Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 02:07 AM EDT

PDB ID	:	3H89
Title	:	A combined crystallographic and molecular dynamics study of cathepsin-L retro-binding inhibitors(compound 4)
Authors	:	Tulsidas, S.R.; Chowdhury, S.F.; Kumar, S.; Joseph, L.; Purisima, E.O.; Sivaraman, J.
Deposited on	:	2009-04-29
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

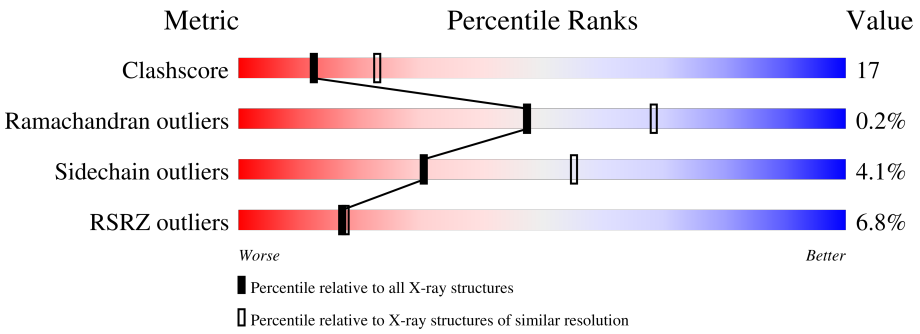
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3%, 74%, 22%, • •
1	B	220	4%, 73%, 23%, • •
1	C	220	4%, 70%, 25%, • •
1	D	220	3%, 75%, 21%, • •
1	E	220	12%, 57%, 39%, • •
1	F	220	14%, 64%, 32%, • •

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	NSX	A	400	-	X	-	-
2	NSX	B	300	-	X	-	-
2	NSX	C	500	-	X	-	-
2	NSX	D	600	-	X	-	-
2	NSX	E	700	-	X	-	-
2	NSX	F	800	-	X	-	-

2 Entry composition (i)

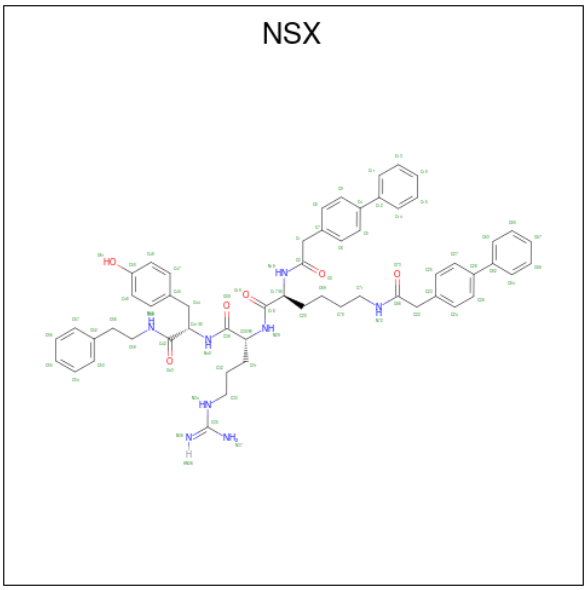
There are 3 unique types of molecules in this entry. The entry contains 10606 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	215	1659	1041	275	330	13	0	0	0
1	B	215	1659	1041	275	330	13	0	0	0
1	C	215	1659	1041	275	330	13	0	0	0
1	D	215	1659	1041	275	330	13	0	0	0
1	E	215	1659	1041	275	330	13	0	0	0
1	F	215	1659	1041	275	330	13	0	0	0

- Molecule 2 is N 2 ,N 6 -bis(biphenyl-4-ylacetyl)-L-lysyl-D-arginyl-N-(2-phenylethyl)-L-tyros inamide (three-letter code: NSX) (formula: $C_{57}H_{64}N_8O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	71	57	8	6	0	0
2	B	1	71	57	8	6	0	0
2	C	1	71	57	8	6	0	0
2	D	1	71	57	8	6	0	0
2	E	1	71	57	8	6	0	0
2	F	1	71	57	8	6	0	0

- Molecule 3 is water.

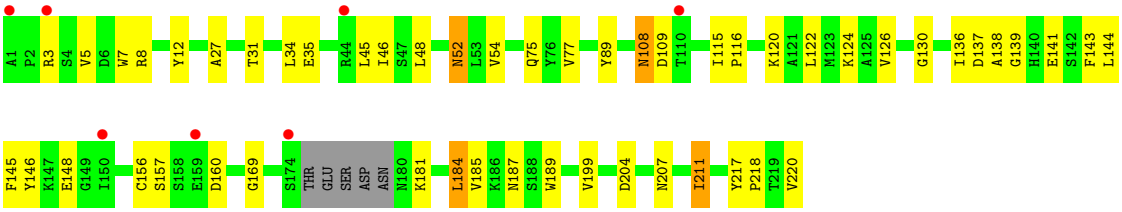
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	41	41	41	0	0
3	B	44	44	44	0	0
3	C	38	38	38	0	0
3	D	39	39	39	0	0
3	E	35	35	35	0	0
3	F	29	29	29	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

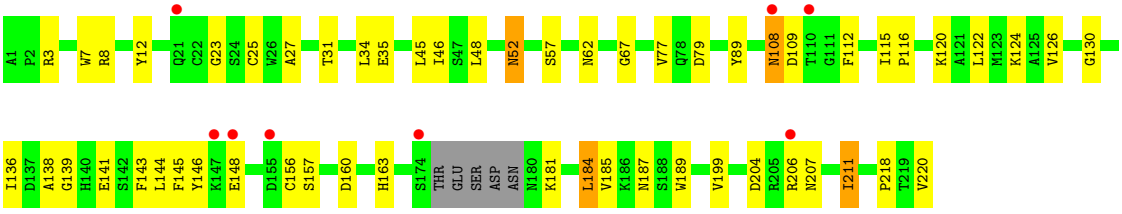
• Molecule 1: Cathepsin L1

Chain A:



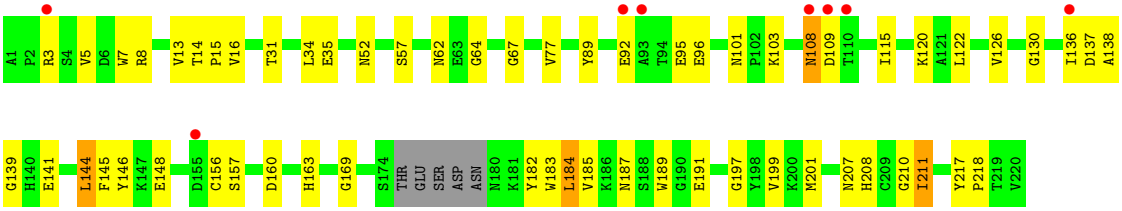
• Molecule 1: Cathepsin L1

Chain B:



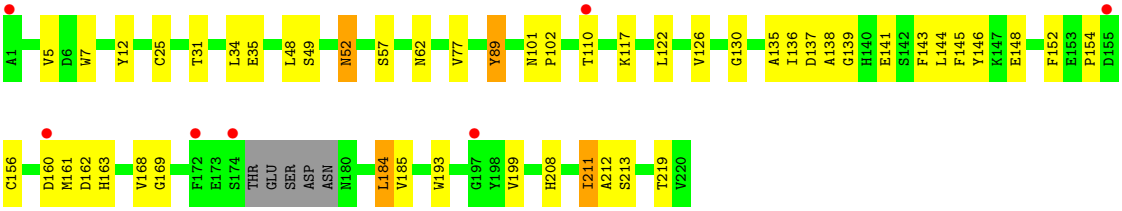
• Molecule 1: Cathepsin L1

Chain C:



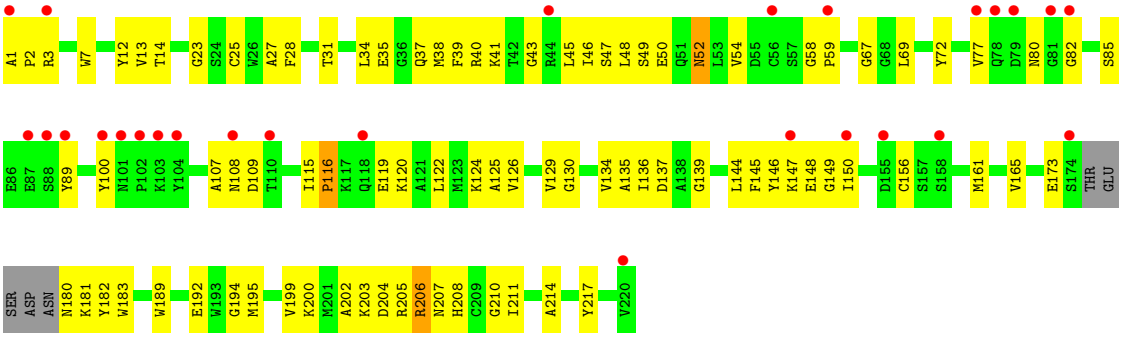
• Molecule 1: Cathepsin L1

Chain D:



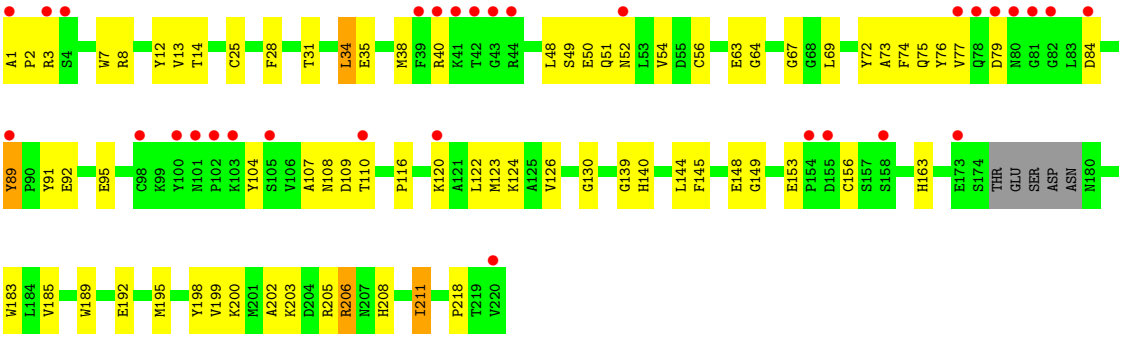
• Molecule 1: Cathepsin L1

Chain E:



• Molecule 1: Cathepsin L1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	99.40Å 61.08Å 205.18Å 90.00° 89.91° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 49.70 – 2.43	Depositor EDS
% Data completeness (in resolution range)	86.1 (25.00-2.50) 89.3 (49.70-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	8.07 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.280 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 19.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.477 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10606	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NSX

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	0.32	0/1700	0.56	0/2296
1	B	0.33	0/1700	0.56	0/2296
1	C	0.34	0/1700	0.58	0/2296
1	D	0.34	0/1700	0.59	0/2296
1	E	0.32	0/1700	0.54	0/2296
1	F	0.31	0/1700	0.54	0/2296
All	All	0.33	0/10200	0.56	0/13776

