Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 01:53 AM EDT

PDB ID	:	2GDD
Title	:	Human beta II tryptase with inhibitor CRA-27592
Authors	:	Somoza, J.R.
Deposited on	:	2006-03-15
Resolution	:	2.35 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:

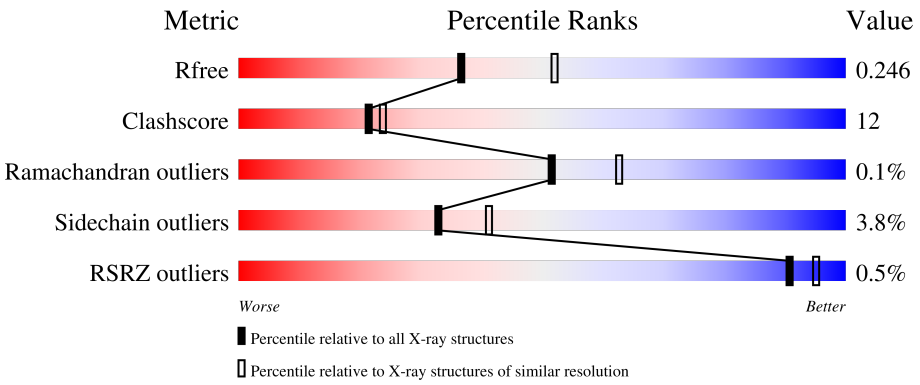
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	245	77% 20% • •
1	B	245	% 76% 21% • •
1	C	245	66% 31% • •
1	D	245	% 72% 26% • •

2 Entry composition (i)

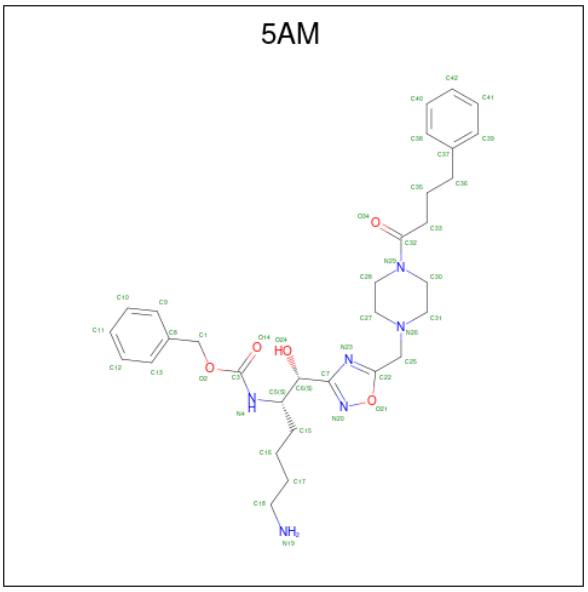
There are 3 unique types of molecules in this entry. The entry contains 7984 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tryptase beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	1920	1230	338	340	12	0	0	0
1	B	243	1920	1230	338	340	12	0	0	0
1	C	243	1920	1230	338	340	12	0	0	0
1	D	243	1920	1230	338	340	12	0	0	0

- Molecule 2 is BENZYL {(1S)-5-AMINO-1-[(S)-HYDROXY(5-{[4-(4-PHENYLBUTANOYL)PIPERAZIN-1-YL]METHYL}-1,2,4-OXADIAZOL-3-YL)METHYL]PENTYL}CARBAMATE (three-letter code: 5AM) (formula: $C_{31}H_{42}N_6O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	42	31	6	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	42	31	6	5	0	0
2	C	1	42	31	6	5	0	0
2	D	1	42	31	6	5	0	0

- Molecule 3 is water.

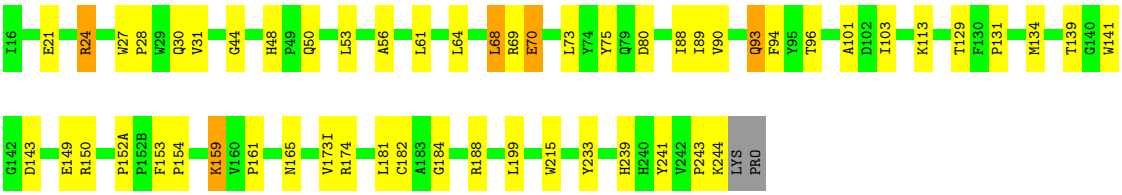
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	43	43	43	0	0
3	B	25	25	25	0	0
3	C	44	44	44	0	0
3	D	24	24	24	0	0

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.

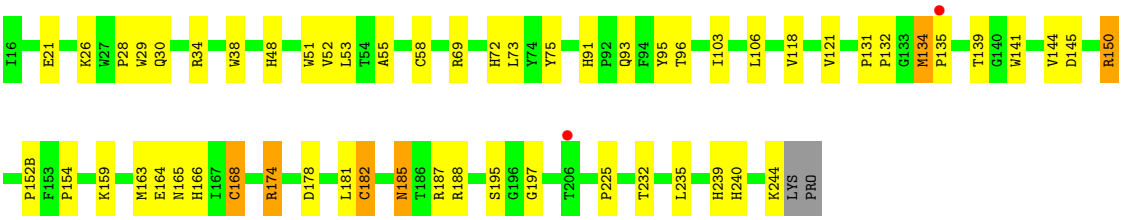
• Molecule 1: Tryptase beta-2

Chain A:



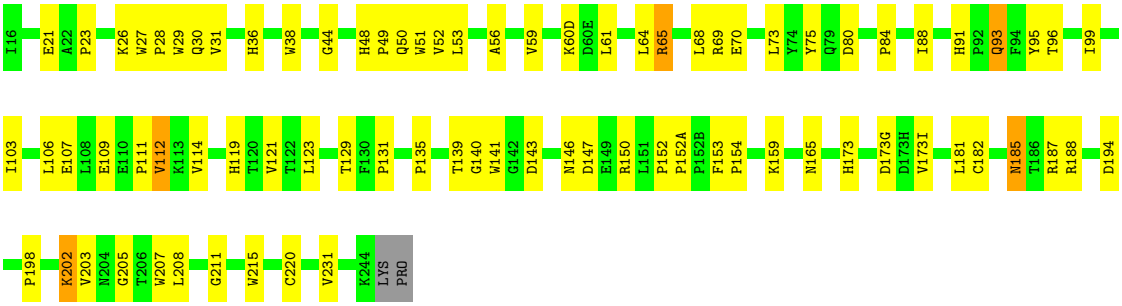
• Molecule 1: Tryptase beta-2

Chain B:



