86
2	B	400	NSY	C1-C7-C6	-6.81	110.63	120.86
2	A	300	NSY	C1-C7-C6	-6.73	110.76	120.86
2	F	800	NSY	C1-C7-C6	-6.38	111.28	120.86
2	E	700	NSY	C1-C7-C6	-6.34	111.34	120.86
2	B	400	NSY	C18-C17-N16	-4.88	97.51	111.26
2	B	400	NSY	C13-C11-C12	-4.70	114.33	120.56
2	A	300	NSY	C13-C11-C12	-4.68	114.37	120.56
2	F	800	NSY	C18-C17-N16	-4.67	98.11	111.26
2	D	600	NSY	C18-C17-N16	-4.64	98.19	111.26
2	A	300	NSY	C18-C17-N16	-4.62	98.24	111.26
2	E	700	NSY	C18-C17-N16	-4.55	98.43	111.26
2	C	500	NSY	C18-C17-N16	-4.55	98.44	111.26
2	A	300	NSY	C71-N72-C68	-4.54	113.87	122.79
2	B	400	NSY	C71-N72-C68	-4.50	113.94	122.79
2	E	700	NSY	C13-C11-C12	-4.31	114.85	120.56
2	F	800	NSY	C13-C11-C12	-4.27	114.91	120.56
2	F	800	NSY	O73-C68-C22	-4.18	110.21	121.88
2	E	700	NSY	O73-C68-C22	-4.12	110.38	121.88
2	F	800	NSY	C71-N72-C68	-4.10	114.73	122.79
2	B	400	NSY	C9-C8-C7	-4.06	115.48	121.04
2	E	700	NSY	C71-N72-C68	-4.05	114.83	122.79
2	E	700	NSY	C9-C8-C7	-4.03	115.52	121.04
2	F	800	NSY	C9-C8-C7	-4.02	115.53	121.04
2	D	600	NSY	O73-C68-C22	-4.01	110.68	121.88
2	C	500	NSY	O73-C68-C22	-4.01	110.68	121.88
2	C	500	NSY	C13-C11-C12	-4.00	115.26	120.56
2	D	600	NSY	C13-C11-C12	-4.00	115.27	120.56
2	D	600	NSY	C9-C8-C7	-3.98	115.59	121.04
2	A	300	NSY	C9-C8-C7	-3.98	115.60	121.04
2	C	500	NSY	C9-C8-C7	-3.92	115.67	121.04
2	C	500	NSY	C71-N72-C68	-3.89	115.14	122.79
2	D	600	NSY	C71-N72-C68	-3.83	115.27	122.79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	NSY	O73-C68-C22	-3.73	111.46	121.88
2	F	800	NSY	C14-C12-C4	-3.72	114.72	121.39
2	B	400	NSY	O73-C68-C22	-3.72	111.50	121.88
2	C	500	NSY	C14-C12-C4	-3.64	114.87	121.39
2	E	700	NSY	C14-C12-C4	-3.64	114.87	121.39
2	D	600	NSY	C14-C12-C4	-3.60	114.93	121.39
2	B	400	NSY	C14-C12-C4	-3.43	115.24	121.39
2	A	300	NSY	C59-N60-C42	-3.39	115.83	122.53
2	A	300	NSY	C14-C12-C4	-3.27	115.52	121.39
2	B	400	NSY	C59-N60-C42	-3.22	116.16	122.53
2	C	500	NSY	C54-C53-C52	-3.16	115.62	120.65
2	D	600	NSY	C54-C53-C52	-3.15	115.64	120.65
2	E	700	NSY	C58-C52-C57	-3.02	113.61	121.25
2	E	700	NSY	C59-N60-C42	-2.90	116.79	122.53
2	F	800	NSY	C59-N60-C42	-2.85	116.89	122.53
2	F	800	NSY	C1-C2-N16	-2.79	111.48	115.96
2	B	400	NSY	C42-C41-N40	-2.77	103.46	111.26
2	A	300	NSY	C54-C53-C52	-2.74	116.28	120.65
2	B	400	NSY	C54-C53-C52	-2.73	116.30	120.65
2	C	500	NSY	C58-C52-C57	-2.72	114.36	121.25
2	F	800	NSY	C58-C52-C57	-2.71	114.39	121.25
2	D	600	NSY	C58-C52-C57	-2.71	114.39	121.25
2	E	700	NSY	C1-C2-N16	-2.70	111.63	115.96
2	A	300	NSY	C42-C41-N40	-2.69	103.69	111.26
2	E	700	NSY	C54-C53-C52	-2.66	116.42	120.65
2	D	600	NSY	C31-C30-C38	-2.64	103.88	110.32
2	F	800	NSY	C54-C53-C52	-2.64	116.44	120.65
2	C	500	NSY	C59-N60-C42	-2.62	117.35	122.53
2	B	400	NSY	C1-C2-N16	-2.56	111.85	115.96