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	1659	0	1542	45	0
1	B	1659	0	1542	54	1
1	C	1659	0	1542	55	0
1	D	1659	0	1542	40	1
1	E	1659	0	1542	74	0
1	F	1659	0	1542	52	0
2	A	71	0	59	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	71	0	59	11	0
2	C	71	0	59	9	0
2	D	71	0	59	13	0
2	E	71	0	59	8	0
2	F	71	0	59	8	0
3	A	41	0	0	5	0
3	B	44	0	0	6	0
3	C	38	0	0	7	0
3	D	39	0	0	1	0
3	E	35	0	0	9	0
3	F	29	0	0	10	0
All	All	10606	0	9606	338	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (338) 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:B:136:ILE:HD11	1:B:211:ILE:HG23	1.36	1.05
1:A:136:ILE:HD11	1:A:211:ILE:HG23	1.35	1.04
1:F:163:HIS:HA	3:F:227:HOH:O	1.59	1.02
1:B:139:GLY:HA2	2:B:300:NSX:H22A	1.38	1.02
2:E:700:NSX:H20A	2:E:700:NSX:H8	1.46	0.98
2:F:800:NSX:H20A	2:F:800:NSX:H8	1.47	0.97
1:C:139:GLY:HA2	2:C:500:NSX:H22A	1.42	0.96
1:E:139:GLY:HA2	2:E:700:NSX:H22A	1.56	0.87
1:C:136:ILE:HD11	1:C:211:ILE:HG23	1.58	0.85
1:A:145:PHE:HZ	2:A:400:NSX:H65	1.40	0.85
1:B:145:PHE:HZ	2:B:300:NSX:H65	1.44	0.83
1:F:140:HIS:HB2	3:F:233:HOH:O	1.80	0.82
1:F:63:GLU:HG3	3:F:237:HOH:O	1.80	0.81
1:A:139:GLY:HA2	2:A:400:NSX:H22A	1.63	0.81
1:B:139:GLY:CA	2:B:300:NSX:H22A	2.10	0.81
1:C:31:THR:O	1:C:35:GLU:HG3	1.81	0.80
1:A:145:PHE:CZ	2:A:400:NSX:H65	2.16	0.80
2:F:800:NSX:H8	2:F:800:NSX:N16	1.97	0.79
2:E:700:NSX:H8	2:E:700:NSX:N16	1.99	0.77
1:C:77:VAL:HG12	1:C:108:ASN:HD22	1.48	0.76
1:F:139:GLY:HA2	2:F:800:NSX:H22A	1.68	0.75
1:B:31:THR:O	1:B:35:GLU:HG3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:GLY:CA	2:C:500:NSX:H22A	2.15	0.74
1:D:145:PHE:CZ	2:D:600:NSX:H65	2.23	0.74
1:E:108:ASN:ND2	1:E:109:ASP:H	1.85	0.74
1:D:139:GLY:HA2	2:D:600:NSX:H22A	1.68	0.73
1:E:31:THR:O	1:E:35:GLU:HG3	1.88	0.73
1:C:145:PHE:HZ	2:C:500:NSX:H65	1.53	0.73
1:F:120:LYS:HD3	1:F:124:LYS:HE3	1.71	0.73
1:B:145:PHE:CZ	2:B:300:NSX:H65	2.25	0.72
1:D:25:CYS:SG	3:D:233:HOH:O	2.48	0.71
1:B:206:ARG:HD3	3:B:262:HOH:O	1.91	0.71
1:A:31:THR:O	1:A:35:GLU:HG3	1.90	0.70
1:D:145:PHE:HZ	2:D:600:NSX:H65	1.57	0.70
1:C:108:ASN:ND2	1:C:109:ASP:H	1.89	0.70
1:E:135:ALA:C	1:E:136:ILE:HD12	2.14	0.68
1:C:141:GLU:HG2	2:C:500:NSX:C63	2.23	0.68
1:E:136:ILE:HG13	1:E:211:ILE:HD13	1.76	0.67
1:B:139:GLY:HA2	2:B:300:NSX:C22	2.21	0.67
1:E:200:LYS:HE2	3:E:224:HOH:O	1.95	0.66
2:F:800:NSX:N16	2:F:800:NSX:C8	2.59	0.66
1:F:195:MET:SD	3:F:245:HOH:O	2.53	0.66
1:E:50:GLU:O	1:E:54:VAL:HG23	1.96	0.65
1:E:208:HIS:O	1:E:211:ILE:HG12	1.96	0.65
1:F:149:GLY:N	3:F:245:HOH:O	2.28	0.65
1:F:38:MET:CE	1:F:107:ALA:HA	2.27	0.65
1:C:197:GLY:HA3	3:C:250:HOH:O	1.97	0.65
1:C:145:PHE:CZ	2:C:500:NSX:H65	2.33	0.64
2:E:700:NSX:N16	2:E:700:NSX:C8	2.60	0.64
1:D:31:THR:O	1:D:35:GLU:HG3	1.99	0.63
1:D:136:ILE:HD11	1:D:211:ILE:HG23	1.79	0.63
1:E:12:TYR:HE2	1:E:40:ARG:HB2	1.64	0.63
1:B:136:ILE:HD11	1:B:211:ILE:CG2	2.23	0.63
1:D:122:LEU:O	1:D:126:VAL:HG23	1.99	0.63
1:D:141:GLU:HG2	2:D:600:NSX:C63	2.28	0.62
1:E:195:MET:SD	3:E:224:HOH:O	2.56	0.62
1:E:108:ASN:HD22	1:E:109:ASP:H	1.48	0.62
1:E:122:LEU:O	1:E:126:VAL:HG23	2.00	0.61
1:B:8:ARG:NH2	1:B:184:LEU:HD11	2.16	0.61
1:A:8:ARG:NH1	3:A:224:HOH:O	2.33	0.61
1:C:31:THR:HB	3:C:236:HOH:O	2.01	0.60
1:D:52:ASN:C	1:D:52:ASN:HD22	2.03	0.60
1:B:34:LEU:HD23	1:B:218:PRO:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:VAL:HG12	1:E:14:THR:O	2.01	0.60
1:E:38:MET:CE	1:E:107:ALA:HA	2.31	0.60
1:E:108:ASN:ND2	1:E:109:ASP:N	2.49	0.60
1:C:8:ARG:NH2	1:C:184:LEU:HD11	2.16	0.60
1:A:8:ARG:NH2	1:A:184:LEU:HD11	2.17	0.59
1:E:202:ALA:HB1	1:E:205:ARG:HG3	1.85	0.59
1:E:146:TYR:CZ	1:E:199:VAL:HG23	2.38	0.59
1:F:50:GLU:O	1:F:54:VAL:HG23	2.03	0.59
1:D:144:LEU:HD23	1:D:145:PHE:CE1	2.38	0.58
1:A:27:ALA:HB2	3:A:246:HOH:O	2.02	0.58
1:E:144:LEU:HD13	1:E:189:TRP:CZ3	2.38	0.58
1:C:77:VAL:CG1	1:C:108:ASN:HA	2.32	0.58
1:C:141:GLU:HG2	2:C:500:NSX:C62	2.33	0.58
1:E:173:GLU:OE2	1:E:200:LYS:NZ	2.29	0.58
1:F:31:THR:O	1:F:35:GLU:HG3	2.04	0.58
1:A:7:TRP:CE2	1:A:130:GLY:HA2	2.40	0.57
1:C:139:GLY:HA2	2:C:500:NSX:C22	2.27	0.57
1:A:45:LEU:C	1:A:46:ILE:HD12	2.25	0.57
1:C:34:LEU:HD23	1:C:218:PRO:HG3	1.87	0.57
1:A:141:GLU:HG2	2:A:400:NSX:C63	2.34	0.57
1:E:49:SER:HB2	1:E:85:SER:O	2.05	0.57
1:E:149:GLY:N	3:E:224:HOH:O	2.37	0.57
1:B:141:GLU:HG2	2:B:300:NSX:C62	2.35	0.57
1:E:115:ILE:HD11	1:E:217:TYR:CE1	2.40	0.57
1:F:13:VAL:HG12	1:F:14:THR:O	2.05	0.57
1:C:77:VAL:HB	1:C:109:ASP:OD2	2.05	0.56
1:D:7:TRP:CE2	1:D:130:GLY:HA2	2.40	0.56
1:E:139:GLY:CA	2:E:700:NSX:H22A	2.32	0.56
1:A:122:LEU:O	1:A:126:VAL:HG23	2.05	0.56
1:C:136:ILE:HG21	1:C:201:MET:HE1	1.87	0.56
1:D:138:ALA:HB1	1:D:143:PHE:CD2	2.40	0.56
1:F:77:VAL:HB	1:F:109:ASP:OD2	2.05	0.56
2:D:600:NSX:H8	2:D:600:NSX:N16	2.21	0.56
1:F:28:PHE:CD2	1:F:50:GLU:HG2	2.40	0.56
1:A:34:LEU:HD23	1:A:218:PRO:HG3	1.88	0.56
1:B:115:ILE:N	1:B:115:ILE:HD12	2.21	0.56
1:E:135:ALA:O	1:E:161:MET:HG2	2.06	0.56
1:E:12:TYR:CE2	1:E:40:ARG:HB2	2.40	0.56
1:A:136:ILE:HD11	1:A:211:ILE:CG2	2.23	0.55
1:B:141:GLU:HG2	2:B:300:NSX:C63	2.36	0.55
1:B:45:LEU:C	1:B:46:ILE:HD12	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:MET:HE1	1:F:107:ALA:HA	1.88	0.55
1:E:67:GLY:HA2	2:E:700:NSX:O39	2.07	0.55
1:B:108:ASN:ND2	1:B:109:ASP:H	2.05	0.54
1:A:157:SER:HB3	1:A:160:ASP:OD1	2.06	0.54
1:B:7:TRP:CE2	1:B:130:GLY:HA2	2.43	0.54
1:C:208:HIS:O	1:C:211:ILE:HG12	2.08	0.54
1:D:136:ILE:HG22	1:D:137:ASP:N	2.23	0.54
1:F:3:ARG:NH1	3:F:247:HOH:O	2.40	0.54
1:F:64:GLY:HA3	1:F:95:GLU:OE1	2.08	0.53
1:B:157:SER:HB3	1:B:160:ASP:OD1	2.09	0.53
1:A:115:ILE:N	1:A:115:ILE:HD12	2.23	0.53
1:B:144:LEU:HD12	1:B:189:TRP:CZ3	2.43	0.53
1:D:7:TRP:NE1	1:D:130:GLY:HA2	2.24	0.53
2:F:800:NSX:H8	2:F:800:NSX:C20	2.30	0.53
1:C:207:ASN:ND2	1:C:210:GLY:HA2	2.23	0.53
1:F:69:LEU:HD12	1:F:72:TYR:CE2	2.44	0.53
1:F:67:GLY:HA2	2:F:800:NSX:O39	2.10	0.52
1:B:120:LYS:CD	1:B:124:LYS:HE3	2.40	0.52
1:C:185:VAL:HB	1:C:199:VAL:HG13	1.92	0.52
1:F:56:CYS:HB2	1:F:76:TYR:CZ	2.44	0.52
1:A:120:LYS:CD	1:A:124:LYS:HE3	2.39	0.52
2:D:600:NSX:N16	2:D:600:NSX:C8	2.73	0.52
1:C:115:ILE:HD11	1:C:217:TYR:CE1	2.44	0.52
1:C:57:SER:HB2	1:C:62:ASN:HD22	1.74	0.52
1:D:49:SER:OG	1:D:89:TYR:HB3	2.10	0.52
2:A:400:NSX:N16	2:A:400:NSX:H8	2.25	0.52
1:A:144:LEU:HD12	1:A:189:TRP:CZ3	2.45	0.52
1:C:191:GLU:HA	3:C:250:HOH:O	2.10	0.51
1:B:122:LEU:O	1:B:126:VAL:HG23	2.10	0.51
1:A:139:GLY:CA	2:A:400:NSX:H22A	2.38	0.51
2:A:400:NSX:H8	2:A:400:NSX:H20A	1.92	0.51
2:D:600:NSX:H8	2:D:600:NSX:HN16	1.75	0.51
1:F:108:ASN:ND2	1:F:109:ASP:N	2.58	0.51
1:F:35:GLU:HG2	1:F:48:LEU:HG	1.93	0.51
1:F:108:ASN:HD22	1:F:109:ASP:H	1.59	0.51
1:A:108:ASN:ND2	1:A:109:ASP:H	2.09	0.51
1:F:75:GLN:HG3	1:F:79:ASP:OD2	2.10	0.51
1:D:185:VAL:HB	1:D:199:VAL:HG13	1.92	0.51
1:A:120:LYS:HD3	1:A:124:LYS:HE3	1.93	0.50
1:A:46:ILE:HD12	1:A:46:ILE:N	2.26	0.50
1:E:38:MET:HE2	1:E:107:ALA:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:VAL:HB	1:B:199:VAL:HG13	1.92	0.50
1:A:187:ASN:HB3	3:A:222:HOH:O	2.10	0.50
1:E:192:GLU:OE2	1:E:192:GLU:HA	2.11	0.50
1:D:146:TYR:CZ	1:D:199:VAL:HG23	2.46	0.50
1:E:145:PHE:O	1:E:147:LYS:HD3	2.11	0.50
1:F:192:GLU:OE2	1:F:192:GLU:HA	2.12	0.50
1:A:52:ASN:C	1:A:52:ASN:HD22	2.15	0.50
1:F:34:LEU:HB3	1:F:48:LEU:CD1	2.42	0.50
1:F:202:ALA:HB1	1:F:205:ARG:HG3	1.92	0.50
1:E:150:ILE:HD12	1:E:182:TYR:HB3	1.94	0.50
1:B:139:GLY:C	2:B:300:NSX:H22A	2.32	0.49
1:D:139:GLY:CA	2:D:600:NSX:H22A	2.38	0.49
1:B:46:ILE:HD12	1:B:46:ILE:N	2.28	0.49
1:C:122:LEU:O	1:C:126:VAL:HG23	2.11	0.49
1:B:120:LYS:HD3	1:B:124:LYS:HE3	1.93	0.49
1:A:185:VAL:HB	1:A:199:VAL:HG13	1.94	0.49
1:C:57:SER:CB	1:C:62:ASN:HD22	2.25	0.49
1:B:3:ARG:HG3	1:B:3:ARG:HH11	1.77	0.49
1:D:136:ILE:CG2	1:D:137:ASP:N	2.76	0.49
1:F:200:LYS:HE2	3:F:245:HOH:O	2.13	0.49
1:E:49:SER:OG	1:E:52:ASN:HB2	2.12	0.49
1:F:108:ASN:HD22	1:F:109:ASP:N	2.11	0.49
1:C:96:GLU:HB2	3:C:255:HOH:O	2.13	0.49
1:C:13:VAL:HG12	1:C:14:THR:O	2.12	0.48
1:F:208:HIS:O	1:F:211:ILE:CG1	2.61	0.48
2:E:700:NSX:H8	2:E:700:NSX:C20	2.31	0.48
1:F:38:MET:HE2	1:F:107:ALA:HA	1.95	0.48
1:F:92:GLU:HG2	3:F:249:HOH:O	2.12	0.48
1:A:3:ARG:HG3	1:A:3:ARG:HH11	1.79	0.48
1:B:35:GLU:HG2	1:B:48:LEU:HG	1.95	0.48
2:D:600:NSX:H13	2:D:600:NSX:C26	2.43	0.48
1:F:51:GLN:HB2	1:F:91:TYR:HA	1.94	0.48
1:F:139:GLY:CA	2:F:800:NSX:H22A	2.40	0.48
1:E:35:GLU:OE2	1:E:47:SER:HA	2.13	0.48
1:C:77:VAL:HG12	1:C:108:ASN:ND2	2.24	0.48
2:D:600:NSX:H8	2:D:600:NSX:H20A	1.95	0.48
1:E:69:LEU:HD12	1:E:72:TYR:CZ	2.49	0.48
1:E:207:ASN:ND2	1:E:210:GLY:HA2	2.28	0.47
1:A:54:VAL:N	3:A:246:HOH:O	2.46	0.47
1:F:122:LEU:O	1:F:126:VAL:HG23	2.14	0.47
1:A:35:GLU:HG2	1:A:48:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LEU:HD13	1:C:144:LEU:HA	1.59	0.47
1:E:28:PHE:CD2	1:E:50:GLU:HG2	2.48	0.47
1:E:115:ILE:HD11	1:E:217:TYR:CD1	2.49	0.47
1:F:120:LYS:HD2	1:F:120:LYS:C	2.34	0.47
1:A:7:TRP:HB3	1:A:12:TYR:HB2	1.97	0.47
1:B:67:GLY:HA2	2:B:300:NSX:O39	2.15	0.47
1:B:207:ASN:OD1	1:B:211:ILE:HD12	2.14	0.47
1:F:25:CYS:SG	3:F:227:HOH:O	2.44	0.47
1:D:5:VAL:O	1:D:169:GLY:HA3	2.15	0.47
1:B:163:HIS:HB2	2:B:300:NSX:C69	2.45	0.46
1:B:77:VAL:HG12	1:B:108:ASN:HD22	1.79	0.46
1:C:187:ASN:HB3	3:C:240:HOH:O	2.14	0.46
1:D:193:TRP:CH2	1:D:199:VAL:HB	2.50	0.46
1:A:207:ASN:OD1	1:A:211:ILE:HD12	2.16	0.46
1:B:139:GLY:HA2	2:B:300:NSX:C68	2.46	0.46
1:F:7:TRP:CE2	1:F:130:GLY:HA2	2.51	0.46
1:B:23:GLY:HA2	3:B:221:HOH:O	2.15	0.46
1:A:138:ALA:HB1	1:A:143:PHE:CD2	2.50	0.46
1:B:112:PHE:HB2	3:B:244:HOH:O	2.16	0.46
1:C:182:TYR:HA	1:C:201:MET:O	2.15	0.46
1:E:1:ALA:HB1	1:E:2:PRO:HD2	1.98	0.46
1:E:144:LEU:HD13	1:E:189:TRP:HZ3	1.78	0.46
2:A:400:NSX:N16	2:A:400:NSX:C8	2.78	0.46
1:C:92:GLU:OE2	1:C:96:GLU:HG3	2.16	0.46
1:D:211:ILE:N	1:D:211:ILE:HD12	2.31	0.46
1:E:7:TRP:CE2	1:E:130:GLY:HA2	2.50	0.45
1:B:187:ASN:HB3	3:B:246:HOH:O	2.17	0.45
1:A:77:VAL:HG12	1:A:108:ASN:HD22	1.82	0.45
1:F:49:SER:OG	1:F:89:TYR:HB3	2.15	0.45
1:C:136:ILE:HD13	1:C:201:MET:CE	2.46	0.45
1:F:40:ARG:HG3	1:F:40:ARG:HH11	1.82	0.45
1:F:145:PHE:CZ	2:F:800:NSX:H65	2.51	0.45
1:B:57:SER:HB2	1:B:62:ASN:HD22	1.81	0.45
1:E:69:LEU:HD11	3:E:239:HOH:O	2.17	0.45
1:A:146:TYR:CZ	1:A:199:VAL:HG23	2.52	0.45
1:C:183:TRP:NE1	1:C:211:ILE:HD12	2.31	0.45
1:F:8:ARG:HD3	1:F:198:TYR:CZ	2.52	0.45
1:F:74:PHE:CZ	1:F:218:PRO:HD3	2.52	0.45
1:B:25:CYS:SG	3:B:222:HOH:O	2.62	0.45
1:A:181:LYS:HD2	1:A:204:ASP:OD2	2.17	0.45
1:B:144:LEU:O	1:B:144:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:LYS:HB2	1:E:203:LYS:O	2.17	0.45
1:E:203:LYS:O	1:E:204:ASP:HB2	2.16	0.45
1:B:138:ALA:HB1	1:B:143:PHE:CD2	2.51	0.44
1:B:146:TYR:CZ	1:B:199:VAL:HG23	2.52	0.44
1:F:183:TRP:NE1	1:F:203:LYS:HG3	2.33	0.44
1:E:45:LEU:O	1:E:46:ILE:HD13	2.18	0.44
1:E:145:PHE:CZ	2:E:700:NSX:H65	2.52	0.44
1:F:205:ARG:O	1:F:206:ARG:HB2	2.17	0.44
1:B:181:LYS:HD2	1:B:204:ASP:OD2	2.18	0.44
1:F:73:ALA:O	1:F:76:TYR:HB3	2.18	0.44
1:E:135:ALA:HB3	1:E:214:ALA:HB3	2.00	0.44
1:C:157:SER:HB3	1:C:160:ASP:OD1	2.17	0.44
1:C:184:LEU:HD23	1:C:184:LEU:HA	1.81	0.44
1:E:77:VAL:HB	1:E:109:ASP:OD2	2.18	0.44
1:E:82:GLY:HA2	1:E:107:ALA:O	2.17	0.44
1:B:7:TRP:HB3	1:B:12:TYR:HB2	2.00	0.44
1:E:25:CYS:SG	3:E:236:HOH:O	2.46	0.44
1:E:120:LYS:HD3	1:E:124:LYS:HE3	2.00	0.44
1:F:153:GLU:HG2	3:F:233:HOH:O	2.17	0.44
1:C:16:VAL:HG11	3:C:250:HOH:O	2.18	0.44
1:A:144:LEU:O	1:A:144:LEU:HG	2.18	0.43
1:D:168:VAL:CG2	1:D:184:LEU:HD13	2.48	0.43
1:E:144:LEU:HD13	1:E:144:LEU:HA	1.81	0.43
1:A:109:ASP:HA	1:A:220:VAL:HA	2.00	0.43
1:A:115:ILE:HG23	1:A:116:PRO:HD2	2.01	0.43
1:B:138:ALA:HA	3:B:229:HOH:O	2.17	0.43
1:D:7:TRP:HB3	1:D:12:TYR:HB2	2.00	0.43
1:C:163:HIS:HB2	2:C:500:NSX:C69	2.48	0.43
1:E:23:GLY:C	3:E:236:HOH:O	2.56	0.43
1:F:144:LEU:HD13	1:F:189:TRP:CZ3	2.54	0.43
1:B:27:ALA:O	1:B:31:THR:HG23	2.19	0.43
1:B:57:SER:CB	1:B:62:ASN:HD22	2.32	0.43
1:B:211:ILE:HD12	1:B:211:ILE:H	1.83	0.43
1:E:27:ALA:O	1:E:31:THR:HG23	2.18	0.43
1:C:5:VAL:O	1:C:169:GLY:HA3	2.18	0.43
1:E:38:MET:HE1	1:E:107:ALA:HA	2.01	0.43
1:F:1:ALA:HB1	1:F:2:PRO:HD2	2.00	0.43
1:C:120:LYS:HD2	1:C:120:LYS:C	2.38	0.43
1:B:52:ASN:HD22	1:B:52:ASN:C	2.19	0.43
1:B:184:LEU:HA	1:B:184:LEU:HD23	1.87	0.43
1:B:211:ILE:HD12	1:B:211:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:ILE:CD1	1:D:211:ILE:HG23	2.47	0.43
1:E:35:GLU:HG2	1:E:48:LEU:HG	2.01	0.43
1:C:183:TRP:CD1	1:C:211:ILE:HD12	2.54	0.43
1:E:147:LYS:HA	1:E:194:GLY:HA2	2.01	0.43
1:C:101:ASN:OD1	1:C:103:LYS:HB3	2.19	0.43
1:E:205:ARG:O	1:E:206:ARG:HB2	2.18	0.43
1:C:3:ARG:HG3	1:C:3:ARG:HH11	1.84	0.42
1:C:146:TYR:CZ	1:C:199:VAL:HG23	2.54	0.42
1:D:161:MET:CE	1:D:213:SER:HB2	2.49	0.42
1:B:34:LEU:HD23	1:B:218:PRO:CG	2.49	0.42
1:D:152:PHE:HA	1:D:208:HIS:NE2	2.34	0.42
1:A:7:TRP:NE1	1:A:130:GLY:HA2	2.34	0.42
1:E:58:GLY:N	1:E:59:PRO:CD	2.82	0.42
1:C:77:VAL:HG12	1:C:108:ASN:HA	1.99	0.42
1:B:3:ARG:HG3	1:B:3:ARG:NH1	2.35	0.42
1:C:108:ASN:ND2	1:C:109:ASP:N	2.62	0.42
1:D:152:PHE:O	1:D:154:PRO:HD3	2.19	0.42
1:D:162:ASP:HB3	2:D:600:NSX:N37	2.34	0.42
1:E:23:GLY:HA2	3:E:236:HOH:O	2.19	0.42
1:E:180:ASN:N	3:E:242:HOH:O	2.52	0.42
1:C:64:GLY:HA3	1:C:95:GLU:OE1	2.18	0.42
1:D:211:ILE:HD12	1:D:211:ILE:H	1.84	0.42
1:E:183:TRP:CE2	1:E:203:LYS:HG3	2.54	0.42
1:F:185:VAL:HB	1:F:199:VAL:HG13	2.01	0.42
1:C:67:GLY:HA2	2:C:500:NSX:O39	2.20	0.42
1:D:110:THR:HG23	1:D:219:THR:OG1	2.20	0.42
1:D:160:ASP:OD1	1:D:160:ASP:O	2.38	0.42
1:E:43:GLY:HA2	3:E:251:HOH:O	2.20	0.42
1:E:125:ALA:O	1:E:129:VAL:HB	2.20	0.41
1:D:101:ASN:HA	1:D:102:PRO:HD2	1.91	0.41
1:E:136:ILE:CG1	1:E:211:ILE:HD13	2.48	0.41
1:E:183:TRP:CD1	1:E:203:LYS:HB2	2.54	0.41
1:A:211:ILE:HD12	1:A:211:ILE:N	2.35	0.41
2:A:400:NSX:H8	2:A:400:NSX:HN16	1.86	0.41
1:D:34:LEU:HD11	1:D:77:VAL:HG21	2.02	0.41
1:D:52:ASN:C	1:D:52:ASN:ND2	2.72	0.41
1:E:3:ARG:HG3	1:E:3:ARG:HH11	1.85	0.41
1:C:138:ALA:HA	3:C:241:HOH:O	2.19	0.41
1:C:144:LEU:HD13	1:C:189:TRP:CZ3	2.55	0.41
1:D:117:LYS:HA	1:D:212:ALA:O	2.20	0.41
1:E:134:VAL:HG23	1:E:165:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:TRP:HB3	1:F:12:TYR:HB2	2.03	0.41
1:F:35:GLU:CG	1:F:48:LEU:HG	2.50	0.41
1:A:115:ILE:HD11	1:A:217:TYR:CD1	2.56	0.41
1:E:119:GLU:OE1	1:E:204:ASP:HA	2.20	0.41
1:A:136:ILE:CG2	1:A:137:ASP:N	2.83	0.41
1:A:75:GLN:HB2	3:A:238:HOH:O	2.19	0.41
2:D:600:NSX:H5	2:D:600:NSX:H14	1.86	0.41
1:E:39:PHE:C	1:E:41:LYS:N	2.74	0.41
1:A:27:ALA:O	1:A:31:THR:HG23	2.21	0.41
1:D:34:LEU:HB3	1:D:48:LEU:CD1	2.51	0.41
1:D:57:SER:HB2	1:D:62:ASN:HD22	1.86	0.41
1:A:211:ILE:HD12	1:A:211:ILE:H	1.86	0.41
1:C:136:ILE:HD11	1:C:211:ILE:CG2	2.39	0.41
1:F:84:ASP:HA	1:F:104:TYR:O	2.21	0.41
1:A:5:VAL:O	1:A:169:GLY:HA3	2.21	0.41
1:E:37:GLN:C	1:E:39:PHE:N	2.73	0.41
1:B:115:ILE:HG23	1:B:116:PRO:HD2	2.03	0.40
1:C:14:THR:HB	1:C:15:PRO:CD	2.51	0.40
1:E:135:ALA:O	1:E:136:ILE:HD12	2.20	0.40
1:C:136:ILE:CG2	1:C:137:ASP:N	2.84	0.40
1:B:109:ASP:HA	1:B:220:VAL:HA	2.03	0.40
1:C:7:TRP:NE1	1:C:130:GLY:HA2	2.36	0.40
1:D:163:HIS:HB2	2:D:600:NSX:C69	2.51	0.40
1:E:1:ALA:HB1	1:E:2:PRO:CD	2.51	0.40
1:E:37:GLN:NE2	1:E:37:GLN:HA	2.36	0.40
1:B:211:ILE:H	1:B:211:ILE:CD1	2.33	0.40
1:E:80:ASN:ND2	1:E:100:TYR:CZ	2.88	0.40
1:E:136:ILE:CG2	1:E:137:ASP:N	2.84	0.40
1:D:135:ALA:O	1:D:161:MET:HG2	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASP:O	1:D:110:THR:OG1[4_646]	2.18	0.02