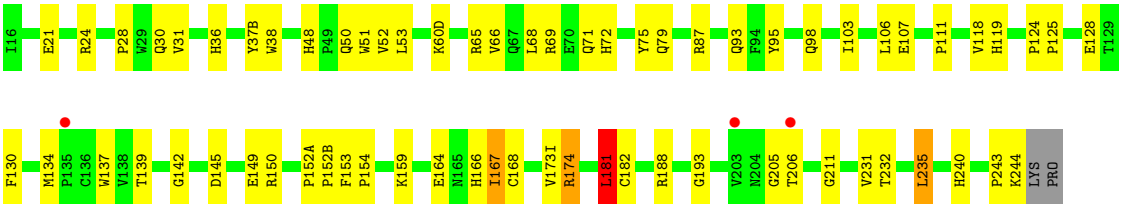
• Molecule 1: Tryptase beta-2

Chain C:



• Molecule 1: Tryptase beta-2

Chain D:


I16
E21
R24
P28
W29
Q30
V31
H36
Y37B
W38
H48
P49
Q50
W51
V52
L53
K60D
R65
V66
Q67
L68
R69
E70
Q71
H72
Y75
Q79
R87
Q93
F94
Y95
Q98
I103
L106
E107
P111
V118
H119
P124
P125
E128
T129
F130
M134
P135
C136
W137
V138
T139
G142
D145
E149
R150
P152A
P152B
F153
P154
K159
E164
N165
H166
I167
C168
V173I
R174
L181
C182
R188
G193
V203
N204
G205
T206
G211
V231
T232
L235
H240
P243
K244
LYS
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	78.02Å 78.02Å 163.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.70 – 2.35 19.74 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.4 (19.70-2.35) 93.5 (19.74-2.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.35Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.254 0.206 , 0.246	Depositor DCC
R_{free} test set	4662 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 11.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l 0.478 for h,-h-k,-l 0.010 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7984	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 4.08% 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: 5AM

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	0.37	0/1985	0.65	0/2720
1	B	0.36	0/1985	0.65	0/2720
1	C	0.36	0/1985	0.64	0/2720
1	D	0.37	0/1985	0.76	3/2720 (0.1%)
All	All	0.37	0/7940	0.68	3/10880 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	87	ARG	NE-CZ-NH1	-15.45	112.58	120.30
1	D	87	ARG	NE-CZ-NH2	13.73	127.16	120.30
1	D	181	LEU	CA-CB-CG	5.43	127.78	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	95	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	D	95	TYR	Sidechain

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	1920	0	1854	43	0
1	B	1920	0	1854	45	0
1	C	1920	0	1854	56	0
1	D	1920	0	1854	48	0
2	A	42	0	41	1	0
2	B	42	0	41	0	0
2	C	42	0	41	1	0
2	D	42	0	41	0	0
3	A	43	0	0	1	0
3	B	25	0	0	2	0
3	C	44	0	0	1	0
3	D	24	0	0	3	0
All	All	7984	0	7580	185	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 12.