2	C	500	NSY	C31-C30-C38	-2.49	104.25	110.32
2	D	600	NSY	C59-N60-C42	-2.46	117.65	122.53
2	A	300	NSY	C1-C2-N16	-2.36	112.17	115.96
2	D	600	NSY	C5-C4-C12	-2.32	117.23	121.39
2	C	500	NSY	C5-C4-C12	-2.32	117.24	121.39
2	F	800	NSY	C5-C4-C12	-2.19	117.46	121.39
2	E	700	NSY	C5-C4-C12	-2.17	117.50	121.39
2	F	800	NSY	C42-C41-N40	-2.15	105.20	111.26
2	E	700	NSY	C31-C30-C38	-2.15	105.08	110.32
2	F	800	NSY	C31-C30-C38	-2.13	105.13	110.32
2	B	400	NSY	C58-C52-C57	-2.10	115.94	121.25
2	E	700	NSY	C42-C41-N40	-2.07	105.44	111.26
2	E	700	NSY	C41-C42-N60	-2.06	112.68	116.72

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	NSY	C58-C52-C57	-2.05	116.07	121.25
2	D	600	NSY	C45-C44-C41	-2.00	107.58	113.41
2	E	700	NSY	C44-C41-N40	2.00	114.99	110.80
2	E	700	NSY	C66-C64-C62	2.03	123.24	120.56
2	E	700	NSY	C7-C1-C2	2.08	119.61	112.84
2	A	300	NSY	C53-C52-C57	2.09	121.48	118.13
2	F	800	NSY	C70-C71-N72	2.12	118.40	112.19
2	D	600	NSY	C22-C23-C24	2.15	124.09	120.86
2	F	800	NSY	C27-C28-C62	2.18	125.29	121.39
2	E	700	NSY	C53-C52-C57	2.19	121.64	118.13
2	E	700	NSY	C70-C71-N72	2.20	118.63	112.19
2	C	500	NSY	C7-C1-C2	2.20	120.02	112.84
2	E	700	NSY	C11-C12-C4	2.21	125.36	121.39
2	B	400	NSY	C53-C52-C57	2.24	121.73	118.13
2	F	800	NSY	C53-C52-C57	2.26	121.75	118.13
2	F	800	NSY	C66-C64-C62	2.27	123.56	120.56
2	E	700	NSY	C27-C28-C62	2.27	125.46	121.39
2	A	300	NSY	C44-C41-N40	2.28	115.56	110.80
2	B	400	NSY	C11-C12-C4	2.30	125.52	121.39
2	F	800	NSY	C11-C12-C4	2.34	125.59	121.39
2	D	600	NSY	C53-C52-C57	2.35	121.89	118.13
2	C	500	NSY	C22-C23-C24	2.38	124.43	120.86
2	B	400	NSY	C44-C41-N40	2.38	115.78	110.80
2	D	600	NSY	C70-C71-N72	2.40	119.21	112.19
2	C	500	NSY	C70-C71-N72	2.42	119.27	112.19
2	F	800	NSY	C32-C33-N34	2.46	120.87	112.35
2	E	700	NSY	C32-C33-N34	2.48	120.94	112.35
2	D	600	NSY	C7-C1-C2	2.50	120.98	112.84
2	D	600	NSY	C32-C33-N34	2.53	121.12	112.35
2	C	500	NSY	C53-C52-C57	2.56	122.23	118.13
2	C	500	NSY	C32-C33-N34	2.57	121.25	112.35
2	D	600	NSY	C69-C70-C71	2.60	126.10	113.69
2	A	300	NSY	C70-C71-N72	2.61	119.83	112.19
2	A	300	NSY	C69-C70-C71	2.63	126.25	113.69
2	C	500	NSY	C69-C70-C71	2.64	126.30	113.69
2	B	400	NSY	C69-C70-C71	2.65	126.36	113.69
2	D	600	NSY	C11-C12-C4	2.74	126.31	121.39
2	A	300	NSY	C69-C20-C17	2.78	122.44	113.91
2	C	500	NSY	C11-C12-C4	2.78	126.37	121.39
2	C	500	NSY	O73-C68-N72	2.79	128.46	122.94
2	A	300	NSY	C7-C1-C2	2.80	121.96	112.84
2	F	800	NSY	C69-C70-C71	2.81	127.13	113.69

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	NSY	C32-C33-N34	2.84	122.19	112.35
2	B	400	NSY	C70-C71-N72	2.84	120.51	112.19
2	E	700	NSY	C69-C70-C71	2.84	127.28	113.69
2	D	600	NSY	O73-C68-N72	2.86	128.60	122.94
2	C	500	NSY	C31-C30-N29	2.87	116.33	110.87