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	211/220 (96%)	199 (94%)	12 (6%)	0	100	100
1	B	211/220 (96%)	199 (94%)	12 (6%)	0	100	100
1	C	211/220 (96%)	200 (95%)	11 (5%)	0	100	100
1	D	211/220 (96%)	198 (94%)	13 (6%)	0	100	100
1	E	211/220 (96%)	196 (93%)	13 (6%)	2 (1%)	17	31
1	F	211/220 (96%)	196 (93%)	14 (7%)	1 (0%)	29	48
All	All	1266/1320 (96%)	1188 (94%)	75 (6%)	3 (0%)	47	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	116	PRO
1	E	206	ARG
1	F	206	ARG

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	174/179 (97%)	167 (96%)	7 (4%)	31	56
1	B	174/179 (97%)	167 (96%)	7 (4%)	31	56
1	C	174/179 (97%)	166 (95%)	8 (5%)	27	50
1	D	174/179 (97%)	168 (97%)	6 (3%)	37	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	174/179 (97%)	168 (97%)	6 (3%)	37	63
1	F	174/179 (97%)	165 (95%)	9 (5%)	23	44
All	All	1044/1074 (97%)	1001 (96%)	43 (4%)	30	55

All (43) 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	148	GLU
1	A	156	CYS
1	A	184	LEU
1	A	211	ILE
1	B	52	ASN
1	B	89	TYR
1	B	108	ASN
1	B	148	GLU
1	B	156	CYS
1	B	184	LEU
1	B	211	ILE
1	C	52	ASN
1	C	89	TYR
1	C	108	ASN
1	C	144	LEU
1	C	148	GLU
1	C	156	CYS
1	C	184	LEU
1	C	211	ILE
1	D	52	ASN
1	D	89	TYR
1	D	148	GLU
1	D	156	CYS
1	D	184	LEU
1	D	211	ILE
1	E	34	LEU
1	E	52	ASN
1	E	89	TYR
1	E	116	PRO
1	E	148	GLU
1	E	156	CYS

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Mol	Chain	Res	Type
1	F	34	LEU
1	F	52	ASN
1	F	89	TYR
1	F	110	THR
1	F	116	PRO
1	F	123	MET
1	F	148	GLU
1	F	156	CYS
1	F	211	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	B	108	ASN
1	C	108	ASN
1	D	108	ASN
1	E	37	GLN
1	E	78	GLN
1	E	108	ASN
1	F	75	GLN
1	F	78	GLN
1	F	108	ASN
1	F	140	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	NSX	F	800	-	74,76,76	5.84	56 (75%)	90,99,99	2.23	31 (34%)
2	NSX	B	300	-	74,76,76	6.26	56 (75%)	90,99,99	3.33	38 (42%)
2	NSX	A	400	-	74,76,76	5.83	56 (75%)	90,99,99	2.28	32 (35%)
2	NSX	E	700	-	74,76,76	5.84	55 (74%)	90,99,99	2.25	29 (32%)
2	NSX	C	500	-	74,76,76	6.20	55 (74%)	90,99,99	3.15	37 (41%)
2	NSX	D	600	-	74,76,76	5.83	57 (77%)	90,99,99	2.27	32 (35%)

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	NSX	F	800	-	-	17/57/65/65	0/6/6/6
2	NSX	B	300	-	-	12/57/65/65	0/6/6/6
2	NSX	A	400	-	-	11/57/65/65	0/6/6/6
2	NSX	E	700	-	-	17/57/65/65	0/6/6/6
2	NSX	C	500	-	-	12/57/65/65	0/6/6/6
2	NSX	D	600	-	-	12/57/65/65	0/6/6/6