All (185) 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:A:24:ARG:HH11	1:A:24:ARG:HB3	1.27	0.99
1:B:239:HIS:HB3	1:B:244:LYS:HE2	1.44	0.99
1:B:185:ASN:ND2	1:B:188:ARG:H	1.69	0.90
1:C:61:LEU:HD21	1:C:88:ILE:HG13	1.54	0.87
1:C:135:PRO:HA	3:C:1029:HOH:O	1.76	0.84
1:B:163:MET:HB2	1:B:182:CYS:SG	2.18	0.82
1:B:91:HIS:HD2	1:B:93:GLN:H	1.26	0.82
1:B:21:GLU:HG3	1:B:154:PRO:HB2	1.65	0.78
1:B:174:ARG:HH11	1:B:174:ARG:HG2	1.49	0.78
1:A:93:GLN:HE21	1:A:93:GLN:HA	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:THR:HG23	1:C:131:PRO:HD3	1.69	0.74
1:A:24:ARG:HB3	1:A:24:ARG:NH1	2.01	0.74
1:C:203:VAL:HG21	1:C:208:LEU:HD12	1.69	0.73
1:A:61:LEU:HD21	1:A:88:ILE:HG12	1.71	0.72
1:C:202:LYS:HE3	1:C:205:GLY:HA2	1.71	0.72
1:A:61:LEU:CD2	1:A:88:ILE:HG12	2.20	0.72
1:B:134:MET:SD	1:B:135:PRO:HD2	2.30	0.70
1:A:129:THR:HG23	1:A:131:PRO:HD3	1.72	0.70
1:C:146:ASN:HD21	1:C:220:CYS:H	1.37	0.70
1:A:21:GLU:HG3	1:A:154:PRO:HB2	1.74	0.70
1:D:164:GLU:O	1:D:167:ILE:HG22	1.93	0.69
1:B:174:ARG:HG2	1:B:174:ARG:NH1	2.05	0.69
1:D:181:LEU:HD12	1:D:182:CYS:N	2.10	0.67
1:B:185:ASN:HD21	1:B:188:ARG:H	1.43	0.67
1:C:114:VAL:HG13	1:C:119:HIS:HB3	1.76	0.65
1:D:181:LEU:HD12	1:D:181:LEU:C	2.16	0.65
1:A:159:LYS:O	1:A:188:ARG:HD3	1.98	0.64
1:C:143:ASP:OD1	1:C:150:ARG:HD3	1.98	0.63
1:D:69:ARG:HH22	1:D:71:GLN:NE2	1.97	0.63
1:C:61:LEU:CD2	1:C:88:ILE:HG13	2.27	0.62
1:A:53:LEU:HD11	1:A:103:ILE:HD11	1.82	0.61
1:C:185:ASN:ND2	1:C:188:ARG:H	1.99	0.61
1:A:64:LEU:CD2	1:A:88:ILE:HD11	2.30	0.60
1:D:145:ASP:HB3	1:D:149:GLU:HG2	1.83	0.59
1:A:48:HIS:HD2	1:A:50:GLN:H	1.49	0.59
1:B:93:GLN:HA	1:C:173(I):VAL:HG21	1.83	0.58
1:B:69:ARG:HD2	3:B:1013:HOH:O	2.03	0.58
1:B:118:VAL:HG23	1:B:118:VAL:O	2.04	0.58
1:A:31:VAL:HG22	1:A:44:GLY:C	2.24	0.58
1:B:174:ARG:NH1	3:B:1002:HOH:O	2.37	0.58
1:B:181:LEU:HD23	1:B:182:CYS:N	2.18	0.58
1:D:48:HIS:HD2	1:D:50:GLN:H	1.52	0.58
1:D:53:LEU:HD11	1:D:103:ILE:HD11	1.86	0.57
1:D:167:ILE:O	1:D:167:ILE:HD13	2.04	0.57
1:A:131:PRO:HD2	1:A:134:MET:CE	2.35	0.57
1:C:31:VAL:HG22	1:C:44:GLY:C	2.25	0.57
1:C:150:ARG:HG2	1:C:150:ARG:HH11	1.69	0.56
1:D:48:HIS:CD2	1:D:50:GLN:H	2.23	0.56
1:C:185:ASN:C	1:C:185:ASN:HD22	2.09	0.56
1:C:48:HIS:HD2	1:C:50:GLN:H	1.52	0.56
1:C:150:ARG:HG2	1:C:150:ARG:NH1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLU:OE1	1:A:80:ASP:OD1	2.25	0.55
1:D:30:GLN:NE2	1:D:139:THR:OG1	2.40	0.54
1:C:114:VAL:HG13	1:C:119:HIS:CB	2.38	0.54
1:D:150:ARG:HG2	3:D:1009:HOH:O	2.07	0.54
1:B:30:GLN:NE2	1:B:139:THR:OG1	2.40	0.53
1:A:48:HIS:CD2	1:A:50:GLN:H	2.27	0.53
1:C:140:GLY:HA3	1:C:194:ASP:OD1	2.09	0.53
1:A:56:ALA:HB2	1:A:103:ILE:O	2.09	0.53
1:D:72:HIS:HB3	1:D:152(B):PRO:O	2.09	0.52
1:A:96:THR:HG21	1:D:98:GLN:HG2	1.91	0.52
1:C:52:VAL:HB	1:C:106:LEU:HB2	1.91	0.52
1:C:173:HIS:CD2	1:C:173(G):ASP:HA	2.44	0.52
1:C:152:PRO:HB3	1:D:37(B):TYR:CD1	2.45	0.51
1:B:174:ARG:HH22	1:B:178:ASP:CG	2.14	0.51
1:A:27:TRP:N	1:A:28:PRO:HD3	2.25	0.51
1:B:53:LEU:HD11	1:B:103:ILE:HD11	1.92	0.51
1:C:36:HIS:HD2	1:C:38:TRP:CZ2	2.29	0.50
1:B:185:ASN:C	1:B:185:ASN:HD22	2.14	0.50
1:B:185:ASN:HD21	1:B:188:ARG:N	2.06	0.50
1:B:240:HIS:O	1:B:240:HIS:ND1	2.44	0.50
1:C:59:VAL:O	1:C:60(D):LYS:HE2	2.12	0.50
1:D:69:ARG:HB3	1:D:118:VAL:HG22	1.92	0.50
1:A:131:PRO:HD2	1:A:134:MET:HE2	1.93	0.50
1:B:185:ASN:HD22	1:B:188:ARG:H	1.51	0.49
1:B:91:HIS:CD2	1:B:93:GLN:H	2.18	0.49
1:B:131:PRO:O	1:B:134:MET:HB2	2.12	0.49
1:C:50:GLN:HG2	1:C:111:PRO:HA	1.94	0.49
1:D:60(D):LYS:HE3	3:D:1003:HOH:O	2.11	0.49
1:D:159:LYS:O	1:D:188:ARG:HD3	2.12	0.49
1:C:84:PRO:HB2	1:C:109:GLU:OE2	2.11	0.49
1:C:202:LYS:HG2	1:C:207:TRP:CE2	2.48	0.49
1:B:144:VAL:O	1:B:145:ASP:HB2	2.13	0.49
1:B:52:VAL:HB	1:B:106:LEU:HB2	1.95	0.48
1:C:181:LEU:HD23	1:C:182:CYS:N	2.28	0.48
1:B:168:CYS:SG	1:B:225:PRO:CG	3.02	0.48
1:C:185:ASN:ND2	1:C:187:ARG:H	2.11	0.48
1:C:185:ASN:HD22	1:C:188:ARG:H	1.60	0.48
1:D:232:THR:HA	1:D:235:LEU:HD22	1.95	0.48
1:D:211:GLY:HA2	1:D:231:VAL:HG23	1.94	0.48
1:C:53:LEU:HD11	1:C:103:ILE:HD11	1.96	0.48
1:D:50:GLN:OE1	1:D:111:PRO:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:GLU:OE2	1:B:166:HIS:HB3	2.14	0.47
1:C:21:GLU:HG3	1:C:154:PRO:HB2	1.96	0.47
1:C:147:ASP:C	1:C:150:ARG:HH12	2.18	0.47
1:D:124:PRO:O	1:D:235:LEU:HD21	2.14	0.47
1:A:56:ALA:HB1	1:A:90:VAL:HG13	1.97	0.47
1:C:73:LEU:HG	1:C:141:TRP:CD1	2.50	0.47
