wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:40 AM GMT

PDB ID	:	2I47
Title	:	Crystal structure of catalytic domain of TACE with inhibitor
Authors	:	Xu, W.; Condon, J.S.; Lovering, F.E.
Deposited on	:	2006-08-21
Resolution	:	1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

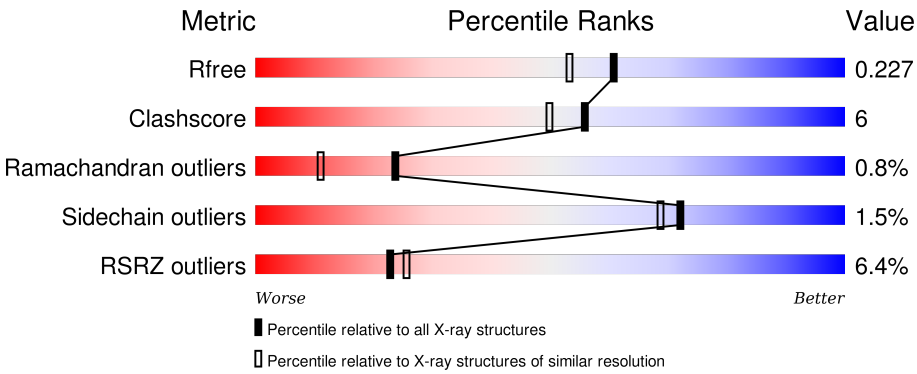
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	288	6% 74% 14% • 11%
1	B	288	3% 76% 11% • 12%
1	C	288	7% 72% 14% • 12%
1	D	288	6% 75% 13% • 11%

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
4	KGY	C	1001	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8926 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 ADAM 17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	255	2023	1273	342	395	13	0	0	0
1	B	254	2016	1268	341	394	13	0	0	0
1	C	254	2016	1268	341	394	13	0	0	0
1	D	255	2023	1273	342	395	13	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	ALA	SER	ENGINEERED	UNP P78536
A	452	GLN	ASN	ENGINEERED	UNP P78536
A	493	SER	-	CLONING ARTIFACT	UNP P78536
A	494	HIS	-	EXPRESSION TAG	UNP P78536
A	495	HIS	-	EXPRESSION TAG	UNP P78536
A	496	HIS	-	EXPRESSION TAG	UNP P78536
A	497	HIS	-	EXPRESSION TAG	UNP P78536
A	498	HIS	-	EXPRESSION TAG	UNP P78536
A	499	HIS	-	EXPRESSION TAG	UNP P78536
B	266	ALA	SER	ENGINEERED	UNP P78536
B	452	GLN	ASN	ENGINEERED	UNP P78536
B	493	SER	-	CLONING ARTIFACT	UNP P78536
B	494	HIS	-	EXPRESSION TAG	UNP P78536
B	495	HIS	-	EXPRESSION TAG	UNP P78536
B	496	HIS	-	EXPRESSION TAG	UNP P78536
B	497	HIS	-	EXPRESSION TAG	UNP P78536
B	498	HIS	-	EXPRESSION TAG	UNP P78536
B	499	HIS	-	EXPRESSION TAG	UNP P78536
C	266	ALA	SER	ENGINEERED	UNP P78536
C	452	GLN	ASN	ENGINEERED	UNP P78536
C	493	SER	-	CLONING ARTIFACT	UNP P78536

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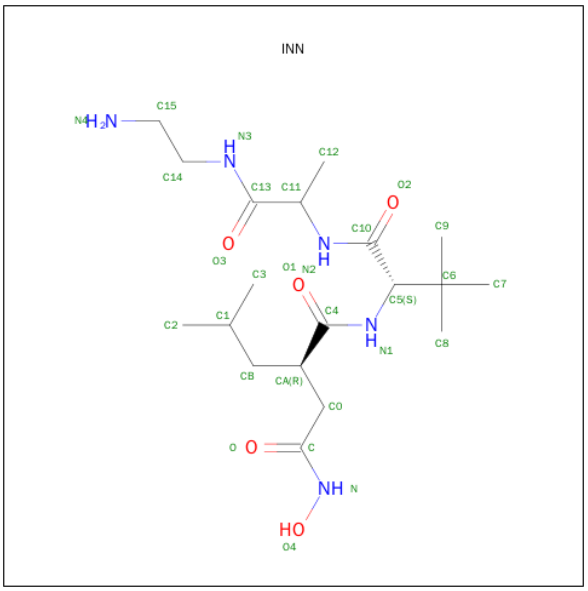
Chain	Residue	Modelled	Actual	Comment	Reference
C	494	HIS	-	EXPRESSION TAG	UNP P78536
C	495	HIS	-	EXPRESSION TAG	UNP P78536
C	496	HIS	-	EXPRESSION TAG	UNP P78536
C	497	HIS	-	EXPRESSION TAG	UNP P78536
C	498	HIS	-	EXPRESSION TAG	UNP P78536
C	499	HIS	-	EXPRESSION TAG	UNP P78536
D	266	ALA	SER	ENGINEERED	UNP P78536
D	452	GLN	ASN	ENGINEERED	UNP P78536
D	493	SER	-	CLONING ARTIFACT	UNP P78536
D	494	HIS	-	EXPRESSION TAG	UNP P78536
D	495	HIS	-	EXPRESSION TAG	UNP P78536
D	496	HIS	-	EXPRESSION TAG	UNP P78536
D	497	HIS	-	EXPRESSION TAG	UNP P78536
D	498	HIS	-	EXPRESSION TAG	UNP P78536
D	499	HIS	-	EXPRESSION TAG	UNP P78536