All (335) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300	NSX	C15-C14	12.82	1.63	1.36
2	C	500	NSX	C53-C52	12.33	1.63	1.38
2	B	300	NSX	C53-C52	12.32	1.63	1.38
2	D	600	NSX	C53-C52	12.24	1.63	1.38
2	A	400	NSX	C53-C52	12.15	1.62	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	700	NSX	C53-C52	12.10	1.62	1.38
2	F	800	NSX	C53-C52	12.03	1.62	1.38
2	B	300	NSX	C14-C12	11.77	1.67	1.42
2	C	500	NSX	C14-C12	11.72	1.67	1.42
2	C	500	NSX	C47-C45	11.45	1.61	1.38
2	B	300	NSX	C47-C45	11.45	1.61	1.38
2	C	500	NSX	C8-C7	11.41	1.61	1.38
2	C	500	NSX	C15-C14	11.41	1.60	1.36
2	D	600	NSX	C47-C45	11.40	1.61	1.38
2	E	700	NSX	C22-C23	-11.40	1.33	1.51
2	B	300	NSX	C8-C7	11.36	1.61	1.38
2	E	700	NSX	C47-C45	11.34	1.61	1.38
2	A	400	NSX	C47-C45	11.21	1.61	1.38
2	F	800	NSX	C47-C45	11.19	1.61	1.38
2	F	800	NSX	C22-C23	-11.10	1.33	1.51
2	A	400	NSX	C22-C23	-10.91	1.34	1.51
2	D	600	NSX	C22-C23	-10.77	1.34	1.51
2	B	300	NSX	C9-C8	10.60	1.59	1.36
2	A	400	NSX	C8-C7	10.56	1.59	1.38
2	D	600	NSX	C8-C7	10.35	1.59	1.38
2	A	400	NSX	C14-C12	10.09	1.64	1.42
2	C	500	NSX	C9-C8	10.06	1.58	1.36
2	D	600	NSX	C14-C12	9.81	1.63	1.42
2	E	700	NSX	C8-C7	9.60	1.57	1.38
2	B	300	NSX	C11-C12	9.58	1.62	1.42
2	B	300	NSX	C54-C53	9.53	1.55	1.38
2	E	700	NSX	C14-C12	9.50	1.62	1.42
2	C	500	NSX	C54-C53	9.50	1.55	1.38
2	F	800	NSX	C14-C12	9.50	1.62	1.42
2	F	800	NSX	C8-C7	9.49	1.57	1.38
2	C	500	NSX	C11-C12	9.47	1.62	1.42
2	F	800	NSX	C6-C7	9.22	1.57	1.38
2	C	500	NSX	C1-C7	9.21	1.66	1.51
2	C	500	NSX	C15-C10	9.19	1.58	1.38
2	E	700	NSX	C15-C10	9.11	1.58	1.38
2	A	400	NSX	C54-C53	9.11	1.54	1.38
2	E	700	NSX	C6-C7	9.10	1.56	1.38
2	D	600	NSX	C54-C53	9.06	1.54	1.38
2	E	700	NSX	C54-C53	9.06	1.54	1.38
2	F	800	NSX	C54-C53	9.06	1.54	1.38
2	B	300	NSX	C1-C7	9.05	1.66	1.51
2	F	800	NSX	C48-C50	9.03	1.55	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	700	NSX	C48-C50	8.96	1.55	1.39
2	C	500	NSX	C48-C50	8.95	1.55	1.39
2	A	400	NSX	C48-C50	8.92	1.55	1.39
2	B	300	NSX	C48-C50	8.92	1.55	1.39
2	F	800	NSX	C15-C10	8.91	1.57	1.38
2	B	300	NSX	C6-C7	8.74	1.56	1.38
2	D	600	NSX	C48-C50	8.73	1.55	1.39
2	A	400	NSX	C13-C11	8.53	1.54	1.36
2	C	500	NSX	C9-C4	8.49	1.60	1.42
2	E	700	NSX	C5-C4	8.42	1.60	1.42
2	F	800	NSX	C5-C4	8.27	1.60	1.42
2	D	600	NSX	C27-C28	8.23	1.59	1.42
2	B	300	NSX	C9-C4	8.18	1.59	1.42
2	C	500	NSX	C13-C11	8.15	1.53	1.36
2	C	500	NSX	C35-N34	8.12	1.48	1.33
2	E	700	NSX	C65-C63	8.12	1.53	1.36
2	D	600	NSX	C5-C4	8.12	1.59	1.42
2	F	800	NSX	C65-C63	8.08	1.53	1.36
2	A	400	NSX	C35-N34	8.03	1.48	1.33
2	D	600	NSX	C35-N34	8.02	1.48	1.33
2	B	300	NSX	C35-N34	8.01	1.48	1.33
2	B	300	NSX	C22-C23	-8.00	1.38	1.51
2	A	400	NSX	C15-C10	7.96	1.55	1.38
2	D	600	NSX	C13-C11	7.93	1.53	1.36
2	A	400	NSX	C65-C63	7.93	1.53	1.36
2	A	400	NSX	C27-C28	7.89	1.59	1.42
2	A	400	NSX	C48-C46	7.89	1.51	1.38
2	F	800	NSX	C48-C46	7.87	1.51	1.38
2	B	300	NSX	C24-C23	7.87	1.54	1.38
2	D	600	NSX	C65-C63	7.83	1.53	1.36
2	C	500	NSX	C48-C46	7.77	1.51	1.38
2	C	500	NSX	C24-C23	7.76	1.54	1.38
2	F	800	NSX	C35-N34	7.75	1.48	1.33
2	E	700	NSX	C35-N34	7.73	1.48	1.33
2	F	800	NSX	C27-C28	7.73	1.58	1.42
2	D	600	NSX	C48-C46	7.68	1.51	1.38
2	C	500	NSX	C27-C28	7.67	1.58	1.42
2	C	500	NSX	C65-C63	7.66	1.52	1.36
2	B	300	NSX	C13-C11	7.64	1.52	1.36
2	E	700	NSX	C48-C46	7.64	1.51	1.38
2	B	300	NSX	C65-C63	7.63	1.52	1.36
2	B	300	NSX	C27-C28	7.59	1.58	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300	NSX	C48-C46	7.59	1.51	1.38
2	C	500	NSX	C22-C23	-7.52	1.39	1.51
2	E	700	NSX	C27-C28	7.52	1.58	1.42
2	A	400	NSX	C25-C23	7.51	1.53	1.38
2	B	300	NSX	C5-C6	7.46	1.52	1.36
2	C	500	NSX	C6-C7	7.46	1.53	1.38
2	A	400	NSX	C6-C7	7.41	1.53	1.38
2	D	600	NSX	C25-C23	7.40	1.53	1.38
2	D	600	NSX	C56-C57	7.33	1.51	1.38
2	F	800	NSX	C25-C23	7.33	1.53	1.38
2	D	600	NSX	C15-C10	7.32	1.54	1.38
2	F	800	NSX	C46-C45	7.32	1.53	1.38
2	B	300	NSX	C56-C57	7.30	1.51	1.38
2	F	800	NSX	C5-C6	7.29	1.52	1.36
2	D	600	NSX	C6-C7	7.29	1.53	1.38
2	D	600	NSX	C13-C10	7.28	1.54	1.38
2	F	800	NSX	C18-N29	7.26	1.49	1.34
2	E	700	NSX	C56-C57	7.22	1.51	1.38
2	A	400	NSX	C56-C57	7.22	1.51	1.38
2	B	300	NSX	C15-C10	7.21	1.54	1.38
2	E	700	NSX	C25-C23	7.19	1.53	1.38
2	C	500	NSX	C56-C57	7.17	1.51	1.38
2	F	800	NSX	C15-C14	7.16	1.51	1.36
2	E	700	NSX	C18-N29	7.13	1.49	1.34
2	C	500	NSX	C63-C62	7.13	1.57	1.42
2	E	700	NSX	C13-C11	7.12	1.51	1.36
2	E	700	NSX	C15-C14	7.10	1.51	1.36
2	F	800	NSX	C56-C57	7.09	1.51	1.38
2	B	300	NSX	C18-N29	7.08	1.49	1.34
2	D	600	NSX	C46-C45	7.06	1.52	1.38
2	E	700	NSX	C5-C6	7.05	1.51	1.36
2	D	600	NSX	C63-C62	7.03	1.57	1.42
2	B	300	NSX	C26-C24	7.02	1.51	1.36
2	B	300	NSX	C1-C2	-6.99	1.37	1.52
2	C	500	NSX	C27-C25	6.97	1.51	1.36
2	A	400	NSX	C18-N29	6.94	1.48	1.34
2	C	500	NSX	C25-C23	6.94	1.52	1.38
2	A	400	NSX	C27-C25	6.92	1.51	1.36
2	D	600	NSX	C18-N29	6.91	1.48	1.34
2	E	700	NSX	C57-C52	6.91	1.52	1.38
2	D	600	NSX	C27-C25	6.91	1.51	1.36
2	A	400	NSX	C46-C45	6.90	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	NSX	C5-C4	6.88	1.57	1.42
2	E	700	NSX	C46-C45	6.88	1.52	1.38
2	B	300	NSX	C25-C23	6.85	1.52	1.38
2	C	500	NSX	C46-C45	6.84	1.52	1.38
2	A	400	NSX	C13-C10	6.83	1.53	1.38
2	F	800	NSX	C13-C11	6.82	1.50	1.36
2	B	300	NSX	C46-C45	6.81	1.52	1.38
2	C	500	NSX	C18-N29	6.78	1.48	1.34
2	A	400	NSX	C63-C62	6.78	1.56	1.42
2	C	500	NSX	C57-C52	6.76	1.52	1.38
2	B	300	NSX	C27-C25	6.70	1.51	1.36
2	F	800	NSX	C57-C52	6.68	1.52	1.38
2	E	700	NSX	C2-N16	6.67	1.48	1.34
2	F	800	NSX	C2-N16	6.67	1.48	1.34
2	D	600	NSX	C1-C2	-6.67	1.38	1.52
2	B	300	NSX	C57-C52	6.66	1.52	1.38
2	E	700	NSX	C63-C62	6.63	1.56	1.42
2	F	800	NSX	C63-C62	6.59	1.56	1.42
2	A	400	NSX	C24-C23	6.56	1.51	1.38
2	A	400	NSX	C1-C2	-6.52	1.38	1.52
2	B	300	NSX	C63-C62	6.51	1.56	1.42
2	D	600	NSX	C24-C23	6.47	1.51	1.38
2	C	500	NSX	C5-C6	6.44	1.50	1.36
2	C	500	NSX	C55-C54	6.44	1.52	1.38
2	D	600	NSX	C9-C8	6.41	1.50	1.36
2	F	800	NSX	C55-C54	6.40	1.52	1.38
2	E	700	NSX	C55-C54	6.40	1.52	1.38
2	F	800	NSX	C27-C25	6.39	1.50	1.36
2	E	700	NSX	C24-C23	6.39	1.51	1.38
2	F	800	NSX	C42-N60	6.38	1.48	1.33
2	A	400	NSX	C11-C12	6.36	1.55	1.42
2	C	500	NSX	C26-C24	6.36	1.50	1.36
2	C	500	NSX	C42-N60	6.35	1.48	1.33
2	B	300	NSX	C64-C62	6.33	1.55	1.42
2	F	800	NSX	C24-C23	6.33	1.51	1.38
2	D	600	NSX	C57-C52	6.32	1.51	1.38
2	F	800	NSX	C66-C64	6.30	1.49	1.36
2	E	700	NSX	C42-N60	6.30	1.48	1.33
2	E	700	NSX	C27-C25	6.30	1.50	1.36
2	A	400	NSX	C9-C8	6.30	1.50	1.36
2	D	600	NSX	C49-C50	6.29	1.50	1.39
2	A	400	NSX	C57-C52	6.28	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300	NSX	C55-C54	6.28	1.52	1.38
2	C	500	NSX	C71-N72	6.27	1.60	1.46
2	B	300	NSX	C49-C47	6.26	1.48	1.38
2	A	400	NSX	C49-C50	6.26	1.50	1.39
2	C	500	NSX	C13-C10	6.25	1.52	1.38
2	D	600	NSX	C49-C47	6.22	1.48	1.38
2	C	500	NSX	C49-C47	6.21	1.48	1.38
2	A	400	NSX	C42-N60	6.21	1.48	1.33
2	A	400	NSX	C2-N16	6.17	1.47	1.34
2	E	700	NSX	C66-C64	6.17	1.49	1.36
2	F	800	NSX	C49-C47	6.16	1.48	1.38
2	D	600	NSX	C42-N60	6.14	1.48	1.33
2	D	600	NSX	C2-N16	6.13	1.47	1.34
2	E	700	NSX	C49-C50	6.12	1.50	1.39
2	B	300	NSX	C71-N72	6.12	1.59	1.46
2	D	600	NSX	C11-C12	6.11	1.55	1.42
2	A	400	NSX	C55-C54	6.06	1.51	1.38
2	D	600	NSX	C55-C54	6.05	1.51	1.38
2	F	800	NSX	C64-C62	6.05	1.55	1.42
2	E	700	NSX	C49-C47	6.05	1.48	1.38
2	D	600	NSX	C56-C55	6.05	1.51	1.38
2	A	400	NSX	C56-C55	6.02	1.51	1.38
2	C	500	NSX	C64-C62	6.01	1.55	1.42
2	B	300	NSX	C49-C50	6.01	1.50	1.39
2	E	700	NSX	C64-C62	5.99	1.55	1.42
2	A	400	NSX	O73-C68	-5.99	1.11	1.23
2	B	300	NSX	C42-N60	5.98	1.47	1.33
2	F	800	NSX	C11-C12	5.97	1.55	1.42
2	E	700	NSX	C56-C55	5.96	1.51	1.38
2	D	600	NSX	C66-C64	5.95	1.49	1.36
2	F	800	NSX	C31-C30	5.95	1.67	1.53
2	D	600	NSX	O73-C68	-5.94	1.11	1.23
2	C	500	NSX	C1-C2	-5.93	1.39	1.52
2	A	400	NSX	C49-C47	5.91	1.48	1.38
2	C	500	NSX	C49-C50	5.88	1.50	1.39
2	E	700	NSX	C31-C30	5.88	1.67	1.53
2	F	800	NSX	C26-C24	5.88	1.49	1.36
2	A	400	NSX	C66-C64	5.87	1.49	1.36
2	C	500	NSX	C56-C55	5.84	1.51	1.38
2	E	700	NSX	C11-C12	5.83	1.54	1.42
2	B	300	NSX	C31-C30	5.82	1.66	1.53
2	F	800	NSX	C56-C55	5.82	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300	NSX	C56-C55	5.81	1.51	1.38
2	F	800	NSX	C13-C10	5.80	1.51	1.38
2	C	500	NSX	C31-C30	5.79	1.66	1.53
2	A	400	NSX	C22-C68	-5.77	1.40	1.52
2	E	700	NSX	C26-C24	5.76	1.49	1.36
2	F	800	NSX	C49-C50	5.73	1.49	1.39
2	A	400	NSX	C64-C62	5.72	1.54	1.42
2	F	800	NSX	O73-C68	-5.68	1.12	1.23
2	D	600	NSX	C15-C14	5.65	1.48	1.36
2	D	600	NSX	C31-C30	5.60	1.66	1.53
2	A	400	NSX	C26-C24	5.55	1.48	1.36
2	D	600	NSX	C22-C68	-5.55	1.40	1.52
2	D	600	NSX	C64-C62	5.54	1.54	1.42
2	E	700	NSX	O73-C68	-5.53	1.12	1.23
2	D	600	NSX	C26-C24	5.51	1.48	1.36
2	E	700	NSX	C13-C10	5.50	1.50	1.38
2	A	400	NSX	C31-C30	5.49	1.66	1.53
2	B	300	NSX	C13-C10	5.48	1.50	1.38
2	C	500	NSX	C66-C64	5.46	1.48	1.36
2	B	300	NSX	C66-C64	5.40	1.48	1.36
2	C	500	NSX	C67-C66	5.35	1.50	1.38
2	B	300	NSX	C5-C4	5.34	1.53	1.42
2	A	400	NSX	C9-C4	5.27	1.53	1.42
2	E	700	NSX	C22-C68	-5.22	1.41	1.52
2	F	800	NSX	C22-C68	-5.20	1.41	1.52
2	F	800	NSX	C67-C66	5.12	1.49	1.38
2	E	700	NSX	C67-C66	5.09	1.49	1.38
2	F	800	NSX	C67-C65	5.08	1.49	1.38
2	A	400	NSX	C67-C65	5.05	1.49	1.38
2	D	600	NSX	C67-C65	5.03	1.49	1.38
2	A	400	NSX	C15-C14	5.02	1.47	1.36
2	E	700	NSX	C67-C65	5.00	1.49	1.38
2	B	300	NSX	C2-N16	4.94	1.44	1.34
2	D	600	NSX	C67-C66	4.91	1.49	1.38
2	B	300	NSX	C67-C66	4.91	1.49	1.38
2	B	300	NSX	O73-C68	-4.89	1.13	1.23
2	C	500	NSX	C67-C65	4.88	1.49	1.38
2	A	400	NSX	C67-C66	4.84	1.48	1.38
2	A	400	NSX	O19-C18	4.80	1.32	1.23
2	E	700	NSX	C9-C8	4.78	1.47	1.36
2	B	300	NSX	C67-C65	4.78	1.48	1.38
2	F	800	NSX	C9-C8	4.74	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	NSX	O73-C68	-4.68	1.14	1.23
2	D	600	NSX	O19-C18	4.67	1.32	1.23
2	E	700	NSX	C1-C2	-4.61	1.42	1.52
2	A	400	NSX	C71-N72	4.56	1.56	1.46
2	C	500	NSX	C70-C69	-4.56	1.29	1.51
2	F	800	NSX	C71-N72	4.51	1.56	1.46
2	E	700	NSX	O19-C18	4.50	1.32	1.23
2	D	600	NSX	C70-C69	-4.49	1.29	1.51
2	B	300	NSX	C70-C69	-4.47	1.29	1.51
2	D	600	NSX	C71-N72	4.46	1.56	1.46
2	A	400	NSX	C70-C69	-4.45	1.29	1.51
2	E	700	NSX	C70-C69	-4.40	1.29	1.51
2	F	800	NSX	O19-C18	4.40	1.31	1.23
2	F	800	NSX	C70-C69	-4.35	1.30	1.51
2	E	700	NSX	C71-N72	4.35	1.56	1.46
2	F	800	NSX	C59-N60	4.33	1.55	1.46
2	C	500	NSX	C2-N16	4.31	1.43	1.34
2	F	800	NSX	C1-C2	-4.28	1.43	1.52
2	D	600	NSX	C9-C4	4.23	1.51	1.42
2	C	500	NSX	C5-C4	4.23	1.51	1.42
2	B	300	NSX	C26-C28	4.19	1.51	1.42
2	D	600	NSX	C5-C6	4.19	1.45	1.36
2	E	700	NSX	C26-C28	4.13	1.51	1.42
2	F	800	NSX	C26-C28	4.10	1.50	1.42
2	E	700	NSX	C59-N60	4.09	1.55	1.46
2	A	400	NSX	C26-C28	4.06	1.50	1.42
2	E	700	NSX	C9-C4	4.01	1.50	1.42
2	C	500	NSX	C30-C38	-3.98	1.42	1.52
2	C	500	NSX	C26-C28	3.95	1.50	1.42
2	B	300	NSX	C30-C38	-3.93	1.42	1.52
2	A	400	NSX	C5-C6	3.93	1.45	1.36
2	F	800	NSX	C9-C4	3.92	1.50	1.42
2	B	300	NSX	C22-C68	-3.86	1.43	1.52
2	C	500	NSX	C59-N60	3.83	1.54	1.46
2	B	300	NSX	C59-N60	3.71	1.54	1.46
2	A	400	NSX	C59-N60	3.66	1.54	1.46
2	D	600	NSX	C59-N60	3.65	1.54	1.46
2	D	600	NSX	C26-C28	3.53	1.49	1.42
2	C	500	NSX	O19-C18	3.44	1.30	1.23
2	E	700	NSX	C30-C38	-3.40	1.44	1.52
2	B	300	NSX	O19-C18	3.40	1.29	1.23
2	C	500	NSX	C22-C68	-3.31	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	800	NSX	C30-C38	-3.29	1.44	1.52
2	D	600	NSX	C30-C38	-3.25	1.44	1.52
2	A	400	NSX	C30-C38	-3.16	1.44	1.52
2	D	600	NSX	C17-N16	-2.98	1.39	1.45
2	F	800	NSX	C44-C45	2.97	1.58	1.51
2	A	400	NSX	C58-C52	-2.96	1.43	1.51
2	C	500	NSX	C44-C45	2.96	1.58	1.51
2	D	600	NSX	C44-C45	2.92	1.58	1.51
2	D	600	NSX	C58-C52	-2.91	1.43	1.51
2	B	300	NSX	O51-C50	-2.88	1.30	1.37
2	E	700	NSX	C44-C45	2.87	1.58	1.51
2	A	400	NSX	C17-N16	-2.86	1.39	1.45
2	E	700	NSX	C58-C52	-2.82	1.43	1.51
2	A	400	NSX	C44-C45	2.77	1.57	1.51
2	F	800	NSX	C58-C52	-2.76	1.43	1.51
2	C	500	NSX	O51-C50	-2.76	1.30	1.37
2	F	800	NSX	O51-C50	-2.72	1.30	1.37
2	C	500	NSX	C58-C52	-2.69	1.44	1.51
2	B	300	NSX	C44-C45	2.66	1.57	1.51
2	B	300	NSX	C58-C52	-2.63	1.44	1.51
2	E	700	NSX	O51-C50	-2.61	1.31	1.37
2	D	600	NSX	O51-C50	-2.54	1.31	1.37
2	D	600	NSX	C20-C17	-2.46	1.47	1.53
2	A	400	NSX	O51-C50	-2.37	1.31	1.37
2	A	400	NSX	C20-C17	-2.30	1.48	1.53
2	E	700	NSX	C20-C17	-2.26	1.48	1.53
2	C	500	NSX	C17-N16	-2.24	1.41	1.45
2	B	300	NSX	O3-C2	-2.15	1.19	1.23
2	B	300	NSX	O39-C38	2.10	1.27	1.23
2	D	600	NSX	O39-C38	2.06	1.27	1.23
2	A	400	NSX	C32-C31	2.05	1.60	1.52
2	F	800	NSX	C20-C17	-2.05	1.48	1.53
2	E	700	NSX	C17-N16	-2.04	1.41	1.45
2	F	800	NSX	C17-N16	-2.03	1.41	1.45
2	D	600	NSX	C32-C31	2.03	1.60	1.52
2	F	800	NSX	C32-C31	2.02	1.60	1.52