1:C:75:TYR:CE2	1:D:75:TYR:HB2	2.49	0.47
1:D:52:VAL:HB	1:D:106:LEU:HB2	1.95	0.47
1:A:24:ARG:HH11	1:A:24:ARG:CB	2.11	0.47
1:C:29:TRP:CG	1:C:121:VAL:HB	2.50	0.47
1:D:181:LEU:CD1	1:D:182:CYS:N	2.77	0.47
1:C:51:TRP:CZ3	1:C:107:GLU:HB2	2.50	0.46
1:C:211:GLY:HA2	1:C:231:VAL:HG23	1.97	0.46
1:C:28:PRO:HG3	1:C:119:HIS:CE1	2.50	0.46
1:D:21:GLU:HG3	1:D:154:PRO:HB2	1.98	0.46
1:B:48:HIS:HB3	1:B:51:TRP:HB2	1.98	0.46
1:D:31:VAL:CG1	1:D:66:VAL:HG13	2.46	0.46
1:D:48:HIS:HB3	1:D:51:TRP:HB2	1.97	0.46
1:D:152(A):PRO:HG3	1:D:153:PHE:CZ	2.51	0.46
1:C:135:PRO:HB3	1:C:159:LYS:HD2	1.98	0.46
1:C:56:ALA:HB2	1:C:103:ILE:O	2.16	0.45
1:D:36:HIS:HB2	1:D:38:TRP:CH2	2.51	0.45
1:A:30:GLN:NE2	1:A:139:THR:OG1	2.49	0.45
1:B:55:ALA:O	1:B:58:CYS:HB2	2.16	0.45
1:B:29:TRP:CG	1:B:121:VAL:HB	2.51	0.45
1:A:48:HIS:CE1	1:A:243:PRO:HG2	2.52	0.45
1:A:64:LEU:HD23	1:A:88:ILE:HD11	1.99	0.45
1:B:187:ARG:HH11	1:B:187:ARG:HG3	1.81	0.45
1:C:48:HIS:CD2	1:C:50:GLN:H	2.32	0.45
1:D:240:HIS:O	1:D:240:HIS:ND1	2.49	0.45
1:B:72:HIS:HB3	1:B:152(B):PRO:O	2.17	0.45
1:B:150:ARG:HD2	1:B:150:ARG:H	1.81	0.45
1:D:24:ARG:HA	1:D:71:GLN:NE2	2.32	0.45
1:A:181:LEU:C	1:A:181:LEU:HD23	2.37	0.45
1:D:79:GLN:NE2	1:D:79:GLN:HA	2.32	0.45
1:D:181:LEU:C	1:D:181:LEU:CD1	2.84	0.45
1:C:70:GLU:OE1	1:C:80:ASP:OD1	2.35	0.44
1:C:215:TRP:HA	2:C:997:5AM:H161	1.99	0.44
1:D:137:TRP:CZ2	1:D:159:LYS:HE3	2.52	0.44
1:A:68:LEU:O	1:A:69:ARG:C	2.55	0.44
1:A:161:PRO:HD2	1:A:184:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:HD23	1:A:182:CYS:N	2.33	0.43
1:C:152(A):PRO:HG3	1:C:153:PHE:CZ	2.54	0.43
1:C:30:GLN:NE2	1:C:139:THR:OG1	2.51	0.43
1:C:91:HIS:CE1	1:C:93:GLN:HB2	2.54	0.43
1:C:203:VAL:CG2	1:C:208:LEU:HD12	2.45	0.43
1:D:28:PRO:HG3	1:D:119:HIS:CE1	2.53	0.43
1:A:215:TRP:HA	2:A:999:5AM:H161	2.00	0.43
1:B:168:CYS:SG	1:B:225:PRO:HG2	2.59	0.43
1:B:185:ASN:ND2	1:B:188:ARG:N	2.50	0.43
1:C:50:GLN:HG2	1:C:111:PRO:CA	2.49	0.43
1:D:164:GLU:OE2	1:D:166:HIS:HB3	2.19	0.43
1:A:93:GLN:HA	1:A:93:GLN:NE2	2.28	0.42
1:C:49:PRO:O	1:C:112:VAL:HG13	2.20	0.42
1:D:142:GLY:HA2	1:D:193:GLY:HA3	2.00	0.42
1:A:24:ARG:HG3	3:A:1041:HOH:O	2.18	0.42
1:A:61:LEU:HD23	1:A:88:ILE:HG12	1.99	0.42
1:A:73:LEU:HG	1:A:141:TRP:CD1	2.55	0.42
1:B:195:SER:C	1:B:197:GLY:H	2.22	0.42
1:A:233:TYR:CD1	1:A:233:TYR:O	2.73	0.42
1:C:27:TRP:CD1	1:C:139:THR:HG21	2.55	0.42
1:A:131:PRO:HD2	1:A:134:MET:HE1	1.99	0.42
1:D:205:GLY:O	1:D:206:THR:HG23	2.20	0.42
1:A:93:GLN:NE2	1:D:173(I):VAL:HG22	2.35	0.42
1:A:152(A):PRO:HA	1:A:153:PHE:N	2.35	0.42
1:D:31:VAL:HG22	1:D:68:LEU:HD23	2.02	0.42
1:D:124:PRO:HB3	1:D:130:PHE:HZ	1.85	0.42
1:A:239:HIS:CG	1:A:244:LYS:HE2	2.55	0.42
1:B:159:LYS:O	1:B:188:ARG:HD3	2.19	0.41
1:C:29:TRP:CD2	1:C:121:VAL:HB	2.55	0.41
1:B:232:THR:HA	1:B:235:LEU:HG	2.02	0.41
1:A:75:TYR:HB2	1:B:75:TYR:CE1	2.55	0.41
1:D:51:TRP:CZ3	1:D:107:GLU:HB2	2.56	0.41
1:A:173(I):VAL:HG21	1:D:93:GLN:HA	2.02	0.41
1:B:95:TYR:CD2	1:B:96:THR:HG23	2.55	0.41
1:D:60(D):LYS:CE	3:D:1003:HOH:O	2.69	0.41
1:A:94:PHE:HB2	1:A:101:ALA:O	2.21	0.41
1:B:29:TRP:CD2	1:B:121:VAL:HB	2.56	0.41
1:B:73:LEU:HG	1:B:141:TRP:CD1	2.55	0.41
1:C:96:THR:OG1	1:C:99:ILE:HG13	2.21	0.41
1:D:125:PRO:HD2	1:D:128:GLU:HB2	2.02	0.41
1:B:28:PRO:HA	1:B:69:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ARG:HD2	1:B:38:TRP:O	2.21	0.41
1:B:131:PRO:HA	1:B:132:PRO:HD3	1.87	0.40
1:C:23:PRO:HG2	1:C:26:LYS:HG3	2.03	0.40
1:D:174:ARG:HB3	1:D:174:ARG:HH21	1.86	0.40
1:C:68:LEU:O	1:C:69:ARG:C	2.59	0.40
1:A:143:ASP:OD2	1:A:150:ARG:NH1	2.51	0.40
1:C:64:LEU:O	1:C:65:ARG:HG2	2.21	0.40
1:D:51:TRP:CH2	1:D:107:GLU:HB2	2.56	0.40
1:A:89:ILE:HD13	1:A:241:TYR:CD1	2.56	0.40
1:C:30:GLN:HE22	1:C:198:PRO:HD2	1.86	0.40
1:D:38:TRP:CZ3	1:D:65:ARG:HG2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	241/245 (98%)	228 (95%)	13 (5%)	0	100	100
1	B	241/245 (98%)	226 (94%)	15 (6%)	0	100	100
1	C	241/245 (98%)	222 (92%)	19 (8%)	0	100	100
1	D	241/245 (98%)	224 (93%)	16 (7%)	1 (0%)	34	38
All	All	964/980 (98%)	900 (93%)	63 (6%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	243	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/210 (99%)	198 (95%)	10 (5%)	25	30
1	B	208/210 (99%)	200 (96%)	8 (4%)	33	41
1	C	208/210 (99%)	201 (97%)	7 (3%)	37	46
1	D	208/210 (99%)	201 (97%)	7 (3%)	37	46
All	All	832/840 (99%)	800 (96%)	32 (4%)	33	41