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

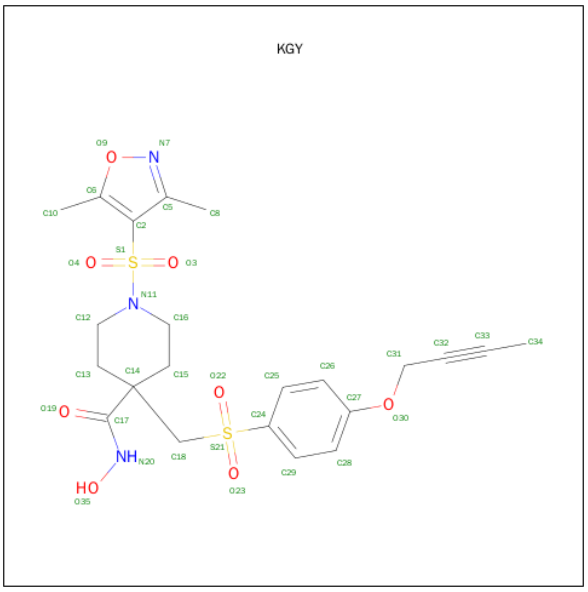
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	B	1	1	1	0	0
2	A	1	1	1	0	0
2	D	1	1	1	0	0
2	C	1	1	1	0	0

- Molecule 3 is N-{(2R)-2-[2-(HYDROXYAMINO)-2-OXOETHYL]-4-METHYLPENTANOYL}-3-METHYL-L-VALYL-N-(2-AMINOETHYL)-L-ALANINAMIDE (three-letter code: INN) (formula: $C_{19}H_{37}N_5O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	29	19	5	5	0	0
			Total	C	N	O		
3	B	1	29	19	5	5	0	0

- Molecule 4 is 4-({[4-(BUT-2-YN-1-YLOXY)PHENYL]SULFONYL}METHYL)-1-[(3,5-DIMETHYLISOXAZOL-4-YL)SULFONYL]-N-HYDROXYPIPERIDINE-4-CARBOXAMIDE (three-letter code: KGY) (formula: $C_{22}H_{27}N_3O_8S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	C	1	35	22	3	8	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	D	1	35	22	3	8	2	0	0

- Molecule 5 is water.

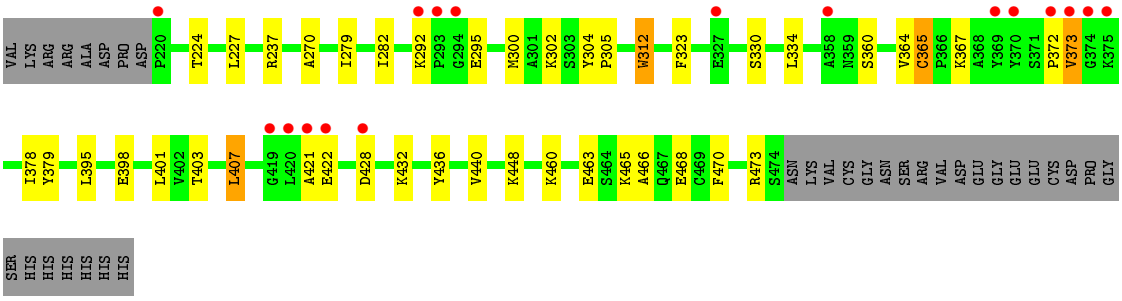
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	213	213	213	0	0
			Total	O		
5	B	165	165	165	0	0
			Total	O		
5	C	169	169	169	0	0
			Total	O		
5	D	169	169	169	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