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	300	NSX	C14-C12-C11	-11.32	108.63	118.81
2	B	300	NSX	C5-C4-C9	-10.02	109.80	118.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	NSX	C14-C12-C11	-9.89	109.92	118.81
2	C	500	NSX	C5-C4-C9	-9.85	109.95	118.81
2	B	300	NSX	C10-C13-C11	8.98	132.41	120.40
2	C	500	NSX	C1-C7-C8	8.41	133.26	120.89
2	B	300	NSX	C1-C7-C8	7.68	132.18	120.89
2	C	500	NSX	C1-C7-C6	-7.53	109.81	120.89
2	B	300	NSX	C8-C9-C4	6.60	130.70	120.84
2	B	300	NSX	C22-C68-N72	6.52	125.10	116.06
2	C	500	NSX	C18-C17-N16	-6.45	93.66	111.11
2	B	300	NSX	C1-C7-C6	-6.32	111.60	120.89
2	B	300	NSX	C18-C17-N16	-6.25	94.19	111.11
2	C	500	NSX	C22-C68-N72	6.14	124.58	116.06
2	B	300	NSX	C23-C22-C68	6.11	130.54	112.33
2	B	300	NSX	C69-C20-C17	6.00	132.26	113.80
2	C	500	NSX	C69-C20-C17	5.92	132.01	113.80
2	C	500	NSX	C23-C22-C68	5.91	129.95	112.33
2	C	500	NSX	C8-C9-C4	5.84	129.55	120.84
2	A	400	NSX	O73-C68-C22	-5.79	109.44	121.99
2	D	600	NSX	C18-C17-N16	-5.78	95.48	111.11
2	D	600	NSX	O73-C68-C22	-5.70	109.65	121.99
2	B	300	NSX	O73-C68-C22	-5.69	109.65	121.99
2	E	700	NSX	O73-C68-C22	-5.68	109.69	121.99
2	F	800	NSX	O73-C68-C22	-5.65	109.75	121.99
2	A	400	NSX	C18-C17-N16	-5.50	96.24	111.11
2	F	800	NSX	C23-C22-C68	5.46	128.61	112.33
2	C	500	NSX	O73-C68-C22	-5.37	110.36	121.99
2	C	500	NSX	C10-C13-C11	5.29	127.48	120.40
2	A	400	NSX	C22-C68-N72	5.25	123.34	116.06
2	B	300	NSX	C59-C58-C52	5.22	124.61	112.83
2	E	700	NSX	C69-C20-C17	5.19	129.76	113.80
2	F	800	NSX	C22-C68-N72	5.19	123.25	116.06
2	E	700	NSX	C22-C68-N72	5.17	123.24	116.06
2	E	700	NSX	C23-C22-C68	5.17	127.74	112.33
2	A	400	NSX	C59-C58-C52	5.14	124.42	112.83
2	D	600	NSX	C22-C68-N72	5.14	123.19	116.06
2	F	800	NSX	C69-C20-C17	5.12	129.54	113.80
2	F	800	NSX	C59-C58-C52	5.06	124.23	112.83
2	D	600	NSX	C59-C58-C52	5.01	124.13	112.83
2	C	500	NSX	C59-C58-C52	5.00	124.10	112.83
2	B	300	NSX	C15-C10-C13	-4.93	113.12	119.87
2	D	600	NSX	C23-C22-C68	4.93	127.02	112.33
2	E	700	NSX	C59-C58-C52	4.89	123.84	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	NSX	C23-C22-C68	4.74	126.46	112.33
2	A	400	NSX	C69-C20-C17	4.50	127.63	113.80
2	E	700	NSX	C14-C12-C11	4.49	122.85	118.81
2	D	600	NSX	C69-C20-C17	4.47	127.56	113.80
2	E	700	NSX	C18-C17-N16	-4.45	99.08	111.11
2	A	400	NSX	C13-C11-C12	-4.44	114.31	120.48
2	A	400	NSX	C71-N72-C68	-4.28	114.85	122.82
2	D	600	NSX	C71-N72-C68	-4.26	114.89	122.82
2	A	400	NSX	C70-C69-C20	4.24	129.59	113.62
2	C	500	NSX	C70-C69-C20	4.18	129.37	113.62
2	E	700	NSX	C71-N72-C68	-4.18	115.04	122.82
2	F	800	NSX	C14-C12-C11	4.18	122.57	118.81
2	D	600	NSX	C1-C7-C6	-4.15	114.78	120.89
2	D	600	NSX	C70-C69-C20	4.13	129.18	113.62
2	B	300	NSX	C71-N72-C68	-4.12	115.15	122.82
2	E	700	NSX	C13-C11-C12	-4.12	114.76	120.48
2	B	300	NSX	C70-C69-C20	4.10	129.08	113.62
2	F	800	NSX	C18-C17-N16	-4.10	100.02	111.11
2	A	400	NSX	C1-C7-C6	-4.08	114.88	120.89
2	D	600	NSX	C13-C11-C12	-4.08	114.81	120.48
2	F	800	NSX	C71-N72-C68	-4.08	115.23	122.82
2	F	800	NSX	C70-C69-C20	4.03	128.81	113.62
2	E	700	NSX	C70-C69-C20	4.01	128.72	113.62
2	A	400	NSX	C7-C1-C2	-3.97	100.48	112.33
2	F	800	NSX	C13-C11-C12	-3.93	115.02	120.48
2	C	500	NSX	C9-C8-C7	-3.92	113.41	121.07
2	C	500	NSX	C20-C17-N16	-3.91	103.16	110.91
2	D	600	NSX	C7-C1-C2	-3.91	100.67	112.33
2	B	300	NSX	C9-C8-C7	-3.81	113.63	121.07
2	C	500	NSX	C42-C41-N40	-3.79	100.86	111.11
2	B	300	NSX	C20-C17-N16	-3.79	103.41	110.91
2	B	300	NSX	C42-C41-N40	-3.79	100.87	111.11
2	A	400	NSX	C64-C62-C63	-3.77	115.42	118.81
2	B	300	NSX	C17-N16-C2	3.76	131.10	121.68
2	C	500	NSX	C17-N16-C2	3.66	130.87	121.68
2	D	600	NSX	C64-C62-C63	-3.64	115.55	118.81
2	B	300	NSX	C15-C14-C12	3.54	125.40	120.48
2	C	500	NSX	C71-N72-C68	-3.53	116.25	122.82
2	E	700	NSX	C42-C41-N40	-3.52	101.59	111.11
2	F	800	NSX	C42-C41-N40	-3.45	101.79	111.11
2	D	600	NSX	C42-C41-N40	-3.41	101.87	111.11
2	A	400	NSX	C10-C13-C11	3.39	124.94	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	300	NSX	C64-C62-C63	-3.34	115.81	118.81
2	D	600	NSX	C10-C13-C11	3.34	124.86	120.40
2	F	800	NSX	C32-C31-C30	3.33	124.04	113.80
2	B	300	NSX	C70-C71-N72	3.30	121.46	112.20
2	E	700	NSX	C32-C31-C30	3.29	123.94	113.80
2	F	800	NSX	C64-C62-C63	-3.29	115.86	118.81
2	C	500	NSX	C64-C62-C63	-3.27	115.87	118.81
2	C	500	NSX	C59-N60-C42	-3.24	116.72	122.55
2	B	300	NSX	C22-C23-C24	3.23	125.64	120.89
2	F	800	NSX	C31-C30-C38	-3.23	102.21	110.11
2	A	400	NSX	C31-C30-C38	-3.22	102.25	110.11
2	A	400	NSX	C42-C41-N40	-3.21	102.42	111.11
2	E	700	NSX	C59-N60-C42	-3.19	116.82	122.55
2	F	800	NSX	C10-C15-C14	-3.13	116.21	120.40
2	E	700	NSX	C31-C30-C38	-3.13	102.47	110.11
2	B	300	NSX	C27-C28-C26	-3.12	116.01	118.81
2	E	700	NSX	C64-C62-C63	-3.08	116.04	118.81
2	D	600	NSX	C31-C30-C38	-3.07	102.60	110.11
2	A	400	NSX	C32-C33-N34	3.05	120.75	112.20
2	C	500	NSX	C15-C14-C12	3.04	124.70	120.48
2	F	800	NSX	C59-N60-C42	-3.03	117.10	122.55
2	E	700	NSX	C17-N16-C2	3.03	129.28	121.68
2	F	800	NSX	C69-C70-C71	3.03	127.55	113.56
2	E	700	NSX	C32-C33-N34	3.03	120.69	112.20
2	C	500	NSX	C15-C10-C13	-3.01	115.75	119.87
2	C	500	NSX	C27-C28-C26	-3.01	116.11	118.81
2	F	800	NSX	C32-C33-N34	2.98	120.56	112.20
2	D	600	NSX	C59-N60-C42	-2.98	117.20	122.55
2	B	300	NSX	C59-N60-C42	-2.97	117.20	122.55
2	E	700	NSX	C70-C71-N72	2.97	120.54	112.20
2	D	600	NSX	C70-C71-N72	2.96	120.50	112.20
2	A	400	NSX	C70-C71-N72	2.95	120.47	112.20
2	E	700	NSX	C69-C70-C71	2.94	127.15	113.56
2	E	700	NSX	C10-C15-C14	-2.94	116.46	120.40
2	D	600	NSX	C32-C33-N34	2.93	120.42	112.20
2	E	700	NSX	C10-C13-C11	2.92	124.31	120.40
2	C	500	NSX	C6-C5-C4	2.91	125.18	120.84
2	F	800	NSX	C70-C71-N72	2.90	120.33	112.20
2	A	400	NSX	C32-C31-C30	2.89	122.68	113.80
2	C	500	NSX	C32-C31-C30	2.89	122.68	113.80
2	B	300	NSX	C32-C31-C30	2.88	122.67	113.80
2	C	500	NSX	C70-C71-N72	2.88	120.26	112.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	NSX	C54-C53-C52	-2.85	116.60	120.61
2	F	800	NSX	C54-C53-C52	-2.85	116.60	120.61
2	C	500	NSX	C22-C23-C24	2.85	125.08	120.89
2	B	300	NSX	C54-C53-C52	-2.84	116.61	120.61
2	A	400	NSX	C14-C12-C11	2.83	121.36	118.81
2	E	700	NSX	C54-C53-C52	-2.83	116.63	120.61
2	A	400	NSX	C59-N60-C42	-2.82	117.47	122.55
2	C	500	NSX	C69-C70-C71	2.80	126.48	113.56
2	A	400	NSX	C69-C70-C71	2.80	126.47	113.56
2	A	400	NSX	C54-C53-C52	-2.79	116.69	120.61
2	D	600	NSX	C32-C31-C30	2.77	122.33	113.80
2	B	300	NSX	C31-C30-C38	-2.77	103.35	110.11
2	B	300	NSX	C32-C33-N34	2.76	119.93	112.20
2	B	300	NSX	C69-C70-C71	2.75	126.27	113.56
2	F	800	NSX	C17-N16-C2	2.75	128.58	121.68
2	D	600	NSX	C69-C70-C71	2.74	126.23	113.56
2	F	800	NSX	C10-C13-C11	2.74	124.06	120.40
2	C	500	NSX	C32-C33-N34	2.73	119.86	112.20
2	C	500	NSX	C31-C30-C38	-2.71	103.48	110.11
2	D	600	NSX	C9-C8-C7	-2.71	115.78	121.07
2	D	600	NSX	C54-C53-C52	-2.70	116.82	120.61
2	B	300	NSX	C45-C44-C41	-2.67	106.25	113.36
2	D	600	NSX	C14-C12-C11	2.65	121.20	118.81
2	A	400	NSX	C17-N16-C2	2.63	128.28	121.68
2	C	500	NSX	O39-C38-N40	2.58	127.58	122.96
2	D	600	NSX	C17-N16-C2	2.53	128.03	121.68
2	F	800	NSX	C6-C5-C4	-2.53	117.06	120.84
2	B	300	NSX	O39-C38-N40	2.52	127.47	122.96
2	D	600	NSX	C8-C7-C6	2.49	121.93	118.23
2	E	700	NSX	C7-C1-C2	-2.48	104.92	112.33
2	E	700	NSX	C6-C5-C4	-2.45	117.18	120.84
2	A	400	NSX	C9-C8-C7	-2.44	116.29	121.07
2	B	300	NSX	N37-C35-N36	-2.43	113.17	120.07
2	F	800	NSX	C7-C1-C2	-2.42	105.12	112.33
2	C	500	NSX	N37-C35-N36	-2.41	113.22	120.07
2	F	800	NSX	N37-C35-N36	-2.41	113.22	120.07
2	C	500	NSX	C45-C44-C41	-2.40	106.97	113.36
2	A	400	NSX	N37-C35-N36	-2.40	113.25	120.07
2	D	600	NSX	C45-C44-C41	-2.39	107.00	113.36
2	D	600	NSX	N37-C35-N36	-2.38	113.31	120.07
2	A	400	NSX	C8-C7-C6	2.38	121.76	118.23
2	E	700	NSX	N37-C35-N36	-2.33	113.43	120.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	700	NSX	C17-C18-N29	-2.31	111.70	116.63
2	B	300	NSX	O3-C2-N16	2.28	126.81	122.95
2	B	300	NSX	C5-C6-C7	2.27	125.51	121.07
2	F	800	NSX	C17-C18-N29	-2.26	111.80	116.63
2	A	400	NSX	C45-C44-C41	-2.24	107.41	113.36
2	A	400	NSX	C27-C28-C26	-2.21	116.83	118.81
2	D	600	NSX	C17-C18-N29	-2.21	111.91	116.63
2	F	800	NSX	C5-C4-C9	2.21	120.80	118.81
2	F	800	NSX	C20-C17-N16	-2.19	106.57	110.91
2	D	600	NSX	C27-C28-C26	-2.19	116.84	118.81
2	A	400	NSX	C17-C18-N29	-2.17	112.00	116.63
2	C	500	NSX	C7-C1-C2	2.17	118.79	112.33
2	B	300	NSX	C6-C5-C4	2.17	124.07	120.84
2	E	700	NSX	C20-C17-N16	-2.15	106.65	110.91
2	F	800	NSX	C27-C28-C26	-2.15	116.89	118.81
2	A	400	NSX	O73-C68-N72	2.13	127.21	123.03
2	D	600	NSX	O73-C68-N72	2.10	127.16	123.03
2	E	700	NSX	C5-C4-C9	2.09	120.69	118.81
2	C	500	NSX	C26-C24-C23	2.08	125.14	121.07
2	A	400	NSX	C58-C52-C57	-2.08	115.86	121.18
2	A	400	NSX	C57-C52-C53	2.07	121.31	118.23
2	C	500	NSX	C44-C41-N40	2.07	115.11	110.83
2	E	700	NSX	O73-C68-N72	2.05	127.06	123.03
2	B	300	NSX	C31-C30-N29	2.05	114.97	110.91
2	D	600	NSX	C58-C59-N60	-2.05	106.06	111.96
2	F	800	NSX	C15-C10-C13	2.04	122.66	119.87
2	B	300	NSX	C44-C41-N40	2.02	115.02	110.83
2	D	600	NSX	C58-C52-C57	-2.02	116.03	121.18
2	F	800	NSX	O73-C68-N72	2.01	126.97	123.03