2	E	700	NSY	C22-C68-N72	2.87	120.14	116.11
2	D	600	NSY	C69-C20-C17	2.91	122.85	113.91
2	B	400	NSY	C7-C1-C2	2.92	122.37	112.84
2	A	300	NSY	C32-C33-N34	2.93	122.49	112.35
2	B	400	NSY	C69-C20-C17	2.95	122.98	113.91
2	D	600	NSY	C31-C30-N29	3.04	116.67	110.87
2	C	500	NSY	C69-C20-C17	3.11	123.46	113.91
2	F	800	NSY	C22-C68-N72	3.13	120.50	116.11
2	E	700	NSY	C31-C30-N29	3.13	116.83	110.87
2	F	800	NSY	O73-C68-N72	3.20	129.28	122.94
2	C	500	NSY	C32-C31-C30	3.22	123.80	113.91
2	D	600	NSY	C17-N16-C2	3.25	129.87	121.58
2	F	800	NSY	C31-C30-N29	3.26	117.08	110.87
2	F	800	NSY	C32-C31-C30	3.27	123.97	113.91
2	D	600	NSY	C22-C68-N72	3.28	120.72	116.11
2	E	700	NSY	O73-C68-N72	3.29	129.47	122.94
2	E	700	NSY	C32-C31-C30	3.30	124.05	113.91
2	E	700	NSY	C69-C20-C17	3.33	124.13	113.91
2	F	800	NSY	C69-C20-C17	3.35	124.22	113.91
2	D	600	NSY	C32-C31-C30	3.38	124.29	113.91
2	C	500	NSY	C22-C68-N72	3.38	120.86	116.11
2	C	500	NSY	C17-N16-C2	3.40	130.25	121.58
2	A	300	NSY	C23-C22-C68	3.52	124.31	112.84
2	B	400	NSY	C23-C22-C68	3.53	124.34	112.84
2	E	700	NSY	C10-C13-C11	3.58	125.42	120.19
2	F	800	NSY	C10-C13-C11	3.59	125.44	120.19
2	A	300	NSY	C17-N16-C2	3.65	130.89	121.58
2	E	700	NSY	C17-N16-C2	3.66	130.91	121.58
2	F	800	NSY	C17-N16-C2	3.72	131.08	121.58
2	D	600	NSY	C10-C13-C11	3.73	125.64	120.19
2	B	400	NSY	C32-C31-C30	3.74	125.40	113.91
2	C	500	NSY	C10-C13-C11	3.74	125.66	120.19
2	B	400	NSY	C17-N16-C2	3.78	131.21	121.58
2	B	400	NSY	C22-C68-N72	3.90	121.59	116.11
2	A	300	NSY	C22-C68-N72	3.98	121.70	116.11
2	A	300	NSY	C10-C13-C11	3.98	126.01	120.19
2	A	300	NSY	C32-C31-C30	4.15	126.67	113.91

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	NSY	C31-C30-N29	4.23	118.93	110.87
2	B	400	NSY	C10-C13-C11	4.27	126.43	120.19
2	E	700	NSY	C23-C22-C68	4.38	127.13	112.84
2	F	800	NSY	C23-C22-C68	4.43	127.27	112.84
2	E	700	NSY	C1-C7-C8	4.47	127.57	120.86
2	A	300	NSY	C31-C30-N29	4.48	119.40	110.87
2	F	800	NSY	C1-C7-C8	4.58	127.74	120.86
2	F	800	NSY	C70-C69-C20	4.67	130.24	113.66
2	D	600	NSY	C23-C22-C68	4.73	128.26	112.84
2	C	500	NSY	C59-C58-C52	4.79	122.77	112.83
2	A	300	NSY	C59-C58-C52	4.80	122.81	112.83
2	E	700	NSY	C70-C69-C20	4.87	130.96	113.66
2	C	500	NSY	C23-C22-C68	4.90	128.80	112.84
2	C	500	NSY	C70-C69-C20	4.91	131.10	113.66
2	D	600	NSY	C70-C69-C20	4.91	131.11	113.66
2	A	300	NSY	C70-C69-C20	5.03	131.52	113.66
2	B	400	NSY	C59-C58-C52	5.03	123.28	112.83
2	B	400	NSY	C70-C69-C20	5.12	131.85	113.66
2	C	500	NSY	C1-C7-C8	5.14	128.58	120.86
2	D	600	NSY	C59-C58-C52	5.17	123.56	112.83
2	A	300	NSY	C1-C7-C8	5.31	128.83	120.86
2	D	600	NSY	C1-C7-C8	5.31	128.84	120.86
2	B	400	NSY	C1-C7-C8	5.63	129.32	120.86
2	F	800	NSY	C59-C58-C52	6.49	126.31	112.83