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	68	LEU
1	A	70	GLU
1	A	93	GLN
1	A	113	LYS
1	A	149	GLU
1	A	159	LYS
1	A	165	ASN
1	A	174	ARG
1	A	199	LEU
1	B	26	LYS
1	B	134	MET
1	B	150	ARG
1	B	165	ASN
1	B	168	CYS
1	B	174	ARG
1	B	182	CYS
1	B	185	ASN
1	C	65	ARG
1	C	93	GLN
1	C	112	VAL
1	C	123	LEU
1	C	165	ASN
1	C	185	ASN

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Mol	Chain	Res	Type
1	C	202	LYS
1	D	134	MET
1	D	167	ILE
1	D	168	CYS
1	D	174	ARG
1	D	181	LEU
1	D	235	LEU
1	D	244	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	48	HIS
1	A	93	GLN
1	A	119	HIS
1	A	165	ASN
1	A	223	ASN
1	B	20	GLN
1	B	30	GLN
1	B	50	GLN
1	B	91	HIS
1	B	185	ASN
1	B	204	ASN
1	B	221(A)	GLN
1	C	30	GLN
1	C	36	HIS
1	C	48	HIS
1	C	72	HIS
1	C	79	GLN
1	C	119	HIS
1	C	146	ASN
1	C	165	ASN
1	C	185	ASN
1	C	221(A)	GLN
1	C	223	ASN
1	D	30	GLN
1	D	48	HIS
1	D	71	GLN
1	D	79	GLN
1	D	93	GLN
1	D	119	HIS

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Mol	Chain	Res	Type
1	D	223	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	5AM	A	999	1	40,45,45	2.46	20 (50%)	51,58,58	1.74	5 (9%)
2	5AM	B	998	1	40,45,45	2.40	21 (52%)	51,58,58	1.79	7 (13%)
2	5AM	C	997	1	40,45,45	2.48	20 (50%)	51,58,58	1.76	8 (15%)
2	5AM	D	996	1	40,45,45	2.47	21 (52%)	51,58,58	1.81	8 (15%)

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	5AM	A	999	1	-	8/31/46/46	0/4/4/4
2	5AM	B	998	1	-	6/31/46/46	0/4/4/4
2	5AM	C	997	1	-	6/31/46/46	0/4/4/4
2	5AM	D	996	1	-	6/31/46/46	0/4/4/4

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	997	5AM	C32-N29	5.86	1.46	1.35
2	A	999	5AM	C32-N29	5.61	1.46	1.35
2	D	996	5AM	C32-N29	5.51	1.45	1.35
2	B	998	5AM	C32-N29	5.50	1.45	1.35
2	D	996	5AM	C3-N4	4.23	1.45	1.34
2	A	999	5AM	C13-C8	4.21	1.47	1.38
2	D	996	5AM	C9-C8	4.20	1.47	1.38
2	A	999	5AM	C9-C8	4.17	1.47	1.38
2	B	998	5AM	C13-C8	4.14	1.47	1.38
2	A	999	5AM	C10-C9	4.13	1.46	1.38
2	B	998	5AM	C10-C9	4.12	1.46	1.38
2	C	997	5AM	C9-C8	4.11	1.47	1.38
2	D	996	5AM	C10-C9	4.10	1.45	1.38
2	B	998	5AM	C3-N4	4.07	1.44	1.34
2	A	999	5AM	C3-N4	4.07	1.44	1.34
2	D	996	5AM	C6-C5	4.06	1.58	1.53
2	C	997	5AM	C13-C8	4.02	1.46	1.38
2	C	997	5AM	C10-C9	4.01	1.45	1.38
2	B	998	5AM	C12-C13	4.01	1.45	1.38
2	D	996	5AM	C13-C8	4.00	1.46	1.38
2	B	998	5AM	C9-C8	3.99	1.46	1.38
2	C	997	5AM	C3-N4	3.98	1.44	1.34
2	A	999	5AM	C12-C13	3.95	1.45	1.38
2	A	999	5AM	C6-C5	3.92	1.58	1.53
2	C	997	5AM	C12-C13	3.85	1.45	1.38
2	C	997	5AM	C6-C5	3.80	1.58	1.53
2	D	996	5AM	C12-C13	3.73	1.45	1.38
2	C	997	5AM	C11-C10	3.61	1.46	1.38
2	B	998	5AM	C6-C5	3.58	1.57	1.53
2	B	998	5AM	C11-C10	3.52	1.46	1.38
2	A	999	5AM	C11-C10	3.50	1.45	1.38
2	D	996	5AM	C11-C10	3.45	1.45	1.38
2	C	997	5AM	C25-C22	-3.13	1.47	1.51
2	D	996	5AM	C25-C22	-2.99	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	997	5AM	C30-N29	2.95	1.52	1.47
2	A	999	5AM	C25-C22	-2.95	1.47	1.51
2	B	998	5AM	C25-C22	-2.92	1.47	1.51
2	D	996	5AM	C38-C37	2.92	1.44	1.38
2	A	999	5AM	C30-N29	2.89	1.52	1.47
2	C	997	5AM	C28-N29	2.82	1.52	1.47
2	C	997	5AM	C38-C37	2.80	1.44	1.38
2	B	998	5AM	C30-N29	2.78	1.52	1.47
2	C	997	5AM	C12-C11	2.78	1.44	1.38
2	C	997	5AM	C39-C37	2.77	1.44	1.38
2	A	999	5AM	C12-C11	2.75	1.44	1.38
2	D	996	5AM	C39-C37	2.74	1.44	1.38
2	A	999	5AM	C39-C37	2.73	1.44	1.38
2	D	996	5AM	C30-N29	2.70	1.51	1.47
2	D	996	5AM	C15-C5	2.67	1.58	1.52
2	D	996	5AM	C12-C11	2.66	1.44	1.38
2	B	998	5AM	C39-C37	2.64	1.44	1.38
2	D	996	5AM	C41-C39	2.63	1.43	1.38
2	A	999	5AM	C28-N29	2.58	1.51	1.47
2	D	996	5AM	C42-C41	2.58	1.43	1.38
2	C	997	5AM	C41-C39	2.57	1.43	1.38
2	A	999	5AM	C38-C37	2.56	1.44	1.38
2	B	998	5AM	C12-C11	2.56	1.43	1.38
2	C	997	5AM	C42-C41	2.53	1.43	1.38
2	A	999	5AM	C41-C39	2.51	1.43	1.38
2	B	998	5AM	C41-C39	2.47	1.43	1.38
2	D	996	5AM	C31-N26	2.46	1.53	1.46
2	B	998	5AM	C38-C37	2.46	1.43	1.38
2	A	999	5AM	C42-C41	2.40	1.43	1.38
2	B	998	5AM	C28-N29	2.38	1.51	1.47
2	C	997	5AM	C27-N26	2.37	1.53	1.46
2	C	997	5AM	C40-C38	2.35	1.42	1.38
2	B	998	5AM	C42-C41	2.34	1.43	1.38
2	D	996	5AM	C40-C38	2.32	1.42	1.38
2	C	997	5AM	C31-N26	2.32	1.53	1.46
2	C	997	5AM	C42-C40	2.32	1.43	1.38
2	A	999	5AM	C40-C38	2.31	1.42	1.38
2	D	996	5AM	C42-C40	2.28	1.43	1.38
2	A	999	5AM	C31-N26	2.28	1.53	1.46
2	A	999	5AM	C27-N26	2.25	1.53	1.46
2	B	998	5AM	C27-N26	2.25	1.53	1.46
2	B	998	5AM	C31-N26	2.19	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	998	5AM	C40-C38	2.17	1.42	1.38
2	B	998	5AM	C42-C40	2.13	1.42	1.38
2	A	999	5AM	C42-C40	2.12	1.42	1.38
2	D	996	5AM	C27-N26	2.09	1.52	1.46
2	D	996	5AM	C28-N29	2.05	1.50	1.47
2	B	998	5AM	C33-C32	-2.04	1.47	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	996	5AM	C1-O2-C3	8.27	134.55	115.93
2	A	999	5AM	C1-O2-C3	8.13	134.23	115.93
2	B	998	5AM	C1-O2-C3	7.98	133.88	115.93
2	C	997	5AM	C1-O2-C3	7.39	132.58	115.93
2	C	997	5AM	C33-C32-N29	5.78	126.84	118.09
2	B	998	5AM	C33-C32-N29	5.57	126.53	118.09
2	D	996	5AM	C33-C32-N29	5.42	126.29	118.09
2	A	999	5AM	C33-C32-N29	5.41	126.29	118.09
2	A	999	5AM	C22-C25-N26	3.37	118.29	113.48
2	C	997	5AM	C22-C25-N26	3.36	118.28	113.48
2	C	997	5AM	O34-C32-C33	-3.30	112.32	121.26
2	C	997	5AM	O14-C3-N4	-3.25	119.54	124.86
2	B	998	5AM	C7-C6-C5	3.24	114.91	111.26
2	D	996	5AM	C7-C6-C5	3.21	114.87	111.26
2	B	998	5AM	O14-C3-N4	-3.14	119.72	124.86
2	B	998	5AM	O34-C32-C33	-3.13	112.78	121.26
2	A	999	5AM	O34-C32-C33	-3.12	112.81	121.26
2	D	996	5AM	O34-C32-C33	-3.01	113.11	121.26
2	A	999	5AM	O14-C3-N4	-2.91	120.09	124.86
2	B	998	5AM	C22-C25-N26	2.88	117.58	113.48
2	C	997	5AM	C7-C6-C5	2.73	114.34	111.26
2	D	996	5AM	O14-C3-N4	-2.69	120.45	124.86
2	D	996	5AM	C22-C25-N26	2.59	117.18	113.48
2	C	997	5AM	C15-C5-N4	-2.39	107.21	110.30
2	D	996	5AM	C15-C5-N4	-2.25	107.39	110.30
2	D	996	5AM	C27-C28-N29	-2.20	106.05	110.42
2	C	997	5AM	O2-C3-N4	2.08	114.91	110.45
2	B	998	5AM	C15-C5-N4	-2.03	107.67	110.30