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	NSX	C20-C69-C70-C71
2	B	300	NSX	C20-C69-C70-C71
2	C	500	NSX	C20-C69-C70-C71
2	D	600	NSX	C20-C69-C70-C71
2	E	700	NSX	C20-C69-C70-C71
2	F	800	NSX	C20-C69-C70-C71
2	A	400	NSX	N16-C17-C20-C69
2	B	300	NSX	N16-C17-C20-C69

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Mol	Chain	Res	Type	Atoms
2	C	500	NSX	N16-C17-C20-C69
2	F	800	NSX	N16-C17-C20-C69
2	B	300	NSX	C18-C17-C20-C69
2	C	500	NSX	C18-C17-C20-C69
2	E	700	NSX	C18-C17-C20-C69
2	D	600	NSX	N16-C17-C20-C69
2	E	700	NSX	N16-C17-C20-C69
2	A	400	NSX	C38-C30-N29-C18
2	D	600	NSX	C38-C30-N29-C18
2	F	800	NSX	C38-C30-N29-C18
2	E	700	NSX	C38-C30-N29-C18
2	D	600	NSX	C18-C17-C20-C69
2	F	800	NSX	C18-C17-C20-C69
2	C	500	NSX	C38-C30-N29-C18
2	B	300	NSX	C38-C30-N29-C18
2	D	600	NSX	N29-C30-C31-C32
2	B	300	NSX	N29-C30-C31-C32
2	C	500	NSX	N29-C30-C31-C32
2	F	800	NSX	C2-C1-C7-C6
2	F	800	NSX	C7-C1-C2-O3
2	E	700	NSX	C2-C1-C7-C6
2	E	700	NSX	C2-C1-C7-C8
2	F	800	NSX	C2-C1-C7-C8
2	A	400	NSX	C18-C17-C20-C69
2	A	400	NSX	N29-C30-C31-C32
2	E	700	NSX	C7-C1-C2-O3
2	B	300	NSX	C38-C30-C31-C32
2	C	500	NSX	C38-C30-C31-C32
2	D	600	NSX	C38-C30-C31-C32
2	F	800	NSX	N29-C30-C31-C32
2	B	300	NSX	C53-C52-C58-C59
2	F	800	NSX	C38-C30-C31-C32
2	B	300	NSX	C57-C52-C58-C59
2	C	500	NSX	C53-C52-C58-C59
2	E	700	NSX	N29-C30-C31-C32
2	F	800	NSX	C7-C1-C2-N16
2	A	400	NSX	C38-C30-C31-C32
2	B	300	NSX	C31-C30-N29-C18
2	D	600	NSX	C53-C52-C58-C59
2	A	400	NSX	N37-C35-N34-C33
2	B	300	NSX	N37-C35-N34-C33
2	C	500	NSX	N37-C35-N34-C33

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Mol	Chain	Res	Type	Atoms
2	D	600	NSX	N37-C35-N34-C33
2	E	700	NSX	N37-C35-N34-C33
2	C	500	NSX	C57-C52-C58-C59
2	D	600	NSX	C57-C52-C58-C59
2	C	500	NSX	C31-C30-N29-C18
2	E	700	NSX	C7-C1-C2-N16
2	E	700	NSX	C38-C30-C31-C32
2	B	300	NSX	C30-C31-C32-C33
2	C	500	NSX	C30-C31-C32-C33
2	D	600	NSX	C30-C31-C32-C33
2	E	700	NSX	C53-C52-C58-C59
2	A	400	NSX	C53-C52-C58-C59
2	A	400	NSX	N36-C35-N34-C33
2	B	300	NSX	N36-C35-N34-C33
2	C	500	NSX	N36-C35-N34-C33
2	D	600	NSX	N36-C35-N34-C33
2	E	700	NSX	N36-C35-N34-C33
2	F	800	NSX	N36-C35-N34-C33
2	E	700	NSX	C57-C52-C58-C59
2	F	800	NSX	C53-C52-C58-C59
2	A	400	NSX	C57-C52-C58-C59
2	F	800	NSX	C30-C31-C32-C33
2	F	800	NSX	C57-C52-C58-C59
2	A	400	NSX	C30-C31-C32-C33
2	E	700	NSX	C30-C31-C32-C33
2	E	700	NSX	C31-C30-N29-C18
2	E	700	NSX	C17-C20-C69-C70
2	F	800	NSX	N37-C35-N34-C33
2	F	800	NSX	C31-C30-N29-C18
2	D	600	NSX	C31-C30-N29-C18
2	F	800	NSX	C17-C20-C69-C70

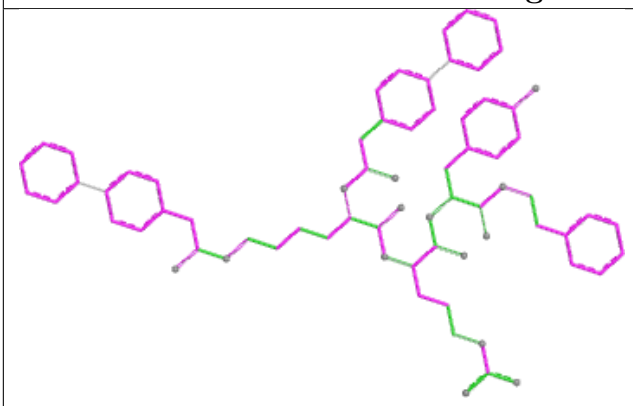
There are no ring outliers.

6 monomers are involved in 58 short contacts:

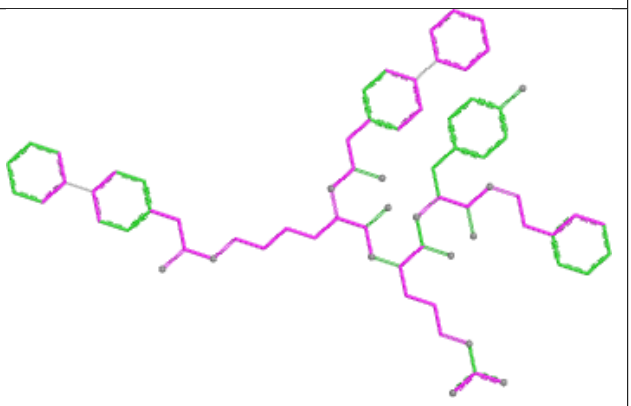
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	800	NSX	8	0
2	B	300	NSX	11	0
2	A	400	NSX	9	0
2	E	700	NSX	8	0
2	C	500	NSX	9	0
2	D	600	NSX	13	0