2	E	700	NSY	C59-C58-C52	7.19	127.76	112.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	NSY	6	0
2	B	400	NSY	9	0
2	C	500	NSY	10	0
2	D	600	NSY	6	0
2	E	700	NSY	14	0
2	F	800	NSY	13	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	215/220 (97%)	0.38	9 (4%)	40 34	12, 19, 40, 58	0
1	B	215/220 (97%)	0.44	13 (6%)	25 20	12, 19, 40, 57	0
1	C	215/220 (97%)	0.61	15 (6%)	19 15	13, 23, 45, 59	0
1	D	215/220 (97%)	0.50	10 (4%)	35 29	13, 23, 47, 59	0
1	E	215/220 (97%)	0.88	22 (10%)	9 6	13, 28, 54, 72	0
1	F	215/220 (97%)	0.89	30 (13%)	4 3	13, 28, 53, 63	0
All	All	1290/1320 (97%)	0.62	99 (7%)	16 13	12, 23, 49, 72	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	ALA	8.1
1	E	104	TYR	5.4
1	E	211	ILE	4.6
1	E	110	THR	4.5
1	F	77	VAL	4.3
1	A	211	ILE	4.2
1	F	103	LYS	4.2
1	E	103	LYS	4.2
1	E	1	ALA	4.0
1	F	110	THR	4.0
1	A	110	THR	3.9
1	B	174	SER	3.9
1	C	154	PRO	3.8
1	F	104	TYR	3.6
1	B	158	SER	3.6
1	E	98	CYS	3.6
1	E	83	LEU	3.5
1	C	174	SER	3.5
1	E	100	TYR	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	84	ASP	3.4
1	B	144	LEU	3.4
1	F	122	LEU	3.3
1	A	108	ASN	3.3
1	A	144	LEU	3.3
1	E	89	TYR	3.2
1	E	77	VAL	3.2
1	E	220	VAL	3.2
1	C	152	PHE	3.2
1	F	118	GLN	3.1
1	C	144	LEU	3.0
1	D	150	ILE	3.0
1	F	120	LYS	3.0
1	C	208	HIS	3.0
1	F	83	LEU	3.0
1	F	3	ARG	2.9
1	C	172	PHE	2.9
1	F	81	GLY	2.9
1	F	98	CYS	2.9
1	B	108	ASN	2.9
1	A	44	ARG	2.9
1	F	44	ARG	2.8
1	D	220	VAL	2.8
1	F	1	ALA	2.8
1	D	206	ARG	2.8
1	D	174	SER	2.7
1	C	136	ILE	2.7
1	B	110	THR	2.7
1	D	172	PHE	2.7
1	F	147	LYS	2.7
1	C	170	TYR	2.7
1	C	155	ASP	2.6
1	F	100	TYR	2.5
1	E	108	ASN	2.5
1	F	211	ILE	2.5
1	C	157	SER	2.5
1	B	147	LYS	2.5
1	E	113	VAL	2.4
1	B	155	ASP	2.4
1	A	136	ILE	2.4
1	E	41	LYS	2.4
1	E	38	MET	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	157	SER	2.4
1	D	144	LEU	2.4
1	F	220	VAL	2.4
1	F	13	VAL	2.3
1	F	152	PHE	2.3
1	B	211	ILE	2.3
1	F	174	SER	2.3
1	A	147	LYS	2.3
1	F	102	PRO	2.3
1	D	110	THR	2.3
1	D	136	ILE	2.3
1	F	172	PHE	2.2
1	C	173	GLU	2.2
1	F	159	GLU	2.2
1	F	42	THR	2.2
1	F	48	LEU	2.2
1	D	5	VAL	2.2
1	B	220	VAL	2.2
1	F	101	ASN	2.2
1	B	118	GLN	2.2
1	E	34	LEU	2.2
1	B	136	ILE	2.1
1	E	147	LYS	2.1
1	C	3	ARG	2.1
1	B	209	CYS	2.1
1	A	3	ARG	2.1
1	E	144	LEU	2.1
1	E	156	CYS	2.1
1	F	41	LYS	2.1
1	F	96	GLU	2.0
1	D	92	GLU	2.0
1	E	75	GLN	2.0
1	F	46	ILE	2.0
1	F	173	GLU	2.0
1	E	42	THR	2.0
1	C	108	ASN	2.0
1	B	160	ASP	2.0
1	C	150	ILE	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	NSY	F	800	70/70	0.70	0.28	5.32	22,43,66,69	0
2	NSY	D	600	70/70	0.75	0.29	4.94	22,43,66,69	0
2	NSY	E	700	70/70	0.70	0.27	4.93	22,43,66,69	0
2	NSY	C	500	70/70	0.73	0.29	4.39	22,43,66,69	0
2	NSY	A	300	70/70	0.81	0.26	4.03	22,43,66,69	0
2	NSY	B	400	70/70	0.71	0.27	3.30	22,43,66,69	0

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

There are no such residues in this entry.