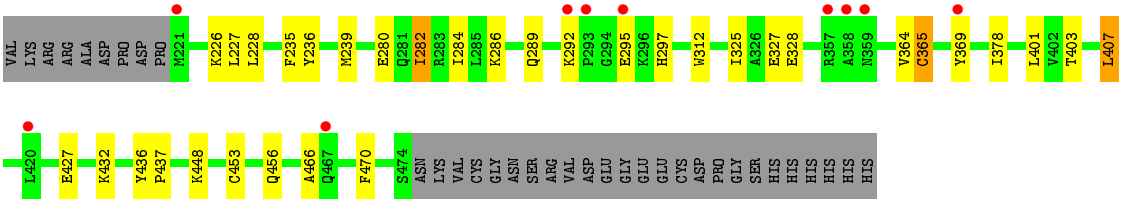
- Molecule 1: ADAM 17

Chain A:



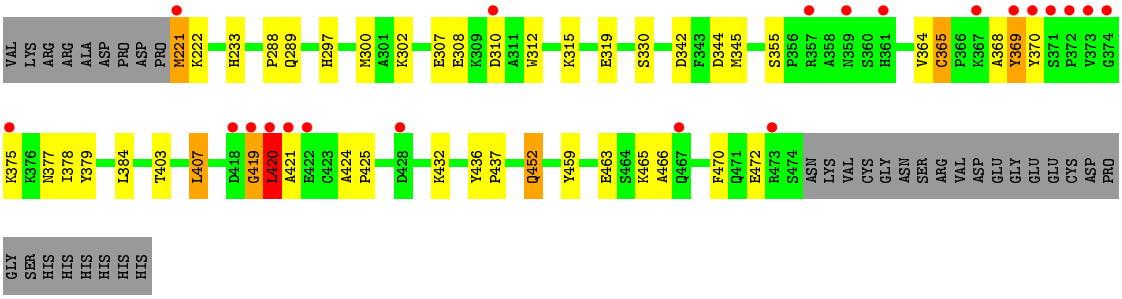
- Molecule 1: ADAM 17

Chain B:



- Molecule 1: ADAM 17

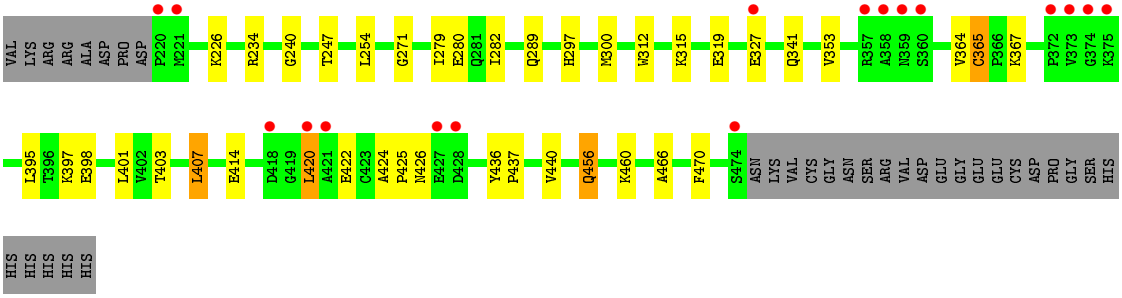
Chain C:



- Molecule 1: ADAM 17

Chain D:

6%
75%
13%
11%


VAL LYS ARG ARG ALA ASP PRO ASP P220 M221 K226 R234 G240 T247 L254 G271 I279 E280 Q281 I282 Q289 H297 M300 W312 K315 E319 E327 Q341 V353 R357 A358 N359 S360 V364 C365 P366 K367 P372 V373 G374 K375
L395 T396 K397 E398 L401 V402 T403 L407 E414 D418 G419 L420 A421 E422 C423 A424 P425 N426 E427 D428 Y436 P437 V440 Q456 K460 A466 F470 S474 ASN LYS VAL CYS GLY ASN SER ARG VAL ASP GLU GLY GLU GLU CYS ASP PRO GLY SER HIS
HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.77Å 126.19Å 81.22Å 90.00° 107.41° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 43.07 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.90) 93.5 (43.07-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 1.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.227 0.199 , 0.227	Depositor DCC
R_{free} test set	4527 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	15.3	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 102366 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8926	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: KGY, ZN, INN

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	0.51	0/2069	0.65	0/2791
1	B	0.50	0/2061	0.64	0/2780
1	C	0.47	0/2061	0.63	0/2780
1	D	0.49	0/2069	0.63	0/2791
All	All	0.49	0/8260	0.64	0/11142

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	A	0	1
1	B	0	2
1	C	0	2
1	D	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	TRP	Peptide
1	B	227	LEU	Peptide
1	B	312	TRP	Peptide
1	C	312	TRP	Peptide
1	C	419	GLY	Peptide

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	2023	0	1940	28	0
1	B	2016	0	1932	18	0
1	C	2016	0	1932	30	0
1	D	2023	0	1940	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	29	0	36	0	0
3	B	29	0	36	0	0
4	C	35	0	26	0	0
4	D	35	0	26	0	0
5	A	213	0	0	3	0
5	B	165	0	0	0	0
5	C	169	0	0	1	0
5	D	169	0	0	3	0
All	All	8926	0	7868	100	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 6.