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

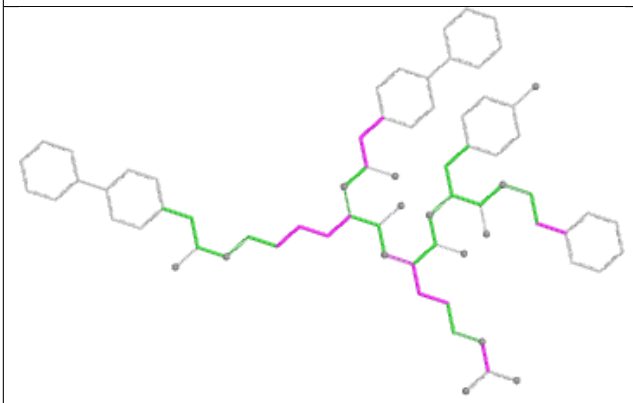
Ligand NSX F 800



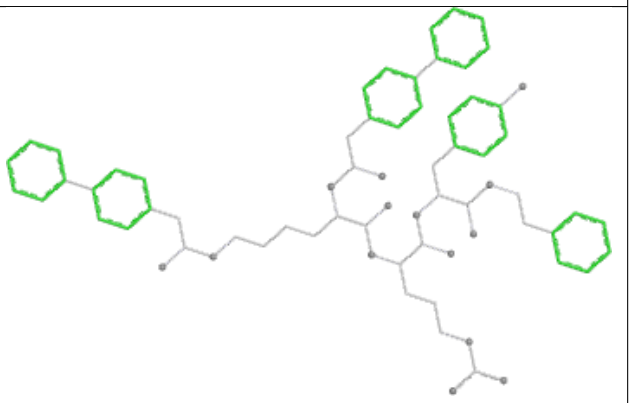
Bond lengths



Bond angles

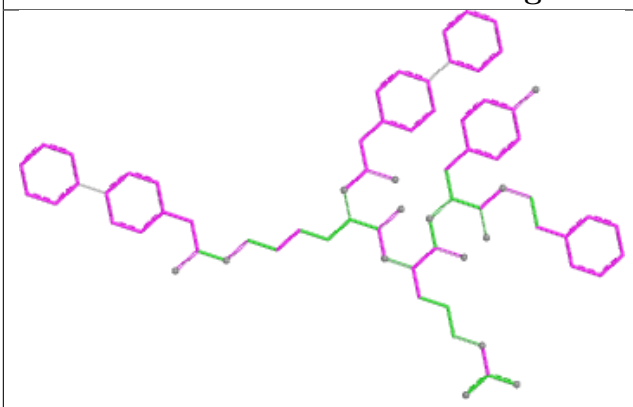


Torsions

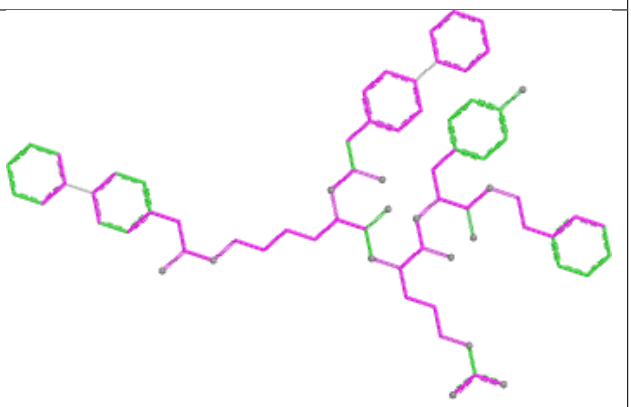


Rings

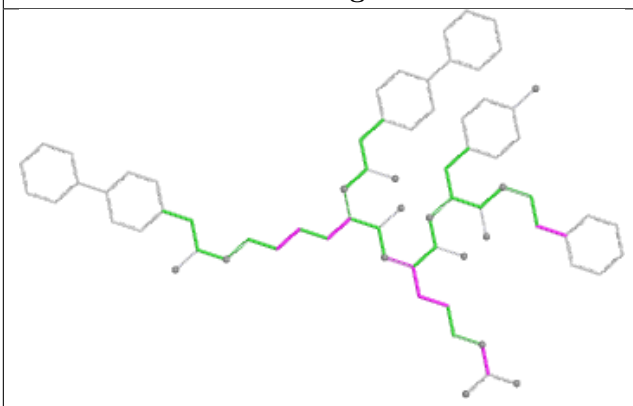
Ligand NSX B 300



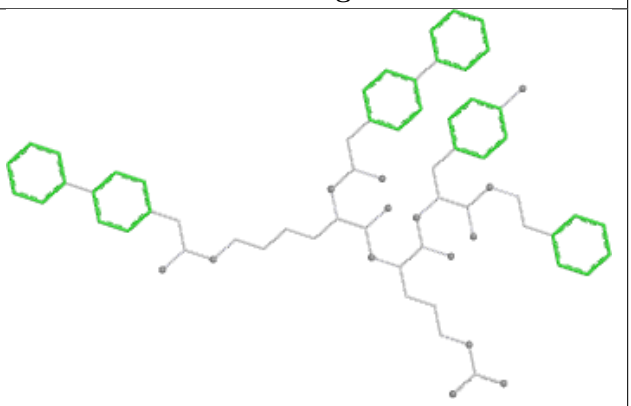
Bond lengths



Bond angles

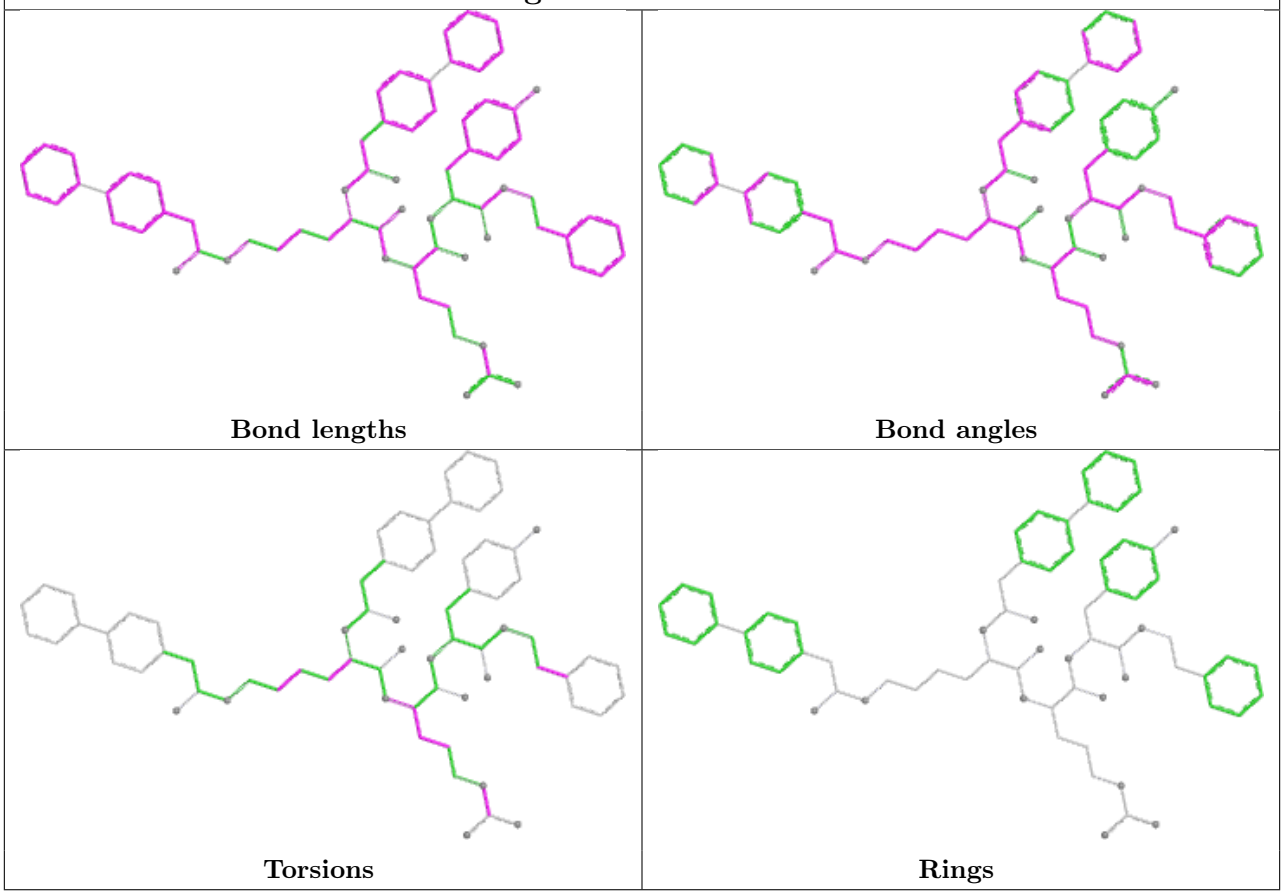


Torsions

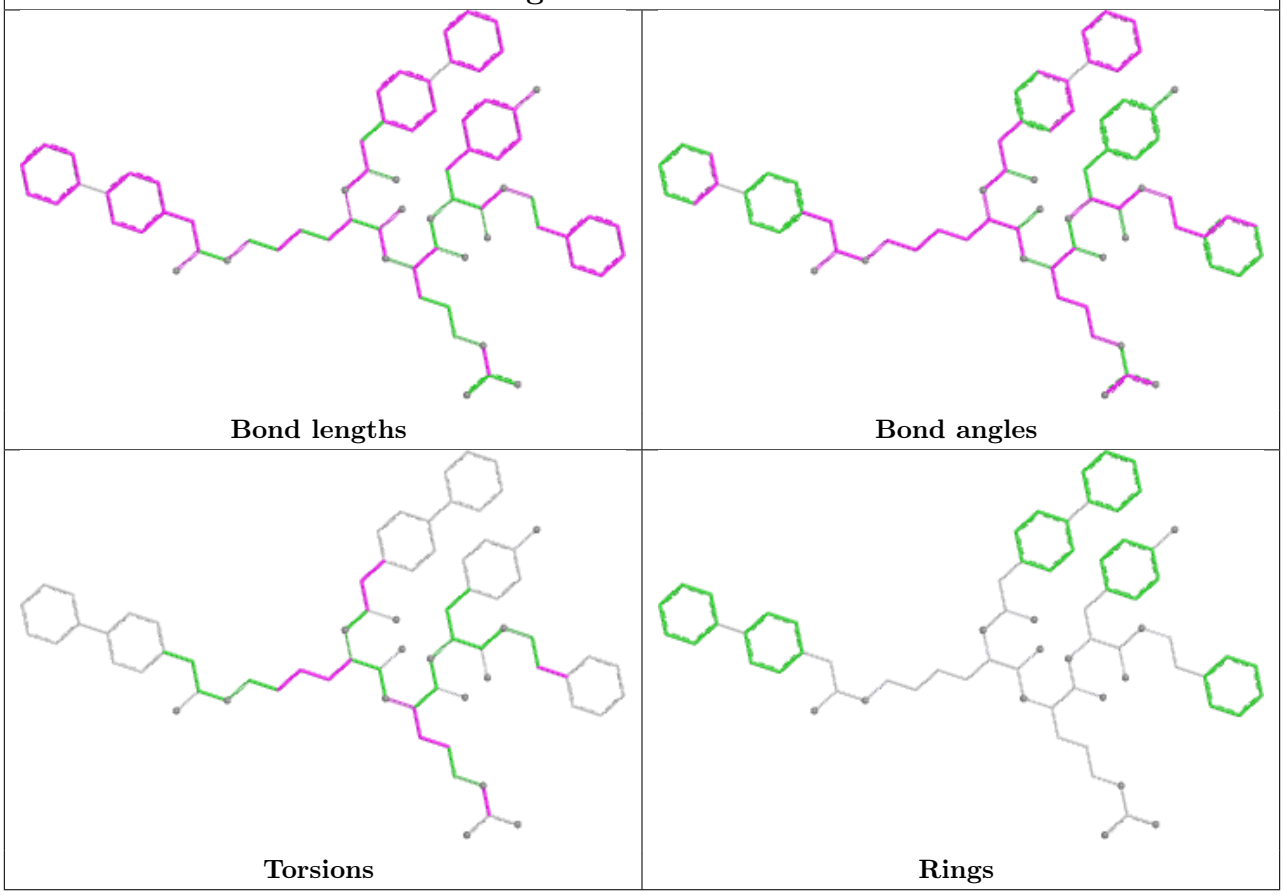


Rings

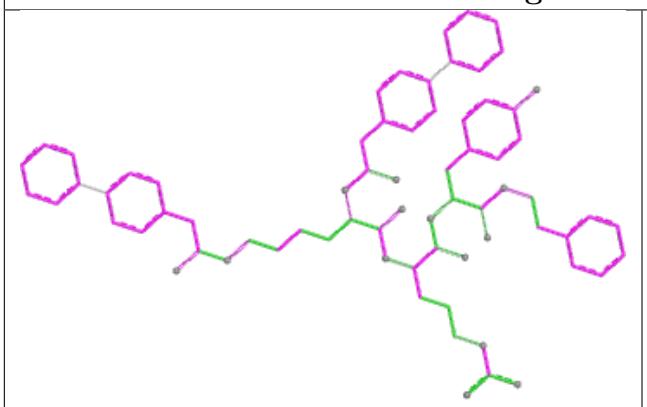
Ligand NSX A 400



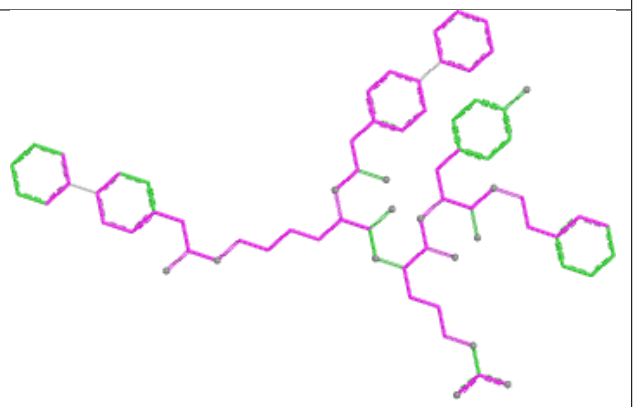
Ligand NSX E 700



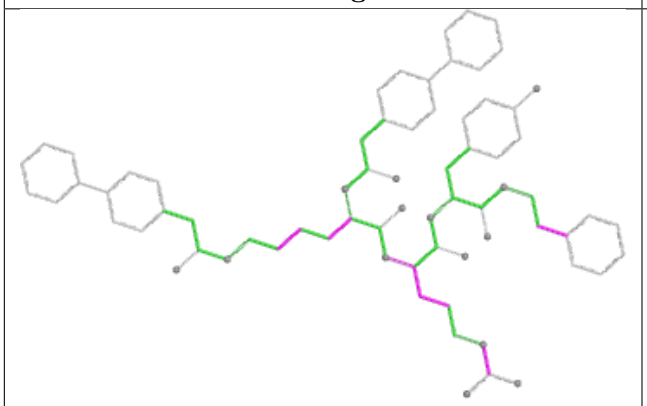
Ligand NSX C 500



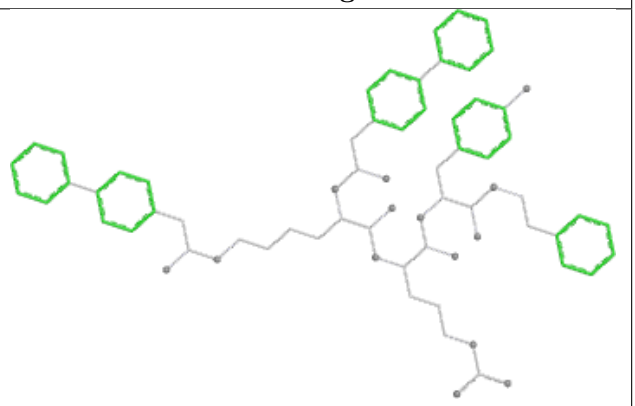
Bond lengths



Bond angles

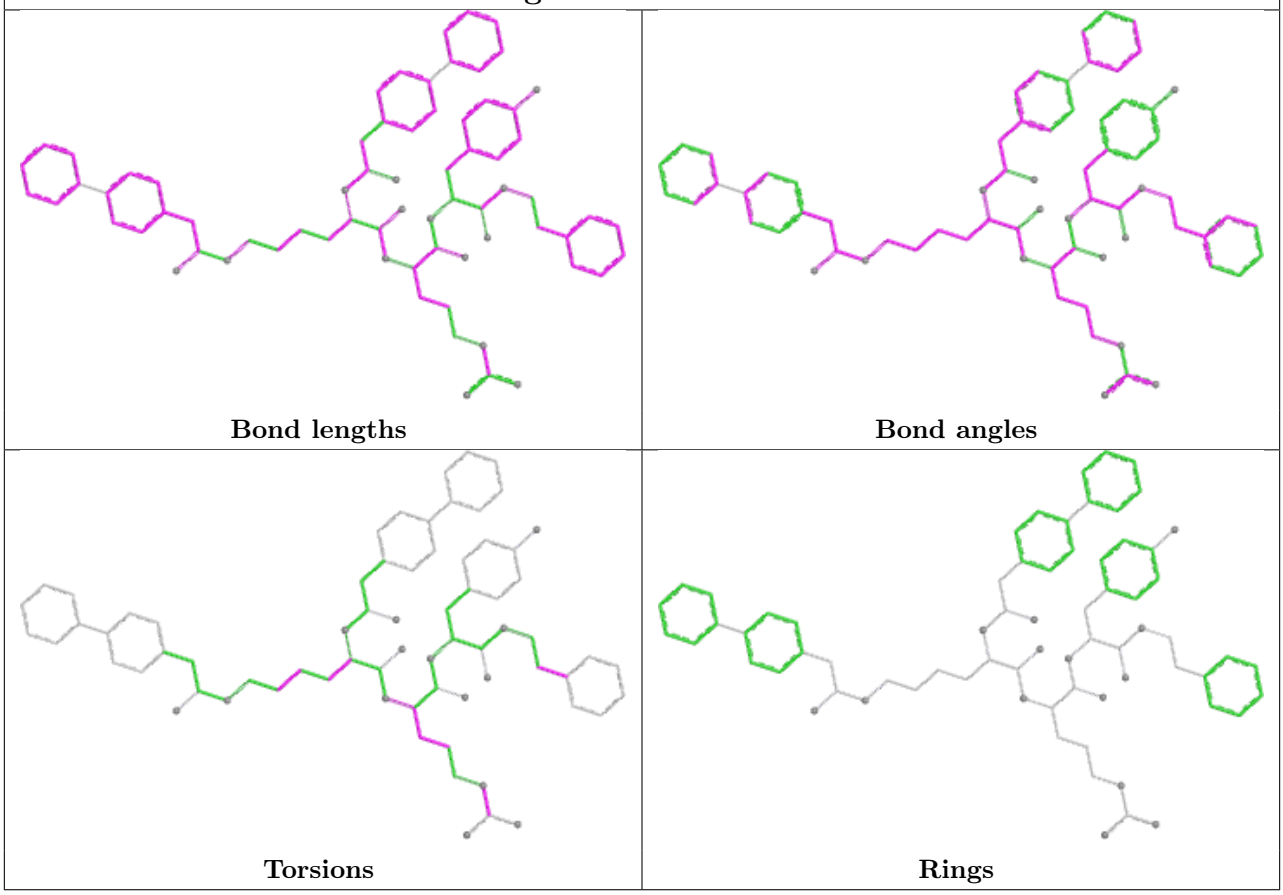


Torsions



Rings

Ligand NSX D 600



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	215/220 (97%)	0.17	7 (3%)	46	50	10, 21, 49, 72	0
1	B	215/220 (97%)	0.15	8 (3%)	41	45	8, 19, 49, 89	0
1	C	215/220 (97%)	0.33	8 (3%)	41	45	9, 20, 44, 75	0
1	D	215/220 (97%)	0.22	7 (3%)	46	50	10, 21, 47, 74	0
1	E	215/220 (97%)	0.69	27 (12%)	3	3	13, 32, 63, 86	0
1	F	215/220 (97%)	0.84	31 (14%)	2	2	13, 30, 62, 100	0
All	All	1290/1320 (97%)	0.40	88 (6%)	17	17	8, 23, 57, 100	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	110	THR	6.5
1	B	174	SER	5.5
1	F	103	LYS	5.5
1	F	89	TYR	5.4
1	F	110	THR	5.0
1	E	88	SER	4.7
1	F	78	GLN	4.4
1	F	82	GLY	4.1
1	E	220	VAL	4.1
1	A	174	SER	4.0
1	D	174	SER	3.8
1	F	154	PRO	3.8
1	A	110	THR	3.7
1	F	100	TYR	3.7
1	F	155	ASP	3.6
1	F	102	PRO	3.6
1	B	147	LYS	3.6
1	A	3	ARG	3.5
1	E	174	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	3	ARG	3.5
1	E	1	ALA	3.5
1	E	147	LYS	3.4
1	E	87	GLU	3.4
1	B	110	THR	3.3
1	E	103	LYS	3.2
1	D	160	ASP	3.2
1	A	1	ALA	3.1
1	E	78	GLN	3.1
1	F	79	ASP	3.1
1	F	1	ALA	3.0
1	E	3	ARG	3.0
1	B	206	ARG	3.0
1	F	101	ASN	3.0
1	F	220	VAL	2.9
1	B	148	GLU	2.9
1	F	3	ARG	2.8
1	E	104	TYR	2.8
1	F	42	THR	2.8
1	E	79	ASP	2.8
1	E	59	PRO	2.8
1	E	155	ASP	2.8
1	E	56	CYS	2.7
1	C	108	ASN	2.7
1	E	100	TYR	2.7
1	F	43	GLY	2.7
1	E	108	ASN	2.6
1	B	108	ASN	2.6
1	F	77	VAL	2.6
1	F	40	ARG	2.6
1	B	21	GLN	2.6
1	D	155	ASP	2.6
1	E	82	GLY	2.6
1	A	44	ARG	2.6