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	999	5AM	C33-C32-N29-C30
2	A	999	5AM	O34-C32-N29-C30
2	A	999	5AM	C33-C32-N29-C28
2	A	999	5AM	O34-C32-N29-C28
2	B	998	5AM	C33-C32-N29-C30
2	B	998	5AM	O34-C32-N29-C30
2	B	998	5AM	C33-C32-N29-C28
2	C	997	5AM	C33-C32-N29-C30
2	D	996	5AM	C33-C32-N29-C30
2	D	996	5AM	O34-C32-N29-C30
2	B	998	5AM	O34-C32-N29-C28
2	C	997	5AM	O34-C32-N29-C30
2	C	997	5AM	O34-C32-N29-C28
2	D	996	5AM	O34-C32-N29-C28
2	C	997	5AM	C33-C32-N29-C28
2	D	996	5AM	C33-C32-N29-C28
2	B	998	5AM	C8-C1-O2-C3
2	A	999	5AM	N29-C32-C33-C35
2	A	999	5AM	O34-C32-C33-C35
2	C	997	5AM	C32-C33-C35-C36
2	C	997	5AM	N4-C5-C6-O24
2	A	999	5AM	C32-C33-C35-C36
2	D	996	5AM	C32-C33-C35-C36
2	A	999	5AM	C8-C1-O2-C3
2	D	996	5AM	N29-C32-C33-C35
2	B	998	5AM	N4-C5-C6-O24

There are no ring outliers.

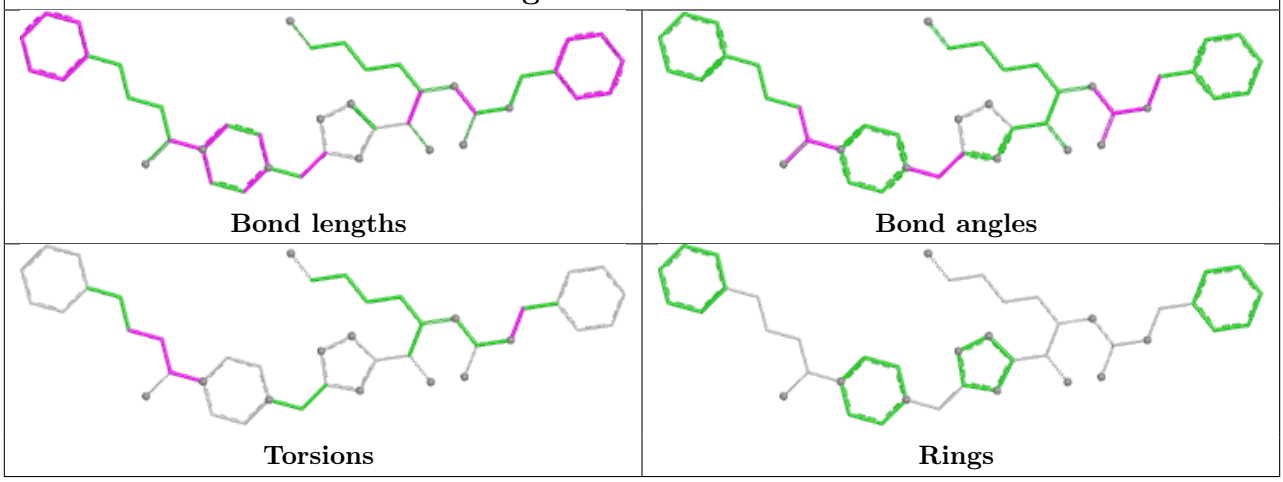
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	5AM	1	0
2	C	997	5AM	1	0