The worst 5 of 100 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:372:PRO:O	1:A:373:VAL:HG23	1.64	0.97
1:B:282:ILE:HD11	1:B:284:ILE:HD11	1.62	0.79
1:A:372:PRO:O	1:A:373:VAL:CG2	2.32	0.78
1:B:466:ALA:O	1:B:470:PHE:HB2	1.97	0.65
1:A:372:PRO:O	1:A:373:VAL:CB	2.47	0.61

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	253/288 (88%)	239 (94%)	11 (4%)	3 (1%)	16	5
1	B	252/288 (88%)	241 (96%)	10 (4%)	1 (0%)	39	27
1	C	252/288 (88%)	243 (96%)	7 (3%)	2 (1%)	24	11
1	D	253/288 (88%)	243 (96%)	8 (3%)	2 (1%)	24	11
All	All	1010/1152 (88%)	966 (96%)	36 (4%)	8 (1%)	24	11

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	VAL
1	C	420	LEU
1	A	312	TRP
1	A	365	CYS
1	B	365	CYS

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	218/247 (88%)	216 (99%)	2 (1%)	84	83
1	B	217/247 (88%)	215 (99%)	2 (1%)	84	83
1	C	217/247 (88%)	211 (97%)	6 (3%)	51	41
1	D	218/247 (88%)	215 (99%)	3 (1%)	74	71
All	All	870/988 (88%)	857 (98%)	13 (2%)	72	69

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	308	GLU
1	C	369	TYR
1	D	407	LEU
1	C	221	MET
1	C	452	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	281	GLN
1	D	361	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
3	INN	A	901	2	28,28,28	0.56	0	33,38,38	1.26	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	INN	B	902	2	28,28,28	0.76	1 (3%)	33,38,38	1.14	3 (9%)
4	KGY	C	1001	2	34,37,37	1.66	8 (23%)	39,55,55	1.86	9 (23%)
4	KGY	D	1002	2	34,37,37	1.65	8 (23%)	39,55,55	1.98	9 (23%)

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
3	INN	A	901	2	-	0/40/40/40	0/0/0/0
3	INN	B	902	2	-	0/40/40/40	0/0/0/0
4	KGY	C	1001	2	-	0/29/49/49	0/2/3/3
4	KGY	D	1002	2	-	0/29/49/49	0/2/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1002	KGY	C2-S1	-4.29	1.71	1.79
4	C	1001	KGY	C2-S1	-4.20	1.71	1.79
4	D	1002	KGY	O35-N20	-2.33	1.35	1.39
3	B	902	INN	C7-C6	2.03	1.57	1.53
4	C	1001	KGY	C29-C28	2.18	1.42	1.38

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	901	INN	C14-N3-C13	-4.51	113.61	122.53
3	B	902	INN	C11-N2-C10	-3.29	113.73	121.27
3	B	902	INN	C14-N3-C13	-3.28	116.04	122.53
4	D	1002	KGY	O22-S21-C24	-2.95	105.15	108.38
4	C	1001	KGY	O3-S1-O4	-2.71	114.79	119.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	255/288 (88%)	0.16	17 (6%)	21	23	7, 19, 44, 54	0
1	B	254/288 (88%)	0.05	10 (3%)	43	47	7, 18, 40, 53	0
1	C	254/288 (88%)	0.15	21 (8%)	14	15	7, 20, 48, 54	0
1	D	255/288 (88%)	-0.02	17 (6%)	21	23	7, 18, 47, 55	0
All	All	1018/1152 (88%)	0.08	65 (6%)	23	25	7, 19, 45, 55	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	420	LEU	15.5
1	D	420	LEU	8.9
1	A	220	PRO	7.8
1	A	420	LEU	7.3
1	B	358	ALA	7.1

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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
4	KGY	C	1001	35/35	0.87	0.18	3.81	17,24,61,62	0
4	KGY	D	1002	35/35	0.93	0.12	1.06	13,21,42,43	0
3	INN	A	901	29/29	0.95	0.09	0.10	6,11,27,34	0
3	INN	B	902	29/29	0.96	0.11	0.06	8,11,26,28	0
2	ZN	A	802	1/1	1.00	0.07	-	11,11,11,11	0
2	ZN	C	804	1/1	0.99	0.06	-	14,14,14,14	0
2	ZN	D	803	1/1	0.99	0.08	-	14,14,14,14	0
2	ZN	B	801	1/1	1.00	0.10	-	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.