1	E	77	VAL	2.5
1	E	102	PRO	2.5
1	E	44	ARG	2.5
1	F	84	ASP	2.5
1	C	109	ASP	2.5
1	D	110	THR	2.4
1	F	39	PHE	2.4
1	C	155	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	4	SER	2.4
1	F	98	CYS	2.4
1	E	118	GLN	2.4
1	C	110	THR	2.4
1	F	105	SER	2.3
1	C	92	GLU	2.3
1	D	197	GLY	2.3
1	E	101	ASN	2.2
1	F	80	ASN	2.2
1	A	159	GLU	2.2
1	E	150	ILE	2.2
1	F	81	GLY	2.2
1	E	81	GLY	2.2
1	C	136	ILE	2.1
1	D	172	PHE	2.1
1	F	44	ARG	2.1
1	F	120	LYS	2.1
1	F	41	LYS	2.1
1	D	1	ALA	2.1
1	E	158	SER	2.1
1	E	89	TYR	2.1
1	F	173	GLU	2.1
1	B	155	ASP	2.1
1	A	150	ILE	2.0
1	F	52	ASN	2.0
1	F	158	SER	2.0
1	C	93	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

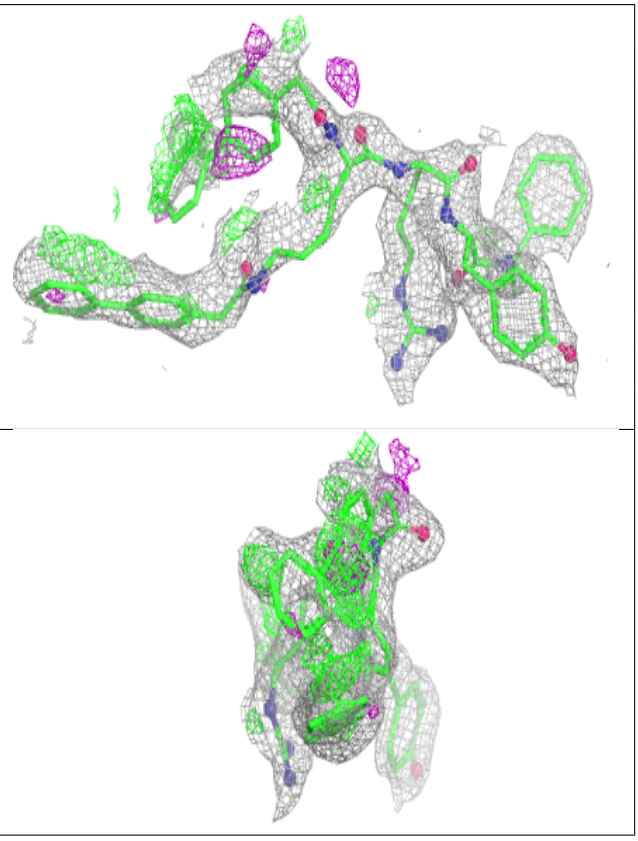
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NSX	E	700	71/71	0.72	0.36	22,43,66,69	0
2	NSX	F	800	71/71	0.73	0.36	22,43,66,69	0
2	NSX	B	300	71/71	0.75	0.39	22,43,66,69	0
2	NSX	A	400	71/71	0.76	0.36	22,43,66,69	0
2	NSX	C	500	71/71	0.76	0.36	22,43,66,69	0
2	NSX	D	600	71/71	0.77	0.33	22,43,66,69	0

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

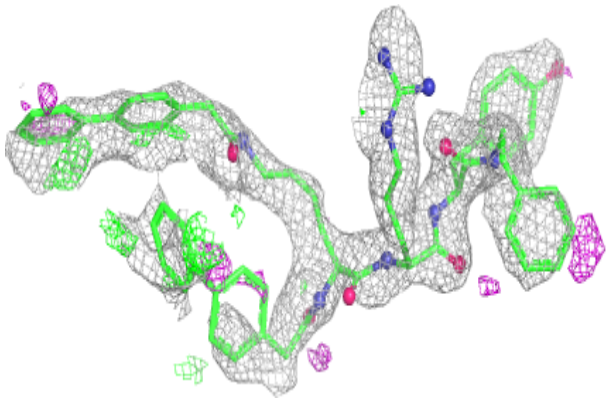
Electron density around NSX E 700:

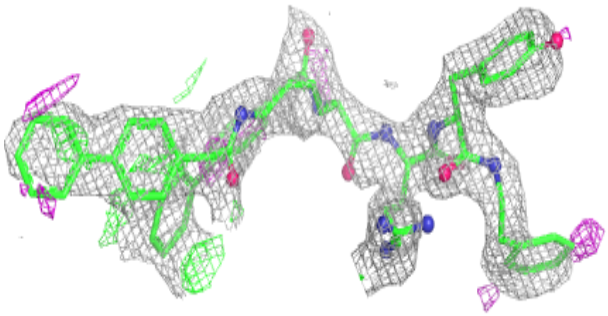
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

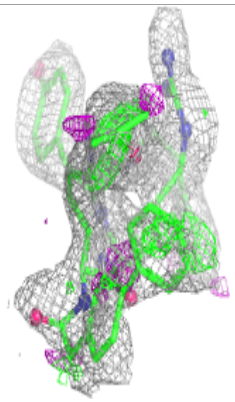


Electron density around NSX F 800:

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

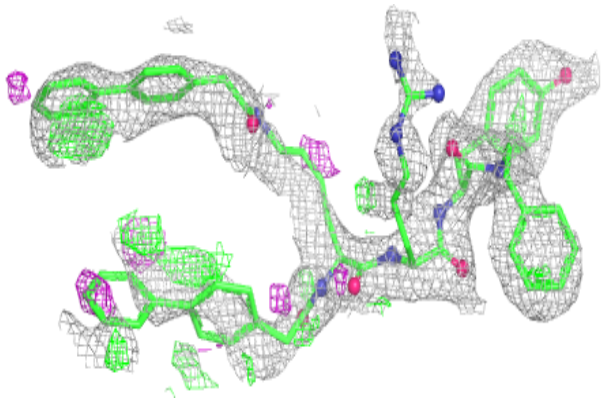


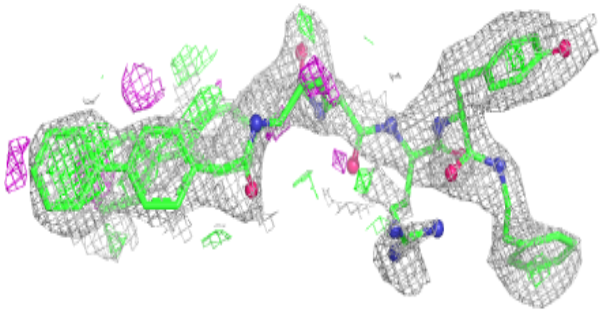


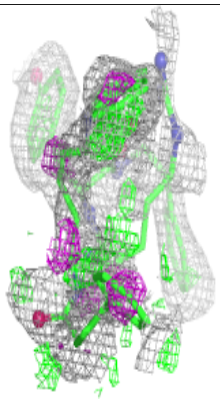


Electron density around NSX B 300:

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

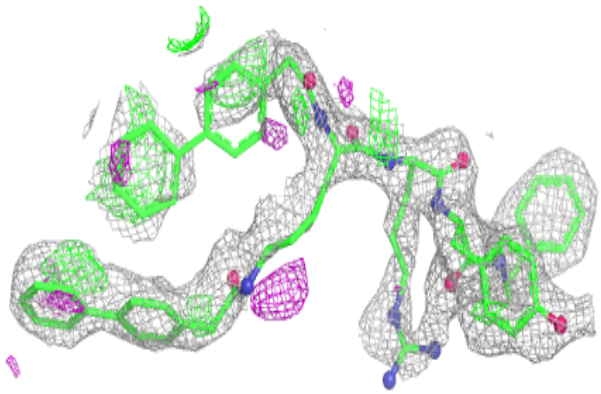


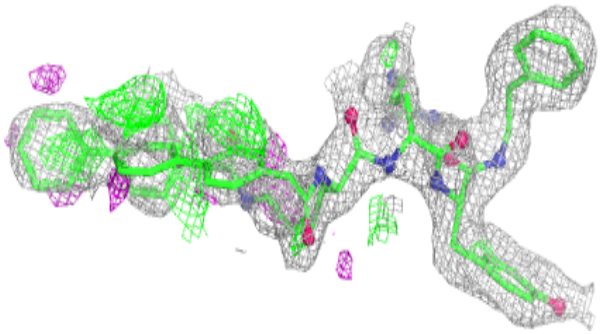


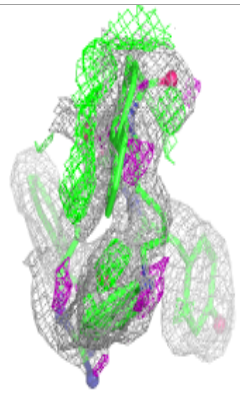


Electron density around NSX A 400:

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

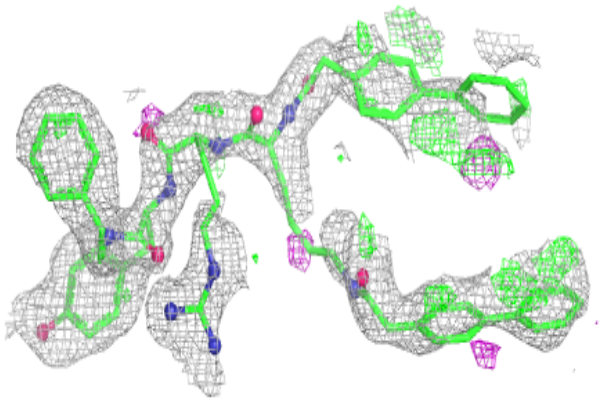


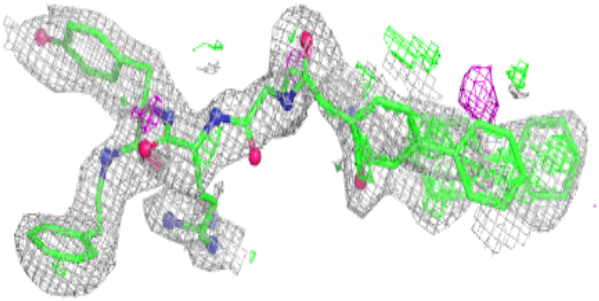


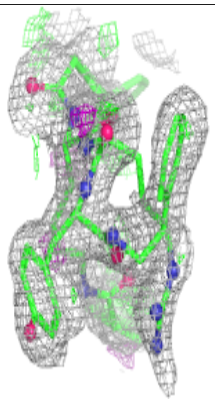


Electron density around NSX C 500:

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

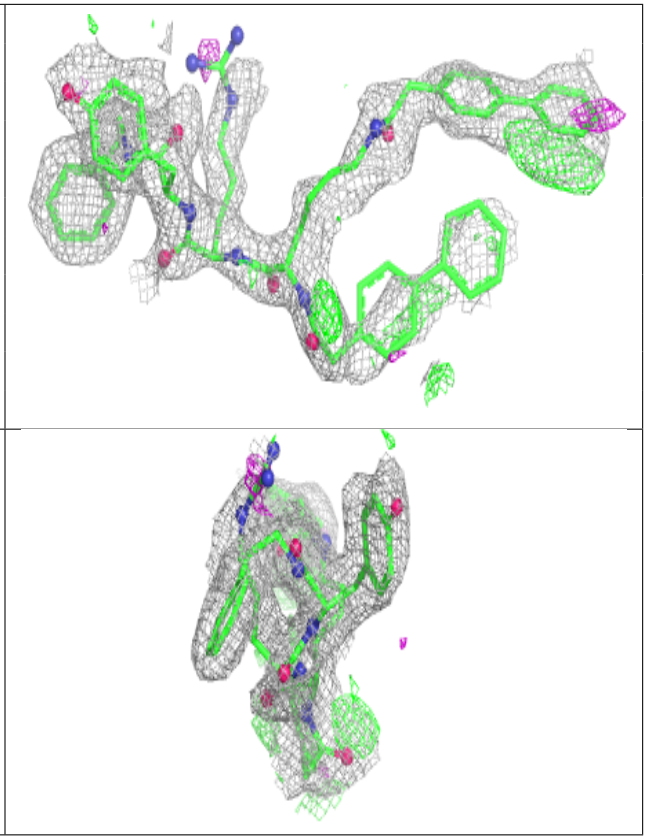






Electron density around NSX D 600:

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



6.5 Other polymers (i)

There are no such residues in this entry.