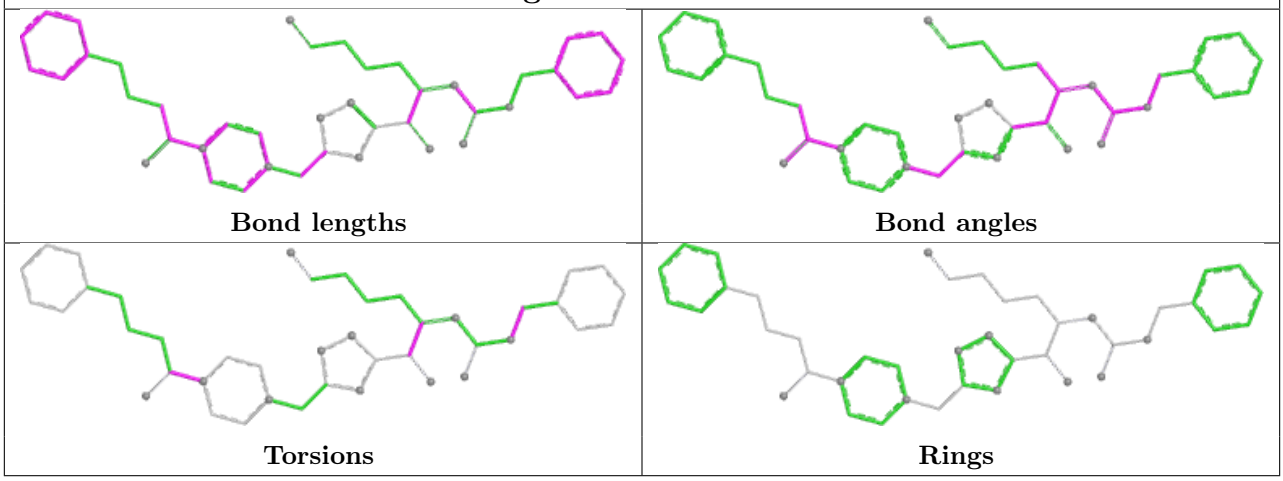
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

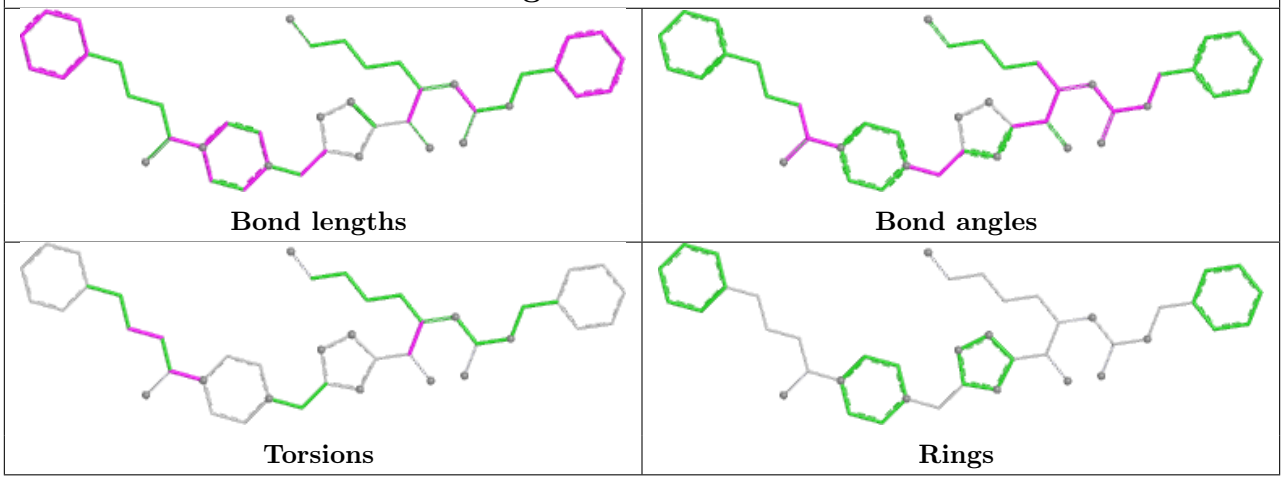
Ligand 5AM A 999

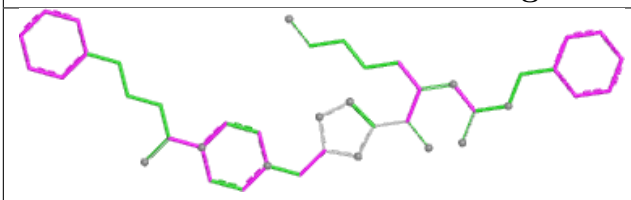
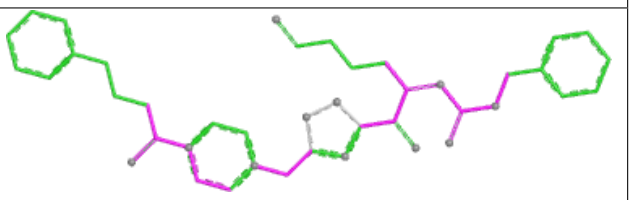
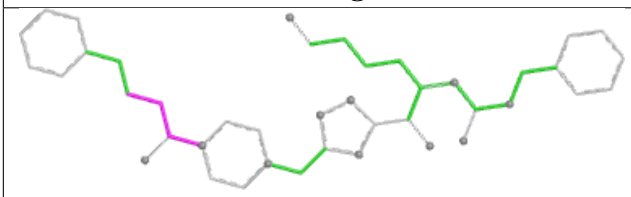
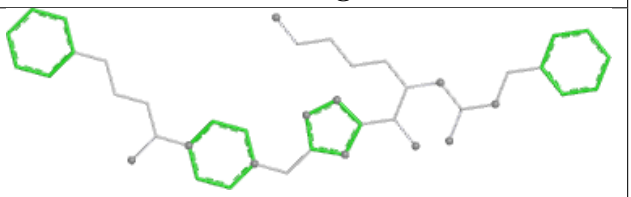


Ligand 5AM B 998



Ligand 5AM C 997



Ligand 5AM D 996	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	243/245 (99%)	-0.60	0 100 100	11, 22, 45, 61	0
1	B	243/245 (99%)	-0.43	2 (0%) 86 91	14, 27, 50, 66	0
1	C	243/245 (99%)	-0.59	0 100 100	10, 23, 43, 62	0
1	D	243/245 (99%)	-0.41	3 (1%) 79 86	14, 26, 52, 66	0
All	All	972/980 (99%)	-0.51	5 (0%) 91 95	10, 24, 49, 66	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	206	THR	3.0
1	D	203	VAL	2.7
1	D	135	PRO	2.4
1	B	135	PRO	2.4
1	D	206	THR	2.2

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,

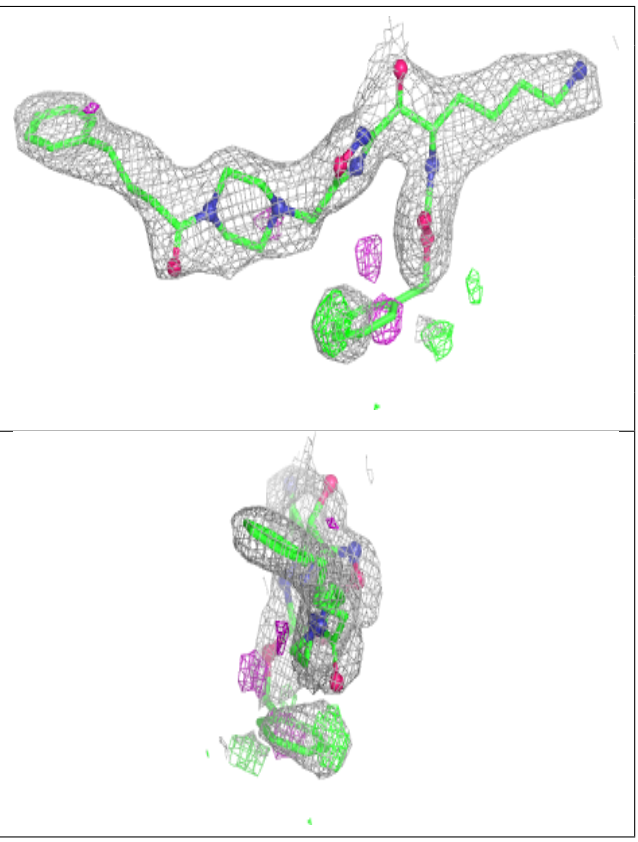
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	5AM	B	998	42/42	0.86	0.21	35,51,69,70	0
2	5AM	D	996	42/42	0.86	0.25	36,50,74,74	0
2	5AM	A	999	42/42	0.87	0.18	18,45,58,60	0
2	5AM	C	997	42/42	0.89	0.18	28,45,77,79	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.

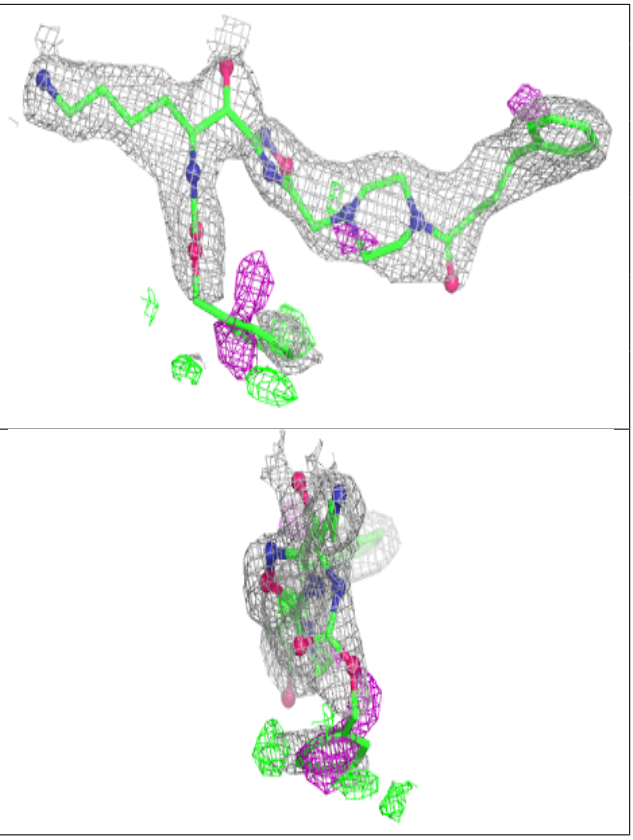
Electron density around 5AM B 998:

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



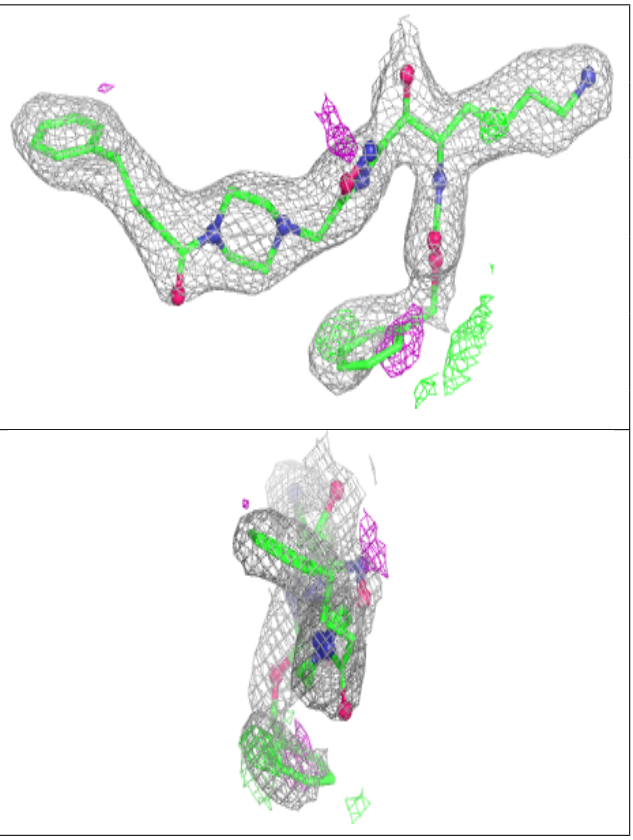
Electron density around 5AM D 996:

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



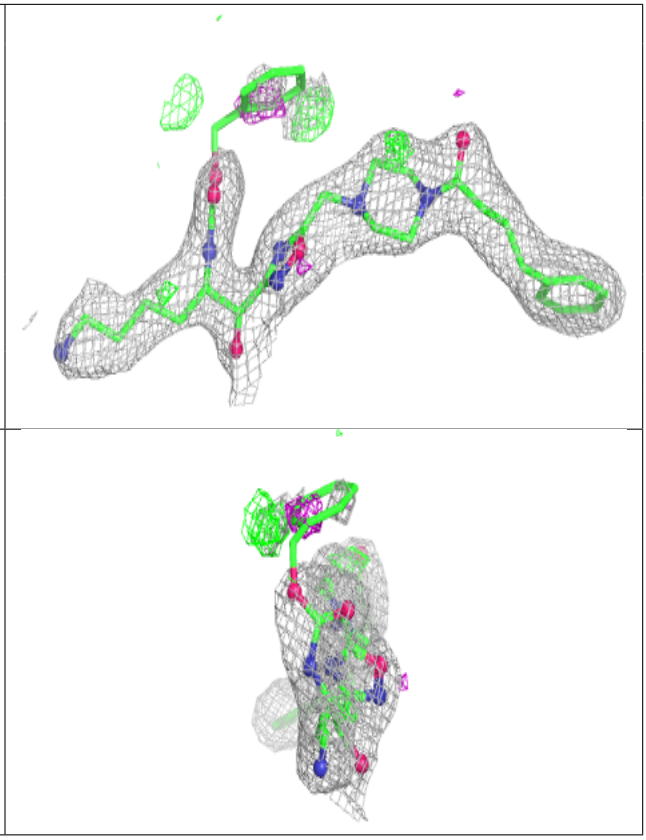
Electron density around 5AM A 999:

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



Electron density around 5AM C 997:

$2mF_o$-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.